



Full wwPDB EM Validation Report ⓘ

Jun 25, 2026 – 03:40 PM EDT

PDB ID : 8FL6 / pdb_00008fl6
EMDB ID : EMD-29268
Title : Human nuclear pre-60S ribosomal subunit (State J1)
Authors : Vanden Broeck, A.; Klinge, S.
Deposited on : 2022-12-21
Resolution : 2.62 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

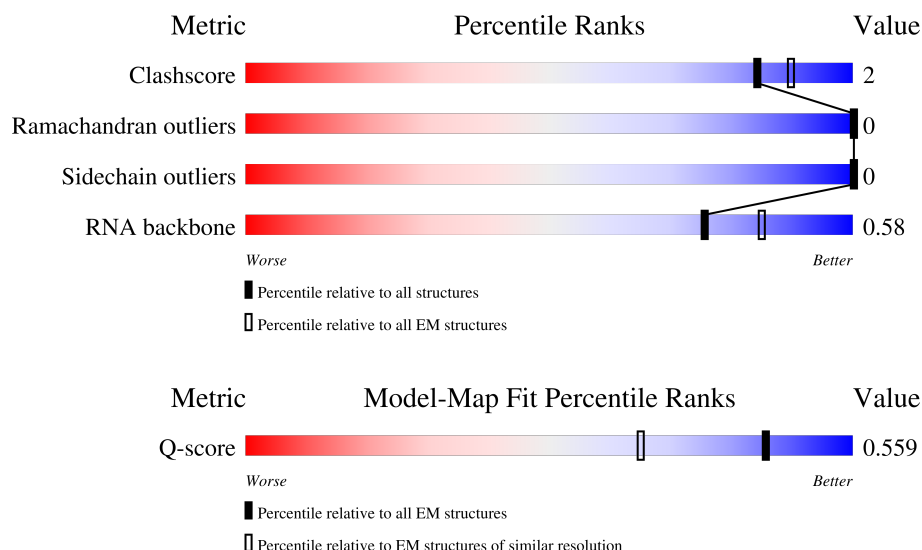
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

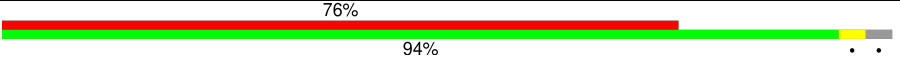
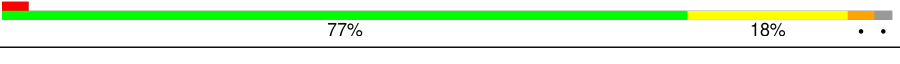
The reported resolution of this entry is 2.62 Å.

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	8810 (2.12 - 3.12)

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	BA	165	
2	L1	157	
3	L2	1167	

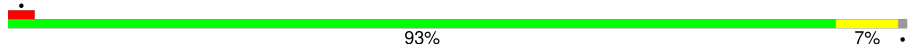
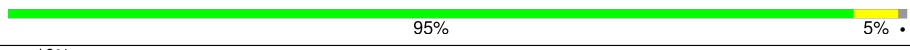
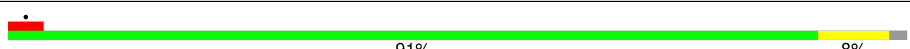
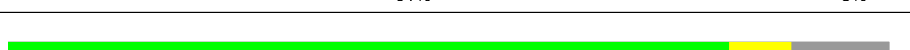
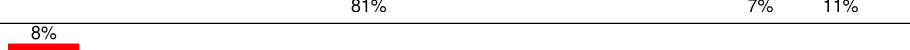
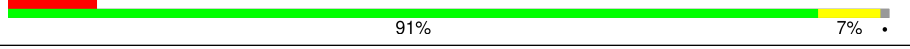
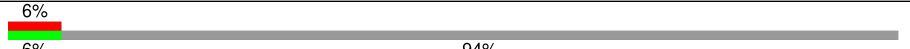
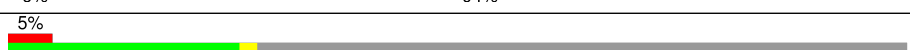
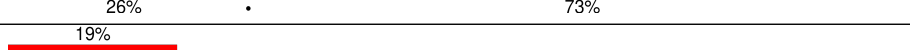
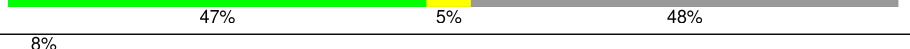
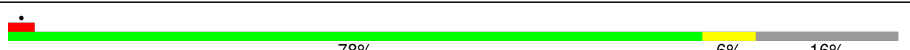
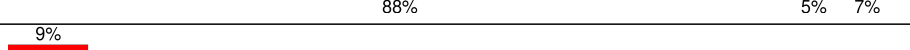
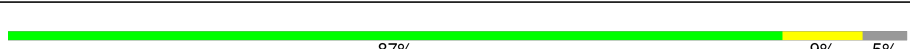
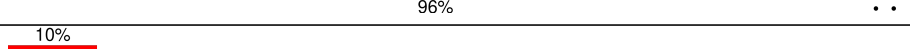
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Mol	Chain	Length	Quality of chain
4	L3	5070	
5	L4	121	
6	L5	178	
7	L6	211	
8	L7	203	
9	L8	215	
10	L9	204	
11	LA	184	
12	LB	188	
13	LC	176	
14	LD	196	
15	LE	160	
16	LF	128	
17	LG	140	
18	LH	156	
19	LI	145	
20	LJ	136	
21	LK	148	
22	LL	137	
23	LM	159	
24	LN	403	
25	LO	115	
26	LP	125	
27	LQ	135	
28	LR	117	

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Mol	Chain	Length	Quality of chain
29	LS	123	
30	LT	110	
31	LU	105	
32	LV	106	
33	LW	97	
34	LX	92	
35	LY	70	
36	LZ	51	
37	NC	731	
38	NF	260	
39	NK	129	
40	NL	478	
41	NP	134	
42	SA	427	
43	SB	297	
44	SC	288	
45	SD	248	
46	SE	266	
47	SF	257	
48	SG	192	
49	SH	293	
50	SI	255	
51	SK	245	
52	SL	490	
53	SM	588	

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Mol	Chain	Length	Quality of chain
54	SQ	239	45% 87% 9%
55	SR	634	15% 88% 6% 5%
56	SV	163	79% 7% 15%

2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 153706 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 L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	BA	160	Total	C	N	O	S	0	0
			954	570	188	193	3		

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L1	154	Total	C	N	O	P	0	0
			3278	1463	581	1080	154		

- Molecule 3 is a RNA chain called ITS2 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L2	72	Total	C	N	O	P	0	0
			1535	683	278	502	72		

- Molecule 4 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L3	3405	Total	C	N	O	P	0	0
			73095	32574	13391	23725	3405		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L4	120	Total	C	N	O	P	0	0
			2561	1141	456	844	120		

- Molecule 6 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L5	168	Total	C	N	O	S	0	0
			1349	853	251	239	6		

- Molecule 7 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L6	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 8 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L7	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 9 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L8	135	Total	C	N	O	S	0	0
			1111	713	213	178	7		

- Molecule 10 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L9	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 11 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LA	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 12 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LB	187	Total	C	N	O	S	0	0
			1512	944	314	249	5		

- Molecule 13 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LC	176	Total	C	N	O	S	0	0
			1461	930	284	236	11		

- Molecule 14 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LD	154	Total	C	N	O	S	0	0
			1289	805	277	198	9		

- Molecule 15 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LE	154	Total	C	N	O	S	0	0
			1264	803	246	210	5		

- Molecule 16 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LF	103	Total	C	N	O	S	0	0
			842	538	148	154	2		

- Molecule 17 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LG	139	Total	C	N	O	S	0	0
			1034	648	199	182	5		

- Molecule 18 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LH	143	Total	C	N	O	S	0	0
			1156	740	220	195	1		

- Molecule 19 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LI	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 20 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LJ	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 21 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LK	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 22 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LL	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 23 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LM	91	Total	C	N	O	S	0	0
			751	469	165	113	4		

- Molecule 24 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LN	402	Total	C	N	O	S	0	0
			3239	2061	608	556	14		

- Molecule 25 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LO	95	Total	C	N	O	S	0	0
			738	468	131	133	6		

- Molecule 26 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LP	106	Total	C	N	O	S	0	0
			879	555	170	152	2		

- Molecule 27 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LQ	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 28 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LR	112	Total	C	N	O	S	0	0
			888	555	183	144	6		

- Molecule 29 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LS	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 30 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LT	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 31 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LU	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 32 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LV	104	Total	C	N	O	S	0	0
			851	533	174	138	6		

- Molecule 33 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LW	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 34 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LX	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 35 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LY	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 36 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LZ	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 37 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	NC	44	Total	C	N	O	S	0	0
			219	131	44	44			

- Molecule 38 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	NF	71	Total	C	N	O	S	0	0
			626	392	129	102	3		

- Molecule 39 is a protein called Protein LLP homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	NK	67	Total	C	N	O	S	0	0
			581	363	128	88	2		

- Molecule 40 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	NL	323	Total	C	N	O	S	0	0
			2666	1658	531	475	2		

- Molecule 41 is a protein called Zinc finger protein 593.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	NP	104	Total	C	N	O	S	0	0
			847	520	178	145	4		

- Molecule 42 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	SA	358	Total	C	N	O	S	0	0
			2853	1797	570	473	13		

- Molecule 43 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	SB	275	Total	C	N	O	S	0	0
			2243	1419	406	404	14		

- Molecule 44 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	SC	217	Total	C	N	O	S	0	0
			1747	1124	332	287	4		

- Molecule 45 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	SD	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

- Molecule 46 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	SE	231	Total	C	N	O	S	1	0
			1869	1191	361	313	4		

- Molecule 47 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SF	245	Total	C	N	O	S	0	0
			1876	1177	383	310	6		

- Molecule 48 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SG	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 49 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SH	150	Total	C	N	O	S	1	0
			1128	721	201	203	3		

- Molecule 50 is a protein called 60S ribosomal protein L7-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SI	234	Total	C	N	O	S	1	0
			1937	1254	363	316	4		

- Molecule 51 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SK	244	Total	C	N	O	S	0	0
			1852	1149	318	372	13		

- Molecule 52 is a protein called Ribosomal L1 domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SL	238	Total	C	N	O	S	0	0
			1917	1227	337	347	6		

- Molecule 53 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SM	399	Total	C	N	O	S	0	0
			3278	2120	576	571	11		

- Molecule 54 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SQ	217	Total	C	N	O	S	0	0
			1771	1129	311	320	11		

- Molecule 55 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SR	601	Total	C	N	O	S	0	0
			4932	3105	899	902	26		

- Molecule 56 is a protein called Probable ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SV	139	Total	C	N	O	S	0	0
			1184	754	229	191	10		

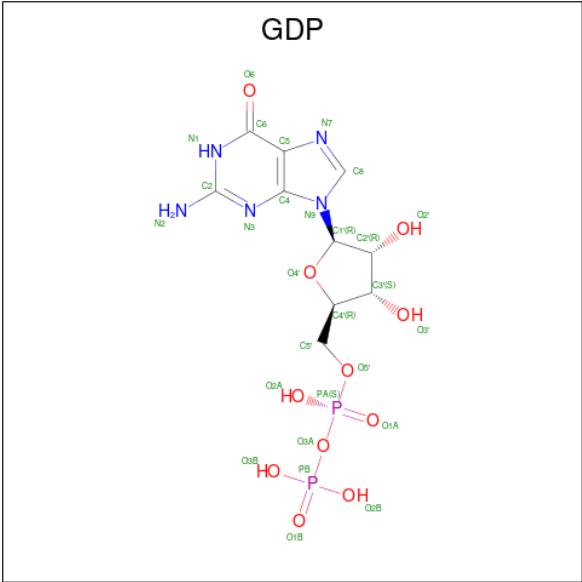
- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	L1	4	Total	Mg	0
			4	4	
57	L3	75	Total	Mg	0
			75	75	
57	L4	3	Total	Mg	0
			3	3	
57	LG	1	Total	Mg	0
			1	1	
57	LQ	1	Total	Mg	0
			1	1	
57	LT	1	Total	Mg	0
			1	1	
57	SA	1	Total	Mg	0
			1	1	
57	SF	1	Total	Mg	0
			1	1	
57	SR	1	Total	Mg	0
			1	1	

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
58	LR	1	Total	Zn	0
			1	1	
58	LV	1	Total	Zn	0
			1	1	
58	LW	1	Total	Zn	0
			1	1	
58	LX	1	Total	Zn	0
			1	1	
58	NP	1	Total	Zn	0
			1	1	
58	SV	1	Total	Zn	0
			1	1	

- Molecule 59 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					AltConf
59	SR	1	Total	C	N	O	P	0
			28	10	5	11	2	

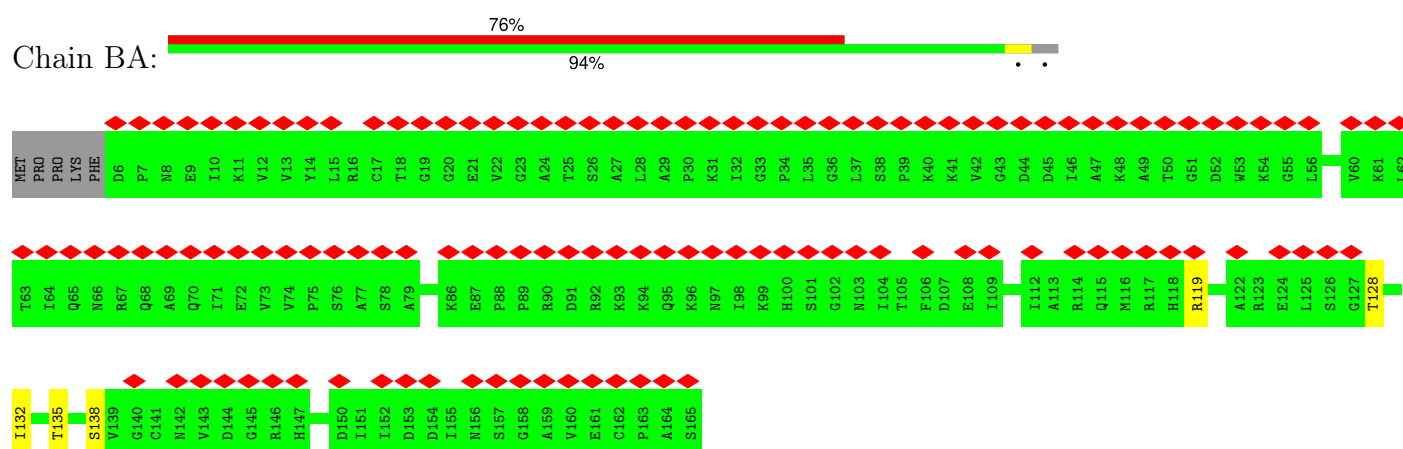
- Molecule 60 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
60	SR	1	Total	K	0
			1	1	

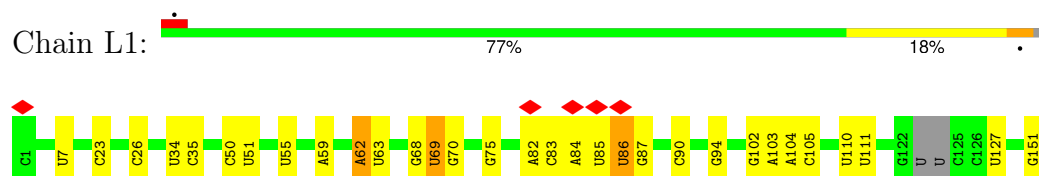
3 Residue-property plots [i](#)

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

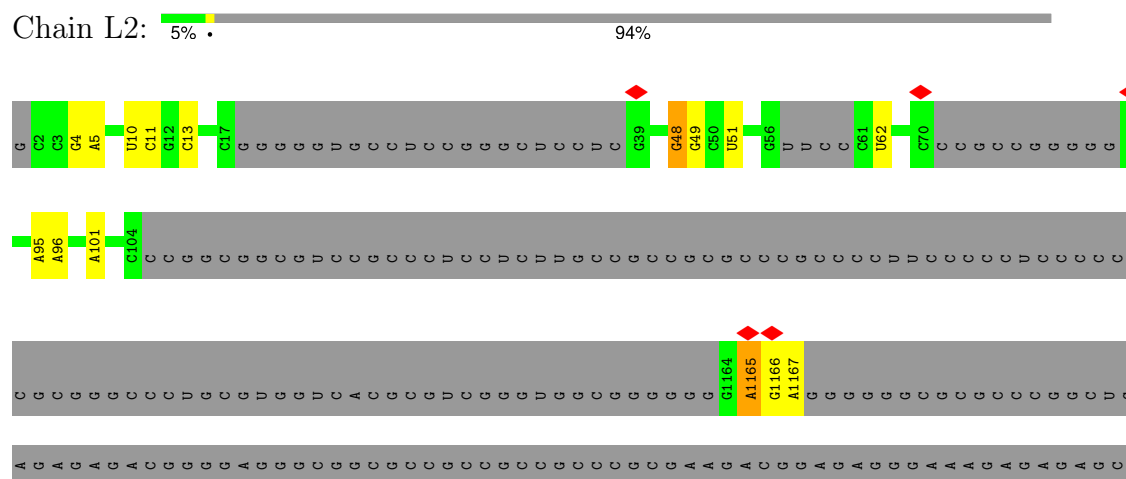
• Molecule 1: 60S ribosomal protein L12

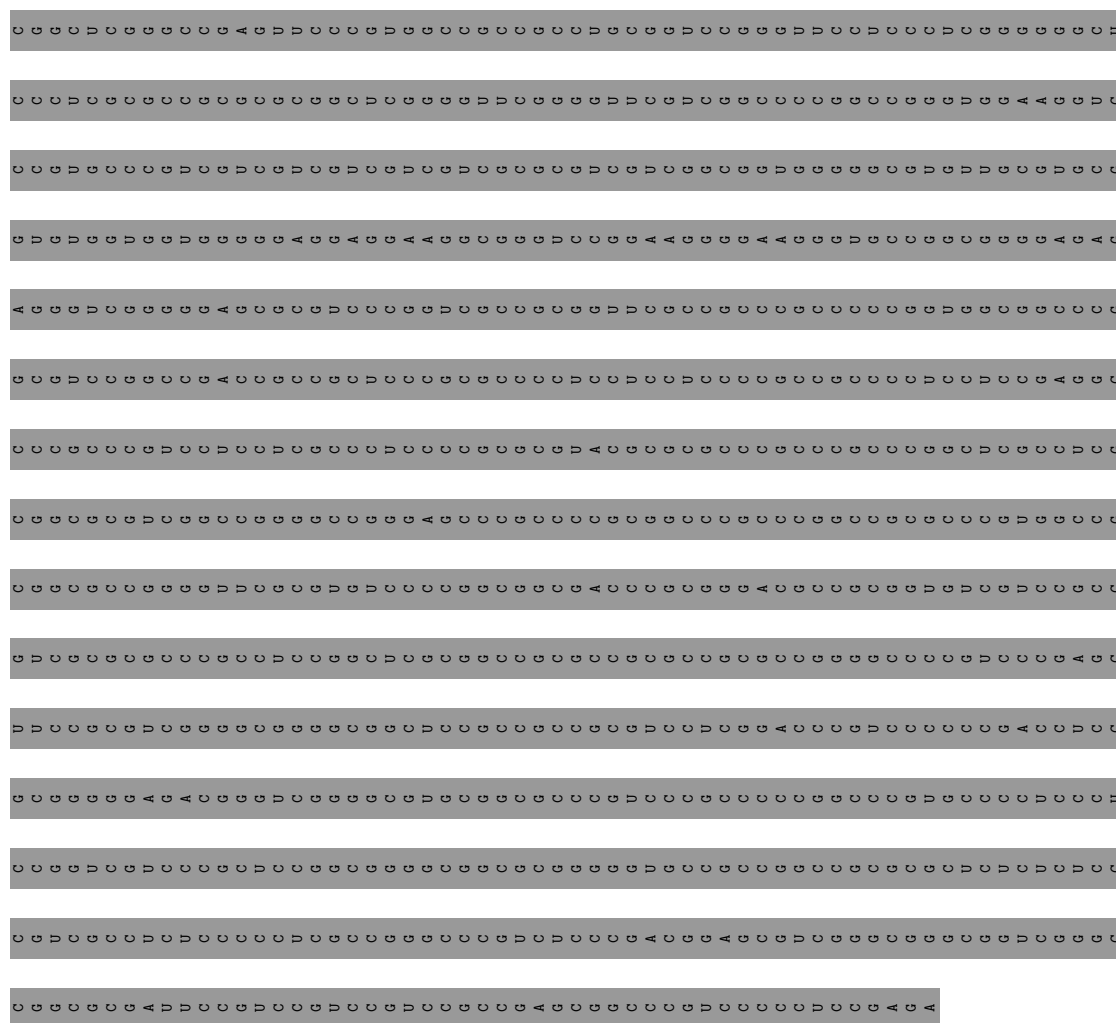


• Molecule 2: 5.8S rRNA

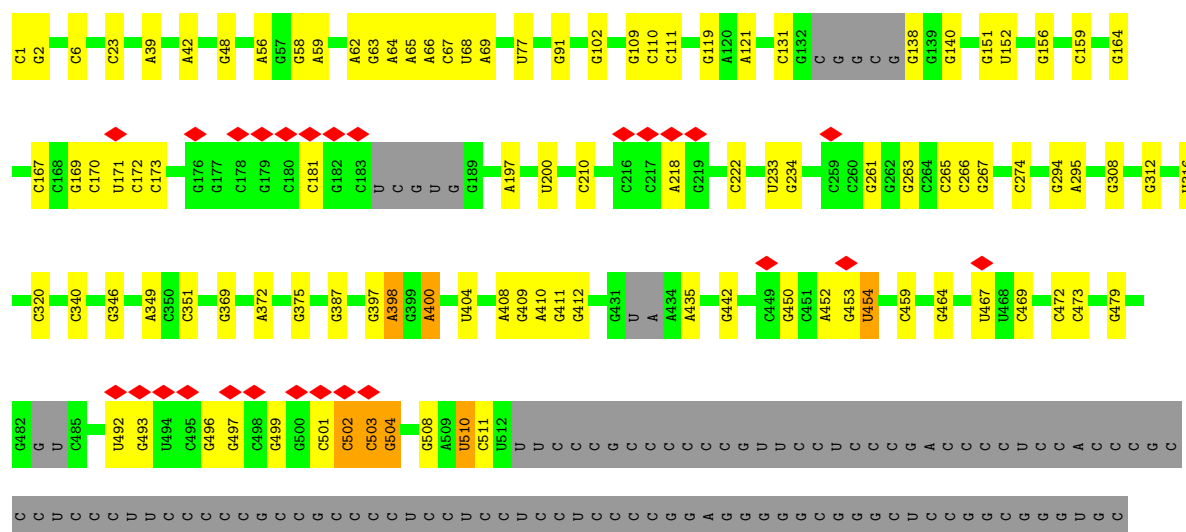


• Molecule 3: ITS2 rRNA

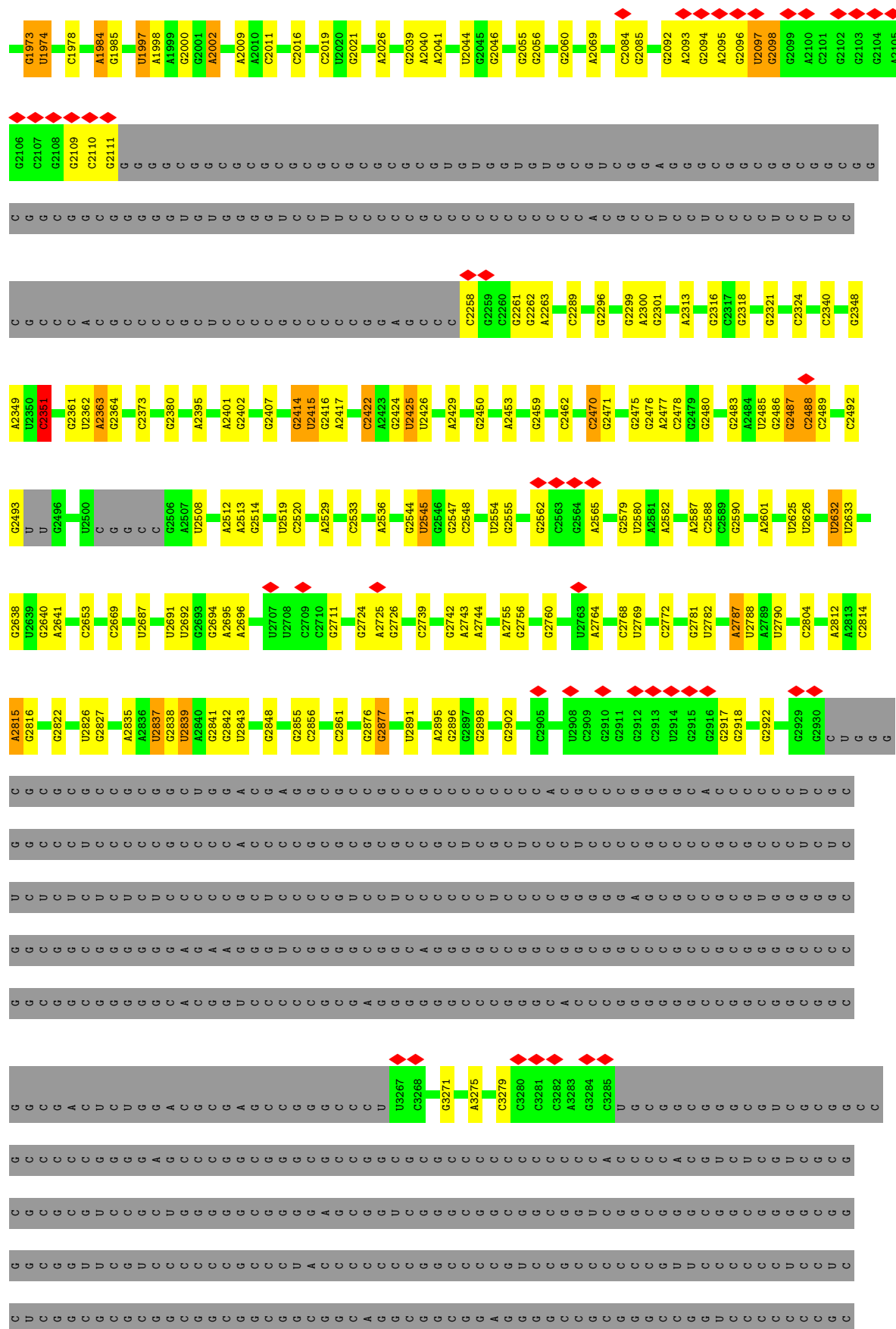




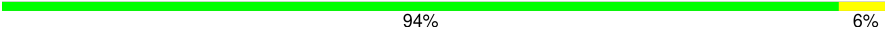
• Molecule 4: 28S rRNA







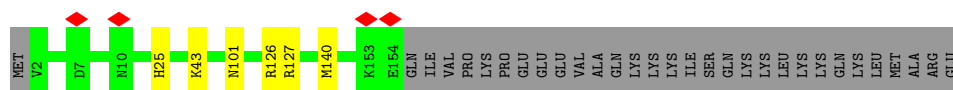


Chain L9:  94% 6%

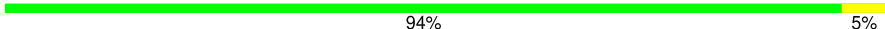


- Molecule 11: 60S ribosomal protein L17

Chain LA:  80% 17%

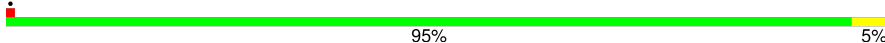


- Molecule 12: 60S ribosomal protein L18

Chain LB:  94% 5%



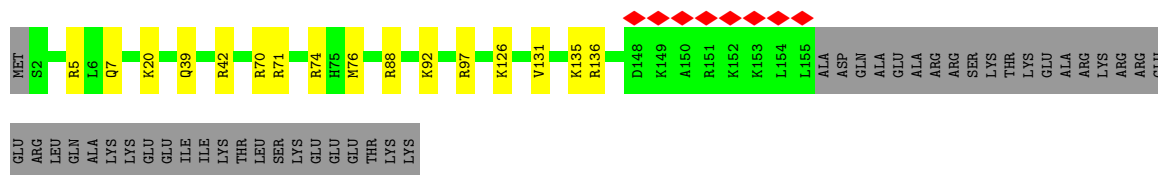
- Molecule 13: 60S ribosomal protein L18a

Chain LC:  95% 5%

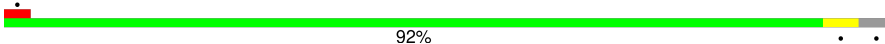


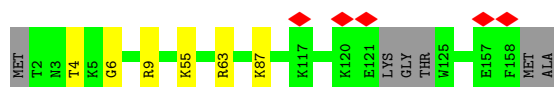
- Molecule 14: 60S ribosomal protein L19

Chain LD:  70% 8% 21%



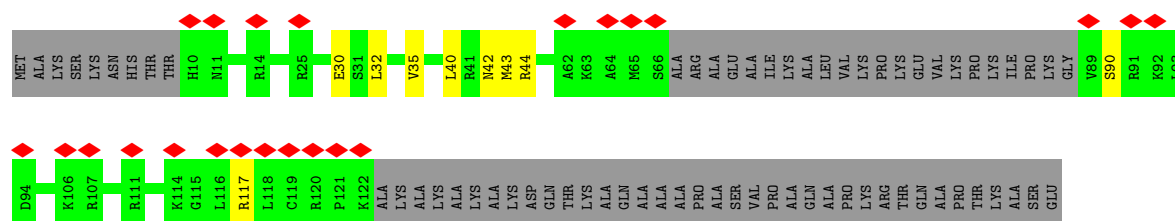
- Molecule 15: 60S ribosomal protein L21

Chain LE:  92%

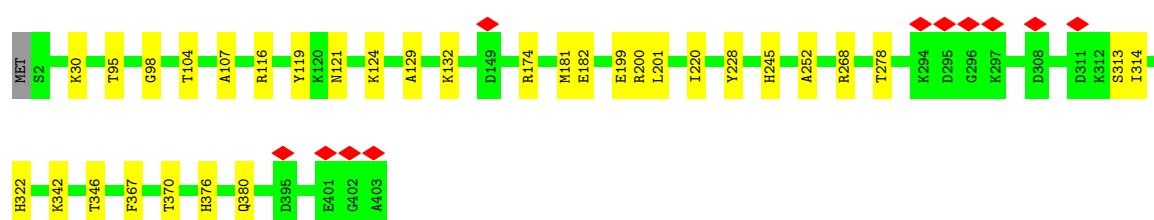


- Molecule 16: 60S ribosomal protein L22

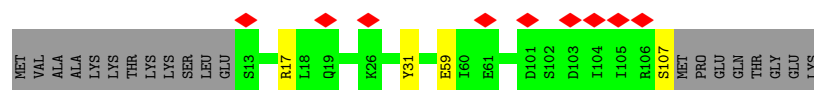
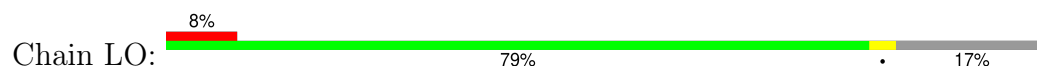
Chain LF:  8% 76% 5% 20%



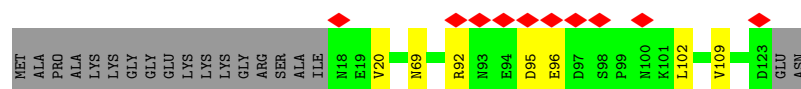
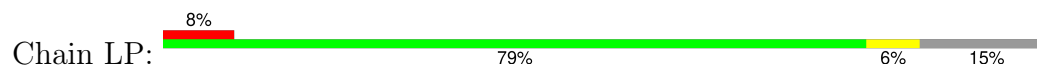
- Molecule 24: 60S ribosomal protein L3



- Molecule 25: 60S ribosomal protein L30



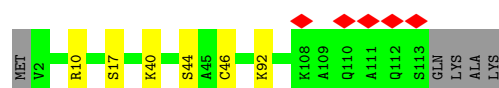
- Molecule 26: 60S ribosomal protein L31



- Molecule 27: 60S ribosomal protein L32



- Molecule 28: 60S ribosomal protein L34

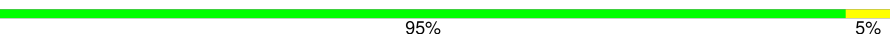


- Molecule 29: 60S ribosomal protein L35

Chain LS:  93% 7%



- Molecule 30: 60S ribosomal protein L35a

Chain LT:  95% 5%



- Molecule 31: 60S ribosomal protein L36

Chain LU:  10% 90% 7%



- Molecule 32: 60S ribosomal protein L36a

Chain LV:  91% 8%

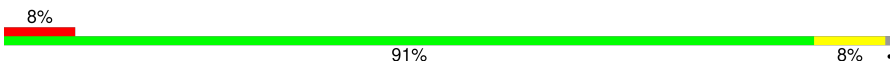


- Molecule 33: 60S ribosomal protein L37

Chain LW:  81% 7% 11%

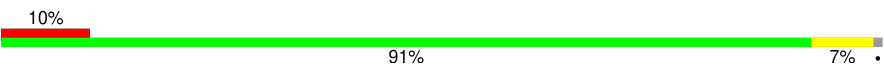


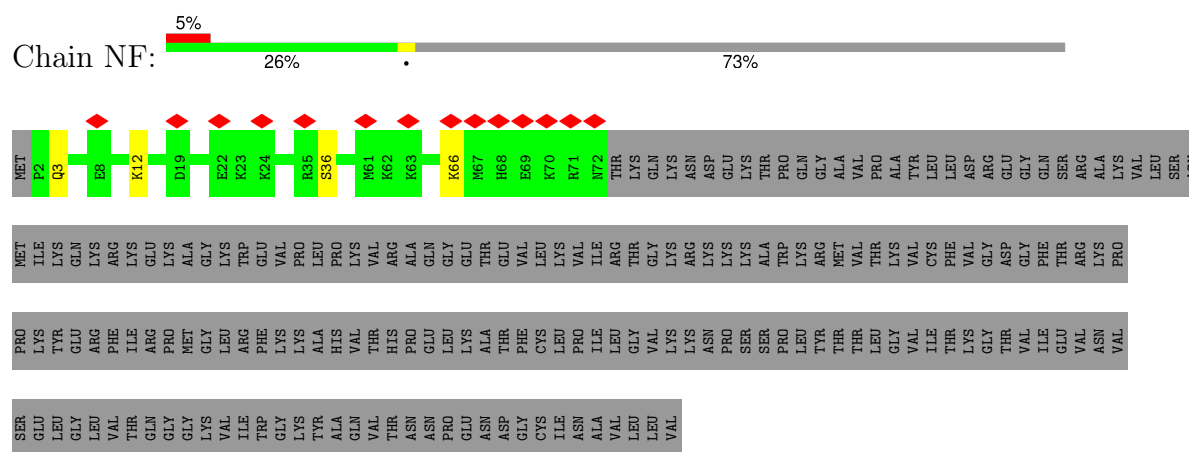
- Molecule 34: 60S ribosomal protein L37a

Chain LX:  8% 91% 8%

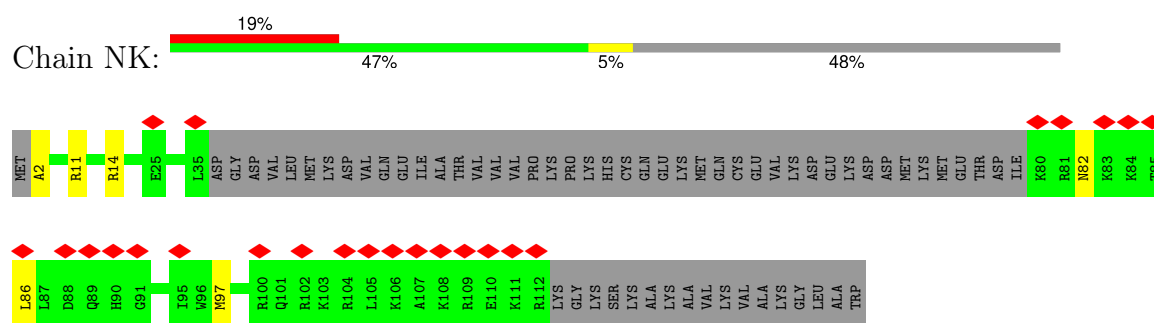


- Molecule 35: 60S ribosomal protein L38

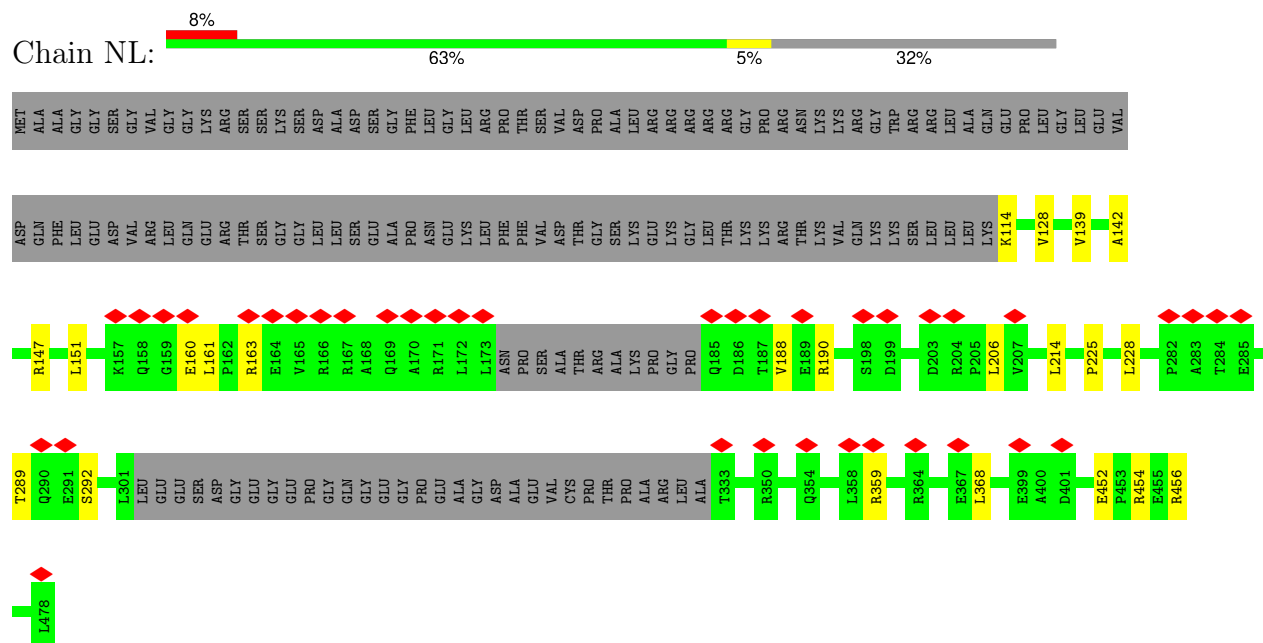
Chain LY:  10% 91% 7%



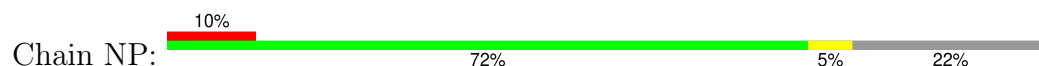
- Molecule 39: Protein LLP homolog



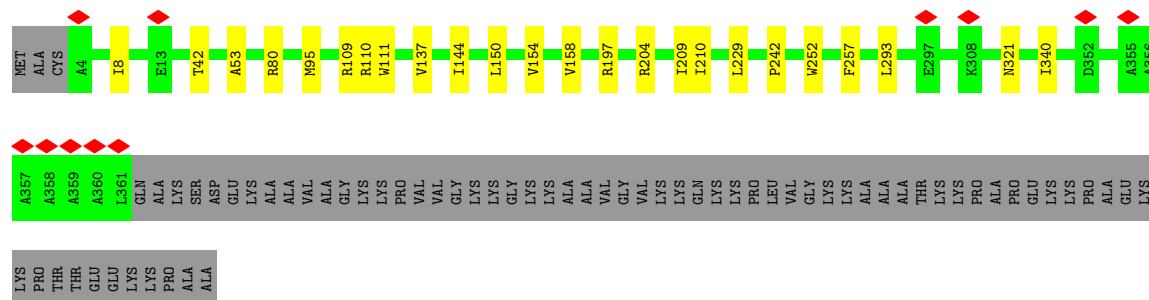
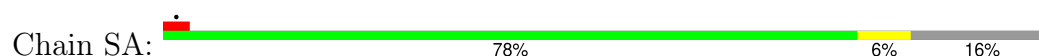
- Molecule 40: Ribosome biogenesis protein NOP53



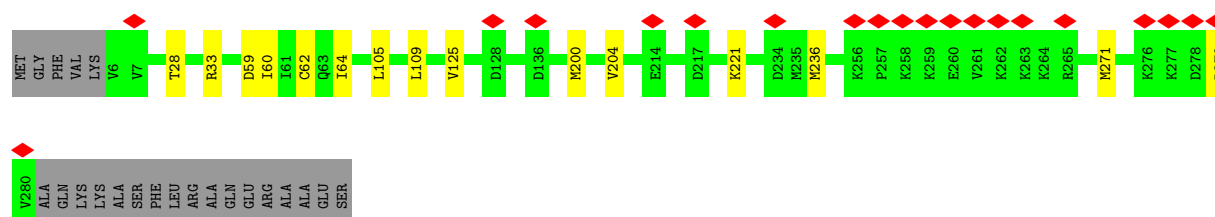
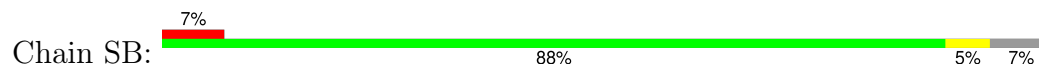
- Molecule 41: Zinc finger protein 593



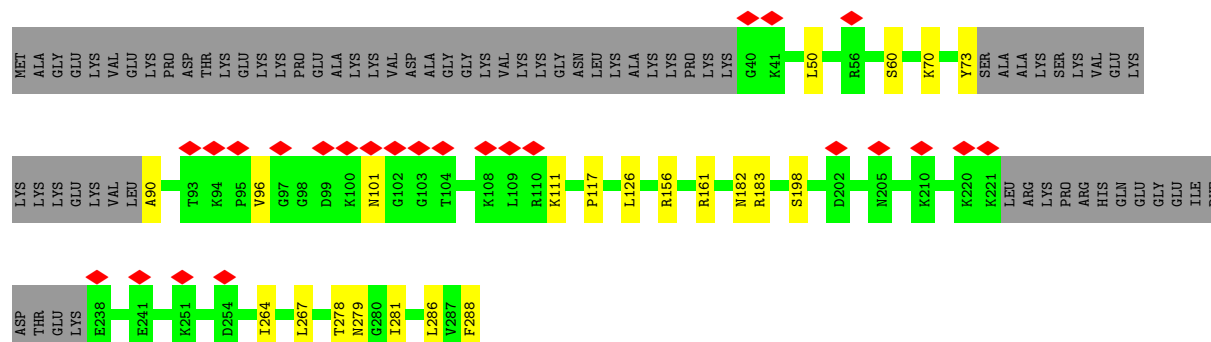
- Molecule 42: 60S ribosomal protein L4



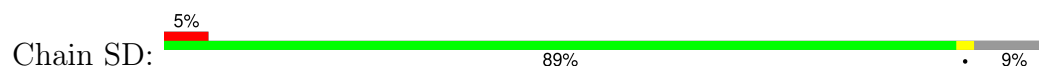
- Molecule 43: 60S ribosomal protein L5



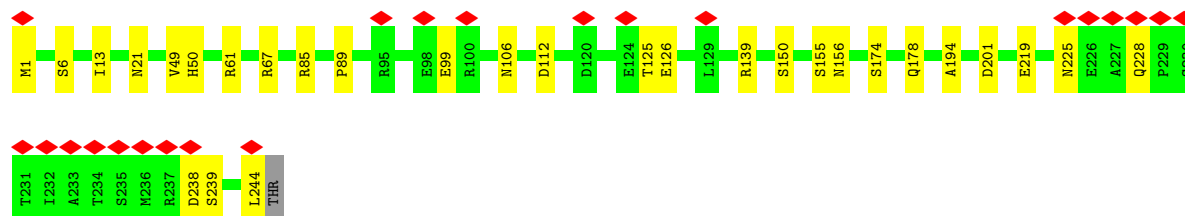
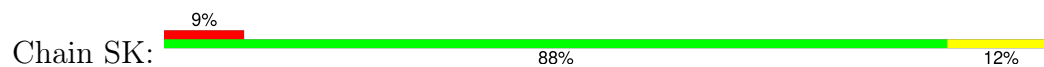
- Molecule 44: 60S ribosomal protein L6



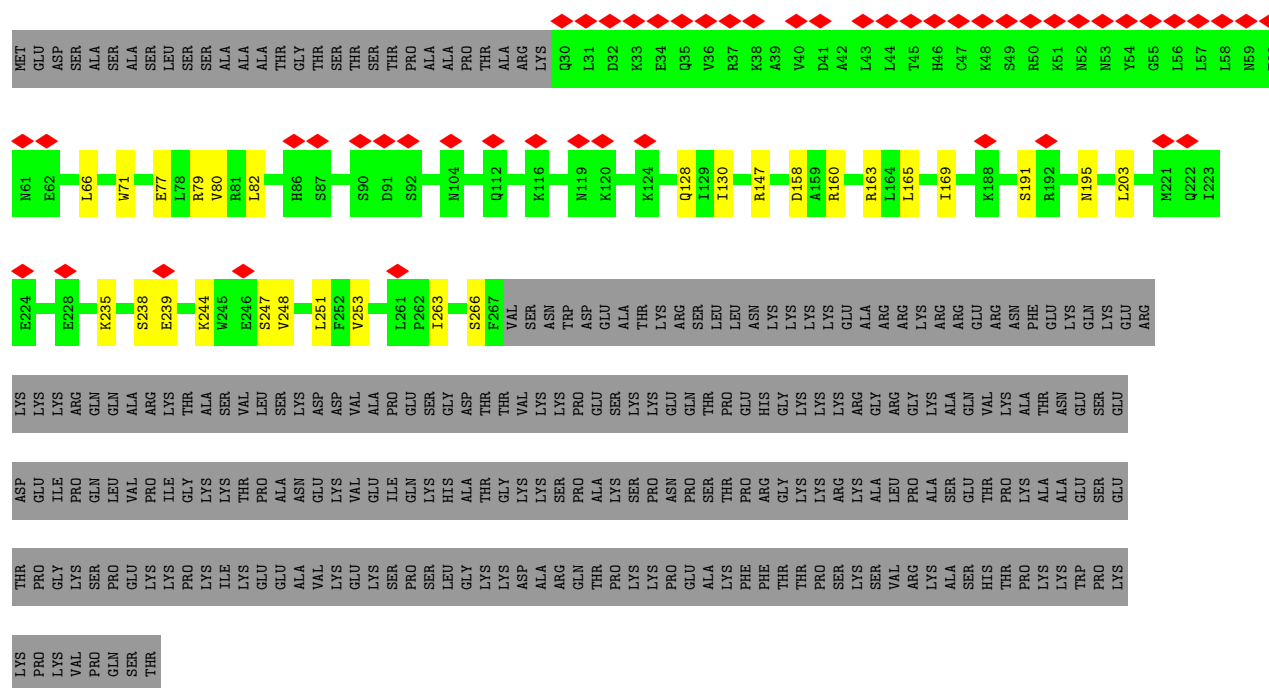
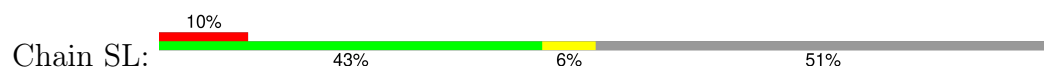
- Molecule 45: 60S ribosomal protein L7



- Molecule 51: Eukaryotic translation initiation factor 6



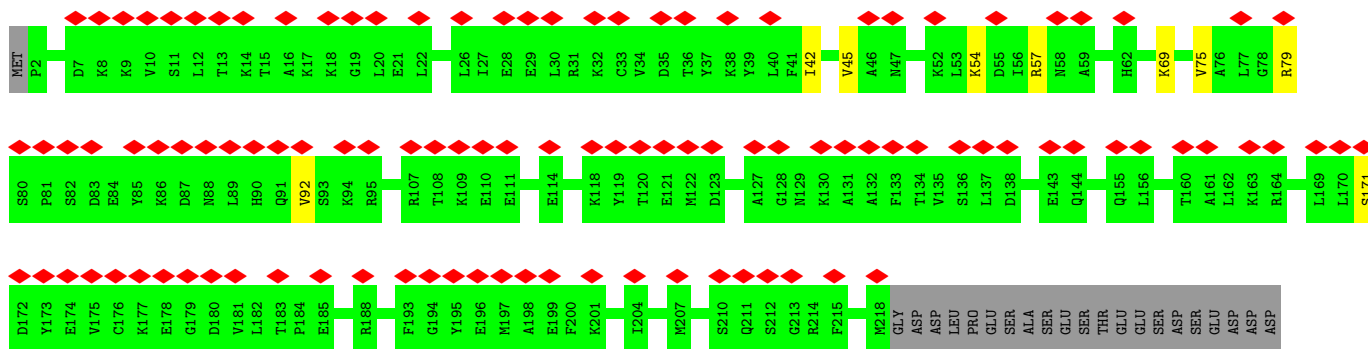
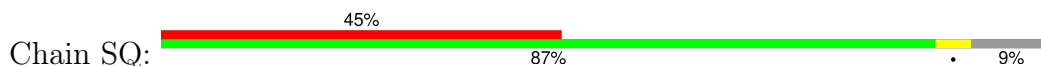
- Molecule 52: Ribosomal L1 domain-containing protein 1



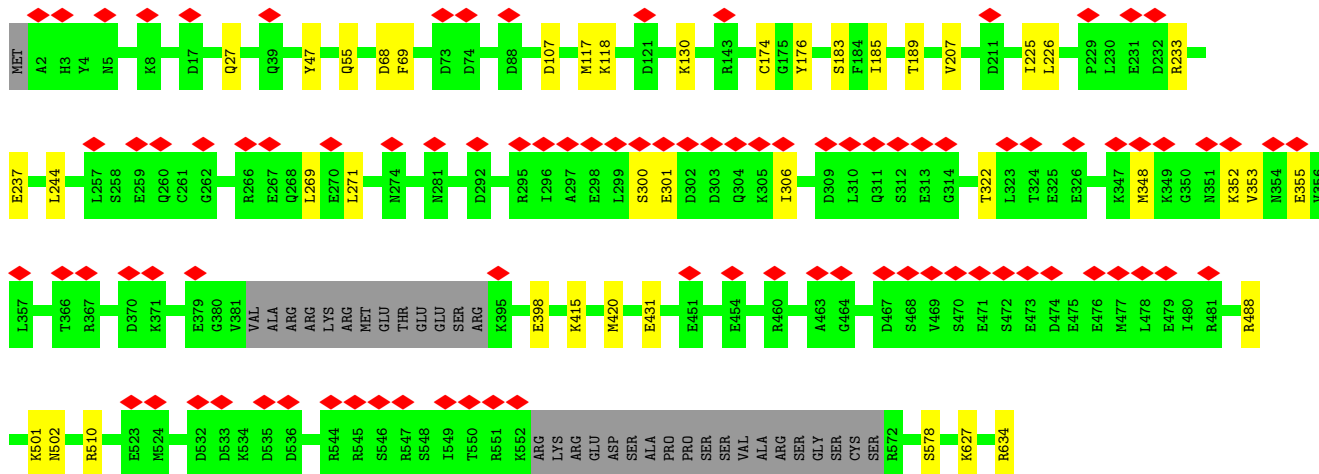
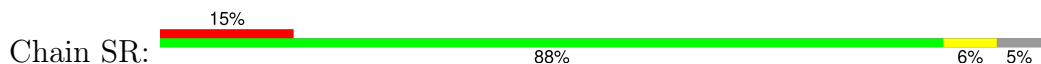
- Molecule 53: Pescadillo homolog



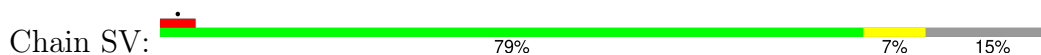
- Molecule 54: mRNA turnover protein 4 homolog

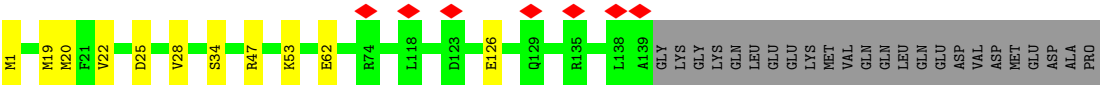


- Molecule 55: GTP-binding protein 4



- Molecule 56: Probable ribosome biogenesis protein RLP24





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	71912	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	9.164	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.048	Depositor
Map value standard deviation	0.186	Depositor
Recommended contour level	1	Depositor
Map size ($\text{\AA}$)	514.56, 514.56, 514.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.072, 1.072, 1.072	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, UR3, PSU, K, OMU, GDP, HIC, MG, 6MZ, A2M, OMC, OMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	BA	0.12	0/959	0.26	0/1312
2	L1	0.26	0/3589	0.27	0/5589
3	L2	0.18	0/1709	0.30	0/2653
4	L3	0.23	0/79296	0.28	0/123670
5	L4	0.31	0/2861	0.31	0/4459
6	L5	0.18	0/1372	0.31	0/1836
7	L6	0.17	0/1732	0.28	0/2315
8	L7	0.20	0/1682	0.31	0/2250
9	L8	0.17	0/1133	0.26	0/1516
10	L9	0.22	0/1746	0.33	0/2338
11	LA	0.19	0/1268	0.33	0/1701
12	LB	0.21	0/1536	0.33	0/2052
13	LC	0.23	0/1501	0.34	0/2013
14	LD	0.17	0/1305	0.29	0/1727
15	LE	0.23	0/1291	0.36	0/1724
16	LF	0.15	0/856	0.29	0/1149
17	LG	0.18	0/1048	0.34	0/1402
18	LH	0.19	0/1175	0.30	0/1572
19	LI	0.19	0/1132	0.30	0/1504
20	LJ	0.20	0/1130	0.29	0/1507
21	LK	0.19	0/1191	0.30	0/1591
22	LL	0.16	0/1017	0.28	0/1364
23	LM	0.18	0/763	0.32	0/1005
24	LN	0.18	0/3294	0.32	0/4406
25	LO	0.15	0/748	0.25	0/1004
26	LP	0.17	0/894	0.31	0/1204
27	LQ	0.19	0/1071	0.30	0/1429
28	LR	0.17	0/898	0.31	0/1197
29	LS	0.19	0/1023	0.28	0/1351
30	LT	0.19	0/895	0.32	0/1198
31	LU	0.15	0/843	0.30	0/1115
32	LV	0.22	0/864	0.32	0/1140

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	LW	0.21	0/720	0.36	0/952
34	LX	0.14	0/718	0.29	0/953
35	LY	0.15	0/575	0.29	0/761
36	LZ	0.19	0/454	0.29	0/599
37	NC	0.10	0/218	0.31	0/303
38	NF	0.14	0/637	0.28	0/834
39	NK	0.14	0/587	0.27	0/767
40	NL	0.16	0/2705	0.29	0/3624
41	NP	0.14	0/864	0.27	0/1154
42	SA	0.19	0/2907	0.31	0/3905
43	SB	0.22	0/2287	0.31	0/3065
44	SC	0.15	0/1781	0.30	0/2388
45	SD	0.19	0/1905	0.30	0/2539
46	SE	0.25	0/1903	0.35	0/2559
47	SF	0.19	0/1914	0.34	0/2567
48	SG	0.18	0/1537	0.29	0/2066
49	SH	0.19	0/1158	0.32	0/1572
50	SI	0.19	0/1980	0.33	0/2656
51	SK	0.16	0/1877	0.30	0/2554
52	SL	0.16	0/1949	0.32	0/2621
53	SM	0.22	0/3357	0.30	0/4529
54	SQ	0.10	0/1806	0.25	0/2420
55	SR	0.14	0/5014	0.28	0/6727
56	SV	0.16	0/1207	0.26	0/1600
All	All	0.21	0/161882	0.29	0/236008

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	BA	954	0	690	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L1	3278	0	1665	16	0
3	L2	1535	0	789	8	0
4	L3	73095	0	37033	330	0
5	L4	2561	0	1295	6	0
6	L5	1349	0	1383	6	0
7	L6	1701	0	1818	13	0
8	L7	1650	0	1794	11	0
9	L8	1111	0	1174	10	0
10	L9	1701	0	1749	12	0
11	LA	1242	0	1269	6	0
12	LB	1512	0	1628	7	0
13	LC	1461	0	1502	7	0
14	LD	1289	0	1429	14	0
15	LE	1264	0	1328	4	0
16	LF	842	0	864	3	0
17	LG	1034	0	1097	5	0
18	LH	1156	0	1268	5	0
19	LI	1115	0	1205	9	0
20	LJ	1107	0	1182	8	0
21	LK	1162	0	1213	8	0
22	LL	1002	0	1068	6	0
23	LM	751	0	820	7	0
24	LN	3239	0	3377	26	0
25	LO	738	0	774	3	0
26	LP	879	0	924	5	0
27	LQ	1053	0	1147	7	0
28	LR	888	0	977	5	0
29	LS	1015	0	1148	9	0
30	LT	876	0	912	4	0
31	LU	832	0	917	6	0
32	LV	851	0	920	7	0
33	LW	705	0	737	6	0
34	LX	708	0	756	8	0
35	LY	569	0	637	3	0
36	LZ	444	0	483	6	0
37	NC	219	0	92	0	0
38	NF	626	0	665	4	0
39	NK	581	0	656	5	0
40	NL	2666	0	2774	16	0
41	NP	847	0	854	6	0
42	SA	2853	0	3028	19	0
43	SB	2243	0	2268	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	SC	1747	0	1897	21	0
45	SD	1870	0	1996	5	0
46	SE	1869	0	2014	14	0
47	SF	1876	0	1970	17	0
48	SG	1518	0	1601	5	0
49	SH	1128	0	1001	1	0
50	SI	1937	0	2070	11	0
51	SK	1852	0	1828	16	0
52	SL	1917	0	2018	16	0
53	SM	3278	0	3332	14	0
54	SQ	1771	0	1810	7	0
55	SR	4932	0	5072	30	0
56	SV	1184	0	1248	12	0
57	L1	4	0	0	0	0
57	L3	75	0	0	0	0
57	L4	3	0	0	0	0
57	LG	1	0	0	0	0
57	LQ	1	0	0	0	0
57	LT	1	0	0	0	0
57	SA	1	0	0	0	0
57	SF	1	0	0	0	0
57	SR	1	0	0	0	0
58	LR	1	0	0	0	0
58	LV	1	0	0	0	0
58	LW	1	0	0	0	0
58	LX	1	0	0	0	0
58	NP	1	0	0	0	0
58	SV	1	0	0	0	0
59	SR	28	0	12	0	0
60	SR	1	0	0	0	0
All	All	153706	0	117178	601	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 2.

All (601) 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)
17:LG:112:MET:HE1	17:LG:117:ILE:HD11	1.53	0.91
5:L4:40:U:O2	6:L5:75:ARG:NH1	2.06	0.89
2:L1:51:U:OP2	36:LZ:21:ARG:NH2	2.07	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:2555:G:O2'	20:LJ:108:ARG:NH2	2.08	0.86
5:L4:30:C:O2'	43:SB:221:LYS:NZ	2.09	0.86
4:L3:2520:C:O2	4:L3:2640:G:N2	2.08	0.86
4:L3:1882:U:O2'	27:LQ:47:ARG:NH1	2.09	0.85
4:L3:3896:C:O2'	24:LN:268:ARG:NH2	2.12	0.83
4:L3:695:G:O2'	4:L3:697:G:OP2	1.96	0.83
4:L3:1889:U:OP1	30:LT:19:ARG:NH1	2.12	0.83
4:L3:2263:A:OP1	22:LL:107:ARG:NH2	2.13	0.82
38:NF:3:GLN:NE2	55:SR:207:VAL:O	2.12	0.82
4:L3:1480:C:O2'	4:L3:1482:G:OP2	1.98	0.81
4:L3:4940:C:OP1	44:SC:156:ARG:NH2	2.13	0.80
2:L1:75:OMG:OP2	19:LI:74:TYR:OH	1.99	0.80
4:L3:4156:G:OP2	4:L3:4157:A:O2'	2.00	0.79
4:L3:4693:C:O2	4:L3:4695:C:N4	2.15	0.78
4:L3:2318:G:N2	4:L3:2321:G:OP2	2.15	0.78
4:L3:295:A:OP2	32:LV:39:ARG:NH1	2.16	0.78
4:L3:151:G:OP1	10:L9:49:ARG:NH2	2.17	0.77
4:L3:2480:G:OP1	53:SM:22:LYS:NZ	2.16	0.77
4:L3:4985:U:O2	24:LN:174:ARG:NH1	2.18	0.77
4:L3:3717:A:OP2	4:L3:3735:G:N2	2.18	0.77
4:L3:4728:U:OP2	24:LN:132:LYS:NZ	2.18	0.77
5:L4:55:A:O2'	6:L5:151:ILE:O	2.03	0.76
4:L3:4415:A:OP1	38:NF:66:LYS:NZ	2.16	0.76
4:L3:4678:G:OP1	39:NK:14:ARG:NH1	2.19	0.76
4:L3:1366:G:N7	7:L6:37:LYS:NZ	2.34	0.75
4:L3:1943:A:OP2	4:L3:2039:G:N2	2.18	0.75
4:L3:1508:A:OP1	42:SA:110:ARG:NH2	2.20	0.75
4:L3:156:G:OP2	29:LS:109:ARG:NH2	2.20	0.75
4:L3:1255:A:OP1	4:L3:1257:A:N6	2.20	0.75
4:L3:502:C:O2'	4:L3:503:C:OP1	2.03	0.75
51:SK:244:LEU:O	55:SR:352:LYS:NZ	2.16	0.74
48:SG:140:GLN:NE2	54:SQ:171:SER:OG	2.21	0.73
4:L3:375:G:OP2	33:LW:52:LYS:NZ	2.21	0.73
4:L3:2626:U:OP2	55:SR:501:LYS:NZ	2.20	0.73
4:L3:1573:G:OP1	14:LD:92:LYS:NZ	2.22	0.72
3:L2:1167:A:O3'	4:L3:1:C:OP2	2.07	0.72
31:LU:66:ASP:OD1	31:LU:87:ARG:NH1	2.23	0.72
2:L1:50:C:O2'	55:SR:578:SER:OG	2.08	0.72
25:LO:17:ARG:NH1	25:LO:107:SER:OG	2.22	0.72
17:LG:96:LEU:HD13	56:SV:20:MET:HE2	1.72	0.72
46:SE:90:GLN:NE2	50:SI:62:GLU:OE2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:SK:21:ASN:ND2	51:SK:112:ASP:OD2	2.23	0.72
51:SK:99:GLU:OE1	51:SK:125:THR:OG1	2.05	0.71
53:SM:33:ASP:OD1	53:SM:36:ARG:NH2	2.23	0.71
4:L3:4449:A:OP1	55:SR:118:LYS:NZ	2.22	0.71
1:BA:119:ARG:NH1	4:L3:1974:U:OP2	2.23	0.71
53:SM:357:ASP:OD2	53:SM:359:SER:OG	2.09	0.70
4:L3:1366:G:N2	4:L3:1371:A:OP2	2.23	0.70
52:SL:191:SER:O	52:SL:195:ASN:ND2	2.25	0.70
40:NL:456:ARG:NH2	53:SM:213:THR:O	2.24	0.70
3:L2:13:C:OP1	50:SI:86:HIS:NE2	2.22	0.70
4:L3:121:A:OP1	46:SE:110:LYS:NZ	2.25	0.69
4:L3:4565:C:O2	24:LN:268:ARG:NH1	2.25	0.69
35:LY:52:LYS:NZ	40:NL:368:LEU:O	2.25	0.69
4:L3:294:G:OP2	32:LV:43:ARG:NH1	2.25	0.69
4:L3:4371:G:OP1	32:LV:59:LYS:NZ	2.26	0.69
20:LJ:9:LYS:NZ	20:LJ:83:THR:O	2.22	0.69
4:L3:2407:G:O6	36:LZ:2:SER:N	2.26	0.69
4:L3:4305:G:O2'	4:L3:4306:OMU:O5'	2.09	0.69
7:L6:127:PHE:O	29:LS:117:ARG:NH2	2.26	0.69
4:L3:2545:U:O2'	4:L3:2547:G:N7	2.27	0.68
4:L3:408:A:O2'	4:L3:411:G:OP2	2.11	0.68
42:SA:8:ILE:HD11	42:SA:257:PHE:CE2	2.29	0.68
4:L3:62:A:N3	4:L3:77:U:O2'	2.26	0.68
4:L3:1364:U:OP2	7:L6:36:ARG:NH2	2.27	0.67
4:L3:1273:G:O5'	23:LM:117:ARG:NH1	2.28	0.67
4:L3:4633:G:O2'	4:L3:4635:A:OP2	2.05	0.67
4:L3:4124:G:N2	46:SE:43:GLN:O	2.28	0.67
4:L3:4663:G:OP1	56:SV:34:SER:OG	2.11	0.67
40:NL:139:VAL:HG23	40:NL:142:ALA:HB2	1.77	0.67
4:L3:4765:G:OP1	48:SG:23:ARG:NE	2.28	0.67
22:LL:112:ARG:NH1	44:SC:117:PRO:O	2.27	0.67
4:L3:1433:A:N6	4:L3:1451:G:O2'	2.28	0.66
4:L3:2299:G:OP2	42:SA:204:ARG:NH1	2.27	0.66
4:L3:1814:C:O2'	23:LM:42:ASN:OD1	2.07	0.66
47:SF:133:TYR:HB3	47:SF:168:VAL:HG12	1.77	0.66
4:L3:4987:C:N4	24:LN:121:ASN:OD1	2.29	0.66
4:L3:2373:C:O4'	26:LP:69:ASN:ND2	2.28	0.66
4:L3:1280:C:O2'	42:SA:321:ASN:OD1	2.12	0.66
4:L3:2848:G:O2'	4:L3:3838:U:O4	2.07	0.66
1:BA:138:SER:OG	4:L3:2002:A:N6	2.29	0.65
4:L3:1998:A:N3	4:L3:2019:C:O2'	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:4717:A:OP2	24:LN:30:LYS:NZ	2.28	0.65
4:L3:3776:G:N2	4:L3:3776:G:OP2	2.28	0.65
1:BA:119:ARG:NH2	4:L3:1973:G:OP1	2.30	0.65
4:L3:308:G:OP2	4:L3:308:G:N2	2.23	0.65
4:L3:1943:A:N6	4:L3:2039:G:O2'	2.29	0.65
4:L3:67:C:OP2	4:L3:312:G:N2	2.28	0.64
4:L3:2841:G:OP1	41:NP:10:HIS:NE2	2.29	0.64
2:L1:152:U:OP1	4:L3:4162:C:N4	2.30	0.64
4:L3:1238:A:O2'	45:SD:52:GLU:OE2	2.16	0.64
4:L3:2822:G:N7	14:LD:20:LYS:NZ	2.46	0.64
4:L3:2876:OMG:HM22	4:L3:2877:G:H5'	1.80	0.64
43:SB:204:VAL:HG13	43:SB:236:MET:HE1	1.79	0.64
4:L3:110:C:OP1	7:L6:89:LYS:NZ	2.29	0.63
4:L3:1369:C:OP2	4:L3:1370:G:O2'	2.12	0.63
4:L3:2009:A:OP1	38:NF:12:LYS:NZ	2.30	0.63
4:L3:3718:A2M:H2	4:L3:3934:G:O4'	1.98	0.63
2:L1:87:G:OP2	29:LS:5:LYS:NZ	2.31	0.63
4:L3:2896:G:OP1	14:LD:136:ARG:NE	2.31	0.63
4:L3:197:A:N3	4:L3:222:C:O2'	2.30	0.63
4:L3:320:C:OP1	31:LU:84:LYS:NZ	2.20	0.63
4:L3:1173:G:N2	4:L3:1188:C:N3	2.46	0.63
52:SL:239:GLU:O	52:SL:244:LYS:NZ	2.32	0.63
5:L4:12:U:O3'	5:L4:109:U:O2'	2.15	0.62
53:SM:337:GLU:OE2	53:SM:380:ARG:NE	2.32	0.62
4:L3:1438:U:O2'	4:L3:1439:C:OP1	2.17	0.62
24:LN:322:HIS:O	24:LN:342:LYS:NZ	2.21	0.62
52:SL:248:VAL:O	52:SL:266:SER:OG	2.14	0.62
4:L3:2262:G:OP2	22:LL:98:ARG:NH2	2.31	0.62
4:L3:23:C:OP1	33:LW:44:LYS:NZ	2.31	0.62
25:LO:31:TYR:OH	25:LO:59:GLU:OE1	2.17	0.62
55:SR:183:SER:HB3	55:SR:322:THR:HG21	1.81	0.62
4:L3:1489:G:OP1	21:LK:131:ARG:NE	2.32	0.61
4:L3:1633:G:O6	4:L3:3918:G:O2'	2.18	0.61
4:L3:3700:C:O2'	4:L3:3774:A:N3	2.32	0.61
40:NL:128:VAL:O	46:SE:150:LYS:NZ	2.27	0.61
51:SK:1:MET:N	51:SK:219:GLU:OE1	2.33	0.61
4:L3:1177:U:OP2	4:L3:1180:C:N4	2.33	0.61
4:L3:1892:A:OP1	4:L3:1893:C:N4	2.19	0.61
4:L3:2562:G:O2'	4:L3:2565:A:N6	2.34	0.61
4:L3:4117:U:O4'	46:SE:43:GLN:NE2	2.33	0.61
4:L3:4987:C:OP2	24:LN:116:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:4220:6MZ:OP2	4:L3:4220:6MZ:H8	2.01	0.61
4:L3:5053:U:O2'	4:L3:5054:C:OP2	2.14	0.61
12:LB:122:THR:OG1	12:LB:124:ASP:OD1	2.15	0.61
2:L1:69:PSU:H2'	2:L1:70:G:O4'	2.00	0.61
4:L3:4927:G:OP2	4:L3:4927:G:N2	2.17	0.60
4:L3:1397:A:O2'	4:L3:1467:C:O2'	2.10	0.60
4:L3:4620:OMU:OP2	4:L3:4670:C:N4	2.30	0.60
41:NP:95:GLU:OE1	41:NP:117:LEU:HD21	2.01	0.60
40:NL:190:ARG:NH2	53:SM:117:ASP:OD1	2.34	0.60
4:L3:454:U:O2	27:LQ:5:ARG:NH1	2.35	0.60
4:L3:2487:G:O6	50:SI:51:LYS:NZ	2.27	0.60
4:L3:3868:G:O2'	4:L3:3869:OMC:H5''	2.00	0.60
4:L3:4910:G:N2	8:L7:106:ASP:O	2.35	0.60
4:L3:3724:A2M:H2'	4:L3:3725:G:C8	2.37	0.60
8:L7:54:TYR:OH	8:L7:73:PHE:O	2.20	0.59
13:LC:84:TYR:CE1	13:LC:93:MET:HE3	2.37	0.59
4:L3:1461:C:OP1	12:LB:144:LYS:NZ	2.34	0.59
4:L3:1481:C:O4'	31:LU:4:ARG:NH2	2.36	0.59
6:L5:93:GLU:OE2	6:L5:175:LEU:HD22	2.02	0.59
4:L3:369:G:N2	4:L3:372:A:OP2	2.31	0.59
4:L3:1238:A:OP2	44:SC:60:SER:OG	2.08	0.59
7:L6:63:THR:HG21	21:LK:66:ASN:HB3	1.83	0.59
14:LD:39:GLN:OE1	14:LD:42:ARG:NH1	2.35	0.59
13:LC:84:TYR:HE1	13:LC:93:MET:HE3	1.67	0.59
4:L3:1548:G:O2'	4:L3:2812:A:N3	2.32	0.58
4:L3:2351:OMC:HM23	42:SA:95:MET:HG3	1.85	0.58
4:L3:2414:G:O2'	4:L3:2415:OMU:H5''	2.02	0.58
4:L3:1595:G:N2	55:SR:634:ARG:OXT	2.32	0.58
31:LU:63:VAL:O	31:LU:64:SER:OG	2.18	0.58
14:LD:70:ARG:NH1	14:LD:76:MET:SD	2.77	0.58
20:LJ:100:VAL:HG13	20:LJ:107:LYS:HA	1.86	0.58
34:LX:26:VAL:HG21	47:SF:180:LEU:HD11	1.85	0.58
4:L3:1629:G:N1	47:SF:208:GLU:OE1	2.36	0.58
4:L3:2922:G:O2'	4:L3:3275:A:N6	2.36	0.58
55:SR:488:ARG:NH1	56:SV:126:GLU:OE1	2.37	0.58
4:L3:2588:C:OP1	4:L3:2768:C:O2'	2.18	0.58
24:LN:107:ALA:HB2	24:LN:201:LEU:HD22	1.86	0.57
52:SL:82:LEU:HD12	52:SL:203:LEU:HD11	1.86	0.57
4:L3:1344:C:O3'	7:L6:8:MET:HE3	2.03	0.57
44:SC:161:ARG:O	44:SC:182:ASN:ND2	2.38	0.57
3:L2:1165:A:O2'	3:L2:1167:A:OP1	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:4546:A:N7	47:SF:215:ASN:ND2	2.52	0.57
4:L3:397:G:H2'	4:L3:398:A2M:H5'	1.86	0.57
55:SR:176:TYR:CE1	55:SR:271:LEU:HD22	2.40	0.57
17:LG:13:LYS:NZ	17:LG:59:ASP:OD1	2.33	0.57
46:SE:136:LEU:HD22	46:SE:202:VAL:CG1	2.35	0.57
4:L3:4593:C:OP2	39:NK:2:ALA:N	2.37	0.56
4:L3:1071:C:O2	44:SC:70:LYS:NZ	2.26	0.56
10:L9:143:ARG:HH11	29:LS:95:LEU:HD23	1.68	0.56
41:NP:33:ARG:NH1	56:SV:25:ASP:OD2	2.38	0.56
43:SB:59:ASP:OD1	43:SB:60:ILE:N	2.37	0.56
3:L2:10:U:OP2	52:SL:163:ARG:NH1	2.38	0.56
50:SI:101:ARG:NH1	50:SI:122:LYS:O	2.39	0.56
51:SK:67:ARG:NH1	51:SK:112:ASP:OD2	2.39	0.56
27:LQ:114:ARG:NH1	27:LQ:117:GLN:OE1	2.39	0.56
2:L1:156:U:OP2	46:SE:89:ARG:NH2	2.39	0.56
4:L3:2415:OMU:HM23	4:L3:2416:G:H8	1.71	0.56
40:NL:225:PRO:HD2	40:NL:228:LEU:HD12	1.87	0.56
2:L1:62:A:OP1	29:LS:52:LYS:NZ	2.39	0.56
4:L3:2361:G:O6	11:LA:25:HIS:ND1	2.39	0.56
4:L3:267:G:N7	40:NL:147:ARG:NH1	2.54	0.55
55:SR:348:MET:HE1	55:SR:353:VAL:HG21	1.88	0.55
4:L3:3651:A:OP2	47:SF:200:ARG:NH1	2.39	0.55
4:L3:131:C:N4	4:L3:138:G:O6	2.39	0.55
4:L3:151:G:OP2	10:L9:4:TYR:OH	2.18	0.55
4:L3:2781:G:O2'	36:LZ:3:SER:O	2.23	0.55
4:L3:4478:G:N2	4:L3:4608:G:O2'	2.39	0.55
40:NL:452:GLU:OE2	40:NL:454:ARG:NH1	2.40	0.55
43:SB:62:CYS:HB3	43:SB:105:LEU:HD22	1.88	0.55
4:L3:2533:C:OP1	18:LH:139:ARG:NH1	2.40	0.55
4:L3:972:C:C6	44:SC:126:LEU:HD23	2.42	0.54
4:L3:1946:G:O2'	38:NF:36:SER:OG	2.25	0.54
4:L3:2838:G:O2'	4:L3:2839:PSU:H5''	2.07	0.54
4:L3:3938:G:N2	4:L3:4171:C:OP2	2.39	0.54
4:L3:2835:A:O2'	24:LN:228:TYR:O	2.23	0.54
6:L5:110:GLN:OE1	6:L5:110:GLN:N	2.40	0.54
4:L3:454:U:O2'	27:LQ:5:ARG:NH2	2.40	0.54
4:L3:4937:C:O3'	44:SC:183:ARG:NH2	2.40	0.54
20:LJ:68:ILE:O	20:LJ:115:LYS:NZ	2.35	0.54
24:LN:199:GLU:OE1	24:LN:200:ARG:NH1	2.40	0.54
4:L3:508:G:O2'	4:L3:510:U:OP2	2.25	0.54
4:L3:5022:U:O2'	4:L3:5023:C:OP2	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LO:59:GLU:OE1	28:LR:92:LYS:NZ	2.23	0.54
4:L3:1493:G:OP1	23:LM:44:ARG:NH2	2.38	0.54
4:L3:2426:U:O3'	14:LD:5:ARG:NH2	2.41	0.54
4:L3:4305:G:HO2'	4:L3:4306:OMU:P	2.29	0.54
4:L3:3825:A2M:HM'2	4:L3:3826:C:O4'	2.08	0.54
4:L3:5066:U:OP1	11:LA:43:LYS:NZ	2.39	0.54
7:L6:62:PRO:O	7:L6:63:THR:OG1	2.24	0.54
42:SA:340:ILE:HG21	44:SC:50:LEU:HD13	1.89	0.54
50:SI:105:ILE:HD13	50:SI:116:ILE:HD13	1.90	0.54
4:L3:1941:A:N6	4:L3:2040:A:OP2	2.41	0.53
5:L4:7:G:OP1	43:SB:33:ARG:NH1	2.41	0.53
4:L3:4088:C:OP1	47:SF:37:ARG:NH2	2.38	0.53
34:LX:8:VAL:O	34:LX:11:VAL:HG22	2.09	0.53
56:SV:53:LYS:NZ	56:SV:62:GLU:OE2	2.41	0.53
26:LP:95:ASP:OD1	26:LP:96:GLU:N	2.41	0.53
42:SA:144:ILE:HD12	42:SA:150:LEU:HD11	1.91	0.53
54:SQ:75:VAL:HG22	54:SQ:79:ARG:HH12	1.74	0.53
4:L3:1325:C:O2'	4:L3:1326:A2M:OP1	2.21	0.53
56:SV:22:VAL:HG22	56:SV:28:VAL:HG22	1.91	0.53
4:L3:4664:A:OP1	24:LN:376:HIS:NE2	2.41	0.53
4:L3:3715:PSU:H2'	4:L3:3716:C:O4'	2.09	0.53
4:L3:3852:A:H2'	4:L3:3853:PSU:H5''	1.89	0.53
4:L3:4761:G:OP1	8:L7:37:ARG:NH2	2.41	0.53
8:L7:190:ASP:OD1	8:L7:191:LYS:N	2.42	0.53
34:LX:73:THR:OG1	47:SF:80:GLU:OE2	2.18	0.53
44:SC:278:THR:HG22	44:SC:279:ASN:H	1.74	0.53
52:SL:165:LEU:HB3	52:SL:169:ILE:HD12	1.91	0.53
3:L2:5:A:N6	3:L2:95:A:O2'	2.42	0.52
4:L3:2756:G:H21	53:SM:59:THR:HG21	1.72	0.52
12:LB:88:ASP:OD1	12:LB:89:ASP:N	2.42	0.52
4:L3:435:A:H61	4:L3:1312:A:H2	1.56	0.52
28:LR:44:SER:OG	28:LR:46:CYS:SG	2.64	0.52
55:SR:420:MET:SD	55:SR:420:MET:N	2.81	0.52
4:L3:4637:OMG:H2'	4:L3:4638:U:C6	2.44	0.52
17:LG:96:LEU:HD11	56:SV:22:VAL:HG23	1.91	0.52
4:L3:1942:A:N6	4:L3:2040:A:OP2	2.42	0.52
4:L3:3724:A2M:H2'	4:L3:3725:G:H8	1.73	0.52
44:SC:281:ILE:HG23	44:SC:286:LEU:HD11	1.91	0.52
55:SR:47:TYR:HB3	55:SR:117:MET:HE1	1.90	0.52
4:L3:4139:G:H21	4:L3:4140:C:N4	2.07	0.52
4:L3:4872:G:O6	9:L8:98:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:SB:64:ILE:HD13	43:SB:109:LEU:HD22	1.92	0.52
51:SK:238:ASP:OD1	51:SK:239:SER:N	2.42	0.52
4:L3:4691:A:OP1	48:SG:75:SER:OG	2.24	0.52
4:L3:4500:PSU:H2'	4:L3:4501:U:C6	2.44	0.52
8:L7:37:ARG:HD2	8:L7:108:ILE:HD11	1.90	0.52
4:L3:2843:U:O2'	4:L3:4632:U:OP1	2.27	0.52
4:L3:398:A2M:O5'	4:L3:398:A2M:H8	2.09	0.52
4:L3:2422:OMC:OP1	11:LA:127:ARG:NH2	2.40	0.52
4:L3:2895:A:O3'	14:LD:136:ARG:NH2	2.42	0.52
55:SR:233:ARG:NE	55:SR:237:GLU:OE2	2.43	0.52
55:SR:269:LEU:HD22	55:SR:306:ILE:HG23	1.91	0.52
4:L3:2590:G:O2'	4:L3:2755:A:N6	2.41	0.51
4:L3:3661:G:N7	47:SF:152:SER:OG	2.41	0.51
4:L3:1100:U:O2'	4:L3:1167:C:OP2	2.17	0.51
4:L3:4523:A2M:H8	4:L3:4523:A2M:OP2	2.10	0.51
4:L3:1646:A:O2'	33:LW:49:TRP:O	2.21	0.51
12:LB:89:ASP:O	12:LB:112:ARG:NH1	2.44	0.51
39:NK:86:LEU:HD23	39:NK:97:MET:HE1	1.93	0.51
51:SK:85:ARG:NH2	51:SK:89:PRO:O	2.44	0.51
4:L3:4524:G:C2	24:LN:252:ALA:HB1	2.46	0.51
7:L6:7:GLY:O	21:LK:49:HIS:NE2	2.42	0.51
18:LH:82:THR:HG22	18:LH:155:ILE:HG23	1.92	0.51
14:LD:7:GLN:N	14:LD:7:GLN:OE1	2.43	0.51
21:LK:38:LEU:O	21:LK:42:ARG:NH1	2.44	0.51
34:LX:69:TRP:NE1	47:SF:173:GLY:O	2.43	0.51
50:SI:182:ILE:HD11	50:SI:194:LEU:HD13	1.92	0.51
51:SK:126:GLU:OE1	51:SK:139:ARG:NH2	2.41	0.51
55:SR:174:CYS:SG	55:SR:244:LEU:HD21	2.51	0.51
4:L3:1577:G:OP1	34:LX:17:ARG:NH2	2.42	0.51
4:L3:3723:A:H2'	4:L3:3724:A2M:H8	1.93	0.51
8:L7:182:GLU:OE2	9:L8:119:ARG:NH2	2.44	0.51
47:SF:23:ARG:NH1	47:SF:52:PRO:O	2.43	0.51
4:L3:1534:A2M:HM'2	4:L3:1535:C:C6	2.46	0.51
7:L6:164:GLU:N	7:L6:164:GLU:OE1	2.44	0.51
24:LN:370:THR:O	24:LN:370:THR:HG22	2.11	0.51
34:LX:26:VAL:HG22	47:SF:178:PRO:HD2	1.93	0.51
4:L3:111:C:OP1	29:LS:110:LYS:NZ	2.43	0.51
43:SB:271:MET:HE1	43:SB:279:ARG:HD2	1.92	0.51
44:SC:198:SER:N	44:SC:288:PHE:O	2.42	0.51
4:L3:1997:U:O3'	54:SQ:57:ARG:NH2	2.43	0.50
4:L3:2876:OMG:C8	34:LX:16:THR:HG22	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:404:U:O3'	19:LI:87:ARG:NH2	2.41	0.50
4:L3:4768:G:OP1	8:L7:168:TYR:OH	2.26	0.50
20:LJ:22:LYS:NZ	20:LJ:132:GLN:O	2.42	0.50
24:LN:181:MET:HE1	24:LN:346:THR:HG23	1.93	0.50
45:SD:26:ALA:O	45:SD:30:ILE:HD12	2.11	0.50
1:BA:128:THR:O	1:BA:132:ILE:HD12	2.11	0.50
4:L3:2000:G:O6	54:SQ:54:LYS:NZ	2.34	0.50
4:L3:2380:G:N2	4:L3:2425:U:OP1	2.39	0.50
4:L3:4311:A:O2'	4:L3:4312:PSU:H5''	2.11	0.50
4:L3:2632:PSU:H2'	4:L3:2633:U:C6	2.46	0.50
4:L3:4580:U:O2'	24:LN:182:GLU:OE2	2.25	0.50
4:L3:4646:U:O2'	55:SR:502:ASN:OD1	2.23	0.50
4:L3:1591:U:OP2	4:L3:2856:C:O2'	2.24	0.50
8:L7:92:THR:O	8:L7:96:GLN:NE2	2.43	0.50
13:LC:173:ASN:ND2	13:LC:175:PHE:O	2.43	0.50
42:SA:137:VAL:CG1	42:SA:144:ILE:HD13	2.42	0.50
4:L3:2562:G:N2	4:L3:2565:A:OP2	2.42	0.50
4:L3:4402:C:H2'	4:L3:4403:PSU:H5''	1.94	0.50
4:L3:4928:C:O4'	9:L8:121:ARG:NH1	2.44	0.50
2:L1:26:C:O2'	42:SA:53:ALA:O	2.30	0.50
36:LZ:28:ARG:NH1	36:LZ:36:ARG:O	2.42	0.50
4:L3:4474:A:OP2	4:L3:4476:C:N4	2.46	0.49
4:L3:2415:OMU:HM22	4:L3:2415:OMU:C2	2.42	0.49
23:LM:35:VAL:HB	23:LM:40:LEU:HD11	1.93	0.49
52:SL:77:GLU:OE2	52:SL:79:ARG:NH2	2.45	0.49
4:L3:459:C:OP1	44:SC:111:LYS:NZ	2.37	0.49
4:L3:972:C:C5	44:SC:126:LEU:HD23	2.47	0.49
30:LT:54:LYS:O	30:LT:66:LYS:NZ	2.41	0.49
51:SK:6:SER:HA	51:SK:13:ILE:HD11	1.95	0.49
3:L2:4:G:O6	50:SI:70:ARG:NH2	2.44	0.49
4:L3:2483:G:O2'	4:L3:2485:U:OP2	2.29	0.49
4:L3:5001:PSU:H2'	4:L3:5002:U:O4'	2.13	0.49
4:L3:2579:G:N2	4:L3:2582:A:OP2	2.29	0.49
4:L3:2601:A:N6	4:L3:2744:A:OP2	2.42	0.49
4:L3:3279:C:OP1	40:NL:359:ARG:NH2	2.45	0.48
24:LN:95:THR:OG1	24:LN:98:GLY:O	2.31	0.48
4:L3:1871:A2M:O5'	4:L3:1871:A2M:H8	2.13	0.48
9:L8:104:MET:HE3	9:L8:109:ARG:HG2	1.94	0.48
4:L3:1314:C:O2'	27:LQ:24:GLN:OE1	2.28	0.48
4:L3:2060:G:O4'	13:LC:118:ARG:NH1	2.45	0.48
4:L3:4389:C:OP2	55:SR:627:LYS:NZ	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L9:143:ARG:NH1	29:LS:95:LEU:HD23	2.27	0.48
4:L3:2363:A2M:H2'	4:L3:2364:OMG:O4'	2.13	0.48
4:L3:3730:PSU:H2'	4:L3:3731:C:H6	1.78	0.48
2:L1:90:C:HO2'	19:LI:24:HIS:HD1	1.60	0.48
55:SR:398:GLU:OE1	55:SR:415:LYS:NZ	2.47	0.48
4:L3:2724:G:O2'	4:L3:2726:G:OP2	2.22	0.48
8:L7:202:LEU:O	8:L7:202:LEU:HD23	2.14	0.48
9:L8:55:MET:O	13:LC:157:ARG:NH2	2.47	0.48
40:NL:114:LYS:O	52:SL:147:ARG:NH1	2.44	0.48
42:SA:109:ARG:HG2	42:SA:111:TRP:CZ2	2.49	0.48
4:L3:4552:PSU:H2'	4:L3:4553:A:C8	2.49	0.48
18:LH:16:GLU:OE1	18:LH:16:GLU:N	2.42	0.48
44:SC:281:ILE:CG2	44:SC:286:LEU:HD11	2.43	0.48
9:L8:11:ARG:NH1	9:L8:58:THR:O	2.46	0.48
24:LN:313:SER:OG	24:LN:314:ILE:N	2.47	0.48
3:L2:4:G:N7	50:SI:70:ARG:NH1	2.59	0.48
4:L3:140:G:OP1	40:NL:163:ARG:NH2	2.47	0.48
24:LN:370:THR:N	24:LN:380:GLN:OE1	2.46	0.48
41:NP:98:SER:OG	41:NP:100:GLU:OE1	2.24	0.48
52:SL:80:VAL:HG13	52:SL:203:LEU:HD12	1.95	0.48
4:L3:1984:A:O2'	4:L3:1985:G:OP1	2.29	0.47
4:L3:4529:G:O2'	4:L3:4530:UR3:H5'	2.14	0.47
15:LE:9:ARG:O	15:LE:55:LYS:NZ	2.42	0.47
42:SA:8:ILE:HD11	42:SA:257:PHE:CZ	2.48	0.47
54:SQ:45:VAL:HG23	54:SQ:45:VAL:O	2.14	0.47
4:L3:2324:C:O2'	27:LQ:98:GLU:OE1	2.32	0.47
4:L3:1214:C:N4	23:LM:90:SER:O	2.47	0.47
4:L3:2296:G:O2'	42:SA:242:PRO:O	2.32	0.47
44:SC:96:VAL:HG11	44:SC:101:ASN:HD22	1.80	0.47
10:L9:22:LEU:HD13	46:SE:165:GLU:OE2	2.14	0.47
3:L2:48:G:O2'	50:SI:79:ARG:NH1	2.47	0.47
7:L6:100:PRO:O	31:LU:25:ARG:NH2	2.43	0.47
4:L3:2782:U:OP2	36:LZ:10:LYS:NZ	2.40	0.47
4:L3:3605:C:OP2	14:LD:71:ARG:NH1	2.48	0.47
55:SR:301:GLU:OE1	55:SR:301:GLU:N	2.46	0.47
14:LD:126:LYS:O	14:LD:131:VAL:HG12	2.15	0.47
46:SE:195:HIS:ND1	53:SM:100:GLU:OE2	2.35	0.47
4:L3:4618:OMG:HM22	4:L3:4619:U:H5'	1.96	0.47
41:NP:95:GLU:O	56:SV:47:ARG:NH1	2.45	0.47
47:SF:126:LEU:HD23	47:SF:150:LEU:HD22	1.96	0.47
4:L3:400:A2M:HM'3	11:LA:101:ASN:OD1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:2815:A2M:H2'	4:L3:2816:G:C8	2.49	0.46
4:L3:3701:OMC:OP1	4:L3:3701:OMC:H3'	2.15	0.46
35:LY:3:ARG:NH2	35:LY:41:TYR:OH	2.49	0.46
55:SR:225:ILE:HG13	55:SR:271:LEU:HD21	1.97	0.46
52:SL:71:TRP:N	52:SL:247:SER:O	2.45	0.46
4:L3:2470:C:O2'	46:SE:56:LYS:NZ	2.48	0.46
32:LV:103:VAL:O	32:LV:103:VAL:HG13	2.14	0.46
51:SK:225:ASN:HB2	51:SK:228:GLN:OE1	2.16	0.46
4:L3:3744:OMG:HM23	4:L3:3744:OMG:H1'	1.67	0.46
4:L3:4156:G:P	4:L3:4157:A:HO2'	2.30	0.46
4:L3:4405:G:OP2	55:SR:130:LYS:NZ	2.34	0.46
19:LI:2:LYS:NZ	19:LI:7:VAL:O	2.46	0.46
47:SF:118:GLU:HG3	47:SF:126:LEU:HD11	1.98	0.46
4:L3:1895:G:OP1	45:SD:96:ARG:NH2	2.49	0.46
4:L3:2601:A:OP1	28:LR:40:LYS:NZ	2.48	0.46
4:L3:4724:A:O2'	24:LN:104:THR:HG22	2.15	0.46
12:LB:34:PHE:CD2	42:SA:293:LEU:HD22	2.51	0.46
47:SF:42:LYS:NZ	47:SF:89:TYR:OH	2.49	0.46
4:L3:2097:U:O3'	4:L3:2098:G:H4'	2.16	0.46
4:L3:3723:A:O2'	4:L3:3724:A2M:H5'	2.16	0.46
26:LP:109:VAL:HG13	26:LP:109:VAL:O	2.16	0.46
4:L3:1279:A:O2'	4:L3:1281:G:N7	2.47	0.46
4:L3:2891:U:OP2	14:LD:74:ARG:NH1	2.49	0.46
4:L3:4575:G:O2'	4:L3:5069:U:OP1	2.33	0.46
10:L9:68:ARG:NH1	10:L9:124:ASP:O	2.44	0.46
53:SM:134:LEU:HD23	53:SM:199:ILE:HD13	1.98	0.46
4:L3:2536:A:O2'	4:L3:2641:A:N1	2.42	0.46
55:SR:226:LEU:O	55:SR:233:ARG:NH2	2.49	0.46
4:L3:2861:OMC:HM23	4:L3:2861:OMC:H1'	1.44	0.45
55:SR:68:ASP:OD1	55:SR:69:PHE:N	2.49	0.45
4:L3:3654:G:O2'	4:L3:3693:U:OP1	2.32	0.45
4:L3:4476:C:O2'	48:SG:173:ARG:NH2	2.48	0.45
46:SE:164:ILE:O	46:SE:168:VAL:HG13	2.16	0.45
4:L3:1328:G:O2'	4:L3:2349:A:OP1	2.33	0.45
4:L3:2739:C:O2	47:SF:188:LYS:NZ	2.45	0.45
46:SE:58:PRO:HD2	46:SE:61:ILE:HD12	1.98	0.45
2:L1:75:OMG:H1'	2:L1:75:OMG:HM23	1.48	0.45
4:L3:2415:OMU:HM23	4:L3:2416:G:C8	2.52	0.45
4:L3:3925:OMU:HM23	4:L3:3925:OMU:H1'	1.50	0.45
4:L3:1797:G:OP1	45:SD:104:LYS:NZ	2.50	0.45
4:L3:4126:C:OP1	46:SE:37:LYS:NZ	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:4227:OMU:HM23	4:L3:4227:OMU:H1'	1.78	0.45
19:LI:34:LEU:HD12	19:LI:44:VAL:HG23	1.98	0.45
52:SL:82:LEU:CD1	52:SL:203:LEU:HD11	2.47	0.45
4:L3:152:U:OP1	10:L9:49:ARG:NH1	2.50	0.45
4:L3:1532:G:OP2	33:LW:31:LYS:NZ	2.47	0.45
4:L3:4249:G:O2'	6:L5:98:ASN:O	2.29	0.45
4:L3:4571:A2M:H8	4:L3:4571:A2M:O5'	2.16	0.45
48:SG:187:VAL:HG12	48:SG:188:GLN:HG3	1.98	0.45
2:L1:7:U:O2'	4:L3:1305:C:OP1	2.34	0.45
4:L3:1645:C:OP1	42:SA:80:ARG:NH2	2.50	0.45
4:L3:3717:A:H2'	4:L3:3718:A2M:H8	1.99	0.45
16:LF:99:TRP:HB2	16:LF:100:LEU:HD12	1.98	0.45
4:L3:3614:G:O6	41:NP:87:LYS:NZ	2.50	0.45
4:L3:5068:G:N2	4:L3:5069:U:O4	2.41	0.45
10:L9:103:GLU:OE1	10:L9:165:THR:HG21	2.17	0.45
22:LL:39:ARG:NH1	22:LL:105:ASP:OD2	2.48	0.45
55:SR:185:ILE:O	55:SR:189:THR:OG1	2.27	0.45
4:L3:982:U:O5'	44:SC:73:TYR:OH	2.35	0.44
24:LN:367:PHE:HB2	56:SV:1:MET:HE1	2.00	0.44
29:LS:91:MET:HE1	33:LW:78:PHE:CD2	2.53	0.44
53:SM:356:TRP:HB2	53:SM:360:LEU:HD23	1.98	0.44
4:L3:351:C:OP2	42:SA:197:ARG:NH1	2.50	0.44
19:LI:62:TYR:CE2	19:LI:97:VAL:HG11	2.52	0.44
51:SK:155:SER:OG	51:SK:201:ASP:OD1	2.36	0.44
4:L3:1677:PSU:H4'	4:L3:1680:G:C2	2.53	0.44
4:L3:3841:OMC:HM23	4:L3:3841:OMC:H1'	1.60	0.44
12:LB:53:MET:SD	12:LB:143:ARG:NH2	2.91	0.44
23:LM:32:LEU:HD13	23:LM:43:MET:HE1	1.99	0.44
4:L3:102:G:OP1	7:L6:71:ARG:NH2	2.45	0.44
4:L3:2402:G:O2'	28:LR:10:ARG:O	2.35	0.44
4:L3:3908:A:O2'	4:L3:4531:U:OP1	2.31	0.44
9:L8:106:ASP:OD1	44:SC:161:ARG:NH2	2.50	0.44
18:LH:155:ILE:H	18:LH:155:ILE:HD12	1.82	0.44
4:L3:508:G:H21	21:LK:85:GLN:HE22	1.66	0.44
4:L3:4670:C:O2'	4:L3:4672:A:OP2	2.31	0.44
4:L3:2415:OMU:HM23	4:L3:2415:OMU:H1'	1.80	0.44
31:LU:63:VAL:O	31:LU:63:VAL:HG12	2.18	0.44
35:LY:5:ILE:HD12	35:LY:10:ASP:OD2	2.17	0.44
4:L3:3852:A:N7	4:L3:3853:PSU:N1	2.66	0.44
11:LA:126:ARG:HB3	11:LA:140:MET:HE1	2.00	0.44
32:LV:17:LYS:NZ	32:LV:19:GLN:OE1	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:SB:125:VAL:CG2	43:SB:200:MET:HE2	2.48	0.44
55:SR:300:SER:OG	55:SR:301:GLU:OE1	2.35	0.44
4:L3:3730:PSU:H2'	4:L3:3731:C:C6	2.51	0.44
4:L3:4571:A2M:HM'2	4:L3:4571:A2M:H1'	1.67	0.44
4:L3:2625:U:OP2	55:SR:510:ARG:NH2	2.51	0.44
40:NL:289:THR:HG23	40:NL:292:SER:H	1.82	0.44
50:SI:90:LEU:HD12	50:SI:90:LEU:H	1.81	0.44
4:L3:1254:A:N1	4:L3:1258:G:N1	2.62	0.43
4:L3:1428:U:OP1	12:LB:42:THR:HG21	2.17	0.43
4:L3:2364:OMG:H1'	4:L3:2364:OMG:HM23	1.47	0.43
4:L3:2580:U:O2'	20:LJ:79:HIS:ND1	2.51	0.43
20:LJ:76:ASN:OD1	20:LJ:77:TYR:N	2.51	0.43
49:SH:46:VAL:HG13	49:SH:121:MET:HB2	2.01	0.43
4:L3:1534:A2M:HM'3	4:L3:1637:A:C4	2.53	0.43
19:LI:19:PHE:O	19:LI:26:ARG:NH2	2.50	0.43
26:LP:20:VAL:O	26:LP:20:VAL:HG13	2.18	0.43
4:L3:3867:A2M:HM'2	4:L3:3867:A2M:H1'	1.63	0.43
5:L4:74:A:N3	13:LC:53:LYS:NZ	2.67	0.43
40:NL:188:VAL:O	53:SM:163:ARG:NH1	2.52	0.43
54:SQ:42:ILE:HD11	54:SQ:92:VAL:HG13	2.00	0.43
4:L3:2815:A2M:H2'	4:L3:2816:G:H8	1.83	0.43
4:L3:4530:UR3:H6	4:L3:4530:UR3:O5'	2.18	0.43
16:LF:91:LEU:O	16:LF:96:LEU:N	2.49	0.43
24:LN:119:TYR:OH	24:LN:129:ALA:N	2.51	0.43
51:SK:49:VAL:HG12	51:SK:50:HIS:O	2.18	0.43
55:SR:355:GLU:N	55:SR:355:GLU:OE1	2.51	0.43
4:L3:2725:A:OP2	14:LD:97:ARG:NH2	2.51	0.43
4:L3:2804:OMC:HM23	4:L3:2804:OMC:H1'	1.64	0.43
4:L3:4536:OMC:HM23	4:L3:4536:OMC:H1'	1.78	0.43
4:L3:4620:OMU:HM23	4:L3:4620:OMU:H1'	1.68	0.43
44:SC:264:ILE:HD12	44:SC:267:LEU:HD22	2.00	0.43
52:SL:253:VAL:HG12	52:SL:263:ILE:HD11	2.01	0.43
2:L1:68:G:O2'	2:L1:69:PSU:H5''	2.18	0.43
4:L3:400:A2M:HM'3	11:LA:101:ASN:CG	2.43	0.43
4:L3:2258:C:N3	44:SC:90:ALA:N	2.66	0.43
33:LW:36:LYS:HA	33:LW:45:ARG:HH21	1.84	0.43
53:SM:170:HIS:HB3	53:SM:283:LEU:HD11	2.01	0.43
4:L3:1316:OMG:HM22	4:L3:1316:OMG:H1'	1.58	0.43
4:L3:2340:C:H4'	42:SA:42:THR:HG23	2.00	0.43
4:L3:3852:A:C2'	4:L3:3853:PSU:H5''	2.48	0.43
4:L3:4872:G:OP2	9:L8:94:LYS:NZ	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:SD:30:ILE:HD12	45:SD:30:ILE:H	1.84	0.43
4:L3:4241:C:OP2	6:L5:145:LYS:NZ	2.44	0.43
4:L3:4678:G:N7	39:NK:11:ARG:NH2	2.66	0.43
15:LE:63:ARG:NH2	23:LM:30:GLU:OE1	2.52	0.43
30:LT:18:LEU:HD23	30:LT:19:ARG:NH2	2.34	0.43
4:L3:5022:U:HO2'	4:L3:5023:C:P	2.40	0.43
7:L6:63:THR:HG22	7:L6:64:VAL:N	2.33	0.43
51:SK:61:ARG:NH1	51:SK:106:ASN:OD1	2.51	0.43
4:L3:2837:OMU:HM23	4:L3:2837:OMU:H1'	1.49	0.43
4:L3:3928:A:OP1	10:L9:90:ASN:ND2	2.52	0.43
4:L3:4305:G:H4'	4:L3:4306:OMU:OP1	2.18	0.43
10:L9:165:THR:HG23	10:L9:168:GLY:H	1.84	0.43
16:LF:60:VAL:HG23	16:LF:61:VAL:HG23	2.00	0.43
22:LL:20:ARG:NH2	27:LQ:84:GLU:OE1	2.46	0.43
24:LN:220:ILE:HG12	24:LN:278:THR:HG23	2.01	0.43
1:BA:135:THR:HG22	4:L3:1974:U:O4	2.19	0.42
4:L3:1676:C:OP2	4:L3:1677:PSU:N1	2.52	0.42
4:L3:2691:U:C2	4:L3:2692:U:C5	3.07	0.42
4:L3:4306:OMU:HM22	4:L3:4307:A:H5'	2.01	0.42
52:SL:66:LEU:HD11	52:SL:251:LEU:HD21	2.01	0.42
4:L3:265:C:H2'	40:NL:151:LEU:HD21	2.02	0.42
42:SA:154:VAL:HG11	42:SA:158:VAL:HG11	2.00	0.42
4:L3:1250:C:N4	4:L3:1261:G:O6	2.52	0.42
43:SB:64:ILE:CD1	43:SB:109:LEU:HD22	2.50	0.42
55:SR:431:GLU:OE2	56:SV:1:MET:HE2	2.20	0.42
2:L1:102:G:OP2	2:L1:104:A:O2'	2.30	0.42
4:L3:1577:G:O2'	4:L3:1612:G:H4'	2.19	0.42
4:L3:2898:G:OP2	14:LD:135:LYS:NZ	2.37	0.42
4:L3:442:G:OP1	30:LT:68:ARG:NH1	2.46	0.42
4:L3:1340:OMC:HM23	4:L3:1340:OMC:H1'	1.49	0.42
4:L3:2514:G:OP1	28:LR:17:SER:OG	2.32	0.42
4:L3:2725:A:N6	14:LD:88:ARG:O	2.52	0.42
40:NL:206:LEU:HD22	40:NL:214:LEU:HD22	2.01	0.42
47:SF:36:GLU:OE2	47:SF:163:ARG:NH1	2.53	0.42
51:SK:174:SER:O	51:SK:178:GLN:N	2.48	0.42
52:SL:158:ASP:OD2	52:SL:160:ARG:NH2	2.51	0.42
2:L1:90:C:O2'	19:LI:24:HIS:ND1	2.45	0.42
4:L3:1397:A:N1	4:L3:1498:G:O2'	2.51	0.42
4:L3:3627:OMG:H1'	4:L3:3627:OMG:HM23	1.76	0.42
4:L3:63:G:OP2	10:L9:169:ARG:NH1	2.49	0.42
4:L3:1677:PSU:H4'	4:L3:1680:G:N1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:LC:45:TRP:HZ3	13:LC:54:MET:HE2	1.84	0.42
42:SA:210:ILE:HG21	42:SA:252:TRP:CZ3	2.55	0.42
56:SV:19:MET:SD	56:SV:19:MET:N	2.93	0.42
4:L3:2487:G:O2'	4:L3:2488:C:O5'	2.38	0.42
4:L3:4280:A:N6	43:SB:28:THR:O	2.49	0.42
44:SC:278:THR:HG22	44:SC:279:ASN:N	2.35	0.42
51:SK:150:SER:HA	51:SK:194:ALA:HB3	2.01	0.42
4:L3:68:U:OP1	10:L9:178:HIS:ND1	2.37	0.41
4:L3:4637:OMG:HM23	4:L3:4637:OMG:H1'	1.72	0.41
4:L3:1326:A2M:HM'3	4:L3:1326:A2M:H1'	1.83	0.41
52:SL:235:LYS:O	52:SL:238:SER:N	2.50	0.41
4:L3:4301:U:OP2	15:LE:87:LYS:NZ	2.31	0.41
20:LJ:96:VAL:HG23	20:LJ:96:VAL:O	2.20	0.41
26:LP:92:ARG:HA	26:LP:102:LEU:HD23	2.02	0.41
40:NL:160:GLU:C	40:NL:161:LEU:HD22	2.45	0.41
4:L3:1961:G:OP1	54:SQ:69:LYS:NZ	2.42	0.41
4:L3:2739:C:OP1	47:SF:177:LYS:NZ	2.51	0.41
4:L3:4457:PSU:O4	24:LN:252:ALA:HB3	2.20	0.41
4:L3:4541:G:N2	4:L3:4544:A:OP2	2.42	0.41
4:L3:503:C:O2'	4:L3:504:G:O5'	2.34	0.41
4:L3:1398:A:H61	4:L3:1501:C:N4	2.17	0.41
4:L3:2362:U:H2'	4:L3:2363:A2M:H8	2.03	0.41
4:L3:4635:A:H3'	4:L3:4636:PSU:H4'	2.01	0.41
8:L7:189:ILE:HD11	9:L8:119:ARG:HG3	2.02	0.41
42:SA:209:ILE:HB	42:SA:229:LEU:HD13	2.02	0.41
4:L3:346:G:OP1	19:LI:8:THR:HG23	2.20	0.41
4:L3:4431:PSU:H2'	4:L3:4432:C:C6	2.54	0.41
50:SI:88:LEU:HD21	50:SI:138:LYS:HD3	2.02	0.41
52:SL:128:GLN:HG2	52:SL:130:ILE:HD11	2.03	0.41
53:SM:150:THR:HG22	53:SM:151:GLY:N	2.36	0.41
2:L1:85:U:H3'	2:L1:86:U:H5'	2.01	0.41
4:L3:3825:A2M:H2'	4:L3:3826:C:O4'	2.20	0.41
18:LH:143:ASP:N	18:LH:143:ASP:OD1	2.54	0.41
32:LV:33:LEU:O	32:LV:33:LEU:HD23	2.21	0.41
4:L3:1860:PSU:H2'	4:L3:1861:U:C6	2.55	0.41
4:L3:4457:PSU:H1'	24:LN:252:ALA:HB3	2.02	0.41
4:L3:4745:G:H22	4:L3:4955:A:H2	1.68	0.41
55:SR:55:GLN:NE2	55:SR:107:ASP:OD1	2.53	0.41
4:L3:1474:C:H2'	4:L3:1475:G:O4'	2.20	0.41
4:L3:2459:G:N2	4:L3:2462:C:OP2	2.51	0.41
4:L3:4162:C:O2'	46:SE:69:ILE:HD11	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:4370:OMG:H5''	32:LV:64:LYS:HG2	2.03	0.41
7:L6:174:LYS:O	21:LK:138:LYS:NZ	2.51	0.41
17:LG:96:LEU:HD11	56:SV:22:VAL:CG2	2.51	0.41
21:LK:140:VAL:O	21:LK:140:VAL:HG12	2.21	0.41
22:LL:64:ILE:HD11	22:LL:96:MET:CE	2.50	0.41
51:SK:155:SER:OG	51:SK:156:ASN:N	2.54	0.41
4:L3:1515:A:OP1	21:LK:33:GLY:N	2.52	0.41
4:L3:3890:A:N6	4:L3:4570:G:O2'	2.51	0.41
4:L3:4266:G:N3	4:L3:4266:G:H2'	2.36	0.41
4:L3:5064:G:O6	24:LN:124:LYS:NZ	2.54	0.41
9:L8:105:THR:HG22	9:L8:106:ASP:N	2.36	0.41
15:LE:4:THR:O	15:LE:6:GLY:N	2.53	0.41
36:LZ:23:ILE:HD12	36:LZ:27:ILE:HD11	2.02	0.41
4:L3:2040:A:N1	55:SR:27:GLN:NE2	2.68	0.40
4:L3:4587:G:OP1	8:L7:61:ARG:NH1	2.53	0.40
29:LS:37:THR:O	29:LS:37:THR:HG22	2.21	0.40
4:L3:1920:C:H3'	4:L3:1921:C:H5''	2.02	0.40
4:L3:2876:OMG:N7	34:LX:16:THR:HG22	2.36	0.40
4:L3:4137:C:H2'	4:L3:4138:C:O4'	2.21	0.40
4:L3:4434:C:H2'	4:L3:4435:U:O4'	2.21	0.40
4:L3:2422:OMC:HM23	4:L3:2422:OMC:H1'	1.42	0.40
44:SC:96:VAL:HG21	44:SC:101:ASN:HD22	1.87	0.40
53:SM:172:ILE:O	53:SM:176:ARG:N	2.55	0.40
39:NK:82:ASN:O	39:NK:86:LEU:N	2.44	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	BA	158/165 (96%)	157 (99%)	1 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	L5	166/178 (93%)	166 (100%)	0	0	100	100
7	L6	208/211 (99%)	204 (98%)	4 (2%)	0	100	100
8	L7	199/203 (98%)	197 (99%)	2 (1%)	0	100	100
9	L8	133/215 (62%)	130 (98%)	3 (2%)	0	100	100
10	L9	201/204 (98%)	194 (96%)	7 (4%)	0	100	100
11	LA	151/184 (82%)	146 (97%)	5 (3%)	0	100	100
12	LB	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
13	LC	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
14	LD	152/196 (78%)	152 (100%)	0	0	100	100
15	LE	150/160 (94%)	144 (96%)	6 (4%)	0	100	100
16	LF	101/128 (79%)	100 (99%)	1 (1%)	0	100	100
17	LG	137/140 (98%)	135 (98%)	2 (2%)	0	100	100
18	LH	141/156 (90%)	141 (100%)	0	0	100	100
19	LI	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
20	LJ	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
21	LK	145/148 (98%)	140 (97%)	5 (3%)	0	100	100
22	LL	123/137 (90%)	122 (99%)	1 (1%)	0	100	100
23	LM	87/159 (55%)	86 (99%)	1 (1%)	0	100	100
24	LN	399/403 (99%)	385 (96%)	14 (4%)	0	100	100
25	LO	93/115 (81%)	93 (100%)	0	0	100	100
26	LP	104/125 (83%)	103 (99%)	1 (1%)	0	100	100
27	LQ	126/135 (93%)	125 (99%)	1 (1%)	0	100	100
28	LR	110/117 (94%)	109 (99%)	1 (1%)	0	100	100
29	LS	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
30	LT	107/110 (97%)	107 (100%)	0	0	100	100
31	LU	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
32	LV	102/106 (96%)	98 (96%)	4 (4%)	0	100	100
33	LW	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
34	LX	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
35	LY	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
36	LZ	48/51 (94%)	47 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	NC	42/731 (6%)	40 (95%)	2 (5%)	0	100	100
38	NF	69/260 (26%)	68 (99%)	1 (1%)	0	100	100
39	NK	63/129 (49%)	63 (100%)	0	0	100	100
40	NL	317/478 (66%)	314 (99%)	3 (1%)	0	100	100
41	NP	100/134 (75%)	100 (100%)	0	0	100	100
42	SA	356/427 (83%)	349 (98%)	7 (2%)	0	100	100
43	SB	273/297 (92%)	271 (99%)	2 (1%)	0	100	100
44	SC	211/288 (73%)	204 (97%)	7 (3%)	0	100	100
45	SD	223/248 (90%)	216 (97%)	7 (3%)	0	100	100
46	SE	228/266 (86%)	226 (99%)	2 (1%)	0	100	100
47	SF	243/257 (95%)	234 (96%)	9 (4%)	0	100	100
48	SG	188/192 (98%)	187 (100%)	1 (0%)	0	100	100
49	SH	149/293 (51%)	145 (97%)	4 (3%)	0	100	100
50	SI	231/255 (91%)	225 (97%)	6 (3%)	0	100	100
51	SK	242/245 (99%)	229 (95%)	13 (5%)	0	100	100
52	SL	236/490 (48%)	227 (96%)	9 (4%)	0	100	100
53	SM	393/588 (67%)	387 (98%)	6 (2%)	0	100	100
54	SQ	215/239 (90%)	213 (99%)	2 (1%)	0	100	100
55	SR	595/634 (94%)	587 (99%)	8 (1%)	0	100	100
56	SV	137/163 (84%)	136 (99%)	1 (1%)	0	100	100
All	All	8936/11492 (78%)	8768 (98%)	168 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BA	53/137 (39%)	53 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	L5	142/149 (95%)	142 (100%)	0	100	100
7	L6	176/177 (99%)	176 (100%)	0	100	100
8	L7	173/174 (99%)	173 (100%)	0	100	100
9	L8	115/161 (71%)	115 (100%)	0	100	100
10	L9	171/172 (99%)	171 (100%)	0	100	100
11	LA	134/163 (82%)	134 (100%)	0	100	100
12	LB	164/165 (99%)	164 (100%)	0	100	100
13	LC	157/157 (100%)	157 (100%)	0	100	100
14	LD	138/175 (79%)	138 (100%)	0	100	100
15	LE	136/140 (97%)	136 (100%)	0	100	100
16	LF	93/115 (81%)	93 (100%)	0	100	100
17	LG	106/107 (99%)	106 (100%)	0	100	100
18	LH	124/133 (93%)	124 (100%)	0	100	100
19	LI	124/135 (92%)	124 (100%)	0	100	100
20	LJ	117/118 (99%)	117 (100%)	0	100	100
21	LK	120/121 (99%)	120 (100%)	0	100	100
22	LL	109/121 (90%)	109 (100%)	0	100	100
23	LM	77/126 (61%)	77 (100%)	0	100	100
24	LN	347/348 (100%)	347 (100%)	0	100	100
25	LO	80/97 (82%)	80 (100%)	0	100	100
26	LP	97/110 (88%)	97 (100%)	0	100	100
27	LQ	114/121 (94%)	114 (100%)	0	100	100
28	LR	96/100 (96%)	96 (100%)	0	100	100
29	LS	109/110 (99%)	109 (100%)	0	100	100
30	LT	88/89 (99%)	88 (100%)	0	100	100
31	LU	86/89 (97%)	86 (100%)	0	100	100
32	LV	92/94 (98%)	92 (100%)	0	100	100
33	LW	73/80 (91%)	73 (100%)	0	100	100
34	LX	74/75 (99%)	74 (100%)	0	100	100
35	LY	64/65 (98%)	64 (100%)	0	100	100
36	LZ	47/48 (98%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	NF	65/228 (28%)	65 (100%)	0	100	100
39	NK	61/115 (53%)	61 (100%)	0	100	100
40	NL	280/402 (70%)	280 (100%)	0	100	100
41	NP	88/114 (77%)	88 (100%)	0	100	100
42	SA	298/348 (86%)	298 (100%)	0	100	100
43	SB	234/250 (94%)	234 (100%)	0	100	100
44	SC	192/252 (76%)	192 (100%)	0	100	100
45	SD	194/215 (90%)	194 (100%)	0	100	100
46	SE	198/223 (89%)	198 (100%)	0	100	100
47	SF	188/199 (94%)	188 (100%)	0	100	100
48	SG	169/171 (99%)	169 (100%)	0	100	100
49	SH	103/274 (38%)	103 (100%)	0	100	100
50	SI	210/228 (92%)	210 (100%)	0	100	100
51	SK	212/213 (100%)	212 (100%)	0	100	100
52	SL	221/437 (51%)	221 (100%)	0	100	100
53	SM	354/509 (70%)	354 (100%)	0	100	100
54	SQ	194/214 (91%)	194 (100%)	0	100	100
55	SR	545/574 (95%)	545 (100%)	0	100	100
56	SV	128/149 (86%)	128 (100%)	0	100	100
All	All	7730/9287 (83%)	7730 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
6	L5	42	GLN
6	L5	112	HIS
6	L5	167	GLN
8	L7	63	ASN
8	L7	90	HIS
9	L8	34	ASN
9	L8	69	HIS
10	L9	86	HIS
10	L9	182	HIS

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Mol	Chain	Res	Type
11	LA	56	GLN
11	LA	72	GLN
11	LA	133	HIS
12	LB	162	HIS
13	LC	77	ASN
14	LD	40	GLN
14	LD	66	ASN
15	LE	58	HIS
17	LG	27	ASN
18	LH	33	HIS
18	LH	35	HIS
19	LI	20	ASN
21	LK	19	HIS
21	LK	28	HIS
21	LK	85	GLN
22	LL	21	ASN
24	LN	42	HIS
24	LN	167	GLN
24	LN	184	GLN
24	LN	209	GLN
25	LO	40	GLN
26	LP	34	HIS
26	LP	116	ASN
27	LQ	126	ASN
30	LT	99	HIS
33	LW	13	ASN
36	LZ	25	GLN
42	SA	178	ASN
42	SA	198	ASN
42	SA	276	ASN
42	SA	299	GLN
42	SA	329	ASN
43	SB	202	GLN
44	SC	136	HIS
44	SC	190	HIS
44	SC	256	GLN
45	SD	239	GLN
46	SE	153	GLN
46	SE	208	ASN
47	SF	139	HIS
48	SG	140	GLN
49	SH	119	HIS

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Mol	Chain	Res	Type
50	SI	136	ASN
51	SK	9	ASN
51	SK	82	GLN
51	SK	83	HIS
52	SL	204	ASN
52	SL	229	ASN
53	SM	170	HIS
53	SM	209	HIS
53	SM	375	HIS
53	SM	384	GLN
54	SQ	47	ASN
54	SQ	186	GLN
55	SR	37	HIS
55	SR	209	HIS
55	SR	354	ASN
55	SR	436	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	L1	152/157 (96%)	18 (11%)	0
3	L2	67/1167 (5%)	9 (13%)	0
4	L3	3373/5070 (66%)	410 (12%)	4 (0%)
5	L4	119/121 (98%)	11 (9%)	1 (0%)
All	All	3711/6515 (56%)	448 (12%)	5 (0%)

All (448) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	L1	23	C
2	L1	34	U
2	L1	35	C
2	L1	59	A
2	L1	62	A
2	L1	63	U
2	L1	82	A
2	L1	83	C
2	L1	84	A
2	L1	86	U
2	L1	94	G
2	L1	103	A

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Mol	Chain	Res	Type
2	L1	105	C
2	L1	110	U
2	L1	111	U
2	L1	127	U
2	L1	151	G
2	L1	156	U
3	L2	11	C
3	L2	48	G
3	L2	49	G
3	L2	51	U
3	L2	62	U
3	L2	96	A
3	L2	101	A
3	L2	1165	A
3	L2	1166	G
4	L3	2	G
4	L3	6	C
4	L3	39	A
4	L3	42	A
4	L3	48	G
4	L3	56	A
4	L3	58	G
4	L3	59	A
4	L3	64	A
4	L3	65	A
4	L3	66	A
4	L3	69	A
4	L3	91	G
4	L3	109	G
4	L3	119	G
4	L3	159	C
4	L3	164	G
4	L3	167	C
4	L3	169	G
4	L3	170	C
4	L3	171	U
4	L3	172	C
4	L3	173	C
4	L3	181	C
4	L3	200	U
4	L3	210	C
4	L3	218	A

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Mol	Chain	Res	Type
4	L3	233	U
4	L3	234	G
4	L3	261	G
4	L3	263	G
4	L3	266	C
4	L3	274	C
4	L3	316	U
4	L3	340	C
4	L3	349	A
4	L3	387	G
4	L3	409	G
4	L3	410	A
4	L3	412	G
4	L3	450	G
4	L3	452	A
4	L3	453	G
4	L3	454	U
4	L3	464	G
4	L3	467	U
4	L3	469	C
4	L3	472	C
4	L3	473	C
4	L3	479	G
4	L3	492	U
4	L3	493	G
4	L3	496	G
4	L3	497	G
4	L3	499	G
4	L3	501	C
4	L3	502	C
4	L3	503	C
4	L3	504	G
4	L3	510	U
4	L3	511	C
4	L3	658	C
4	L3	660	A
4	L3	667	A
4	L3	668	C
4	L3	669	C
4	L3	686	A
4	L3	704	C
4	L3	730	G

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Mol	Chain	Res	Type
4	L3	731	G
4	L3	739	G
4	L3	741	C
4	L3	742	G
4	L3	746	A
4	L3	913	U
4	L3	915	A
4	L3	916	C
4	L3	917	A
4	L3	918	G
4	L3	926	G
4	L3	932	A
4	L3	933	G
4	L3	944	A
4	L3	945	U
4	L3	956	A
4	L3	959	G
4	L3	960	A
4	L3	971	U
4	L3	972	C
4	L3	1066	G
4	L3	1072	C
4	L3	1080	C
4	L3	1100	U
4	L3	1167	C
4	L3	1169	G
4	L3	1171	G
4	L3	1173	G
4	L3	1174	G
4	L3	1178	G
4	L3	1180	C
4	L3	1181	C
4	L3	1182	C
4	L3	1201	U
4	L3	1203	G
4	L3	1211	G
4	L3	1214	C
4	L3	1215	C
4	L3	1216	C
4	L3	1253	G
4	L3	1254	A
4	L3	1255	A

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Mol	Chain	Res	Type
4	L3	1266	G
4	L3	1269	G
4	L3	1270	A
4	L3	1273	G
4	L3	1280	C
4	L3	1284	G
4	L3	1287	G
4	L3	1294	A
4	L3	1295	C
4	L3	1301	C
4	L3	1314	C
4	L3	1319	U
4	L3	1325	C
4	L3	1326	A2M
4	L3	1354	A
4	L3	1358	G
4	L3	1359	G
4	L3	1365	C
4	L3	1366	G
4	L3	1379	C
4	L3	1397	A
4	L3	1420	A
4	L3	1439	C
4	L3	1443	A
4	L3	1497	A
4	L3	1498	G
4	L3	1502	G
4	L3	1523	A
4	L3	1534	A2M
4	L3	1547	A
4	L3	1578	U
4	L3	1581	G
4	L3	1592	G
4	L3	1613	A
4	L3	1624	G
4	L3	1625	OMG
4	L3	1631	A
4	L3	1633	G
4	L3	1634	A
4	L3	1642	A
4	L3	1654	G
4	L3	1661	C

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Mol	Chain	Res	Type
4	L3	1670	G
4	L3	1671	U
4	L3	1676	C
4	L3	1677	PSU
4	L3	1678	C
4	L3	1721	G
4	L3	1726	U
4	L3	1734	G
4	L3	1791	U
4	L3	1804	A
4	L3	1811	G
4	L3	1815	G
4	L3	1821	G
4	L3	1822	U
4	L3	1836	G
4	L3	1837	A
4	L3	1842	G
4	L3	1854	G
4	L3	1875	C
4	L3	1880	G
4	L3	1882	U
4	L3	1887	G
4	L3	1888	A
4	L3	1897	A
4	L3	1910	G
4	L3	1919	G
4	L3	1921	C
4	L3	1922	G
4	L3	1925	G
4	L3	1973	G
4	L3	1974	U
4	L3	1978	C
4	L3	1984	A
4	L3	1997	U
4	L3	2002	A
4	L3	2011	C
4	L3	2016	C
4	L3	2021	G
4	L3	2026	A
4	L3	2041	A
4	L3	2044	U
4	L3	2046	G

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Mol	Chain	Res	Type
4	L3	2055	G
4	L3	2056	G
4	L3	2069	A
4	L3	2084	C
4	L3	2085	G
4	L3	2092	G
4	L3	2093	A
4	L3	2094	G
4	L3	2095	A
4	L3	2096	G
4	L3	2097	U
4	L3	2098	G
4	L3	2109	G
4	L3	2110	C
4	L3	2111	G
4	L3	2261	G
4	L3	2289	C
4	L3	2300	A
4	L3	2301	G
4	L3	2313	A
4	L3	2316	G
4	L3	2348	G
4	L3	2351	OMC
4	L3	2395	A
4	L3	2414	G
4	L3	2417	A
4	L3	2422	OMC
4	L3	2424	OMG
4	L3	2425	U
4	L3	2429	A
4	L3	2450	G
4	L3	2453	A
4	L3	2470	C
4	L3	2471	G
4	L3	2475	G
4	L3	2476	G
4	L3	2477	A
4	L3	2478	C
4	L3	2486	G
4	L3	2487	G
4	L3	2488	C
4	L3	2489	C

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Mol	Chain	Res	Type
4	L3	2492	C
4	L3	2493	G
4	L3	2512	A
4	L3	2513	A
4	L3	2519	U
4	L3	2529	A
4	L3	2544	G
4	L3	2545	U
4	L3	2548	C
4	L3	2554	U
4	L3	2587	A
4	L3	2638	G
4	L3	2653	C
4	L3	2669	C
4	L3	2687	U
4	L3	2694	G
4	L3	2695	A
4	L3	2696	A
4	L3	2711	G
4	L3	2742	G
4	L3	2743	A
4	L3	2760	G
4	L3	2764	A
4	L3	2769	U
4	L3	2772	C
4	L3	2787	A2M
4	L3	2788	U
4	L3	2790	U
4	L3	2814	C
4	L3	2826	U
4	L3	2827	G
4	L3	2842	G
4	L3	2855	G
4	L3	2877	G
4	L3	2902	G
4	L3	2917	G
4	L3	2918	G
4	L3	3271	G
4	L3	3593	C
4	L3	3595	U
4	L3	3597	G
4	L3	3626	G

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Mol	Chain	Res	Type
4	L3	3635	A
4	L3	3644	U
4	L3	3653	A
4	L3	3662	A
4	L3	3696	C
4	L3	3697	U
4	L3	3701	OMC
4	L3	3838	U
4	L3	3840	U
4	L3	3868	G
4	L3	3872	A
4	L3	3875	G
4	L3	3887	OMC
4	L3	3905	A
4	L3	3915	U
4	L3	4069	U
4	L3	4076	G
4	L3	4084	G
4	L3	4085	A
4	L3	4119	C
4	L3	4122	G
4	L3	4127	A
4	L3	4133	C
4	L3	4139	G
4	L3	4140	C
4	L3	4142	C
4	L3	4143	G
4	L3	4144	C
4	L3	4145	C
4	L3	4147	G
4	L3	4150	G
4	L3	4154	G
4	L3	4162	C
4	L3	4170	A
4	L3	4183	G
4	L3	4184	G
4	L3	4191	G
4	L3	4194	U
4	L3	4202	U
4	L3	4205	A
4	L3	4220	6MZ
4	L3	4222	G

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Mol	Chain	Res	Type
4	L3	4229	U
4	L3	4233	A
4	L3	4251	A
4	L3	4254	G
4	L3	4266	G
4	L3	4268	A
4	L3	4273	A
4	L3	4281	A
4	L3	4305	G
4	L3	4306	OMU
4	L3	4329	G
4	L3	4330	G
4	L3	4332	C
4	L3	4373	G
4	L3	4376	A
4	L3	4377	G
4	L3	4378	A
4	L3	4387	C
4	L3	4418	G
4	L3	4453	C
4	L3	4464	A
4	L3	4466	C
4	L3	4475	G
4	L3	4491	G
4	L3	4498	OMU
4	L3	4512	U
4	L3	4513	A
4	L3	4519	C
4	L3	4523	A2M
4	L3	4524	G
4	L3	4545	G
4	L3	4548	A
4	L3	4549	G
4	L3	4555	U
4	L3	4556	U
4	L3	4558	U
4	L3	4560	C
4	L3	4584	A
4	L3	4590	A2M
4	L3	4608	G
4	L3	4627	U
4	L3	4636	PSU

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Mol	Chain	Res	Type
4	L3	4637	OMG
4	L3	4656	A
4	L3	4670	C
4	L3	4672	A
4	L3	4678	G
4	L3	4701	A
4	L3	4708	A
4	L3	4709	U
4	L3	4719	G
4	L3	4720	C
4	L3	4740	G
4	L3	4741	C
4	L3	4742	G
4	L3	4750	G
4	L3	4751	G
4	L3	4754	G
4	L3	4757	C
4	L3	4759	C
4	L3	4765	G
4	L3	4772	C
4	L3	4773	C
4	L3	4870	G
4	L3	4871	C
4	L3	4882	U
4	L3	4883	C
4	L3	4900	C
4	L3	4901	G
4	L3	4910	G
4	L3	4914	C
4	L3	4916	G
4	L3	4937	C
4	L3	4943	A
4	L3	4976	U
4	L3	5014	A
4	L3	5020	G
4	L3	5022	U
4	L3	5023	C
4	L3	5026	U
4	L3	5027	C
4	L3	5031	G
4	L3	5041	G
4	L3	5050	C

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Mol	Chain	Res	Type
4	L3	5054	C
4	L3	5055	G
4	L3	5061	A
4	L3	5062	G
4	L3	5069	U
5	L4	7	G
5	L4	24	C
5	L4	49	A
5	L4	53	U
5	L4	54	A
5	L4	64	G
5	L4	66	G
5	L4	89	G
5	L4	110	G
5	L4	111	C
5	L4	120	U

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	L3	496	G
4	L3	502	C
4	L3	503	C
4	L3	2095	A
5	L4	109	U

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

107 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
4	PSU	L3	1683	4	18,21,22	1.08	2 (11%)	21,30,33	1.87	4 (19%)
4	A2M	L3	3867	4	22,25,26	0.85	0	30,36,39	2.11	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A2M	L3	3825	4	22,25,26	0.87	0	30,36,39	2.10	7 (23%)
4	OMG	L3	1522	4	23,26,27	0.55	0	32,38,41	0.53	0
4	OMG	L3	4499	4	23,26,27	0.46	0	32,38,41	0.47	0
4	OMC	L3	2804	4	19,22,23	0.58	0	25,31,34	0.62	0
4	A2M	L3	3830	4	22,25,26	0.89	1 (4%)	30,36,39	2.08	7 (23%)
4	A2M	L3	4590	4	22,25,26	0.92	1 (4%)	30,36,39	2.02	8 (26%)
4	OMC	L3	4536	4	19,22,23	0.57	0	25,31,34	0.68	0
4	OMG	L3	4494	4	23,26,27	0.55	0	32,38,41	0.54	0
4	OMG	L3	4228	4	23,26,27	0.61	0	32,38,41	0.60	0
4	OMU	L3	4620	4	19,22,23	1.94	5 (26%)	25,31,34	1.71	4 (16%)
4	PSU	L3	1536	4	18,21,22	1.08	1 (5%)	21,30,33	1.94	5 (23%)
4	A2M	L3	4523	4	22,25,26	0.88	0	30,36,39	2.08	8 (26%)
4	OMG	L3	2876	4	23,26,27	0.48	0	32,38,41	0.50	0
4	PSU	L3	4457	4	18,21,22	1.12	1 (5%)	21,30,33	1.98	4 (19%)
4	PSU	L3	3715	4	18,21,22	1.11	1 (5%)	21,30,33	1.95	5 (23%)
4	OMG	L3	3899	4	23,26,27	0.54	0	32,38,41	0.57	0
4	OMG	L3	4623	4	23,26,27	0.52	0	32,38,41	0.57	0
4	A2M	L3	1871	4	22,25,26	0.83	0	30,36,39	2.13	9 (30%)
4	PSU	L3	4500	4	18,21,22	1.09	1 (5%)	21,30,33	1.94	4 (19%)
4	PSU	L3	3639	4	18,21,22	1.08	2 (11%)	21,30,33	2.02	6 (28%)
4	PSU	L3	2839	4	18,21,22	1.12	1 (5%)	21,30,33	1.89	4 (19%)
4	A2M	L3	1326	4	22,25,26	0.88	0	30,36,39	2.01	7 (23%)
4	PSU	L3	2632	4	18,21,22	1.09	1 (5%)	21,30,33	1.90	5 (23%)
4	PSU	L3	4576	4	18,21,22	1.10	1 (5%)	21,30,33	1.94	4 (19%)
4	A2M	L3	3724	4	22,25,26	0.87	0	30,36,39	2.03	7 (23%)
4	PSU	L3	3884	4	18,21,22	1.07	2 (11%)	21,30,33	1.93	4 (19%)
4	PSU	L3	4521	4	18,21,22	1.03	2 (11%)	21,30,33	1.91	4 (19%)
4	PSU	L3	5010	4	18,21,22	1.09	1 (5%)	21,30,33	1.92	5 (23%)
4	PSU	L3	4353	4	18,21,22	1.01	1 (5%)	21,30,33	2.08	6 (28%)
4	OMU	L3	4227	4	19,22,23	1.97	6 (31%)	25,31,34	1.83	4 (16%)
4	OMG	L3	3744	4	23,26,27	0.46	0	32,38,41	0.49	0
4	PSU	L3	4493	4	18,21,22	1.06	2 (11%)	21,30,33	1.95	5 (23%)
4	A2M	L3	1524	4	22,25,26	0.89	0	30,36,39	2.11	7 (23%)
24	HIC	LN	245	24	10,11,12	1.46	1 (10%)	9,14,16	1.26	1 (11%)
4	PSU	L3	3637	4	18,21,22	1.06	1 (5%)	21,30,33	1.96	5 (23%)
4	PSU	L3	3822	4	18,21,22	1.14	1 (5%)	21,30,33	1.98	5 (23%)
4	PSU	L3	2508	4	18,21,22	1.05	1 (5%)	21,30,33	1.96	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PSU	L3	3853	4	18,21,22	1.05	1 (5%)	21,30,33	1.86	5 (23%)
4	PSU	L3	1792	4	18,21,22	1.07	1 (5%)	21,30,33	1.93	4 (19%)
4	OMC	L3	1340	4	19,22,23	0.65	0	25,31,34	0.76	0
4	UR3	L3	4530	4	19,22,23	1.12	3 (15%)	26,32,35	1.52	2 (7%)
4	PSU	L3	4628	4	18,21,22	1.02	2 (11%)	21,30,33	1.93	5 (23%)
4	A2M	L3	2787	4	22,25,26	0.90	1 (4%)	30,36,39	2.10	7 (23%)
4	PSU	L3	4471	4	18,21,22	1.10	1 (5%)	21,30,33	1.97	5 (23%)
4	OMU	L3	4498	4	19,22,23	2.12	7 (36%)	25,31,34	1.85	5 (20%)
4	OMC	L3	2351	4,57	19,22,23	0.66	0	25,31,34	0.84	1 (4%)
4	OMC	L3	3869	4	19,22,23	0.59	0	25,31,34	0.69	0
4	PSU	L3	4312	4	18,21,22	1.03	1 (5%)	21,30,33	2.02	4 (19%)
4	OMG	L3	4392	4	23,26,27	0.52	0	32,38,41	0.50	0
4	OMG	L3	3627	4	23,26,27	0.53	0	32,38,41	0.62	0
4	OMC	L3	2365	4	19,22,23	0.58	0	25,31,34	0.67	0
4	A2M	L3	4571	4	22,25,26	0.89	1 (4%)	30,36,39	1.99	7 (23%)
4	OMU	L3	2415	4	19,22,23	2.01	6 (31%)	25,31,34	1.91	5 (20%)
4	PSU	L3	1677	4	18,21,22	1.04	1 (5%)	21,30,33	1.90	5 (23%)
4	PSU	L3	4532	4	18,21,22	1.08	1 (5%)	21,30,33	2.00	5 (23%)
4	PSU	L3	3851	4	18,21,22	1.09	2 (11%)	21,30,33	1.92	5 (23%)
4	OMG	L3	4618	4	23,26,27	0.53	0	32,38,41	0.58	0
4	OMU	L3	2837	4	19,22,23	2.04	6 (31%)	25,31,34	1.90	5 (20%)
2	PSU	L1	69	2	18,21,22	1.10	1 (5%)	21,30,33	1.92	5 (23%)
2	OMG	L1	75	2	23,26,27	0.50	0	32,38,41	0.49	0
4	A2M	L3	2815	4	22,25,26	0.87	0	30,36,39	2.12	7 (23%)
4	OMG	L3	4370	4	23,26,27	0.62	0	32,38,41	0.56	0
4	A2M	L3	1534	4,57	22,25,26	0.89	1 (4%)	30,36,39	2.08	9 (30%)
4	A2M	L3	398	4	22,25,26	0.88	1 (4%)	30,36,39	2.15	8 (26%)
4	OMG	L3	2364	4	23,26,27	0.53	0	32,38,41	0.49	0
4	OMU	L3	3925	4	19,22,23	1.97	6 (31%)	25,31,34	1.90	5 (20%)
4	OMC	L3	2422	4,57	19,22,23	0.56	0	25,31,34	0.70	0
4	PSU	L3	1860	4	18,21,22	1.05	1 (5%)	21,30,33	1.94	6 (28%)
4	OMG	L3	4637	4	23,26,27	0.53	0	32,38,41	0.52	0
4	PSU	L3	1862	4	18,21,22	1.11	1 (5%)	21,30,33	1.91	5 (23%)
4	OMC	L3	3887	4	19,22,23	0.59	0	25,31,34	0.63	0
4	PSU	L3	4431	4	18,21,22	1.13	1 (5%)	21,30,33	2.02	5 (23%)
4	PSU	L3	4579	4	18,21,22	1.03	2 (11%)	21,30,33	1.87	4 (19%)
4	A2M	L3	2401	4	22,25,26	0.91	1 (4%)	30,36,39	2.11	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OMC	L3	2824	4	19,22,23	0.57	0	25,31,34	0.64	0
4	A2M	L3	2363	4,57	22,25,26	0.92	1 (4%)	30,36,39	2.04	7 (23%)
4	PSU	L3	4361	4	18,21,22	1.00	1 (5%)	21,30,33	1.97	5 (23%)
4	OMC	L3	4456	4	19,22,23	0.59	0	25,31,34	0.62	0
4	OMU	L3	4306	4	19,22,23	1.97	5 (26%)	25,31,34	1.94	5 (20%)
4	PSU	L3	3695	4	18,21,22	1.11	1 (5%)	21,30,33	1.96	5 (23%)
4	PSU	L3	4673	4	18,21,22	1.10	2 (11%)	21,30,33	1.97	5 (23%)
4	PSU	L3	4972	4	18,21,22	1.04	1 (5%)	21,30,33	1.93	4 (19%)
4	A2M	L3	400	4	22,25,26	0.85	0	30,36,39	2.11	8 (26%)
4	6MZ	L3	4220	4	22,25,26	1.13	2 (9%)	29,36,39	2.17	9 (31%)
4	PSU	L3	4636	4	18,21,22	1.08	1 (5%)	21,30,33	2.05	6 (28%)
4	PSU	L3	1582	4	18,21,22	1.06	1 (5%)	21,30,33	1.95	4 (19%)
4	OMC	L3	2861	4	19,22,23	0.55	0	25,31,34	0.63	0
4	OMC	L3	3841	4	19,22,23	0.56	0	25,31,34	0.66	0
4	A2M	L3	3718	4	22,25,26	0.91	1 (4%)	30,36,39	1.94	7 (23%)
4	PSU	L3	3730	4	18,21,22	1.10	1 (5%)	21,30,33	1.93	5 (23%)
4	PSU	L3	3734	4	18,21,22	1.11	1 (5%)	21,30,33	1.99	6 (28%)
4	PSU	L3	4689	4	18,21,22	1.08	1 (5%)	21,30,33	1.96	4 (19%)
4	PSU	L3	4299	4	18,21,22	0.99	2 (11%)	21,30,33	2.08	5 (23%)
4	OMG	L3	1316	4	23,26,27	0.52	0	32,38,41	0.50	0
4	OMG	L3	1625	4	23,26,27	0.54	0	32,38,41	0.49	0
4	PSU	L3	4296	4	18,21,22	1.01	2 (11%)	21,30,33	2.11	5 (23%)
4	PSU	L3	4552	4	18,21,22	1.05	1 (5%)	21,30,33	1.93	5 (23%)
4	PSU	L3	4293	4	18,21,22	1.00	2 (11%)	21,30,33	1.78	4 (19%)
4	PSU	L3	3920	4,57	18,21,22	1.04	2 (11%)	21,30,33	1.96	5 (23%)
2	PSU	L1	55	2	18,21,22	1.06	2 (11%)	21,30,33	2.01	5 (23%)
4	OMG	L3	2424	4	23,26,27	0.53	0	32,38,41	0.46	0
4	PSU	L3	4403	4	18,21,22	1.08	1 (5%)	21,30,33	1.93	5 (23%)
4	OMC	L3	3701	4	19,22,23	0.52	0	25,31,34	0.61	0
4	PSU	L3	3844	4	18,21,22	1.11	1 (5%)	21,30,33	1.88	5 (23%)
4	PSU	L3	5001	4	18,21,22	1.09	2 (11%)	21,30,33	2.00	5 (23%)

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
4	PSU	L3	1683	4	-	0/7/25/26	0/2/2/2
4	A2M	L3	3867	4	-	1/9/27/28	0/3/3/3
4	A2M	L3	3825	4	-	0/9/27/28	0/3/3/3
4	OMG	L3	1522	4	-	0/9/27/28	0/3/3/3
4	OMG	L3	4499	4	-	0/9/27/28	0/3/3/3
4	OMC	L3	2804	4	-	1/9/27/28	0/2/2/2
4	A2M	L3	3830	4	-	1/9/27/28	0/3/3/3
4	A2M	L3	4590	4	-	4/9/27/28	0/3/3/3
4	OMC	L3	4536	4	-	1/9/27/28	0/2/2/2
4	OMG	L3	4494	4	-	0/9/27/28	0/3/3/3
4	OMG	L3	4228	4	-	0/9/27/28	0/3/3/3
4	OMU	L3	4620	4	-	1/9/27/28	0/2/2/2
4	PSU	L3	1536	4	-	0/7/25/26	0/2/2/2
4	A2M	L3	4523	4	-	2/9/27/28	0/3/3/3
4	OMG	L3	2876	4	-	1/9/27/28	0/3/3/3
4	PSU	L3	4457	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	3715	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	3899	4	-	0/9/27/28	0/3/3/3
4	OMG	L3	4623	4	-	0/9/27/28	0/3/3/3
4	A2M	L3	1871	4	-	0/9/27/28	0/3/3/3
4	PSU	L3	4500	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	3639	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	2839	4	-	3/7/25/26	0/2/2/2
4	A2M	L3	1326	4	-	3/9/27/28	0/3/3/3
4	PSU	L3	2632	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4576	4	-	0/7/25/26	0/2/2/2
4	A2M	L3	3724	4	-	1/9/27/28	0/3/3/3
4	PSU	L3	3884	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4521	4	-	2/7/25/26	0/2/2/2
4	PSU	L3	5010	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4353	4	-	0/7/25/26	0/2/2/2
4	OMU	L3	4227	4	-	1/9/27/28	0/2/2/2
4	OMG	L3	3744	4	-	1/9/27/28	0/3/3/3
4	PSU	L3	4493	4	-	0/7/25/26	0/2/2/2
4	A2M	L3	1524	4	-	3/9/27/28	0/3/3/3
24	HIC	LN	245	24	-	2/5/6/8	0/1/1/1
4	PSU	L3	3637	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	3822	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	2508	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	3853	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	1792	4	-	0/7/25/26	0/2/2/2
4	OMC	L3	1340	4	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	UR3	L3	4530	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4628	4	-	0/7/25/26	0/2/2/2
4	A2M	L3	2787	4	-	6/9/27/28	0/3/3/3
4	PSU	L3	4471	4	-	0/7/25/26	0/2/2/2
4	OMU	L3	4498	4	-	1/9/27/28	0/2/2/2
4	OMC	L3	2351	4,57	-	2/9/27/28	0/2/2/2
4	OMC	L3	3869	4	-	0/9/27/28	0/2/2/2
4	PSU	L3	4312	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	4392	4	-	1/9/27/28	0/3/3/3
4	OMG	L3	3627	4	-	0/9/27/28	0/3/3/3
4	OMC	L3	2365	4	-	0/9/27/28	0/2/2/2
4	A2M	L3	4571	4	-	1/9/27/28	0/3/3/3
4	OMU	L3	2415	4	-	1/9/27/28	0/2/2/2
4	PSU	L3	1677	4	-	4/7/25/26	0/2/2/2
4	PSU	L3	4532	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	3851	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	4618	4	-	2/9/27/28	0/3/3/3
4	OMU	L3	2837	4	-	1/9/27/28	0/2/2/2
2	PSU	L1	69	2	-	0/7/25/26	0/2/2/2
2	OMG	L1	75	2	-	1/9/27/28	0/3/3/3
4	A2M	L3	2815	4	-	2/9/27/28	0/3/3/3
4	OMG	L3	4370	4	-	0/9/27/28	0/3/3/3
4	A2M	L3	1534	4,57	-	0/9/27/28	0/3/3/3
4	A2M	L3	398	4	-	1/9/27/28	0/3/3/3
4	OMG	L3	2364	4	-	2/9/27/28	0/3/3/3
4	OMU	L3	3925	4	-	1/9/27/28	0/2/2/2
4	OMC	L3	2422	4,57	-	2/9/27/28	0/2/2/2
4	PSU	L3	1860	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	4637	4	-	3/9/27/28	0/3/3/3
4	PSU	L3	1862	4	-	2/7/25/26	0/2/2/2
4	OMC	L3	3887	4	-	2/9/27/28	0/2/2/2
4	PSU	L3	4431	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4579	4	-	0/7/25/26	0/2/2/2
4	A2M	L3	2401	4	-	2/9/27/28	0/3/3/3
4	OMC	L3	2824	4	-	0/9/27/28	0/2/2/2
4	A2M	L3	2363	4,57	-	1/9/27/28	0/3/3/3
4	PSU	L3	4361	4	-	0/7/25/26	0/2/2/2
4	OMC	L3	4456	4	-	1/9/27/28	0/2/2/2
4	OMU	L3	4306	4	-	4/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PSU	L3	3695	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4673	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4972	4	-	0/7/25/26	0/2/2/2
4	A2M	L3	400	4	-	1/9/27/28	0/3/3/3
4	6MZ	L3	4220	4	-	3/9/27/28	0/3/3/3
4	PSU	L3	4636	4	-	3/7/25/26	0/2/2/2
4	PSU	L3	1582	4	-	0/7/25/26	0/2/2/2
4	OMC	L3	2861	4	-	1/9/27/28	0/2/2/2
4	OMC	L3	3841	4	-	1/9/27/28	0/2/2/2
4	A2M	L3	3718	4	-	1/9/27/28	0/3/3/3
4	PSU	L3	3730	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	3734	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4689	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4299	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	1316	4	-	1/9/27/28	0/3/3/3
4	OMG	L3	1625	4	-	2/9/27/28	0/3/3/3
4	PSU	L3	4296	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4552	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4293	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	3920	4,57	-	0/7/25/26	0/2/2/2
2	PSU	L1	55	2	-	0/7/25/26	0/2/2/2
4	OMG	L3	2424	4	-	2/9/27/28	0/3/3/3
4	PSU	L3	4403	4	-	0/7/25/26	0/2/2/2
4	OMC	L3	3701	4	-	7/9/27/28	0/2/2/2
4	PSU	L3	3844	4	-	1/7/25/26	0/2/2/2
4	PSU	L3	5001	4	-	0/7/25/26	0/2/2/2

All (119) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L3	4498	OMU	C6-N1	4.80	1.49	1.38
4	L3	4620	OMU	C6-N1	4.68	1.49	1.38
4	L3	2837	OMU	C6-N1	4.61	1.49	1.38
4	L3	2415	OMU	C6-N1	4.60	1.49	1.38
4	L3	4306	OMU	C6-N1	4.60	1.49	1.38
4	L3	4498	OMU	C2-N1	4.52	1.45	1.38
4	L3	4227	OMU	C6-N1	4.51	1.48	1.38
4	L3	3925	OMU	C6-N1	4.46	1.48	1.38
4	L3	2837	OMU	C2-N1	4.20	1.45	1.38
4	L3	4498	OMU	C5-C4	4.18	1.52	1.43
4	L3	2415	OMU	C5-C4	4.02	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L3	2837	OMU	C5-C4	4.01	1.52	1.43
4	L3	4227	OMU	C2-N1	3.99	1.44	1.38
4	L3	2415	OMU	C2-N1	3.98	1.44	1.38
4	L3	4306	OMU	C2-N1	3.90	1.44	1.38
4	L3	3925	OMU	C5-C4	3.88	1.52	1.43
4	L3	3925	OMU	C2-N1	3.88	1.44	1.38
4	L3	4227	OMU	C5-C4	3.81	1.52	1.43
4	L3	4620	OMU	C2-N1	3.79	1.44	1.38
4	L3	3822	PSU	C6-C5	3.73	1.39	1.35
4	L3	4620	OMU	C5-C4	3.72	1.51	1.43
4	L3	4220	6MZ	C6-N6	3.64	1.38	1.34
4	L3	4306	OMU	C5-C4	3.64	1.51	1.43
4	L3	2839	PSU	C6-C5	3.61	1.39	1.35
4	L3	4431	PSU	C6-C5	3.60	1.39	1.35
4	L3	4457	PSU	C6-C5	3.56	1.39	1.35
4	L3	1862	PSU	C6-C5	3.55	1.39	1.35
4	L3	3715	PSU	C6-C5	3.52	1.39	1.35
4	L3	3734	PSU	C6-C5	3.52	1.39	1.35
4	L3	3730	PSU	C6-C5	3.50	1.39	1.35
4	L3	4500	PSU	C6-C5	3.50	1.39	1.35
4	L3	3695	PSU	C6-C5	3.50	1.39	1.35
4	L3	4576	PSU	C6-C5	3.47	1.39	1.35
4	L3	3844	PSU	C6-C5	3.44	1.39	1.35
2	L1	69	PSU	C6-C5	3.42	1.39	1.35
4	L3	5010	PSU	C6-C5	3.41	1.39	1.35
4	L3	4403	PSU	C6-C5	3.40	1.39	1.35
4	L3	4471	PSU	C6-C5	3.39	1.39	1.35
4	L3	2632	PSU	C6-C5	3.38	1.39	1.35
4	L3	4532	PSU	C6-C5	3.36	1.39	1.35
4	L3	4673	PSU	C6-C5	3.35	1.39	1.35
4	L3	4636	PSU	C6-C5	3.34	1.39	1.35
4	L3	1792	PSU	C6-C5	3.33	1.39	1.35
4	L3	1860	PSU	C6-C5	3.31	1.39	1.35
4	L3	3637	PSU	C6-C5	3.27	1.38	1.35
4	L3	2508	PSU	C6-C5	3.27	1.38	1.35
4	L3	1582	PSU	C6-C5	3.27	1.38	1.35
4	L3	3851	PSU	C6-C5	3.27	1.38	1.35
4	L3	4552	PSU	C6-C5	3.25	1.38	1.35
4	L3	3884	PSU	C6-C5	3.25	1.38	1.35
4	L3	1536	PSU	C6-C5	3.24	1.38	1.35
4	L3	3853	PSU	C6-C5	3.21	1.38	1.35
4	L3	4972	PSU	C6-C5	3.21	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L3	5001	PSU	C6-C5	3.20	1.38	1.35
4	L3	3639	PSU	C6-C5	3.16	1.38	1.35
4	L3	4689	PSU	C6-C5	3.16	1.38	1.35
2	L1	55	PSU	C6-C5	3.15	1.38	1.35
4	L3	4493	PSU	C6-C5	3.13	1.38	1.35
4	L3	4306	OMU	O4-C4	-3.07	1.18	1.24
4	L3	4312	PSU	C6-C5	3.06	1.38	1.35
4	L3	4521	PSU	C6-C5	3.02	1.38	1.35
4	L3	4353	PSU	C6-C5	2.99	1.38	1.35
4	L3	4361	PSU	C6-C5	2.98	1.38	1.35
4	L3	4620	OMU	O4-C4	-2.96	1.18	1.24
24	LN	245	HIC	CD2-CG	2.95	1.41	1.36
4	L3	1683	PSU	C6-C5	2.94	1.38	1.35
4	L3	3920	PSU	C6-C5	2.93	1.38	1.35
4	L3	4579	PSU	C6-C5	2.92	1.38	1.35
4	L3	4530	UR3	C2-N1	-2.90	1.34	1.38
4	L3	4227	OMU	O4-C4	-2.90	1.18	1.24
4	L3	4628	PSU	C6-C5	2.85	1.38	1.35
4	L3	4530	UR3	C4-N3	-2.84	1.34	1.40
4	L3	1677	PSU	C6-C5	2.82	1.38	1.35
4	L3	2415	OMU	O4-C4	-2.82	1.19	1.24
4	L3	2837	OMU	O4-C4	-2.82	1.19	1.24
4	L3	4293	PSU	C6-C5	2.82	1.38	1.35
4	L3	3925	OMU	O4-C4	-2.79	1.19	1.24
4	L3	4498	OMU	O4-C4	-2.73	1.19	1.24
4	L3	4306	OMU	O2-C2	-2.73	1.18	1.23
4	L3	4296	PSU	C6-C5	2.72	1.38	1.35
4	L3	4498	OMU	C2-N3	2.59	1.42	1.38
4	L3	2837	OMU	C2-N3	2.54	1.42	1.38
4	L3	4299	PSU	C6-C5	2.53	1.38	1.35
4	L3	4227	OMU	O2-C2	-2.47	1.18	1.23
4	L3	4620	OMU	O2-C2	-2.39	1.18	1.23
4	L3	2415	OMU	O2-C2	-2.36	1.18	1.23
4	L3	2415	OMU	C2-N3	2.35	1.42	1.38
4	L3	3925	OMU	O2-C2	-2.34	1.18	1.23
4	L3	3925	OMU	C2-N3	2.30	1.42	1.38
4	L3	4530	UR3	C2-N3	-2.26	1.34	1.39
4	L3	2837	OMU	O2-C2	-2.22	1.19	1.23
4	L3	1683	PSU	C4-C5	-2.21	1.38	1.44
4	L3	2787	A2M	C5-N7	-2.20	1.35	1.39
4	L3	4299	PSU	C4-C5	-2.18	1.38	1.44
4	L3	4498	OMU	O2-C2	-2.16	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L3	2363	A2M	C5-N7	-2.16	1.35	1.39
4	L3	4628	PSU	C4-C5	-2.14	1.38	1.44
4	L3	1534	A2M	C5-N7	-2.14	1.35	1.39
4	L3	4673	PSU	C4-C5	-2.14	1.38	1.44
4	L3	3718	A2M	C5-N7	-2.13	1.35	1.39
4	L3	4571	A2M	C5-N7	-2.12	1.35	1.39
4	L3	4220	6MZ	C5-N7	-2.12	1.35	1.39
4	L3	4579	PSU	C4-C5	-2.12	1.38	1.44
4	L3	2401	A2M	C5-N7	-2.11	1.35	1.39
4	L3	4296	PSU	C4-C5	-2.09	1.38	1.44
2	L1	55	PSU	C4-C5	-2.09	1.38	1.44
4	L3	4498	OMU	C4-N3	2.08	1.42	1.38
4	L3	4493	PSU	C4-C5	-2.08	1.38	1.44
4	L3	4293	PSU	C4-C5	-2.07	1.38	1.44
4	L3	4227	OMU	C2-N3	2.07	1.41	1.38
4	L3	4590	A2M	C5-N7	-2.06	1.35	1.39
4	L3	3639	PSU	C4-C5	-2.05	1.38	1.44
4	L3	3920	PSU	C4-C5	-2.05	1.38	1.44
4	L3	5001	PSU	C4-C5	-2.02	1.38	1.44
4	L3	3830	A2M	C5-N7	-2.02	1.35	1.39
4	L3	4521	PSU	C4-C5	-2.02	1.38	1.44
4	L3	3884	PSU	C4-C5	-2.01	1.38	1.44
4	L3	3851	PSU	C4-C5	-2.01	1.38	1.44
4	L3	398	A2M	C5-N7	-2.01	1.35	1.39

All (412) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	2837	OMU	C4-N3-C2	-5.72	119.52	126.61
4	L3	2415	OMU	C4-N3-C2	-5.69	119.55	126.61
4	L3	4306	OMU	C4-N3-C2	-5.69	119.55	126.61
4	L3	3825	A2M	C5-C4-N3	-5.68	118.89	126.72
4	L3	3925	OMU	C4-N3-C2	-5.67	119.57	126.61
4	L3	2815	A2M	C5-C4-N3	-5.65	118.94	126.72
4	L3	2787	A2M	C5-C4-N3	-5.63	118.97	126.72
4	L3	398	A2M	C5-C4-N3	-5.59	119.02	126.72
4	L3	4498	OMU	C4-N3-C2	-5.58	119.68	126.61
4	L3	1871	A2M	C5-C4-N3	-5.57	119.05	126.72
4	L3	4227	OMU	C4-N3-C2	-5.56	119.71	126.61
4	L3	1534	A2M	C5-C4-N3	-5.54	119.08	126.72
4	L3	4523	A2M	C5-C4-N3	-5.51	119.12	126.72
4	L3	4296	PSU	C4-N3-C2	-5.51	118.78	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	3718	A2M	C5-C4-N3	-5.49	119.16	126.72
4	L3	4571	A2M	C5-C4-N3	-5.49	119.16	126.72
4	L3	2363	A2M	C5-C4-N3	-5.48	119.17	126.72
4	L3	400	A2M	C5-C4-N3	-5.47	119.19	126.72
4	L3	1524	A2M	C5-C4-N3	-5.44	119.22	126.72
4	L3	1326	A2M	C5-C4-N3	-5.43	119.24	126.72
4	L3	4220	6MZ	C5-C4-N3	-5.42	119.26	126.72
4	L3	3830	A2M	C5-C4-N3	-5.38	119.31	126.72
4	L3	4299	PSU	C4-N3-C2	-5.33	119.03	126.37
4	L3	3867	A2M	C5-C4-N3	-5.33	119.38	126.72
4	L3	4530	UR3	C4-N3-C2	-5.32	120.30	124.58
4	L3	2401	A2M	C5-C4-N3	-5.30	119.42	126.72
4	L3	4353	PSU	N1-C2-N3	5.26	120.71	115.17
4	L3	4312	PSU	C4-N3-C2	-5.21	119.19	126.37
4	L3	4636	PSU	C4-N3-C2	-5.18	119.23	126.37
4	L3	3724	A2M	C5-C4-N3	-5.18	119.59	126.72
4	L3	4299	PSU	N1-C2-N3	5.15	120.60	115.17
4	L3	4353	PSU	C4-N3-C2	-5.13	119.30	126.37
4	L3	4431	PSU	C4-N3-C2	-5.12	119.32	126.37
4	L3	4312	PSU	N1-C2-N3	5.10	120.55	115.17
4	L3	4532	PSU	C4-N3-C2	-5.08	119.38	126.37
4	L3	1582	PSU	C4-N3-C2	-5.07	119.38	126.37
4	L3	4296	PSU	N1-C2-N3	5.07	120.52	115.17
4	L3	4361	PSU	N1-C2-N3	5.06	120.50	115.17
4	L3	4457	PSU	N1-C2-N3	5.04	120.48	115.17
4	L3	2508	PSU	C4-N3-C2	-5.04	119.44	126.37
4	L3	4636	PSU	N1-C2-N3	5.02	120.47	115.17
4	L3	3637	PSU	C4-N3-C2	-5.02	119.46	126.37
4	L3	3639	PSU	N1-C2-N3	5.02	120.46	115.17
4	L3	3851	PSU	C4-N3-C2	-4.99	119.50	126.37
4	L3	2632	PSU	C4-N3-C2	-4.99	119.50	126.37
4	L3	4493	PSU	C4-N3-C2	-4.99	119.50	126.37
2	L1	55	PSU	C4-N3-C2	-4.98	119.51	126.37
4	L3	4403	PSU	C4-N3-C2	-4.97	119.52	126.37
4	L3	5001	PSU	N1-C2-N3	4.97	120.41	115.17
4	L3	4532	PSU	N1-C2-N3	4.96	120.40	115.17
4	L3	4689	PSU	C4-N3-C2	-4.96	119.54	126.37
4	L3	4673	PSU	C4-N3-C2	-4.95	119.55	126.37
4	L3	4521	PSU	C4-N3-C2	-4.94	119.57	126.37
4	L3	3695	PSU	C4-N3-C2	-4.93	119.58	126.37
4	L3	4689	PSU	N1-C2-N3	4.93	120.37	115.17
4	L3	3637	PSU	N1-C2-N3	4.93	120.36	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	5010	PSU	C4-N3-C2	-4.92	119.60	126.37
4	L3	3822	PSU	N1-C2-N3	4.92	120.35	115.17
4	L3	3920	PSU	C4-N3-C2	-4.91	119.61	126.37
4	L3	4361	PSU	C4-N3-C2	-4.91	119.61	126.37
4	L3	4471	PSU	N1-C2-N3	4.91	120.34	115.17
4	L3	1677	PSU	N1-C2-N3	4.90	120.33	115.17
4	L3	3639	PSU	C4-N3-C2	-4.89	119.63	126.37
4	L3	4431	PSU	N1-C2-N3	4.88	120.32	115.17
4	L3	1677	PSU	C4-N3-C2	-4.88	119.65	126.37
4	L3	1792	PSU	N1-C2-N3	4.87	120.31	115.17
4	L3	1683	PSU	C4-N3-C2	-4.87	119.66	126.37
4	L3	4457	PSU	C4-N3-C2	-4.87	119.66	126.37
4	L3	4972	PSU	C4-N3-C2	-4.87	119.66	126.37
2	L1	55	PSU	N1-C2-N3	4.87	120.30	115.17
4	L3	4673	PSU	N1-C2-N3	4.87	120.30	115.17
4	L3	4500	PSU	C4-N3-C2	-4.86	119.67	126.37
4	L3	4552	PSU	C4-N3-C2	-4.86	119.67	126.37
4	L3	5001	PSU	C4-N3-C2	-4.86	119.67	126.37
4	L3	3715	PSU	C4-N3-C2	-4.86	119.68	126.37
4	L3	4471	PSU	C4-N3-C2	-4.85	119.69	126.37
4	L3	3884	PSU	N1-C2-N3	4.85	120.28	115.17
4	L3	1860	PSU	C4-N3-C2	-4.84	119.70	126.37
4	L3	4576	PSU	C4-N3-C2	-4.84	119.71	126.37
4	L3	3734	PSU	C4-N3-C2	-4.83	119.71	126.37
4	L3	1862	PSU	C4-N3-C2	-4.83	119.71	126.37
4	L3	1536	PSU	C4-N3-C2	-4.83	119.72	126.37
4	L3	4576	PSU	N1-C2-N3	4.83	120.26	115.17
4	L3	4493	PSU	N1-C2-N3	4.81	120.24	115.17
4	L3	3734	PSU	N1-C2-N3	4.81	120.24	115.17
4	L3	4972	PSU	N1-C2-N3	4.81	120.24	115.17
4	L3	4628	PSU	C4-N3-C2	-4.80	119.75	126.37
4	L3	2839	PSU	C4-N3-C2	-4.79	119.77	126.37
4	L3	1792	PSU	C4-N3-C2	-4.79	119.77	126.37
4	L3	3730	PSU	C4-N3-C2	-4.79	119.77	126.37
4	L3	4500	PSU	N1-C2-N3	4.79	120.22	115.17
4	L3	3825	A2M	N3-C4-N9	4.79	135.31	127.17
4	L3	1860	PSU	N1-C2-N3	4.78	120.21	115.17
4	L3	3695	PSU	N1-C2-N3	4.78	120.21	115.17
4	L3	3822	PSU	C4-N3-C2	-4.77	119.80	126.37
4	L3	3730	PSU	N1-C2-N3	4.77	120.20	115.17
4	L3	3715	PSU	N1-C2-N3	4.77	120.20	115.17
2	L1	69	PSU	C4-N3-C2	-4.76	119.81	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	2508	PSU	N1-C2-N3	4.76	120.19	115.17
4	L3	1536	PSU	N1-C2-N3	4.75	120.18	115.17
4	L3	4620	OMU	C4-N3-C2	-4.73	120.74	126.61
4	L3	4552	PSU	N1-C2-N3	4.73	120.16	115.17
4	L3	3920	PSU	N1-C2-N3	4.72	120.15	115.17
4	L3	4403	PSU	N1-C2-N3	4.72	120.15	115.17
4	L3	1582	PSU	N1-C2-N3	4.72	120.15	115.17
4	L3	2839	PSU	N1-C2-N3	4.72	120.14	115.17
4	L3	1862	PSU	N1-C2-N3	4.71	120.13	115.17
4	L3	5010	PSU	N1-C2-N3	4.70	120.13	115.17
4	L3	4628	PSU	N1-C2-N3	4.68	120.11	115.17
2	L1	69	PSU	N1-C2-N3	4.68	120.11	115.17
4	L3	4521	PSU	N1-C2-N3	4.67	120.09	115.17
4	L3	3844	PSU	N1-C2-N3	4.67	120.09	115.17
4	L3	3884	PSU	C4-N3-C2	-4.66	119.95	126.37
4	L3	4571	A2M	N3-C4-N9	4.65	135.08	127.17
4	L3	4579	PSU	C4-N3-C2	-4.65	119.97	126.37
4	L3	3851	PSU	N1-C2-N3	4.64	120.07	115.17
4	L3	398	A2M	N3-C4-N9	4.64	135.06	127.17
4	L3	2632	PSU	N1-C2-N3	4.64	120.06	115.17
4	L3	3844	PSU	C4-N3-C2	-4.63	119.99	126.37
4	L3	4306	OMU	N3-C2-N1	4.62	120.91	114.89
4	L3	3853	PSU	C4-N3-C2	-4.62	120.00	126.37
4	L3	2787	A2M	N3-C4-N9	4.59	134.98	127.17
4	L3	2363	A2M	N3-C4-N9	4.59	134.97	127.17
4	L3	3718	A2M	N3-C4-N9	4.59	134.97	127.17
4	L3	4590	A2M	N3-C2-N1	-4.58	121.66	128.58
4	L3	3867	A2M	N3-C4-N9	4.57	134.93	127.17
4	L3	3853	PSU	N1-C2-N3	4.56	119.98	115.17
4	L3	4590	A2M	C5-C4-N3	-4.56	120.44	126.72
4	L3	4523	A2M	N3-C4-N9	4.55	134.91	127.17
4	L3	1871	A2M	N3-C4-N9	4.54	134.89	127.17
4	L3	4579	PSU	N1-C2-N3	4.52	119.94	115.17
4	L3	400	A2M	N3-C4-N9	4.52	134.86	127.17
4	L3	2815	A2M	N3-C4-N9	4.51	134.83	127.17
4	L3	1683	PSU	N1-C2-N3	4.50	119.92	115.17
4	L3	4293	PSU	C4-N3-C2	-4.48	120.20	126.37
4	L3	4293	PSU	N1-C2-N3	4.48	119.89	115.17
4	L3	1534	A2M	N3-C4-N9	4.48	134.79	127.17
4	L3	3830	A2M	N3-C4-N9	4.48	134.78	127.17
4	L3	2415	OMU	N3-C2-N1	4.46	120.69	114.89
4	L3	1524	A2M	N3-C4-N9	4.44	134.73	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	2401	A2M	N3-C4-N9	4.38	134.62	127.17
4	L3	3724	A2M	N3-C2-N1	-4.37	121.96	128.58
4	L3	3925	OMU	N3-C2-N1	4.37	120.58	114.89
4	L3	4220	6MZ	N3-C4-N9	4.37	134.60	127.17
4	L3	3724	A2M	N3-C4-N9	4.34	134.54	127.17
4	L3	3830	A2M	N3-C2-N1	-4.31	122.06	128.58
4	L3	1326	A2M	N3-C4-N9	4.30	134.49	127.17
4	L3	2837	OMU	N3-C2-N1	4.29	120.47	114.89
4	L3	2363	A2M	N3-C2-N1	-4.25	122.14	128.58
4	L3	1524	A2M	N3-C2-N1	-4.23	122.19	128.58
4	L3	400	A2M	N3-C2-N1	-4.20	122.22	128.58
4	L3	4498	OMU	N3-C2-N1	4.14	120.28	114.89
4	L3	2401	A2M	N3-C2-N1	-4.11	122.36	128.58
4	L3	4523	A2M	N3-C2-N1	-4.10	122.37	128.58
4	L3	1326	A2M	N3-C2-N1	-4.10	122.38	128.58
4	L3	3867	A2M	N3-C2-N1	-4.09	122.39	128.58
4	L3	4227	OMU	C5-C4-N3	4.08	120.51	114.80
4	L3	1871	A2M	N3-C2-N1	-4.06	122.43	128.58
4	L3	2787	A2M	N3-C2-N1	-4.06	122.43	128.58
4	L3	3825	A2M	N3-C2-N1	-4.06	122.43	128.58
4	L3	2815	A2M	N3-C2-N1	-4.05	122.46	128.58
4	L3	4220	6MZ	N1-C2-N3	-3.98	122.56	128.58
4	L3	398	A2M	N3-C2-N1	-3.96	122.58	128.58
4	L3	2815	A2M	C5-N7-C8	3.93	109.62	103.45
4	L3	1534	A2M	N3-C2-N1	-3.92	122.65	128.58
4	L3	4571	A2M	N3-C2-N1	-3.89	122.70	128.58
4	L3	1524	A2M	C5-N7-C8	3.87	109.53	103.45
4	L3	4590	A2M	C5-N7-C8	3.87	109.53	103.45
4	L3	4227	OMU	N3-C2-N1	3.84	119.89	114.89
4	L3	2837	OMU	C5-C4-N3	3.79	120.11	114.80
4	L3	4220	6MZ	C5-N7-C8	3.78	109.39	103.45
4	L3	4498	OMU	C5-C4-N3	3.77	120.09	114.80
4	L3	3825	A2M	C5-N7-C8	3.77	109.37	103.45
4	L3	4620	OMU	C5-C4-N3	3.77	120.07	114.80
4	L3	400	A2M	C5-N7-C8	3.75	109.35	103.45
4	L3	4523	A2M	C5-N7-C8	3.75	109.35	103.45
4	L3	4306	OMU	C5-C4-N3	3.73	120.03	114.80
4	L3	398	A2M	C5-N7-C8	3.71	109.28	103.45
4	L3	1534	A2M	C5-N7-C8	3.71	109.28	103.45
4	L3	1326	A2M	C5-N7-C8	3.71	109.28	103.45
4	L3	3718	A2M	N3-C2-N1	-3.71	122.97	128.58
4	L3	3830	A2M	C5-N7-C8	3.71	109.27	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	2363	A2M	C5-N7-C8	3.70	109.27	103.45
4	L3	3825	A2M	C2-N3-C4	3.69	120.85	111.83
4	L3	2415	OMU	C5-C4-N3	3.69	119.97	114.80
4	L3	3867	A2M	C5-N7-C8	3.68	109.23	103.45
4	L3	2787	A2M	C5-N7-C8	3.66	109.21	103.45
4	L3	2815	A2M	C2-N3-C4	3.66	120.77	111.83
4	L3	1871	A2M	C5-N7-C8	3.66	109.20	103.45
4	L3	4620	OMU	N3-C2-N1	3.65	119.64	114.89
4	L3	3925	OMU	C5-C4-N3	3.65	119.91	114.80
4	L3	400	A2M	C2-N3-C4	3.64	120.73	111.83
4	L3	1524	A2M	C2-N3-C4	3.63	120.69	111.83
4	L3	2363	A2M	C2-N3-C4	3.62	120.68	111.83
4	L3	2787	A2M	C2-N3-C4	3.61	120.65	111.83
4	L3	1871	A2M	C2-N3-C4	3.60	120.63	111.83
4	L3	3830	A2M	C2-N3-C4	3.60	120.63	111.83
4	L3	4523	A2M	C2-N3-C4	3.60	120.63	111.83
4	L3	3724	A2M	C5-N7-C8	3.59	109.09	103.45
4	L3	398	A2M	C2-N3-C4	3.57	120.56	111.83
4	L3	2401	A2M	C5-N7-C8	3.57	109.06	103.45
4	L3	1326	A2M	C2-N3-C4	3.57	120.55	111.83
4	L3	4590	A2M	N3-C4-N9	3.56	133.23	127.17
4	L3	3867	A2M	C2-N3-C4	3.55	120.51	111.83
4	L3	3724	A2M	C2-N3-C4	3.54	120.47	111.83
4	L3	1534	A2M	C2-N3-C4	3.53	120.45	111.83
4	L3	4571	A2M	C5-N7-C8	3.53	109.00	103.45
4	L3	4220	6MZ	C9-N6-C6	-3.53	119.58	122.85
4	L3	4220	6MZ	C2-N3-C4	3.53	120.44	111.83
4	L3	2401	A2M	C2-N3-C4	3.52	120.43	111.83
4	L3	2401	A2M	C2'-C1'-N9	-3.50	108.00	113.75
4	L3	4571	A2M	C2-N3-C4	3.48	120.34	111.83
4	L3	4590	A2M	C2-N3-C4	3.40	120.14	111.83
4	L3	3718	A2M	C5-N7-C8	3.39	108.78	103.45
4	L3	3718	A2M	C2-N3-C4	3.38	120.09	111.83
4	L3	4296	PSU	O2-C2-N1	-3.36	119.33	122.79
4	L3	4530	UR3	C5-C4-N3	3.31	119.40	115.04
4	L3	4590	A2M	C4-C5-N7	-3.25	106.87	110.58
4	L3	2815	A2M	C4-C5-N7	-3.22	106.90	110.58
4	L3	4227	OMU	O4-C4-C5	-3.19	119.67	125.16
4	L3	398	A2M	C2'-C1'-N9	-3.18	108.51	113.75
4	L3	3853	PSU	O2-C2-N1	-3.16	119.53	122.79
4	L3	4628	PSU	O2-C2-N1	-3.13	119.56	122.79
4	L3	4220	6MZ	C4-C5-N7	-3.11	107.03	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	1536	PSU	O2-C2-N1	-3.10	119.59	122.79
24	LN	245	HIC	NE2-CE1-ND1	-3.09	111.48	112.66
4	L3	2837	OMU	O4-C4-C5	-3.09	119.83	125.16
4	L3	1534	A2M	C4-C5-N7	-3.09	107.05	110.58
4	L3	1524	A2M	C4-C5-N7	-3.08	107.06	110.58
4	L3	1326	A2M	C4-C5-N7	-3.08	107.06	110.58
4	L3	2508	PSU	O2-C2-N1	-3.07	119.63	122.79
4	L3	3925	OMU	O4-C4-C5	-3.04	119.92	125.16
4	L3	4457	PSU	O2-C2-N1	-3.04	119.66	122.79
4	L3	3639	PSU	O2-C2-N1	-3.03	119.67	122.79
2	L1	55	PSU	O2-C2-N1	-3.03	119.67	122.79
4	L3	4498	OMU	O4-C4-C5	-3.02	119.95	125.16
4	L3	3734	PSU	O2-C2-N1	-3.00	119.69	122.79
4	L3	4523	A2M	C4-C5-N7	-2.99	107.16	110.58
4	L3	400	A2M	C4-C5-N7	-2.98	107.17	110.58
4	L3	3884	PSU	C6-N1-C2	-2.98	119.92	122.69
4	L3	3822	PSU	O2-C2-N1	-2.98	119.72	122.79
4	L3	4579	PSU	O2-C2-N1	-2.97	119.73	122.79
4	L3	1524	A2M	N9-C8-N7	-2.96	109.73	113.94
4	L3	4500	PSU	O2-C2-N1	-2.94	119.76	122.79
4	L3	4532	PSU	O2-C2-N1	-2.94	119.76	122.79
4	L3	398	A2M	C4-C5-N7	-2.93	107.23	110.58
4	L3	3867	A2M	N9-C8-N7	-2.90	109.82	113.94
4	L3	1862	PSU	O2-C2-N1	-2.90	119.80	122.79
4	L3	3884	PSU	O2-C2-N1	-2.90	119.80	122.79
2	L1	69	PSU	O2-C2-N1	-2.90	119.80	122.79
4	L3	3715	PSU	O2-C2-N1	-2.90	119.80	122.79
4	L3	4590	A2M	N9-C8-N7	-2.89	109.83	113.94
4	L3	1871	A2M	C4-C5-N7	-2.89	107.28	110.58
4	L3	4576	PSU	O2-C2-N1	-2.88	119.82	122.79
4	L3	3920	PSU	O2-C2-N1	-2.87	119.82	122.79
4	L3	3830	A2M	C4-C5-N7	-2.87	107.30	110.58
4	L3	4620	OMU	O4-C4-C5	-2.86	120.23	125.16
4	L3	2415	OMU	O4-C4-C5	-2.86	120.24	125.16
4	L3	2363	A2M	C4-C5-N7	-2.85	107.32	110.58
4	L3	3830	A2M	N9-C8-N7	-2.84	109.90	113.94
4	L3	2815	A2M	N9-C8-N7	-2.84	109.90	113.94
4	L3	2787	A2M	C4-C5-N7	-2.84	107.33	110.58
4	L3	5001	PSU	O2-C2-N1	-2.84	119.86	122.79
4	L3	3825	A2M	C4-C5-N7	-2.83	107.35	110.58
4	L3	4972	PSU	O2-C2-N1	-2.82	119.88	122.79
4	L3	4353	PSU	O2-C2-N1	-2.82	119.89	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	1677	PSU	O2-C2-N1	-2.81	119.89	122.79
4	L3	3724	A2M	C4-C5-N7	-2.81	107.37	110.58
4	L3	1860	PSU	O2-C2-N1	-2.81	119.89	122.79
4	L3	4579	PSU	C6-N1-C2	-2.80	120.09	122.69
4	L3	4571	A2M	C4-C5-N7	-2.79	107.39	110.58
4	L3	3730	PSU	O2-C2-N1	-2.79	119.91	122.79
4	L3	4312	PSU	O2-C2-N1	-2.79	119.91	122.79
4	L3	3825	A2M	N9-C8-N7	-2.79	109.98	113.94
4	L3	2401	A2M	C4-C5-N7	-2.78	107.40	110.58
4	L3	400	A2M	N9-C8-N7	-2.77	110.00	113.94
4	L3	4306	OMU	O4-C4-C5	-2.77	120.39	125.16
4	L3	1582	PSU	O2-C2-N1	-2.76	119.94	122.79
4	L3	4471	PSU	O2-C2-N1	-2.76	119.94	122.79
4	L3	5001	PSU	C6-N1-C2	-2.76	120.13	122.69
4	L3	4299	PSU	O2-C2-N1	-2.75	119.96	122.79
4	L3	4636	PSU	C6-C5-C4	2.75	120.03	118.17
4	L3	3844	PSU	O2-C2-N1	-2.74	119.96	122.79
4	L3	4523	A2M	N9-C8-N7	-2.74	110.05	113.94
4	L3	3867	A2M	C4-C5-N7	-2.73	107.47	110.58
4	L3	3724	A2M	N9-C8-N7	-2.72	110.08	113.94
4	L3	4403	PSU	O2-C2-N1	-2.72	119.99	122.79
4	L3	1792	PSU	O2-C2-N1	-2.71	119.99	122.79
4	L3	3851	PSU	O2-C2-N1	-2.71	119.99	122.79
4	L3	3718	A2M	C4-C5-N7	-2.70	107.49	110.58
4	L3	3867	A2M	C2'-C1'-N9	-2.70	109.31	113.75
4	L3	4431	PSU	O2-C2-N1	-2.70	120.01	122.79
4	L3	4521	PSU	O2-C2-N1	-2.69	120.01	122.79
4	L3	3734	PSU	C6-C5-C4	2.69	119.99	118.17
4	L3	2401	A2M	N9-C8-N7	-2.69	110.13	113.94
4	L3	4457	PSU	C6-N1-C2	-2.67	120.21	122.69
4	L3	2839	PSU	O2-C2-N1	-2.67	120.04	122.79
4	L3	4353	PSU	C6-C5-C4	2.66	119.97	118.17
4	L3	1326	A2M	N9-C8-N7	-2.66	110.17	113.94
4	L3	4220	6MZ	N9-C8-N7	-2.66	110.17	113.94
4	L3	3639	PSU	C6-N1-C2	-2.65	120.23	122.69
4	L3	398	A2M	N9-C8-N7	-2.65	110.18	113.94
4	L3	4431	PSU	C6-C5-C4	2.65	119.96	118.17
4	L3	3695	PSU	O2-C2-N1	-2.64	120.07	122.79
4	L3	4293	PSU	C6-N1-C2	-2.63	120.25	122.69
4	L3	2363	A2M	N9-C8-N7	-2.63	110.21	113.94
4	L3	4636	PSU	O2-C2-N1	-2.63	120.08	122.79
4	L3	4552	PSU	O2-C2-N1	-2.62	120.08	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	1677	PSU	C6-N1-C2	-2.62	120.26	122.69
4	L3	3822	PSU	C6-C5-C4	2.61	119.93	118.17
4	L3	1534	A2M	N9-C8-N7	-2.60	110.25	113.94
4	L3	4689	PSU	O2-C2-N1	-2.59	120.12	122.79
4	L3	5010	PSU	O2-C2-N1	-2.58	120.13	122.79
4	L3	2787	A2M	N9-C8-N7	-2.57	110.29	113.94
4	L3	4299	PSU	C6-C5-C4	2.56	119.90	118.17
4	L3	4576	PSU	C6-N1-C2	-2.55	120.32	122.69
4	L3	4972	PSU	C6-N1-C2	-2.55	120.33	122.69
4	L3	3637	PSU	C6-C5-C4	2.54	119.89	118.17
4	L3	4689	PSU	C6-N1-C2	-2.54	120.33	122.69
4	L3	4628	PSU	C6-N1-C2	-2.54	120.33	122.69
4	L3	3730	PSU	C6-N1-C2	-2.54	120.34	122.69
4	L3	1871	A2M	N9-C8-N7	-2.53	110.34	113.94
4	L3	4361	PSU	O2-C2-N1	-2.53	120.18	122.79
4	L3	3822	PSU	C6-N1-C2	-2.51	120.36	122.69
4	L3	4673	PSU	C6-N1-C2	-2.51	120.36	122.69
4	L3	4500	PSU	C6-N1-C2	-2.50	120.37	122.69
4	L3	2415	OMU	O2-C2-N1	-2.49	119.55	122.80
4	L3	3925	OMU	O2-C2-N1	-2.49	119.56	122.80
4	L3	4571	A2M	N9-C8-N7	-2.47	110.44	113.94
4	L3	3695	PSU	C6-C5-C4	2.46	119.83	118.17
4	L3	3715	PSU	C6-N1-C2	-2.45	120.41	122.69
4	L3	3844	PSU	C6-N1-C2	-2.45	120.42	122.69
4	L3	3920	PSU	C6-C5-C4	2.44	119.82	118.17
2	L1	69	PSU	C6-N1-C2	-2.43	120.44	122.69
4	L3	1792	PSU	C6-N1-C2	-2.42	120.44	122.69
4	L3	4673	PSU	O2-C2-N1	-2.42	120.29	122.79
4	L3	4361	PSU	C6-N1-C2	-2.42	120.45	122.69
4	L3	4471	PSU	C6-N1-C2	-2.42	120.45	122.69
4	L3	1860	PSU	C6-N1-C2	-2.41	120.45	122.69
4	L3	5001	PSU	C6-C5-C4	2.41	119.80	118.17
4	L3	1683	PSU	O2-C2-N1	-2.41	120.31	122.79
2	L1	55	PSU	C6-C5-C4	2.40	119.79	118.17
4	L3	3734	PSU	C6-N1-C2	-2.40	120.47	122.69
4	L3	4471	PSU	C6-C5-C4	2.40	119.79	118.17
4	L3	4532	PSU	C6-C5-C4	2.39	119.79	118.17
4	L3	2839	PSU	C6-N1-C2	-2.39	120.47	122.69
4	L3	4353	PSU	C6-N1-C2	-2.39	120.47	122.69
4	L3	4590	A2M	C2-N1-C6	2.39	122.65	118.73
4	L3	3853	PSU	C6-N1-C2	-2.38	120.48	122.69
4	L3	3639	PSU	C6-C5-C4	2.38	119.78	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	4293	PSU	O2-C2-N1	-2.36	120.35	122.79
2	L1	55	PSU	C6-N1-C2	-2.36	120.50	122.69
4	L3	1536	PSU	C6-N1-C2	-2.35	120.51	122.69
4	L3	2632	PSU	O2-C2-N1	-2.33	120.39	122.79
4	L3	2837	OMU	O2-C2-N1	-2.31	119.79	122.80
4	L3	1862	PSU	C6-N1-C2	-2.31	120.55	122.69
4	L3	4312	PSU	C6-N1-C2	-2.30	120.56	122.69
4	L3	4552	PSU	C6-N1-C2	-2.30	120.56	122.69
4	L3	3695	PSU	C6-N1-C2	-2.29	120.56	122.69
4	L3	5010	PSU	C6-N1-C2	-2.29	120.56	122.69
4	L3	4493	PSU	C6-N1-C2	-2.29	120.56	122.69
4	L3	4299	PSU	C6-N1-C2	-2.27	120.58	122.69
2	L1	69	PSU	O4'-C1'-C2'	2.27	108.29	105.15
4	L3	4532	PSU	C6-N1-C2	-2.25	120.60	122.69
4	L3	4493	PSU	O2-C2-N1	-2.25	120.47	122.79
4	L3	2351	OMC	C1'-N1-C2	2.25	123.40	118.44
4	L3	4296	PSU	C6-C5-C4	2.21	119.66	118.17
4	L3	4306	OMU	O2-C2-N1	-2.20	119.93	122.80
4	L3	3637	PSU	O2-C2-N1	-2.20	120.52	122.79
4	L3	1871	A2M	C2'-C1'-N9	-2.20	110.14	113.75
4	L3	3920	PSU	C6-N1-C2	-2.19	120.66	122.69
4	L3	400	A2M	C2'-C1'-N9	-2.19	110.15	113.75
4	L3	4521	PSU	C6-N1-C2	-2.19	120.66	122.69
4	L3	4431	PSU	C6-N1-C2	-2.18	120.67	122.69
4	L3	3715	PSU	O4'-C1'-C2'	2.18	108.17	105.15
4	L3	3718	A2M	N9-C8-N7	-2.18	110.85	113.94
4	L3	3844	PSU	C6-C5-C4	2.18	119.64	118.17
4	L3	5010	PSU	C6-C5-C4	2.15	119.63	118.17
4	L3	4552	PSU	C6-C5-C4	2.15	119.62	118.17
4	L3	4220	6MZ	C6-C5-N7	2.15	134.77	132.43
4	L3	3730	PSU	C6-C5-C4	2.15	119.62	118.17
4	L3	4403	PSU	C6-C5-C4	2.15	119.62	118.17
4	L3	4493	PSU	C6-C5-C4	2.15	119.62	118.17
4	L3	1534	A2M	O4'-C1'-C2'	-2.14	102.90	106.59
4	L3	1582	PSU	C6-C5-C4	2.13	119.61	118.17
4	L3	1860	PSU	O4'-C1'-C2'	2.11	108.07	105.15
4	L3	4628	PSU	O4'-C1'-C2'	2.11	108.07	105.15
4	L3	2632	PSU	C6-N1-C2	-2.10	120.74	122.69
4	L3	4353	PSU	O4'-C1'-C2'	2.09	108.04	105.15
4	L3	1536	PSU	C6-C5-C4	2.09	119.58	118.17
4	L3	3637	PSU	C6-N1-C2	-2.08	120.76	122.69
4	L3	4673	PSU	C6-C5-C4	2.08	119.58	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	3853	PSU	O4'-C1'-C2'	2.08	108.03	105.15
4	L3	4523	A2M	C2'-C1'-N9	-2.08	110.33	113.75
4	L3	1860	PSU	C6-C5-C4	2.08	119.58	118.17
4	L3	4361	PSU	C6-C5-C4	2.08	119.58	118.17
4	L3	3851	PSU	O4'-C1'-C2'	2.07	108.02	105.15
4	L3	3851	PSU	C6-N1-C2	-2.07	120.77	122.69
4	L3	4636	PSU	C6-N1-C2	-2.07	120.77	122.69
4	L3	4498	OMU	O2-C2-N1	-2.07	120.11	122.80
4	L3	4403	PSU	C6-N1-C2	-2.06	120.78	122.69
4	L3	4636	PSU	O4'-C1'-C2'	2.06	108.00	105.15
4	L3	1534	A2M	C3'-C2'-C1'	-2.06	98.86	102.81
4	L3	2632	PSU	O4'-C1'-C2'	2.05	107.99	105.15
4	L3	4296	PSU	C6-N1-C2	-2.05	120.79	122.69
4	L3	3734	PSU	O4'-C1'-C2'	2.04	107.97	105.15
4	L3	1683	PSU	C6-N1-C2	-2.04	120.80	122.69
4	L3	1677	PSU	C6-C5-C4	2.01	119.53	118.17
4	L3	1862	PSU	C6-C5-C4	2.01	119.53	118.17
4	L3	2508	PSU	C6-N1-C2	-2.01	120.83	122.69
4	L3	3639	PSU	O4'-C1'-C2'	2.01	107.93	105.15
4	L3	1871	A2M	C3'-C2'-C1'	-2.01	98.96	102.81

There are no chirality outliers.

All (95) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L1	75	OMG	C1'-C2'-O2'-CM2
4	L3	398	A2M	C1'-C2'-O2'-CM'
4	L3	400	A2M	C1'-C2'-O2'-CM'
4	L3	1316	OMG	C1'-C2'-O2'-CM2
4	L3	1326	A2M	O4'-C4'-C5'-O5'
4	L3	1326	A2M	C3'-C4'-C5'-O5'
4	L3	1326	A2M	C1'-C2'-O2'-CM'
4	L3	1340	OMC	C1'-C2'-O2'-CM2
4	L3	2363	A2M	C1'-C2'-O2'-CM'
4	L3	2364	OMG	C1'-C2'-O2'-CM2
4	L3	2415	OMU	C1'-C2'-O2'-CM2
4	L3	2422	OMC	C1'-C2'-O2'-CM2
4	L3	2787	A2M	C3'-C4'-C5'-O5'
4	L3	2787	A2M	C1'-C2'-O2'-CM'
4	L3	2804	OMC	C1'-C2'-O2'-CM2
4	L3	2815	A2M	C1'-C2'-O2'-CM'
4	L3	2837	OMU	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
4	L3	2839	PSU	C2'-C1'-C5-C4
4	L3	2861	OMC	C1'-C2'-O2'-CM2
4	L3	3701	OMC	C2'-C1'-N1-C2
4	L3	3701	OMC	C2'-C1'-N1-C6
4	L3	3718	A2M	C1'-C2'-O2'-CM'
4	L3	3724	A2M	C1'-C2'-O2'-CM'
4	L3	3744	OMG	C1'-C2'-O2'-CM2
4	L3	3830	A2M	C1'-C2'-O2'-CM'
4	L3	3841	OMC	C1'-C2'-O2'-CM2
4	L3	3867	A2M	C1'-C2'-O2'-CM'
4	L3	3887	OMC	O4'-C4'-C5'-O5'
4	L3	3925	OMU	C1'-C2'-O2'-CM2
4	L3	4392	OMG	C1'-C2'-O2'-CM2
4	L3	4456	OMC	C1'-C2'-O2'-CM2
4	L3	4571	A2M	C1'-C2'-O2'-CM'
4	L3	4590	A2M	O4'-C4'-C5'-O5'
4	L3	4590	A2M	C3'-C4'-C5'-O5'
4	L3	4620	OMU	C1'-C2'-O2'-CM2
4	L3	4636	PSU	C2'-C1'-C5-C4
4	L3	4637	OMG	O4'-C4'-C5'-O5'
4	L3	4637	OMG	C1'-C2'-O2'-CM2
4	L3	3887	OMC	C3'-C4'-C5'-O5'
4	L3	4220	6MZ	O4'-C4'-C5'-O5'
4	L3	4523	A2M	C3'-C4'-C5'-O5'
4	L3	4618	OMG	O4'-C4'-C5'-O5'
4	L3	2401	A2M	O4'-C4'-C5'-O5'
4	L3	2401	A2M	C3'-C4'-C5'-O5'
4	L3	2424	OMG	O4'-C4'-C5'-O5'
4	L3	2787	A2M	O4'-C4'-C5'-O5'
4	L3	4306	OMU	C3'-C4'-C5'-O5'
4	L3	4306	OMU	O4'-C4'-C5'-O5'
4	L3	4523	A2M	O4'-C4'-C5'-O5'
4	L3	1625	OMG	C3'-C4'-C5'-O5'
4	L3	1862	PSU	C3'-C4'-C5'-O5'
4	L3	3701	OMC	C3'-C4'-C5'-O5'
4	L3	4220	6MZ	C3'-C4'-C5'-O5'
4	L3	4637	OMG	C3'-C4'-C5'-O5'
4	L3	1677	PSU	O4'-C4'-C5'-O5'
4	L3	3701	OMC	O4'-C4'-C5'-O5'
24	LN	245	HIC	CA-CB-CG-ND1
4	L3	1677	PSU	C3'-C4'-C5'-O5'
4	L3	4618	OMG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	L3	4590	A2M	C4'-C5'-O5'-P
24	LN	245	HIC	CA-CB-CG-CD2
4	L3	1862	PSU	O4'-C4'-C5'-O5'
4	L3	2787	A2M	C2'-C1'-N9-C8
4	L3	4227	OMU	C1'-C2'-O2'-CM2
4	L3	4590	A2M	C1'-C2'-O2'-CM'
4	L3	2424	OMG	C3'-C4'-C5'-O5'
4	L3	1625	OMG	O4'-C4'-C5'-O5'
4	L3	3701	OMC	C4'-C5'-O5'-P
4	L3	4220	6MZ	C4'-C5'-O5'-P
4	L3	4306	OMU	C4'-C5'-O5'-P
4	L3	2839	PSU	O4'-C1'-C5-C4
4	L3	4521	PSU	O4'-C1'-C5-C4
4	L3	4636	PSU	O4'-C1'-C5-C4
4	L3	2787	A2M	C2'-C1'-N9-C4
4	L3	2422	OMC	O4'-C4'-C5'-O5'
4	L3	1524	A2M	C3'-C2'-O2'-CM'
4	L3	2876	OMG	C3'-C2'-O2'-CM2
4	L3	3844	PSU	C4'-C5'-O5'-P
4	L3	2815	A2M	O4'-C4'-C5'-O5'
4	L3	3701	OMC	O4'-C1'-N1-C6
4	L3	2351	OMC	C2'-C1'-N1-C6
4	L3	4536	OMC	C1'-C2'-O2'-CM2
4	L3	4636	PSU	C4'-C5'-O5'-P
4	L3	1677	PSU	O4'-C1'-C5-C6
4	L3	4521	PSU	O4'-C1'-C5-C6
4	L3	2787	A2M	O4'-C1'-N9-C8
4	L3	2351	OMC	C2'-C1'-N1-C2
4	L3	3701	OMC	O4'-C1'-N1-C2
4	L3	2364	OMG	O4'-C4'-C5'-O5'
4	L3	1524	A2M	O4'-C1'-N9-C4
4	L3	1677	PSU	C2'-C1'-C5-C6
4	L3	1524	A2M	O4'-C1'-N9-C8
4	L3	4498	OMU	C4'-C5'-O5'-P
4	L3	4306	OMU	C2'-C1'-N1-C2
4	L3	2839	PSU	C3'-C4'-C5'-O5'

There are no ring outliers.

55 monomers are involved in 88 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L3	3867	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L3	3825	A2M	2	0
4	L3	2804	OMC	1	0
4	L3	4536	OMC	1	0
4	L3	4620	OMU	2	0
4	L3	4523	A2M	1	0
4	L3	2876	OMG	3	0
4	L3	4457	PSU	2	0
4	L3	3715	PSU	1	0
4	L3	1871	A2M	1	0
4	L3	4500	PSU	1	0
4	L3	2839	PSU	1	0
4	L3	1326	A2M	2	0
4	L3	2632	PSU	1	0
4	L3	3724	A2M	4	0
4	L3	4227	OMU	1	0
4	L3	3744	OMG	1	0
4	L3	3853	PSU	3	0
4	L3	1340	OMC	1	0
4	L3	4530	UR3	2	0
4	L3	2351	OMC	1	0
4	L3	3869	OMC	1	0
4	L3	4312	PSU	1	0
4	L3	3627	OMG	1	0
4	L3	4571	A2M	2	0
4	L3	2415	OMU	5	0
4	L3	1677	PSU	3	0
4	L3	4618	OMG	1	0
4	L3	2837	OMU	1	0
2	L1	69	PSU	2	0
2	L1	75	OMG	2	0
4	L3	2815	A2M	2	0
4	L3	4370	OMG	1	0
4	L3	1534	A2M	2	0
4	L3	398	A2M	2	0
4	L3	2364	OMG	2	0
4	L3	3925	OMU	1	0
4	L3	2422	OMC	2	0
4	L3	1860	PSU	1	0
4	L3	4637	OMG	2	0
4	L3	4431	PSU	1	0
4	L3	2363	A2M	2	0
4	L3	4306	OMU	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L3	400	A2M	2	0
4	L3	4220	6MZ	1	0
4	L3	4636	PSU	1	0
4	L3	2861	OMC	1	0
4	L3	3841	OMC	1	0
4	L3	3718	A2M	2	0
4	L3	3730	PSU	2	0
4	L3	1316	OMG	1	0
4	L3	4552	PSU	1	0
4	L3	4403	PSU	1	0
4	L3	3701	OMC	1	0
4	L3	5001	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 96 ligands modelled in this entry, 95 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
59	GDP	SR	1001	60,57	29,30,30	3.04	12 (41%)	45,47,47	2.69	17 (37%)

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
59	GDP	SR	1001	60,57	-	0/16/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	SR	1001	GDP	O6-C6	8.81	1.40	1.23
59	SR	1001	GDP	C5-N7	6.51	1.52	1.39
59	SR	1001	GDP	PA-O3A	5.17	1.65	1.59
59	SR	1001	GDP	C2-N2	4.81	1.45	1.34
59	SR	1001	GDP	C8-N9	-4.06	1.28	1.37
59	SR	1001	GDP	C4-N9	-3.90	1.28	1.38
59	SR	1001	GDP	C5-C4	3.77	1.49	1.38
59	SR	1001	GDP	C4-N3	2.74	1.40	1.34
59	SR	1001	GDP	PB-O3B	-2.32	1.46	1.54
59	SR	1001	GDP	PB-O2B	-2.32	1.46	1.54
59	SR	1001	GDP	O4'-C1'	2.25	1.47	1.42
59	SR	1001	GDP	C2'-C3'	-2.12	1.47	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	SR	1001	GDP	C8-N9-C4	7.95	120.92	106.03
59	SR	1001	GDP	N9-C4-N3	6.66	139.27	125.95
59	SR	1001	GDP	C5-C4-N3	-6.61	117.88	128.39
59	SR	1001	GDP	C2-N3-C4	5.32	121.47	112.30
59	SR	1001	GDP	C6-C5-N7	4.81	139.04	130.29
59	SR	1001	GDP	C4-C5-N7	-4.59	103.39	110.67
59	SR	1001	GDP	N9-C8-N7	-3.13	107.59	113.40
59	SR	1001	GDP	C3'-C2'-C1'	3.05	107.23	101.46
59	SR	1001	GDP	C2-N1-C6	-2.97	119.72	125.11
59	SR	1001	GDP	O2B-PB-O3A	2.87	114.25	104.64
59	SR	1001	GDP	O3B-PB-O3A	2.69	113.65	104.64
59	SR	1001	GDP	C2'-C3'-C4'	2.64	107.71	102.61
59	SR	1001	GDP	C5-C6-N1	2.57	119.81	113.25
59	SR	1001	GDP	C1'-N9-C4	-2.57	118.88	126.49
59	SR	1001	GDP	O6-C6-C5	-2.50	119.95	126.53
59	SR	1001	GDP	O2A-PA-O1A	-2.32	101.64	112.44
59	SR	1001	GDP	C1'-N9-C8	-2.31	120.18	126.73

There are no chirality outliers.

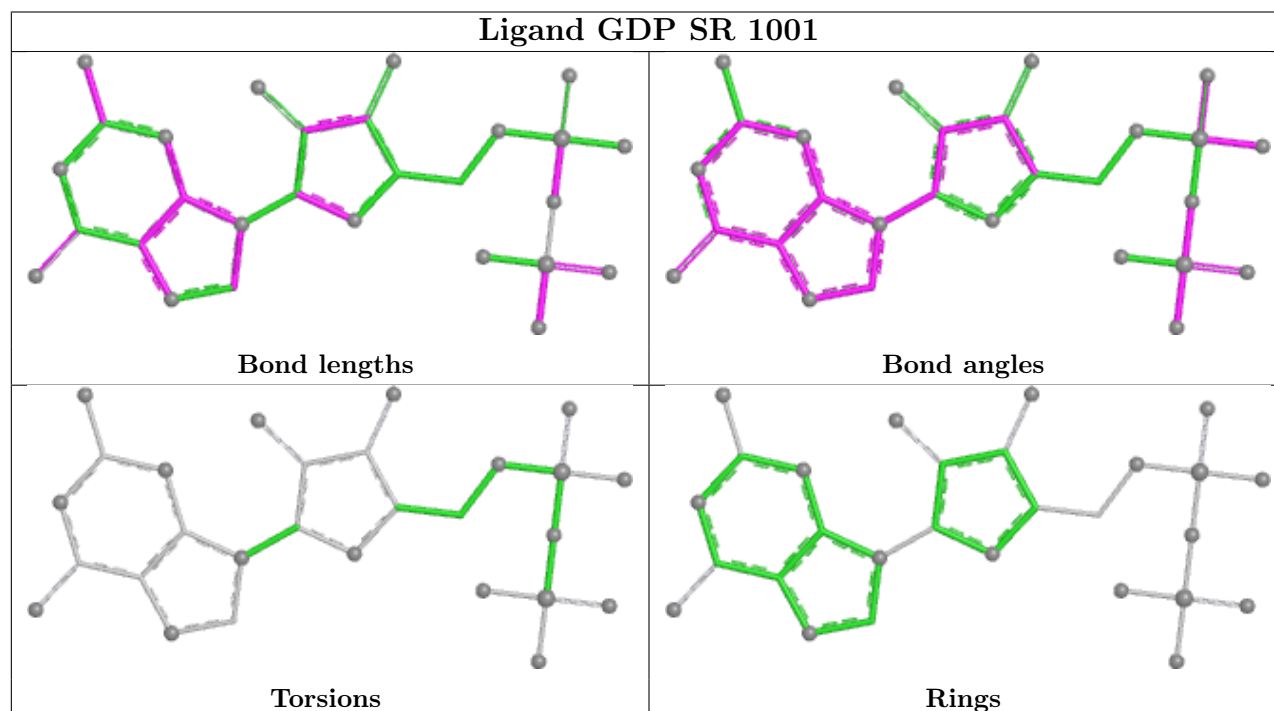
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

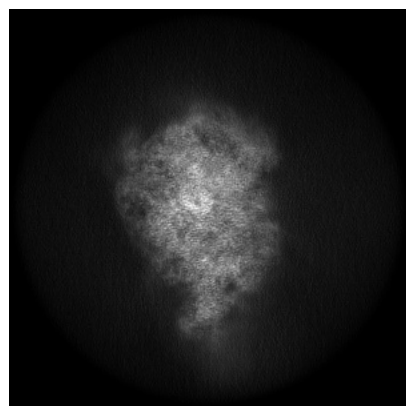
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29268. These allow visual inspection of the internal detail of the map and identification of artifacts.

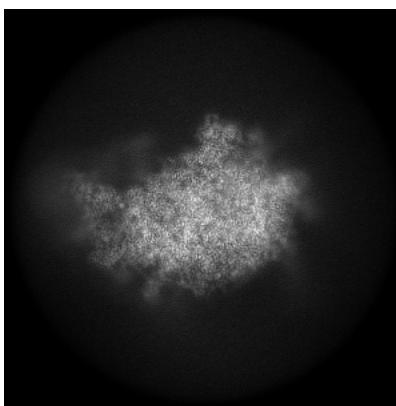
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

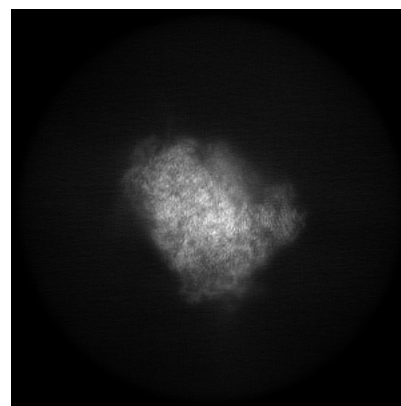
6.1.1 Primary map



X

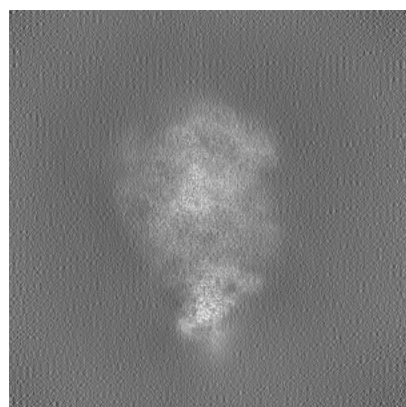


Y

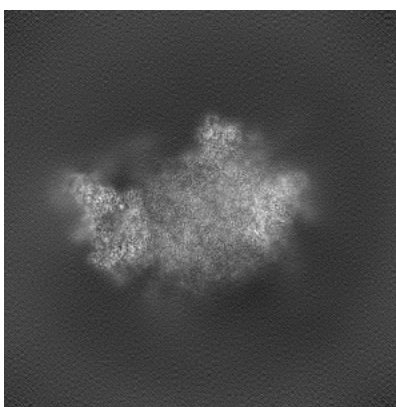


Z

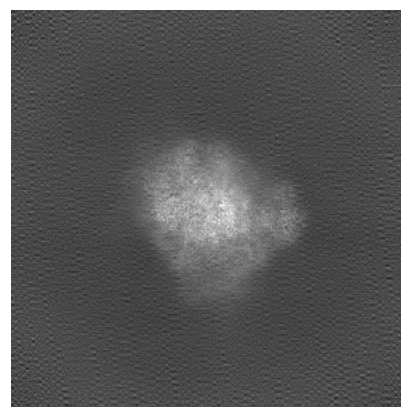
6.1.2 Raw map



X



Y

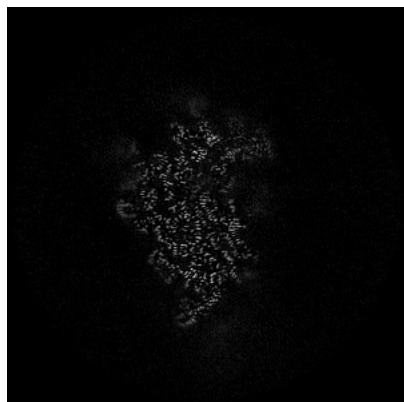


Z

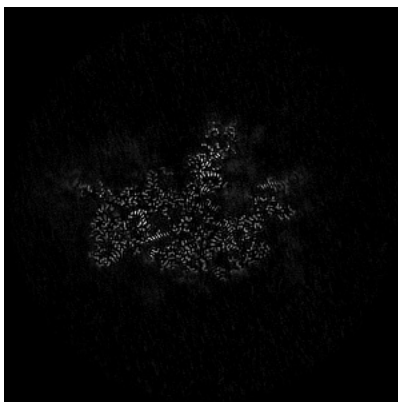
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

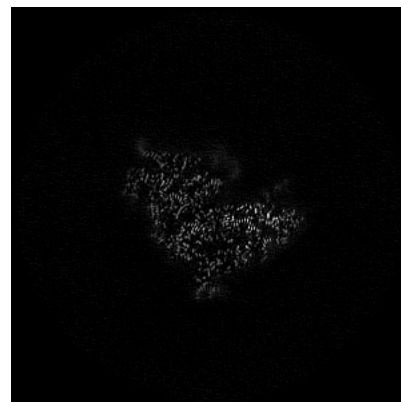
6.2.1 Primary map



X Index: 240

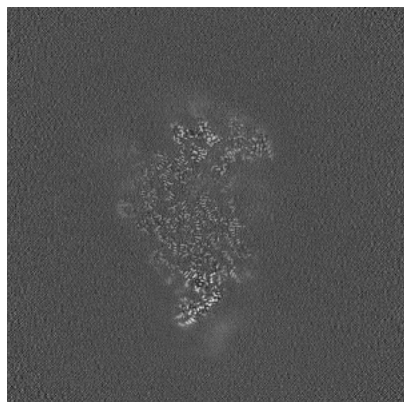


Y Index: 240

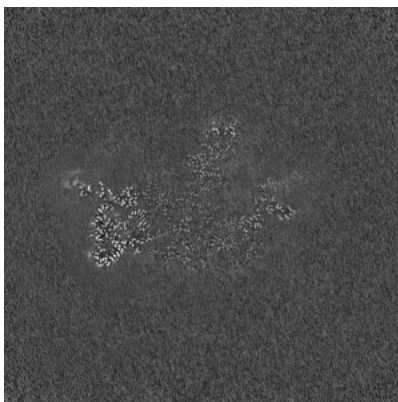


Z Index: 240

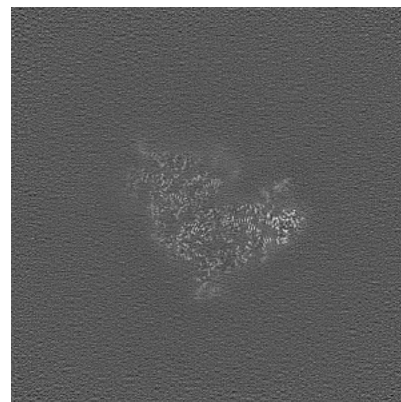
6.2.2 Raw map



X Index: 240



Y Index: 240

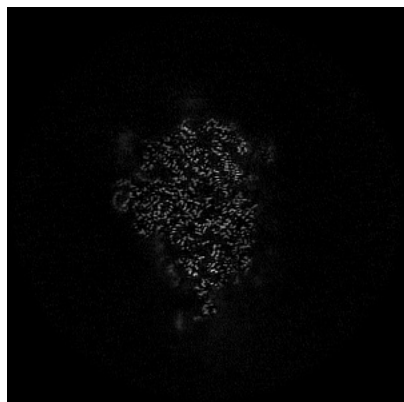


Z Index: 240

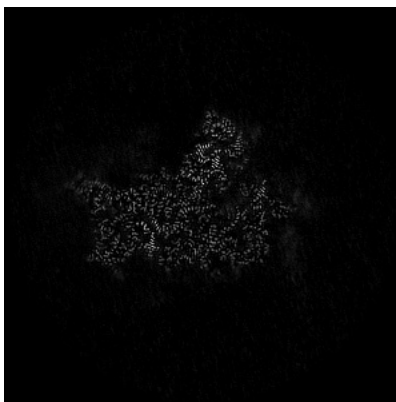
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

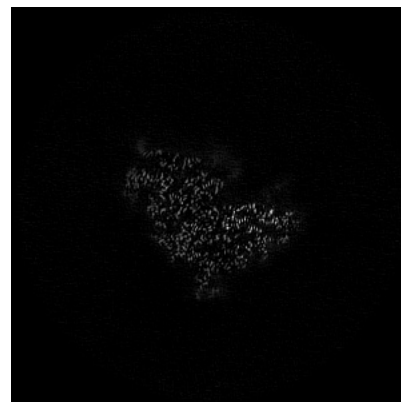
6.3.1 Primary map



X Index: 226

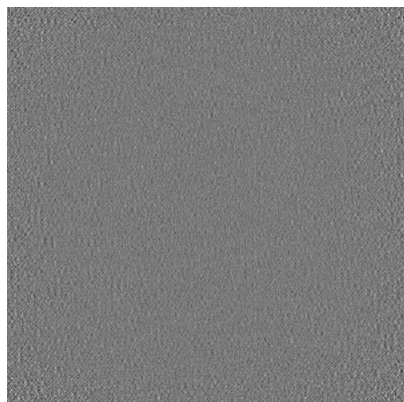


Y Index: 233

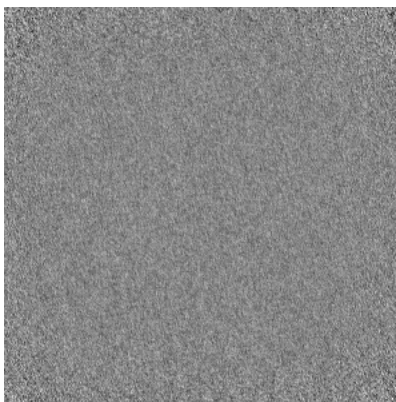


Z Index: 239

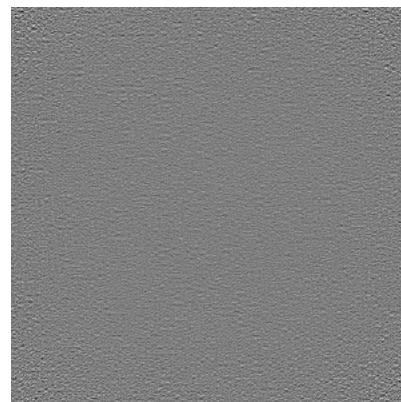
6.3.2 Raw map



X Index: 0



Y Index: 0

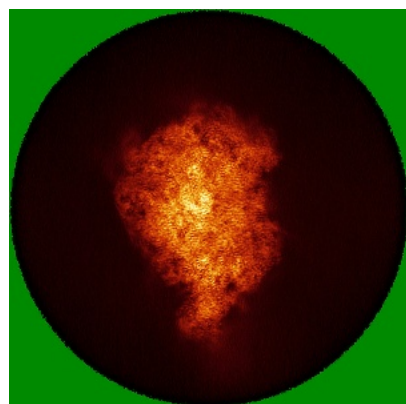


Z Index: 0

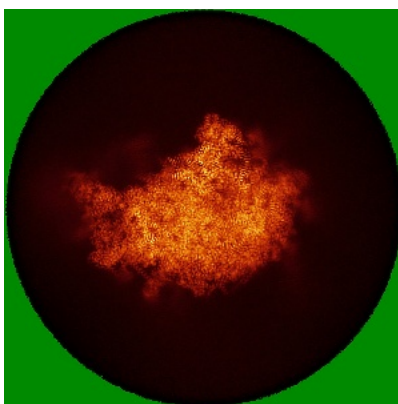
The images above show the largest variance slices of the map in three orthogonal directions.

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

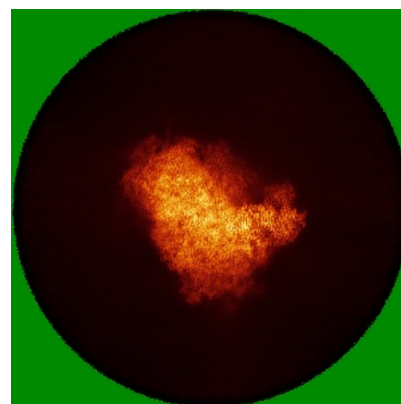
6.4.1 Primary map



X

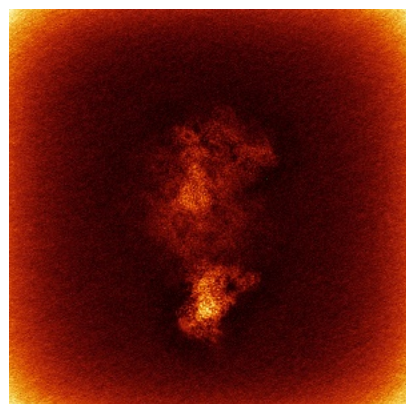


Y

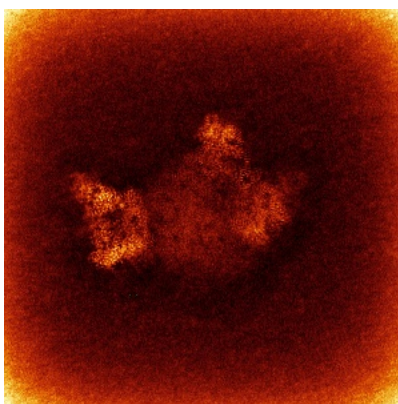


Z

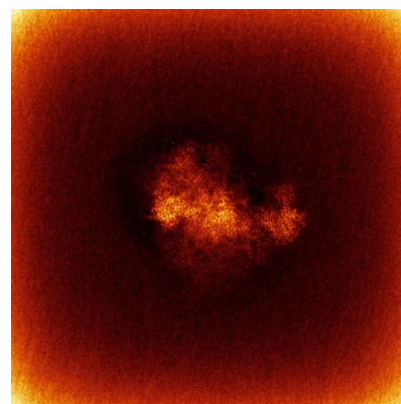
6.4.2 Raw map



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](#)

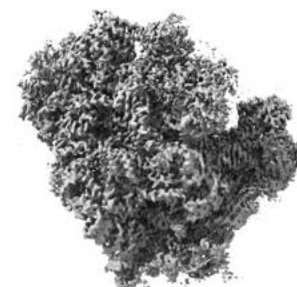
6.5.1 Primary map



X



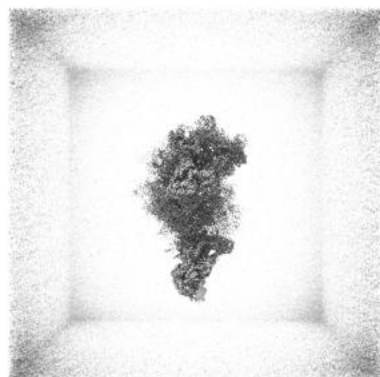
Y



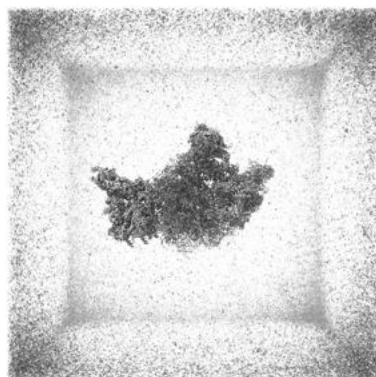
Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

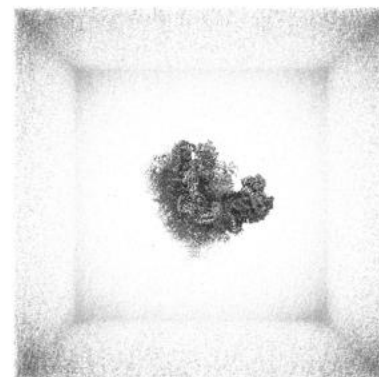
6.5.2 Raw map



X



Y



Z

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

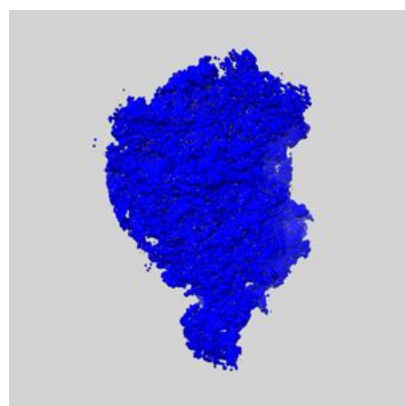
6.6 Mask visualisation [i](#)

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

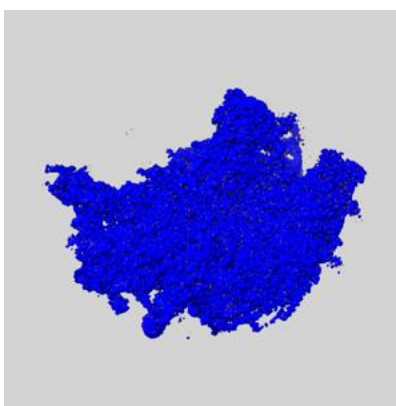
A mask typically either:

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

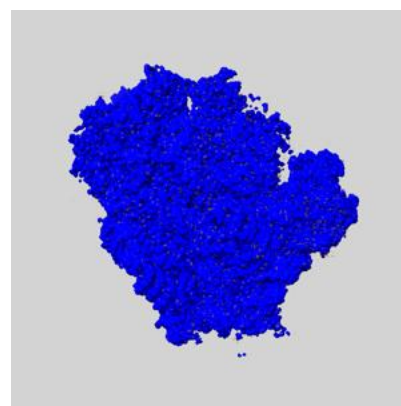
6.6.1 emd_29268_msk_1.map [i](#)



X



Y

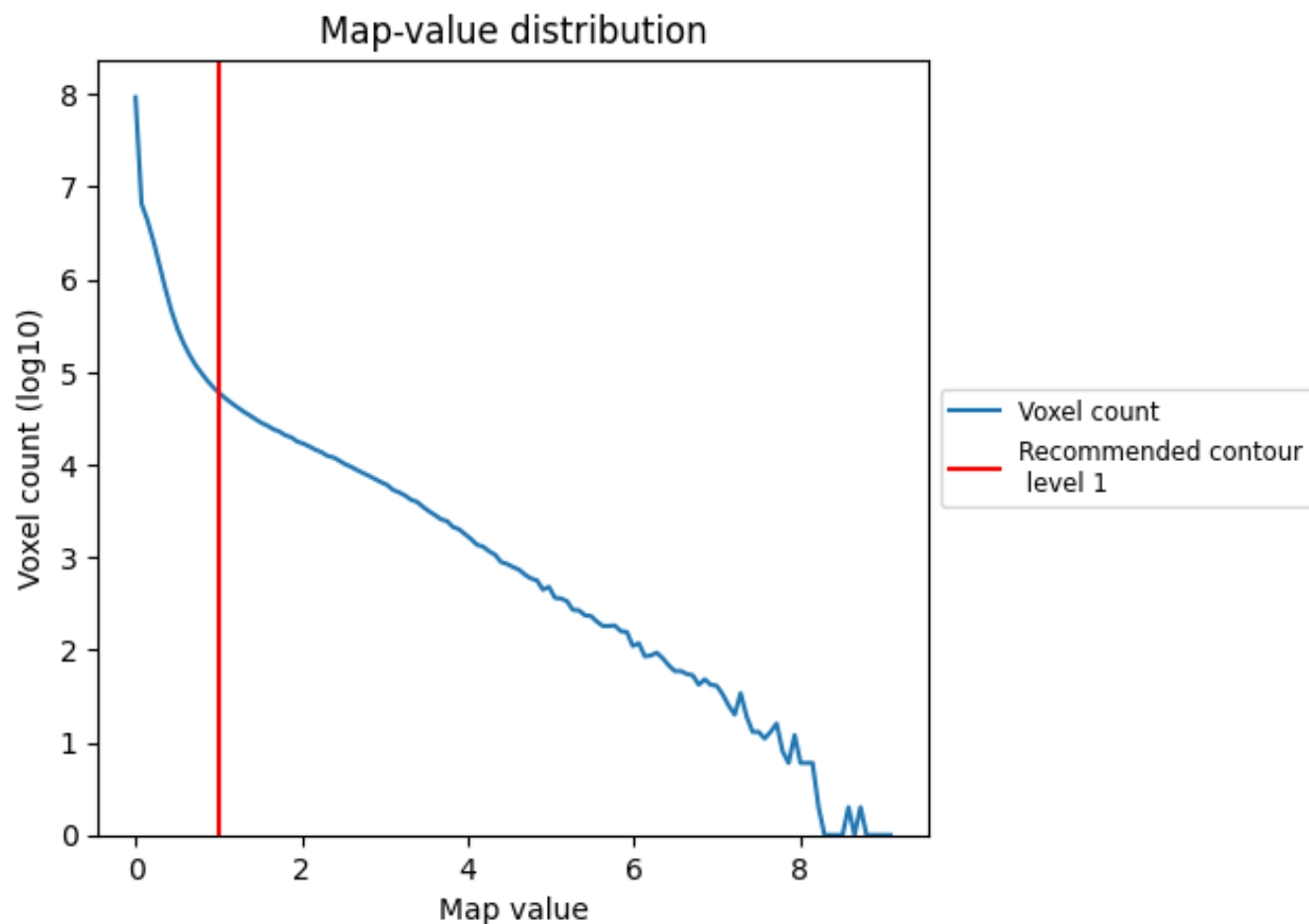


Z

7 Map analysis [i](#)

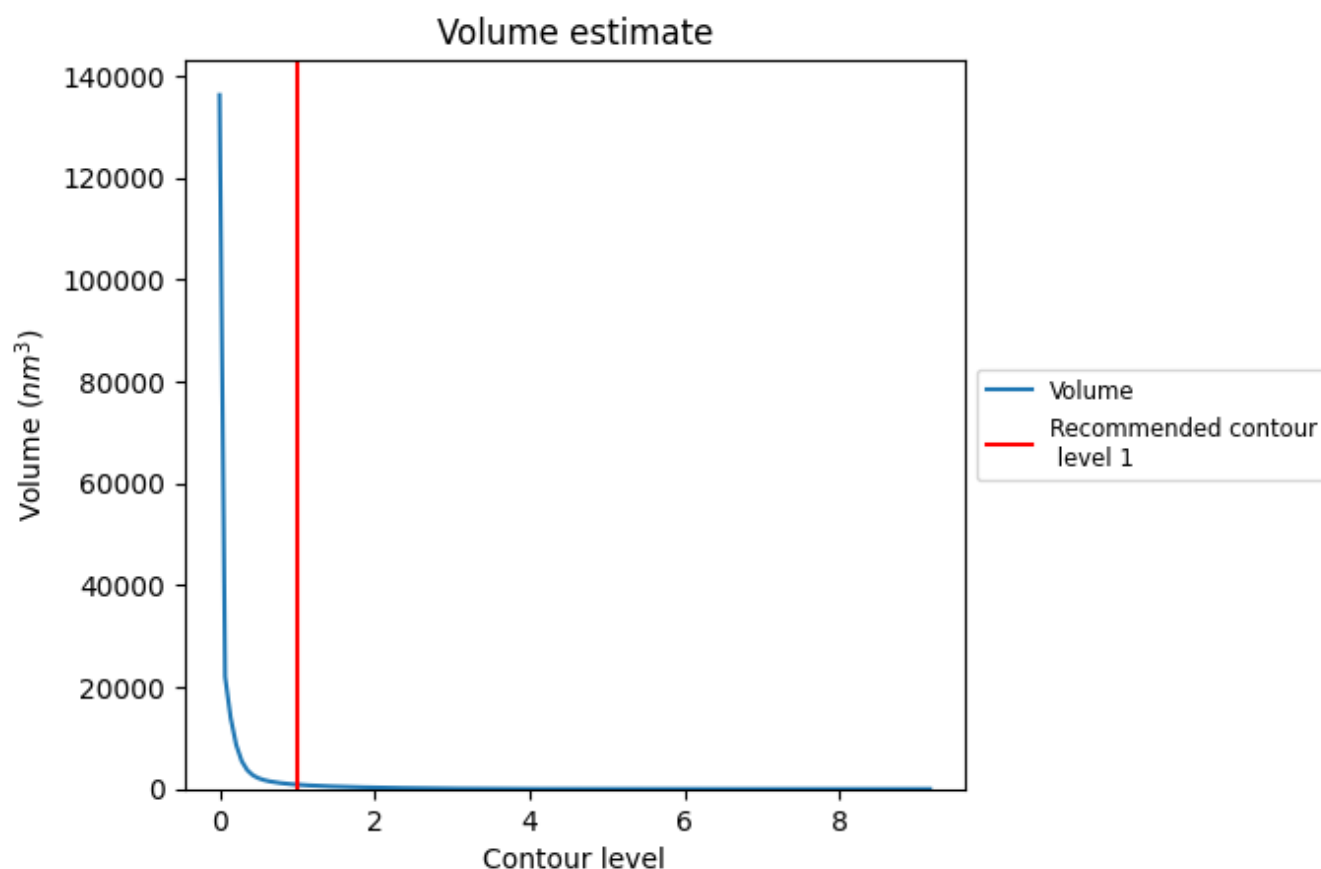
This section contains the results of statistical analysis of the map.

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.

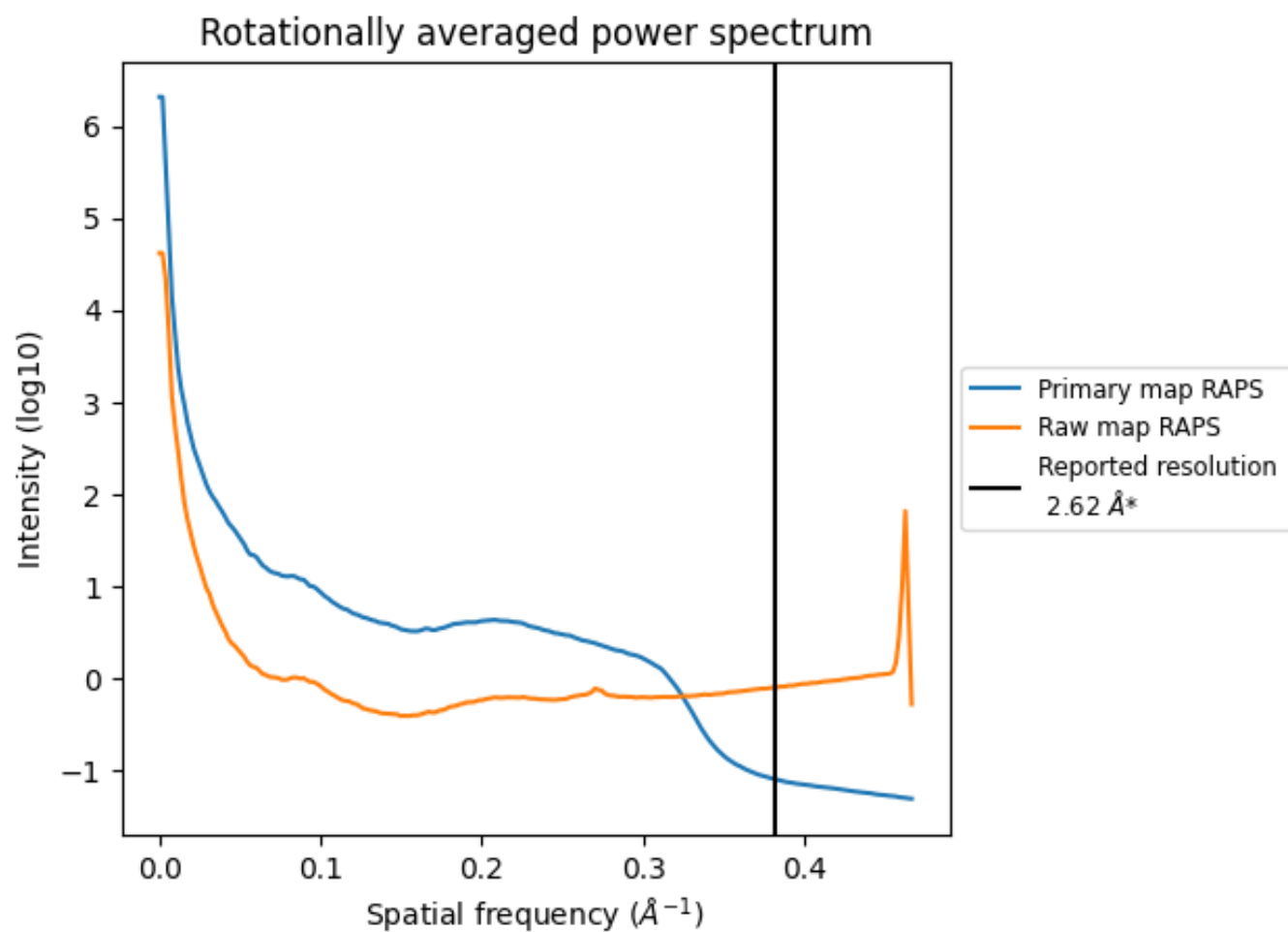
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 849 nm^3 ; this corresponds to an approximate mass of 767 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 ⓘ

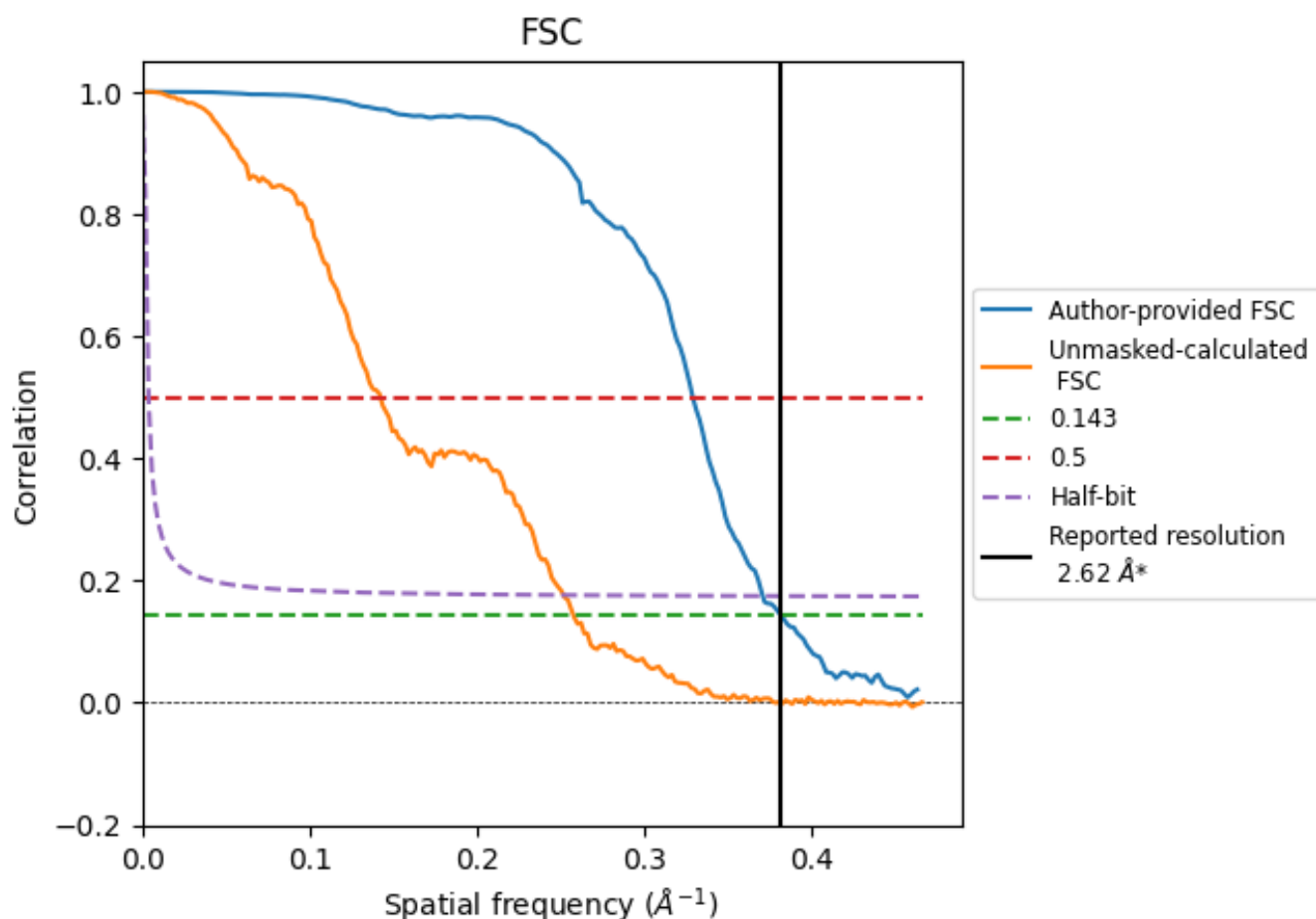


*Reported resolution corresponds to spatial frequency of 0.382 Å⁻¹

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 0.382 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

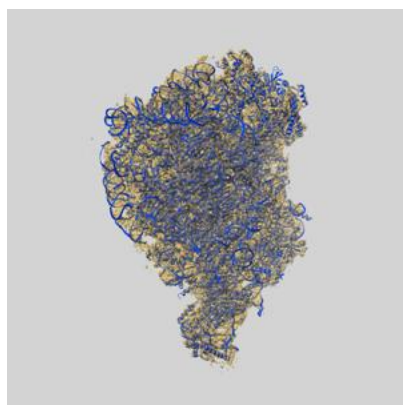
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.62	-	-
Author-provided FSC curve	2.62	3.04	2.69
Unmasked-calculated*	3.88	7.02	3.97

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.88 differs from the reported value 2.62 by more than 10 %

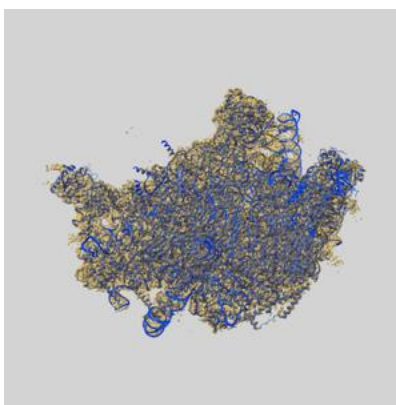
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29268 and PDB model 8FL6. Per-residue inclusion information can be found in section [3](#) on page [16](#).

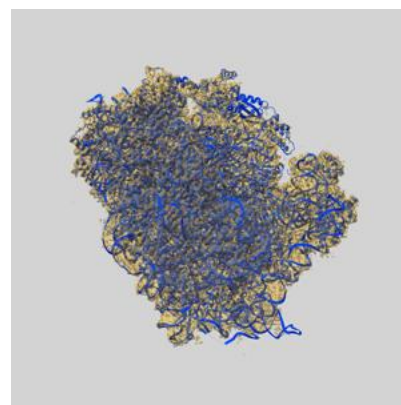
9.1 Map-model overlay [i](#)



X



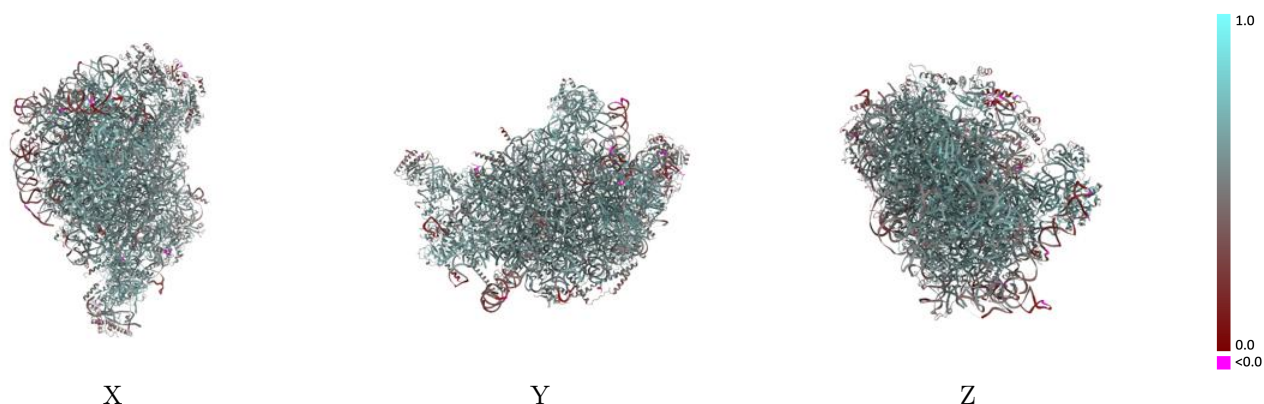
Y



Z

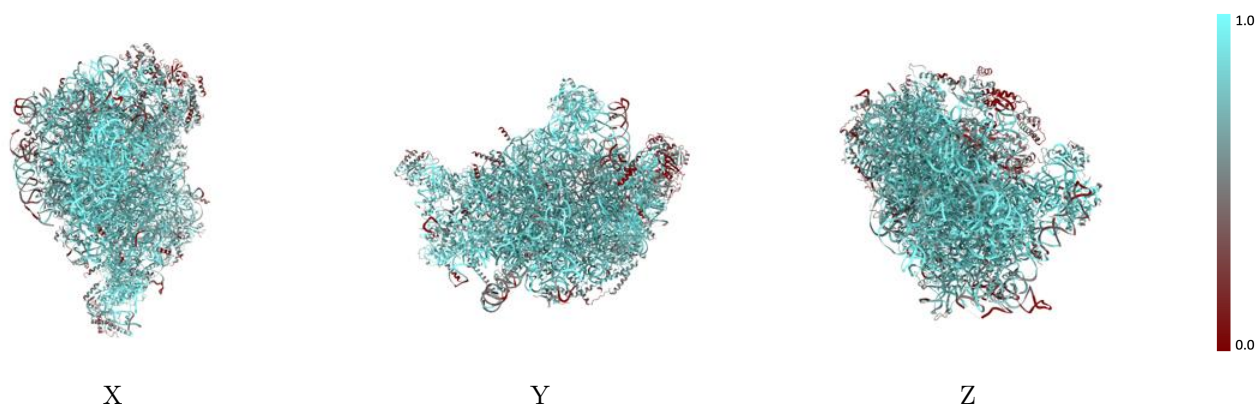
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



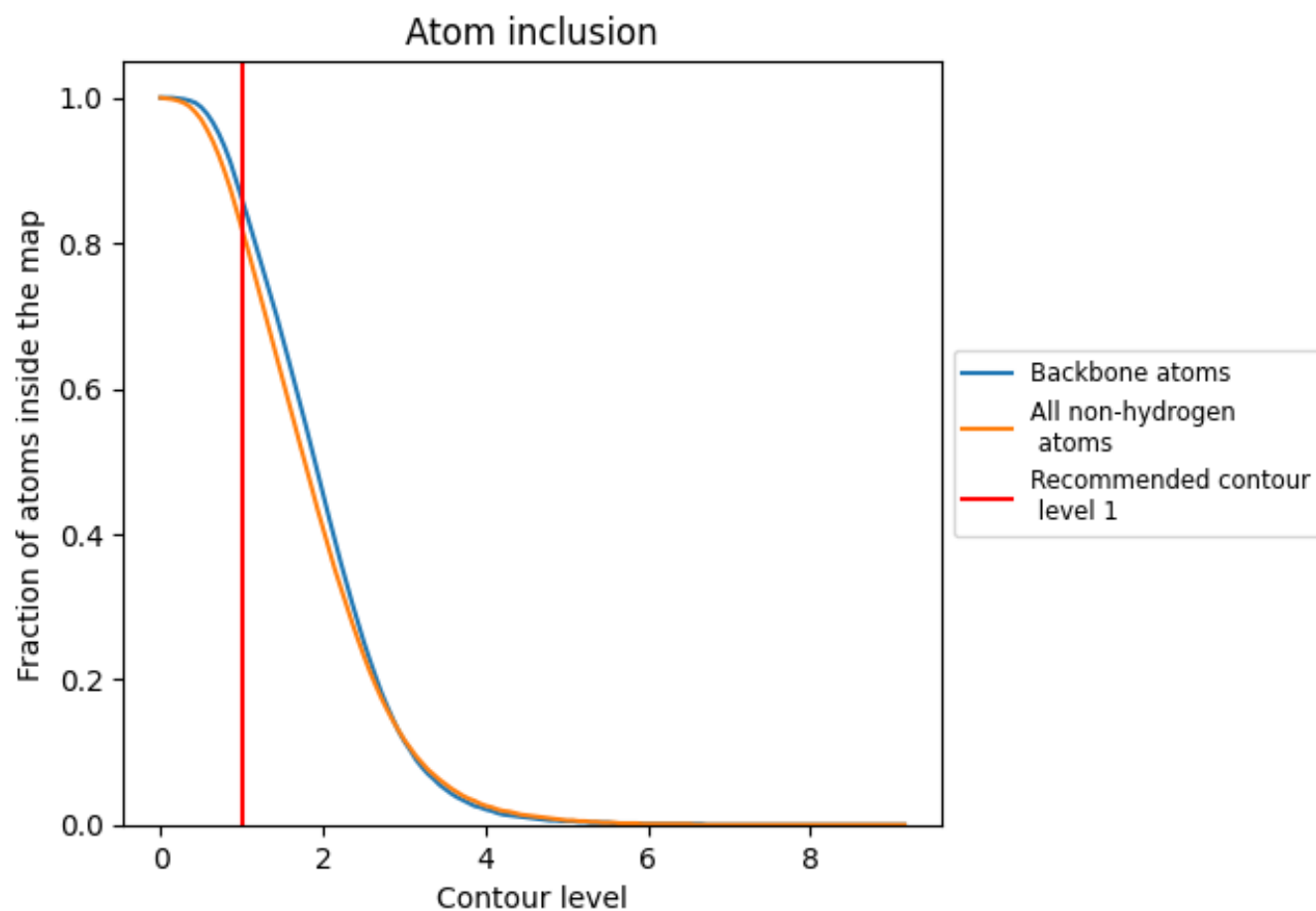
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8200	 0.5590
BA	 0.2310	 0.3430
L1	 0.9330	 0.6010
L2	 0.8160	 0.5310
L3	 0.8610	 0.5490
L4	 0.9670	 0.6220
L5	 0.7430	 0.5440
L6	 0.7590	 0.5550
L7	 0.8690	 0.6080
L8	 0.8730	 0.5960
L9	 0.9230	 0.6270
LA	 0.8140	 0.5700
LB	 0.8580	 0.5940
LC	 0.9370	 0.6420
LD	 0.7600	 0.5530
LE	 0.8420	 0.5770
LF	 0.6660	 0.5130
LG	 0.8260	 0.6010
LH	 0.8240	 0.5940
LI	 0.7730	 0.5560
LJ	 0.8300	 0.5900
LK	 0.8680	 0.6010
LL	 0.8070	 0.5730
LM	 0.6630	 0.5450
LN	 0.8140	 0.5760
LO	 0.7020	 0.5320
LP	 0.7370	 0.5530
LQ	 0.8170	 0.5890
LR	 0.8150	 0.5920
LS	 0.7950	 0.5730
LT	 0.8730	 0.6000
LU	 0.7160	 0.5400
LV	 0.8310	 0.6000
LW	 0.8970	 0.6010
LX	 0.7200	 0.5570



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Chain	Atom inclusion	Q-score
LY	 0.6710	 0.5280
LZ	 0.8820	 0.6060
NC	 0.0000	 0.3340
NF	 0.6020	 0.5570
NK	 0.5700	 0.4890
NL	 0.7140	 0.5480
NP	 0.6830	 0.5250
SA	 0.8230	 0.5830
SB	 0.8380	 0.5910
SC	 0.7000	 0.5270
SD	 0.8410	 0.5820
SE	 0.8420	 0.5920
SF	 0.8310	 0.5920
SG	 0.8530	 0.6110
SH	 0.7610	 0.5460
SI	 0.8020	 0.5800
SK	 0.7600	 0.5560
SL	 0.6080	 0.4760
SM	 0.8730	 0.6160
SQ	 0.4280	 0.4810
SR	 0.6600	 0.5330
SV	 0.7440	 0.5370