



wwPDB EM Validation Summary Report ⓘ

Mar 22, 2026 – 11:12 AM UTC

PDB ID : 8AZW / pdb_00008azw
EMDB ID : EMD-15773
Title : Cryo-EM structure of the plant 60S subunit
Authors : Smirnova, J.; Loerke, J.; Kleinau, G.; Schmidt, A.; Buerger, J.; Meyer, E.H.;
Mielke, T.; Scheerer, P.; Bock, R.; Spahn, C.M.T.; Zoschke, R.
Deposited on : 2022-09-06
Resolution : 2.14 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:

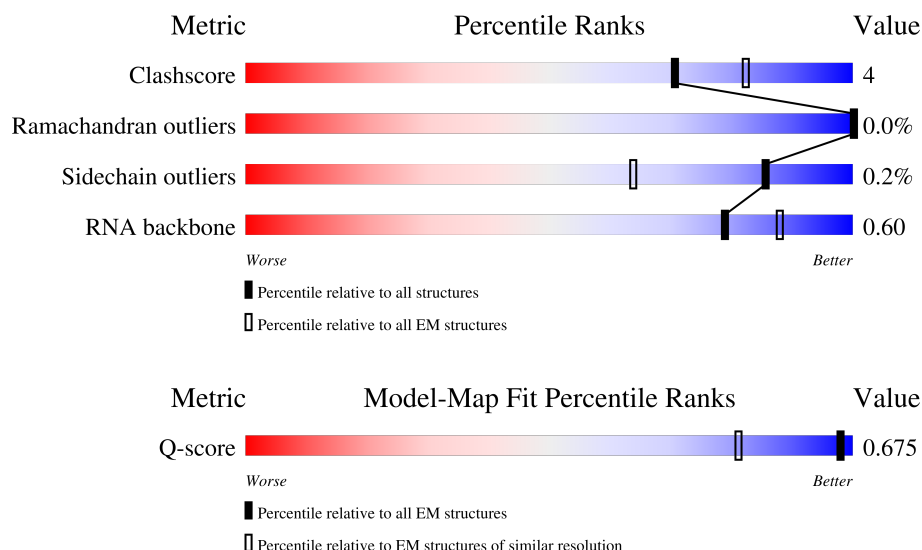
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 2.14 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.



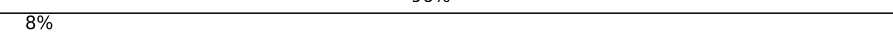
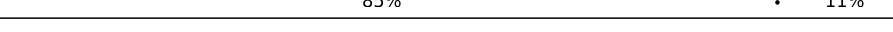
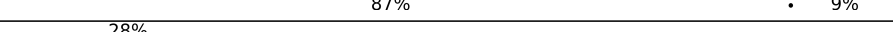
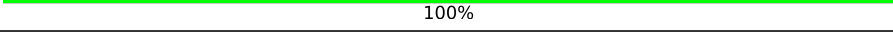
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	2493 (1.66 - 2.64)

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	C	119	 81% 18% 6% 5%
2	D	206	 92% 5% 3% 2%
3	E	134	 88% 9% 3% 2%

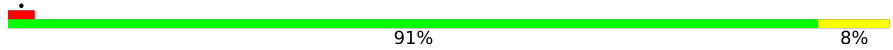
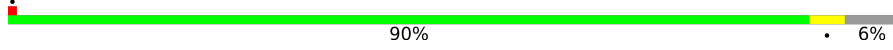
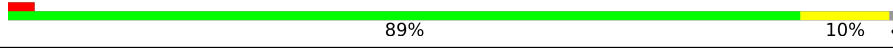
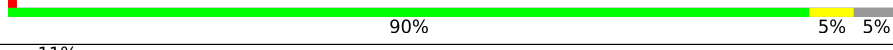
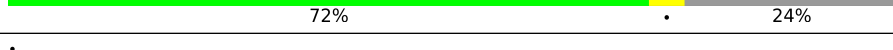
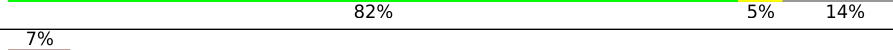
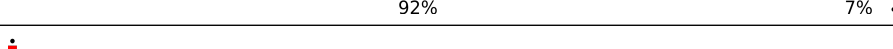
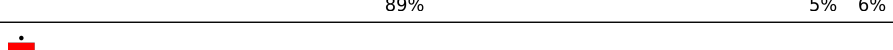
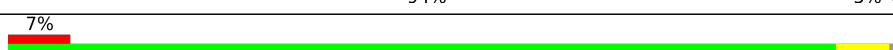
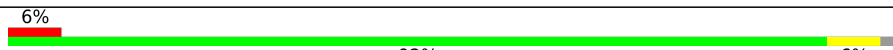
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Mol	Chain	Length	Quality of chain
4	F	204	
5	G	187	
6	H	214	
7	I	178	
8	J	164	
9	K	127	
10	L	164	
11	M	135	
12	N	143	
13	O	61	
14	P	113	
15	Q	120	
16	R	133	
17	S	112	
18	T	120	
19	U	110	
20	V	95	
21	W	69	
22	X	51	
23	Y	128	
24	p	25	
25	Z	105	
26	a	92	
27	b	230	
28	c	258	

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Mol	Chain	Length	Quality of chain
29	d	206	
30	e	140	
31	f	148	
32	g	221	
33	h	301	
34	j	175	
35	k	154	
36	m	146	
37	n	123	
38	o	260	
39	q	242	
40	r	389	
41	s	405	
42	t	181	
43	u	194	
44	l	24	
45	A	3390	
46	B	163	

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 223261 atoms, of which 92404 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 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	C	119	Total	C	H	N	O	P	0	0
			3823	1133	1285	457	829	119		

- Molecule 2 is a protein called eL13 (60S ribosomal protein L13).

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	200	Total	C	H	N	O	S	0	0
			3296	1007	1691	324	270	4		

- Molecule 3 is a protein called eL14 (60S ribosomal protein L14).

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	130	Total	C	H	N	O	S	0	0
			2206	678	1150	196	179	3		

- Molecule 4 is a protein called eL15 (60S ribosomal protein L15).

Mol	Chain	Residues	Atoms						AltConf	Trace
4	F	203	Total	C	H	N	O	S	0	0
			3469	1071	1768	350	277	3		

- Molecule 5 is a protein called eL18 (60S ribosomal protein L18).

Mol	Chain	Residues	Atoms						AltConf	Trace
5	G	186	Total	C	H	N	O	S	0	0
			3042	931	1580	283	245	3		

- Molecule 6 is a protein called eL19 (60S ribosomal protein L19).

Mol	Chain	Residues	Atoms						AltConf	Trace
6	H	182	Total	C	H	N	O	S	0	0
			3181	946	1652	327	247	9		

- Molecule 7 is a protein called eL20 (60S ribosomal protein L18a).

Mol	Chain	Residues	Atoms						AltConf	Trace
7	I	177	Total	C	H	N	O	S	0	0
			3061	969	1556	277	251	8		

- Molecule 8 is a protein called eL21 (60S ribosomal protein L21).

Mol	Chain	Residues	Atoms						AltConf	Trace
8	J	163	Total	C	H	N	O	S	0	0
			2672	823	1366	255	224	4		

- Molecule 9 is a protein called eL22 (60S ribosomal protein L22).

Mol	Chain	Residues	Atoms						AltConf	Trace
9	K	99	Total	C	H	N	O	S	0	0
			1653	515	845	141	150	2		

- Molecule 10 is a protein called eL24 (60S ribosomal protein L24).

Mol	Chain	Residues	Atoms						AltConf	Trace
10	L	62	Total	C	H	N	O	S	0	0
			1079	341	553	101	81	3		

- Molecule 11 is a protein called eL27 (60S ribosomal protein L27).

Mol	Chain	Residues	Atoms						AltConf	Trace
11	M	134	Total	C	H	N	O	S	0	0
			2283	708	1184	206	183	2		

- Molecule 12 is a protein called eL28 (60S ribosomal protein L28).

Mol	Chain	Residues	Atoms						AltConf	Trace
12	N	142	Total	C	H	N	O	S	0	0
			2298	701	1187	207	201	2		

- Molecule 13 is a protein called eL29 (60S ribosomal protein L29).

Mol	Chain	Residues	Atoms						AltConf	Trace
13	O	49	Total	C	H	N	O	S	0	0
			831	250	419	95	66	1		

- Molecule 14 is a protein called eL30 (60S ribosomal protein L30).

Mol	Chain	Residues	Atoms						AltConf	Trace
14	P	97	Total	C	H	N	O	S	0	0
			1526	475	781	130	135	5		

- Molecule 15 is a protein called eL31 (60S ribosomal protein L31).

Mol	Chain	Residues	Atoms						AltConf	Trace
15	Q	108	Total	C	H	N	O	S	0	0
			1809	549	934	168	156	2		

- Molecule 16 is a protein called eL32 (60S ribosomal protein L32).

Mol	Chain	Residues	Atoms						AltConf	Trace
16	R	126	Total	C	H	N	O	S	0	0
			2151	655	1115	207	169	5		

- Molecule 17 is a protein called eL33 (60S ribosomal protein L35a).

Mol	Chain	Residues	Atoms						AltConf	Trace
17	S	111	Total	C	H	N	O	S	0	0
			1832	571	932	171	153	5		

- Molecule 18 is a protein called eL34 (60S ribosomal protein L34).

Mol	Chain	Residues	Atoms						AltConf	Trace
18	T	114	Total	C	H	N	O	S	0	0
			1939	579	1013	193	153	1		

- Molecule 19 is a protein called eL36 (60S ribosomal protein L36).

Mol	Chain	Residues	Atoms						AltConf	Trace
19	U	98	Total	C	H	N	O	S	0	0
			1650	489	868	162	129	2		

- Molecule 20 is a protein called eL37 (60S ribosomal protein L37).

Mol	Chain	Residues	Atoms						AltConf	Trace
20	V	86	Total	C	H	N	O	S	0	0
			1427	429	726	155	112	5		

- Molecule 21 is a protein called eL38 (60S ribosomal protein L38).

Mol	Chain	Residues	Atoms						AltConf	Trace
21	W	68	Total	C	H	N	O	S	0	0
			1160	358	602	99	98	3		

- Molecule 22 is a protein called eL39 (60S ribosomal protein L39).

Mol	Chain	Residues	Atoms						AltConf	Trace
22	X	50	Total	C	H	N	O	S	0	0
			928	286	480	96	64	2		

- Molecule 23 is a protein called eL40 (60S ribosomal protein L40).

Mol	Chain	Residues	Atoms						AltConf	Trace
23	Y	51	Total	C	H	N	O	S	0	0
			881	262	460	88	65	6		

- Molecule 24 is a protein called eL41 (60S ribosomal protein L41).

Mol	Chain	Residues	Atoms						AltConf	Trace
24	p	25	Total	C	H	N	O	S	0	0
			527	145	289	62	28	3		

- Molecule 25 is a protein called eL42 (60S ribosomal protein L42).

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Z	98	Total	C	H	N	O	S	0	0
			1629	494	842	157	131	5		

- Molecule 26 is a protein called eL43 (60S ribosomal protein L37a).

Mol	Chain	Residues	Atoms						AltConf	Trace
26	a	91	Total	C	H	N	O	S	0	0
			1453	443	745	136	124	5		

- Molecule 27 is a protein called eL6 (60S ribosomal protein L6).

Mol	Chain	Residues	Atoms						AltConf	Trace
27	b	208	Total	C	H	N	O	S	0	0
			3360	1046	1749	290	271	4		

- Molecule 28 is a protein called eL8 (60S ribosomal protein L7a).

Mol	Chain	Residues	Atoms						AltConf	Trace
28	c	233	Total	C	H	N	O	S	0	0
			3907	1206	2028	347	319	7		

- Molecule 29 is a protein called uL13 (60S ribosomal protein L13a).

Mol	Chain	Residues	Atoms						AltConf	Trace
29	d	205	Total	C	H	N	O	S	0	0
			3414	1046	1774	318	268	8		

- Molecule 30 is a protein called uL14 (60S ribosomal protein L23).

Mol	Chain	Residues	Atoms						AltConf	Trace
30	e	131	Total	C	H	N	O	S	0	0
			2029	623	1044	183	170	9		

- Molecule 31 is a protein called uL15 (60S ribosomal protein L27a).

Mol	Chain	Residues	Atoms						AltConf	Trace
31	f	147	Total	C	H	N	O	S	0	0
			2361	740	1200	228	190	3		

- Molecule 32 is a protein called uL16 (60S ribosomal protein L10).

Mol	Chain	Residues	Atoms						AltConf	Trace
32	g	209	Total	C	H	N	O	S	0	0
			3397	1058	1726	329	273	11		

- Molecule 33 is a protein called uL18 (60S ribosomal protein L5).

Mol	Chain	Residues	Atoms						AltConf	Trace
33	h	288	Total	C	H	N	O	S	0	0
			4715	1481	2374	426	429	5		

- Molecule 34 is a protein called uL22 (60S ribosomal protein L17).

Mol	Chain	Residues	Atoms						AltConf	Trace
34	j	154	Total	C	H	N	O	S	0	0
			2515	775	1270	246	219	5		

- Molecule 35 is a protein called uL23 (60S ribosomal protein L23a).

Mol	Chain	Residues	Atoms						AltConf	Trace
35	k	117	Total	C	H	N	O	S	0	0
			1980	609	1030	170	169	2		

- Molecule 36 is a protein called uL24 (60S ribosomal protein L26).

Mol	Chain	Residues	Atoms						AltConf	Trace
36	m	126	Total	C	H	N	O	S	0	0
			2124	634	1103	209	175	3		

- Molecule 37 is a protein called uL29 (60S ribosomal protein L35).

Mol	Chain	Residues	Atoms						AltConf	Trace
37	n	122	Total	C	H	N	O	S	0	0
			2140	642	1141	191	165	1		

- Molecule 38 is a protein called uL2 (60S ribosomal protein L8).

Mol	Chain	Residues	Atoms						AltConf	Trace
38	o	245	Total	C	H	N	O	S	0	0
			3791	1174	1911	381	315	10		

- Molecule 39 is a protein called uL30 (60S ribosomal protein L7).

Mol	Chain	Residues	Atoms						AltConf	Trace
39	q	238	Total	C	H	N	O	S	0	0
			4016	1256	2058	359	339	4		

- Molecule 40 is a protein called uL3 (60S ribosomal protein L3).

Mol	Chain	Residues	Atoms						AltConf	Trace
40	r	386	Total	C	H	N	O	S	0	0
			6327	1981	3223	578	530	15		

- Molecule 41 is a protein called uL4 (60S ribosomal protein L4).

Mol	Chain	Residues	Atoms						AltConf	Trace
41	s	398	Total	C	H	N	O	S	0	0
			6324	1956	3227	583	548	10		

- Molecule 42 is a protein called uL5 (60S ribosomal protein L11).

Mol	Chain	Residues	Atoms						AltConf	Trace
42	t	172	Total	C	H	N	O	S	0	0
			2836	882	1444	259	244	7		

- Molecule 43 is a protein called uL6 (60S ribosomal protein L9).

Mol	Chain	Residues	Atoms						AltConf	Trace
43	u	191	Total	C	H	N	O	S	0	0
			3124	963	1604	276	276	5		

- Molecule 44 is a protein called nascent chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	l	4	Total	C	H	N	O		
			29	12	9	4	4	0	0

- Molecule 45 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	A	3196	Total	C	H	N	O	P	0	0
			103169	30602	34651	12456	22264	3196		

- Molecule 46 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	B	163	Total	C	H	N	O	P	0	0
			5243	1555	1763	627	1135	163		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	85	U	C	conflict	GB 1782605526

- Molecule 47 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
47	C	4	Total	Mg	0
			4	4	
47	V	1	Total	Mg	0
			1	1	
47	e	1	Total	Mg	0
			1	1	
47	j	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
47	q	1	Total 1	Mg 1	0
47	r	2	Total 2	Mg 2	0
47	A	50	Total 50	Mg 50	0

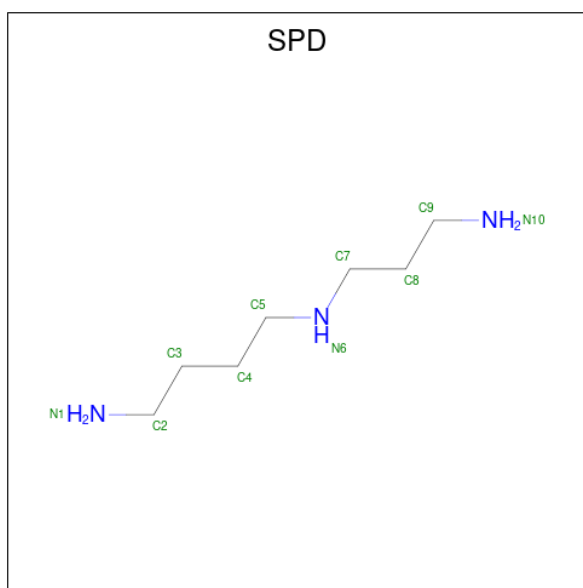
- Molecule 48 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
48	D	1	Total 1	K 1	0
48	R	1	Total 1	K 1	0
48	T	1	Total 1	K 1	0
48	Z	1	Total 1	K 1	0
48	f	1	Total 1	K 1	0
48	g	1	Total 1	K 1	0
48	o	2	Total 2	K 2	0
48	r	1	Total 1	K 1	0
48	A	83	Total 83	K 83	0
48	B	2	Total 2	K 2	0

- Molecule 49 is ZINC ION (CCD ID: ZN) (formula: Zn).

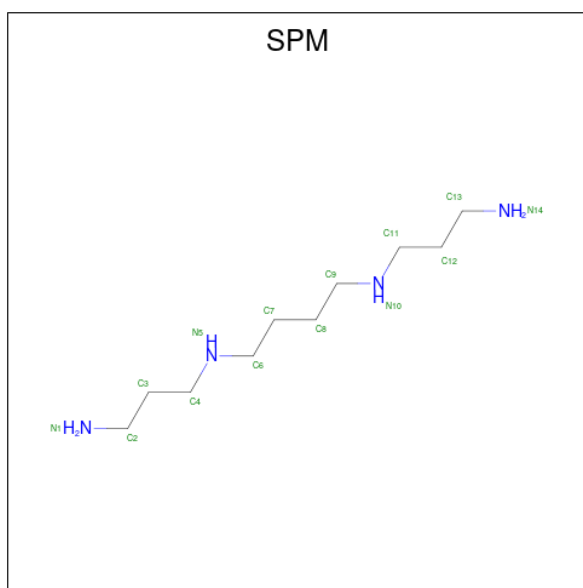
Mol	Chain	Residues	Atoms		AltConf
49	V	1	Total 1	Zn 1	0
49	Y	1	Total 1	Zn 1	0
49	Z	1	Total 1	Zn 1	0
49	a	1	Total 1	Zn 1	0

- Molecule 50 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			AltConf
50	A	1	Total	C	N	0
			10	7	3	

- Molecule 51 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms				AltConf
51	A	1	Total	C	H	N	0
			40	10	26	4	
51	A	1	Total	C	H	N	0
			40	10	26	4	

- Molecule 52 is water.

Mol	Chain	Residues	Atoms		AltConf
52	C	88	Total 88	O 88	0
52	D	47	Total 47	O 47	0
52	F	105	Total 105	O 105	0
52	G	53	Total 53	O 53	0
52	H	11	Total 11	O 11	0
52	I	13	Total 13	O 13	0
52	J	27	Total 27	O 27	0
52	M	2	Total 2	O 2	0
52	N	8	Total 8	O 8	0
52	O	26	Total 26	O 26	0
52	Q	3	Total 3	O 3	0
52	R	42	Total 42	O 42	0
52	S	5	Total 5	O 5	0
52	T	12	Total 12	O 12	0
52	U	3	Total 3	O 3	0
52	V	30	Total 30	O 30	0
52	W	1	Total 1	O 1	0
52	X	6	Total 6	O 6	0
52	Y	2	Total 2	O 2	0
52	Z	25	Total 25	O 25	0
52	a	6	Total 6	O 6	0

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Mol	Chain	Residues	Atoms		AltConf
52	b	1	Total 1	O 1	0
52	c	10	Total 10	O 10	0
52	d	12	Total 12	O 12	0
52	e	13	Total 13	O 13	0
52	f	41	Total 41	O 41	0
52	g	16	Total 16	O 16	0
52	h	19	Total 19	O 19	0
52	j	15	Total 15	O 15	0
52	k	16	Total 16	O 16	0
52	m	8	Total 8	O 8	0
52	n	17	Total 17	O 17	0
52	o	56	Total 56	O 56	0
52	q	27	Total 27	O 27	0
52	r	27	Total 27	O 27	0
52	s	66	Total 66	O 66	0
52	t	1	Total 1	O 1	0
52	u	2	Total 2	O 2	0
52	A	3376	Total 3376	O 3376	0
52	B	168	Total 168	O 168	0

3 Residue-property plots [i](#)

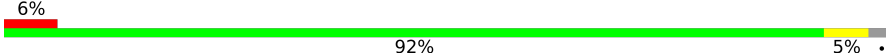
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

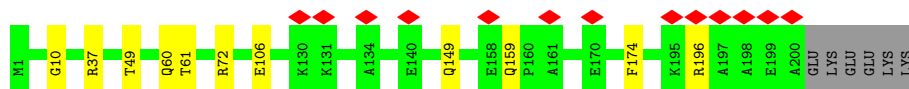
- Molecule 1: 5S rRNA

Chain C: 



- Molecule 2: eL13 (60S ribosomal protein L13)

Chain D: 



- Molecule 3: eL14 (60S ribosomal protein L14)

Chain E: 

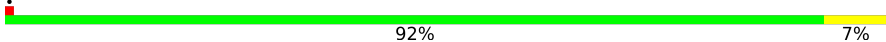


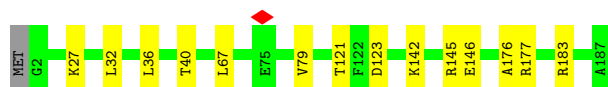
- Molecule 4: eL15 (60S ribosomal protein L15)

Chain F: 

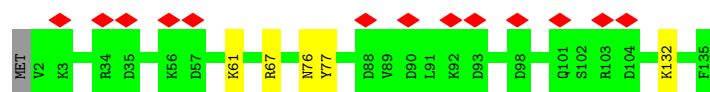


- Molecule 5: eL18 (60S ribosomal protein L18)

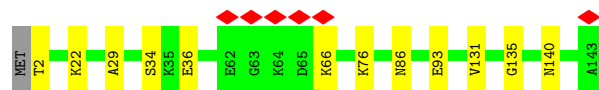
Chain G: 



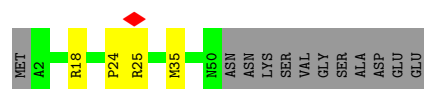
- Molecule 6: eL19 (60S ribosomal protein L19)



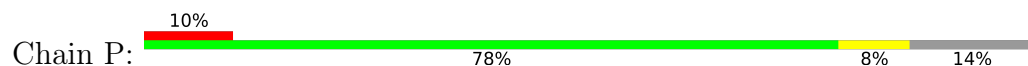
- Molecule 12: eL28 (60S ribosomal protein L28)



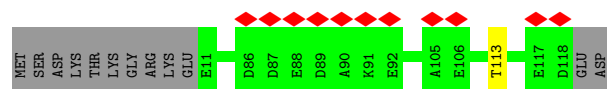
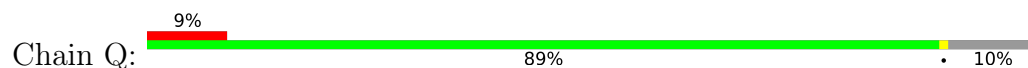
- Molecule 13: eL29 (60S ribosomal protein L29)



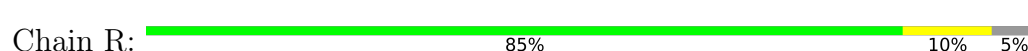
- Molecule 14: eL30 (60S ribosomal protein L30)



- Molecule 15: eL31 (60S ribosomal protein L31)



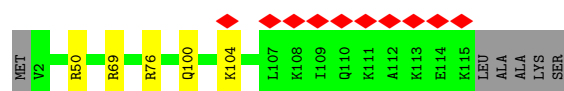
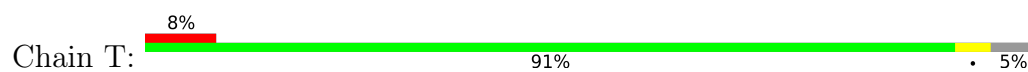
- Molecule 16: eL32 (60S ribosomal protein L32)



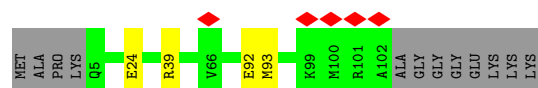
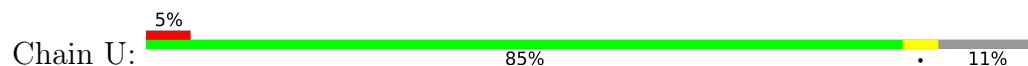
- Molecule 17: eL33 (60S ribosomal protein L35a)



- Molecule 18: eL34 (60S ribosomal protein L34)



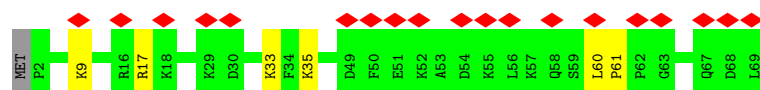
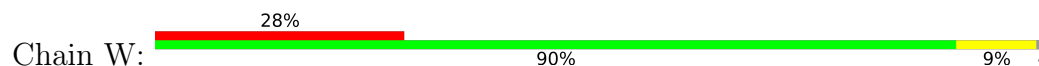
- Molecule 19: eL36 (60S ribosomal protein L36)



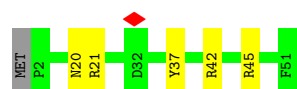
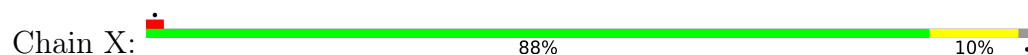
- Molecule 20: eL37 (60S ribosomal protein L37)



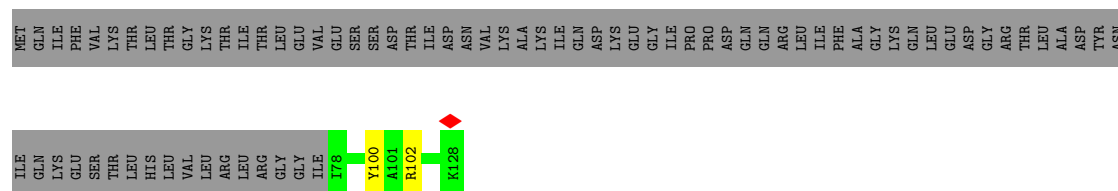
- Molecule 21: eL38 (60S ribosomal protein L38)



- Molecule 22: eL39 (60S ribosomal protein L39)



- Molecule 23: eL40 (60S ribosomal protein L40)

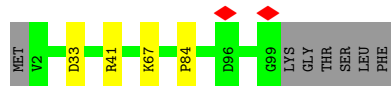
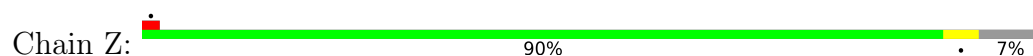


- Molecule 24: eL41 (60S ribosomal protein L41)

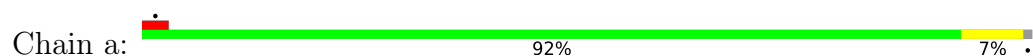




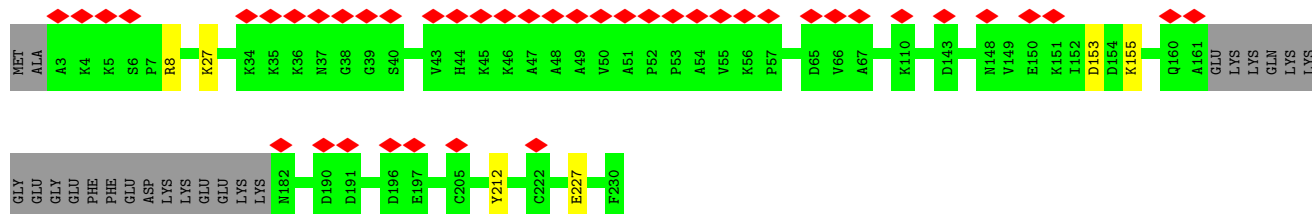
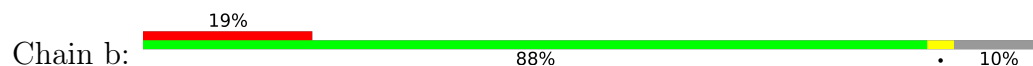
- Molecule 25: eL42 (60S ribosomal protein L42)



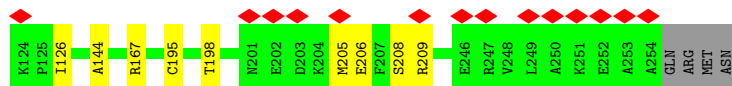
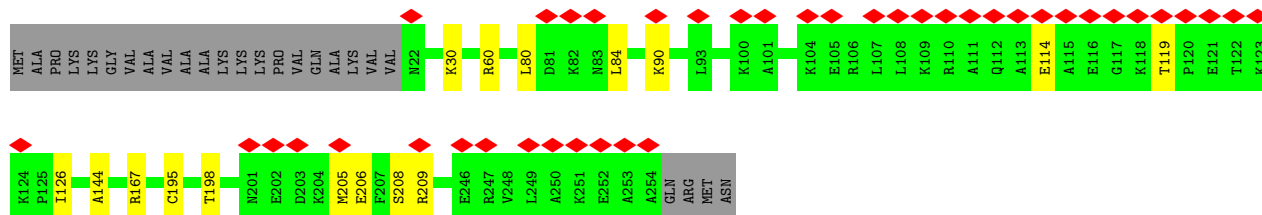
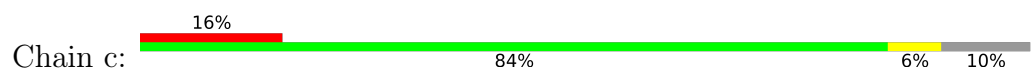
- Molecule 26: eL43 (60S ribosomal protein L37a)



- Molecule 27: eL6 (60S ribosomal protein L6)



- Molecule 28: eL8 (60S ribosomal protein L7a)

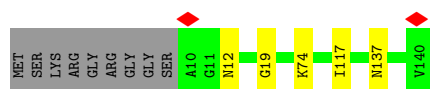


- Molecule 29: uL13 (60S ribosomal protein L13a)



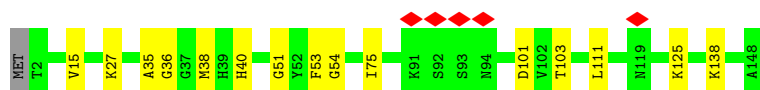
- Molecule 30: uL14 (60S ribosomal protein L23)

Chain e:  90% 6%



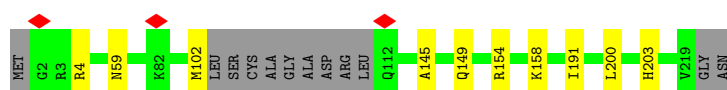
- Molecule 31: uL15 (60S ribosomal protein L27a)

Chain f:  89% 10%



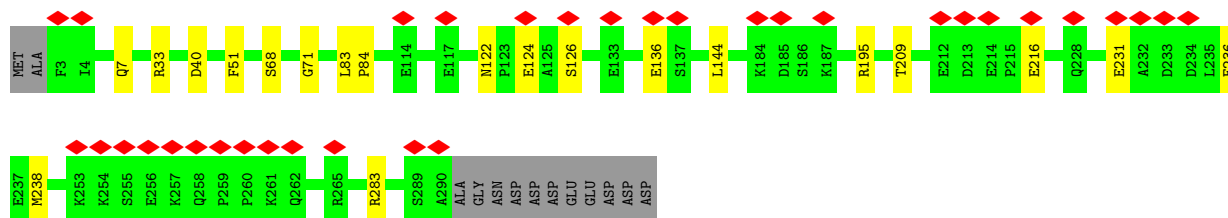
- Molecule 32: uL16 (60S ribosomal protein L10)

Chain g:  90% 5% 5%



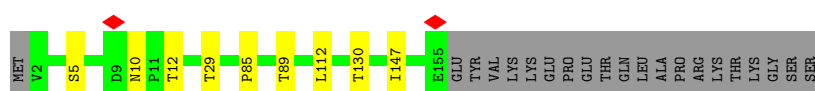
- Molecule 33: uL18 (60S ribosomal protein L5)

Chain h:  11% 89% 7%



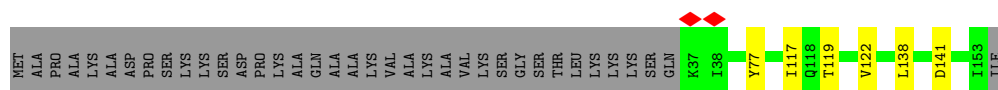
- Molecule 34: uL22 (60S ribosomal protein L17)

Chain j:  83% 5% 12%

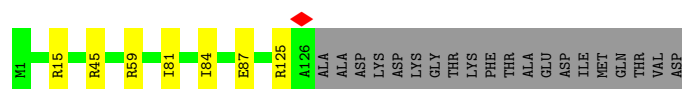
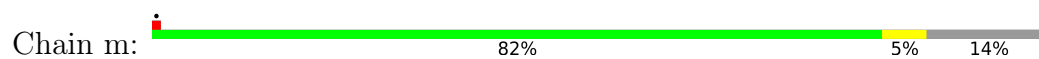


- Molecule 35: uL23 (60S ribosomal protein L23a)

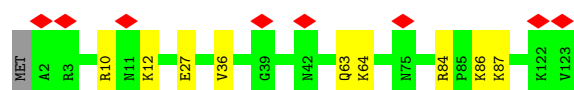
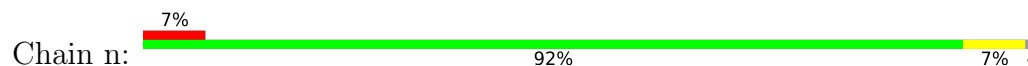
Chain k:  72% 24%



- Molecule 36: uL24 (60S ribosomal protein L26)



- Molecule 37: uL29 (60S ribosomal protein L35)



- Molecule 38: uL2 (60S ribosomal protein L8)



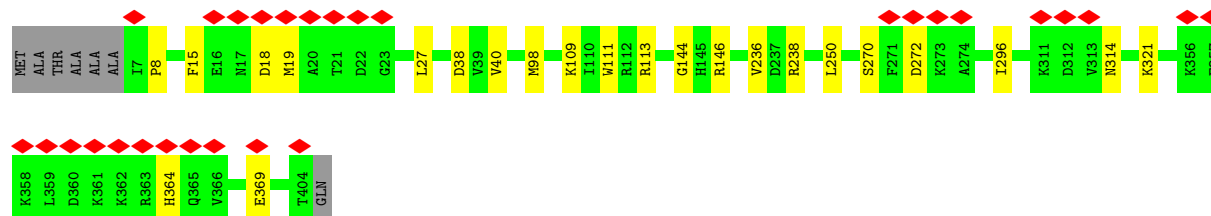
- Molecule 39: uL30 (60S ribosomal protein L7)



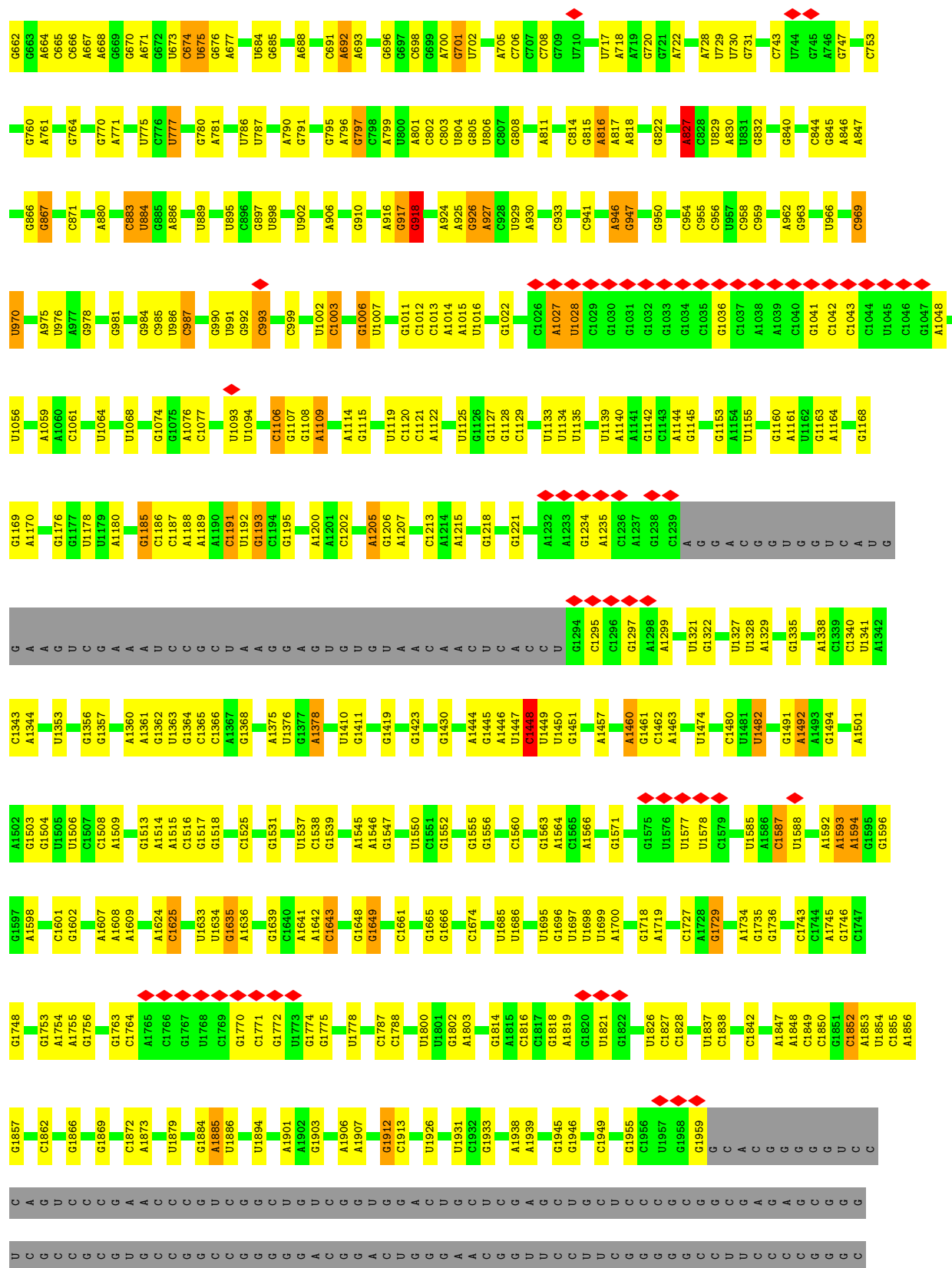
- Molecule 40: uL3 (60S ribosomal protein L3)



- Molecule 41: uL4 (60S ribosomal protein L4)

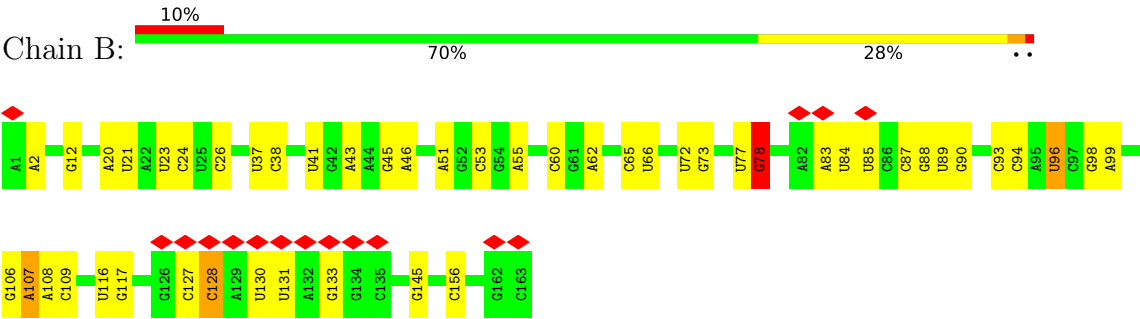


- Molecule 42: uL5 (60S ribosomal protein L11)





● Molecule 46: 5.8S rRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	335291	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 ($e^-/\text{\AA}^2$)	27	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	15.519	Depositor
Minimum map value	-7.827	Depositor
Average map value	0.020	Depositor
Map value standard deviation	0.314	Depositor
Recommended contour level	1.05	Depositor
Map size ($\text{\AA}$)	381.6, 381.6, 381.6	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.848, 0.848, 0.848	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, SPD, 5MC, OMG, OMC, 1MA, K, A2M, ZN, MG, UR3, SPM, OMU, UY1

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	C	0.08	0/2837	0.22	0/4420
2	D	0.09	0/1635	0.23	0/2194
3	E	0.09	0/1069	0.23	0/1427
4	F	0.12	0/1740	0.26	0/2333
5	G	0.11	0/1487	0.26	0/1989
6	H	0.09	0/1548	0.22	0/2042
7	I	0.11	0/1544	0.25	0/2071
8	J	0.09	0/1331	0.24	0/1784
9	K	0.10	0/819	0.23	0/1098
10	L	0.11	0/539	0.23	0/716
11	M	0.10	0/1118	0.22	0/1492
12	N	0.12	0/1126	0.29	0/1508
13	O	0.13	0/422	0.26	0/558
14	P	0.10	0/757	0.23	0/1018
15	Q	0.12	0/885	0.24	0/1184
16	R	0.10	0/1053	0.26	0/1408
17	S	0.10	0/920	0.23	0/1232
18	T	0.10	0/939	0.22	0/1251
19	U	0.12	0/791	0.25	0/1047
20	V	0.18	0/714	0.30	0/949
21	W	0.10	0/566	0.27	0/752
22	X	0.08	0/460	0.20	0/611
23	Y	0.11	0/427	0.26	0/562
24	p	0.08	0/239	0.19	0/302
25	Z	0.10	0/801	0.21	0/1058
26	a	0.10	0/717	0.22	0/952
27	b	0.11	0/1645	0.24	0/2210
28	c	0.10	0/1912	0.24	0/2562
29	d	0.11	0/1669	0.24	0/2235
30	e	0.10	0/1001	0.26	0/1345
31	f	0.10	0/1190	0.24	0/1591
32	g	0.10	0/1707	0.22	0/2283

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	h	0.09	0/2386	0.24	0/3200
34	j	0.14	0/1270	0.33	0/1704
35	k	0.10	0/965	0.22	0/1295
36	m	0.09	0/1035	0.25	0/1383
37	n	0.11	0/1009	0.27	0/1343
38	o	0.10	0/1924	0.25	0/2585
39	q	0.17	0/1992	0.30	0/2670
40	r	0.09	0/3172	0.25	0/4249
41	s	0.11	0/3159	0.28	0/4259
42	t	0.10	0/1414	0.23	0/1890
43	u	0.09	0/1539	0.25	0/2059
45	A	0.16	7/73586 (0.0%)	0.27	5/114785 (0.0%)
46	B	0.13	1/3772 (0.0%)	0.26	0/5878
All	All	0.14	8/132831 (0.0%)	0.26	5/195484 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	2972	A	O3'-P	7.24	1.72	1.61
45	A	654	U	O3'-P	5.88	1.70	1.61
45	A	2284	A2M	O3'-P	5.15	1.61	1.56
46	B	46	A2M	O3'-P	5.12	1.61	1.56
45	A	675	OMU	O3'-P	5.11	1.61	1.56

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	A	654	U	P-O3'-C3'	8.00	132.19	120.20
45	A	2972	A	P-O3'-C3'	7.71	131.76	120.20
45	A	808	G	P-O3'-C3'	6.46	129.90	120.20
45	A	1491	G	P-O3'-C3'	5.81	128.91	120.20
45	A	657	A	C2'-C3'-O3'	5.18	121.46	113.70

There are no chirality outliers.

There are no planarity outliers.

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	C	2538	1285	1285	16	0
2	D	1605	1691	1691	9	0
3	E	1056	1150	1150	10	0
4	F	1701	1768	1769	11	0
5	G	1462	1580	1581	11	0
6	H	1529	1652	1652	9	0
7	I	1505	1556	1557	9	0
8	J	1306	1366	1367	13	0
9	K	808	845	845	6	0
10	L	526	553	554	0	0
11	M	1099	1184	1184	4	0
12	N	1111	1187	1186	9	0
13	O	412	419	418	4	0
14	P	745	781	783	6	0
15	Q	875	934	934	1	0
16	R	1036	1115	1116	11	0
17	S	900	932	933	3	0
18	T	926	1013	1013	5	0
19	U	782	868	867	3	0
20	V	701	726	725	3	0
21	W	558	602	604	4	0
22	X	448	480	480	4	0
23	Y	421	460	459	2	0
24	p	238	289	289	0	0
25	Z	787	842	842	4	0
26	a	708	745	744	6	0
27	b	1611	1749	1749	6	0
28	c	1879	2028	2030	13	0
29	d	1640	1774	1776	11	0
30	e	985	1044	1046	4	0
31	f	1161	1200	1200	11	0
32	g	1671	1726	1731	8	0
33	h	2341	2374	2374	14	0
34	j	1245	1270	1272	6	0
35	k	950	1030	1029	4	0
36	m	1021	1103	1103	6	0
37	n	999	1141	1140	7	0
38	o	1880	1911	1915	12	0
39	q	1958	2058	2058	17	0
40	r	3104	3223	3229	15	0
41	s	3097	3227	3228	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	t	1392	1444	1446	12	0
43	u	1520	1604	1605	8	0
44	l	20	9	6	0	0
45	A	68518	34651	34636	521	0
46	B	3480	1763	1764	20	0
47	A	50	0	0	0	0
47	C	4	0	0	0	0
47	V	1	0	0	0	0
47	e	1	0	0	0	0
47	j	1	0	0	0	0
47	q	1	0	0	0	0
47	r	2	0	0	0	0
48	A	83	0	0	0	0
48	B	2	0	0	0	0
48	D	1	0	0	0	0
48	R	1	0	0	0	0
48	T	1	0	0	0	0
48	Z	1	0	0	0	0
48	f	1	0	0	0	0
48	g	1	0	0	0	0
48	o	2	0	0	0	0
48	r	1	0	0	0	0
49	V	1	0	0	0	0
49	Y	1	0	0	0	0
49	Z	1	0	0	0	0
49	a	1	0	0	0	0
50	A	10	0	19	3	0
51	A	28	52	52	1	0
52	A	3376	0	0	161	0
52	B	168	0	0	8	0
52	C	88	0	0	2	0
52	D	47	0	0	1	0
52	F	105	0	0	2	0
52	G	53	0	0	0	0
52	H	11	0	0	0	0
52	I	13	0	0	0	0
52	J	27	0	0	2	0
52	M	2	0	0	0	0
52	N	8	0	0	1	0
52	O	26	0	0	2	0
52	Q	3	0	0	0	0
52	R	42	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	S	5	0	0	0	0
52	T	12	0	0	0	0
52	U	3	0	0	0	0
52	V	30	0	0	1	0
52	W	1	0	0	0	0
52	X	6	0	0	0	0
52	Y	2	0	0	1	0
52	Z	25	0	0	1	0
52	a	6	0	0	1	0
52	b	1	0	0	0	0
52	c	10	0	0	1	0
52	d	12	0	0	0	0
52	e	13	0	0	0	0
52	f	41	0	0	1	0
52	g	16	0	0	2	0
52	h	19	0	0	0	0
52	j	15	0	0	1	0
52	k	16	0	0	0	0
52	m	8	0	0	0	0
52	n	17	0	0	1	0
52	o	56	0	0	2	0
52	q	27	0	0	1	0
52	r	27	0	0	2	0
52	s	66	0	0	3	0
52	t	1	0	0	0	0
52	u	2	0	0	0	0
All	All	130857	92404	92436	753	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 4.

The worst 5 of 753 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)
1:C:39:C:C6	42:t:48:VAL:HG21	1.97	0.98
45:A:2468:G:O2'	45:A:2469:G:O5'	1.81	0.97
45:A:884:U:OP2	45:A:1913:C:O2'	1.89	0.91
45:A:40:OMC:HM22	45:A:2806:A:H61	1.37	0.89
45:A:3094:C:O2'	45:A:3096:G:OP2	1.91	0.88

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	198/206 (96%)	195 (98%)	3 (2%)	0	100	100
3	E	128/134 (96%)	127 (99%)	1 (1%)	0	100	100
4	F	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
5	G	184/187 (98%)	182 (99%)	2 (1%)	0	100	100
6	H	180/214 (84%)	180 (100%)	0	0	100	100
7	I	175/178 (98%)	174 (99%)	1 (1%)	0	100	100
8	J	161/164 (98%)	158 (98%)	3 (2%)	0	100	100
9	K	97/127 (76%)	96 (99%)	1 (1%)	0	100	100
10	L	60/164 (37%)	60 (100%)	0	0	100	100
11	M	132/135 (98%)	131 (99%)	1 (1%)	0	100	100
12	N	140/143 (98%)	137 (98%)	3 (2%)	0	100	100
13	O	47/61 (77%)	44 (94%)	3 (6%)	0	100	100
14	P	95/113 (84%)	94 (99%)	1 (1%)	0	100	100
15	Q	106/120 (88%)	106 (100%)	0	0	100	100
16	R	124/133 (93%)	124 (100%)	0	0	100	100
17	S	109/112 (97%)	108 (99%)	1 (1%)	0	100	100
18	T	112/120 (93%)	112 (100%)	0	0	100	100
19	U	96/110 (87%)	96 (100%)	0	0	100	100
20	V	84/95 (88%)	83 (99%)	1 (1%)	0	100	100
21	W	66/69 (96%)	66 (100%)	0	0	100	100
22	X	48/51 (94%)	48 (100%)	0	0	100	100
23	Y	49/128 (38%)	49 (100%)	0	0	100	100
24	p	23/25 (92%)	23 (100%)	0	0	100	100
25	Z	96/105 (91%)	95 (99%)	1 (1%)	0	100	100
26	a	89/92 (97%)	85 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	b	204/230 (89%)	200 (98%)	4 (2%)	0	100	100
28	c	231/258 (90%)	229 (99%)	2 (1%)	0	100	100
29	d	203/206 (98%)	203 (100%)	0	0	100	100
30	e	129/140 (92%)	126 (98%)	3 (2%)	0	100	100
31	f	145/148 (98%)	138 (95%)	6 (4%)	1 (1%)	18	13
32	g	205/221 (93%)	202 (98%)	3 (2%)	0	100	100
33	h	286/301 (95%)	281 (98%)	5 (2%)	0	100	100
34	j	152/175 (87%)	150 (99%)	2 (1%)	0	100	100
35	k	115/154 (75%)	115 (100%)	0	0	100	100
36	m	124/146 (85%)	122 (98%)	2 (2%)	0	100	100
37	n	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
38	o	243/260 (94%)	234 (96%)	9 (4%)	0	100	100
39	q	236/242 (98%)	231 (98%)	5 (2%)	0	100	100
40	r	384/389 (99%)	379 (99%)	5 (1%)	0	100	100
41	s	396/405 (98%)	391 (99%)	5 (1%)	0	100	100
42	t	170/181 (94%)	168 (99%)	2 (1%)	0	100	100
43	u	189/194 (97%)	188 (100%)	1 (0%)	0	100	100
All	All	6332/6963 (91%)	6244 (99%)	87 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
31	f	15	VAL

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	D	165/171 (96%)	165 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	114/117 (97%)	114 (100%)	0	100	100
4	F	176/177 (99%)	175 (99%)	1 (1%)	78	84
5	G	154/155 (99%)	154 (100%)	0	100	100
6	H	160/182 (88%)	160 (100%)	0	100	100
7	I	163/164 (99%)	162 (99%)	1 (1%)	78	84
8	J	140/141 (99%)	139 (99%)	1 (1%)	76	81
9	K	91/109 (84%)	91 (100%)	0	100	100
10	L	57/133 (43%)	57 (100%)	0	100	100
11	M	117/118 (99%)	117 (100%)	0	100	100
12	N	123/124 (99%)	122 (99%)	1 (1%)	73	79
13	O	43/53 (81%)	43 (100%)	0	100	100
14	P	85/98 (87%)	85 (100%)	0	100	100
15	Q	95/106 (90%)	95 (100%)	0	100	100
16	R	114/121 (94%)	114 (100%)	0	100	100
17	S	98/99 (99%)	98 (100%)	0	100	100
18	T	100/104 (96%)	100 (100%)	0	100	100
19	U	83/90 (92%)	83 (100%)	0	100	100
20	V	72/77 (94%)	72 (100%)	0	100	100
21	W	64/65 (98%)	63 (98%)	1 (2%)	55	61
22	X	47/48 (98%)	47 (100%)	0	100	100
23	Y	46/114 (40%)	46 (100%)	0	100	100
24	p	24/24 (100%)	24 (100%)	0	100	100
25	Z	86/92 (94%)	86 (100%)	0	100	100
26	a	73/74 (99%)	73 (100%)	0	100	100
27	b	175/194 (90%)	175 (100%)	0	100	100
28	c	202/221 (91%)	202 (100%)	0	100	100
29	d	173/174 (99%)	172 (99%)	1 (1%)	78	84
30	e	103/109 (94%)	103 (100%)	0	100	100
31	f	119/120 (99%)	119 (100%)	0	100	100
32	g	173/181 (96%)	173 (100%)	0	100	100
33	h	244/254 (96%)	243 (100%)	1 (0%)	84	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	j	135/154 (88%)	135 (100%)	0	100	100
35	k	106/134 (79%)	106 (100%)	0	100	100
36	m	115/131 (88%)	115 (100%)	0	100	100
37	n	109/110 (99%)	109 (100%)	0	100	100
38	o	190/197 (96%)	189 (100%)	1 (0%)	81	86
39	q	207/209 (99%)	207 (100%)	0	100	100
40	r	330/332 (99%)	329 (100%)	1 (0%)	86	90
41	s	326/329 (99%)	326 (100%)	0	100	100
42	t	149/157 (95%)	148 (99%)	1 (1%)	76	81
43	u	167/170 (98%)	167 (100%)	0	100	100
All	All	5513/5932 (93%)	5503 (100%)	10 (0%)	85	91

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	o	208	GLU
40	r	327	LEU
42	t	45	GLN
12	N	66	LYS
21	W	17	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
34	j	56	GLN
41	s	334	ASN
34	j	122	GLN
38	o	168	GLN
17	S	6	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	118/119 (99%)	8 (6%)	0
45	A	3192/3390 (94%)	418 (13%)	16 (0%)
46	B	162/163 (99%)	26 (16%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	3472/3672 (94%)	452 (13%)	16 (0%)

5 of 452 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	2	G
1	C	25	G
1	C	33	U
1	C	38	U
1	C	53	U

5 of 16 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
45	A	2543	A
45	A	2503	U
45	A	1027	A
45	A	2496	A
45	A	990	G

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

135 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
45	5MC	A	2873	45,48	19,22,23	4.57	8 (42%)	26,32,35	1.10	2 (7%)
45	OMC	A	2962	45	19,22,23	3.28	8 (42%)	25,31,34	0.74	0
45	OMC	A	1448	45	19,22,23	3.30	8 (42%)	25,31,34	0.74	0
45	A2M	A	1460	45	22,25,26	4.02	9 (40%)	30,36,39	2.98	13 (43%)
45	OMU	A	2424	45	19,22,23	3.27	8 (42%)	25,31,34	1.79	5 (20%)
45	A2M	A	2949	45	22,25,26	4.02	9 (40%)	30,36,39	3.03	15 (50%)
45	1MA	A	656	45	21,25,26	1.38	3 (14%)	30,37,40	1.79	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	PSU	A	2139	45	18,21,22	4.81	8 (44%)	21,30,33	1.96	5 (23%)
45	PSU	A	1133	45	18,21,22	4.83	8 (44%)	21,30,33	1.97	5 (23%)
45	PSU	A	2857	45	18,21,22	4.80	8 (44%)	21,30,33	2.03	5 (23%)
45	OMC	A	674	45	19,22,23	3.26	8 (42%)	25,31,34	0.67	0
45	PSU	A	2263	45	18,21,22	4.83	8 (44%)	21,30,33	1.98	6 (28%)
45	PSU	A	786	45	18,21,22	4.82	8 (44%)	21,30,33	1.88	5 (23%)
46	OMG	B	78	46	23,26,27	2.59	8 (34%)	32,38,41	2.27	11 (34%)
45	OMG	A	2654	45	23,26,27	2.55	9 (39%)	32,38,41	2.15	13 (40%)
45	PSU	A	2958	45	18,21,22	4.84	8 (44%)	21,30,33	1.98	5 (23%)
45	PSU	A	2978	45	18,21,22	4.81	8 (44%)	21,30,33	1.92	5 (23%)
45	PSU	A	2829	45	18,21,22	4.79	8 (44%)	21,30,33	2.01	6 (28%)
45	PSU	A	311	45,48	18,21,22	4.83	8 (44%)	21,30,33	1.91	5 (23%)
45	OMC	A	2200	45,48	19,22,23	3.31	8 (42%)	25,31,34	0.81	0
45	PSU	A	2435	45	18,21,22	4.81	8 (44%)	21,30,33	2.05	6 (28%)
45	OMG	A	2920	45	23,26,27	2.58	8 (34%)	32,38,41	2.25	11 (34%)
45	PSU	A	2317	45,48	18,21,22	4.83	8 (44%)	21,30,33	2.05	6 (28%)
45	5MC	A	2281	45	19,22,23	4.58	8 (42%)	26,32,35	0.98	2 (7%)
45	OMG	A	918	45,48	23,26,27	2.60	8 (34%)	32,38,41	2.30	10 (31%)
46	A2M	B	46	46	22,25,26	4.00	9 (40%)	30,36,39	3.01	14 (46%)
46	PSU	B	77	46	18,21,22	4.82	8 (44%)	21,30,33	2.01	5 (23%)
45	PSU	A	34	45	18,21,22	4.80	8 (44%)	21,30,33	2.06	5 (23%)
45	OMG	A	296	45	23,26,27	2.60	8 (34%)	32,38,41	2.25	11 (34%)
45	PSU	A	2261	45	18,21,22	4.83	8 (44%)	21,30,33	1.95	5 (23%)
45	UR3	A	2956	45	19,22,23	2.85	8 (42%)	26,32,35	1.62	3 (11%)
45	PSU	A	2214	45	18,21,22	4.82	8 (44%)	21,30,33	1.99	6 (28%)
45	OMG	A	1461	45	23,26,27	2.57	8 (34%)	32,38,41	2.30	12 (37%)
45	PSU	A	1002	45	18,21,22	4.84	8 (44%)	21,30,33	2.00	6 (28%)
45	PSU	A	2267	45	18,21,22	4.81	8 (44%)	21,30,33	1.98	5 (23%)
45	OMG	A	2818	45	23,26,27	2.56	9 (39%)	32,38,41	2.21	12 (37%)
45	OMU	A	2720	45	19,22,23	3.26	8 (42%)	25,31,34	1.77	5 (20%)
45	PSU	A	2137	45,48	18,21,22	4.82	8 (44%)	21,30,33	2.08	5 (23%)
45	PSU	A	464	45	18,21,22	4.84	8 (44%)	21,30,33	1.94	6 (28%)
45	A2M	A	817	45	22,25,26	3.98	9 (40%)	30,36,39	3.04	14 (46%)
45	OMU	A	2924	45,48	19,22,23	3.26	8 (42%)	25,31,34	1.79	5 (20%)
45	OMU	A	2350	45	19,22,23	3.28	8 (42%)	25,31,34	1.77	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	OMU	A	44	45,48	19,22,23	3.29	8 (42%)	25,31,34	1.74	4 (16%)
45	PSU	A	2747	45	18,21,22	4.80	8 (44%)	21,30,33	1.92	5 (23%)
45	OMU	A	2413	45,48	19,22,23	3.24	8 (42%)	25,31,34	1.68	4 (16%)
45	PSU	A	2883	45	18,21,22	4.81	8 (44%)	21,30,33	2.00	6 (28%)
45	OMG	A	2794	45	23,26,27	2.58	9 (39%)	32,38,41	2.19	11 (34%)
45	PSU	A	970	45	18,21,22	4.83	8 (44%)	21,30,33	2.01	6 (28%)
45	PSU	A	42	45,48	18,21,22	4.81	8 (44%)	21,30,33	1.96	5 (23%)
45	OMU	A	3304	45	19,22,23	3.26	8 (42%)	25,31,34	1.75	5 (20%)
45	OMG	A	2127	45	23,26,27	2.57	9 (39%)	32,38,41	2.22	13 (40%)
45	PSU	A	2926	45,48	18,21,22	4.82	8 (44%)	21,30,33	2.03	5 (23%)
45	A2M	A	2129	45	22,25,26	4.03	9 (40%)	30,36,39	3.00	13 (43%)
45	A2M	A	1144	45	22,25,26	4.01	9 (40%)	30,36,39	3.02	15 (50%)
45	OMC	A	2685	45	19,22,23	3.31	8 (42%)	25,31,34	0.72	0
45	A2M	A	2329	45	22,25,26	4.01	9 (40%)	30,36,39	2.96	15 (50%)
45	OMU	A	48	45	19,22,23	3.23	8 (42%)	25,31,34	1.71	4 (16%)
45	OMC	A	2951	45	19,22,23	3.26	8 (42%)	25,31,34	0.77	0
45	OMG	A	2394	45	23,26,27	2.58	9 (39%)	32,38,41	2.22	13 (40%)
45	A2M	A	369	45	22,25,26	4.01	9 (40%)	30,36,39	3.01	13 (43%)
45	OMU	A	787	45	19,22,23	3.26	8 (42%)	25,31,34	1.74	5 (20%)
45	PSU	A	976	45,48	18,21,22	4.83	8 (44%)	21,30,33	1.97	5 (23%)
46	PSU	B	96	46,48	18,21,22	4.83	8 (44%)	21,30,33	1.90	5 (23%)
45	OMG	A	2239	45	23,26,27	2.61	8 (34%)	32,38,41	2.29	10 (31%)
45	OMG	A	2796	45	23,26,27	2.58	8 (34%)	32,38,41	2.25	11 (34%)
45	PSU	A	2269	45	18,21,22	4.86	8 (44%)	21,30,33	1.92	5 (23%)
45	OMU	A	1068	45	19,22,23	3.27	8 (42%)	25,31,34	1.82	5 (20%)
45	PSU	A	1056	45	18,21,22	4.82	8 (44%)	21,30,33	1.99	5 (23%)
45	PSU	A	277	45	18,21,22	4.78	8 (44%)	21,30,33	1.98	5 (23%)
45	PSU	A	510	45	18,21,22	4.82	8 (44%)	21,30,33	1.99	5 (23%)
45	OMG	A	815	45	23,26,27	2.60	8 (34%)	32,38,41	2.31	11 (34%)
45	A2M	A	2914	45	22,25,26	4.01	9 (40%)	30,36,39	3.06	13 (43%)
45	OMG	A	2126	45	23,26,27	2.57	9 (39%)	32,38,41	2.24	11 (34%)
46	PSU	B	21	46,45	18,21,22	4.77	8 (44%)	21,30,33	1.98	5 (23%)
45	OMU	A	144	45	19,22,23	3.26	8 (42%)	25,31,34	1.75	4 (16%)
45	OMU	A	804	45	19,22,23	3.25	8 (42%)	25,31,34	1.77	5 (20%)
45	PSU	A	717	45	18,21,22	4.82	8 (44%)	21,30,33	1.97	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	OMC	A	2839	45	19,22,23	3.30	8 (42%)	25,31,34	0.78	0
45	PSU	A	1064	45,48	18,21,22	4.81	8 (44%)	21,30,33	1.99	5 (23%)
45	PSU	A	228	45	18,21,22	4.83	8 (44%)	21,30,33	1.99	5 (23%)
45	PSU	A	1474	45	18,21,22	4.80	8 (44%)	21,30,33	1.96	6 (28%)
45	PSU	A	2194	45,48	18,21,22	4.82	8 (44%)	21,30,33	1.96	5 (23%)
45	OMG	A	2291	45	23,26,27	2.60	8 (34%)	32,38,41	2.30	10 (31%)
45	PSU	A	2947	45,48	18,21,22	4.80	9 (50%)	21,30,33	2.01	6 (28%)
45	OMU	A	675	45	19,22,23	3.27	8 (42%)	25,31,34	1.78	5 (20%)
45	OMU	A	1894	45	19,22,23	3.26	8 (42%)	25,31,34	1.83	5 (20%)
45	PSU	A	902	45,48,47	18,21,22	4.81	8 (44%)	21,30,33	1.97	5 (23%)
45	A2M	A	886	45	22,25,26	4.01	9 (40%)	30,36,39	2.91	13 (43%)
45	OMG	A	2398	45	23,26,27	2.56	9 (39%)	32,38,41	2.21	13 (40%)
45	A2M	A	1378	45	22,25,26	4.01	9 (40%)	30,36,39	2.94	12 (40%)
45	A2M	A	2284	45	22,25,26	3.98	9 (40%)	30,36,39	3.18	15 (50%)
45	PSU	A	966	45	18,21,22	4.78	8 (44%)	21,30,33	1.87	5 (23%)
45	OMC	A	2368	45	19,22,23	3.28	8 (42%)	25,31,34	0.70	0
45	OMC	A	1849	45	19,22,23	3.27	8 (42%)	25,31,34	0.73	0
45	OMC	A	1862	45	19,22,23	3.26	8 (42%)	25,31,34	0.67	0
45	OMU	A	3289	45	19,22,23	3.26	8 (42%)	25,31,34	1.78	5 (20%)
45	PSU	A	829	45	18,21,22	4.80	8 (44%)	21,30,33	2.01	5 (23%)
45	OMC	A	1852	45	19,22,23	3.32	8 (42%)	25,31,34	0.76	0
45	OMG	A	399	45	23,26,27	2.63	8 (34%)	32,38,41	2.35	10 (31%)
45	OMU	A	2732	45	19,22,23	3.24	8 (42%)	25,31,34	1.72	4 (16%)
45	OMU	A	2738	45	19,22,23	3.27	8 (42%)	25,31,34	1.80	5 (20%)
45	PSU	A	2868	45	18,21,22	4.81	8 (44%)	21,30,33	2.01	6 (28%)
45	PSU	A	684	45	18,21,22	4.80	8 (44%)	21,30,33	1.94	5 (23%)
45	A2M	A	2643	45	22,25,26	4.01	9 (40%)	30,36,39	2.95	12 (40%)
45	PSU	A	150	45,48	18,21,22	4.81	8 (44%)	21,30,33	2.02	6 (28%)
45	OMU	A	1537	45	19,22,23	3.26	8 (42%)	25,31,34	1.72	4 (16%)
45	A2M	A	660	45	22,25,26	4.01	9 (40%)	30,36,39	3.12	15 (50%)
45	A2M	A	2259	45	22,25,26	4.05	9 (40%)	30,36,39	3.06	14 (46%)
45	PSU	A	1016	45,48	18,21,22	4.83	8 (44%)	21,30,33	2.00	5 (23%)
45	PSU	A	1134	45	18,21,22	4.78	8 (44%)	21,30,33	2.01	5 (23%)
45	UY1	A	2653	45	19,22,23	4.34	7 (36%)	21,31,34	1.99	5 (23%)
45	PSU	A	1482	45	18,21,22	4.82	8 (44%)	21,30,33	1.95	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	PSU	A	3113	45	18,21,22	4.79	8 (44%)	21,30,33	1.90	5 (23%)
45	A2M	A	2324	45	22,25,26	4.00	9 (40%)	30,36,39	3.01	14 (46%)
45	OMC	A	2340	45	19,22,23	3.28	8 (42%)	25,31,34	0.68	0
45	PSU	A	895	45	18,21,22	4.78	8 (44%)	21,30,33	1.94	5 (23%)
45	PSU	A	2419	45	18,21,22	4.81	8 (44%)	21,30,33	1.94	5 (23%)
45	OMU	A	2886	45	19,22,23	3.27	8 (42%)	25,31,34	1.74	5 (20%)
45	OMG	A	2925	45	23,26,27	2.59	8 (34%)	32,38,41	2.30	10 (31%)
45	A2M	A	827	45,48,47	22,25,26	4.04	9 (40%)	30,36,39	3.03	13 (43%)
45	OMC	A	1480	45	19,22,23	3.32	8 (42%)	25,31,34	0.72	0
45	A2M	A	2804	45	22,25,26	3.98	9 (40%)	30,36,39	3.21	15 (50%)
45	OMC	A	2882	45	19,22,23	3.29	8 (42%)	25,31,34	0.76	0
45	OMG	A	1857	45	23,26,27	2.58	8 (34%)	32,38,41	2.23	11 (34%)
45	PSU	A	2257	45	18,21,22	4.83	8 (44%)	21,30,33	2.00	5 (23%)
45	PSU	A	1685	45	18,21,22	4.83	8 (44%)	21,30,33	2.04	6 (28%)
45	PSU	A	2897	45	18,21,22	4.82	8 (44%)	21,30,33	1.94	5 (23%)
45	OMG	A	2622	45	23,26,27	2.60	8 (34%)	32,38,41	2.28	10 (31%)
45	OMC	A	40	45	19,22,23	3.27	8 (42%)	25,31,34	0.91	1 (4%)
45	A2M	A	946	45	22,25,26	4.01	9 (40%)	30,36,39	3.09	16 (53%)
45	PSU	A	2321	45,47	18,21,22	4.80	8 (44%)	21,30,33	2.02	5 (23%)
45	OMG	A	2412	45,48	23,26,27	2.59	8 (34%)	32,38,41	2.28	11 (34%)
45	PSU	A	1135	45	18,21,22	4.82	8 (44%)	21,30,33	2.00	5 (23%)
45	A2M	A	2223	45	22,25,26	4.04	9 (40%)	30,36,39	2.94	11 (36%)
45	OMC	A	2296	45	19,22,23	3.31	8 (42%)	25,31,34	0.75	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	5MC	A	2873	45,48	-	4/7/25/26	0/2/2/2
45	OMC	A	2962	45	-	0/9/27/28	0/2/2/2
45	OMC	A	1448	45	-	2/9/27/28	0/2/2/2
45	A2M	A	1460	45	-	0/9/27/28	0/3/3/3
45	OMU	A	2424	45	-	0/9/27/28	0/2/2/2
45	A2M	A	2949	45	-	0/9/27/28	0/3/3/3
45	1MA	A	656	45	-	2/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	PSU	A	2139	45	-	0/7/25/26	0/2/2/2
45	PSU	A	1133	45	-	0/7/25/26	0/2/2/2
45	PSU	A	2857	45	-	0/7/25/26	0/2/2/2
45	OMC	A	674	45	-	0/9/27/28	0/2/2/2
45	PSU	A	2263	45	-	0/7/25/26	0/2/2/2
45	PSU	A	786	45	-	1/7/25/26	0/2/2/2
46	OMG	B	78	46	-	2/9/27/28	0/3/3/3
45	OMG	A	2654	45	-	0/9/27/28	0/3/3/3
45	PSU	A	2958	45	-	0/7/25/26	0/2/2/2
45	PSU	A	2978	45	-	0/7/25/26	0/2/2/2
45	PSU	A	2829	45	-	0/7/25/26	0/2/2/2
45	PSU	A	311	45,48	-	0/7/25/26	0/2/2/2
45	OMC	A	2200	45,48	-	4/9/27/28	0/2/2/2
45	PSU	A	2435	45	-	0/7/25/26	0/2/2/2
45	OMG	A	2920	45	-	0/9/27/28	0/3/3/3
45	PSU	A	2317	45,48	-	3/7/25/26	0/2/2/2
45	5MC	A	2281	45	-	0/7/25/26	0/2/2/2
45	OMG	A	918	45,48	-	2/9/27/28	0/3/3/3
46	A2M	B	46	46	-	0/9/27/28	0/3/3/3
46	PSU	B	77	46	-	0/7/25/26	0/2/2/2
45	PSU	A	34	45	-	0/7/25/26	0/2/2/2
45	OMG	A	296	45	-	2/9/27/28	0/3/3/3
45	PSU	A	2261	45	-	1/7/25/26	0/2/2/2
45	UR3	A	2956	45	-	2/7/25/26	0/2/2/2
45	PSU	A	2214	45	-	0/7/25/26	0/2/2/2
45	OMG	A	1461	45	-	1/9/27/28	0/3/3/3
45	PSU	A	1002	45	-	2/7/25/26	0/2/2/2
45	PSU	A	2267	45	-	0/7/25/26	0/2/2/2
45	OMG	A	2818	45	-	0/9/27/28	0/3/3/3
45	OMU	A	2720	45	-	0/9/27/28	0/2/2/2
45	PSU	A	2137	45,48	-	0/7/25/26	0/2/2/2
45	PSU	A	464	45	-	0/7/25/26	0/2/2/2
45	A2M	A	817	45	-	0/9/27/28	0/3/3/3
45	OMU	A	2924	45,48	-	0/9/27/28	0/2/2/2
45	OMU	A	2350	45	-	0/9/27/28	0/2/2/2
45	OMU	A	44	45,48	-	0/9/27/28	0/2/2/2
45	PSU	A	2747	45	-	0/7/25/26	0/2/2/2
45	OMU	A	2413	45,48	-	2/9/27/28	0/2/2/2
45	PSU	A	2883	45	-	0/7/25/26	0/2/2/2
45	OMG	A	2794	45	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	PSU	A	970	45	-	1/7/25/26	0/2/2/2
45	PSU	A	42	45,48	-	0/7/25/26	0/2/2/2
45	OMU	A	3304	45	-	0/9/27/28	0/2/2/2
45	OMG	A	2127	45	-	0/9/27/28	0/3/3/3
45	PSU	A	2926	45,48	-	3/7/25/26	0/2/2/2
45	A2M	A	2129	45	-	0/9/27/28	0/3/3/3
45	A2M	A	1144	45	-	0/9/27/28	0/3/3/3
45	OMC	A	2685	45	-	0/9/27/28	0/2/2/2
45	A2M	A	2329	45	-	0/9/27/28	0/3/3/3
45	OMU	A	48	45	-	0/9/27/28	0/2/2/2
45	OMC	A	2951	45	-	0/9/27/28	0/2/2/2
45	OMG	A	2394	45	-	0/9/27/28	0/3/3/3
45	A2M	A	369	45	-	1/9/27/28	0/3/3/3
45	OMU	A	787	45	-	0/9/27/28	0/2/2/2
45	PSU	A	976	45,48	-	0/7/25/26	0/2/2/2
46	PSU	B	96	46,48	-	2/7/25/26	0/2/2/2
45	OMG	A	2239	45	-	0/9/27/28	0/3/3/3
45	OMG	A	2796	45	-	0/9/27/28	0/3/3/3
45	PSU	A	2269	45	-	2/7/25/26	0/2/2/2
45	OMU	A	1068	45	-	0/9/27/28	0/2/2/2
45	PSU	A	1056	45	-	0/7/25/26	0/2/2/2
45	PSU	A	277	45	-	0/7/25/26	0/2/2/2
45	PSU	A	510	45	-	0/7/25/26	0/2/2/2
45	OMG	A	815	45	-	0/9/27/28	0/3/3/3
45	A2M	A	2914	45	-	5/9/27/28	0/3/3/3
45	OMG	A	2126	45	-	0/9/27/28	0/3/3/3
46	PSU	B	21	46,45	-	0/7/25/26	0/2/2/2
45	OMU	A	144	45	-	1/9/27/28	0/2/2/2
45	OMU	A	804	45	-	0/9/27/28	0/2/2/2
45	PSU	A	717	45	-	0/7/25/26	0/2/2/2
45	OMC	A	2839	45	-	0/9/27/28	0/2/2/2
45	PSU	A	1064	45,48	-	0/7/25/26	0/2/2/2
45	PSU	A	228	45	-	2/7/25/26	0/2/2/2
45	PSU	A	1474	45	-	0/7/25/26	0/2/2/2
45	PSU	A	2194	45,48	-	0/7/25/26	0/2/2/2
45	OMG	A	2291	45	-	2/9/27/28	0/3/3/3
45	PSU	A	2947	45,48	-	2/7/25/26	0/2/2/2
45	OMU	A	675	45	-	0/9/27/28	0/2/2/2
45	OMU	A	1894	45	-	0/9/27/28	0/2/2/2
45	PSU	A	902	45,48,47	-	0/7/25/26	0/2/2/2
45	A2M	A	886	45	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	OMG	A	2398	45	-	0/9/27/28	0/3/3/3
45	A2M	A	1378	45	-	2/9/27/28	0/3/3/3
45	A2M	A	2284	45	-	3/9/27/28	0/3/3/3
45	PSU	A	966	45	-	0/7/25/26	0/2/2/2
45	OMC	A	2368	45	-	2/9/27/28	0/2/2/2
45	OMC	A	1849	45	-	0/9/27/28	0/2/2/2
45	OMC	A	1862	45	-	0/9/27/28	0/2/2/2
45	OMU	A	3289	45	-	0/9/27/28	0/2/2/2
45	PSU	A	829	45	-	0/7/25/26	0/2/2/2
45	OMC	A	1852	45	-	0/9/27/28	0/2/2/2
45	OMG	A	399	45	-	2/9/27/28	0/3/3/3
45	OMU	A	2732	45	-	0/9/27/28	0/2/2/2
45	OMU	A	2738	45	-	0/9/27/28	0/2/2/2
45	PSU	A	2868	45	-	0/7/25/26	0/2/2/2
45	PSU	A	684	45	-	0/7/25/26	0/2/2/2
45	A2M	A	2643	45	-	0/9/27/28	0/3/3/3
45	PSU	A	150	45,48	-	0/7/25/26	0/2/2/2
45	OMU	A	1537	45	-	0/9/27/28	0/2/2/2
45	A2M	A	660	45	-	2/9/27/28	0/3/3/3
45	A2M	A	2259	45	-	2/9/27/28	0/3/3/3
45	PSU	A	1016	45,48	-	0/7/25/26	0/2/2/2
45	PSU	A	1134	45	-	0/7/25/26	0/2/2/2
45	UY1	A	2653	45	-	0/9/27/28	0/2/2/2
45	PSU	A	1482	45	-	0/7/25/26	0/2/2/2
45	PSU	A	3113	45	-	0/7/25/26	0/2/2/2
45	A2M	A	2324	45	-	0/9/27/28	0/3/3/3
45	OMC	A	2340	45	-	0/9/27/28	0/2/2/2
45	PSU	A	895	45	-	0/7/25/26	0/2/2/2
45	PSU	A	2419	45	-	0/7/25/26	0/2/2/2
45	OMU	A	2886	45	-	0/9/27/28	0/2/2/2
45	OMG	A	2925	45	-	0/9/27/28	0/3/3/3
45	A2M	A	827	45,48,47	-	2/9/27/28	0/3/3/3
45	OMC	A	1480	45	-	0/9/27/28	0/2/2/2
45	A2M	A	2804	45	-	4/9/27/28	0/3/3/3
45	OMC	A	2882	45	-	0/9/27/28	0/2/2/2
45	OMG	A	1857	45	-	0/9/27/28	0/3/3/3
45	PSU	A	2257	45	-	0/7/25/26	0/2/2/2
45	PSU	A	1685	45	-	0/7/25/26	0/2/2/2
45	PSU	A	2897	45	-	0/7/25/26	0/2/2/2
45	OMG	A	2622	45	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	OMC	A	40	45	-	1/9/27/28	0/2/2/2
45	A2M	A	946	45	-	0/9/27/28	0/3/3/3
45	PSU	A	2321	45,47	-	2/7/25/26	0/2/2/2
45	OMG	A	2412	45,48	-	1/9/27/28	0/3/3/3
45	PSU	A	1135	45	-	0/7/25/26	0/2/2/2
45	A2M	A	2223	45	-	0/9/27/28	0/3/3/3
45	OMC	A	2296	45	-	0/9/27/28	0/2/2/2

The worst 5 of 1102 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	2269	PSU	C6-C5	12.93	1.49	1.35
45	A	1002	PSU	C6-C5	12.89	1.49	1.35
45	A	2317	PSU	C6-C5	12.89	1.49	1.35
45	A	311	PSU	C6-C5	12.87	1.49	1.35
45	A	2137	PSU	C6-C5	12.87	1.49	1.35

The worst 5 of 902 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	A	2284	A2M	N6-C6-N1	-7.01	102.76	118.38
45	A	946	A2M	N6-C6-N1	-6.91	102.99	118.38
45	A	2804	A2M	C4-N9-C1'	-6.78	110.78	126.63
45	A	817	A2M	N6-C6-N1	-6.78	103.29	118.38
45	A	660	A2M	N6-C6-N1	-6.74	103.36	118.38

There are no chirality outliers.

5 of 74 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	B	78	OMG	O4'-C4'-C5'-O5'
46	B	78	OMG	C3'-C4'-C5'-O5'
46	B	96	PSU	O4'-C4'-C5'-O5'
45	A	40	OMC	C3'-C2'-O2'-CM2
45	A	296	OMG	O4'-C4'-C5'-O5'

There are no ring outliers.

38 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	A	2873	5MC	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	A	2962	OMC	1	0
45	A	1448	OMC	3	0
45	A	1460	A2M	1	0
45	A	656	1MA	1	0
45	A	674	OMC	3	0
46	B	78	OMG	1	0
45	A	2317	PSU	1	0
45	A	918	OMG	1	0
45	A	34	PSU	1	0
45	A	2261	PSU	1	0
45	A	464	PSU	1	0
45	A	2747	PSU	1	0
45	A	2413	OMU	1	0
45	A	2883	PSU	1	0
45	A	2794	OMG	1	0
45	A	2127	OMG	1	0
45	A	2951	OMC	1	0
45	A	369	A2M	2	0
45	A	2839	OMC	1	0
45	A	2947	PSU	1	0
45	A	675	OMU	1	0
45	A	2398	OMG	1	0
45	A	1378	A2M	1	0
45	A	2284	A2M	2	0
45	A	2368	OMC	1	0
45	A	3289	OMU	1	0
45	A	2732	OMU	1	0
45	A	660	A2M	2	0
45	A	2653	UY1	1	0
45	A	1482	PSU	1	0
45	A	2886	OMU	3	0
45	A	827	A2M	1	0
45	A	2804	A2M	2	0
45	A	2882	OMC	1	0
45	A	40	OMC	3	0
45	A	2412	OMG	1	0
45	A	2223	A2M	2	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 161 ligands modelled in this entry, 158 are monoatomic - leaving 3 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
51	SPM	A	3452	-	13,13,13	0.37	0	12,12,12	1.02	0
51	SPM	A	3453	-	13,13,13	0.37	0	12,12,12	1.01	0
50	SPD	A	3451	-	9,9,9	0.32	0	8,8,8	0.50	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	SPM	A	3452	-	-	5/11/11/11	-
51	SPM	A	3453	-	-	6/11/11/11	-
50	SPD	A	3451	-	-	2/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
51	A	3453	SPM	N10-C11-C12-C13
51	A	3453	SPM	C7-C8-C9-N10
51	A	3453	SPM	C2-C3-C4-N5
51	A	3453	SPM	N5-C6-C7-C8
51	A	3452	SPM	C3-C4-N5-C6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	A	3452	SPM	1	0
50	A	3451	SPD	3	0

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.

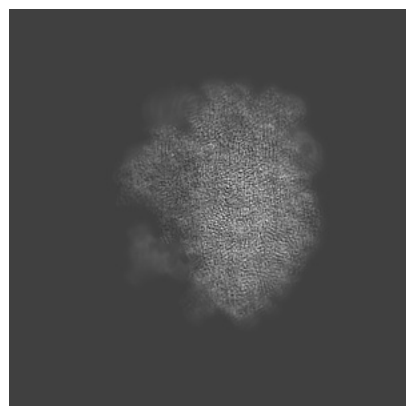
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15773. These allow visual inspection of the internal detail of the map and identification of artifacts.

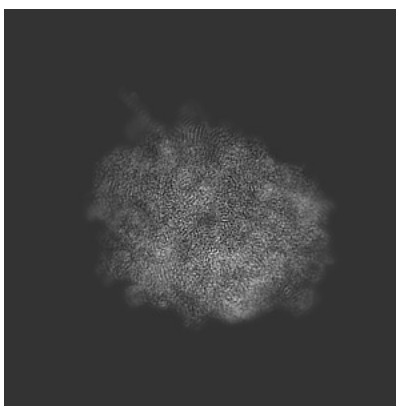
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

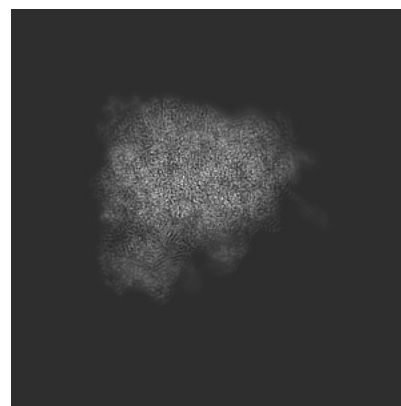
6.1.1 Primary map



X

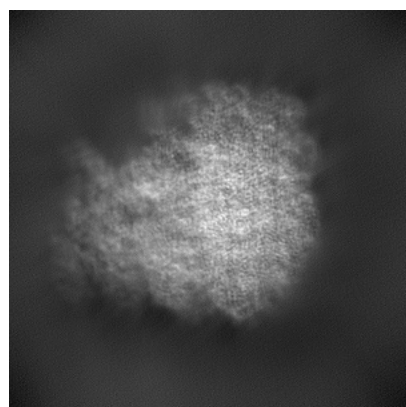


Y

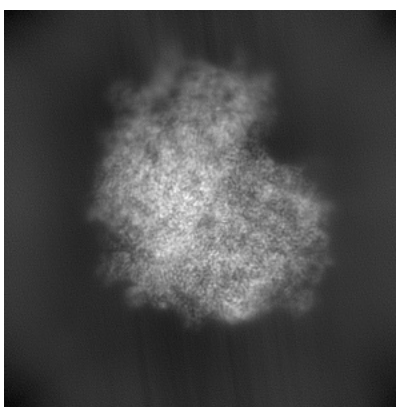


Z

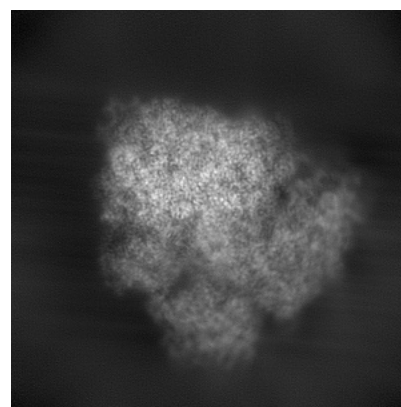
6.1.2 Raw map



X



Y

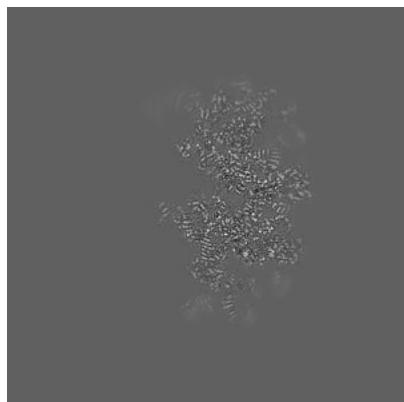


Z

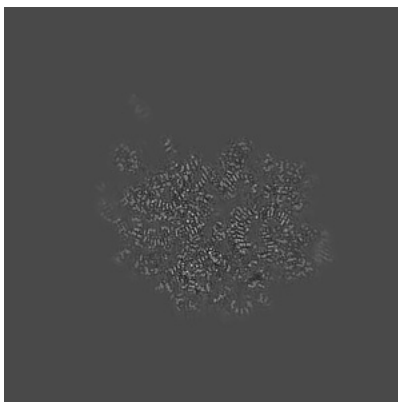
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

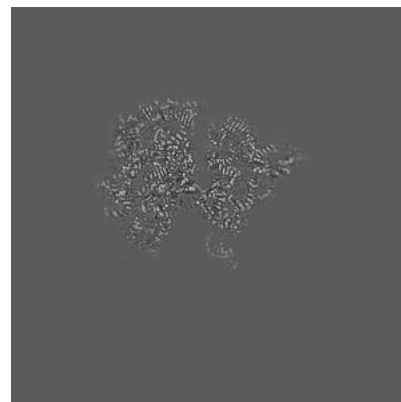
6.2.1 Primary map



X Index: 225

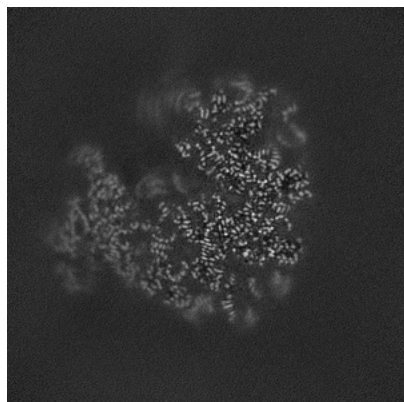


Y Index: 225

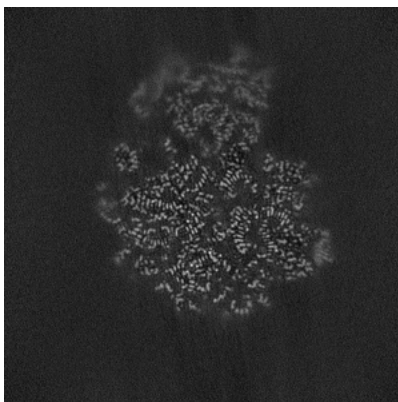


Z Index: 225

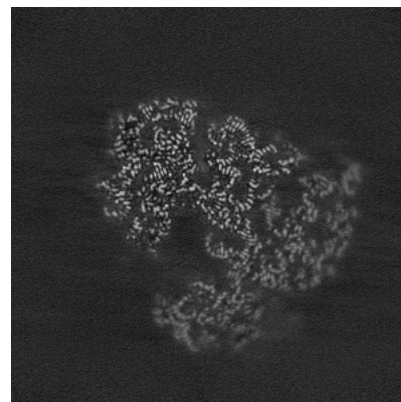
6.2.2 Raw map



X Index: 225



Y Index: 225

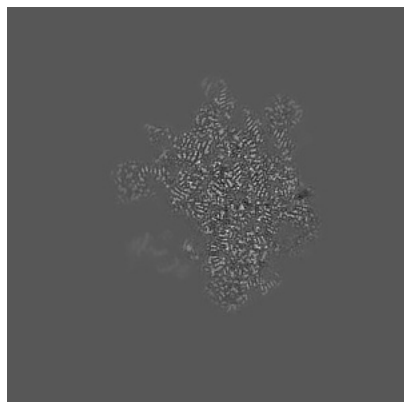


Z Index: 225

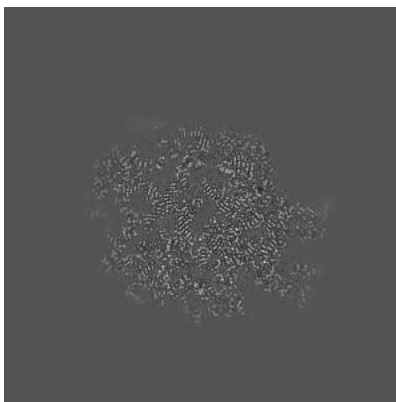
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

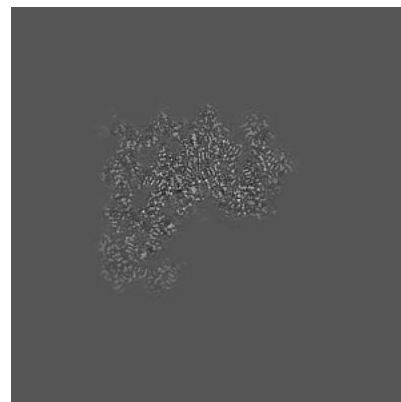
6.3.1 Primary map



X Index: 169

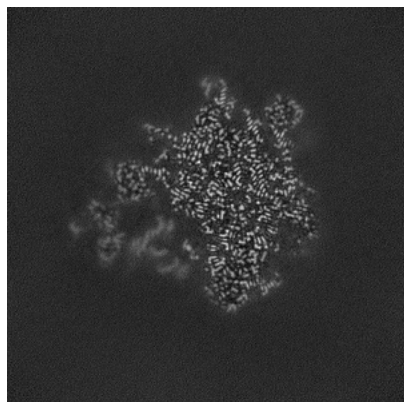


Y Index: 262

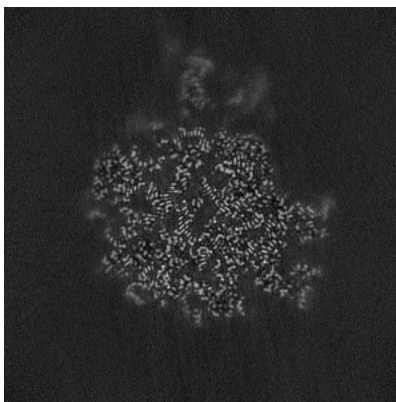


Z Index: 250

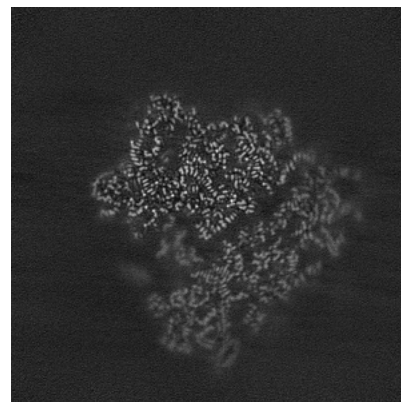
6.3.2 Raw map



X Index: 169



Y Index: 262

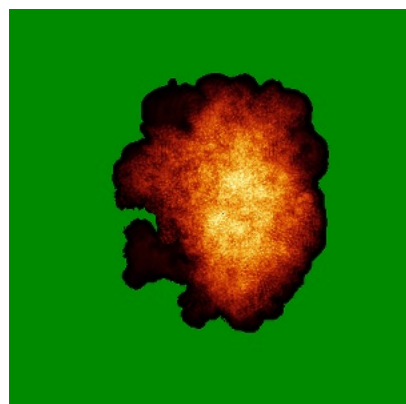


Z Index: 206

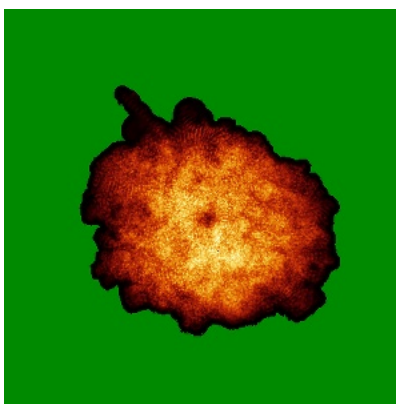
The images above show the largest variance slices of the map in three orthogonal directions.

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

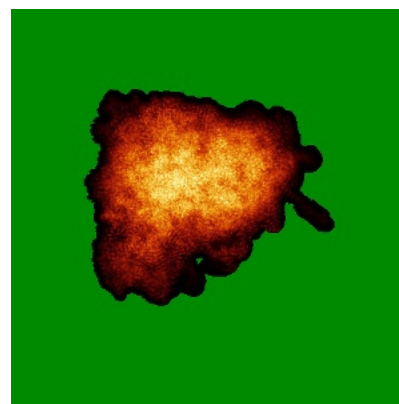
6.4.1 Primary map



X

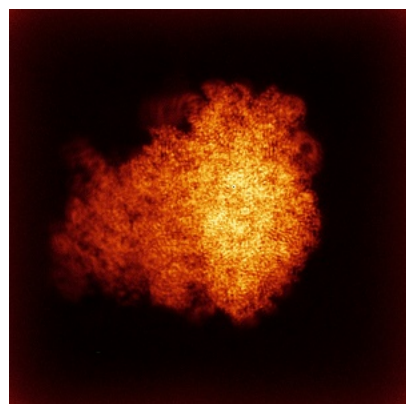


Y

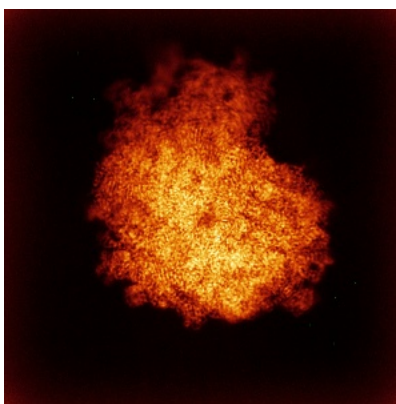


Z

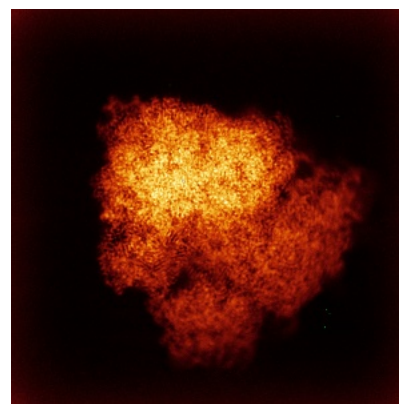
6.4.2 Raw map



X



Y

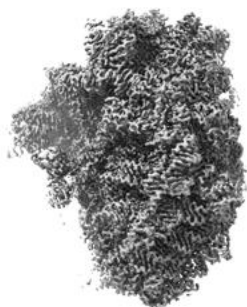


Z

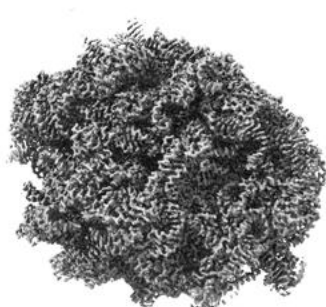
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

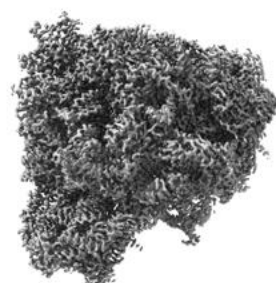
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

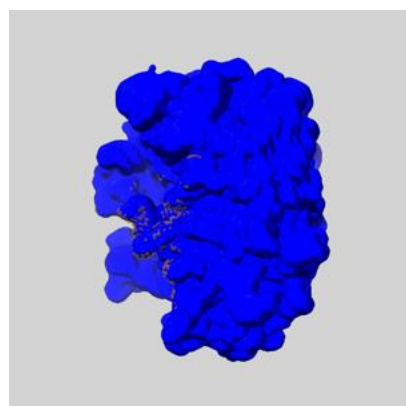
6.6 Mask visualisation [i](#)

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

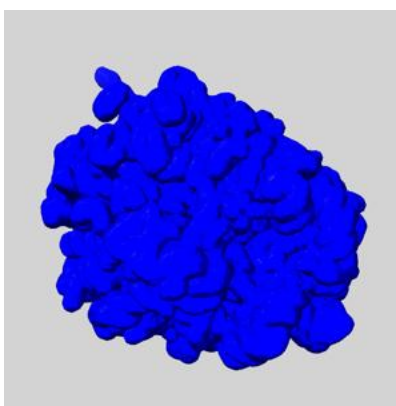
A mask typically either:

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

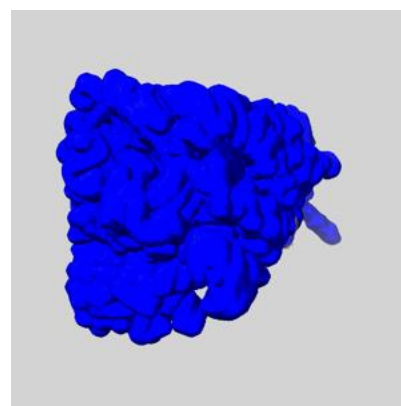
6.6.1 emd_15773_msk_1.map [i](#)



X



Y

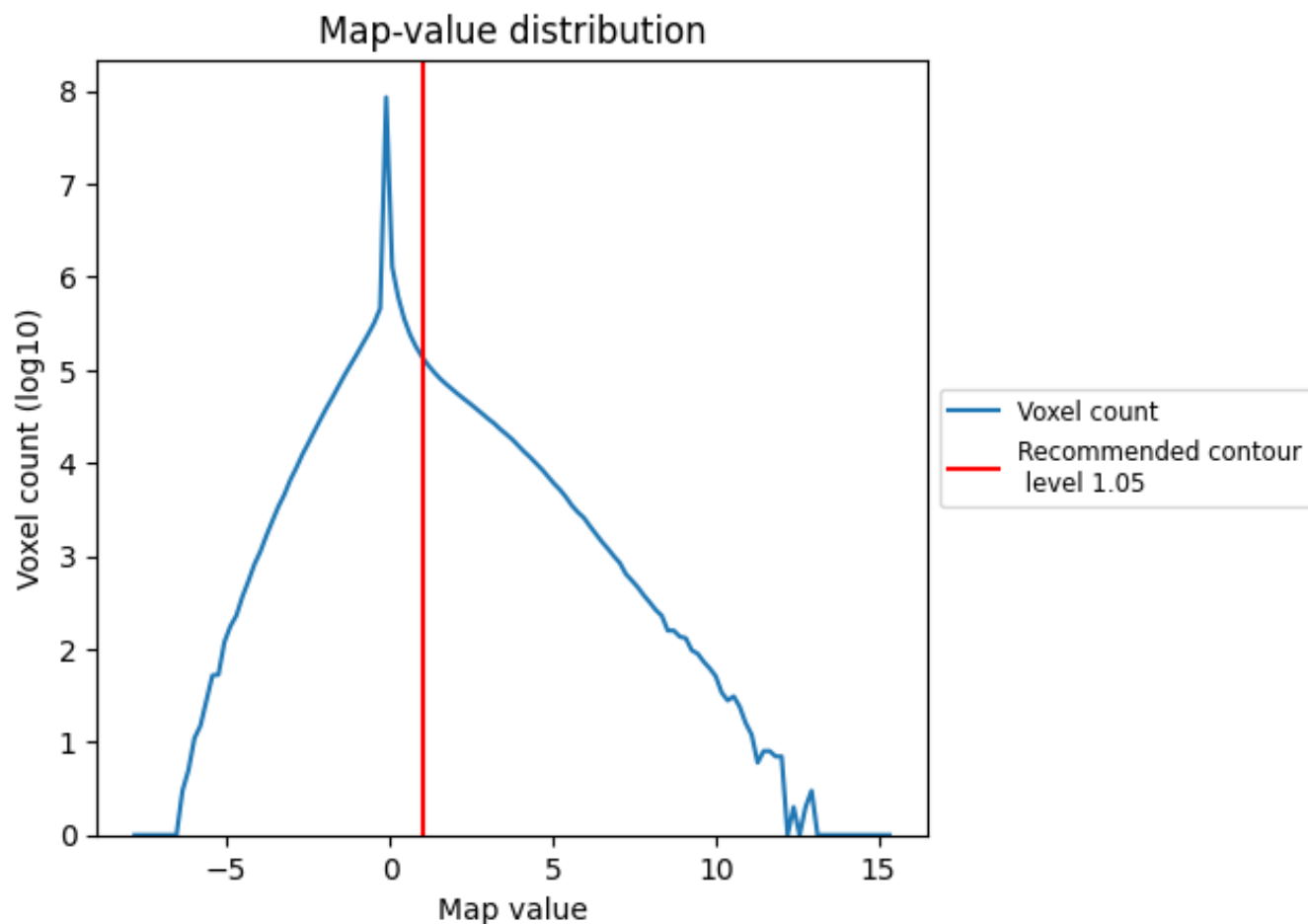


Z

7 Map analysis [i](#)

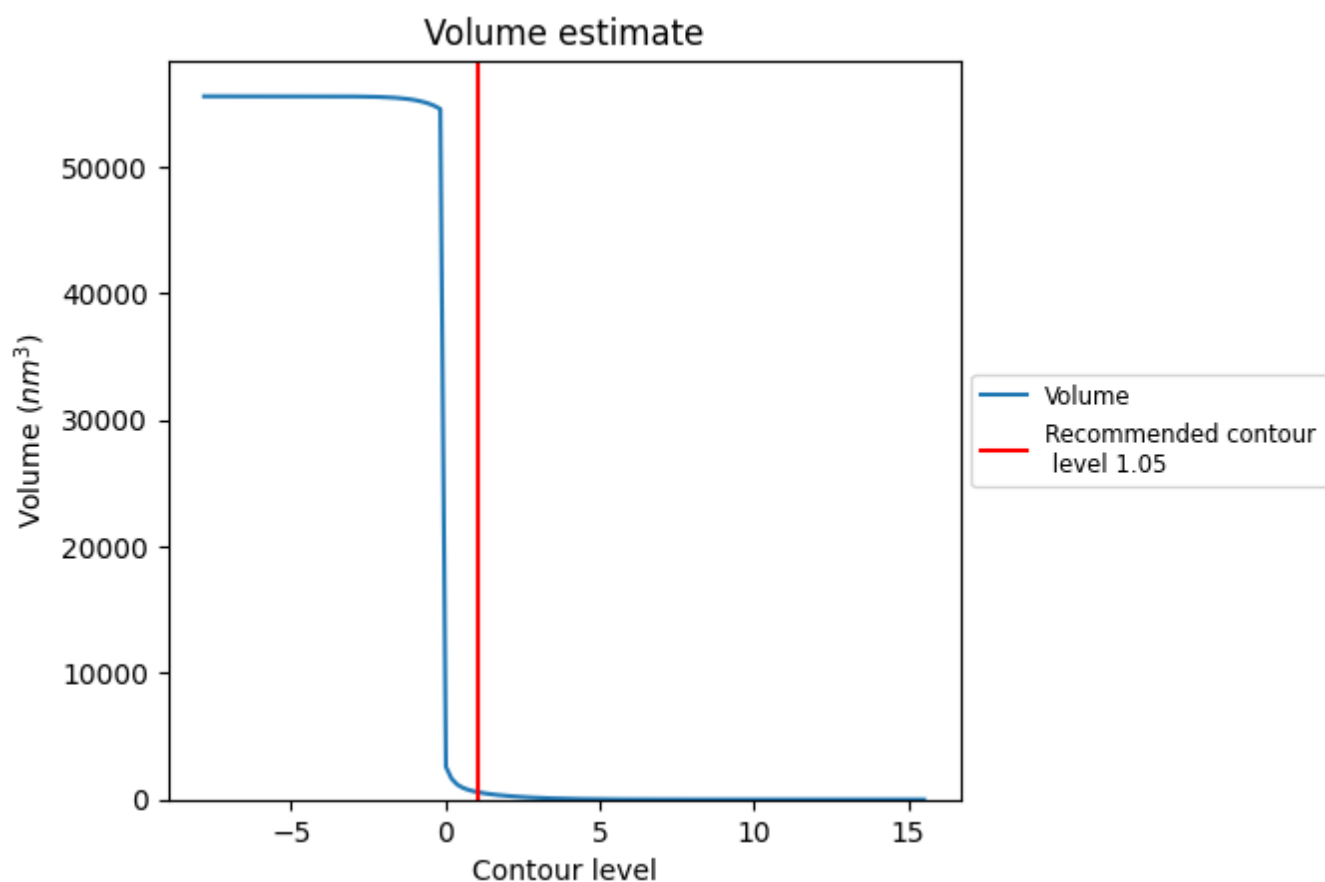
This section contains the results of statistical analysis of the map.

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.

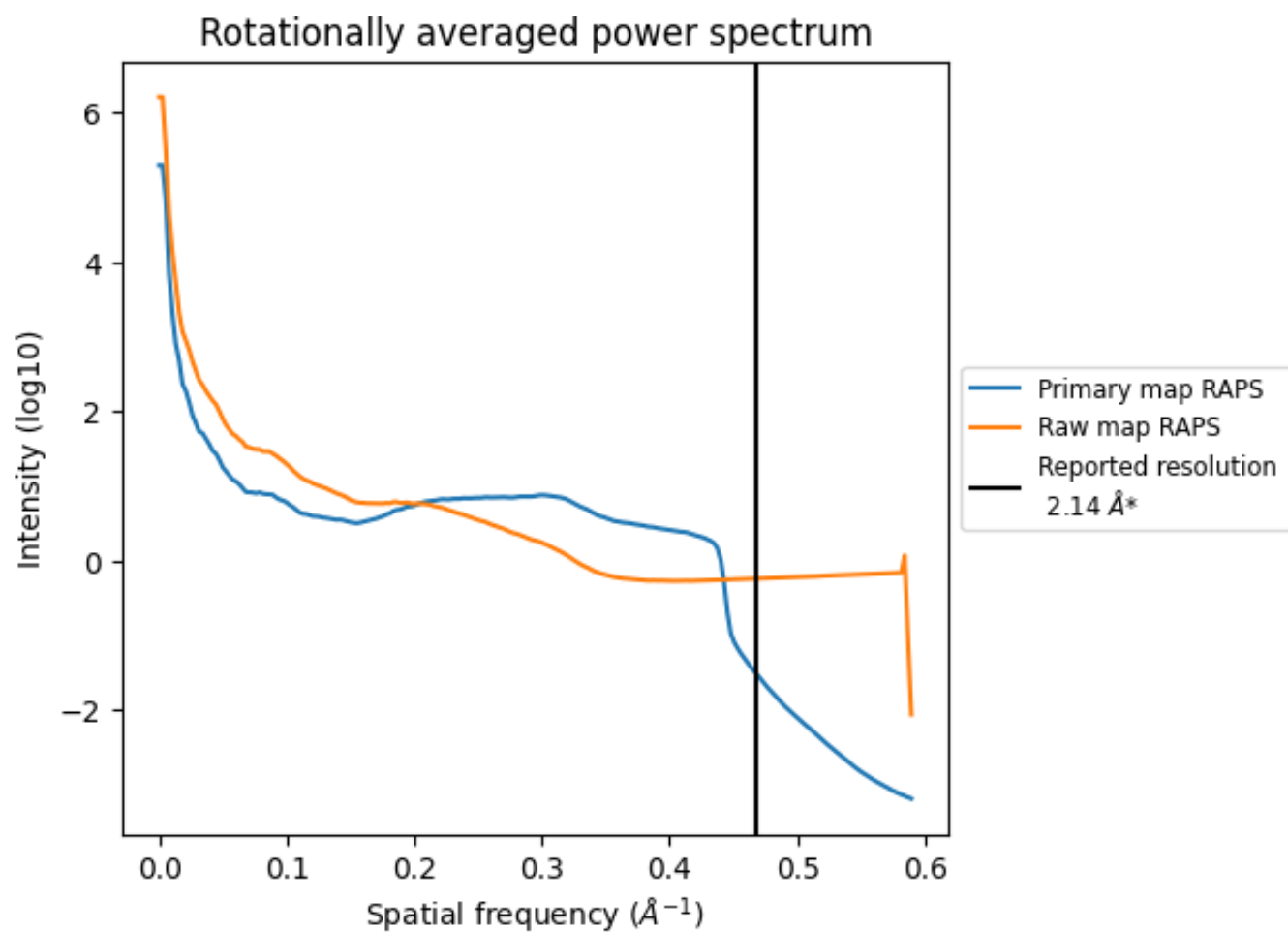
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 586 nm³; this corresponds to an approximate mass of 530 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 ⓘ

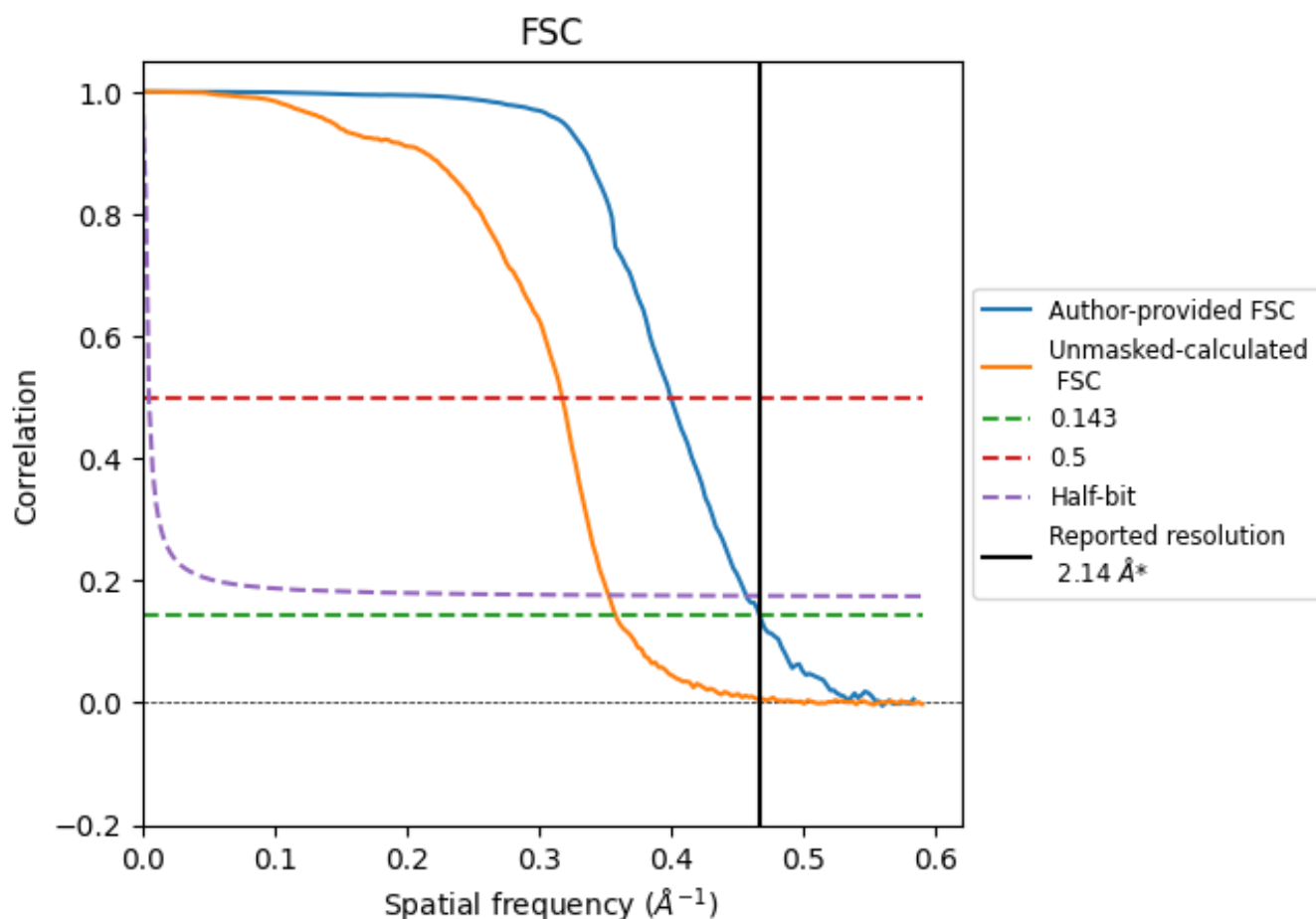


*Reported resolution corresponds to spatial frequency of $0.467 \text{ \AA}^{-1}$

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 $0.467 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

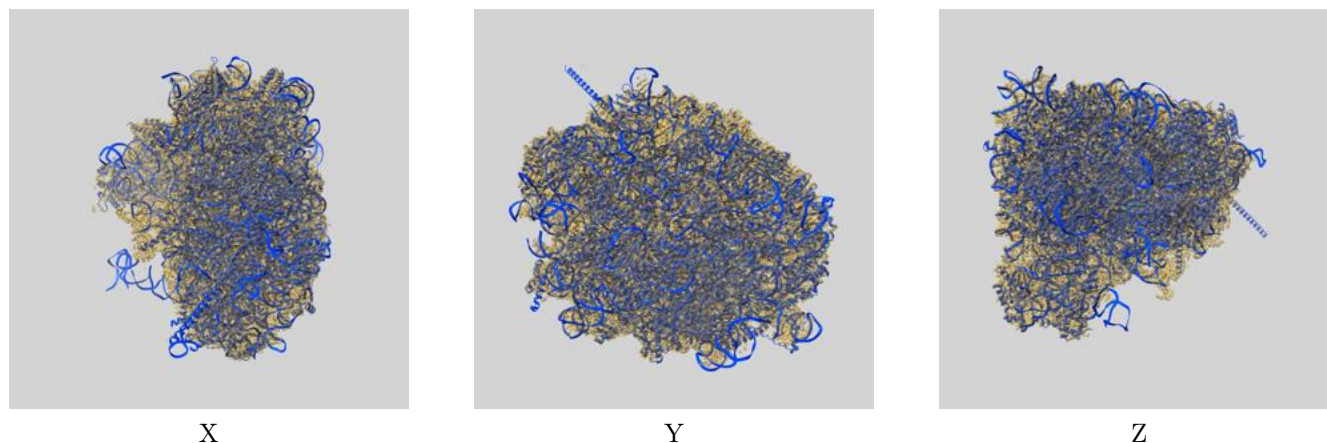
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.14	-	-
Author-provided FSC curve	2.14	2.50	2.19
Unmasked-calculated*	2.79	3.15	2.84

*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 2.14 by more than 10 %

9 Map-model fit [i](#)

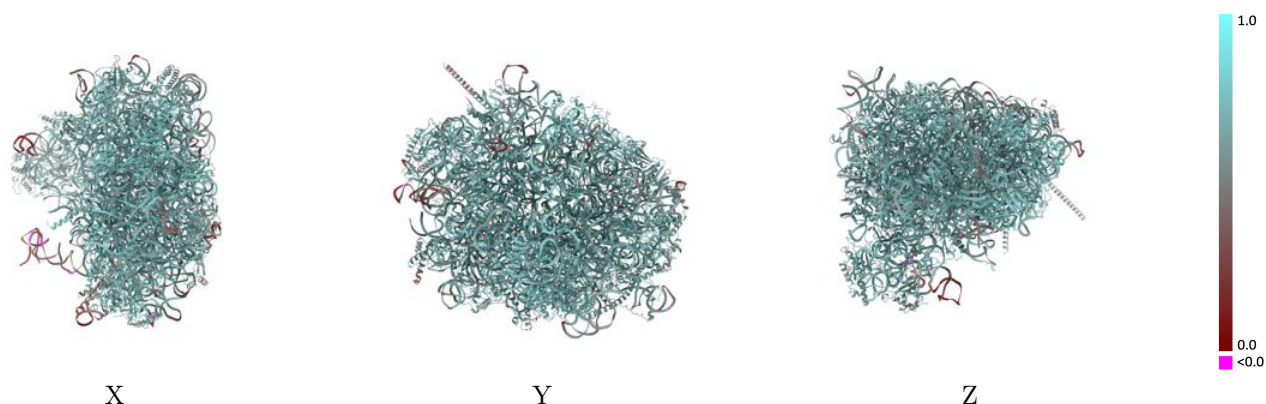
This section contains information regarding the fit between EMDB map EMD-15773 and PDB model 8AZW. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



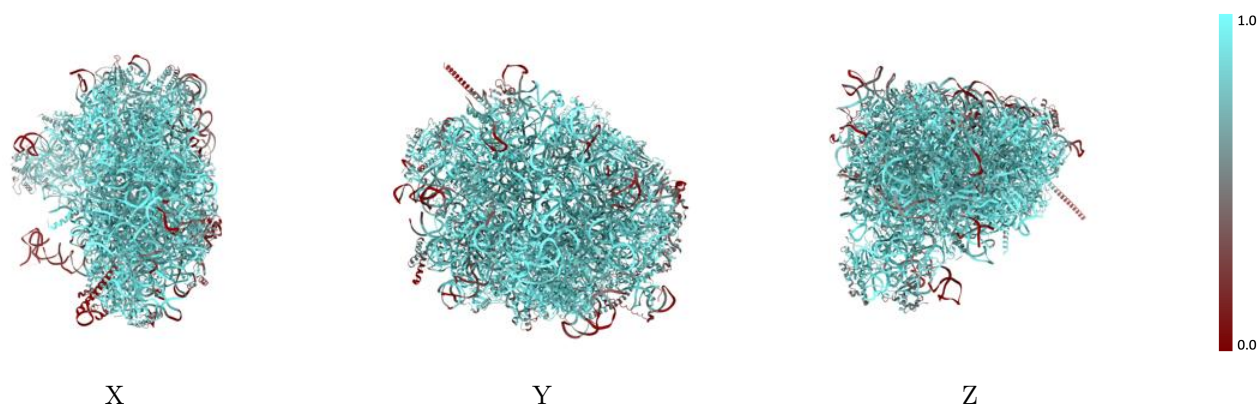
The images above show the 3D surface view of the map at the recommended contour level 1.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



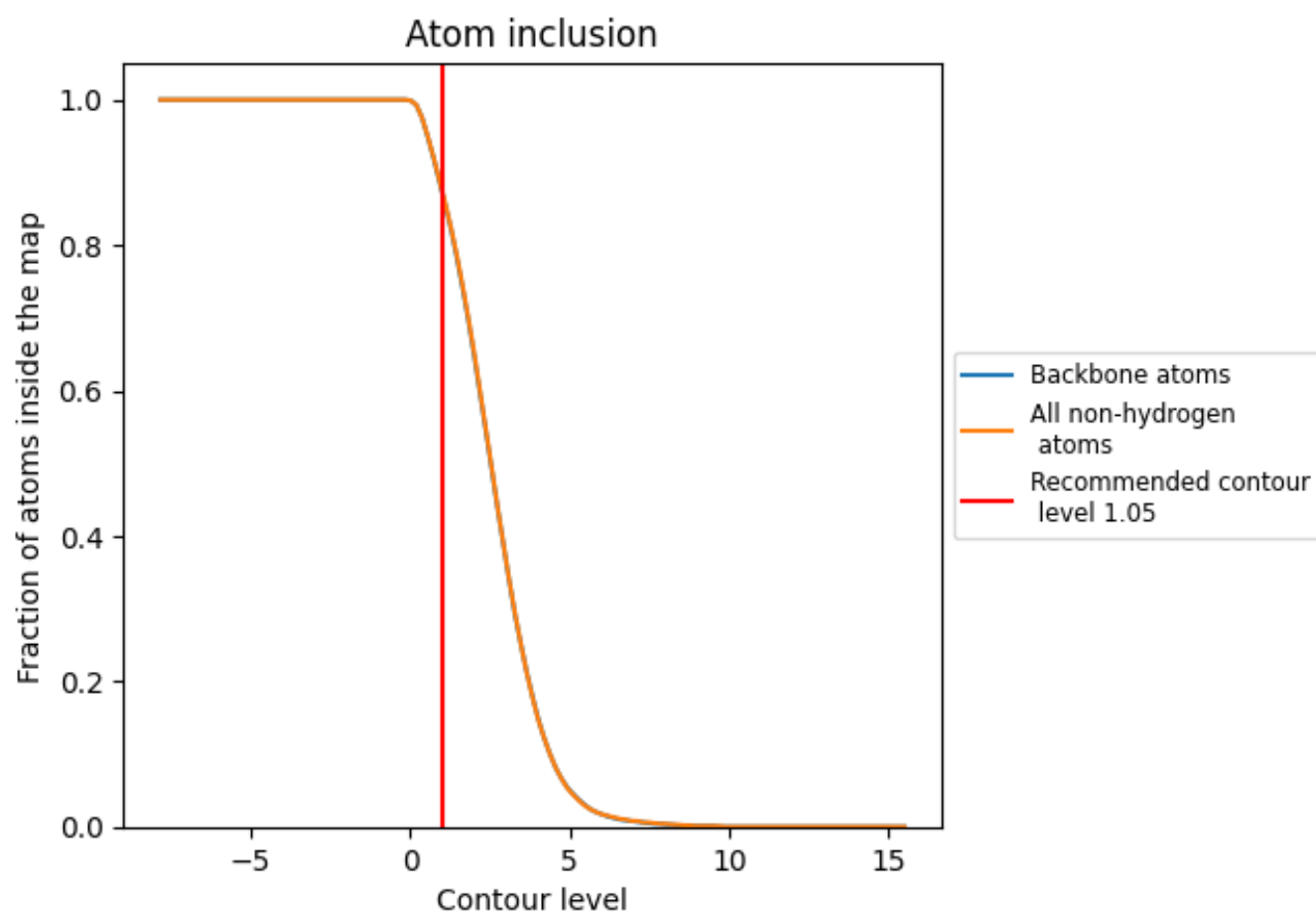
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 87% 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 (1.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8680	 0.6750
A	 0.8750	 0.6650
B	 0.8640	 0.6600
C	 0.9510	 0.6770
D	 0.8720	 0.6980
E	 0.8390	 0.6830
F	 0.9900	 0.7400
G	 0.9570	 0.7290
H	 0.7360	 0.6410
I	 0.9230	 0.7090
J	 0.9000	 0.7040
K	 0.4530	 0.5630
L	 0.9020	 0.7060
M	 0.8090	 0.6660
N	 0.8800	 0.6960
O	 0.9370	 0.7180
P	 0.8020	 0.6560
Q	 0.8100	 0.6730
R	 0.9530	 0.7270
S	 0.9520	 0.7200
T	 0.8750	 0.6860
U	 0.8550	 0.6790
V	 0.9760	 0.7370
W	 0.6570	 0.6140
X	 0.9530	 0.7270
Y	 0.9170	 0.7030
Z	 0.9240	 0.7210
a	 0.8980	 0.7110
b	 0.6980	 0.6420
c	 0.7390	 0.6490
d	 0.9140	 0.7150
e	 0.9160	 0.7120
f	 0.9170	 0.7130
g	 0.8950	 0.6980
h	 0.7670	 0.6560



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
j	 0.9210	 0.7100
k	 0.8620	 0.6920
l	 0.3000	 0.3230
m	 0.9060	 0.6940
n	 0.8290	 0.6700
o	 0.9710	 0.7300
p	 0.7670	 0.6500
q	 0.8870	 0.7030
r	 0.9320	 0.7210
s	 0.8690	 0.6930
t	 0.6530	 0.6230
u	 0.8140	 0.6700