



Full wwPDB EM Validation Report ⓘ

Jun 26, 2026 – 02:53 AM EDT

PDB ID : 8FL3 / pdb_00008fl3
EMDB ID : EMD-29266
Title : Human nuclear pre-60S ribosomal subunit (State I2)
Authors : Vanden Broeck, A.; Klinge, S.
Deposited on : 2022-12-21
Resolution : 2.53 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:

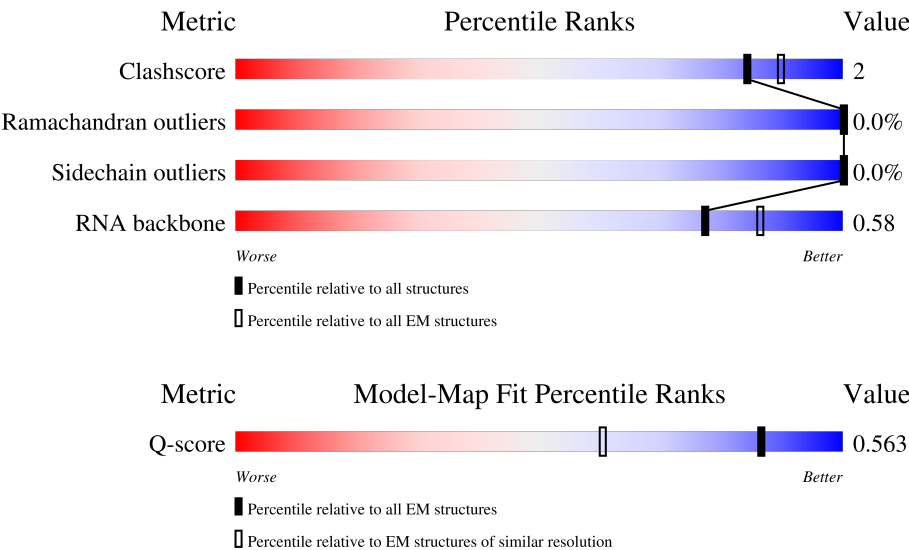
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 2.53 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.



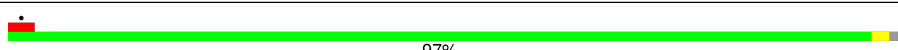
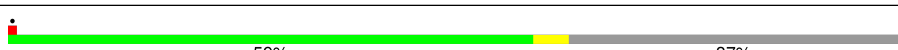
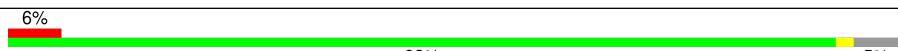
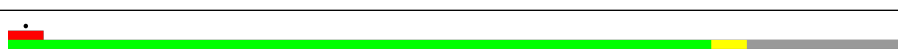
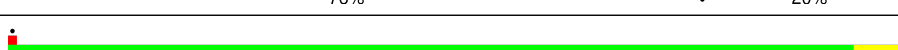
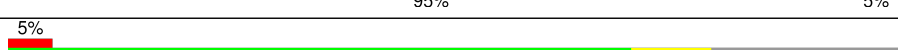
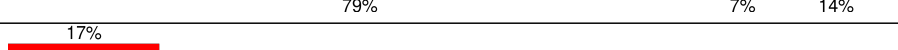
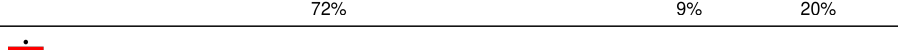
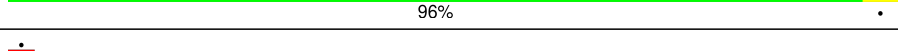
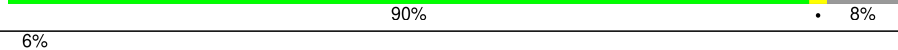
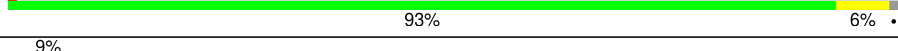
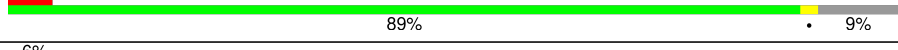
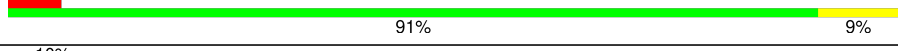
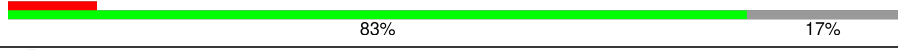
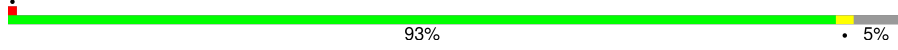
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7309 (2.03 - 3.03)

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	41% 87% 10% .
2	BB	217	11% 84% 15%
3	BD	734	97%

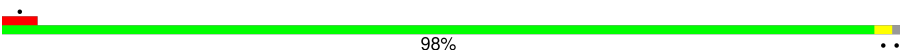
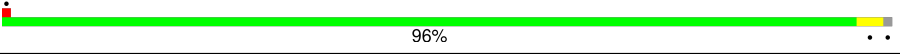
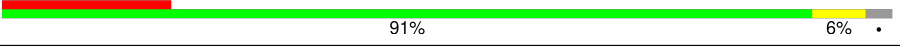
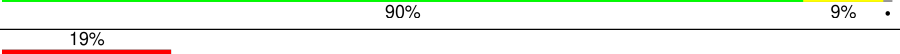
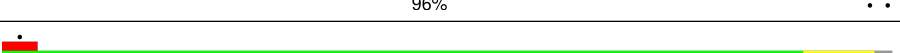
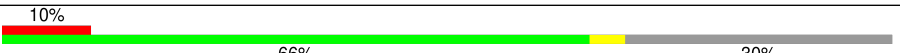
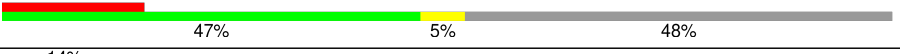
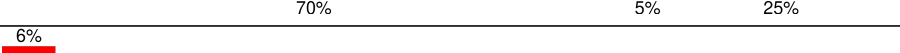
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Mol	Chain	Length	Quality of chain
4	L1	157	
5	L3	5070	
6	L4	121	
7	L5	178	
8	L6	211	
9	L7	203	
10	L8	215	
11	L9	204	
12	LA	184	
13	LB	188	
14	LC	176	
15	LD	196	
16	LE	160	
17	LF	128	
18	LG	140	
19	LH	156	
20	LI	145	
21	LJ	136	
22	LK	148	
23	LL	137	
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	LW	97	
33	LX	92	
34	LY	70	
35	LZ	51	
36	NB	549	
37	NC	731	
38	NF	260	
39	NJ	485	
40	NK	129	
41	NL	478	
42	NP	134	
43	NT	687	
44	NU	929	
45	NV	432	
45	NW	432	
46	NX	1130	
46	NY	1130	
47	NZ	360	
48	SA	427	
49	SB	297	
50	SC	288	
51	SD	248	

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Mol	Chain	Length	Quality of chain
52	SE	266	
53	SF	257	
54	SG	192	
55	SH	293	
56	SI	255	
57	SK	245	
58	SM	588	
59	SQ	239	
60	SR	634	
61	SV	163	

2 Entry composition

There are 66 unique types of molecules in this entry. The entry contains 185196 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
			1208	749	226	229	4		

- Molecule 2 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BB	216	Total	C	N	O	S	0	0
			1736	1109	313	306	8		

- Molecule 3 is a protein called Ribosomal biogenesis protein LAS1L.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	BD	19	Total	C	N	O	0	0
			149	98	26	25		

- Molecule 4 is a RNA chain called 5.8S rRNA.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L3	3494	Total	C	N	O	P	0	0
			75007	33439	13731	24343	3494		

- Molecule 6 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L4	117	Total	C	N	O	P	0	0
			2494	1111	441	825	117		

- Molecule 7 is a protein called 60S ribosomal protein L11.

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

- Molecule 8 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L6	203	Total	C	N	O	S	0	0
			1652	1036	341	272	3		

- Molecule 9 is a protein called 60S ribosomal protein L13a.

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

- Molecule 10 is a protein called 60S ribosomal protein L14.

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

- Molecule 11 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L9	194	Total	C	N	O	S	0	0
			1635	1030	345	256	4		

- Molecule 12 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LA	153	Total	C	N	O	S	1	0
			1249	781	243	216	9		

- Molecule 13 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LB	151	Total	C	N	O	S	0	0
			1223	768	247	203	5		

- Molecule 14 is a protein called 60S ribosomal protein L18a.

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

- Molecule 15 is a protein called 60S ribosomal protein L19.

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

- Molecule 16 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LE	137	Total	C	N	O	S	1	0
			1119	714	213	187	5		

- Molecule 17 is a protein called 60S ribosomal protein L22.

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

- Molecule 18 is a protein called 60S ribosomal protein L23.

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

- Molecule 19 is a protein called 60S ribosomal protein L23a.

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

- Molecule 20 is a protein called 60S ribosomal protein L26.

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

- Molecule 21 is a protein called 60S ribosomal protein L27.

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

- Molecule 22 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LK	117	Total	C	N	O	S	0	0
			918	583	183	149	3		

- Molecule 23 is a protein called 60S ribosomal protein L28.

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

- 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 L37.

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

- Molecule 33 is a protein called 60S ribosomal protein L37a.

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

- Molecule 34 is a protein called 60S ribosomal protein L38.

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

- Molecule 35 is a protein called 60S ribosomal protein L39.

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

- Molecule 36 is a protein called Guanine nucleotide-binding protein-like 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	NB	81	Total	C	N	O	S	0	0
			691	431	148	109	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	NC	511	Total	C	N	O	S	0	0
			4097	2595	729	757	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	NF	233	Total	C	N	O	S	0	0
			1891	1210	355	318	8		

- Molecule 39 is a protein called Notchless protein homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	NJ	379	Total	C	N	O	S	0	0
			2951	1849	544	547	11		

- Molecule 40 is a protein called Protein LLP homolog.

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

- Molecule 41 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	NL	304	Total	C	N	O	S	0	0
			2519	1564	505	448	2		

- Molecule 42 is a protein called Zinc finger protein 593.

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

- Molecule 43 is a protein called Protein SDA1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	NT	501	Total	C	N	O	S	0	0
			4072	2610	706	727	29		

- Molecule 44 is a protein called Testis-expressed protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	NU	833	Total	C	N	O	S	0	0
			6469	4154	1128	1165	22		

- Molecule 45 is a protein called WD repeat-containing protein 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	NV	381	Total	C	N	O	S	1	0
			2915	1849	506	540	20		
45	NW	367	Total	C	N	O	S	0	0
			2789	1771	482	516	20		

- Molecule 46 is a protein called Proline-, glutamic acid- and leucine-rich protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	NX	518	Total	C	N	O	S	0	0
			3926	2491	698	708	29		
46	NY	526	Total	C	N	O	S	0	0
			3983	2528	708	718	29		

- Molecule 47 is a protein called Coiled-coil domain-containing protein 86.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	NZ	117	Total	C	N	O	S	0	0
			1010	624	216	168	2		

- Molecule 48 is a protein called 60S ribosomal protein L4.

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

- Molecule 49 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SB	254	Total	C	N	O	S	0	0
			2057	1303	365	376	13		

- Molecule 50 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SC	217	Total	C	N	O	S	0	0
			1743	1121	332	286	4		

- Molecule 51 is a protein called 60S ribosomal protein L7.

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

- Molecule 52 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SE	233	Total	C	N	O	S	1	0
			1885	1202	364	315	4		

- Molecule 53 is a protein called 60S ribosomal protein L8.

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

- Molecule 54 is a protein called 60S ribosomal protein L9.

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

- Molecule 55 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SH	93	Total	C	N	O	S	0	0
			773	501	130	139	3		

- Molecule 56 is a protein called 60S ribosomal protein L7-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SI	234	Total	C	N	O	S	3	0
			1952	1267	365	316	4		

- Molecule 57 is a protein called Eukaryotic translation initiation factor 6.

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

- Molecule 58 is a protein called Pescadillo homolog.

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

- Molecule 59 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SQ	217	Total	C	N	O	S	1	0
			1778	1134	313	320	11		

- Molecule 60 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SR	601	Total	C	N	O	S	1	0
			4939	3110	901	902	26		

- Molecule 61 is a protein called Probable ribosome biogenesis protein RLP24.

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

- Molecule 62 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
62	L1	4	Total	Mg	0
			4	4	
62	L3	86	Total	Mg	0
			86	86	
62	L4	1	Total	Mg	0
			1	1	

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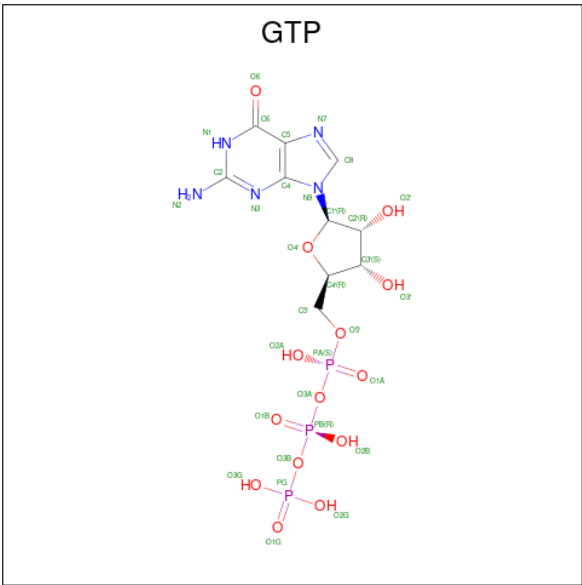
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
62	L9	1	Total 1	Mg 1	0
62	LQ	1	Total 1	Mg 1	0
62	LR	1	Total 1	Mg 1	0
62	LT	1	Total 1	Mg 1	0
62	LW	1	Total 1	Mg 1	0
62	NC	1	Total 1	Mg 1	0
62	SA	1	Total 1	Mg 1	0
62	SF	1	Total 1	Mg 1	0
62	SR	1	Total 1	Mg 1	0

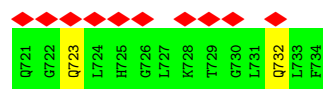
- Molecule 63 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

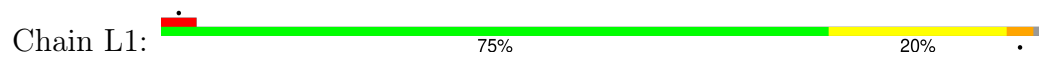
- Molecule 64 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



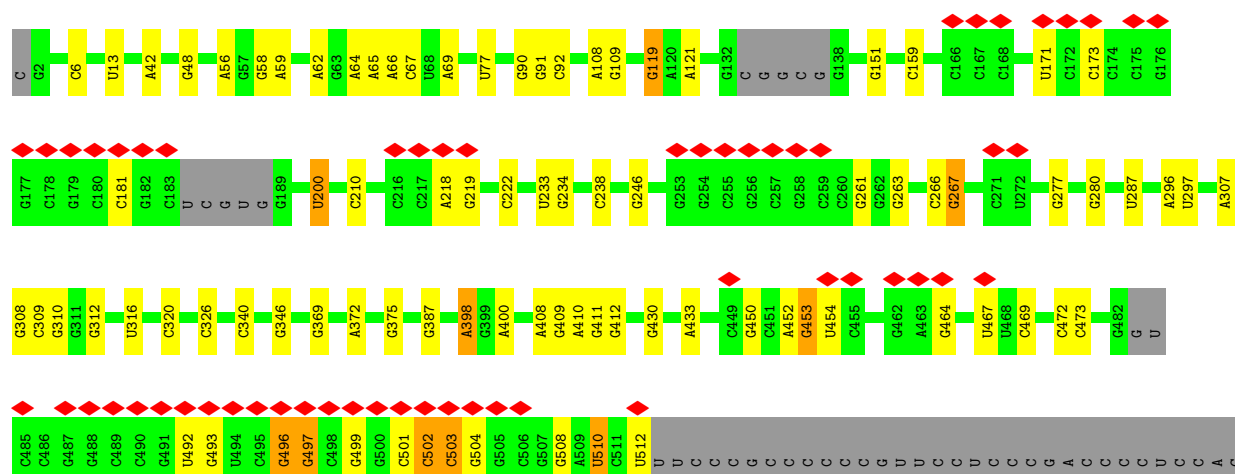
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
66	SR	1	28	10	5	11	2	0



- Molecule 4: 5.8S rRNA

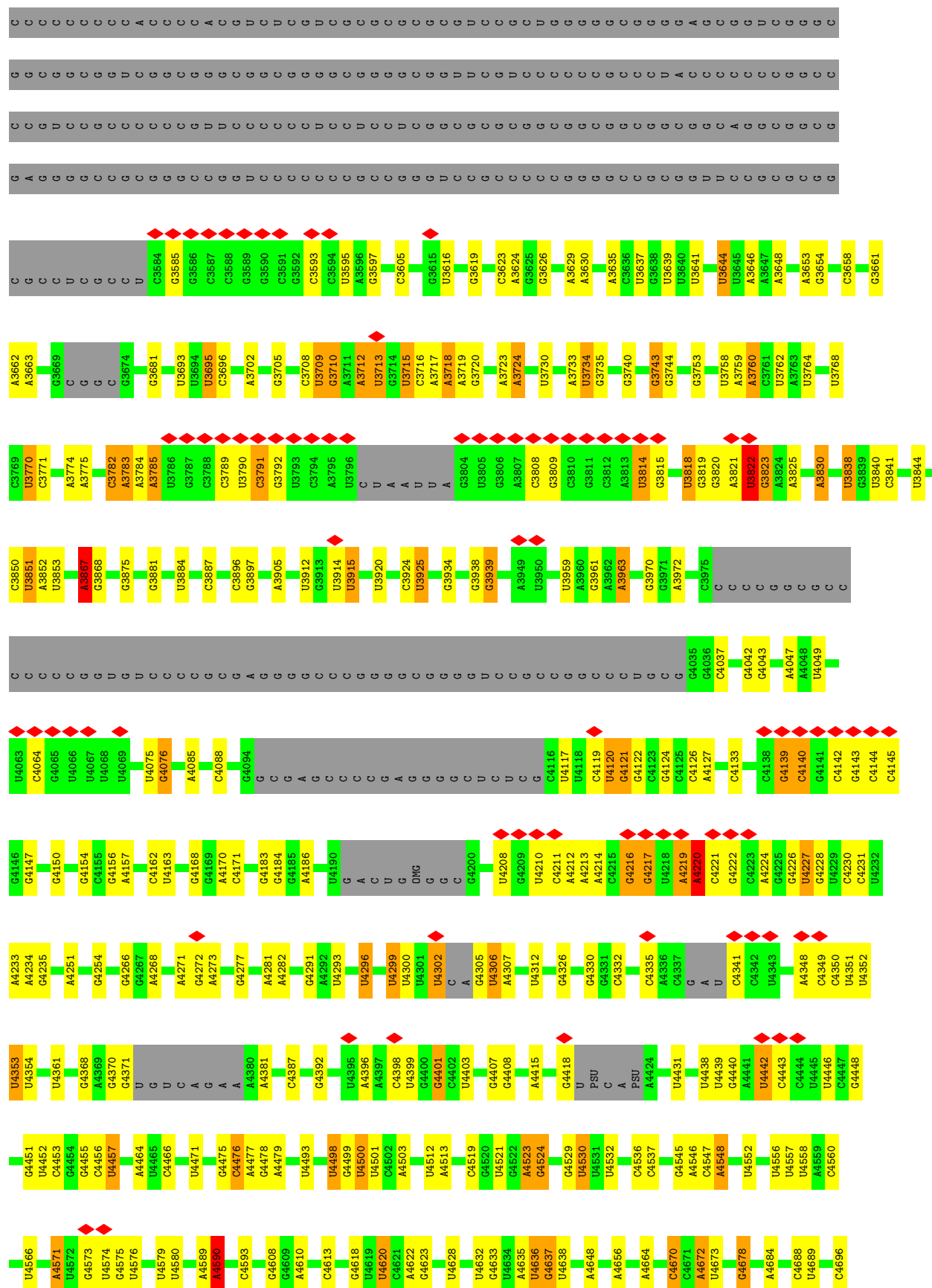


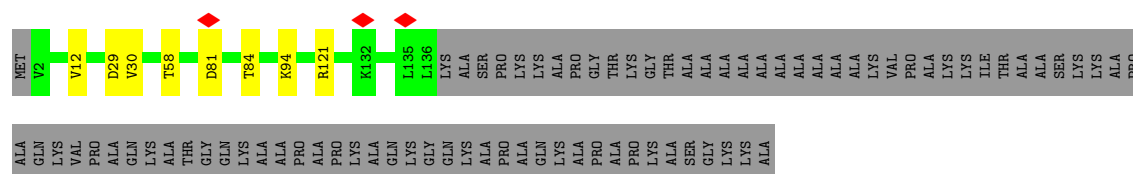
- Molecule 5: 28S rRNA



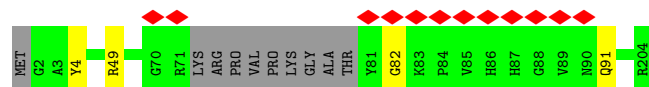




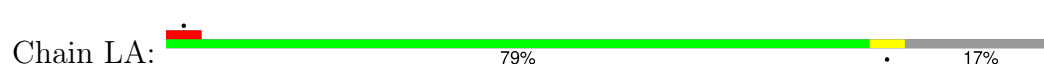




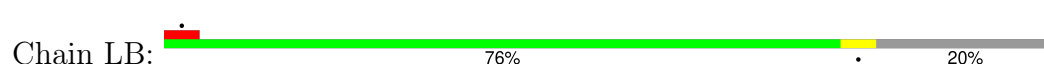
- Molecule 11: 60S ribosomal protein L15



- Molecule 12: 60S ribosomal protein L17



- Molecule 13: 60S ribosomal protein L18



- Molecule 14: 60S ribosomal protein L18a

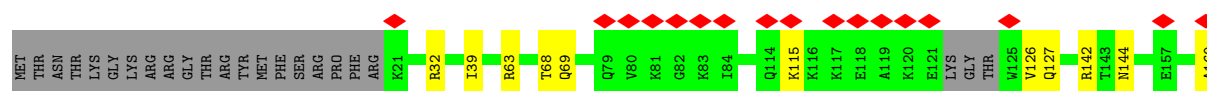
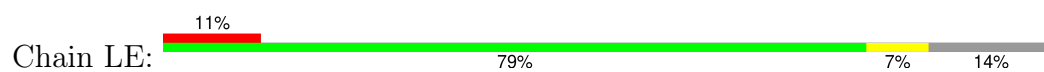


- Molecule 15: 60S ribosomal protein L19

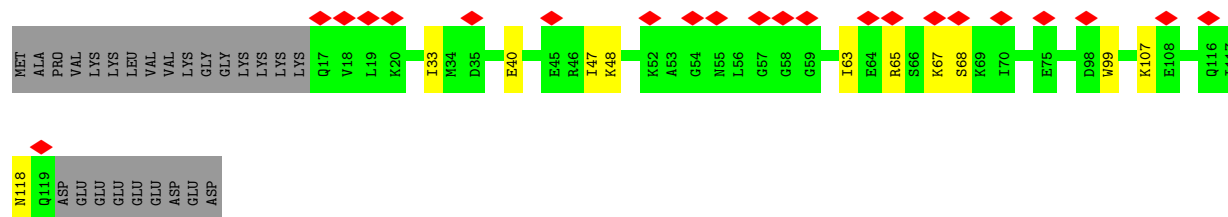


- Molecule 16: 60S ribosomal protein L21





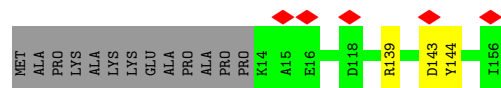
- Molecule 17: 60S ribosomal protein L22



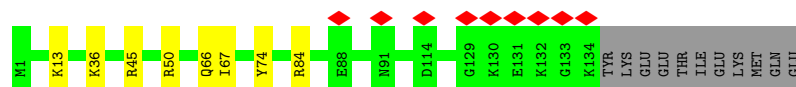
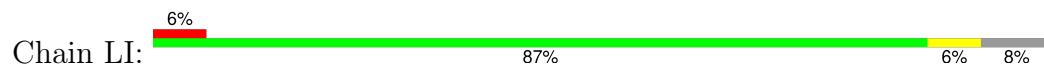
- Molecule 18: 60S ribosomal protein L23



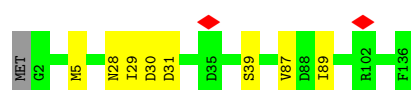
- Molecule 19: 60S ribosomal protein L23a



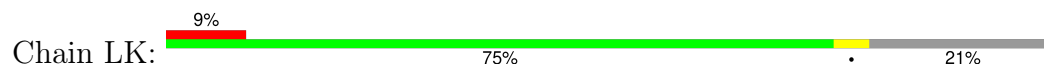
- Molecule 20: 60S ribosomal protein L26

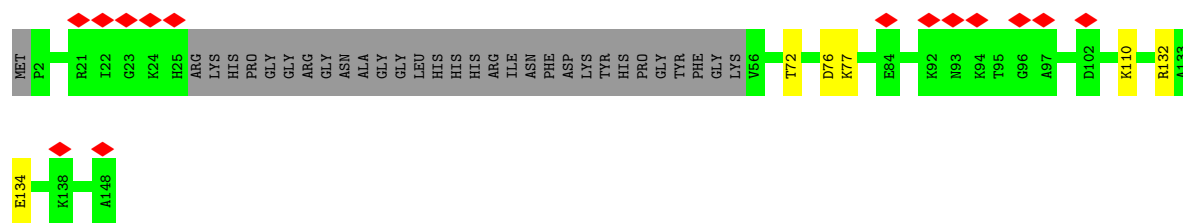


- Molecule 21: 60S ribosomal protein L27

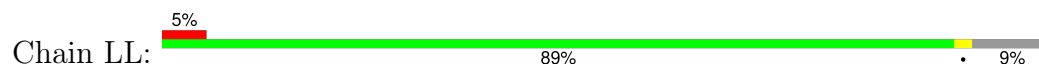


- Molecule 22: 60S ribosomal protein L27a

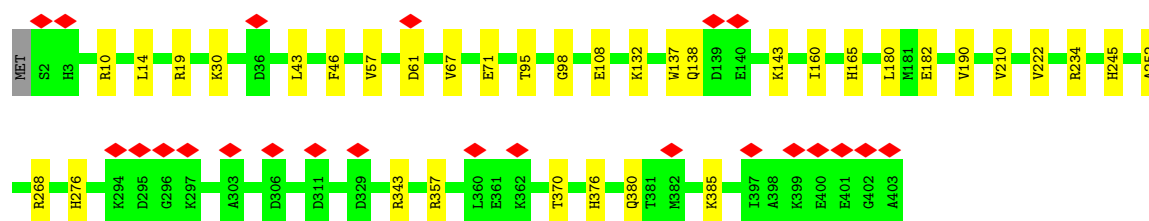




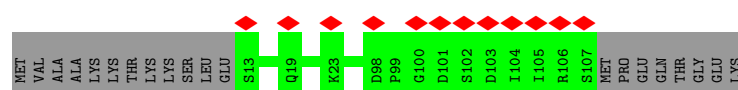
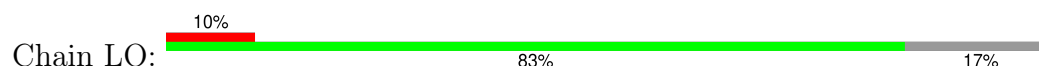
- Molecule 23: 60S ribosomal protein L28



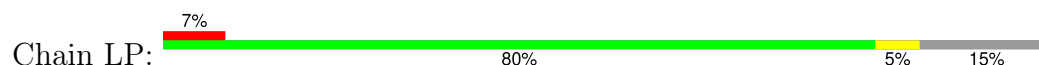
- Molecule 24: 60S ribosomal protein L3



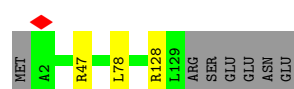
- Molecule 25: 60S ribosomal protein L30



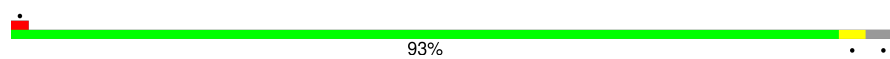
- Molecule 26: 60S ribosomal protein L31

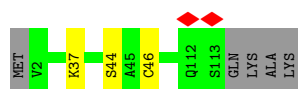


- Molecule 27: 60S ribosomal protein L32

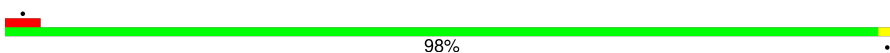


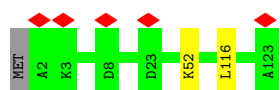
- Molecule 28: 60S ribosomal protein L34

Chain LR:  93%

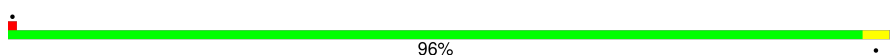


- Molecule 29: 60S ribosomal protein L35

Chain LS:  98%

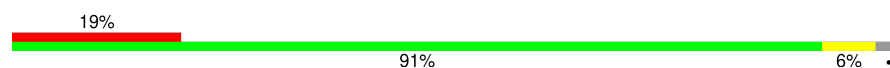


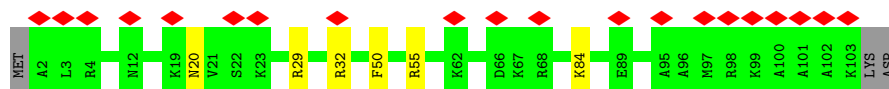
- Molecule 30: 60S ribosomal protein L35a

Chain LT:  96%



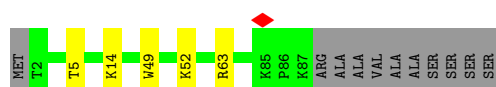
- Molecule 31: 60S ribosomal protein L36

Chain LU:  19% 91% 6%



- Molecule 32: 60S ribosomal protein L37

Chain LW:  84% 5% 11%

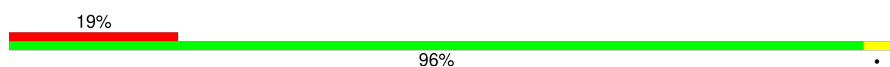


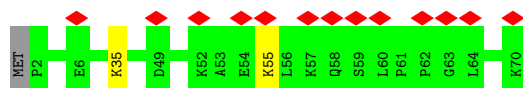
- Molecule 33: 60S ribosomal protein L37a

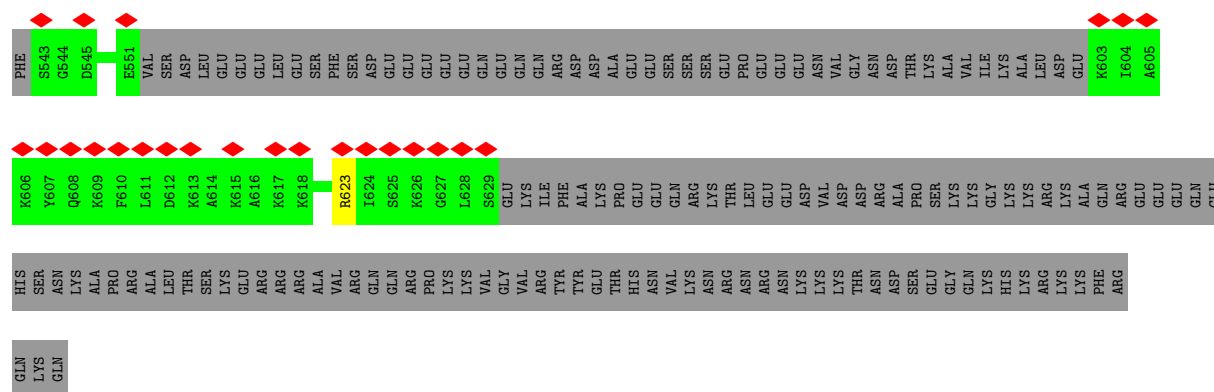
Chain LX:  90% 9%



- Molecule 34: 60S ribosomal protein L38

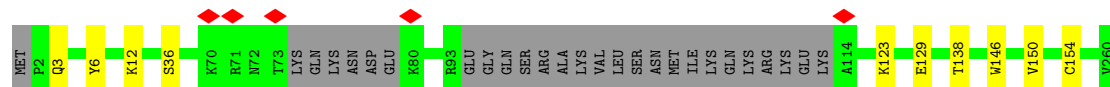
Chain LY:  19% 96%





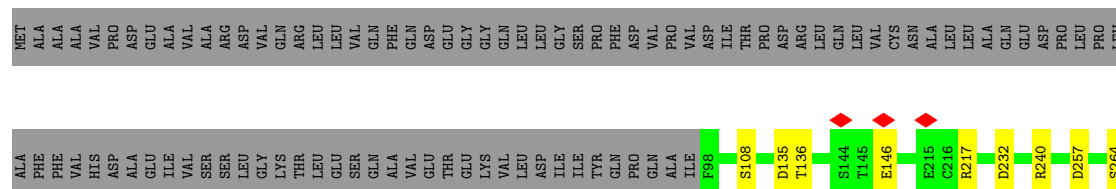
• Molecule 38: Ribosome biogenesis protein NSA2 homolog

Chain NF: 86% 10%



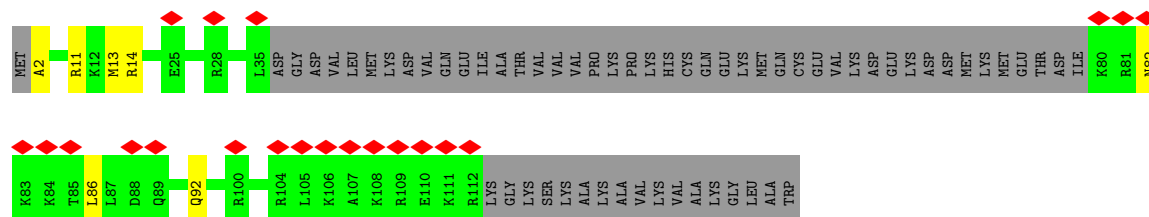
• Molecule 39: Notchless protein homolog 1

Chain NJ: 74% 22%



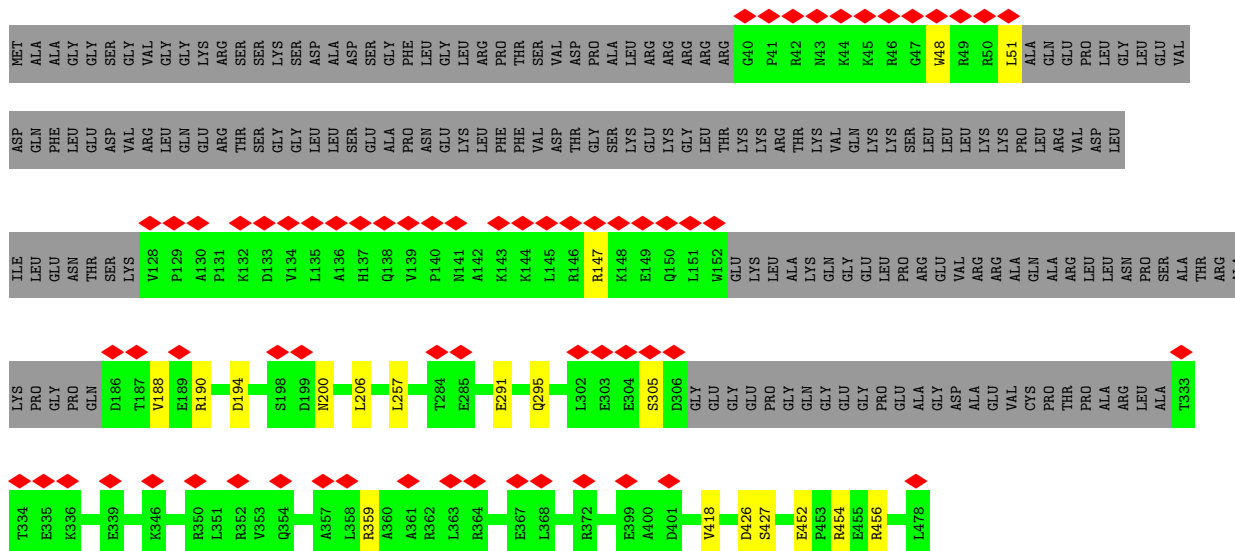
• Molecule 40: Protein LLP homolog

Chain NK: 16% 47% 5% 48%

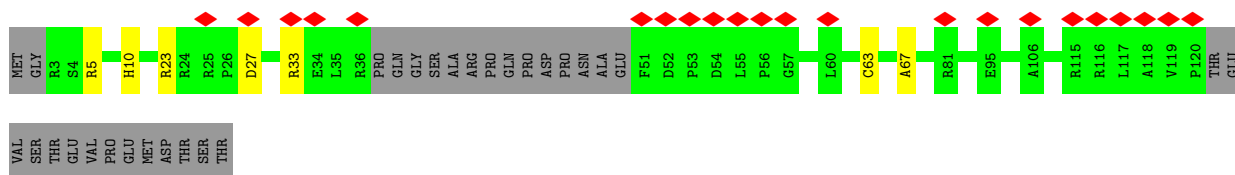


• Molecule 41: Ribosome biogenesis protein NOP53

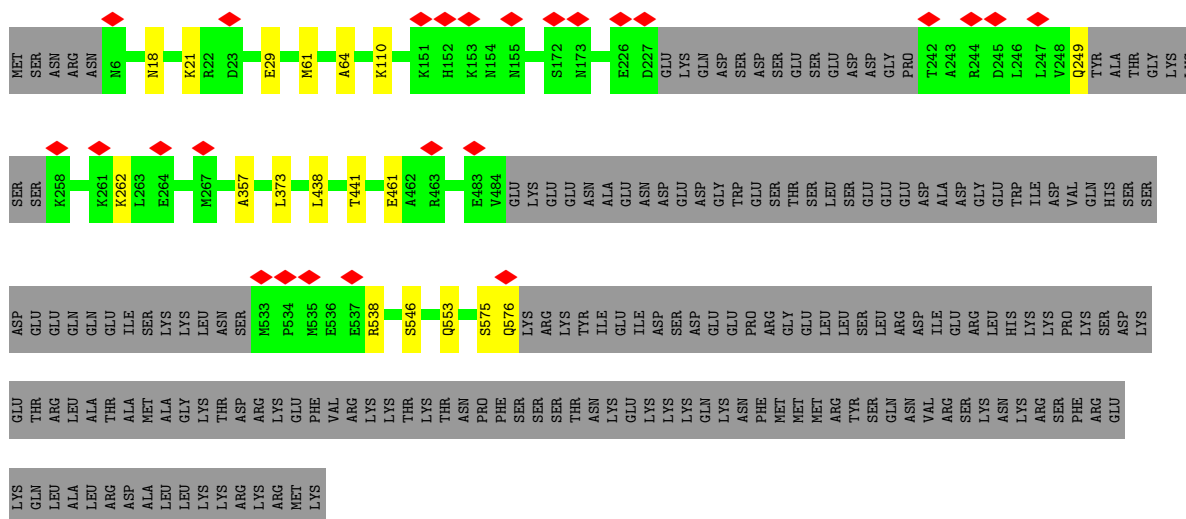
Chain NL: 14% 60% 36%



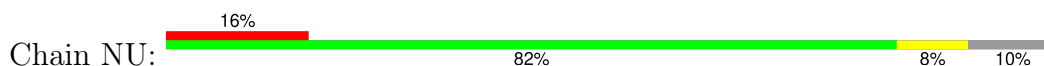
- Molecule 42: Zinc finger protein 593

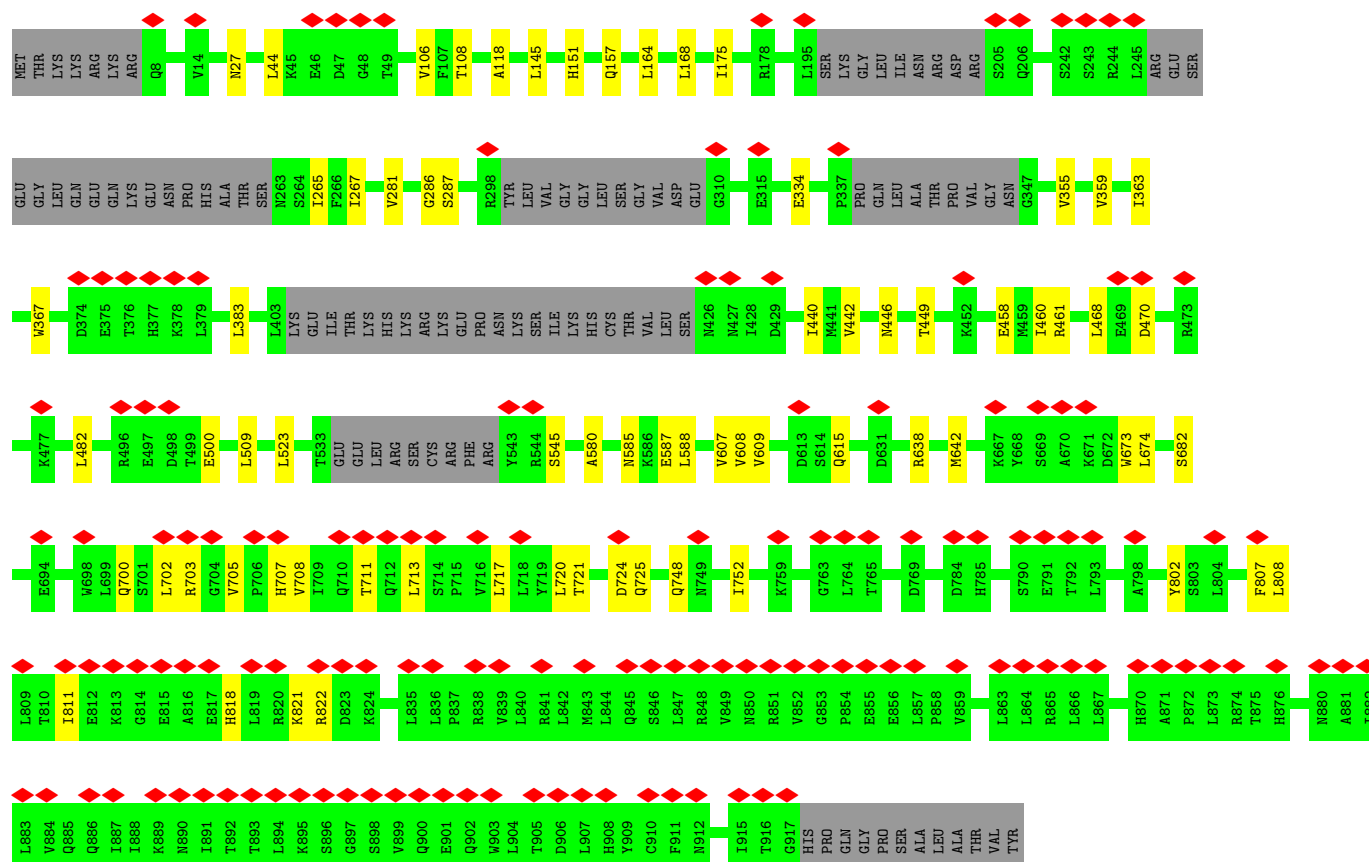


- Molecule 43: Protein SDA1 homolog

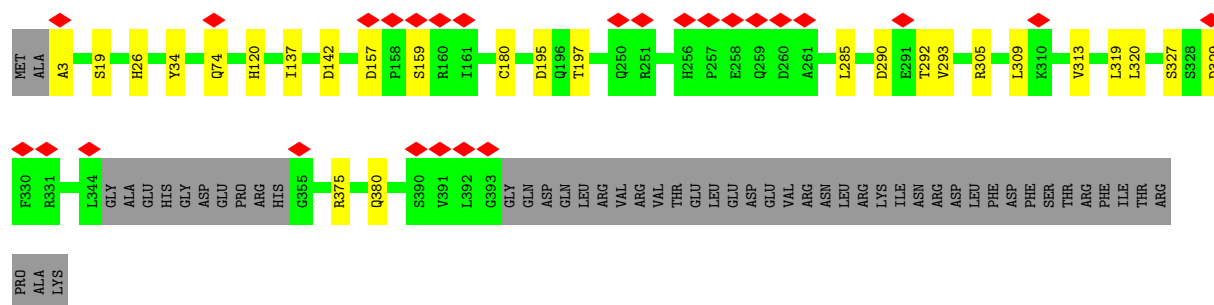
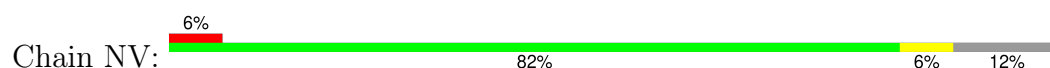


- Molecule 44: Testis-expressed protein 10

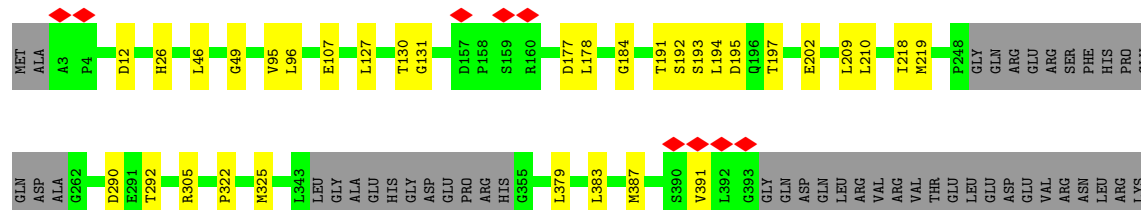
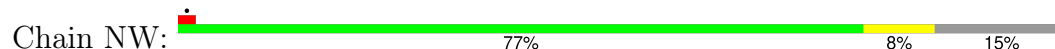




• Molecule 45: WD repeat-containing protein 18



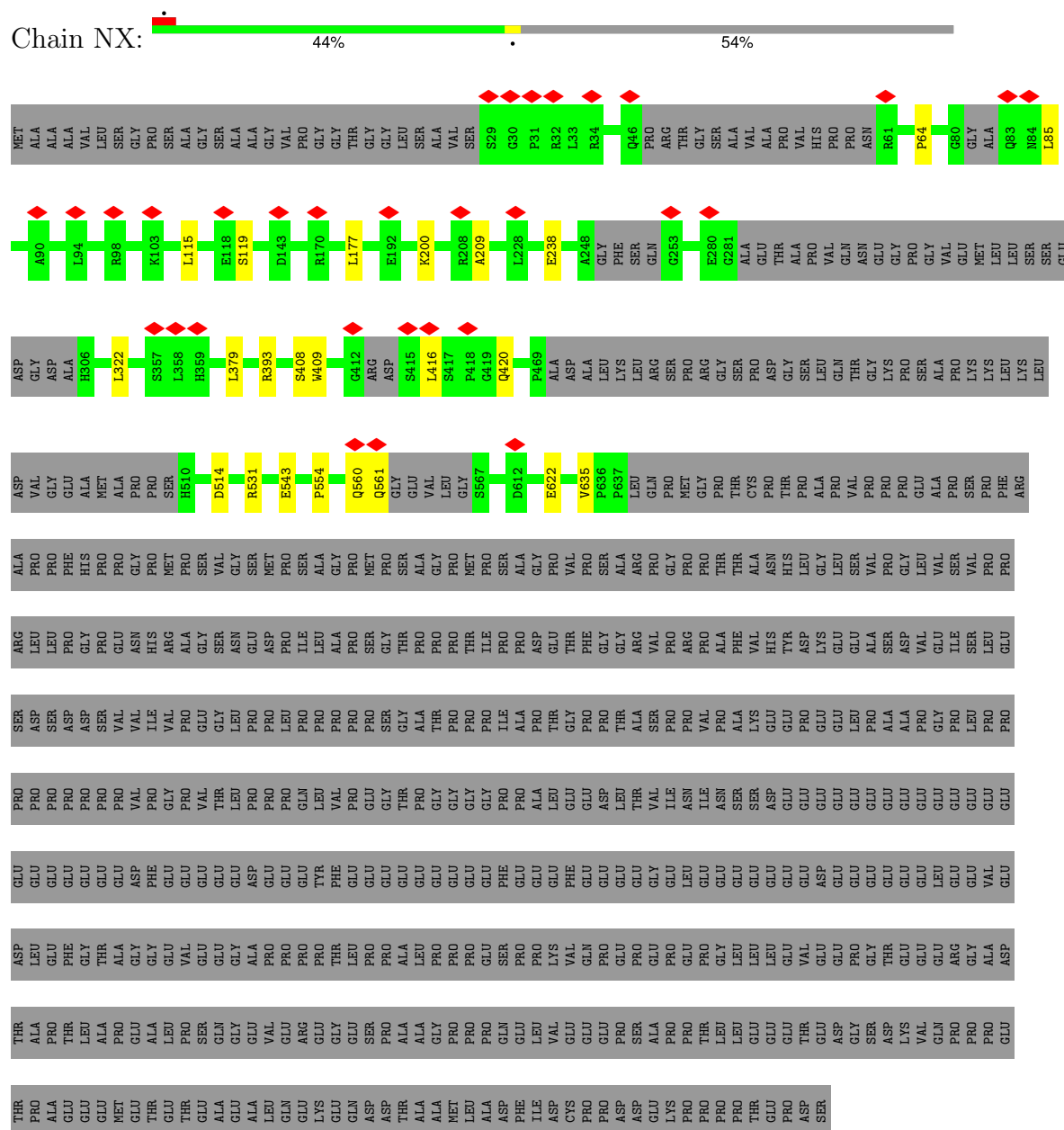
• Molecule 45: WD repeat-containing protein 18



TLE
ASN
ARG
ASP
LEU
PHE
ASP
PHE
SER
THR
ARG
PHE
TLE
THR
ARG
PRO
ALA
LYS

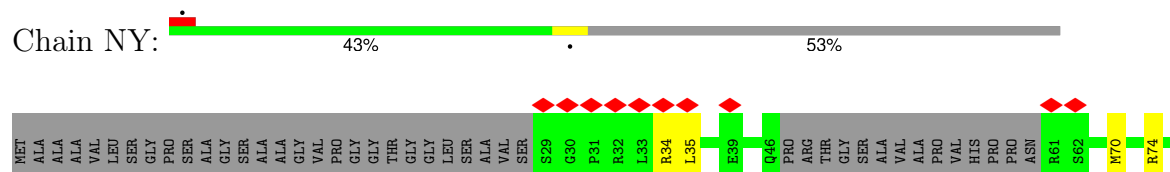
- Molecule 46: Proline-, glutamic acid- and leucine-rich protein 1

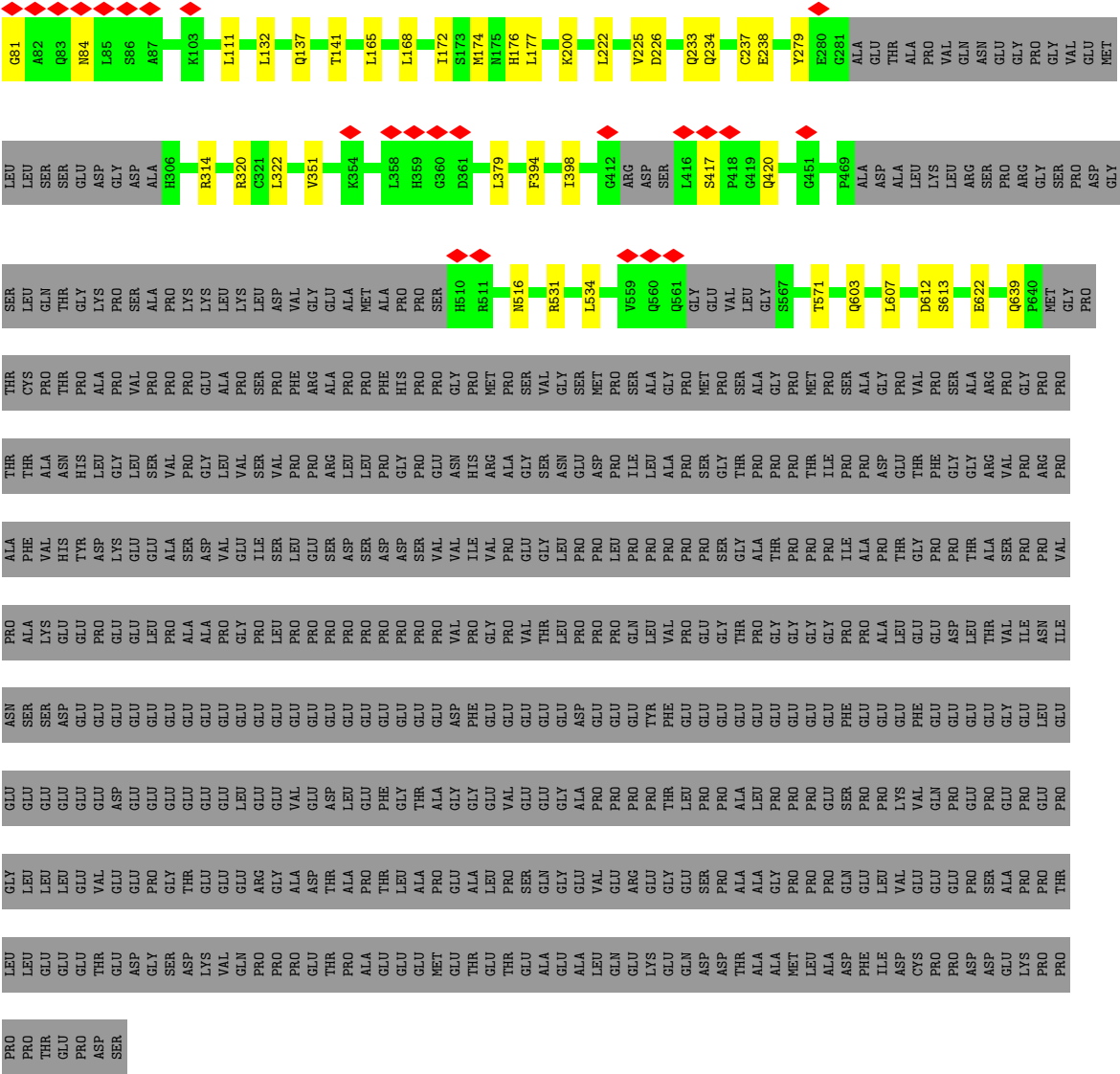
Chain NX:



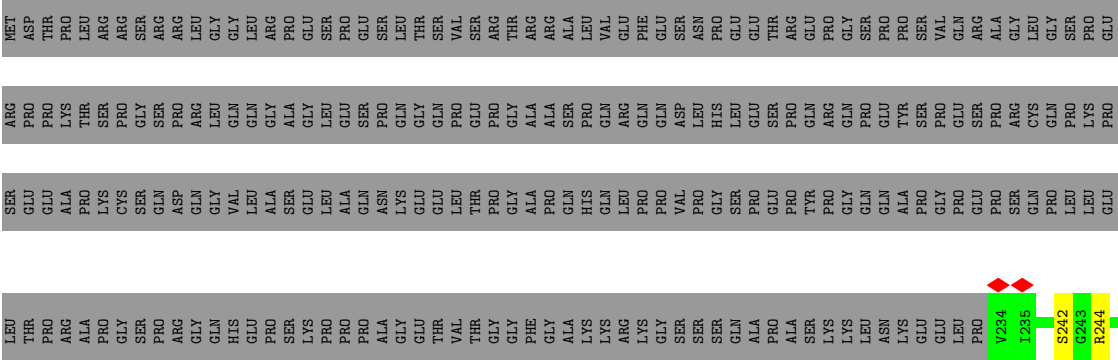
- Molecule 46: Proline-, glutamic acid- and leucine-rich protein 1

Chain NY:





● Molecule 47: Coiled-coil domain-containing protein 86



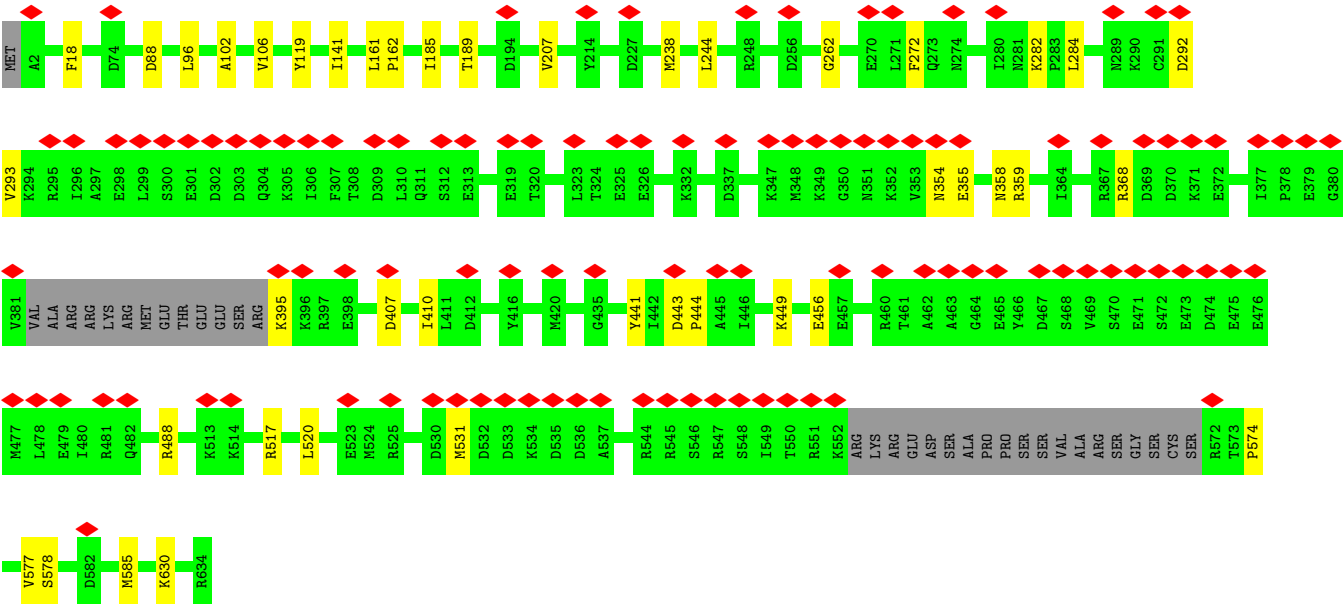
Chain SR:

18%

88%

7%

5%



• Molecule 61: Probable ribosome biogenesis protein RLP24

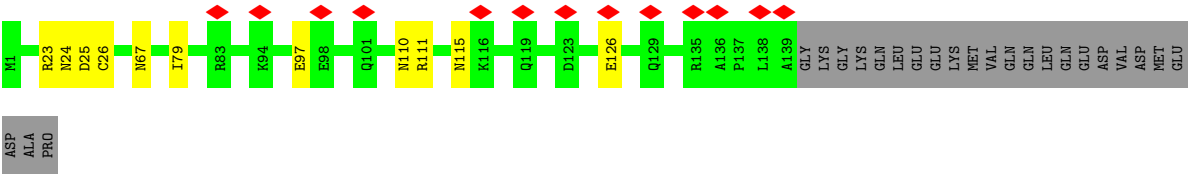
Chain SV:

8%

79%

7%

15%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	107973	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	8.345	Depositor
Minimum map value	-0.193	Depositor
Average map value	0.044	Depositor
Map value standard deviation	0.180	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: MG, 1MA, GTP, ZN, PSU, OMG, K, HIC, 6MZ, A2M, 5MC, UR3, OMU, GDP, OMC

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	0.18	0/1224	0.33	0/1651
2	BB	0.13	0/1764	0.31	0/2365
3	BD	0.11	0/152	0.23	0/202
4	L1	0.15	0/3589	0.24	0/5589
5	L3	0.16	0/80922	0.27	0/126208
6	L4	0.14	0/2784	0.26	0/4336
7	L5	0.13	0/1372	0.29	0/1836
8	L6	0.12	0/1682	0.27	0/2248
9	L7	0.12	0/1682	0.27	0/2250
10	L8	0.11	0/1133	0.24	0/1516
11	L9	0.15	0/1677	0.28	0/2243
12	LA	0.12	0/1279	0.30	0/1716
13	LB	0.11	0/1239	0.26	0/1658
14	LC	0.15	0/1501	0.29	0/2013
15	LD	0.10	0/1305	0.24	0/1727
16	LE	0.14	0/1146	0.30	0/1533
17	LF	0.12	0/856	0.30	0/1149
18	LG	0.12	0/1048	0.29	0/1402
19	LH	0.12	0/1175	0.26	0/1572
20	LI	0.13	0/1132	0.26	0/1504
21	LJ	0.15	0/1130	0.26	0/1507
22	LK	0.10	0/935	0.23	0/1249
23	LL	0.12	0/1017	0.26	0/1364
24	LN	0.14	0/3294	0.30	0/4406
25	LO	0.10	0/748	0.24	0/1004
26	LP	0.12	0/894	0.26	0/1204
27	LQ	0.12	0/1071	0.25	0/1429
28	LR	0.12	0/898	0.28	0/1197
29	LS	0.11	0/1023	0.25	0/1351
30	LT	0.13	0/895	0.28	0/1198
31	LU	0.12	0/843	0.27	0/1115
32	LW	0.13	0/720	0.30	0/952

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	LX	0.11	0/718	0.26	0/953
34	LY	0.11	0/575	0.23	0/761
35	LZ	0.14	0/454	0.26	0/599
36	NB	0.14	0/701	0.26	0/920
37	NC	0.12	0/4175	0.27	0/5621
38	NF	0.15	0/1929	0.29	0/2579
39	NJ	0.16	0/3024	0.32	0/4099
40	NK	0.10	0/587	0.24	0/767
41	NL	0.12	0/2558	0.25	0/3424
42	NP	0.10	0/864	0.26	0/1154
43	NT	0.13	0/4144	0.25	0/5575
44	NU	0.14	0/6590	0.27	0/8941
45	NV	0.13	0/2987	0.29	0/4065
45	NW	0.17	0/2853	0.31	0/3883
46	NX	0.11	0/3993	0.24	0/5410
46	NY	0.12	0/4054	0.25	0/5496
47	NZ	0.11	0/1020	0.25	0/1343
48	SA	0.13	0/2907	0.27	0/3905
49	SB	0.14	0/2098	0.28	0/2817
50	SC	0.12	0/1776	0.28	0/2381
51	SD	0.14	0/1905	0.28	0/2539
52	SE	0.16	0/1919	0.31	0/2580
53	SF	0.14	0/1914	0.31	0/2567
54	SG	0.12	0/1537	0.26	0/2066
55	SH	0.11	0/794	0.24	0/1071
56	SI	0.12	0/2003	0.28	0/2688
57	SK	0.12	0/1877	0.29	0/2554
58	SM	0.15	0/3357	0.28	0/4529
59	SQ	0.10	0/1817	0.26	0/2435
60	SR	0.12	0/5025	0.28	0/6742
61	SV	0.12	0/1207	0.28	0/1600
All	All	0.14	0/193492	0.27	0/278758

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 ⓘ

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	1208	0	1257	12	0
2	BB	1736	0	1847	21	0
3	BD	149	0	152	3	0
4	L1	3278	0	1665	18	0
5	L3	75007	0	38003	325	0
6	L4	2494	0	1263	10	0
7	L5	1349	0	1383	7	0
8	L6	1652	0	1770	11	0
9	L7	1650	0	1794	4	0
10	L8	1111	0	1174	5	0
11	L9	1635	0	1671	4	0
12	LA	1249	0	1276	6	0
13	LB	1223	0	1330	6	0
14	LC	1461	0	1502	7	0
15	LD	1289	0	1429	12	0
16	LE	1119	0	1177	8	0
17	LF	842	0	864	8	0
18	LG	1034	0	1097	4	0
19	LH	1156	0	1268	2	0
20	LI	1115	0	1205	7	0
21	LJ	1107	0	1182	4	0
22	LK	918	0	985	4	0
23	LL	1002	0	1068	3	0
24	LN	3239	0	3377	27	0
25	LO	738	0	774	0	0
26	LP	879	0	924	4	0
27	LQ	1053	0	1147	3	0
28	LR	888	0	977	2	0
29	LS	1015	0	1148	2	0
30	LT	876	0	912	2	0
31	LU	832	0	917	5	0
32	LW	705	0	737	5	0
33	LX	708	0	756	8	0
34	LY	569	0	637	2	0
35	LZ	444	0	483	5	0
36	NB	691	0	770	2	0
37	NC	4097	0	4176	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	NF	1891	0	2015	9	0
39	NJ	2951	0	2895	11	0
40	NK	581	0	656	7	0
41	NL	2519	0	2598	13	0
42	NP	847	0	854	6	0
43	NT	4072	0	4225	12	0
44	NU	6469	0	6478	51	0
45	NV	2915	0	2896	15	0
45	NW	2789	0	2781	23	0
46	NX	3926	0	4073	17	0
46	NY	3983	0	4129	31	0
47	NZ	1010	0	1106	6	0
48	SA	2853	0	3028	20	0
49	SB	2057	0	2050	10	0
50	SC	1743	0	1899	9	0
51	SD	1870	0	1996	6	0
52	SE	1885	0	2036	18	0
53	SF	1876	0	1970	19	0
54	SG	1518	0	1601	7	0
55	SH	773	0	755	2	0
56	SI	1952	0	2086	7	0
57	SK	1852	0	1828	20	0
58	SM	3278	0	3332	19	0
59	SQ	1778	0	1817	8	0
60	SR	4939	0	5077	33	0
61	SV	1184	0	1248	10	0
62	L1	4	0	0	0	0
62	L3	86	0	0	0	0
62	L4	1	0	0	0	0
62	L9	1	0	0	0	0
62	LQ	1	0	0	0	0
62	LR	1	0	0	0	0
62	LT	1	0	0	0	0
62	LW	1	0	0	0	0
62	NC	1	0	0	0	0
62	SA	1	0	0	0	0
62	SF	1	0	0	0	0
62	SR	1	0	0	0	0
63	LR	1	0	0	0	0
63	LW	1	0	0	0	0
63	LX	1	0	0	0	0
63	NP	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	SV	1	0	0	0	0
64	NC	32	0	12	0	0
65	NC	1	0	0	0	0
65	SR	1	0	0	0	0
66	SR	28	0	12	0	0
All	All	185196	0	149550	755	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 (755) 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)
2:BB:87:ILE:HD13	2:BB:116:LEU:HD11	1.57	0.86
17:LF:40:GLU:OE1	17:LF:65:ARG:NH1	2.08	0.86
5:L3:3713:U:O4	5:L3:3740:G:N2	2.09	0.85
6:L4:40:U:O2	7:L5:75:ARG:NH1	2.09	0.84
5:L3:512:U:OP2	8:L6:165:LYS:NZ	2.12	0.82
58:SM:357:ASP:OD2	58:SM:359:SER:OG	1.97	0.82
5:L3:4156:G:OP2	5:L3:4157:A:O2'	1.99	0.81
57:SK:100:ARG:NH1	61:SV:26:CYS:SG	2.53	0.81
1:BA:50:THR:HG22	1:BA:58:ILE:HD11	1.63	0.80
5:L3:62:A:N3	5:L3:77:U:O2'	2.14	0.80
60:SR:443:ASP:OD2	60:SR:449:LYS:NZ	2.13	0.80
4:L1:51:U:OP2	35:LZ:21:ARG:NH2	2.14	0.80
2:BB:207:LYS:NZ	2:BB:208:SER:O	2.14	0.80
44:NU:700:GLN:O	44:NU:703:ARG:NH1	2.14	0.80
5:L3:4227:OMU:HM22	5:L3:4228:OMG:H5'	1.62	0.79
5:L3:2487:G:OP1	41:NL:456:ARG:NH2	2.16	0.79
2:BB:156:LYS:NZ	2:BB:158:GLN:OE1	2.17	0.78
5:L3:2520:C:O2	5:L3:2640:G:N2	2.15	0.78
5:L3:4962:C:O2'	40:NK:92:GLN:NE2	2.16	0.78
3:BD:720:SER:OG	3:BD:723:GLN:OE1	2.01	0.78
5:L3:2695:A:OP1	34:LY:35:LYS:NZ	2.17	0.78
5:L3:2848:G:O2'	5:L3:3838:U:O4	2.01	0.78
2:BB:33:GLU:OE2	5:L3:3970:G:O2'	2.02	0.77
37:NC:64:SER:OG	38:NF:129:GLU:OE1	2.02	0.77
46:NY:200:LYS:NZ	46:NY:238:GLU:OE1	2.17	0.77
5:L3:4768:G:OP1	9:L7:168:TYR:OH	2.03	0.77
7:L5:158:SER:OG	7:L5:161:GLU:OE1	2.03	0.77
5:L3:695:G:O2'	5:L3:697:G:OP2	2.02	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L3:3717:A:OP2	5:L3:3735:G:N2	2.17	0.77
5:L3:4717:A:OP2	24:LN:30:LYS:NZ	2.18	0.77
1:BA:123:ARG:NH1	59:SQ:61:LYS:O	2.18	0.76
5:L3:1480:C:O2'	5:L3:1482:G:OP2	2.02	0.76
5:L3:4620:OMU:OP2	5:L3:4670:C:N4	2.16	0.76
56:SI:249:GLN:OE1	58:SM:267:LEU:HD21	1.85	0.76
2:BB:41:TYR:OH	2:BB:47:LYS:O	2.02	0.76
5:L3:151:G:OP1	11:L9:49:ARG:NH2	2.18	0.76
5:L3:2892:C:OP2	15:LD:72:LYS:NZ	2.18	0.76
5:L3:3709:U:OP2	43:NT:18:ASN:ND2	2.19	0.76
5:L3:1508:A:OP1	48:SA:110:ARG:NH2	2.19	0.76
5:L3:2009:A:OP1	38:NF:12:LYS:NZ	2.18	0.75
46:NY:234:GLN:OE1	46:NY:320:ARG:NH1	2.19	0.75
6:L4:55:A:O2'	7:L5:151:ILE:O	2.05	0.74
5:L3:508:G:O2'	5:L3:510:U:OP2	2.05	0.74
5:L3:375:G:OP2	32:LW:52:LYS:NZ	2.20	0.73
32:LW:14:LYS:NZ	35:LZ:51:LEU:OXT	2.21	0.73
5:L3:67:C:OP2	5:L3:312:G:N2	2.20	0.73
5:L3:1293:G:OP2	5:L3:1293:G:N2	2.16	0.73
5:L3:1883:G:OP1	27:LQ:47:ARG:NH1	2.21	0.73
5:L3:408:A:O2'	5:L3:411:G:OP2	2.06	0.73
46:NY:237:CYS:SG	46:NY:320:ARG:NH2	2.61	0.73
6:L4:23:A:N3	6:L4:118:C:O2'	2.21	0.72
16:LE:115:LYS:NZ	16:LE:127:GLN:O	2.21	0.72
5:L3:1783:C:OP1	47:NZ:329:LYS:NZ	2.21	0.72
24:LN:108:GLU:OE2	24:LN:138:GLN:NE2	2.22	0.72
5:L3:1397:A:O2'	5:L3:1467:C:O2'	2.08	0.72
5:L3:4688:C:O2'	54:SG:155:SER:OG	2.04	0.72
57:SK:39:GLU:O	60:SR:395:LYS:NZ	2.23	0.72
5:L3:309:C:OP2	31:LU:32:ARG:NH2	2.21	0.72
5:L3:5002:U:OP2	24:LN:385:LYS:NZ	2.20	0.72
1:BA:92:ARG:NH2	5:L3:1980:U:OP2	2.23	0.71
2:BB:23:ARG:NH1	2:BB:24:LYS:O	2.22	0.71
5:L3:502:C:O2'	5:L3:503:C:OP1	2.05	0.71
5:L3:1420:A:O2'	5:L3:1500:A:O2'	2.03	0.71
16:LE:69:GLN:OE1	49:SB:42:ASN:ND2	2.24	0.71
5:L3:2262:G:OP2	23:LL:98:ARG:NH1	2.24	0.71
39:NJ:108:SER:OG	39:NJ:146:GLU:OE1	2.04	0.70
44:NU:446:ASN:OD1	44:NU:449:THR:OG1	2.04	0.70
5:L3:3770:PSU:H2'	5:L3:3771:C:C6	2.26	0.70
5:L3:3961:G:O2'	5:L3:4043:G:N2	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:25:THR:OG1	60:SR:262:GLY:O	2.04	0.69
5:L3:4216:G:N2	5:L3:4219:A:OP2	2.25	0.69
46:NX:200:LYS:NZ	46:NX:238:GLU:OE1	2.23	0.69
5:L3:1568:C:OP2	33:LX:3:LYS:NZ	2.22	0.69
5:L3:3695:PSU:H2'	5:L3:3696:C:C6	2.28	0.68
46:NX:622:GLU:OE2	46:NY:531:ARG:NH1	2.26	0.68
57:SK:126:GLU:OE1	57:SK:139:ARG:NH2	2.26	0.68
5:L3:2471:G:OP1	52:SE:59:ARG:NH2	2.26	0.68
5:L3:308:G:OP2	5:L3:308:G:N2	2.16	0.68
5:L3:3896:C:O2'	24:LN:268:ARG:NH1	2.27	0.68
5:L3:934:C:O2'	5:L3:935:A:O5'	2.12	0.67
42:NP:33:ARG:NH1	61:SV:25:ASP:OD2	2.28	0.67
46:NX:531:ARG:NH1	46:NY:622:GLU:OE2	2.27	0.67
53:SF:15:VAL:O	53:SF:194:ASN:ND2	2.27	0.67
5:L3:5039:U:O2'	61:SV:115:ASN:OD1	2.12	0.67
2:BB:101:LYS:NZ	5:L3:4047:A:OP1	2.26	0.67
13:LB:40:ASN:OD1	13:LB:132:LYS:NZ	2.28	0.67
16:LE:68:THR:HG22	16:LE:69:GLN:H	1.59	0.67
37:NC:25:GLN:NE2	37:NC:26:GLY:O	2.27	0.67
39:NJ:240:ARG:NH2	39:NJ:275:HIS:O	2.28	0.67
5:L3:3867:A2M:H2'	5:L3:3868:G:C8	2.31	0.66
5:L3:4299:PSU:H2'	5:L3:4300:U:C6	2.31	0.66
44:NU:367:TRP:NE1	44:NU:383:LEU:HD13	2.10	0.66
1:BA:37:LEU:HD12	1:BA:42:VAL:HG21	1.78	0.66
5:L3:151:G:OP2	11:L9:4:TYR:OH	2.13	0.66
15:LD:39:GLN:OE1	15:LD:42:ARG:NH1	2.29	0.65
5:L3:3605:C:OP2	15:LD:71:ARG:NH1	2.28	0.65
5:L3:4670:C:O2'	5:L3:4672:A:OP2	2.15	0.65
33:LX:26:VAL:HG21	53:SF:180:LEU:HD11	1.78	0.65
46:NY:172:ILE:HG22	46:NY:177:LEU:CD2	2.25	0.65
4:L1:75:OMG:OP2	20:LI:74:TYR:OH	2.15	0.65
5:L3:3623:C:O2	15:LD:82:LYS:NZ	2.30	0.65
5:L3:3644:U:OP2	60:SR:630:LYS:NZ	2.22	0.65
16:LE:32:ARG:O	49:SB:41:LYS:NZ	2.23	0.65
38:NF:3:GLN:NE2	60:SR:207:VAL:O	2.30	0.65
45:NW:202:GLU:OE2	45:NW:209:LEU:HD21	1.97	0.65
5:L3:4124:G:N2	52:SE:43:GLN:O	2.30	0.65
5:L3:4940:C:OP1	50:SC:156:ARG:NH1	2.29	0.65
48:SA:204:ARG:NH1	48:SA:205:ARG:O	2.30	0.65
5:L3:1677:PSU:H5''	5:L3:1678:C:O5'	1.96	0.64
5:L3:2630:U:OP1	17:LF:48:LYS:NZ	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:SR:441:TYR:OH	61:SV:97:GLU:OE2	2.10	0.64
5:L3:1468:C:OP1	22:LK:132:ARG:NH2	2.31	0.64
5:L3:1670:G:N2	5:L3:1670:G:OP2	2.31	0.64
37:NC:623:ARG:NH1	41:NL:305:SER:OG	2.31	0.64
5:L3:4305:G:O2'	5:L3:4306:OMU:H5''	1.98	0.64
5:L3:2422:OMC:OP1	12:LA:127:ARG:NH2	2.31	0.64
5:L3:2922:G:O2'	5:L3:3275:A:N6	2.30	0.64
46:NY:516:ASN:OD1	46:NY:571:THR:OG1	2.14	0.64
5:L3:3708:C:O2'	5:L3:3710:G:OP2	2.17	0.63
57:SK:107:VAL:HG23	57:SK:108:THR:HG23	1.81	0.63
5:L3:1255:A:OP1	5:L3:1257:A:N6	2.31	0.63
24:LN:61:ASP:OD2	60:SR:410:ILE:HD12	1.98	0.63
60:SR:185:ILE:O	60:SR:189:THR:OG1	2.15	0.63
21:LJ:30:ASP:O	21:LJ:39:SER:OG	2.07	0.63
1:BA:128:THR:O	1:BA:132:ILE:HD12	1.98	0.63
5:L3:4370:OMG:H2'	5:L3:4371:G:C8	2.33	0.63
45:NV:120:HIS:ND1	45:NV:142:ASP:OD2	2.30	0.63
46:NY:417:SER:OG	46:NY:420:GLN:OE1	2.17	0.63
5:L3:4117:U:O4'	52:SE:43:GLN:NE2	2.32	0.63
41:NL:206:LEU:O	41:NL:206:LEU:HD23	1.99	0.63
58:SM:150:THR:HG1	58:SM:153:CYS:HG	1.40	0.63
39:NJ:257:ASP:OD1	39:NJ:337:ARG:NH1	2.32	0.62
5:L3:4696:C:OP1	47:NZ:242:SER:OG	2.15	0.62
18:LG:99:GLU:OE1	61:SV:24:ASN:ND2	2.32	0.62
5:L3:1548:G:O2'	5:L3:2812:A:N3	2.31	0.62
5:L3:2545:U:O2'	5:L3:2547:G:N7	2.28	0.62
60:SR:272:PHE:HE1	60:SR:284:LEU:HD21	1.64	0.62
5:L3:2876:OMG:HM22	5:L3:2877:G:H5'	1.80	0.62
5:L3:3912:U:OP1	37:NC:49:ARG:NH2	2.33	0.62
5:L3:4524:G:C2	24:LN:252:ALA:HB1	2.33	0.62
37:NC:528:ARG:O	37:NC:532:ASN:N	2.33	0.62
41:NL:194:ASP:O	41:NL:200:ASN:ND2	2.32	0.62
5:L3:1754:U:O2'	5:L3:1755:C:O5'	2.17	0.61
24:LN:43:LEU:HB2	24:LN:210:VAL:HG11	1.82	0.61
9:L7:190:ASP:OD1	9:L7:191:LYS:N	2.33	0.61
46:NY:34:ARG:NH1	46:NY:81:GLY:O	2.32	0.61
52:SE:90:GLN:NE2	56:SI:62:GLU:OE2	2.33	0.61
37:NC:117:PRO:HB2	37:NC:120:LEU:HD12	1.83	0.61
5:L3:2373:C:O4'	26:LP:69:ASN:ND2	2.34	0.61
58:SM:183:LEU:HD23	58:SM:188:ILE:HG12	1.83	0.61
5:L3:1364:U:OP2	8:L6:36:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L3:4216:G:N3	5:L3:4217:G:O2'	2.34	0.61
5:L3:5022:U:O2'	5:L3:5025:C:N4	2.32	0.61
46:NY:165:LEU:HD12	46:NY:168:LEU:HD12	1.83	0.61
24:LN:57:VAL:HG12	24:LN:71:GLU:OE2	2.01	0.61
5:L3:3681:G:OP2	53:SF:128:ARG:NH2	2.34	0.60
6:L4:27:G:OP1	7:L5:146:ARG:NH2	2.33	0.60
5:L3:369:G:N2	5:L3:372:A:OP2	2.29	0.60
5:L3:2363:A2M:H2'	5:L3:2364:OMG:O4'	2.01	0.60
5:L3:1818:G:O2'	5:L3:1820:C:OP2	2.16	0.60
43:NT:29:GLU:OE1	53:SF:155:LYS:NZ	2.35	0.60
5:L3:3924:C:O2'	5:L3:3925:OMU:H5''	2.01	0.60
5:L3:4696:C:OP2	47:NZ:244:ARG:NH2	2.34	0.60
5:L3:4120:U:O2'	5:L3:4121:G:OP1	2.19	0.60
5:L3:4637:OMG:H2'	5:L3:4638:U:C6	2.37	0.60
31:LU:50:PHE:O	31:LU:55:ARG:NH1	2.34	0.60
5:L3:4442:PSU:H2'	5:L3:4443:C:O2	2.02	0.59
39:NJ:422:TRP:CZ3	39:NJ:443:VAL:HG21	2.37	0.59
44:NU:458:GLU:OE1	44:NU:461:ARG:NH2	2.34	0.59
45:NV:290:ASP:OD1	45:NV:292:THR:HG22	2.03	0.59
4:L1:12:G:OP1	12:LA:3:ARG:NH1	2.35	0.59
4:L1:102:G:OP2	4:L1:104:A:O2'	2.17	0.59
5:L3:5001:PSU:H2'	5:L3:5002:U:O4'	2.03	0.59
44:NU:363:ILE:HG22	44:NU:367:TRP:HZ3	1.66	0.59
5:L3:4664:A:OP1	24:LN:376:HIS:NE2	2.33	0.59
20:LI:67:ILE:O	20:LI:84:ARG:NH2	2.35	0.59
44:NU:724:ASP:OD1	44:NU:725:GLN:N	2.35	0.59
5:L3:2872:C:HO2'	5:L3:3823:G:HO2'	1.48	0.58
5:L3:1279:A:O2'	5:L3:1281:G:N7	2.31	0.58
5:L3:4088:C:OP1	53:SF:37:ARG:NH2	2.36	0.58
5:L3:2590:G:O2'	5:L3:2755:A:N6	2.37	0.58
14:LC:95:ARG:NH2	14:LC:112:ASP:OD2	2.35	0.58
54:SG:187:VAL:HG12	54:SG:188:GLN:HG3	1.86	0.58
24:LN:95:THR:OG1	24:LN:98:GLY:O	2.20	0.58
5:L3:2601:A:N6	5:L3:2744:A:OP2	2.34	0.58
5:L3:2296:G:O2'	48:SA:242:PRO:O	2.20	0.58
24:LN:222:VAL:O	24:LN:343:ARG:NH1	2.37	0.58
37:NC:155:LEU:HD11	60:SR:238:MET:HE2	1.85	0.58
5:L3:3759:A:C6	5:L3:4220:6MZ:H9	2.39	0.57
23:LL:20:ARG:NH1	27:LQ:78:LEU:O	2.36	0.57
4:L1:156:U:OP2	52:SE:89:ARG:NH2	2.38	0.57
5:L3:1865:G:OP1	38:NF:123:LYS:NZ	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:NX:115:LEU:O	46:NX:119:SER:OG	2.05	0.57
57:SK:85:ARG:NH2	57:SK:89:PRO:O	2.37	0.57
2:BB:8:ASP:OD1	2:BB:9:THR:N	2.37	0.57
16:LE:142:ARG:NH1	16:LE:144:ASN:OD1	2.38	0.57
5:L3:2306:G:OP1	27:LQ:128:ARG:NH1	2.37	0.57
43:NT:249:GLN:O	43:NT:262:LYS:NZ	2.36	0.57
5:L3:2533:C:OP1	19:LH:139:ARG:NH1	2.38	0.57
45:NV:137:ILE:HD13	45:NV:180:CYS:SG	2.45	0.57
44:NU:286:GLY:O	44:NU:287:SER:OG	2.17	0.57
3:BD:732:GLN:O	44:NU:682:SER:OG	2.23	0.57
39:NJ:297:THR:OG1	39:NJ:342:GLU:OE2	2.23	0.57
44:NU:748:GLN:O	44:NU:752:ILE:HD12	2.05	0.57
5:L3:4299:PSU:H2'	5:L3:4300:U:H6	1.70	0.57
5:L3:4580:U:O2'	24:LN:182:GLU:OE2	2.21	0.57
41:NL:426:ASP:OD1	41:NL:427:SER:N	2.37	0.57
1:BA:90:ARG:CZ	1:BA:98:ILE:HD13	2.35	0.56
5:L3:1564:A:N3	5:L3:3789:C:O2'	2.33	0.56
5:L3:4529:G:O2'	5:L3:4530:UR3:H5'	2.06	0.56
16:LE:39:ILE:HD13	16:LE:63:ARG:HG2	1.87	0.56
59:SQ:64:ARG:NH1	59:SQ:65:MET:O	2.38	0.56
5:L3:119:G:O4'	52:SE:132:ARG:NH1	2.38	0.56
5:L3:2705:G:O6	15:LD:46:LYS:NZ	2.39	0.56
5:L3:4678:G:OP1	40:NK:14:ARG:NH1	2.38	0.56
2:BB:93:LEU:HD22	2:BB:99:LEU:HB3	1.86	0.56
5:L3:1683:PSU:H2'	5:L3:1684:A:H8	1.71	0.56
45:NV:380:GLN:OE1	46:NY:74:ARG:NH1	2.38	0.56
57:SK:157:GLN:O	57:SK:223:LYS:NZ	2.34	0.56
5:L3:3867:A2M:HM'2	5:L3:3867:A2M:N3	2.21	0.56
5:L3:4126:C:OP1	52:SE:37:LYS:NZ	2.33	0.56
24:LN:160:ILE:HD11	24:LN:190:VAL:HG13	1.87	0.56
5:L3:90:G:OP2	5:L3:92:C:N4	2.39	0.56
5:L3:4910:G:N2	9:L7:106:ASP:O	2.38	0.56
59:SQ:42:ILE:HD11	59:SQ:92:VAL:HG13	1.87	0.56
15:LD:75:HIS:O	15:LD:76:MET:HE2	2.05	0.56
39:NJ:135:ASP:O	39:NJ:136:THR:OG1	2.21	0.56
48:SA:35:ASP:OD1	48:SA:36:ILE:N	2.38	0.56
21:LJ:5:MET:O	21:LJ:28:ASN:ND2	2.39	0.56
37:NC:382:VAL:HG11	37:NC:387:ILE:HD11	1.88	0.56
5:L3:200:U:OP1	20:LI:36:LYS:NZ	2.38	0.55
5:L3:1322:1MA:H2'	5:L3:1323:A:O4'	2.05	0.55
5:L3:4075:U:OP1	52:SE:249:ARG:NH2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L3:4928:C:O4'	10:L8:121:ARG:NH1	2.39	0.55
6:L4:97:G:OP1	51:SD:134:ARG:NH1	2.39	0.55
17:LF:99:TRP:CD2	60:SR:520:LEU:HD13	2.42	0.55
5:L3:4448:G:OP2	60:SR:119:TYR:OH	2.22	0.55
44:NU:673:TRP:CD1	44:NU:674:LEU:HD12	2.41	0.55
52:SE:101:LYS:NZ	52:SE:211:ASP:OD1	2.32	0.55
57:SK:21:ASN:ND2	57:SK:201:ASP:OD2	2.39	0.55
24:LN:165:HIS:HB3	24:LN:180:LEU:HD23	1.89	0.55
5:L3:3782:5MC:H4'	5:L3:3783:A:O5'	2.07	0.55
5:L3:4457:PSU:OP1	18:LG:50:ASN:ND2	2.39	0.55
44:NU:585:ASN:ND2	44:NU:587:GLU:OE1	2.40	0.55
44:NU:807:PHE:CZ	44:NU:811:ILE:HD11	2.42	0.55
5:L3:4765:G:OP1	54:SG:23:ARG:NE	2.40	0.55
46:NX:560:GLN:OE1	46:NX:561:GLN:NE2	2.39	0.55
37:NC:206:ILE:HG22	37:NC:365:VAL:HG12	1.89	0.54
5:L3:267:G:N7	41:NL:147:ARG:NH1	2.55	0.54
8:L6:62:PRO:O	8:L6:63:THR:OG1	2.20	0.54
5:L3:4186:A:O2'	11:L9:82:GLY:O	2.23	0.54
5:L3:4571:A2M:H8	5:L3:4571:A2M:O5'	2.07	0.54
46:NX:416:LEU:HD11	46:NX:420:GLN:OE1	2.08	0.54
10:L8:12:VAL:O	10:L8:58:THR:OG1	2.15	0.54
58:SM:175:ALA:HB2	58:SM:242:LEU:HD11	1.90	0.54
5:L3:1359:G:OP1	48:SA:114:ARG:NH1	2.40	0.54
43:NT:461:GLU:OE2	43:NT:538:ARG:NH2	2.40	0.54
45:NW:194:LEU:HD23	45:NW:219:MET:HE1	1.89	0.54
60:SR:292:ASP:OD1	60:SR:293:VAL:N	2.40	0.54
5:L3:2361:G:O6	12:LA:25:HIS:ND1	2.41	0.54
1:BA:37:LEU:CD1	1:BA:42:VAL:HG21	2.37	0.54
5:L3:1740:C:N4	5:L3:1741:G:O6	2.41	0.54
5:L3:121:A:OP1	52:SE:110:LYS:NZ	2.32	0.54
46:NY:35:LEU:HD11	46:NY:84:ASN:HD21	1.73	0.54
5:L3:3814:U:OP1	33:LX:6:LYS:NZ	2.41	0.53
4:L1:69:PSU:H2'	4:L1:70:G:O4'	2.08	0.53
37:NC:522:MET:SD	44:NU:702:LEU:HD12	2.48	0.53
44:NU:721:THR:O	44:NU:821:LYS:NZ	2.41	0.53
2:BB:77:ALA:O	2:BB:81:ASP:N	2.41	0.53
45:NV:157:ASP:OD2	45:NV:159:SER:OG	2.17	0.53
57:SK:44:ASP:OD1	57:SK:45:THR:N	2.41	0.53
28:LR:44:SER:OG	28:LR:46:CYS:SG	2.64	0.53
39:NJ:217:ARG:NE	39:NJ:232:ASP:OD1	2.42	0.53
5:L3:4302:U:O2	5:L3:4306:OMU:H5	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:NY:70:MET:HE1	46:NY:111:LEU:HD23	1.91	0.53
2:BB:151:VAL:O	2:BB:154:THR:HG22	2.09	0.53
5:L3:3718:A2M:H2	5:L3:3934:G:O4'	2.08	0.53
41:NL:291:GLU:OE2	41:NL:295:GLN:NE2	2.42	0.53
10:L8:81:ASP:OD2	10:L8:84:THR:OG1	2.27	0.53
57:SK:228:GLN:OE1	57:SK:228:GLN:N	2.42	0.53
5:L3:3938:G:N2	5:L3:4171:C:OP2	2.42	0.53
45:NW:193:SER:OG	45:NW:195:ASP:OD1	2.16	0.53
5:L3:2407:G:O6	35:LZ:2:SER:N	2.42	0.52
5:L3:1271:G:O2'	51:SD:34:ARG:NH2	2.39	0.52
5:L3:4306:OMU:HM22	5:L3:4306:OMU:O2	2.09	0.52
5:L3:1326:A2M:H2'	5:L3:1327:C:H6	1.75	0.52
5:L3:4457:PSU:O4	24:LN:252:ALA:HB3	2.09	0.52
37:NC:86:VAL:HG22	44:NU:27:ASN:HB3	1.91	0.52
5:L3:2562:G:O2'	5:L3:2565:A:N6	2.42	0.52
5:L3:2861:OMC:HM22	5:L3:2861:OMC:O2	2.10	0.52
5:L3:4623:OMG:OP1	24:LN:19:ARG:NH2	2.42	0.52
46:NY:137:GLN:O	46:NY:141:THR:HG23	2.10	0.52
4:L1:60:G:O6	4:L1:96:C:O2'	2.24	0.52
5:L3:453:G:O2'	5:L3:705:G:OP1	2.25	0.52
52:SE:105:GLU:OE2	52:SE:113:ARG:NH1	2.43	0.52
5:L3:3629:A:OP1	37:NC:431:LYS:NZ	2.40	0.52
56:SI:101:ARG:NH1	56:SI:122:LYS:O	2.43	0.52
5:L3:4548:A:OP2	38:NF:138:THR:OG1	2.12	0.52
4:L1:83:C:H41	20:LI:50:ARG:NH2	2.06	0.52
4:L1:50:C:O2'	60:SR:578:SER:OG	2.08	0.52
5:L3:4476:C:O2'	5:L3:4478:G:OP2	2.27	0.52
41:NL:452:GLU:OE2	41:NL:454:ARG:NH1	2.42	0.51
46:NY:132:LEU:HD13	46:NY:172:ILE:HD12	1.91	0.51
5:L3:1215:C:OP2	51:SD:59:LYS:NZ	2.43	0.51
5:L3:3760:A2M:O5'	5:L3:3760:A2M:H8	2.10	0.51
43:NT:357:ALA:HB1	43:NT:373:LEU:HD21	1.91	0.51
5:L3:4970:C:O4'	12:LA:75:GLN:NE2	2.42	0.51
2:BB:191:VAL:O	2:BB:197:ASN:ND2	2.41	0.51
5:L3:1325:C:H3'	5:L3:1326:A2M:H8	1.93	0.51
5:L3:2366:A:N3	5:L3:3850:C:O2'	2.42	0.51
24:LN:370:THR:O	24:LN:370:THR:HG22	2.11	0.51
60:SR:18:PHE:HD2	60:SR:141:ILE:HG21	1.76	0.51
5:L3:66:A:O2'	5:L3:326:C:O2	2.28	0.51
44:NU:808:LEU:HA	44:NU:811:ILE:HD12	1.91	0.51
5:L3:222:C:OP2	48:SA:165:LYS:NZ	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L3:1772:C:O2'	5:L3:1773:OMU:H5''	2.10	0.51
5:L3:2924:A:OP1	34:LY:55:LYS:NZ	2.43	0.51
46:NY:35:LEU:HD11	46:NY:84:ASN:ND2	2.26	0.51
57:SK:136:GLU:OE1	60:SR:368:ARG:NH2	2.44	0.51
5:L3:1921:C:O2'	14:LC:160:ARG:NH2	2.44	0.51
5:L3:4633:G:O2'	5:L3:4635:A:OP2	2.22	0.51
5:L3:3648:A:N6	5:L3:3830:A2M:O4'	2.44	0.51
46:NX:543:GLU:OE1	46:NX:543:GLU:N	2.41	0.51
5:L3:307:A:N3	5:L3:310:G:O2'	2.44	0.51
13:LB:53:MET:SD	13:LB:143:ARG:NH2	2.84	0.50
60:SR:272:PHE:CE1	60:SR:284:LEU:HD21	2.46	0.50
5:L3:3715:PSU:H2'	5:L3:3716:C:O4'	2.10	0.50
5:L3:3734:PSU:H2'	5:L3:3735:G:O4'	2.11	0.50
5:L3:2318:G:N2	5:L3:2321:G:OP2	2.31	0.50
5:L3:4352:U:O2'	5:L3:4353:PSU:H5''	2.11	0.50
6:L4:11:A:O2'	6:L4:13:A:OP2	2.20	0.50
41:NL:190:ARG:NH2	58:SM:117:ASP:OD1	2.45	0.50
44:NU:267:ILE:HD12	45:NW:210:LEU:HD11	1.93	0.50
5:L3:4351:U:OP1	8:L6:190:ARG:NH2	2.44	0.50
46:NY:222:LEU:O	46:NY:225:VAL:HG12	2.11	0.50
46:NY:226:ASP:OD2	46:NY:314:ARG:NH2	2.44	0.50
5:L3:4872:G:OP2	10:L8:94:LYS:NZ	2.35	0.50
44:NU:500:GLU:OE2	44:NU:545:SER:OG	2.23	0.50
45:NV:285:LEU:HD11	45:NV:293:VAL:CG1	2.42	0.50
45:NW:387:MET:HE3	45:NW:391:VAL:HG23	1.94	0.50
50:SC:91:THR:OG1	50:SC:106:VAL:HG22	2.11	0.50
5:L3:4042:OMG:H2'	5:L3:4043:G:C8	2.47	0.50
5:L3:4613:C:H4'	40:NK:13:MET:HE2	1.93	0.50
35:LZ:9:ILE:HG23	35:LZ:51:LEU:HD21	1.94	0.50
44:NU:468:LEU:HG	44:NU:482:LEU:HD21	1.93	0.50
45:NW:192:SER:OG	45:NW:218:ILE:O	2.30	0.50
2:BB:171:HIS:CE1	2:BB:174:MET:HE3	2.47	0.49
44:NU:638:ARG:HE	44:NU:642:MET:HE3	1.77	0.49
58:SM:265:TYR:HB3	58:SM:362:ILE:HD11	1.94	0.49
5:L3:4536:OMC:H2'	5:L3:4537:C:C6	2.47	0.49
15:LD:95:TRP:CH2	15:LD:99:MET:HE3	2.47	0.49
45:NV:309:LEU:HD12	45:NV:313:VAL:HG22	1.94	0.49
5:L3:3838:U:OP2	42:NP:23:ARG:NH2	2.44	0.49
5:L3:1645:C:OP1	48:SA:80:ARG:NH2	2.44	0.49
5:L3:4219:A:O3'	5:L3:4220:6MZ:H4'	2.12	0.49
5:L3:5007:A:N7	5:L3:5042:A:O2'	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:NU:708:VAL:HG13	44:NU:717:LEU:HD21	1.94	0.49
44:NU:367:TRP:CD1	44:NU:383:LEU:HD13	2.46	0.49
57:SK:115:ALA:HB2	57:SK:135:VAL:HG11	1.93	0.49
5:L3:3759:A:N6	5:L3:4220:6MZ:H9	2.27	0.49
45:NW:379:LEU:O	45:NW:383:LEU:HD12	2.12	0.49
57:SK:49:VAL:HG12	57:SK:50:HIS:O	2.12	0.49
46:NY:279:TYR:CE2	46:NY:351:VAL:HG21	2.47	0.49
53:SF:147:ARG:HG2	53:SF:157:VAL:HG22	1.95	0.49
5:L3:3723:A:H2'	5:L3:3724:A2M:H8	1.95	0.49
6:L4:12:U:OP2	6:L4:67:C:O2'	2.31	0.49
18:LG:134:SER:O	57:SK:106:ASN:ND2	2.46	0.49
44:NU:367:TRP:CH2	44:NU:440:ILE:HG23	2.48	0.49
44:NU:509:LEU:HD22	44:NU:523:LEU:HD11	1.95	0.49
5:L3:277:G:OP2	31:LU:29:ARG:NH2	2.42	0.49
5:L3:2424:OMG:HM23	5:L3:2424:OMG:H1'	1.57	0.49
5:L3:3791:C:O2'	5:L3:3792:OMG:H5'	2.12	0.49
45:NW:12:ASP:OD1	45:NW:12:ASP:N	2.45	0.48
17:LF:67:LYS:O	17:LF:68:SER:OG	2.28	0.48
20:LI:66:GLN:OE1	20:LI:66:GLN:N	2.44	0.48
60:SR:102:ALA:O	60:SR:106:VAL:HG23	2.12	0.48
5:L3:4536:OMC:H2'	5:L3:4537:C:H6	1.77	0.48
56:SI:193:CYS:SG	56:SI:194:LEU:N	2.85	0.48
15:LD:7:GLN:OE1	15:LD:7:GLN:N	2.46	0.48
4:L1:75:OMG:HM21	60:SR:585:MET:CE	2.43	0.48
5:L3:1952:G:H4'	14:LC:93:MET:HE3	1.95	0.48
5:L3:2414:G:O2'	5:L3:2415:OMU:H5''	2.14	0.48
44:NU:265:ILE:HD12	44:NU:281:VAL:HG12	1.94	0.48
44:NU:355:VAL:O	44:NU:359:VAL:HG23	2.12	0.48
51:SD:171:ASP:OD1	51:SD:172:ASN:N	2.47	0.48
44:NU:711:THR:HG22	44:NU:713:LEU:H	1.79	0.48
5:L3:1562:G:N2	5:L3:1565:A:OP2	2.27	0.48
5:L3:2742:G:OP1	53:SF:24:LYS:NZ	2.47	0.48
8:L6:129:ARG:NH1	29:LS:116:LEU:O	2.46	0.48
5:L3:4042:OMG:H2'	5:L3:4043:G:H8	1.78	0.48
7:L5:160:GLU:N	7:L5:160:GLU:OE1	2.47	0.48
5:L3:5024:C:OP2	5:L3:5025:C:N4	2.46	0.48
43:NT:575:SER:OG	43:NT:576:GLN:OE1	2.31	0.48
44:NU:363:ILE:HG22	44:NU:367:TRP:CZ3	2.47	0.48
44:NU:580:ALA:HB3	44:NU:588:LEU:HD22	1.96	0.48
45:NW:96:LEU:HB3	45:NW:127:LEU:HD21	1.96	0.48
5:L3:1280:C:O2'	48:SA:321:ASN:OD1	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L3:1996:C:O2	59:SQ:54:LYS:NZ	2.47	0.48
16:LE:160:ALA:O	47:NZ:287:LEU:HD22	2.13	0.48
50:SC:161:ARG:O	50:SC:182:ASN:ND2	2.46	0.48
5:L3:3818:OMU:O5'	5:L3:3818:OMU:H6	2.14	0.47
33:LX:8:VAL:O	33:LX:11:VAL:HG22	2.13	0.47
46:NX:635:VAL:HG11	46:NY:639:GLN:HG2	1.96	0.47
46:NY:172:ILE:HD13	46:NY:176:HIS:HD2	1.77	0.47
52:SE:45:ILE:HD12	52:SE:45:ILE:H	1.79	0.47
21:LJ:29:ILE:O	21:LJ:31:ASP:N	2.46	0.47
5:L3:1950:U:O2'	14:LC:116:ARG:NH1	2.47	0.47
40:NK:92:GLN:OE1	40:NK:92:GLN:N	2.47	0.47
5:L3:3717:A:H2'	5:L3:3718:A2M:H8	1.96	0.47
39:NJ:422:TRP:HZ3	39:NJ:443:VAL:HG21	1.75	0.47
54:SG:113:GLU:OE1	54:SG:115:ARG:NH2	2.48	0.47
41:NL:188:VAL:O	58:SM:163:ARG:NH1	2.47	0.47
44:NU:608:VAL:HG23	44:NU:609:VAL:HG13	1.95	0.47
45:NV:3:ALA:HB2	46:NX:554:PRO:HB3	1.97	0.47
45:NV:19:SER:N	45:NV:34:TYR:O	2.46	0.47
45:NW:387:MET:HE2	46:NX:64:PRO:HA	1.97	0.47
5:L3:238:C:OP2	20:LI:45:ARG:NH2	2.48	0.47
5:L3:709:C:OP1	30:LT:89:ARG:NH2	2.47	0.47
5:L3:934:C:HO2'	5:L3:935:A:P	2.37	0.47
5:L3:1946:G:O2'	38:NF:36:SER:OG	2.29	0.47
5:L3:2843:U:O2'	5:L3:4632:U:OP1	2.32	0.47
5:L3:3770:PSU:H2'	5:L3:3771:C:H6	1.75	0.47
5:L3:4139:G:H21	5:L3:4140:C:N4	2.13	0.47
5:L3:4341:C:H42	5:L3:4371:G:H1	1.63	0.47
60:SR:488:ARG:NH1	61:SV:126:GLU:OE1	2.47	0.47
37:NC:404:GLU:OE1	37:NC:404:GLU:N	2.46	0.47
46:NX:322:LEU:HD23	46:NX:379:LEU:HD21	1.95	0.47
46:NY:612:ASP:OD1	46:NY:613:SER:N	2.47	0.47
48:SA:211:TYR:OH	48:SA:218:ILE:HD11	2.15	0.47
49:SB:152:ARG:HG3	49:SB:154:THR:HG23	1.96	0.47
60:SR:444:PRO:HD3	61:SV:79:ILE:HD11	1.97	0.47
1:BA:135:THR:HG22	5:L3:1974:U:O4	2.15	0.47
44:NU:367:TRP:HE1	44:NU:383:LEU:HD13	1.79	0.47
45:NV:327:SER:OG	45:NV:329:ASP:OD1	2.32	0.47
5:L3:1862:PSU:H2'	5:L3:1863:U:C6	2.50	0.47
5:L3:1961:G:N7	59:SQ:71:LYS:NZ	2.63	0.47
5:L3:2351:OMC:HM22	48:SA:95:MET:HG3	1.97	0.47
14:LC:93:MET:HE2	14:LC:95:ARG:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:NC:413:ASP:OD1	37:NC:414:SER:N	2.47	0.47
44:NU:470:ASP:OD1	44:NU:470:ASP:N	2.46	0.47
5:L3:2562:G:N2	5:L3:2565:A:OP2	2.47	0.47
5:L3:4392:OMG:HM23	5:L3:4392:OMG:H1'	1.50	0.47
5:L3:4590:A2M:HM'3	5:L3:4590:A2M:H1'	1.67	0.47
5:L3:1316:OMG:H1'	5:L3:1316:OMG:HM23	1.49	0.46
41:NL:48:TRP:HA	41:NL:51:LEU:HD13	1.97	0.46
44:NU:106:VAL:HG11	44:NU:118:ALA:HB2	1.97	0.46
2:BB:41:TYR:CD2	2:BB:159:MET:HE1	2.50	0.46
5:L3:2841:G:OP1	42:NP:10:HIS:NE2	2.46	0.46
59:SQ:172:ASP:N	59:SQ:172:ASP:OD1	2.48	0.46
60:SR:244:LEU:O	60:SR:282:LYS:NZ	2.47	0.46
5:L3:1522:OMG:HM22	5:L3:1523:A:H5''	1.98	0.46
5:L3:2815:A2M:H2'	5:L3:2816:G:C8	2.50	0.46
5:L3:3963:A:H1'	46:NY:174:MET:HE3	1.97	0.46
5:L3:4593:C:OP2	40:NK:2:ALA:N	2.48	0.46
48:SA:124:ILE:HG21	48:SA:264:TYR:OH	2.15	0.46
58:SM:150:THR:OG1	58:SM:153:CYS:SG	2.59	0.46
58:SM:274:GLU:HB3	58:SM:362:ILE:HD12	1.97	0.46
2:BB:54:ARG:NE	2:BB:150:GLU:OE1	2.46	0.46
5:L3:1646:A:O2'	32:LW:49:TRP:O	2.27	0.46
5:L3:3695:PSU:O2'	37:NC:286:THR:HG23	2.15	0.46
22:LK:76:ASP:OD1	22:LK:77:LYS:N	2.48	0.46
24:LN:357:ARG:NE	60:SR:407:ASP:OD1	2.48	0.46
44:NU:108:THR:O	44:NU:108:THR:HG22	2.15	0.46
44:NU:509:LEU:CD2	44:NU:523:LEU:HD11	2.45	0.46
1:BA:95:GLN:HB3	1:BA:98:ILE:HD11	1.97	0.46
2:BB:197:ASN:O	43:NT:553:GLN:NE2	2.49	0.46
5:L3:3718:A2M:HM'3	5:L3:3718:A2M:H1'	1.68	0.46
5:L3:4622:A:O2'	5:L3:4623:OMG:H5'	2.15	0.46
44:NU:580:ALA:HB3	44:NU:588:LEU:CD2	2.45	0.46
53:SF:101:VAL:C	53:SF:102:LEU:HD12	2.41	0.46
57:SK:95:ARG:HH11	57:SK:128:ILE:HD12	1.80	0.46
5:L3:947:C:OP1	48:SA:336:ARG:NH1	2.49	0.46
5:L3:3744:OMG:HM23	5:L3:3744:OMG:H1'	1.57	0.46
36:NB:73:GLU:OE2	36:NB:77:GLN:NE2	2.49	0.46
38:NF:150:VAL:HG11	38:NF:154:CYS:SG	2.56	0.46
45:NW:194:LEU:CD2	45:NW:219:MET:HE1	2.46	0.46
6:L4:7:G:OP1	49:SB:33:ARG:NH1	2.49	0.46
45:NW:195:ASP:O	45:NW:197:THR:N	2.47	0.46
5:L3:3720:G:H22	5:L3:3733:A:H2	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L3:4589:A:N3	5:L3:4590:A2M:HM'3	2.31	0.46
42:NP:27:ASP:OD2	61:SV:23:ARG:NH1	2.48	0.46
44:NU:811:ILE:HD13	44:NU:822:ARG:HD3	1.98	0.46
45:NV:26:HIS:O	45:NV:305:ARG:NH2	2.49	0.46
49:SB:232:THR:OG1	49:SB:234:ASP:OD1	2.31	0.46
53:SF:129:ALA:O	53:SF:169:VAL:HG11	2.15	0.46
58:SM:170:HIS:HB3	58:SM:283:LEU:HD11	1.98	0.46
5:L3:1238:A:OP2	50:SC:60:SER:OG	2.15	0.46
5:L3:1854:G:HO2'	5:L3:1855:G:P	2.38	0.46
5:L3:2340:C:H4'	48:SA:42:THR:HG23	1.97	0.46
5:L3:3841:OMC:HM23	5:L3:3841:OMC:H1'	1.48	0.46
46:NY:394:PHE:O	46:NY:398:ILE:HD12	2.16	0.46
50:SC:50:LEU:HD12	50:SC:51:VAL:HG22	1.97	0.46
58:SM:140:MET:HE1	58:SM:220:MET:HE3	1.97	0.46
5:L3:1354:A:OP1	13:LB:108:ARG:NH2	2.49	0.45
5:L3:1625:OMG:H4'	5:L3:1626:G:O5'	2.16	0.45
5:L3:2515:G:OP1	28:LR:37:LYS:NZ	2.43	0.45
8:L6:164:GLU:N	8:L6:164:GLU:OE1	2.49	0.45
5:L3:4156:G:P	5:L3:4157:A:HO2'	2.28	0.45
37:NC:155:LEU:CD1	60:SR:238:MET:HE2	2.46	0.45
44:NU:705:VAL:HG21	44:NU:707:HIS:CE1	2.50	0.45
45:NW:107:GLU:OE1	46:NX:393:ARG:NH1	2.48	0.45
45:NW:290:ASP:O	45:NW:292:THR:N	2.48	0.45
49:SB:133:GLU:N	49:SB:133:GLU:OE1	2.49	0.45
5:L3:1892:A:OP2	5:L3:3875:G:N1	2.41	0.45
5:L3:3939:G:O2'	5:L3:4076:G:N2	2.44	0.45
45:NW:178:LEU:CD2	45:NW:191:THR:HG22	2.47	0.45
56:SI:182:ILE:HD11	56:SI:194:LEU:HD13	1.99	0.45
2:BB:188:ASN:ND2	43:NT:546:SER:O	2.50	0.45
5:L3:287:U:O2'	11:L9:91:GLN:OE1	2.33	0.45
37:NC:46:GLN:OE1	37:NC:61:GLN:NE2	2.48	0.45
49:SB:93:THR:HG22	49:SB:93:THR:O	2.17	0.45
5:L3:1522:OMG:H4'	48:SA:75:ARG:O	2.16	0.45
5:L3:2632:PSU:H2'	5:L3:2633:U:C6	2.51	0.45
5:L3:4728:U:OP1	24:LN:132:LYS:NZ	2.48	0.45
5:L3:4761:G:OP1	9:L7:37:ARG:NH2	2.43	0.45
35:LZ:9:ILE:HD12	35:LZ:51:LEU:HD21	1.99	0.45
58:SM:120:ILE:HD11	58:SM:229:THR:HB	1.99	0.45
5:L3:4566:U:O2'	24:LN:234:ARG:NH1	2.49	0.45
44:NU:711:THR:HG21	44:NU:802:TYR:HE2	1.82	0.45
49:SB:51:MET:HE2	49:SB:53:VAL:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L3:1982:G:O6	5:L3:1983:A:N6	2.50	0.45
5:L3:4042:OMG:HM23	5:L3:4042:OMG:H1'	1.78	0.45
5:L3:4546:A:N7	53:SF:215:ASN:ND2	2.64	0.45
58:SM:265:TYR:OH	58:SM:358:LYS:O	2.32	0.45
5:L3:1340:OMC:HM23	5:L3:1340:OMC:H1'	1.53	0.45
5:L3:3709:U:OP1	43:NT:21:LYS:NZ	2.25	0.45
24:LN:137:TRP:O	24:LN:143:LYS:NZ	2.33	0.45
55:SH:81:ARG:HG3	55:SH:82:THR:HG23	1.99	0.45
4:L1:46:G:O2'	4:L1:61:A:N1	2.48	0.45
5:L3:3619:G:H22	5:L3:3624:A:H1'	1.81	0.45
48:SA:209:ILE:HB	48:SA:229:LEU:HD13	1.99	0.45
59:SQ:47:ASN:ND2	59:SQ:129:ASN:OD1	2.49	0.45
4:L1:71:A:O2'	4:L1:83:C:N4	2.50	0.45
5:L3:1501:C:O2'	13:LB:68:ARG:NH1	2.50	0.45
5:L3:2364:OMG:HM23	5:L3:2364:OMG:H1'	1.47	0.45
17:LF:118:ASN:O	60:SR:517:ARG:N	2.47	0.45
21:LJ:87:VAL:HG11	21:LJ:89:ILE:HD12	1.99	0.45
45:NW:177:ASP:OD1	45:NW:178:LEU:N	2.50	0.45
3:BD:717:LEU:HD22	44:NU:748:GLN:NE2	2.32	0.44
5:L3:1590:C:O2'	42:NP:5:ARG:NH2	2.51	0.44
37:NC:262:THR:HG23	44:NU:44:LEU:CD2	2.47	0.44
45:NW:130:THR:HG21	45:NW:184:GLY:HA2	1.98	0.44
55:SH:123:PRO:O	55:SH:126:VAL:HG12	2.17	0.44
6:L4:48:G:OP1	49:SB:226:TYR:OH	2.33	0.44
50:SC:95:PRO:HA	50:SC:104:THR:HG22	1.99	0.44
58:SM:282:SER:OG	58:SM:348:ARG:NH2	2.48	0.44
5:L3:2088:A:OP2	13:LB:38:ARG:NH1	2.50	0.44
5:L3:4306:OMU:HM22	5:L3:4306:OMU:C2	2.47	0.44
5:L3:4716:C:OP1	24:LN:276:HIS:ND1	2.50	0.44
37:NC:532:ASN:OD1	44:NU:642:MET:HE1	2.18	0.44
45:NW:95:VAL:C	45:NW:96:LEU:HD12	2.42	0.44
58:SM:271:SER:OG	58:SM:275:LYS:NZ	2.50	0.44
5:L3:1326:A2M:HM'3	5:L3:1326:A2M:H1'	1.66	0.44
5:L3:2368:A:N6	5:L3:2827:G:O2'	2.50	0.44
5:L3:2588:C:OP1	5:L3:2768:C:O2'	2.24	0.44
58:SM:358:LYS:HD2	58:SM:364:ALA:HB3	2.00	0.44
59:SQ:45:VAL:HG23	59:SQ:45:VAL:O	2.17	0.44
5:L3:1322:1MA:H5'	5:L3:1880:G:O2'	2.17	0.44
5:L3:2724:G:O2'	5:L3:2726:G:OP2	2.27	0.44
5:L3:3925:OMU:HM23	5:L3:3925:OMU:H1'	1.49	0.44
10:L8:29:ASP:OD1	10:L8:30:VAL:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:LG:29:ALA:HB3	18:LG:82:ILE:HD11	1.98	0.44
24:LN:67:VAL:O	24:LN:67:VAL:HG22	2.17	0.44
45:NV:74:GLN:OE1	45:NV:74:GLN:N	2.43	0.44
46:NY:398:ILE:HD12	46:NY:398:ILE:H	1.82	0.44
52:SE:87:LEU:N	52:SE:183:ILE:O	2.46	0.44
5:L3:2639:U:O2'	5:L3:2694:G:O6	2.23	0.44
5:L3:3808:OMC:HM23	5:L3:3808:OMC:H1'	1.49	0.44
17:LF:47:ILE:HD12	17:LF:63:ILE:HD11	1.99	0.44
43:NT:438:LEU:O	43:NT:441:THR:OG1	2.32	0.44
46:NX:85:LEU:H	46:NX:85:LEU:HD23	1.83	0.44
4:L1:75:OMG:H1'	4:L1:75:OMG:HM23	1.45	0.44
5:L3:1524:A2M:H2	5:L3:3915:U:O2	2.18	0.44
5:L3:3641:U:OP2	5:L3:3646:A:N6	2.41	0.44
5:L3:3654:G:O2'	5:L3:3693:U:OP1	2.25	0.44
5:L3:3822:PSU:H1'	5:L3:3823:G:P	2.57	0.44
5:L3:4217:G:O4'	5:L3:4222:G:N2	2.51	0.44
45:NV:319:LEU:HD23	45:NV:320:LEU:O	2.18	0.44
45:NV:375:ARG:NH2	46:NX:514:ASP:OD2	2.51	0.44
51:SD:41:MET:SD	51:SD:41:MET:N	2.91	0.44
5:L3:3808:OMC:H2'	5:L3:3809:G:C8	2.53	0.44
26:LP:42:ALA:HB3	26:LP:43:PRO:HD3	1.99	0.44
43:NT:64:ALA:O	43:NT:110:LYS:NZ	2.49	0.44
52:SE:136:LEU:HD22	52:SE:202:VAL:CG1	2.48	0.44
5:L3:3851:PSU:H3'	5:L3:3852:A:H8	1.83	0.44
33:LX:69:TRP:NE1	53:SF:173:GLY:O	2.50	0.44
19:LH:143:ASP:OD1	19:LH:144:TYR:N	2.51	0.43
26:LP:65:ASP:OD1	26:LP:66:THR:N	2.50	0.43
30:LT:40:GLU:OE2	30:LT:109:ARG:NH2	2.52	0.43
45:NV:195:ASP:O	45:NV:197:THR:N	2.50	0.43
5:L3:4401:G:OP1	36:NB:20:LYS:NZ	2.51	0.43
24:LN:61:ASP:OD2	60:SR:410:ILE:HG23	2.18	0.43
45:NW:130:THR:HG22	45:NW:131:GLY:N	2.33	0.43
4:L1:62:A:OP1	29:LS:52:LYS:NZ	2.48	0.43
5:L3:1927:U:OP1	5:L3:1949:U:O2'	2.31	0.43
5:L3:2380:G:N2	5:L3:2425:U:OP1	2.44	0.43
5:L3:4536:OMC:HM22	5:L3:4537:C:O4'	2.18	0.43
5:L3:4745:G:H22	5:L3:4955:A:H2	1.64	0.43
47:NZ:290:GLU:OE1	47:NZ:293:ARG:NH2	2.52	0.43
49:SB:33:ARG:O	49:SB:37:VAL:HG22	2.17	0.43
57:SK:103:ALA:O	57:SK:107:VAL:HG22	2.18	0.43
5:L3:1326:A2M:H2'	5:L3:1327:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L3:2052:G:O2'	5:L3:2057:A:N1	2.48	0.43
5:L3:3712:A:HO2'	5:L3:3713:U:P	2.41	0.43
8:L6:63:THR:HG22	8:L6:64:VAL:N	2.34	0.43
8:L6:208:GLU:OE1	8:L6:208:GLU:N	2.52	0.43
16:LE:115:LYS:NZ	16:LE:126:VAL:HG22	2.34	0.43
44:NU:151:HIS:O	44:NU:157:GLN:NE2	2.51	0.43
54:SG:12:ILE:HG12	54:SG:18:ILE:HD12	2.00	0.43
56:SI:135:GLN:OE1	56:SI:135:GLN:N	2.48	0.43
5:L3:398:A2M:H1'	5:L3:398:A2M:HM'3	1.73	0.43
5:L3:496:G:O2'	5:L3:497:G:OP1	2.29	0.43
5:L3:4216:G:O3'	5:L3:4217:G:H4'	2.19	0.43
5:L3:5009:G:O2'	5:L3:5010:PSU:H5''	2.19	0.43
5:L3:3867:A2M:HM'3	5:L3:3867:A2M:H1'	1.50	0.43
7:L5:136:ARG:NH1	7:L5:156:ARG:O	2.52	0.43
44:NU:705:VAL:HG21	44:NU:707:HIS:NE2	2.33	0.43
60:SR:574:PRO:HG2	60:SR:577:VAL:HG22	2.01	0.43
5:L3:1760:OMG:H1'	5:L3:1760:OMG:HM23	1.55	0.43
5:L3:2351:OMC:H1'	5:L3:2351:OMC:HM23	1.53	0.43
5:L3:2878:G:OP2	5:L3:2879:A:O2'	2.33	0.43
5:L3:4678:G:N7	40:NK:11:ARG:NH2	2.67	0.43
14:LC:173:ASN:OD1	14:LC:174:THR:N	2.52	0.43
33:LX:26:VAL:HG22	53:SF:178:PRO:HD2	2.01	0.43
42:NP:63:CYS:O	42:NP:67:ALA:N	2.49	0.43
44:NU:720:LEU:HD21	44:NU:818:HIS:NE2	2.34	0.43
60:SR:456:GLU:OE1	61:SV:67:ASN:ND2	2.44	0.43
61:SV:110:ASN:OD1	61:SV:111:ARG:N	2.52	0.43
5:L3:320:C:OP1	31:LU:84:LYS:NZ	2.42	0.43
5:L3:1773:OMU:HM22	5:L3:1773:OMU:H1'	1.66	0.43
5:L3:4455:G:O2'	5:L3:4456:OMC:H5''	2.19	0.43
37:NC:111:MET:SD	37:NC:304:LEU:HD22	2.59	0.43
45:NW:26:HIS:O	45:NW:305:ARG:NH2	2.51	0.43
53:SF:132:ASN:O	53:SF:169:VAL:HG12	2.18	0.43
5:L3:1754:U:H4'	5:L3:1755:C:OP1	2.18	0.43
5:L3:4456:OMC:HM23	5:L3:4456:OMC:H1'	1.58	0.43
5:L3:4477:A:OP1	38:NF:6:TYR:OH	2.36	0.43
5:L3:4479:A:OP1	5:L3:4610:A:O2'	2.30	0.43
45:NW:322:PRO:HD2	45:NW:325:MET:HE3	2.00	0.43
46:NX:177:LEU:HD23	46:NX:209:ALA:HB3	2.01	0.43
5:L3:2716:C:O3'	17:LF:107:LYS:NZ	2.46	0.43
5:L3:2872:C:HO2'	5:L3:2873:U:H5'	1.82	0.43
5:L3:3718:A2M:H2'	5:L3:3719:A:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:LA:40:HIS:NE2	12:LA:110:ASP:O	2.45	0.42
41:NL:257:LEU:HD23	41:NL:418:VAL:HG23	2.00	0.42
53:SF:131:GLY:H	53:SF:169:VAL:HG13	1.84	0.42
5:L3:3663:A:N6	5:L3:4168:G:O2'	2.52	0.42
15:LD:126:LYS:O	15:LD:131:VAL:HG22	2.19	0.42
39:NJ:264:SER:OG	39:NJ:265:GLN:N	2.52	0.42
46:NX:622:GLU:HG2	46:NY:534:LEU:HD23	2.00	0.42
5:L3:346:G:OP2	20:LI:13:LYS:NZ	2.45	0.42
5:L3:3743:G:O2'	43:NT:61:MET:HE2	2.19	0.42
8:L6:79:GLU:OE2	31:LU:20:ASN:ND2	2.46	0.42
52:SE:58:PRO:HD2	52:SE:61:ILE:HD12	2.00	0.42
57:SK:160:LEU:HG	57:SK:193:ILE:HD13	2.01	0.42
5:L3:1534:A2M:HM'3	5:L3:1637:A:C4	2.53	0.42
5:L3:2837:OMU:HM23	5:L3:2837:OMU:H1'	1.70	0.42
12:LA:125:MET:HE3	12:LA:143:PRO:HG3	2.02	0.42
17:LF:33:ILE:HG22	60:SR:531:MET:HE1	2.01	0.42
23:LL:71:ARG:NE	48:SA:149:GLU:OE2	2.51	0.42
52:SE:108:GLN:OE1	52:SE:108:GLN:N	2.50	0.42
2:BB:80:VAL:O	2:BB:80:VAL:HG12	2.18	0.42
5:L3:219:G:O6	48:SA:181:LYS:NZ	2.35	0.42
45:NW:46:LEU:HD21	45:NW:49:GLY:HA2	2.00	0.42
58:SM:253:GLN:NE2	58:SM:272:CYS:SG	2.91	0.42
5:L3:2691:U:C2	5:L3:2692:U:C5	3.07	0.42
22:LK:72:THR:HG22	22:LK:110:LYS:HB3	2.01	0.42
26:LP:20:VAL:O	26:LP:20:VAL:HG23	2.19	0.42
39:NJ:292:THR:HG23	39:NJ:378:VAL:HG12	2.02	0.42
5:L3:2422:OMC:H1'	5:L3:2422:OMC:HM23	1.49	0.42
6:L4:39:C:N3	7:L5:73:THR:HG22	2.35	0.42
37:NC:43:MET:HE3	38:NF:146:TRP:CE3	2.55	0.42
57:SK:121:LEU:O	57:SK:139:ARG:NH1	2.43	0.42
2:BB:11:TYR:CE1	2:BB:180:VAL:HG21	2.55	0.42
5:L3:2362:U:H2'	5:L3:2363:A2M:H8	2.02	0.42
5:L3:4648:A:OP1	15:LD:62:ARG:NH2	2.50	0.42
60:SR:161:LEU:HD12	60:SR:162:PRO:HD2	2.01	0.42
5:L3:2378:G:N2	5:L3:2381:A:OP2	2.52	0.42
5:L3:2804:OMC:HM22	5:L3:2805:C:O4'	2.19	0.42
5:L3:4277:G:O2'	5:L3:4282:A:N1	2.44	0.42
5:L3:4407:G:H2'	5:L3:4408:G:C8	2.55	0.42
14:LC:44:PHE:O	14:LC:48:VAL:HG12	2.20	0.42
33:LX:85:ARG:NH1	44:NU:334:GLU:OE2	2.46	0.42
44:NU:145:LEU:HD21	44:NU:164:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SC:203:ILE:O	50:SC:203:ILE:HG22	2.19	0.42
5:L3:1950:U:OP2	54:SG:64:ARG:NH2	2.43	0.42
5:L3:2519:U:C2	5:L3:2520:C:C5	3.07	0.42
5:L3:4440:G:C2	60:SR:96:LEU:HD13	2.55	0.42
48:SA:143:ARG:NH1	48:SA:145:GLU:OE2	2.53	0.42
56:SI:98:PHE:HB2	56:SI:152:PRO:HG3	2.01	0.42
5:L3:5022:U:C2'	5:L3:5025:C:H42	2.33	0.41
46:NY:279:TYR:CD2	46:NY:351:VAL:HG21	2.55	0.41
1:BA:146:ARG:NH1	1:BA:154:ASP:OD2	2.53	0.41
5:L3:2824:OMC:HM23	5:L3:2824:OMC:H1'	1.80	0.41
5:L3:3661:G:N7	53:SF:152:SER:OG	2.43	0.41
46:NY:603:GLN:HE22	46:NY:607:LEU:HD11	1.85	0.41
52:SE:159:HIS:ND1	52:SE:185:LYS:HA	2.35	0.41
4:L1:30:U:OP1	8:L6:34:ARG:NH2	2.54	0.41
5:L3:1601:A:OP1	32:LW:5:THR:OG1	2.29	0.41
5:L3:1677:PSU:H5''	5:L3:1678:C:P	2.60	0.41
5:L3:1831:G:H3'	5:L3:1832:C:H5''	2.02	0.41
44:NU:442:VAL:HG23	44:NU:460:ILE:HD13	2.02	0.41
57:SK:6:SER:HA	57:SK:13:ILE:HD11	2.03	0.41
57:SK:177:LEU:HD12	57:SK:181:LEU:HD11	2.02	0.41
1:BA:120:SER:CB	1:BA:128:THR:HG22	2.50	0.41
2:BB:99:LEU:HD23	2:BB:102:LYS:NZ	2.35	0.41
5:L3:4637:OMG:HM23	5:L3:4637:OMG:H1'	1.41	0.41
24:LN:46:PHE:HE2	24:LN:210:VAL:HG22	1.86	0.41
40:NK:82:ASN:O	40:NK:86:LEU:N	2.45	0.41
46:NY:322:LEU:HD22	46:NY:379:LEU:HD22	2.02	0.41
50:SC:67:ALA:O	50:SC:71:ARG:NH1	2.53	0.41
60:SR:358:ASN:OD1	60:SR:359:ARG:N	2.52	0.41
5:L3:3658:C:OP1	53:SF:242:ARG:NH1	2.54	0.41
52:SE:103:ARG:NH2	52:SE:192:ARG:O	2.53	0.41
13:LB:28:LEU:HG	48:SA:284:MET:HE3	2.03	0.41
53:SF:2:GLY:HA2	53:SF:207:VAL:HG23	2.02	0.41
57:SK:233:ALA:O	57:SK:237:ARG:HG3	2.20	0.41
5:L3:2667:C:OP1	15:LD:100:ARG:NE	2.42	0.41
5:L3:3705:G:H21	53:SF:224:THR:HG21	1.85	0.41
37:NC:397:VAL:HG13	37:NC:451:TRP:CE3	2.56	0.41
47:NZ:258:LEU:HD23	54:SG:67:LEU:HD12	2.02	0.41
58:SM:189:TYR:CZ	58:SM:202:ILE:HD12	2.56	0.41
5:L3:5000:G:O2'	5:L3:5001:PSU:H5''	2.21	0.41
24:LN:370:THR:N	24:LN:380:GLN:OE1	2.52	0.41
60:SR:354:ASN:OD1	60:SR:355:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L1:68:G:O2'	4:L1:69:PSU:H5''	2.20	0.41
5:L3:1773:OMU:H2'	5:L3:1774:C:C6	2.56	0.41
5:L3:1854:G:O2'	5:L3:1855:G:P	2.78	0.41
5:L3:2363:A2M:H1'	5:L3:2363:A2M:HM'3	1.66	0.41
5:L3:3279:C:OP1	41:NL:359:ARG:NH2	2.54	0.41
33:LX:22:LEU:O	33:LX:26:VAL:HG23	2.21	0.41
45:NW:178:LEU:HD23	45:NW:191:THR:HG22	2.01	0.41
46:NX:408:SER:HG	46:NX:409:TRP:CD1	2.39	0.41
46:NY:172:ILE:HD13	46:NY:176:HIS:CD2	2.55	0.41
5:L3:4227:OMU:O5'	5:L3:4227:OMU:H6	2.21	0.41
46:NY:233:GLN:HG2	46:NY:320:ARG:NH2	2.36	0.41
2:BB:176:ASP:O	2:BB:180:VAL:HG23	2.21	0.40
4:L1:58:G:O6	32:LW:63:ARG:NH1	2.54	0.40
5:L3:1210:C:H41	51:SD:66:ARG:CZ	2.34	0.40
39:NJ:281:ARG:NE	39:NJ:358:PRO:O	2.53	0.40
44:NU:168:LEU:HD23	44:NU:175:ILE:HG21	2.02	0.40
44:NU:367:TRP:CZ3	44:NU:440:ILE:HG23	2.56	0.40
48:SA:295:SER:OG	48:SA:297:GLU:OE1	2.37	0.40
4:L1:28:C:O2'	5:L3:1371:A:N1	2.51	0.40
5:L3:1683:PSU:H2'	5:L3:1684:A:C8	2.53	0.40
5:L3:3924:C:H2'	5:L3:3925:OMU:H6	2.04	0.40
37:NC:197:ILE:HG13	37:NC:382:VAL:HG13	2.03	0.40
5:L3:433:A:C2	5:L3:3867:A2M:H4'	2.55	0.40
5:L3:1071:C:O2	50:SC:70:LYS:NZ	2.37	0.40
5:L3:1426:G:N1	5:L3:1458:C:OP2	2.43	0.40
53:SF:29:LEU:O	53:SF:123:ARG:NE	2.52	0.40
8:L6:178:ALA:N	22:LK:134:GLU:OE2	2.49	0.40
15:LD:23:TRP:CZ3	15:LD:51:ILE:HD12	2.56	0.40
24:LN:10:ARG:NH2	24:LN:14:LEU:HD21	2.35	0.40
44:NU:607:VAL:O	44:NU:615:GLN:NE2	2.54	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%)	158 (100%)	0	0	100	100
2	BB	214/217 (99%)	209 (98%)	5 (2%)	0	100	100
3	BD	17/734 (2%)	16 (94%)	1 (6%)	0	100	100
7	L5	166/178 (93%)	165 (99%)	1 (1%)	0	100	100
8	L6	201/211 (95%)	197 (98%)	4 (2%)	0	100	100
9	L7	199/203 (98%)	198 (100%)	1 (0%)	0	100	100
10	L8	133/215 (62%)	132 (99%)	1 (1%)	0	100	100
11	L9	190/204 (93%)	188 (99%)	2 (1%)	0	100	100
12	LA	152/184 (83%)	149 (98%)	3 (2%)	0	100	100
13	LB	149/188 (79%)	149 (100%)	0	0	100	100
14	LC	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
15	LD	152/196 (78%)	152 (100%)	0	0	100	100
16	LE	134/160 (84%)	131 (98%)	3 (2%)	0	100	100
17	LF	101/128 (79%)	100 (99%)	1 (1%)	0	100	100
18	LG	137/140 (98%)	135 (98%)	2 (2%)	0	100	100
19	LH	141/156 (90%)	140 (99%)	1 (1%)	0	100	100
20	LI	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
21	LJ	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
22	LK	113/148 (76%)	112 (99%)	1 (1%)	0	100	100
23	LL	123/137 (90%)	122 (99%)	1 (1%)	0	100	100
24	LN	399/403 (99%)	386 (97%)	13 (3%)	0	100	100
25	LO	93/115 (81%)	93 (100%)	0	0	100	100
26	LP	104/125 (83%)	104 (100%)	0	0	100	100
27	LQ	126/135 (93%)	126 (100%)	0	0	100	100
28	LR	110/117 (94%)	110 (100%)	0	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%)	100 (100%)	0	0	100	100
32	LW	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
33	LX	89/92 (97%)	87 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	LY	67/70 (96%)	67 (100%)	0	0	100	100
35	LZ	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
36	NB	79/549 (14%)	79 (100%)	0	0	100	100
37	NC	501/731 (68%)	498 (99%)	3 (1%)	0	100	100
38	NF	227/260 (87%)	225 (99%)	2 (1%)	0	100	100
39	NJ	375/485 (77%)	360 (96%)	15 (4%)	0	100	100
40	NK	63/129 (49%)	63 (100%)	0	0	100	100
41	NL	296/478 (62%)	294 (99%)	2 (1%)	0	100	100
42	NP	100/134 (75%)	100 (100%)	0	0	100	100
43	NT	493/687 (72%)	488 (99%)	5 (1%)	0	100	100
44	NU	819/929 (88%)	809 (99%)	10 (1%)	0	100	100
45	NV	378/432 (88%)	374 (99%)	4 (1%)	0	100	100
45	NW	361/432 (84%)	354 (98%)	7 (2%)	0	100	100
46	NX	502/1130 (44%)	499 (99%)	3 (1%)	0	100	100
46	NY	514/1130 (46%)	510 (99%)	4 (1%)	0	100	100
47	NZ	115/360 (32%)	115 (100%)	0	0	100	100
48	SA	356/427 (83%)	351 (99%)	5 (1%)	0	100	100
49	SB	252/297 (85%)	248 (98%)	4 (2%)	0	100	100
50	SC	211/288 (73%)	205 (97%)	6 (3%)	0	100	100
51	SD	223/248 (90%)	218 (98%)	5 (2%)	0	100	100
52	SE	230/266 (86%)	228 (99%)	2 (1%)	0	100	100
53	SF	243/257 (95%)	235 (97%)	8 (3%)	0	100	100
54	SG	188/192 (98%)	186 (99%)	2 (1%)	0	100	100
55	SH	91/293 (31%)	90 (99%)	1 (1%)	0	100	100
56	SI	233/255 (91%)	230 (99%)	3 (1%)	0	100	100
57	SK	242/245 (99%)	236 (98%)	6 (2%)	0	100	100
58	SM	393/588 (67%)	389 (99%)	4 (1%)	0	100	100
59	SQ	216/239 (90%)	213 (99%)	3 (1%)	0	100	100
60	SR	596/634 (94%)	585 (98%)	10 (2%)	1 (0%)	43	62
61	SV	137/163 (84%)	136 (99%)	1 (1%)	0	100	100
All	All	12800/17822 (72%)	12632 (99%)	167 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
60	SR	88	ASP

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	132/137 (96%)	132 (100%)	0	100	100
2	BB	195/196 (100%)	195 (100%)	0	100	100
3	BD	15/641 (2%)	15 (100%)	0	100	100
7	L5	142/149 (95%)	142 (100%)	0	100	100
8	L6	171/177 (97%)	171 (100%)	0	100	100
9	L7	173/174 (99%)	173 (100%)	0	100	100
10	L8	115/161 (71%)	115 (100%)	0	100	100
11	L9	164/172 (95%)	164 (100%)	0	100	100
12	LA	135/163 (83%)	135 (100%)	0	100	100
13	LB	136/165 (82%)	136 (100%)	0	100	100
14	LC	157/157 (100%)	157 (100%)	0	100	100
15	LD	138/175 (79%)	138 (100%)	0	100	100
16	LE	121/140 (86%)	121 (100%)	0	100	100
17	LF	93/115 (81%)	93 (100%)	0	100	100
18	LG	106/107 (99%)	106 (100%)	0	100	100
19	LH	124/133 (93%)	124 (100%)	0	100	100
20	LI	124/135 (92%)	124 (100%)	0	100	100
21	LJ	117/118 (99%)	117 (100%)	0	100	100
22	LK	98/121 (81%)	98 (100%)	0	100	100
23	LL	109/121 (90%)	109 (100%)	0	100	100
24	LN	347/348 (100%)	347 (100%)	0	100	100
25	LO	80/97 (82%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	LW	73/80 (91%)	73 (100%)	0	100	100
33	LX	74/75 (99%)	74 (100%)	0	100	100
34	LY	64/65 (98%)	64 (100%)	0	100	100
35	LZ	47/48 (98%)	47 (100%)	0	100	100
36	NB	74/485 (15%)	74 (100%)	0	100	100
37	NC	455/654 (70%)	455 (100%)	0	100	100
38	NF	203/228 (89%)	203 (100%)	0	100	100
39	NJ	314/404 (78%)	314 (100%)	0	100	100
40	NK	61/115 (53%)	61 (100%)	0	100	100
41	NL	263/402 (65%)	263 (100%)	0	100	100
42	NP	88/114 (77%)	88 (100%)	0	100	100
43	NT	457/629 (73%)	457 (100%)	0	100	100
44	NU	694/843 (82%)	694 (100%)	0	100	100
45	NV	324/368 (88%)	324 (100%)	0	100	100
45	NW	311/368 (84%)	311 (100%)	0	100	100
46	NX	440/944 (47%)	440 (100%)	0	100	100
46	NY	445/944 (47%)	445 (100%)	0	100	100
47	NZ	108/312 (35%)	108 (100%)	0	100	100
48	SA	298/348 (86%)	297 (100%)	1 (0%)	86	94
49	SB	213/250 (85%)	213 (100%)	0	100	100
50	SC	192/252 (76%)	192 (100%)	0	100	100
51	SD	194/215 (90%)	194 (100%)	0	100	100
52	SE	200/223 (90%)	200 (100%)	0	100	100
53	SF	188/199 (94%)	188 (100%)	0	100	100
54	SG	169/171 (99%)	169 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	SH	85/274 (31%)	85 (100%)	0	100	100
56	SI	212/228 (93%)	212 (100%)	0	100	100
57	SK	212/213 (100%)	212 (100%)	0	100	100
58	SM	354/509 (70%)	354 (100%)	0	100	100
59	SQ	195/214 (91%)	195 (100%)	0	100	100
60	SR	546/574 (95%)	546 (100%)	0	100	100
61	SV	128/149 (86%)	128 (100%)	0	100	100
All	All	11263/15418 (73%)	11262 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
48	SA	109	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	BA	149	HIS
9	L7	150	GLN
9	L7	199	HIS
10	L8	48	GLN
10	L8	56	GLN
10	L8	125	ASN
11	L9	196	ASN
12	LA	133	HIS
15	LD	27	ASN
15	LD	66	ASN
18	LG	135	ASN
19	LH	107	HIS
20	LI	20	ASN
21	LJ	127	ASN
22	LK	62	HIS
23	LL	6	GLN
24	LN	184	GLN
24	LN	203	GLN
24	LN	354	GLN
25	LO	72	HIS
27	LQ	126	ASN

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Mol	Chain	Res	Type
30	LT	20	ASN
30	LT	56	ASN
30	LT	99	HIS
31	LU	80	HIS
33	LX	56	HIS
34	LY	28	ASN
36	NB	41	HIS
37	NC	31	ASN
37	NC	133	HIS
37	NC	282	HIS
38	NF	68	HIS
39	NJ	149	HIS
39	NJ	291	ASN
39	NJ	323	GLN
41	NL	365	HIS
42	NP	99	GLN
43	NT	89	HIS
43	NT	291	HIS
43	NT	415	GLN
43	NT	445	GLN
44	NU	357	GLN
44	NU	658	HIS
44	NU	725	GLN
44	NU	845	GLN
45	NV	48	ASN
45	NV	179	HIS
45	NV	256	HIS
45	NV	342	HIS
45	NW	166	HIS
45	NW	315	ASN
46	NX	461	HIS
46	NY	65	HIS
46	NY	164	GLN
46	NY	175	ASN
46	NY	176	HIS
46	NY	313	GLN
46	NY	561	GLN
46	NY	632	HIS
47	NZ	275	GLN
48	SA	212	ASN
49	SB	17	GLN
49	SB	45	ASN

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Mol	Chain	Res	Type
50	SC	136	HIS
50	SC	190	HIS
50	SC	211	HIS
52	SE	90	GLN
53	SF	8	GLN
53	SF	22	HIS
54	SG	156	ASN
54	SG	163	GLN
55	SH	67	GLN
56	SI	94	HIS
57	SK	82	GLN
57	SK	83	HIS
58	SM	50	HIS
58	SM	154	HIS
58	SM	211	HIS
58	SM	253	GLN
59	SQ	47	ASN
59	SQ	50	ASN
60	SR	91	HIS
60	SR	100	ASN
60	SR	246	HIS
60	SR	263	HIS
60	SR	426	HIS
60	SR	612	HIS
61	SV	17	HIS
61	SV	39	ASN
61	SV	132	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	L1	152/157 (96%)	18 (11%)	0
5	L3	3463/5070 (68%)	468 (13%)	14 (0%)
6	L4	115/121 (95%)	12 (10%)	1 (0%)
All	All	3730/5348 (69%)	498 (13%)	15 (0%)

All (498) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	L1	23	C
4	L1	34	U

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Mol	Chain	Res	Type
4	L1	35	C
4	L1	59	A
4	L1	62	A
4	L1	63	U
4	L1	82	A
4	L1	83	C
4	L1	84	A
4	L1	86	U
4	L1	94	G
4	L1	103	A
4	L1	105	C
4	L1	110	U
4	L1	111	U
4	L1	114	G
4	L1	151	G
4	L1	156	U
5	L3	6	C
5	L3	13	U
5	L3	42	A
5	L3	48	G
5	L3	56	A
5	L3	58	G
5	L3	59	A
5	L3	64	A
5	L3	65	A
5	L3	69	A
5	L3	91	G
5	L3	108	A
5	L3	109	G
5	L3	119	G
5	L3	159	C
5	L3	171	U
5	L3	173	C
5	L3	181	C
5	L3	200	U
5	L3	210	C
5	L3	218	A
5	L3	233	U
5	L3	234	G
5	L3	246	G
5	L3	261	G
5	L3	263	G

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Mol	Chain	Res	Type
5	L3	266	C
5	L3	267	G
5	L3	280	G
5	L3	296	A
5	L3	297	U
5	L3	316	U
5	L3	340	C
5	L3	387	G
5	L3	409	G
5	L3	410	A
5	L3	412	G
5	L3	430	G
5	L3	450	G
5	L3	452	A
5	L3	453	G
5	L3	454	U
5	L3	464	G
5	L3	467	U
5	L3	469	C
5	L3	472	C
5	L3	473	C
5	L3	492	U
5	L3	493	G
5	L3	496	G
5	L3	497	G
5	L3	499	G
5	L3	501	C
5	L3	502	C
5	L3	503	C
5	L3	504	G
5	L3	510	U
5	L3	658	C
5	L3	660	A
5	L3	667	A
5	L3	669	C
5	L3	686	A
5	L3	704	C
5	L3	729	G
5	L3	730	G
5	L3	731	G
5	L3	739	G
5	L3	741	C

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Mol	Chain	Res	Type
5	L3	742	G
5	L3	746	A
5	L3	913	U
5	L3	915	A
5	L3	916	C
5	L3	917	A
5	L3	926	G
5	L3	932	A
5	L3	933	G
5	L3	935	A
5	L3	943	A
5	L3	944	A
5	L3	945	U
5	L3	956	A
5	L3	959	G
5	L3	960	A
5	L3	1066	G
5	L3	1070	G
5	L3	1072	C
5	L3	1080	C
5	L3	1211	G
5	L3	1214	C
5	L3	1253	G
5	L3	1254	A
5	L3	1255	A
5	L3	1256	G
5	L3	1266	G
5	L3	1269	G
5	L3	1270	A
5	L3	1272	C
5	L3	1273	G
5	L3	1280	C
5	L3	1284	G
5	L3	1287	G
5	L3	1294	A
5	L3	1295	C
5	L3	1301	C
5	L3	1313	C
5	L3	1314	C
5	L3	1315	C
5	L3	1319	U
5	L3	1320	U

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Mol	Chain	Res	Type
5	L3	1322	1MA
5	L3	1354	A
5	L3	1358	G
5	L3	1359	G
5	L3	1365	C
5	L3	1366	G
5	L3	1379	C
5	L3	1397	A
5	L3	1399	G
5	L3	1420	A
5	L3	1497	A
5	L3	1498	G
5	L3	1502	G
5	L3	1523	A
5	L3	1534	A2M
5	L3	1547	A
5	L3	1578	U
5	L3	1592	G
5	L3	1596	U
5	L3	1597	G
5	L3	1613	A
5	L3	1624	G
5	L3	1625	OMG
5	L3	1631	A
5	L3	1633	G
5	L3	1634	A
5	L3	1640	C
5	L3	1654	G
5	L3	1661	C
5	L3	1671	U
5	L3	1676	C
5	L3	1677	PSU
5	L3	1678	C
5	L3	1680	G
5	L3	1684	A
5	L3	1694	C
5	L3	1726	U
5	L3	1734	G
5	L3	1735	U
5	L3	1736	A
5	L3	1737	A
5	L3	1739	G

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Mol	Chain	Res	Type
5	L3	1743	A
5	L3	1744	PSU
5	L3	1747	U
5	L3	1748	U
5	L3	1749	A
5	L3	1750	G
5	L3	1754	U
5	L3	1755	C
5	L3	1756	U
5	L3	1758	G
5	L3	1775	A
5	L3	1781	PSU
5	L3	1804	A
5	L3	1806	G
5	L3	1813	U
5	L3	1815	G
5	L3	1827	C
5	L3	1829	G
5	L3	1832	C
5	L3	1833	G
5	L3	1835	G
5	L3	1836	G
5	L3	1837	A
5	L3	1842	G
5	L3	1852	U
5	L3	1854	G
5	L3	1855	G
5	L3	1881	C
5	L3	1883	G
5	L3	1891	A
5	L3	1897	A
5	L3	1910	G
5	L3	1919	G
5	L3	1921	C
5	L3	1922	G
5	L3	1925	G
5	L3	1931	C
5	L3	1935	C
5	L3	1941	A
5	L3	1943	A
5	L3	1969	G
5	L3	1973	G

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Mol	Chain	Res	Type
5	L3	1974	U
5	L3	1978	C
5	L3	1984	A
5	L3	2002	A
5	L3	2025	A
5	L3	2026	A
5	L3	2041	A
5	L3	2042	A
5	L3	2046	G
5	L3	2055	G
5	L3	2056	G
5	L3	2069	A
5	L3	2084	C
5	L3	2289	C
5	L3	2300	A
5	L3	2301	G
5	L3	2313	A
5	L3	2348	G
5	L3	2351	OMC
5	L3	2395	A
5	L3	2398	U
5	L3	2417	A
5	L3	2422	OMC
5	L3	2424	OMG
5	L3	2425	U
5	L3	2450	G
5	L3	2453	A
5	L3	2469	C
5	L3	2470	C
5	L3	2471	G
5	L3	2475	G
5	L3	2476	G
5	L3	2477	A
5	L3	2478	C
5	L3	2480	G
5	L3	2486	G
5	L3	2487	G
5	L3	2488	C
5	L3	2489	C
5	L3	2492	C
5	L3	2512	A
5	L3	2513	A

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Mol	Chain	Res	Type
5	L3	2519	U
5	L3	2529	A
5	L3	2544	G
5	L3	2545	U
5	L3	2548	C
5	L3	2554	U
5	L3	2587	A
5	L3	2601	A
5	L3	2627	C
5	L3	2653	C
5	L3	2669	C
5	L3	2687	U
5	L3	2694	G
5	L3	2695	A
5	L3	2696	A
5	L3	2711	G
5	L3	2742	G
5	L3	2743	A
5	L3	2760	G
5	L3	2764	A
5	L3	2769	U
5	L3	2771	G
5	L3	2787	A2M
5	L3	2788	U
5	L3	2790	U
5	L3	2814	C
5	L3	2826	U
5	L3	2827	G
5	L3	2829	U
5	L3	2850	A
5	L3	2855	G
5	L3	2877	G
5	L3	2902	G
5	L3	2917	G
5	L3	2918	G
5	L3	3271	G
5	L3	3585	G
5	L3	3593	C
5	L3	3595	U
5	L3	3597	G
5	L3	3616	U
5	L3	3626	G

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Mol	Chain	Res	Type
5	L3	3630	A
5	L3	3635	A
5	L3	3644	U
5	L3	3653	A
5	L3	3662	A
5	L3	3702	A
5	L3	3709	U
5	L3	3710	G
5	L3	3713	U
5	L3	3743	G
5	L3	3753	G
5	L3	3774	A
5	L3	3775	A
5	L3	3782	5MC
5	L3	3783	A
5	L3	3784	A
5	L3	3785	A2M
5	L3	3790	U
5	L3	3791	C
5	L3	3814	U
5	L3	3815	G
5	L3	3820	G
5	L3	3821	A
5	L3	3822	PSU
5	L3	3823	G
5	L3	3838	U
5	L3	3840	U
5	L3	3867	A2M
5	L3	3881	G
5	L3	3887	OMC
5	L3	3897	G
5	L3	3905	A
5	L3	3914	U
5	L3	3915	U
5	L3	3939	G
5	L3	3963	A
5	L3	3972	A
5	L3	4037	C
5	L3	4049	U
5	L3	4064	C
5	L3	4076	G
5	L3	4085	A

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Mol	Chain	Res	Type
5	L3	4119	C
5	L3	4120	U
5	L3	4121	G
5	L3	4122	G
5	L3	4127	A
5	L3	4133	C
5	L3	4139	G
5	L3	4140	C
5	L3	4142	C
5	L3	4143	G
5	L3	4144	C
5	L3	4145	C
5	L3	4147	G
5	L3	4150	G
5	L3	4154	G
5	L3	4162	C
5	L3	4163	U
5	L3	4170	A
5	L3	4183	G
5	L3	4184	G
5	L3	4208	U
5	L3	4210	U
5	L3	4211	C
5	L3	4212	A
5	L3	4213	A
5	L3	4214	A
5	L3	4216	G
5	L3	4217	G
5	L3	4219	A
5	L3	4220	6MZ
5	L3	4221	C
5	L3	4224	A
5	L3	4226	G
5	L3	4230	C
5	L3	4231	C
5	L3	4233	A
5	L3	4234	A
5	L3	4235	G
5	L3	4251	A
5	L3	4254	G
5	L3	4266	G
5	L3	4268	A

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Mol	Chain	Res	Type
5	L3	4271	A
5	L3	4272	G
5	L3	4273	A
5	L3	4281	A
5	L3	4291	G
5	L3	4296	PSU
5	L3	4302	U
5	L3	4307	A
5	L3	4326	G
5	L3	4330	G
5	L3	4332	C
5	L3	4335	C
5	L3	4348	A
5	L3	4349	C
5	L3	4350	C
5	L3	4354	U
5	L3	4368	G
5	L3	4381	A
5	L3	4387	C
5	L3	4396	A
5	L3	4398	C
5	L3	4399	U
5	L3	4401	G
5	L3	4415	A
5	L3	4418	G
5	L3	4438	U
5	L3	4439	U
5	L3	4446	U
5	L3	4451	G
5	L3	4452	U
5	L3	4453	C
5	L3	4464	A
5	L3	4466	C
5	L3	4475	G
5	L3	4476	C
5	L3	4498	OMU
5	L3	4499	OMG
5	L3	4500	PSU
5	L3	4501	U
5	L3	4503	A
5	L3	4512	U
5	L3	4513	A

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Mol	Chain	Res	Type
5	L3	4519	C
5	L3	4523	A2M
5	L3	4524	G
5	L3	4545	G
5	L3	4547	C
5	L3	4548	A
5	L3	4556	U
5	L3	4557	U
5	L3	4558	U
5	L3	4560	C
5	L3	4573	G
5	L3	4574	U
5	L3	4575	G
5	L3	4590	A2M
5	L3	4608	G
5	L3	4618	OMG
5	L3	4636	PSU
5	L3	4637	OMG
5	L3	4656	A
5	L3	4670	C
5	L3	4672	A
5	L3	4678	G
5	L3	4684	A
5	L3	4700	A
5	L3	4708	A
5	L3	4709	U
5	L3	4719	G
5	L3	4720	C
5	L3	4740	G
5	L3	4741	C
5	L3	4742	G
5	L3	4750	G
5	L3	4751	G
5	L3	4754	G
5	L3	4757	C
5	L3	4759	C
5	L3	4765	G
5	L3	4773	C
5	L3	4870	G
5	L3	4871	C
5	L3	4882	U
5	L3	4883	C

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Mol	Chain	Res	Type
5	L3	4900	C
5	L3	4901	G
5	L3	4910	G
5	L3	4916	G
5	L3	4943	A
5	L3	4976	U
5	L3	5006	U
5	L3	5007	A
5	L3	5014	A
5	L3	5020	G
5	L3	5022	U
5	L3	5024	C
5	L3	5025	C
5	L3	5026	U
5	L3	5027	C
5	L3	5031	G
5	L3	5041	G
5	L3	5050	C
5	L3	5054	C
5	L3	5061	A
5	L3	5062	G
5	L3	5069	U
6	L4	7	G
6	L4	18	C
6	L4	22	A
6	L4	53	U
6	L4	54	A
6	L4	64	G
6	L4	66	G
6	L4	84	U
6	L4	97	G
6	L4	100	A
6	L4	106	G
6	L4	110	G

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	L3	496	G
5	L3	502	C
5	L3	503	C
5	L3	934	C

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Mol	Chain	Res	Type
5	L3	1677	PSU
5	L3	1742	A
5	L3	1754	U
5	L3	1831	G
5	L3	3712	A
5	L3	3819	G
5	L3	3822	PSU
5	L3	4213	A
5	L3	4500	PSU
5	L3	4699	U
6	L4	109	U

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

129 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	$\# Z > 2$
5	A2M	L3	3718	5	22,25,26	0.89	0	30,36,39	2.05	8 (26%)
5	OMG	L3	4623	5	23,26,27	0.47	0	32,38,41	0.54	0
5	PSU	L3	4636	5	18,21,22	1.09	1 (5%)	21,30,33	2.01	5 (23%)
5	PSU	L3	3695	5	18,21,22	1.10	1 (5%)	21,30,33	1.94	6 (28%)
5	A2M	L3	3825	5	22,25,26	0.85	0	30,36,39	2.06	7 (23%)
5	PSU	L3	2839	5	18,21,22	1.06	1 (5%)	21,30,33	1.96	5 (23%)
5	PSU	L3	5010	5	18,21,22	1.10	1 (5%)	21,30,33	1.94	5 (23%)
5	PSU	L3	1582	5	18,21,22	1.05	1 (5%)	21,30,33	1.94	5 (23%)
5	OMG	L3	4228	5	23,26,27	0.45	0	32,38,41	0.48	0
5	OMG	L3	3627	5	23,26,27	0.47	0	32,38,41	0.58	0
5	PSU	L3	3851	5	18,21,22	1.09	1 (5%)	21,30,33	1.99	5 (23%)
5	OMC	L3	2804	5	19,22,23	0.54	0	25,31,34	0.71	0
5	PSU	L3	1860	5	18,21,22	1.06	1 (5%)	21,30,33	1.97	5 (23%)
5	OMU	L3	4498	5	19,22,23	2.08	7 (36%)	25,31,34	1.81	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	A2M	L3	4523	5	22,25,26	0.86	0	30,36,39	2.08	8 (26%)
5	PSU	L3	4312	5	18,21,22	1.07	1 (5%)	21,30,33	1.92	5 (23%)
5	A2M	L3	2787	5	22,25,26	0.86	1 (4%)	30,36,39	2.11	7 (23%)
5	PSU	L3	3853	5	18,21,22	1.05	1 (5%)	21,30,33	1.91	4 (19%)
5	A2M	L3	1326	5	22,25,26	0.87	0	30,36,39	2.05	7 (23%)
5	PSU	L3	4552	5	18,21,22	1.09	1 (5%)	21,30,33	1.98	5 (23%)
5	1MA	L3	1322	5	21,25,26	0.41	0	30,37,40	0.74	1 (3%)
5	A2M	L3	1524	5	22,25,26	0.87	0	30,36,39	2.13	8 (26%)
5	PSU	L3	3637	5	18,21,22	1.10	1 (5%)	21,30,33	2.00	5 (23%)
5	A2M	L3	3785	5	22,25,26	0.85	0	30,36,39	2.06	7 (23%)
5	A2M	L3	4590	5	22,25,26	0.84	0	30,36,39	2.03	8 (26%)
5	PSU	L3	1862	5	18,21,22	1.08	1 (5%)	21,30,33	1.91	5 (23%)
5	A2M	L3	3867	5	22,25,26	0.89	0	30,36,39	2.09	7 (23%)
5	5MC	L3	3782	5	19,22,23	0.50	0	26,32,35	0.63	0
5	PSU	L3	3920	62,5	18,21,22	1.10	1 (5%)	21,30,33	1.97	6 (28%)
5	PSU	L3	4521	5	18,21,22	1.11	1 (5%)	21,30,33	1.93	5 (23%)
5	PSU	L3	1683	5	18,21,22	1.14	1 (5%)	21,30,33	1.98	5 (23%)
5	OMG	L3	2424	5	23,26,27	0.48	0	32,38,41	0.46	0
5	PSU	L3	1782	5	18,21,22	1.10	1 (5%)	21,30,33	1.99	5 (23%)
5	PSU	L3	2632	5	18,21,22	1.11	1 (5%)	21,30,33	1.84	4 (19%)
5	OMG	L3	3899	5	23,26,27	0.47	0	32,38,41	0.53	0
5	OMC	L3	2861	5	19,22,23	0.53	0	25,31,34	0.68	0
5	PSU	L3	3639	5	18,21,22	1.10	1 (5%)	21,30,33	1.94	5 (23%)
5	PSU	L3	3734	5	18,21,22	1.14	1 (5%)	21,30,33	1.97	6 (28%)
5	PSU	L3	1779	5	18,21,22	1.12	1 (5%)	21,30,33	1.89	4 (19%)
5	OMG	L3	1522	5	23,26,27	0.47	0	32,38,41	0.50	0
5	A2M	L3	400	5	22,25,26	0.85	0	30,36,39	2.12	8 (26%)
5	PSU	L3	1781	5	18,21,22	1.21	3 (16%)	21,30,33	1.96	5 (23%)
5	OMC	L3	3701	5	19,22,23	0.53	0	25,31,34	0.59	0
5	OMC	L3	2422	62,5	19,22,23	0.51	0	25,31,34	0.68	0
5	OMU	L3	3818	5	19,22,23	2.09	7 (36%)	25,31,34	1.80	5 (20%)
5	PSU	L3	1744	5	18,21,22	1.14	1 (5%)	21,30,33	1.94	5 (23%)
5	OMC	L3	4456	5	19,22,23	0.52	0	25,31,34	0.67	0
5	OMG	L3	2364	5	23,26,27	0.48	0	32,38,41	0.45	0
5	A2M	L3	4571	5	22,25,26	0.86	0	30,36,39	2.03	7 (23%)
5	PSU	L3	4576	5	18,21,22	1.12	1 (5%)	21,30,33	1.90	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	A2M	L3	398	5	22,25,26	0.85	0	30,36,39	2.13	8 (26%)
5	PSU	L3	4532	5	18,21,22	1.09	1 (5%)	21,30,33	1.98	5 (23%)
5	OMG	L3	4637	5	23,26,27	0.48	0	32,38,41	0.49	0
5	OMU	L3	2837	5	19,22,23	2.05	7 (36%)	25,31,34	1.86	5 (20%)
5	OMU	L3	3925	5	19,22,23	2.04	7 (36%)	25,31,34	1.77	5 (20%)
5	PSU	L3	4628	5	18,21,22	1.07	1 (5%)	21,30,33	1.87	5 (23%)
5	OMC	L3	2351	62,5	19,22,23	0.55	0	25,31,34	0.75	1 (4%)
5	PSU	L3	3770	5	18,21,22	1.11	1 (5%)	21,30,33	1.91	4 (19%)
5	OMC	L3	2824	5	19,22,23	0.51	0	25,31,34	0.71	0
5	OMG	L3	4618	5	23,26,27	0.48	0	32,38,41	0.57	0
5	PSU	L3	3884	5	18,21,22	1.09	1 (5%)	21,30,33	1.93	4 (19%)
24	HIC	LN	245	24	10,11,12	0.55	0	9,14,16	0.83	1 (11%)
5	PSU	L3	4353	5	18,21,22	1.11	1 (5%)	21,30,33	1.94	5 (23%)
5	OMC	L3	3887	5	19,22,23	0.49	0	25,31,34	0.70	0
5	PSU	L3	3822	5	18,21,22	1.09	1 (5%)	21,30,33	1.72	4 (19%)
5	A2M	L3	2363	62,5	22,25,26	0.87	0	30,36,39	2.03	7 (23%)
5	A2M	L3	3760	5	22,25,26	0.86	0	30,36,39	2.07	7 (23%)
5	OMG	L3	1760	5	23,26,27	0.44	0	32,38,41	0.53	0
5	PSU	L3	4293	5	18,21,22	1.11	1 (5%)	21,30,33	1.97	5 (23%)
4	PSU	L1	55	4	18,21,22	1.11	1 (5%)	21,30,33	1.97	5 (23%)
5	A2M	L3	1534	62,5	22,25,26	0.85	0	30,36,39	2.08	7 (23%)
5	PSU	L3	4500	5	18,21,22	1.10	1 (5%)	21,30,33	1.88	5 (23%)
5	PSU	L3	4361	5	18,21,22	1.11	1 (5%)	21,30,33	2.00	5 (23%)
5	OMC	L3	1340	5	19,22,23	0.52	0	25,31,34	0.72	0
5	PSU	L3	3758	5	18,21,22	1.09	1 (5%)	21,30,33	1.97	5 (23%)
5	OMC	L3	4536	5	19,22,23	0.53	0	25,31,34	0.70	0
5	OMG	L3	4494	5	23,26,27	0.48	0	32,38,41	0.49	0
4	OMG	L1	75	4	23,26,27	0.48	0	32,38,41	0.47	0
5	OMG	L3	1316	5	23,26,27	0.48	0	32,38,41	0.51	0
5	OMG	L3	1625	5	23,26,27	0.47	0	32,38,41	0.49	0
5	OMC	L3	4054	5	19,22,23	0.52	0	25,31,34	0.78	0
4	PSU	L1	69	4	18,21,22	1.12	1 (5%)	21,30,33	2.02	6 (28%)
5	PSU	L3	5001	5	18,21,22	1.10	1 (5%)	21,30,33	1.97	5 (23%)
5	A2M	L3	2401	5	22,25,26	0.87	0	30,36,39	2.11	8 (26%)
5	PSU	L3	4403	5	18,21,22	1.08	1 (5%)	21,30,33	1.96	6 (28%)
5	OMU	L3	1773	5	19,22,23	2.08	7 (36%)	25,31,34	1.81	5 (20%)
5	PSU	L3	3762	5	18,21,22	1.06	1 (5%)	21,30,33	1.91	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PSU	L3	4689	62,5	18,21,22	1.09	1 (5%)	21,30,33	1.97	4 (19%)
5	A2M	L3	2815	5	22,25,26	0.85	0	30,36,39	2.09	8 (26%)
5	A2M	L3	3724	5	22,25,26	0.85	0	30,36,39	2.03	7 (23%)
5	OMC	L3	2365	5	19,22,23	0.52	0	25,31,34	0.70	0
5	PSU	L3	4493	5	18,21,22	1.12	2 (11%)	21,30,33	1.99	5 (23%)
5	PSU	L3	4296	5	18,21,22	1.13	1 (5%)	21,30,33	1.94	5 (23%)
5	PSU	L3	4471	5	18,21,22	1.11	1 (5%)	21,30,33	2.01	5 (23%)
5	OMU	L3	4306	5	19,22,23	2.08	7 (36%)	25,31,34	1.86	5 (20%)
5	PSU	L3	4972	5	18,21,22	1.09	1 (5%)	21,30,33	1.97	5 (23%)
5	PSU	L3	3844	5	18,21,22	1.13	1 (5%)	21,30,33	1.90	5 (23%)
5	PSU	L3	1677	5	18,21,22	1.12	1 (5%)	21,30,33	1.97	6 (28%)
5	OMU	L3	4227	5	19,22,23	2.12	7 (36%)	25,31,34	1.84	5 (20%)
5	6MZ	L3	4220	5	22,25,26	1.11	1 (4%)	29,36,39	2.20	8 (27%)
5	PSU	L3	2508	5	18,21,22	1.12	1 (5%)	21,30,33	1.94	5 (23%)
5	OMG	L3	4042	5	23,26,27	0.48	0	32,38,41	0.46	0
5	OMG	L3	3744	5	23,26,27	0.50	0	32,38,41	0.48	0
5	PSU	L3	3959	5	18,21,22	1.10	1 (5%)	21,30,33	2.00	5 (23%)
5	UR3	L3	4530	5	19,22,23	1.10	3 (15%)	26,32,35	1.50	2 (7%)
5	PSU	L3	4299	5	18,21,22	1.11	1 (5%)	21,30,33	2.01	6 (28%)
5	PSU	L3	4673	5	18,21,22	1.09	1 (5%)	21,30,33	1.91	5 (23%)
5	OMU	L3	4620	5	19,22,23	2.00	6 (31%)	25,31,34	1.72	5 (20%)
5	OMG	L3	4370	5	23,26,27	0.47	0	32,38,41	0.45	0
5	OMC	L3	3808	5	19,22,23	0.47	0	25,31,34	0.69	0
5	PSU	L3	4579	5	18,21,22	1.05	1 (5%)	21,30,33	1.90	4 (19%)
5	PSU	L3	3768	5	18,21,22	1.05	1 (5%)	21,30,33	1.94	5 (23%)
5	PSU	L3	4457	5	18,21,22	1.10	1 (5%)	21,30,33	1.99	5 (23%)
5	OMG	L3	3792	5	23,26,27	0.47	0	32,38,41	0.45	0
5	OMC	L3	3841	5	19,22,23	0.49	0	25,31,34	0.70	0
5	PSU	L3	4431	5	18,21,22	1.11	2 (11%)	21,30,33	1.99	5 (23%)
5	OMC	L3	3869	5	19,22,23	0.53	0	25,31,34	0.69	0
5	A2M	L3	3830	5	22,25,26	0.86	0	30,36,39	2.07	8 (26%)
5	A2M	L3	1871	5	22,25,26	0.90	0	30,36,39	2.12	8 (26%)
5	PSU	L3	4442	5	18,21,22	1.11	1 (5%)	21,30,33	1.89	5 (23%)
5	OMU	L3	2415	5	19,22,23	2.06	7 (36%)	25,31,34	1.81	5 (20%)
5	5MC	L3	4447	5	19,22,23	0.52	0	26,32,35	0.64	0
5	OMG	L3	4392	5	23,26,27	0.48	0	32,38,41	0.50	0
5	PSU	L3	3764	5	18,21,22	1.11	1 (5%)	21,30,33	1.91	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	OMG	L3	4499	5	23,26,27	0.46	0	32,38,41	0.48	0
5	OMG	L3	2876	5	23,26,27	0.47	0	32,38,41	0.46	0
5	PSU	L3	1536	5	18,21,22	1.09	1 (5%)	21,30,33	1.98	5 (23%)
5	PSU	L3	3730	5	18,21,22	1.10	1 (5%)	21,30,33	1.98	5 (23%)
5	PSU	L3	3715	5	18,21,22	1.11	1 (5%)	21,30,33	1.97	6 (28%)

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
5	A2M	L3	3718	5	-	1/9/27/28	0/3/3/3
5	OMG	L3	4623	5	-	0/9/27/28	0/3/3/3
5	PSU	L3	4636	5	-	3/7/25/26	0/2/2/2
5	PSU	L3	3695	5	-	0/7/25/26	0/2/2/2
5	A2M	L3	3825	5	-	1/9/27/28	0/3/3/3
5	PSU	L3	2839	5	-	0/7/25/26	0/2/2/2
5	PSU	L3	5010	5	-	0/7/25/26	0/2/2/2
5	PSU	L3	1582	5	-	0/7/25/26	0/2/2/2
5	OMG	L3	4228	5	-	0/9/27/28	0/3/3/3
5	OMG	L3	3627	5	-	1/9/27/28	0/3/3/3
5	PSU	L3	3851	5	-	0/7/25/26	0/2/2/2
5	OMC	L3	2804	5	-	0/9/27/28	0/2/2/2
5	PSU	L3	1860	5	-	0/7/25/26	0/2/2/2
5	OMU	L3	4498	5	-	5/9/27/28	0/2/2/2
5	A2M	L3	4523	5	-	2/9/27/28	0/3/3/3
5	PSU	L3	4312	5	-	0/7/25/26	0/2/2/2
5	A2M	L3	2787	5	-	5/9/27/28	0/3/3/3
5	PSU	L3	3853	5	-	0/7/25/26	0/2/2/2
5	A2M	L3	1326	5	-	3/9/27/28	0/3/3/3
5	PSU	L3	4552	5	-	0/7/25/26	0/2/2/2
5	1MA	L3	1322	5	-	2/7/25/26	0/3/3/3
5	A2M	L3	1524	5	-	0/9/27/28	0/3/3/3
5	PSU	L3	3637	5	-	0/7/25/26	0/2/2/2
5	A2M	L3	3785	5	-	3/9/27/28	0/3/3/3
5	A2M	L3	4590	5	-	4/9/27/28	0/3/3/3
5	PSU	L3	1862	5	-	0/7/25/26	0/2/2/2
5	A2M	L3	3867	5	-	4/9/27/28	0/3/3/3
5	5MC	L3	3782	5	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PSU	L3	3920	62,5	-	0/7/25/26	0/2/2/2
5	PSU	L3	4521	5	-	2/7/25/26	0/2/2/2
5	PSU	L3	1683	5	-	0/7/25/26	0/2/2/2
5	OMG	L3	2424	5	-	3/9/27/28	0/3/3/3
5	PSU	L3	1782	5	-	0/7/25/26	0/2/2/2
5	PSU	L3	2632	5	-	0/7/25/26	0/2/2/2
5	OMG	L3	3899	5	-	1/9/27/28	0/3/3/3
5	OMC	L3	2861	5	-	1/9/27/28	0/2/2/2
5	PSU	L3	3639	5	-	0/7/25/26	0/2/2/2
5	PSU	L3	3734	5	-	0/7/25/26	0/2/2/2
5	PSU	L3	1779	5	-	0/7/25/26	0/2/2/2
5	OMG	L3	1522	5	-	1/9/27/28	0/3/3/3
5	A2M	L3	400	5	-	1/9/27/28	0/3/3/3
5	PSU	L3	1781	5	-	2/7/25/26	0/2/2/2
5	OMC	L3	3701	5	-	4/9/27/28	0/2/2/2
5	OMC	L3	2422	62,5	-	2/9/27/28	0/2/2/2
5	OMU	L3	3818	5	-	1/9/27/28	0/2/2/2
5	PSU	L3	1744	5	-	2/7/25/26	0/2/2/2
5	OMC	L3	4456	5	-	1/9/27/28	0/2/2/2
5	OMG	L3	2364	5	-	2/9/27/28	0/3/3/3
5	A2M	L3	4571	5	-	1/9/27/28	0/3/3/3
5	PSU	L3	4576	5	-	0/7/25/26	0/2/2/2
5	A2M	L3	398	5	-	1/9/27/28	0/3/3/3
5	PSU	L3	4532	5	-	0/7/25/26	0/2/2/2
5	OMG	L3	4637	5	-	3/9/27/28	0/3/3/3
5	OMU	L3	2837	5	-	1/9/27/28	0/2/2/2
5	OMU	L3	3925	5	-	1/9/27/28	0/2/2/2
5	PSU	L3	4628	5	-	0/7/25/26	0/2/2/2
5	OMC	L3	2351	62,5	-	3/9/27/28	0/2/2/2
5	PSU	L3	3770	5	-	0/7/25/26	0/2/2/2
5	OMC	L3	2824	5	-	0/9/27/28	0/2/2/2
5	OMG	L3	4618	5	-	2/9/27/28	0/3/3/3
5	PSU	L3	3884	5	-	0/7/25/26	0/2/2/2
24	HIC	LN	245	24	-	3/5/6/8	0/1/1/1
5	PSU	L3	4353	5	-	0/7/25/26	0/2/2/2
5	OMC	L3	3887	5	-	2/9/27/28	0/2/2/2
5	PSU	L3	3822	5	-	2/7/25/26	0/2/2/2
5	A2M	L3	2363	62,5	-	1/9/27/28	0/3/3/3
5	A2M	L3	3760	5	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OMG	L3	1760	5	-	1/9/27/28	0/3/3/3
5	PSU	L3	4293	5	-	0/7/25/26	0/2/2/2
4	PSU	L1	55	4	-	0/7/25/26	0/2/2/2
5	A2M	L3	1534	62,5	-	1/9/27/28	0/3/3/3
5	PSU	L3	4500	5	-	5/7/25/26	0/2/2/2
5	PSU	L3	4361	5	-	0/7/25/26	0/2/2/2
5	OMC	L3	1340	5	-	1/9/27/28	0/2/2/2
5	PSU	L3	3758	5	-	0/7/25/26	0/2/2/2
5	OMC	L3	4536	5	-	0/9/27/28	0/2/2/2
5	OMG	L3	4494	5	-	0/9/27/28	0/3/3/3
4	OMG	L1	75	4	-	1/9/27/28	0/3/3/3
5	OMG	L3	1316	5	-	1/9/27/28	0/3/3/3
5	OMG	L3	1625	5	-	0/9/27/28	0/3/3/3
5	OMC	L3	4054	5	-	1/9/27/28	0/2/2/2
4	PSU	L1	69	4	-	0/7/25/26	0/2/2/2
5	PSU	L3	5001	5	-	0/7/25/26	0/2/2/2
5	A2M	L3	2401	5	-	4/9/27/28	0/3/3/3
5	PSU	L3	4403	5	-	0/7/25/26	0/2/2/2
5	OMU	L3	1773	5	-	1/9/27/28	0/2/2/2
5	PSU	L3	3762	5	-	0/7/25/26	0/2/2/2
5	PSU	L3	4689	62,5	-	0/7/25/26	0/2/2/2
5	A2M	L3	2815	5	-	0/9/27/28	0/3/3/3
5	A2M	L3	3724	5	-	1/9/27/28	0/3/3/3
5	OMC	L3	2365	5	-	0/9/27/28	0/2/2/2
5	PSU	L3	4493	5	-	0/7/25/26	0/2/2/2
5	PSU	L3	4296	5	-	2/7/25/26	0/2/2/2
5	PSU	L3	4471	5	-	0/7/25/26	0/2/2/2
5	OMU	L3	4306	5	-	1/9/27/28	0/2/2/2
5	PSU	L3	4972	5	-	0/7/25/26	0/2/2/2
5	PSU	L3	3844	5	-	1/7/25/26	0/2/2/2
5	PSU	L3	1677	5	-	0/7/25/26	0/2/2/2
5	OMU	L3	4227	5	-	1/9/27/28	0/2/2/2
5	6MZ	L3	4220	5	-	6/9/27/28	0/3/3/3
5	PSU	L3	2508	5	-	0/7/25/26	0/2/2/2
5	OMG	L3	4042	5	-	1/9/27/28	0/3/3/3
5	OMG	L3	3744	5	-	1/9/27/28	0/3/3/3
5	PSU	L3	3959	5	-	0/7/25/26	0/2/2/2
5	UR3	L3	4530	5	-	0/7/25/26	0/2/2/2
5	PSU	L3	4299	5	-	0/7/25/26	0/2/2/2
5	PSU	L3	4673	5	-	0/7/25/26	0/2/2/2
5	OMU	L3	4620	5	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OMG	L3	4370	5	-	1/9/27/28	0/3/3/3
5	OMC	L3	3808	5	-	1/9/27/28	0/2/2/2
5	PSU	L3	4579	5	-	0/7/25/26	0/2/2/2
5	PSU	L3	3768	5	-	0/7/25/26	0/2/2/2
5	PSU	L3	4457	5	-	0/7/25/26	0/2/2/2
5	OMG	L3	3792	5	-	1/9/27/28	0/3/3/3
5	OMC	L3	3841	5	-	1/9/27/28	0/2/2/2
5	PSU	L3	4431	5	-	0/7/25/26	0/2/2/2
5	OMC	L3	3869	5	-	0/9/27/28	0/2/2/2
5	A2M	L3	3830	5	-	0/9/27/28	0/3/3/3
5	A2M	L3	1871	5	-	0/9/27/28	0/3/3/3
5	PSU	L3	4442	5	-	0/7/25/26	0/2/2/2
5	OMU	L3	2415	5	-	2/9/27/28	0/2/2/2
5	5MC	L3	4447	5	-	0/7/25/26	0/2/2/2
5	OMG	L3	4392	5	-	1/9/27/28	0/3/3/3
5	PSU	L3	3764	5	-	0/7/25/26	0/2/2/2
5	OMG	L3	4499	5	-	2/9/27/28	0/3/3/3
5	OMG	L3	2876	5	-	2/9/27/28	0/3/3/3
5	PSU	L3	1536	5	-	0/7/25/26	0/2/2/2
5	PSU	L3	3730	5	-	0/7/25/26	0/2/2/2
5	PSU	L3	3715	5	-	0/7/25/26	0/2/2/2

All (129) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L3	4227	OMU	C6-N1	4.88	1.49	1.38
5	L3	1773	OMU	C6-N1	4.80	1.49	1.38
5	L3	4498	OMU	C6-N1	4.80	1.49	1.38
5	L3	3818	OMU	C6-N1	4.78	1.49	1.38
5	L3	2415	OMU	C6-N1	4.77	1.49	1.38
5	L3	4306	OMU	C6-N1	4.74	1.49	1.38
5	L3	4620	OMU	C6-N1	4.70	1.49	1.38
5	L3	2837	OMU	C6-N1	4.69	1.49	1.38
5	L3	3925	OMU	C6-N1	4.69	1.49	1.38
5	L3	4227	OMU	C2-N1	4.39	1.45	1.38
5	L3	4306	OMU	C2-N1	4.37	1.45	1.38
5	L3	3818	OMU	C2-N1	4.31	1.45	1.38
5	L3	1773	OMU	C2-N1	4.29	1.45	1.38
5	L3	4498	OMU	C2-N1	4.25	1.45	1.38
5	L3	2837	OMU	C2-N1	4.24	1.45	1.38
5	L3	2415	OMU	C2-N1	4.18	1.45	1.38
5	L3	4227	OMU	C5-C4	4.15	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L3	1773	OMU	C5-C4	4.14	1.52	1.43
5	L3	3925	OMU	C2-N1	4.12	1.44	1.38
5	L3	3818	OMU	C5-C4	4.10	1.52	1.43
5	L3	2415	OMU	C5-C4	4.10	1.52	1.43
5	L3	4498	OMU	C5-C4	4.07	1.52	1.43
5	L3	4306	OMU	C5-C4	4.04	1.52	1.43
5	L3	2837	OMU	C5-C4	4.03	1.52	1.43
5	L3	4620	OMU	C2-N1	4.01	1.44	1.38
5	L3	3925	OMU	C5-C4	3.98	1.52	1.43
5	L3	4620	OMU	C5-C4	3.93	1.52	1.43
5	L3	4220	6MZ	C6-N6	3.92	1.38	1.34
5	L3	3822	PSU	C6-C5	3.79	1.39	1.35
5	L3	1683	PSU	C6-C5	3.75	1.39	1.35
5	L3	4296	PSU	C6-C5	3.74	1.39	1.35
5	L3	1781	PSU	C6-C5	3.72	1.39	1.35
5	L3	2632	PSU	C6-C5	3.72	1.39	1.35
5	L3	1779	PSU	C6-C5	3.69	1.39	1.35
5	L3	1744	PSU	C6-C5	3.68	1.39	1.35
5	L3	1677	PSU	C6-C5	3.65	1.39	1.35
5	L3	2508	PSU	C6-C5	3.64	1.39	1.35
5	L3	4576	PSU	C6-C5	3.64	1.39	1.35
5	L3	3734	PSU	C6-C5	3.63	1.39	1.35
5	L3	3764	PSU	C6-C5	3.62	1.39	1.35
5	L3	4442	PSU	C6-C5	3.60	1.39	1.35
5	L3	3770	PSU	C6-C5	3.59	1.39	1.35
5	L3	3730	PSU	C6-C5	3.58	1.39	1.35
5	L3	4500	PSU	C6-C5	3.56	1.39	1.35
5	L3	4353	PSU	C6-C5	3.55	1.39	1.35
5	L3	4636	PSU	C6-C5	3.54	1.39	1.35
5	L3	4293	PSU	C6-C5	3.54	1.39	1.35
5	L3	4431	PSU	C6-C5	3.54	1.39	1.35
5	L3	3844	PSU	C6-C5	3.54	1.39	1.35
4	L1	55	PSU	C6-C5	3.54	1.39	1.35
5	L3	4471	PSU	C6-C5	3.53	1.39	1.35
5	L3	4361	PSU	C6-C5	3.52	1.39	1.35
5	L3	3715	PSU	C6-C5	3.52	1.39	1.35
5	L3	4521	PSU	C6-C5	3.52	1.39	1.35
5	L3	3959	PSU	C6-C5	3.52	1.39	1.35
5	L3	4552	PSU	C6-C5	3.51	1.39	1.35
5	L3	1782	PSU	C6-C5	3.51	1.39	1.35
5	L3	3920	PSU	C6-C5	3.51	1.39	1.35
5	L3	5001	PSU	C6-C5	3.51	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L3	3884	PSU	C6-C5	3.51	1.39	1.35
5	L3	3758	PSU	C6-C5	3.51	1.39	1.35
5	L3	1862	PSU	C6-C5	3.50	1.39	1.35
5	L3	3639	PSU	C6-C5	3.50	1.39	1.35
5	L3	4299	PSU	C6-C5	3.50	1.39	1.35
5	L3	3851	PSU	C6-C5	3.49	1.39	1.35
5	L3	3695	PSU	C6-C5	3.49	1.39	1.35
5	L3	5010	PSU	C6-C5	3.49	1.39	1.35
5	L3	4532	PSU	C6-C5	3.48	1.39	1.35
5	L3	4493	PSU	C6-C5	3.48	1.39	1.35
4	L1	69	PSU	C6-C5	3.47	1.39	1.35
5	L3	3637	PSU	C6-C5	3.47	1.39	1.35
5	L3	4689	PSU	C6-C5	3.46	1.39	1.35
5	L3	4972	PSU	C6-C5	3.46	1.39	1.35
5	L3	4673	PSU	C6-C5	3.46	1.39	1.35
5	L3	4403	PSU	C6-C5	3.44	1.39	1.35
5	L3	4457	PSU	C6-C5	3.44	1.39	1.35
5	L3	4312	PSU	C6-C5	3.43	1.39	1.35
5	L3	1536	PSU	C6-C5	3.41	1.39	1.35
5	L3	1860	PSU	C6-C5	3.38	1.39	1.35
5	L3	1582	PSU	C6-C5	3.37	1.39	1.35
5	L3	3853	PSU	C6-C5	3.36	1.39	1.35
5	L3	4628	PSU	C6-C5	3.36	1.39	1.35
5	L3	3762	PSU	C6-C5	3.35	1.39	1.35
5	L3	2839	PSU	C6-C5	3.29	1.38	1.35
5	L3	4579	PSU	C6-C5	3.28	1.38	1.35
5	L3	3768	PSU	C6-C5	3.27	1.38	1.35
5	L3	4530	UR3	C2-N1	-2.85	1.34	1.38
5	L3	4530	UR3	C4-N3	-2.81	1.35	1.40
5	L3	2415	OMU	O4-C4	-2.74	1.19	1.24
5	L3	3925	OMU	O4-C4	-2.72	1.19	1.24
5	L3	4620	OMU	O4-C4	-2.72	1.19	1.24
5	L3	2837	OMU	O4-C4	-2.71	1.19	1.24
5	L3	4498	OMU	O4-C4	-2.70	1.19	1.24
5	L3	3818	OMU	O4-C4	-2.69	1.19	1.24
5	L3	4227	OMU	O4-C4	-2.69	1.19	1.24
5	L3	4306	OMU	O4-C4	-2.67	1.19	1.24
5	L3	1773	OMU	C2-N3	2.66	1.42	1.38
5	L3	1773	OMU	O4-C4	-2.65	1.19	1.24
5	L3	4227	OMU	C2-N3	2.64	1.42	1.38
5	L3	3818	OMU	C2-N3	2.63	1.42	1.38
5	L3	3925	OMU	C2-N3	2.62	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L3	4306	OMU	C2-N3	2.61	1.42	1.38
5	L3	4498	OMU	C2-N3	2.60	1.42	1.38
5	L3	2415	OMU	C2-N3	2.52	1.42	1.38
5	L3	2837	OMU	C2-N3	2.52	1.42	1.38
5	L3	4620	OMU	C2-N3	2.35	1.42	1.38
5	L3	4620	OMU	O2-C2	-2.25	1.19	1.23
5	L3	2837	OMU	O2-C2	-2.23	1.19	1.23
5	L3	3925	OMU	O2-C2	-2.23	1.19	1.23
5	L3	3818	OMU	C4-N3	2.22	1.42	1.38
5	L3	4306	OMU	O2-C2	-2.21	1.19	1.23
5	L3	4227	OMU	C4-N3	2.20	1.42	1.38
5	L3	4498	OMU	O2-C2	-2.20	1.19	1.23
5	L3	4498	OMU	C4-N3	2.18	1.42	1.38
5	L3	4306	OMU	C4-N3	2.15	1.42	1.38
5	L3	4227	OMU	O2-C2	-2.14	1.19	1.23
5	L3	4530	UR3	C2-N3	-2.14	1.34	1.39
5	L3	3818	OMU	O2-C2	-2.13	1.19	1.23
5	L3	2415	OMU	O2-C2	-2.13	1.19	1.23
5	L3	1773	OMU	O2-C2	-2.11	1.19	1.23
5	L3	1773	OMU	C4-N3	2.10	1.42	1.38
5	L3	1781	PSU	O4'-C1'	-2.08	1.41	1.43
5	L3	2415	OMU	C4-N3	2.06	1.42	1.38
5	L3	1781	PSU	C4-C5	-2.06	1.38	1.44
5	L3	3925	OMU	C4-N3	2.06	1.42	1.38
5	L3	4493	PSU	C4-C5	-2.04	1.38	1.44
5	L3	2837	OMU	C4-N3	2.01	1.42	1.38
5	L3	2787	A2M	C5-N7	-2.01	1.35	1.39
5	L3	4431	PSU	C4-C5	-2.00	1.38	1.44

All (498) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L3	3867	A2M	C5-C4-N3	-5.81	118.71	126.72
5	L3	1524	A2M	C5-C4-N3	-5.66	118.92	126.72
5	L3	2363	A2M	C5-C4-N3	-5.59	119.02	126.72
5	L3	4220	6MZ	C5-C4-N3	-5.59	119.02	126.72
5	L3	3718	A2M	C5-C4-N3	-5.59	119.03	126.72
5	L3	4306	OMU	C4-N3-C2	-5.57	119.69	126.61
5	L3	3825	A2M	C5-C4-N3	-5.57	119.05	126.72
5	L3	3760	A2M	C5-C4-N3	-5.56	119.06	126.72
5	L3	2787	A2M	C5-C4-N3	-5.55	119.08	126.72
5	L3	4571	A2M	C5-C4-N3	-5.54	119.08	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L3	2401	A2M	C5-C4-N3	-5.53	119.11	126.72
5	L3	2815	A2M	C5-C4-N3	-5.49	119.15	126.72
5	L3	2837	OMU	C4-N3-C2	-5.49	119.79	126.61
5	L3	1534	A2M	C5-C4-N3	-5.47	119.18	126.72
5	L3	4523	A2M	C5-C4-N3	-5.45	119.21	126.72
5	L3	1326	A2M	C5-C4-N3	-5.45	119.21	126.72
5	L3	400	A2M	C5-C4-N3	-5.43	119.24	126.72
5	L3	4498	OMU	C4-N3-C2	-5.41	119.90	126.61
5	L3	398	A2M	C5-C4-N3	-5.40	119.28	126.72
5	L3	1773	OMU	C4-N3-C2	-5.39	119.92	126.61
5	L3	3785	A2M	C5-C4-N3	-5.39	119.30	126.72
5	L3	2415	OMU	C4-N3-C2	-5.38	119.93	126.61
5	L3	4530	UR3	C4-N3-C2	-5.38	120.25	124.58
5	L3	3724	A2M	C5-C4-N3	-5.37	119.32	126.72
5	L3	3818	OMU	C4-N3-C2	-5.36	119.96	126.61
5	L3	4227	OMU	C4-N3-C2	-5.34	119.98	126.61
5	L3	3830	A2M	C5-C4-N3	-5.33	119.38	126.72
5	L3	3925	OMU	C4-N3-C2	-5.25	120.09	126.61
5	L3	1871	A2M	C5-C4-N3	-5.18	119.59	126.72
5	L3	3851	PSU	N1-C2-N3	5.07	120.52	115.17
5	L3	4471	PSU	N1-C2-N3	5.07	120.51	115.17
5	L3	3637	PSU	N1-C2-N3	5.05	120.50	115.17
5	L3	1782	PSU	N1-C2-N3	5.02	120.47	115.17
5	L3	4636	PSU	C4-N3-C2	-4.99	119.50	126.37
5	L3	4457	PSU	N1-C2-N3	4.98	120.42	115.17
5	L3	4636	PSU	N1-C2-N3	4.98	120.42	115.17
5	L3	4590	A2M	C5-C4-N3	-4.95	119.89	126.72
5	L3	1536	PSU	N1-C2-N3	4.94	120.38	115.17
5	L3	4361	PSU	N1-C2-N3	4.94	120.38	115.17
5	L3	3959	PSU	N1-C2-N3	4.94	120.38	115.17
5	L3	3637	PSU	C4-N3-C2	-4.94	119.57	126.37
5	L3	4552	PSU	N1-C2-N3	4.94	120.38	115.17
5	L3	4620	OMU	C4-N3-C2	-4.94	120.48	126.61
5	L3	1683	PSU	N1-C2-N3	4.94	120.38	115.17
5	L3	5001	PSU	N1-C2-N3	4.93	120.37	115.17
5	L3	4293	PSU	N1-C2-N3	4.92	120.36	115.17
5	L3	4299	PSU	N1-C2-N3	4.92	120.36	115.17
5	L3	4431	PSU	C4-N3-C2	-4.91	119.60	126.37
5	L3	4431	PSU	N1-C2-N3	4.91	120.34	115.17
5	L3	4471	PSU	C4-N3-C2	-4.90	119.62	126.37
5	L3	4689	PSU	N1-C2-N3	4.90	120.34	115.17
5	L3	3730	PSU	N1-C2-N3	4.90	120.33	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L3	2839	PSU	N1-C2-N3	4.90	120.33	115.17
5	L3	4532	PSU	N1-C2-N3	4.89	120.33	115.17
5	L3	4532	PSU	C4-N3-C2	-4.89	119.64	126.37
5	L3	3730	PSU	C4-N3-C2	-4.89	119.64	126.37
5	L3	4552	PSU	C4-N3-C2	-4.88	119.64	126.37
5	L3	1582	PSU	C4-N3-C2	-4.88	119.65	126.37
4	L1	55	PSU	N1-C2-N3	4.88	120.32	115.17
5	L3	1860	PSU	N1-C2-N3	4.88	120.31	115.17
5	L3	3758	PSU	C4-N3-C2	-4.88	119.65	126.37
5	L3	1536	PSU	C4-N3-C2	-4.87	119.66	126.37
5	L3	4403	PSU	N1-C2-N3	4.87	120.31	115.17
5	L3	4493	PSU	N1-C2-N3	4.87	120.31	115.17
5	L3	4972	PSU	N1-C2-N3	4.87	120.31	115.17
5	L3	4972	PSU	C4-N3-C2	-4.87	119.66	126.37
5	L3	3920	PSU	N1-C2-N3	4.87	120.30	115.17
4	L1	69	PSU	N1-C2-N3	4.86	120.30	115.17
5	L3	1683	PSU	C4-N3-C2	-4.86	119.68	126.37
4	L1	69	PSU	C4-N3-C2	-4.86	119.68	126.37
5	L3	1744	PSU	N1-C2-N3	4.86	120.29	115.17
5	L3	4361	PSU	C4-N3-C2	-4.85	119.68	126.37
5	L3	4493	PSU	C4-N3-C2	-4.85	119.68	126.37
5	L3	3758	PSU	N1-C2-N3	4.85	120.29	115.17
5	L3	3884	PSU	N1-C2-N3	4.85	120.29	115.17
5	L3	1677	PSU	C4-N3-C2	-4.85	119.69	126.37
5	L3	3959	PSU	C4-N3-C2	-4.85	119.69	126.37
5	L3	2508	PSU	C4-N3-C2	-4.85	119.69	126.37
5	L3	1781	PSU	N1-C2-N3	4.85	120.28	115.17
5	L3	3715	PSU	C4-N3-C2	-4.85	119.70	126.37
5	L3	4299	PSU	C4-N3-C2	-4.85	119.70	126.37
5	L3	3920	PSU	C4-N3-C2	-4.84	119.70	126.37
5	L3	1782	PSU	C4-N3-C2	-4.84	119.70	126.37
5	L3	4521	PSU	N1-C2-N3	4.84	120.27	115.17
5	L3	3867	A2M	N3-C4-N9	4.83	135.38	127.17
5	L3	3734	PSU	C4-N3-C2	-4.83	119.72	126.37
5	L3	4293	PSU	C4-N3-C2	-4.83	119.72	126.37
5	L3	4353	PSU	C4-N3-C2	-4.83	119.72	126.37
5	L3	1860	PSU	C4-N3-C2	-4.83	119.72	126.37
5	L3	4296	PSU	N1-C2-N3	4.82	120.25	115.17
5	L3	3715	PSU	N1-C2-N3	4.82	120.25	115.17
5	L3	1582	PSU	N1-C2-N3	4.82	120.25	115.17
4	L1	55	PSU	C4-N3-C2	-4.82	119.74	126.37
5	L3	3695	PSU	C4-N3-C2	-4.82	119.74	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L3	5001	PSU	C4-N3-C2	-4.82	119.74	126.37
5	L3	1677	PSU	N1-C2-N3	4.81	120.25	115.17
5	L3	3853	PSU	N1-C2-N3	4.81	120.24	115.17
5	L3	4457	PSU	C4-N3-C2	-4.81	119.75	126.37
5	L3	3768	PSU	N1-C2-N3	4.81	120.24	115.17
5	L3	1862	PSU	C4-N3-C2	-4.80	119.76	126.37
5	L3	3734	PSU	N1-C2-N3	4.80	120.23	115.17
5	L3	4353	PSU	N1-C2-N3	4.80	120.23	115.17
5	L3	3639	PSU	N1-C2-N3	4.80	120.23	115.17
5	L3	2508	PSU	N1-C2-N3	4.80	120.23	115.17
5	L3	4500	PSU	N1-C2-N3	4.80	120.23	115.17
5	L3	5010	PSU	N1-C2-N3	4.79	120.22	115.17
5	L3	4296	PSU	C4-N3-C2	-4.79	119.77	126.37
5	L3	3770	PSU	C4-N3-C2	-4.79	119.77	126.37
5	L3	3639	PSU	C4-N3-C2	-4.79	119.78	126.37
5	L3	4689	PSU	C4-N3-C2	-4.78	119.78	126.37
5	L3	4500	PSU	C4-N3-C2	-4.78	119.78	126.37
5	L3	4521	PSU	C4-N3-C2	-4.78	119.79	126.37
5	L3	4673	PSU	C4-N3-C2	-4.77	119.79	126.37
5	L3	4312	PSU	N1-C2-N3	4.77	120.20	115.17
5	L3	4403	PSU	C4-N3-C2	-4.77	119.80	126.37
5	L3	3884	PSU	C4-N3-C2	-4.76	119.81	126.37
5	L3	3764	PSU	N1-C2-N3	4.76	120.19	115.17
5	L3	5010	PSU	C4-N3-C2	-4.75	119.82	126.37
5	L3	3762	PSU	N1-C2-N3	4.75	120.18	115.17
5	L3	3770	PSU	N1-C2-N3	4.75	120.18	115.17
5	L3	2632	PSU	C4-N3-C2	-4.75	119.83	126.37
5	L3	3768	PSU	C4-N3-C2	-4.75	119.83	126.37
5	L3	2839	PSU	C4-N3-C2	-4.74	119.84	126.37
5	L3	4442	PSU	C4-N3-C2	-4.72	119.86	126.37
5	L3	3851	PSU	C4-N3-C2	-4.72	119.87	126.37
5	L3	4576	PSU	C4-N3-C2	-4.72	119.87	126.37
5	L3	1524	A2M	N3-C4-N9	4.71	135.18	127.17
5	L3	4312	PSU	C4-N3-C2	-4.71	119.88	126.37
5	L3	1862	PSU	N1-C2-N3	4.71	120.13	115.17
5	L3	3695	PSU	N1-C2-N3	4.71	120.13	115.17
5	L3	3764	PSU	C4-N3-C2	-4.70	119.89	126.37
5	L3	3844	PSU	N1-C2-N3	4.70	120.13	115.17
5	L3	3762	PSU	C4-N3-C2	-4.70	119.90	126.37
5	L3	4579	PSU	N1-C2-N3	4.70	120.12	115.17
5	L3	1744	PSU	C4-N3-C2	-4.70	119.90	126.37
5	L3	2787	A2M	N3-C4-N9	4.69	135.14	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L3	4576	PSU	N1-C2-N3	4.67	120.10	115.17
5	L3	4673	PSU	N1-C2-N3	4.67	120.09	115.17
5	L3	4220	6MZ	N3-C4-N9	4.67	135.11	127.17
5	L3	3825	A2M	N3-C4-N9	4.65	135.08	127.17
5	L3	1779	PSU	N1-C2-N3	4.65	120.07	115.17
5	L3	1779	PSU	C4-N3-C2	-4.65	119.97	126.37
5	L3	3853	PSU	C4-N3-C2	-4.65	119.97	126.37
5	L3	1781	PSU	C4-N3-C2	-4.65	119.97	126.37
5	L3	3760	A2M	N3-C4-N9	4.65	135.07	127.17
5	L3	4628	PSU	C4-N3-C2	-4.65	119.97	126.37
5	L3	4579	PSU	C4-N3-C2	-4.63	119.99	126.37
5	L3	4571	A2M	N3-C4-N9	4.63	135.04	127.17
5	L3	4442	PSU	N1-C2-N3	4.63	120.05	115.17
5	L3	2363	A2M	N3-C4-N9	4.62	135.02	127.17
5	L3	2632	PSU	N1-C2-N3	4.62	120.04	115.17
5	L3	2815	A2M	N3-C4-N9	4.60	135.00	127.17
5	L3	3844	PSU	C4-N3-C2	-4.58	120.06	126.37
5	L3	2401	A2M	N3-C4-N9	4.55	134.91	127.17
5	L3	4523	A2M	N3-C4-N9	4.55	134.91	127.17
5	L3	400	A2M	N3-C4-N9	4.53	134.88	127.17
5	L3	4628	PSU	N1-C2-N3	4.53	119.95	115.17
5	L3	3718	A2M	N3-C4-N9	4.53	134.87	127.17
5	L3	1534	A2M	N3-C4-N9	4.52	134.85	127.17
5	L3	398	A2M	N3-C4-N9	4.51	134.84	127.17
5	L3	3830	A2M	N3-C4-N9	4.51	134.84	127.17
5	L3	3785	A2M	N3-C4-N9	4.50	134.82	127.17
5	L3	3822	PSU	N1-C2-N3	4.48	119.89	115.17
5	L3	3822	PSU	C4-N3-C2	-4.46	120.23	126.37
5	L3	3724	A2M	N3-C4-N9	4.44	134.72	127.17
5	L3	1326	A2M	N3-C4-N9	4.40	134.65	127.17
5	L3	1871	A2M	N3-C4-N9	4.36	134.59	127.17
5	L3	1871	A2M	N3-C2-N1	-4.36	121.99	128.58
5	L3	4590	A2M	N3-C2-N1	-4.28	122.10	128.58
5	L3	400	A2M	N3-C2-N1	-4.18	122.25	128.58
5	L3	4590	A2M	N3-C4-N9	4.16	134.25	127.17
5	L3	3724	A2M	N3-C2-N1	-4.16	122.29	128.58
5	L3	3830	A2M	N3-C2-N1	-4.12	122.34	128.58
5	L3	2401	A2M	N3-C2-N1	-4.12	122.35	128.58
5	L3	1326	A2M	N3-C2-N1	-4.11	122.36	128.58
5	L3	398	A2M	N3-C2-N1	-4.08	122.40	128.58
5	L3	4220	6MZ	N1-C2-N3	-4.08	122.40	128.58
5	L3	1534	A2M	N3-C2-N1	-4.07	122.42	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L3	4306	OMU	N3-C2-N1	4.05	120.17	114.89
5	L3	2815	A2M	N3-C2-N1	-4.05	122.45	128.58
5	L3	3760	A2M	N3-C2-N1	-4.04	122.47	128.58
5	L3	2787	A2M	N3-C2-N1	-4.03	122.48	128.58
5	L3	4571	A2M	N3-C2-N1	-4.03	122.48	128.58
5	L3	4523	A2M	N3-C2-N1	-4.03	122.49	128.58
5	L3	3785	A2M	N3-C2-N1	-4.02	122.49	128.58
5	L3	2415	OMU	N3-C2-N1	4.00	120.10	114.89
5	L3	1773	OMU	N3-C2-N1	4.00	120.09	114.89
5	L3	4498	OMU	N3-C2-N1	3.99	120.08	114.89
5	L3	2837	OMU	N3-C2-N1	3.98	120.07	114.89
5	L3	3825	A2M	N3-C2-N1	-3.98	122.56	128.58
5	L3	2363	A2M	N3-C2-N1	-3.98	122.56	128.58
5	L3	3925	OMU	N3-C2-N1	3.95	120.04	114.89
5	L3	4227	OMU	N3-C2-N1	3.92	119.99	114.89
5	L3	1524	A2M	N3-C2-N1	-3.89	122.69	128.58
5	L3	3867	A2M	N3-C2-N1	-3.89	122.70	128.58
5	L3	3718	A2M	N3-C2-N1	-3.88	122.71	128.58
5	L3	4220	6MZ	C5-N7-C8	3.84	109.49	103.45
5	L3	2837	OMU	C5-C4-N3	3.82	120.16	114.80
5	L3	2815	A2M	C5-N7-C8	3.82	109.45	103.45
5	L3	2787	A2M	C5-N7-C8	3.81	109.44	103.45
5	L3	398	A2M	C5-N7-C8	3.80	109.42	103.45
5	L3	3785	A2M	C5-N7-C8	3.80	109.42	103.45
5	L3	3818	OMU	N3-C2-N1	3.80	119.84	114.89
5	L3	400	A2M	C5-N7-C8	3.79	109.40	103.45
5	L3	4523	A2M	C5-N7-C8	3.79	109.40	103.45
5	L3	4227	OMU	C5-C4-N3	3.78	120.10	114.80
5	L3	3825	A2M	C5-N7-C8	3.78	109.39	103.45
5	L3	2363	A2M	C5-N7-C8	3.78	109.39	103.45
5	L3	1534	A2M	C5-N7-C8	3.78	109.38	103.45
5	L3	2401	A2M	C5-N7-C8	3.77	109.38	103.45
5	L3	3818	OMU	C5-C4-N3	3.77	120.08	114.80
5	L3	4620	OMU	N3-C2-N1	3.74	119.77	114.89
5	L3	4590	A2M	C5-N7-C8	3.74	109.33	103.45
5	L3	4498	OMU	C5-C4-N3	3.74	120.04	114.80
5	L3	1773	OMU	C5-C4-N3	3.73	120.03	114.80
5	L3	3760	A2M	C5-N7-C8	3.73	109.31	103.45
5	L3	3867	A2M	C5-N7-C8	3.73	109.31	103.45
5	L3	4306	OMU	C5-C4-N3	3.73	120.02	114.80
5	L3	1524	A2M	C5-N7-C8	3.72	109.30	103.45
5	L3	1871	A2M	C5-N7-C8	3.72	109.29	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L3	2415	OMU	C5-C4-N3	3.70	119.98	114.80
5	L3	1326	A2M	C5-N7-C8	3.70	109.26	103.45
5	L3	3724	A2M	C5-N7-C8	3.68	109.23	103.45
5	L3	3830	A2M	C5-N7-C8	3.68	109.23	103.45
5	L3	3718	A2M	C5-N7-C8	3.66	109.20	103.45
5	L3	3925	OMU	C5-C4-N3	3.65	119.91	114.80
5	L3	4571	A2M	C5-N7-C8	3.65	109.18	103.45
5	L3	3867	A2M	C2-N3-C4	3.64	120.71	111.83
5	L3	4220	6MZ	C2-N3-C4	3.62	120.67	111.83
5	L3	2401	A2M	C2-N3-C4	3.62	120.67	111.83
5	L3	4620	OMU	C5-C4-N3	3.61	119.86	114.80
5	L3	3760	A2M	C2-N3-C4	3.61	120.65	111.83
5	L3	3825	A2M	C2-N3-C4	3.61	120.64	111.83
5	L3	4571	A2M	C2-N3-C4	3.60	120.63	111.83
5	L3	1534	A2M	C2-N3-C4	3.60	120.63	111.83
5	L3	2787	A2M	C2-N3-C4	3.60	120.62	111.83
5	L3	1524	A2M	C2-N3-C4	3.60	120.62	111.83
5	L3	400	A2M	C2-N3-C4	3.59	120.60	111.83
5	L3	2815	A2M	C2-N3-C4	3.58	120.57	111.83
5	L3	2363	A2M	C2-N3-C4	3.58	120.57	111.83
5	L3	1326	A2M	C2-N3-C4	3.57	120.56	111.83
5	L3	398	A2M	C2-N3-C4	3.56	120.53	111.83
5	L3	1871	A2M	C2-N3-C4	3.55	120.51	111.83
5	L3	3785	A2M	C2-N3-C4	3.55	120.50	111.83
5	L3	4523	A2M	C2-N3-C4	3.55	120.49	111.83
5	L3	3718	A2M	C2-N3-C4	3.54	120.48	111.83
5	L3	3724	A2M	C2-N3-C4	3.54	120.47	111.83
5	L3	3830	A2M	C2-N3-C4	3.51	120.40	111.83
5	L3	4590	A2M	C2-N3-C4	3.46	120.28	111.83
5	L3	4530	UR3	C5-C4-N3	3.36	119.46	115.04
5	L3	4220	6MZ	C9-N6-C6	-3.23	119.85	122.85
5	L3	3959	PSU	O2-C2-N1	-3.11	119.58	122.79
5	L3	4306	OMU	O4-C4-C5	-3.09	119.83	125.16
5	L3	1781	PSU	O2-C2-N1	-3.08	119.61	122.79
5	L3	3818	OMU	O4-C4-C5	-3.05	119.90	125.16
5	L3	4227	OMU	O4-C4-C5	-3.04	119.92	125.16
5	L3	1326	A2M	C4-C5-N7	-3.03	107.12	110.58
5	L3	3920	PSU	O2-C2-N1	-3.02	119.67	122.79
5	L3	2837	OMU	O4-C4-C5	-3.02	119.95	125.16
5	L3	4498	OMU	O4-C4-C5	-3.02	119.96	125.16
5	L3	2401	A2M	C4-C5-N7	-3.01	107.14	110.58
5	L3	4590	A2M	N9-C8-N7	-3.01	109.67	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L3	4689	PSU	O2-C2-N1	-2.99	119.70	122.79
5	L3	2363	A2M	C4-C5-N7	-2.99	107.16	110.58
5	L3	3718	A2M	C4-C5-N7	-2.99	107.17	110.58
5	L3	5010	PSU	O2-C2-N1	-2.98	119.72	122.79
5	L3	398	A2M	C4-C5-N7	-2.98	107.18	110.58
5	L3	1534	A2M	C4-C5-N7	-2.97	107.18	110.58
5	L3	4523	A2M	C4-C5-N7	-2.96	107.19	110.58
5	L3	3785	A2M	C4-C5-N7	-2.96	107.20	110.58
5	L3	1773	OMU	O4-C4-C5	-2.96	120.06	125.16
5	L3	3724	A2M	C4-C5-N7	-2.95	107.21	110.58
5	L3	2815	A2M	C4-C5-N7	-2.95	107.21	110.58
5	L3	3825	A2M	C4-C5-N7	-2.94	107.22	110.58
5	L3	1536	PSU	O2-C2-N1	-2.94	119.75	122.79
5	L3	3925	OMU	O4-C4-C5	-2.94	120.09	125.16
5	L3	4220	6MZ	C4-C5-N7	-2.93	107.23	110.58
5	L3	3853	PSU	O2-C2-N1	-2.92	119.77	122.79
5	L3	400	A2M	C4-C5-N7	-2.92	107.24	110.58
5	L3	4571	A2M	C4-C5-N7	-2.92	107.24	110.58
5	L3	1524	A2M	C4-C5-N7	-2.92	107.24	110.58
5	L3	2415	OMU	O4-C4-C5	-2.92	120.12	125.16
5	L3	2839	PSU	O2-C2-N1	-2.92	119.78	122.79
5	L3	3867	A2M	C4-C5-N7	-2.92	107.25	110.58
5	L3	4590	A2M	C4-C5-N7	-2.92	107.25	110.58
5	L3	1781	PSU	C6-N1-C2	-2.92	119.98	122.69
5	L3	3758	PSU	O2-C2-N1	-2.91	119.79	122.79
5	L3	5001	PSU	O2-C2-N1	-2.91	119.79	122.79
5	L3	4579	PSU	O2-C2-N1	-2.90	119.80	122.79
5	L3	1860	PSU	O2-C2-N1	-2.89	119.80	122.79
5	L3	2787	A2M	C4-C5-N7	-2.89	107.28	110.58
5	L3	3764	PSU	O2-C2-N1	-2.89	119.81	122.79
5	L3	2815	A2M	N9-C8-N7	-2.88	109.84	113.94
5	L3	1871	A2M	N9-C8-N7	-2.88	109.85	113.94
5	L3	400	A2M	N9-C8-N7	-2.88	109.85	113.94
5	L3	4403	PSU	O2-C2-N1	-2.86	119.84	122.79
5	L3	1871	A2M	C4-C5-N7	-2.86	107.31	110.58
5	L3	3760	A2M	C4-C5-N7	-2.86	107.31	110.58
5	L3	4431	PSU	O2-C2-N1	-2.86	119.84	122.79
5	L3	4293	PSU	O2-C2-N1	-2.85	119.85	122.79
5	L3	3730	PSU	O2-C2-N1	-2.84	119.86	122.79
5	L3	3851	PSU	O2-C2-N1	-2.84	119.86	122.79
5	L3	3785	A2M	N9-C8-N7	-2.84	109.90	113.94
5	L3	398	A2M	N9-C8-N7	-2.84	109.90	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L3	1779	PSU	O2-C2-N1	-2.84	119.86	122.79
5	L3	4457	PSU	O2-C2-N1	-2.84	119.86	122.79
5	L3	4636	PSU	O2-C2-N1	-2.84	119.86	122.79
5	L3	3830	A2M	C4-C5-N7	-2.83	107.34	110.58
5	L3	4361	PSU	O2-C2-N1	-2.83	119.86	122.79
5	L3	4579	PSU	C6-N1-C2	-2.83	120.07	122.69
5	L3	4523	A2M	N9-C8-N7	-2.82	109.93	113.94
5	L3	4312	PSU	O2-C2-N1	-2.82	119.88	122.79
5	L3	4500	PSU	O2-C2-N1	-2.82	119.88	122.79
5	L3	4442	PSU	O2-C2-N1	-2.81	119.89	122.79
5	L3	3639	PSU	O2-C2-N1	-2.81	119.89	122.79
5	L3	1782	PSU	O2-C2-N1	-2.80	119.90	122.79
5	L3	3825	A2M	N9-C8-N7	-2.80	109.96	113.94
5	L3	3734	PSU	O2-C2-N1	-2.80	119.90	122.79
5	L3	2787	A2M	N9-C8-N7	-2.80	109.96	113.94
5	L3	4689	PSU	C6-N1-C2	-2.80	120.09	122.69
5	L3	1677	PSU	O2-C2-N1	-2.80	119.90	122.79
5	L3	4471	PSU	O2-C2-N1	-2.79	119.91	122.79
5	L3	4299	PSU	C6-C5-C4	2.78	120.05	118.17
5	L3	1534	A2M	N9-C8-N7	-2.78	109.99	113.94
5	L3	1524	A2M	C2'-C1'-N9	-2.78	109.17	113.75
5	L3	4220	6MZ	N9-C8-N7	-2.78	109.99	113.94
5	L3	4457	PSU	C6-N1-C2	-2.78	120.11	122.69
5	L3	3830	A2M	N9-C8-N7	-2.78	110.00	113.94
5	L3	4620	OMU	O4-C4-C5	-2.78	120.37	125.16
5	L3	4628	PSU	O2-C2-N1	-2.78	119.92	122.79
5	L3	4972	PSU	O2-C2-N1	-2.78	119.92	122.79
5	L3	3851	PSU	C6-N1-C2	-2.78	120.11	122.69
5	L3	3768	PSU	O2-C2-N1	-2.76	119.94	122.79
5	L3	4493	PSU	O2-C2-N1	-2.76	119.94	122.79
5	L3	3715	PSU	O2-C2-N1	-2.76	119.94	122.79
5	L3	2401	A2M	N9-C8-N7	-2.76	110.02	113.94
4	L1	69	PSU	O2-C2-N1	-2.76	119.94	122.79
5	L3	4296	PSU	O2-C2-N1	-2.76	119.94	122.79
5	L3	1744	PSU	O2-C2-N1	-2.75	119.95	122.79
5	L3	3695	PSU	O2-C2-N1	-2.74	119.96	122.79
5	L3	4552	PSU	O2-C2-N1	-2.74	119.96	122.79
5	L3	3760	A2M	N9-C8-N7	-2.74	110.05	113.94
5	L3	4299	PSU	O2-C2-N1	-2.74	119.97	122.79
5	L3	3884	PSU	O2-C2-N1	-2.73	119.97	122.79
5	L3	2839	PSU	C6-N1-C2	-2.73	120.16	122.69
5	L3	3853	PSU	C6-N1-C2	-2.73	120.16	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L3	1524	A2M	N9-C8-N7	-2.72	110.07	113.94
5	L3	3762	PSU	O2-C2-N1	-2.72	119.98	122.79
5	L3	4673	PSU	O2-C2-N1	-2.72	119.98	122.79
5	L3	4521	PSU	O2-C2-N1	-2.72	119.98	122.79
5	L3	3822	PSU	O2-C2-N1	-2.71	119.99	122.79
5	L3	3724	A2M	N9-C8-N7	-2.70	110.10	113.94
5	L3	4471	PSU	C6-N1-C2	-2.70	120.19	122.69
5	L3	3851	PSU	C6-C5-C4	2.69	119.99	118.17
5	L3	4353	PSU	O2-C2-N1	-2.68	120.02	122.79
4	L1	55	PSU	O2-C2-N1	-2.68	120.02	122.79
5	L3	1326	A2M	N9-C8-N7	-2.68	110.14	113.94
5	L3	4532	PSU	O2-C2-N1	-2.67	120.03	122.79
5	L3	3762	PSU	C6-N1-C2	-2.67	120.22	122.69
4	L1	69	PSU	C6-C5-C4	2.66	119.97	118.17
5	L3	2363	A2M	N9-C8-N7	-2.64	110.19	113.94
5	L3	3768	PSU	C6-N1-C2	-2.64	120.24	122.69
5	L3	2508	PSU	O2-C2-N1	-2.64	120.07	122.79
5	L3	4293	PSU	C6-N1-C2	-2.64	120.24	122.69
5	L3	1744	PSU	C6-N1-C2	-2.64	120.25	122.69
5	L3	1683	PSU	O2-C2-N1	-2.63	120.07	122.79
5	L3	3639	PSU	C6-N1-C2	-2.63	120.25	122.69
5	L3	3637	PSU	C6-C5-C4	2.62	119.94	118.17
5	L3	1862	PSU	O2-C2-N1	-2.62	120.08	122.79
5	L3	1782	PSU	C6-N1-C2	-2.62	120.26	122.69
5	L3	5001	PSU	C6-N1-C2	-2.61	120.27	122.69
5	L3	3884	PSU	C6-N1-C2	-2.61	120.27	122.69
5	L3	3844	PSU	C6-N1-C2	-2.59	120.28	122.69
5	L3	4521	PSU	C6-N1-C2	-2.59	120.28	122.69
5	L3	4361	PSU	C6-C5-C4	2.59	119.92	118.17
5	L3	3770	PSU	O2-C2-N1	-2.59	120.12	122.79
5	L3	1536	PSU	C6-N1-C2	-2.58	120.30	122.69
5	L3	1683	PSU	C6-N1-C2	-2.58	120.30	122.69
5	L3	4403	PSU	C6-N1-C2	-2.58	120.30	122.69
5	L3	3867	A2M	N9-C8-N7	-2.58	110.28	113.94
5	L3	4493	PSU	C6-C5-C4	2.58	119.91	118.17
5	L3	4493	PSU	C6-N1-C2	-2.57	120.30	122.69
5	L3	400	A2M	C2'-C1'-N9	-2.57	109.52	113.75
5	L3	4312	PSU	C6-N1-C2	-2.57	120.31	122.69
5	L3	4361	PSU	C6-N1-C2	-2.57	120.31	122.69
5	L3	3959	PSU	C6-N1-C2	-2.56	120.31	122.69
5	L3	5010	PSU	C6-N1-C2	-2.56	120.31	122.69
5	L3	4576	PSU	O2-C2-N1	-2.55	120.15	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L3	3844	PSU	O2-C2-N1	-2.55	120.15	122.79
5	L3	3764	PSU	C6-N1-C2	-2.55	120.32	122.69
5	L3	3920	PSU	C6-N1-C2	-2.55	120.32	122.69
5	L3	398	A2M	C2'-C1'-N9	-2.55	109.56	113.75
5	L3	3637	PSU	C6-N1-C2	-2.54	120.33	122.69
5	L3	3730	PSU	C6-N1-C2	-2.52	120.35	122.69
4	L1	55	PSU	C6-N1-C2	-2.52	120.35	122.69
5	L3	4431	PSU	C6-N1-C2	-2.52	120.35	122.69
5	L3	4571	A2M	N9-C8-N7	-2.52	110.36	113.94
5	L3	3715	PSU	C6-C5-C4	2.52	119.87	118.17
4	L1	55	PSU	C6-C5-C4	2.51	119.87	118.17
5	L3	4636	PSU	C6-C5-C4	2.50	119.86	118.17
5	L3	4972	PSU	C6-N1-C2	-2.50	120.37	122.69
5	L3	1860	PSU	C6-N1-C2	-2.49	120.38	122.69
4	L1	69	PSU	C6-N1-C2	-2.49	120.38	122.69
5	L3	4552	PSU	C6-N1-C2	-2.49	120.38	122.69
5	L3	1779	PSU	C6-N1-C2	-2.48	120.39	122.69
5	L3	3734	PSU	C6-C5-C4	2.48	119.85	118.17
5	L3	4500	PSU	C6-N1-C2	-2.48	120.39	122.69
5	L3	3770	PSU	C6-N1-C2	-2.48	120.39	122.69
5	L3	3822	PSU	C6-N1-C2	-2.48	120.39	122.69
5	L3	4296	PSU	C6-N1-C2	-2.47	120.40	122.69
5	L3	4628	PSU	C6-N1-C2	-2.46	120.40	122.69
5	L3	4299	PSU	C6-N1-C2	-2.46	120.41	122.69
5	L3	4457	PSU	C6-C5-C4	2.46	119.83	118.17
5	L3	1582	PSU	O2-C2-N1	-2.45	120.26	122.79
5	L3	3715	PSU	C6-N1-C2	-2.45	120.42	122.69
5	L3	3718	A2M	N9-C8-N7	-2.45	110.47	113.94
5	L3	4532	PSU	C6-N1-C2	-2.44	120.42	122.69
5	L3	2632	PSU	O2-C2-N1	-2.44	120.27	122.79
5	L3	4471	PSU	C6-C5-C4	2.44	119.82	118.17
5	L3	3734	PSU	C6-N1-C2	-2.43	120.43	122.69
5	L3	1582	PSU	C6-C5-C4	2.42	119.80	118.17
5	L3	4532	PSU	C6-C5-C4	2.41	119.80	118.17
5	L3	4431	PSU	C6-C5-C4	2.41	119.80	118.17
5	L3	1782	PSU	C6-C5-C4	2.40	119.80	118.17
5	L3	3758	PSU	C6-N1-C2	-2.40	120.46	122.69
5	L3	4442	PSU	C6-N1-C2	-2.40	120.46	122.69
5	L3	4673	PSU	C6-N1-C2	-2.39	120.47	122.69
5	L3	1677	PSU	C6-C5-C4	2.39	119.79	118.17
5	L3	3730	PSU	C6-C5-C4	2.39	119.79	118.17
5	L3	4576	PSU	C6-N1-C2	-2.39	120.47	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L3	4353	PSU	C6-N1-C2	-2.39	120.47	122.69
5	L3	4552	PSU	C6-C5-C4	2.38	119.78	118.17
5	L3	1860	PSU	C6-C5-C4	2.38	119.78	118.17
5	L3	2508	PSU	C6-N1-C2	-2.38	120.48	122.69
5	L3	1871	A2M	C2'-C1'-N9	-2.38	109.84	113.75
5	L3	1683	PSU	C6-C5-C4	2.37	119.77	118.17
5	L3	3844	PSU	C6-C5-C4	2.37	119.77	118.17
4	L1	69	PSU	O4'-C1'-C2'	2.35	108.40	105.15
5	L3	4636	PSU	C6-N1-C2	-2.35	120.51	122.69
5	L3	3959	PSU	C6-C5-C4	2.34	119.75	118.17
5	L3	4403	PSU	C6-C5-C4	2.34	119.75	118.17
5	L3	4972	PSU	C6-C5-C4	2.34	119.75	118.17
5	L3	1677	PSU	C6-N1-C2	-2.33	120.53	122.69
5	L3	4353	PSU	C6-C5-C4	2.33	119.74	118.17
5	L3	3758	PSU	C6-C5-C4	2.33	119.74	118.17
5	L3	2632	PSU	C6-N1-C2	-2.32	120.54	122.69
5	L3	1536	PSU	C6-C5-C4	2.32	119.74	118.17
5	L3	1862	PSU	C6-N1-C2	-2.31	120.55	122.69
5	L3	1781	PSU	C6-C5-C4	2.31	119.73	118.17
5	L3	2401	A2M	C2'-C1'-N9	-2.31	109.96	113.75
5	L3	1322	1MA	N1-C6-N6	2.30	125.50	119.71
5	L3	3695	PSU	C6-N1-C2	-2.30	120.56	122.69
5	L3	3768	PSU	C6-C5-C4	2.29	119.72	118.17
5	L3	4306	OMU	O2-C2-N1	-2.28	119.83	122.80
5	L3	5001	PSU	C6-C5-C4	2.27	119.71	118.17
5	L3	5010	PSU	C6-C5-C4	2.27	119.70	118.17
5	L3	3695	PSU	C6-C5-C4	2.26	119.70	118.17
5	L3	4500	PSU	C6-C5-C4	2.25	119.69	118.17
5	L3	3718	A2M	C2'-C1'-N9	-2.24	110.07	113.75
5	L3	3818	OMU	O2-C2-N1	-2.23	119.89	122.80
5	L3	3637	PSU	O2-C2-N1	-2.23	120.49	122.79
5	L3	2415	OMU	O2-C2-N1	-2.22	119.91	122.80
5	L3	2839	PSU	C6-C5-C4	2.22	119.67	118.17
5	L3	1582	PSU	C6-N1-C2	-2.22	120.63	122.69
5	L3	4299	PSU	O4'-C1'-C2'	2.21	108.21	105.15
5	L3	3925	OMU	O2-C2-N1	-2.20	119.94	122.80
5	L3	2508	PSU	C6-C5-C4	2.19	119.65	118.17
5	L3	1744	PSU	C6-C5-C4	2.18	119.65	118.17
5	L3	1677	PSU	O4'-C1'-C2'	2.17	108.16	105.15
5	L3	3762	PSU	C6-C5-C4	2.17	119.64	118.17
5	L3	3734	PSU	O4'-C1'-C2'	2.16	108.13	105.15
5	L3	2837	OMU	O2-C2-N1	-2.15	120.00	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L3	4293	PSU	C6-C5-C4	2.15	119.62	118.17
5	L3	3695	PSU	O4'-C1'-C2'	2.14	108.11	105.15
5	L3	4498	OMU	O2-C2-N1	-2.13	120.02	122.80
5	L3	4521	PSU	C6-C5-C4	2.13	119.61	118.17
5	L3	4227	OMU	O2-C2-N1	-2.12	120.04	122.80
5	L3	3830	A2M	C2'-C1'-N9	-2.12	110.27	113.75
5	L3	1773	OMU	O2-C2-N1	-2.10	120.06	122.80
5	L3	4296	PSU	C6-C5-C4	2.08	119.58	118.17
5	L3	3920	PSU	C6-C5-C4	2.06	119.56	118.17
5	L3	4620	OMU	O2-C2-N1	-2.06	120.12	122.80
5	L3	3715	PSU	O4'-C1'-C2'	2.06	108.00	105.15
5	L3	4576	PSU	O4'-C1'-C2'	2.06	108.00	105.15
5	L3	4673	PSU	C6-C5-C4	2.06	119.56	118.17
5	L3	4590	A2M	C4-N9-C8	2.05	107.89	105.74
5	L3	4403	PSU	O4'-C1'-C2'	2.05	107.99	105.15
24	LN	245	HIC	NE2-CE1-ND1	-2.04	111.88	112.66
5	L3	4523	A2M	C2'-C1'-N9	-2.04	110.40	113.75
5	L3	4312	PSU	C6-C5-C4	2.03	119.55	118.17
5	L3	4628	PSU	O4'-C1'-C2'	2.03	107.96	105.15
5	L3	3639	PSU	C6-C5-C4	2.03	119.54	118.17
5	L3	2815	A2M	C2'-C1'-N9	-2.02	110.42	113.75
5	L3	3920	PSU	O4'-C1'-C2'	2.01	107.94	105.15
5	L3	4576	PSU	C6-C5-C4	2.01	119.53	118.17
5	L3	2351	OMC	C1'-N1-C2	2.01	122.87	118.44
5	L3	1862	PSU	C6-C5-C4	2.00	119.53	118.17
5	L3	4442	PSU	C6-C5-C4	2.00	119.53	118.17

There are no chirality outliers.

All (120) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L1	75	OMG	C1'-C2'-O2'-CM2
5	L3	398	A2M	C1'-C2'-O2'-CM'
5	L3	400	A2M	C1'-C2'-O2'-CM'
5	L3	1316	OMG	C1'-C2'-O2'-CM2
5	L3	1322	1MA	O4'-C4'-C5'-O5'
5	L3	1326	A2M	C1'-C2'-O2'-CM'
5	L3	1340	OMC	C1'-C2'-O2'-CM2
5	L3	1744	PSU	O4'-C4'-C5'-O5'
5	L3	1760	OMG	C1'-C2'-O2'-CM2
5	L3	1773	OMU	C1'-C2'-O2'-CM2
5	L3	2351	OMC	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
5	L3	2363	A2M	C1'-C2'-O2'-CM'
5	L3	2364	OMG	C1'-C2'-O2'-CM2
5	L3	2422	OMC	C1'-C2'-O2'-CM2
5	L3	2424	OMG	O4'-C4'-C5'-O5'
5	L3	2424	OMG	C1'-C2'-O2'-CM2
5	L3	2837	OMU	C1'-C2'-O2'-CM2
5	L3	2861	OMC	C1'-C2'-O2'-CM2
5	L3	3627	OMG	C1'-C2'-O2'-CM2
5	L3	3701	OMC	C2'-C1'-N1-C2
5	L3	3701	OMC	C2'-C1'-N1-C6
5	L3	3718	A2M	C1'-C2'-O2'-CM'
5	L3	3724	A2M	C1'-C2'-O2'-CM'
5	L3	3744	OMG	C1'-C2'-O2'-CM2
5	L3	3782	5MC	O4'-C4'-C5'-O5'
5	L3	3785	A2M	C1'-C2'-O2'-CM'
5	L3	3808	OMC	C1'-C2'-O2'-CM2
5	L3	3822	PSU	C2'-C1'-C5-C4
5	L3	3825	A2M	C1'-C2'-O2'-CM'
5	L3	3841	OMC	C1'-C2'-O2'-CM2
5	L3	3867	A2M	O4'-C4'-C5'-O5'
5	L3	3867	A2M	C3'-C4'-C5'-O5'
5	L3	3867	A2M	C1'-C2'-O2'-CM'
5	L3	3887	OMC	O4'-C4'-C5'-O5'
5	L3	3899	OMG	C1'-C2'-O2'-CM2
5	L3	3925	OMU	C1'-C2'-O2'-CM2
5	L3	4054	OMC	C1'-C2'-O2'-CM2
5	L3	4220	6MZ	C5-C6-N6-C9
5	L3	4220	6MZ	N1-C6-N6-C9
5	L3	4220	6MZ	C4'-C5'-O5'-P
5	L3	4306	OMU	C1'-C2'-O2'-CM2
5	L3	4370	OMG	C1'-C2'-O2'-CM2
5	L3	4392	OMG	C1'-C2'-O2'-CM2
5	L3	4456	OMC	C1'-C2'-O2'-CM2
5	L3	4500	PSU	O4'-C1'-C5-C4
5	L3	4500	PSU	C2'-C1'-C5-C6
5	L3	4500	PSU	O4'-C1'-C5-C6
5	L3	4523	A2M	O4'-C4'-C5'-O5'
5	L3	4571	A2M	C1'-C2'-O2'-CM'
5	L3	4590	A2M	O4'-C4'-C5'-O5'
5	L3	4590	A2M	C3'-C4'-C5'-O5'
5	L3	4590	A2M	C1'-C2'-O2'-CM'
5	L3	4636	PSU	C2'-C1'-C5-C4

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Mol	Chain	Res	Type	Atoms
5	L3	4637	OMG	O4'-C4'-C5'-O5'
5	L3	4637	OMG	C1'-C2'-O2'-CM2
5	L3	2787	A2M	C3'-C4'-C5'-O5'
5	L3	3782	5MC	C3'-C4'-C5'-O5'
5	L3	3887	OMC	C3'-C4'-C5'-O5'
5	L3	4220	6MZ	C3'-C4'-C5'-O5'
5	L3	4618	OMG	O4'-C4'-C5'-O5'
5	L3	1744	PSU	C3'-C4'-C5'-O5'
5	L3	1781	PSU	O4'-C4'-C5'-O5'
5	L3	2401	A2M	O4'-C4'-C5'-O5'
5	L3	2401	A2M	C3'-C4'-C5'-O5'
5	L3	4500	PSU	C3'-C4'-C5'-O5'
5	L3	4500	PSU	O4'-C4'-C5'-O5'
5	L3	4523	A2M	C3'-C4'-C5'-O5'
5	L3	1322	1MA	C3'-C4'-C5'-O5'
5	L3	1781	PSU	C3'-C4'-C5'-O5'
5	L3	2876	OMG	C3'-C4'-C5'-O5'
5	L3	4498	OMU	O4'-C4'-C5'-O5'
5	L3	4590	A2M	C4'-C5'-O5'-P
5	L3	2424	OMG	C3'-C4'-C5'-O5'
5	L3	4296	PSU	C3'-C4'-C5'-O5'
5	L3	4618	OMG	C3'-C4'-C5'-O5'
5	L3	4637	OMG	C3'-C4'-C5'-O5'
5	L3	2787	A2M	O4'-C4'-C5'-O5'
5	L3	2876	OMG	O4'-C4'-C5'-O5'
5	L3	4220	6MZ	O4'-C4'-C5'-O5'
5	L3	4296	PSU	O4'-C4'-C5'-O5'
5	L3	2787	A2M	C2'-C1'-N9-C8
5	L3	4498	OMU	C3'-C4'-C5'-O5'
5	L3	2415	OMU	O4'-C4'-C5'-O5'
24	LN	245	HIC	C-CA-CB-CG
5	L3	2401	A2M	C3'-C2'-O2'-CM'
5	L3	4498	OMU	C2'-C1'-N1-C6
5	L3	4521	PSU	O4'-C1'-C5-C4
5	L3	2787	A2M	C2'-C1'-N9-C4
5	L3	4499	OMG	C3'-C4'-C5'-O5'
24	LN	245	HIC	CA-CB-CG-ND1
5	L3	3701	OMC	O4'-C1'-N1-C6
5	L3	4499	OMG	O4'-C4'-C5'-O5'
24	LN	245	HIC	CA-CB-CG-CD2
5	L3	3701	OMC	O4'-C1'-N1-C2
5	L3	3785	A2M	C3'-C2'-O2'-CM'

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Mol	Chain	Res	Type	Atoms
5	L3	1326	A2M	C3'-C4'-C5'-O5'
5	L3	3785	A2M	O4'-C4'-C5'-O5'
5	L3	4498	OMU	O4'-C1'-N1-C6
5	L3	3867	A2M	C4'-C5'-O5'-P
5	L3	2401	A2M	C1'-C2'-O2'-CM'
5	L3	3792	OMG	C1'-C2'-O2'-CM2
5	L3	4042	OMG	C1'-C2'-O2'-CM2
5	L3	3844	PSU	C4'-C5'-O5'-P
5	L3	4521	PSU	O4'-C1'-C5-C6
5	L3	1522	OMG	C3'-C2'-O2'-CM2
5	L3	4227	OMU	C3'-C4'-C5'-O5'
5	L3	2787	A2M	O4'-C1'-N9-C8
5	L3	2364	OMG	O4'-C4'-C5'-O5'
5	L3	4636	PSU	O4'-C4'-C5'-O5'
5	L3	3822	PSU	C2'-C1'-C5-C6
5	L3	4220	6MZ	O4'-C1'-N9-C8
5	L3	2351	OMC	C2'-C1'-N1-C6
5	L3	3818	OMU	C3'-C2'-O2'-CM2
5	L3	1326	A2M	O4'-C4'-C5'-O5'
5	L3	4498	OMU	O4'-C1'-N1-C2
5	L3	2415	OMU	C3'-C4'-C5'-O5'
5	L3	1534	A2M	C4'-C5'-O5'-P
5	L3	4636	PSU	C4'-C5'-O5'-P
5	L3	2351	OMC	O4'-C4'-C5'-O5'
5	L3	2422	OMC	O4'-C4'-C5'-O5'

There are no ring outliers.

68 monomers are involved in 111 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L3	3718	A2M	4	0
5	L3	4623	OMG	2	0
5	L3	3695	PSU	2	0
5	L3	5010	PSU	1	0
5	L3	4228	OMG	1	0
5	L3	3851	PSU	1	0
5	L3	2804	OMC	1	0
5	L3	1326	A2M	4	0
5	L3	1322	1MA	2	0
5	L3	1524	A2M	1	0
5	L3	4590	A2M	2	0
5	L3	1862	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L3	3867	A2M	4	0
5	L3	3782	5MC	1	0
5	L3	1683	PSU	2	0
5	L3	2424	OMG	1	0
5	L3	2632	PSU	1	0
5	L3	2861	OMC	1	0
5	L3	3734	PSU	1	0
5	L3	1522	OMG	2	0
5	L3	2422	OMC	2	0
5	L3	3818	OMU	1	0
5	L3	4456	OMC	2	0
5	L3	2364	OMG	2	0
5	L3	4571	A2M	1	0
5	L3	398	A2M	1	0
5	L3	4637	OMG	2	0
5	L3	2837	OMU	1	0
5	L3	3925	OMU	3	0
5	L3	2351	OMC	2	0
5	L3	3770	PSU	2	0
5	L3	2824	OMC	1	0
5	L3	4353	PSU	1	0
5	L3	3822	PSU	1	0
5	L3	2363	A2M	3	0
5	L3	3760	A2M	1	0
5	L3	1760	OMG	1	0
5	L3	1534	A2M	1	0
5	L3	1340	OMC	1	0
5	L3	4536	OMC	3	0
4	L1	75	OMG	3	0
5	L3	1316	OMG	1	0
5	L3	1625	OMG	1	0
4	L1	69	PSU	2	0
5	L3	5001	PSU	2	0
5	L3	1773	OMU	3	0
5	L3	2815	A2M	1	0
5	L3	3724	A2M	1	0
5	L3	4306	OMU	4	0
5	L3	1677	PSU	2	0
5	L3	4227	OMU	2	0
5	L3	4220	6MZ	3	0
5	L3	4042	OMG	3	0
5	L3	3744	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L3	4530	UR3	1	0
5	L3	4299	PSU	2	0
5	L3	4620	OMU	1	0
5	L3	4370	OMG	1	0
5	L3	3808	OMC	2	0
5	L3	4457	PSU	2	0
5	L3	3792	OMG	1	0
5	L3	3841	OMC	1	0
5	L3	3830	A2M	1	0
5	L3	4442	PSU	1	0
5	L3	2415	OMU	1	0
5	L3	4392	OMG	1	0
5	L3	2876	OMG	1	0
5	L3	3715	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 109 ligands modelled in this entry, 107 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
66	GDP	SR	1001	65,62	29,30,30	3.03	12 (41%)	45,47,47	2.66	17 (37%)
64	GTP	NC	1000	65,62	33,34,34	3.23	15 (45%)	50,54,54	1.77	13 (26%)

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
66	GDP	SR	1001	65,62	-	0/16/32/32	0/3/3/3
64	GTP	NC	1000	65,62	-	3/22/38/38	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	SR	1001	GDP	O6-C6	8.84	1.40	1.23
64	NC	1000	GTP	O6-C6	8.72	1.40	1.23
64	NC	1000	GTP	C5-N7	6.57	1.52	1.39
66	SR	1001	GDP	C5-N7	6.50	1.52	1.39
66	SR	1001	GDP	PA-O3A	5.18	1.65	1.59
64	NC	1000	GTP	PB-O3A	5.12	1.65	1.59
64	NC	1000	GTP	PA-O3A	4.99	1.64	1.59
64	NC	1000	GTP	PB-O3B	4.90	1.64	1.59
64	NC	1000	GTP	C2-N2	4.79	1.45	1.34
66	SR	1001	GDP	C2-N2	4.78	1.45	1.34
64	NC	1000	GTP	C2-N1	4.58	1.48	1.37
64	NC	1000	GTP	C2-N3	4.30	1.43	1.33
64	NC	1000	GTP	C8-N9	-4.16	1.28	1.37
66	SR	1001	GDP	C8-N9	-4.04	1.28	1.37
66	SR	1001	GDP	C4-N9	-3.87	1.28	1.38
66	SR	1001	GDP	C5-C4	3.75	1.49	1.38
64	NC	1000	GTP	C4-N9	-3.65	1.28	1.38
66	SR	1001	GDP	C4-N3	2.85	1.40	1.34
64	NC	1000	GTP	O4'-C1'	2.59	1.48	1.42
64	NC	1000	GTP	C2'-C3'	-2.43	1.46	1.53
64	NC	1000	GTP	C4-N3	2.38	1.39	1.34
66	SR	1001	GDP	PB-O2B	-2.30	1.46	1.54
64	NC	1000	GTP	PG-O3G	-2.30	1.46	1.54
66	SR	1001	GDP	PB-O3B	-2.28	1.46	1.54
64	NC	1000	GTP	PG-O2G	-2.27	1.46	1.54
66	SR	1001	GDP	O4'-C1'	2.18	1.47	1.42
66	SR	1001	GDP	C2'-C3'	-2.14	1.47	1.53

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	SR	1001	GDP	C8-N9-C4	7.84	120.71	106.03
64	NC	1000	GTP	C8-N9-C4	6.75	118.68	106.03
66	SR	1001	GDP	N9-C4-N3	6.70	139.35	125.95
66	SR	1001	GDP	C5-C4-N3	-6.69	117.74	128.39
66	SR	1001	GDP	C2-N3-C4	5.31	121.45	112.30
66	SR	1001	GDP	C6-C5-N7	4.73	138.89	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	SR	1001	GDP	C4-C5-N7	-4.55	103.47	110.67
64	NC	1000	GTP	C2-N1-C6	-3.36	119.01	125.11
66	SR	1001	GDP	N9-C8-N7	-3.04	107.76	113.40
66	SR	1001	GDP	C2-N1-C6	-2.99	119.69	125.11
66	SR	1001	GDP	O2B-PB-O3A	2.91	114.39	104.64
64	NC	1000	GTP	O3G-PG-O3B	2.90	114.37	104.64
64	NC	1000	GTP	O2G-PG-O3B	2.83	114.12	104.64
66	SR	1001	GDP	O3B-PB-O3A	2.81	114.06	104.64
66	SR	1001	GDP	C1'-N9-C4	-2.63	118.70	126.49
66	SR	1001	GDP	C5-C6-N1	2.61	119.89	113.25
66	SR	1001	GDP	C3'-C2'-C1'	2.58	106.34	101.46
64	NC	1000	GTP	N9-C4-N3	2.53	131.02	125.95
64	NC	1000	GTP	C5-C6-N1	2.52	119.66	113.25
66	SR	1001	GDP	O6-C6-C5	-2.46	120.05	126.53
64	NC	1000	GTP	O6-C6-C5	-2.42	120.13	126.53
64	NC	1000	GTP	O2A-PA-O1A	-2.40	101.26	112.44
66	SR	1001	GDP	O2A-PA-O1A	-2.37	101.42	112.44
66	SR	1001	GDP	C2'-C3'-C4'	2.35	107.14	102.61
64	NC	1000	GTP	O2B-PB-O1B	-2.32	101.67	112.44
66	SR	1001	GDP	C1'-N9-C8	-2.17	120.55	126.73
64	NC	1000	GTP	C3'-C2'-C1'	2.15	105.53	101.46
64	NC	1000	GTP	C1'-N9-C8	-2.11	120.74	126.73
64	NC	1000	GTP	C8-N7-C5	-2.04	100.62	104.26
64	NC	1000	GTP	C1'-N9-C4	-2.01	120.56	126.49

There are no chirality outliers.

All (3) torsion outliers are listed below:

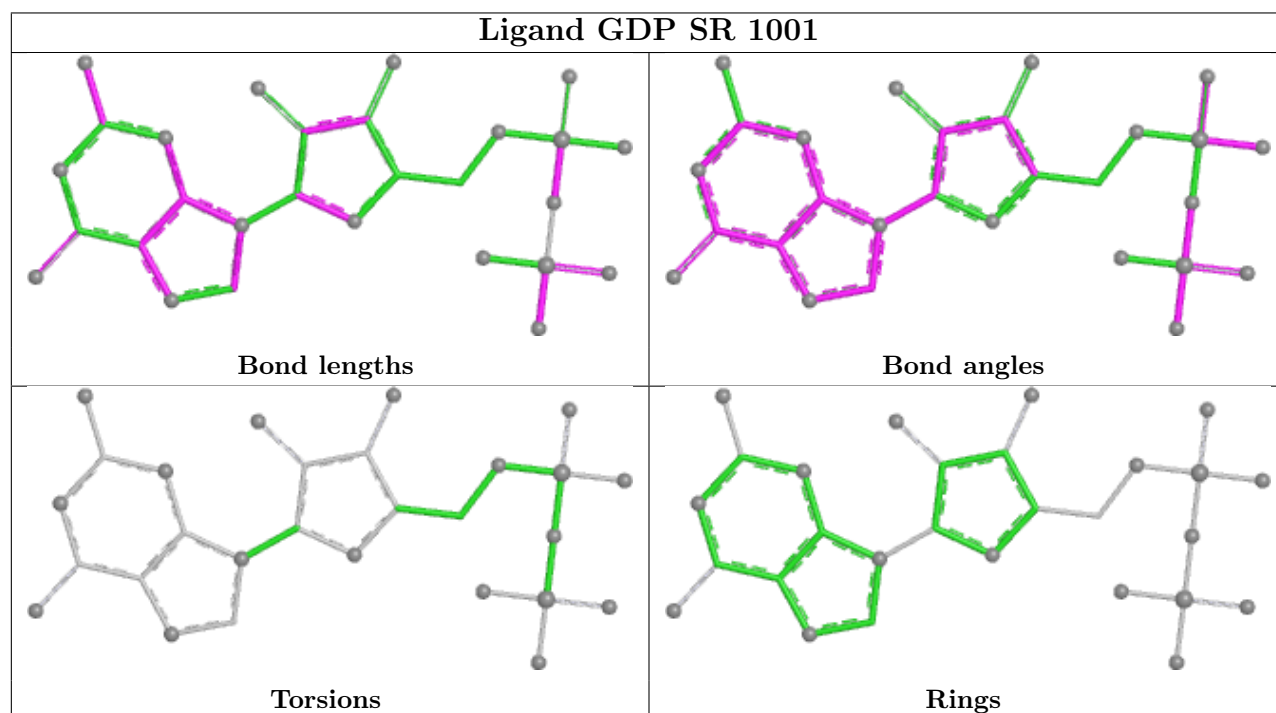
Mol	Chain	Res	Type	Atoms
64	NC	1000	GTP	PB-O3A-PA-O1A
64	NC	1000	GTP	O4'-C4'-C5'-O5'
64	NC	1000	GTP	PG-O3B-PB-O2B

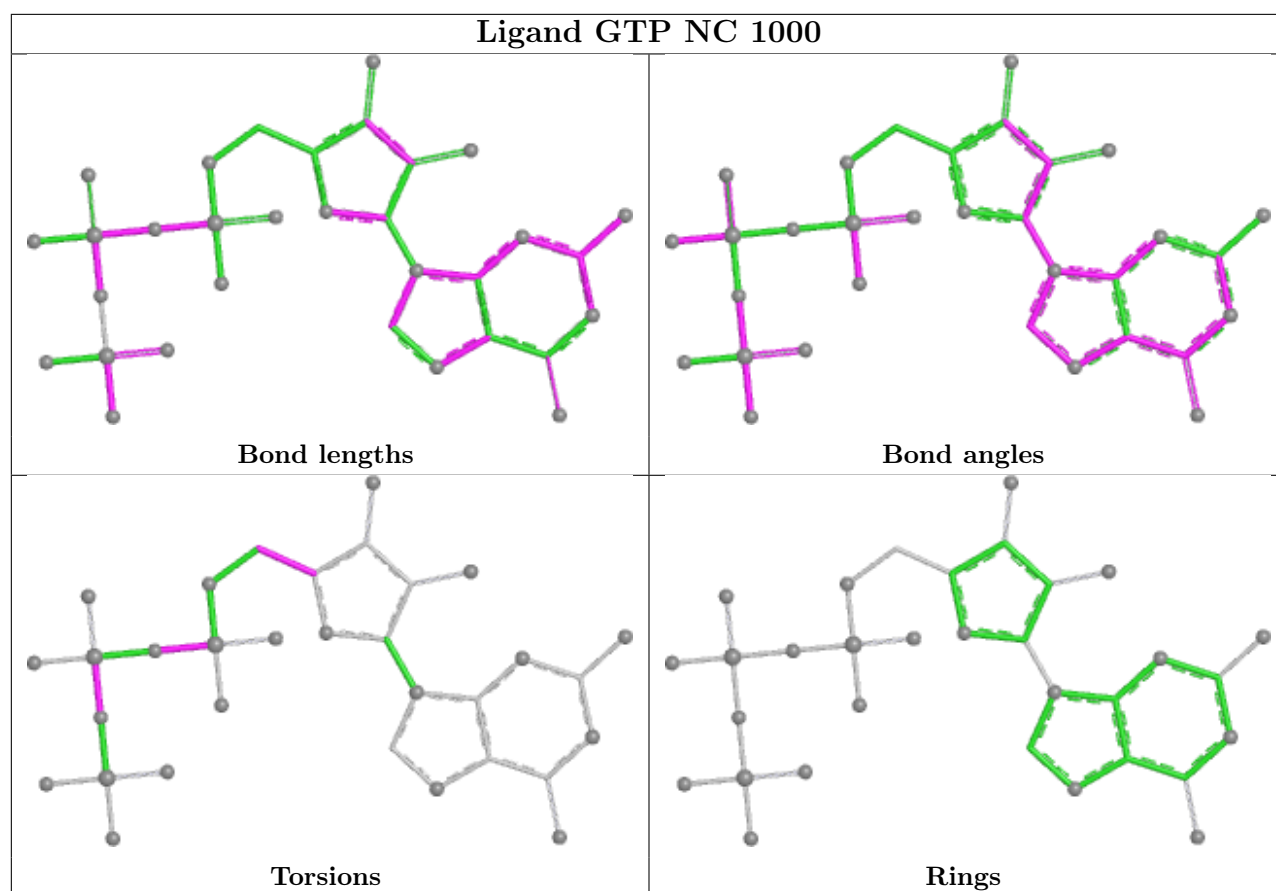
There are no ring outliers.

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.

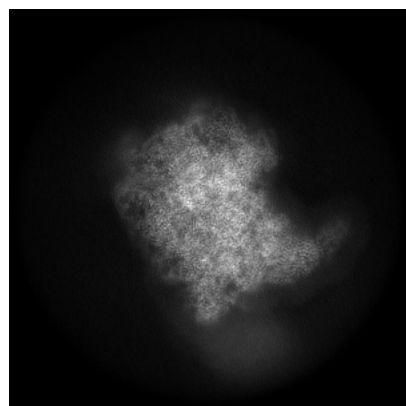
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29266. These allow visual inspection of the internal detail of the map and identification of artifacts.

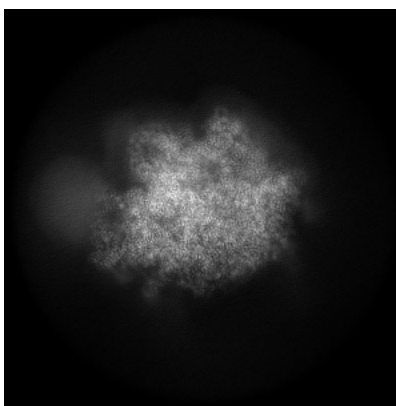
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

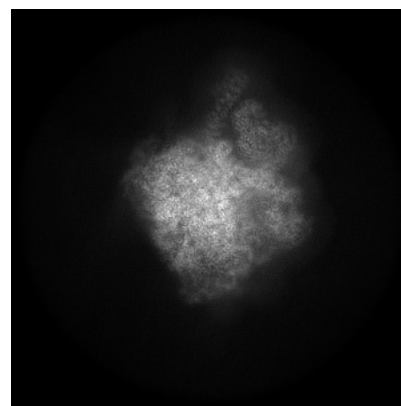
6.1.1 Primary map



X

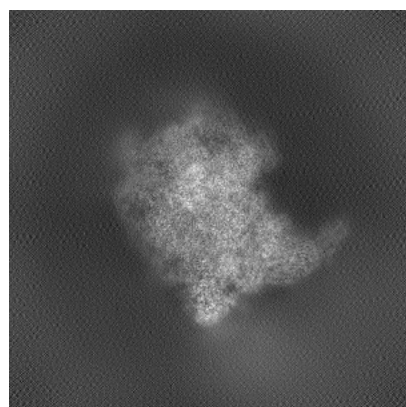


Y

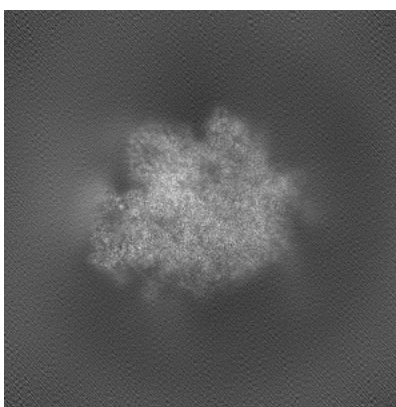


Z

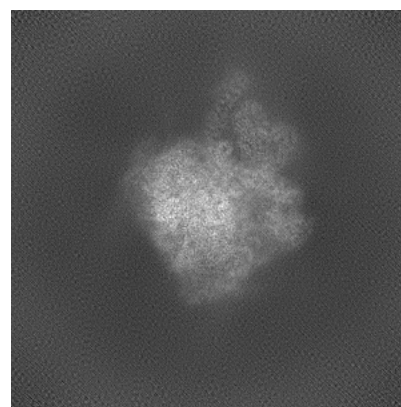
6.1.2 Raw map



X



Y

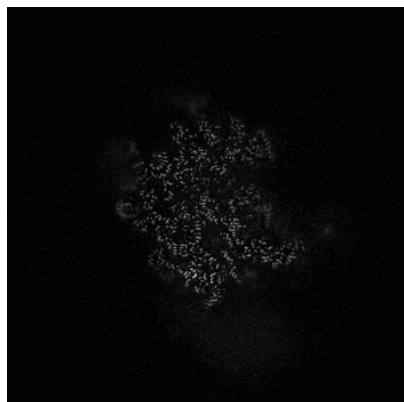


Z

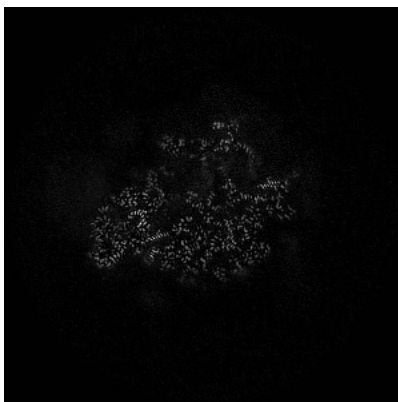
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

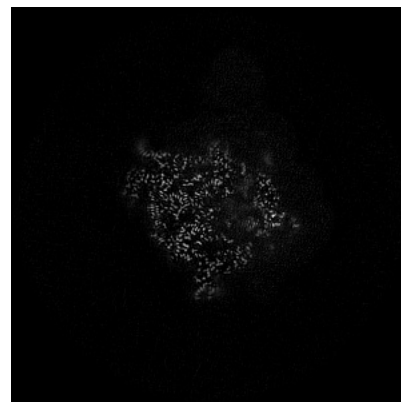
6.2.1 Primary map



X Index: 240

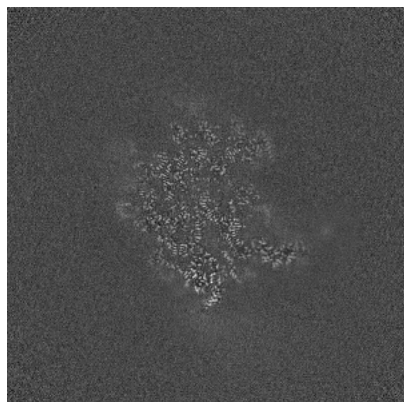


Y Index: 240

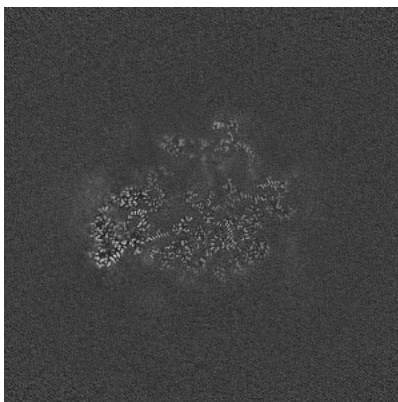


Z Index: 240

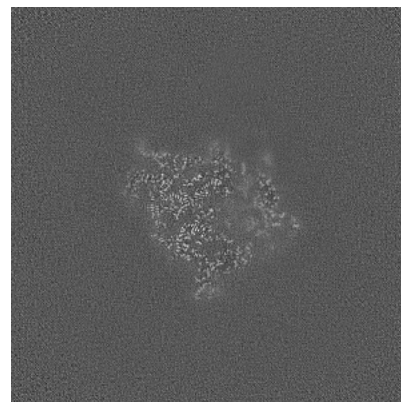
6.2.2 Raw map



X Index: 240



Y Index: 240

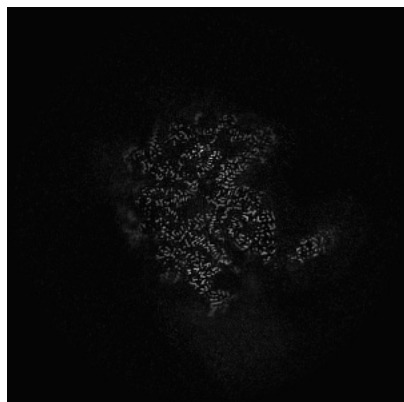


Z Index: 240

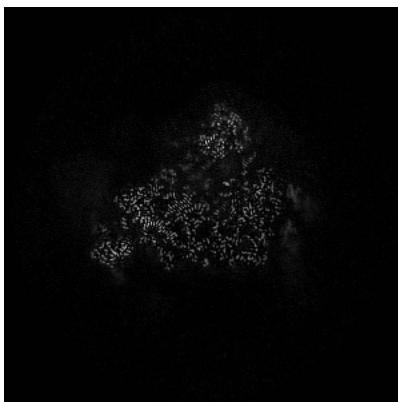
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

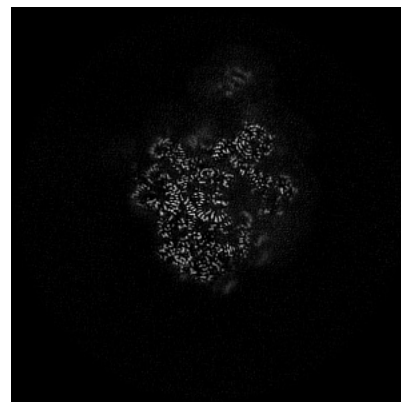
6.3.1 Primary map



X Index: 254

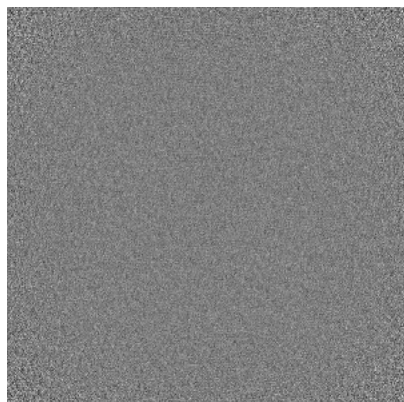


Y Index: 227

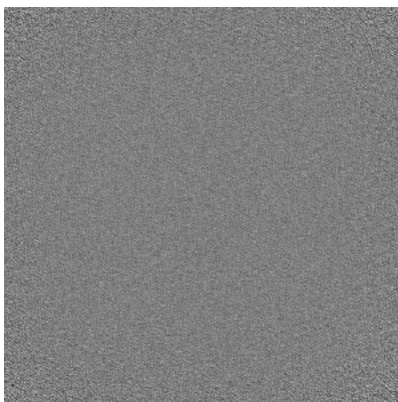


Z Index: 217

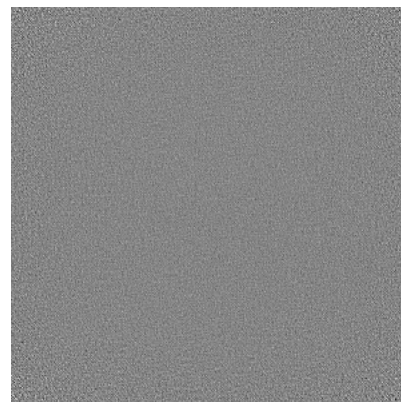
6.3.2 Raw map



X Index: 0



Y Index: 0

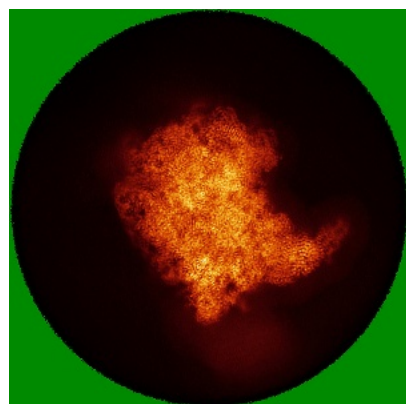


Z Index: 0

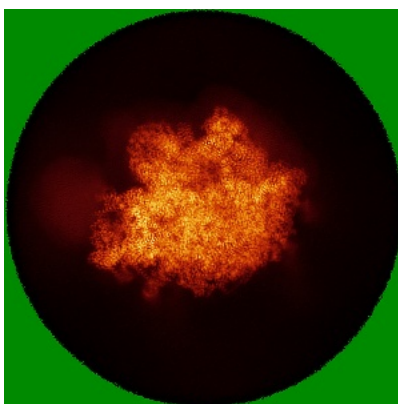
The images above show the largest variance slices of the map in three orthogonal directions.

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

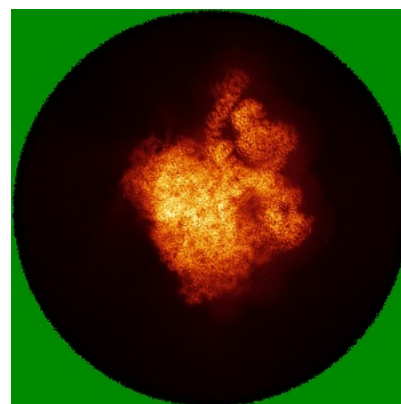
6.4.1 Primary map



X

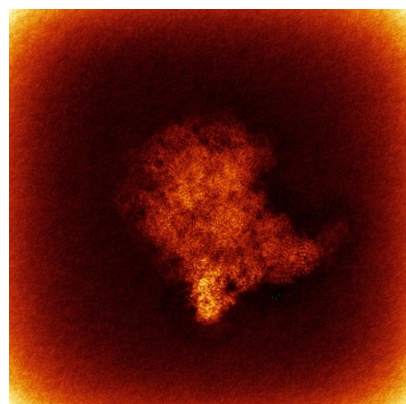


Y

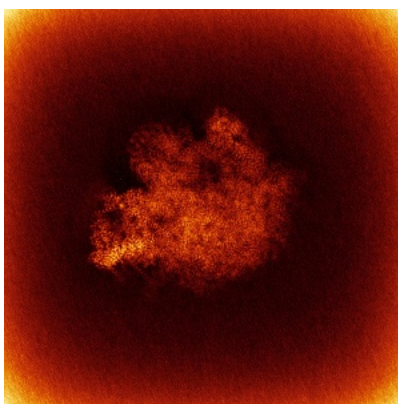


Z

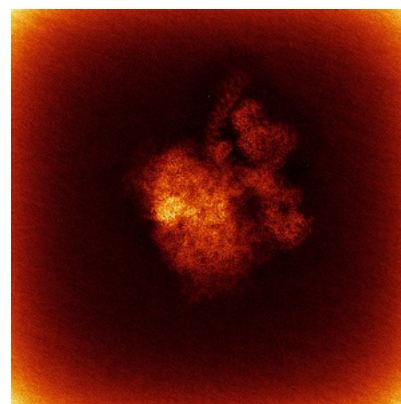
6.4.2 Raw map



X



Y

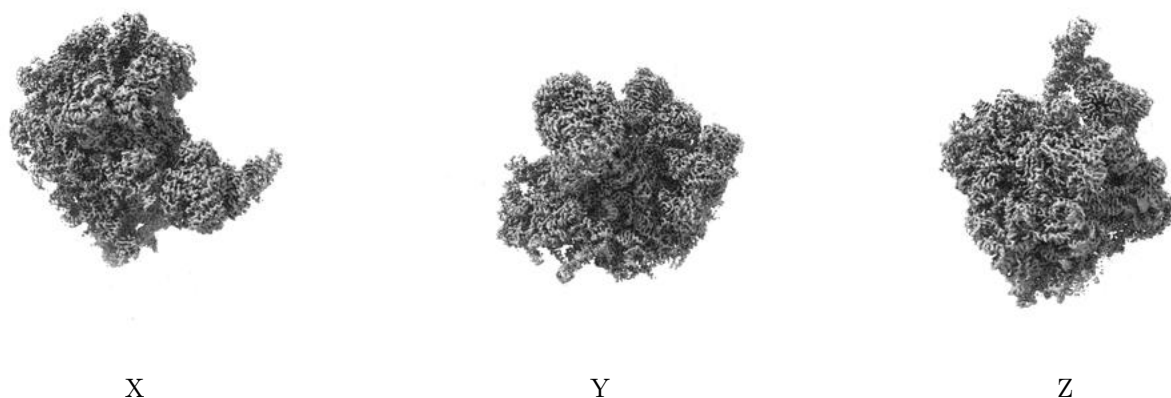


Z

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.

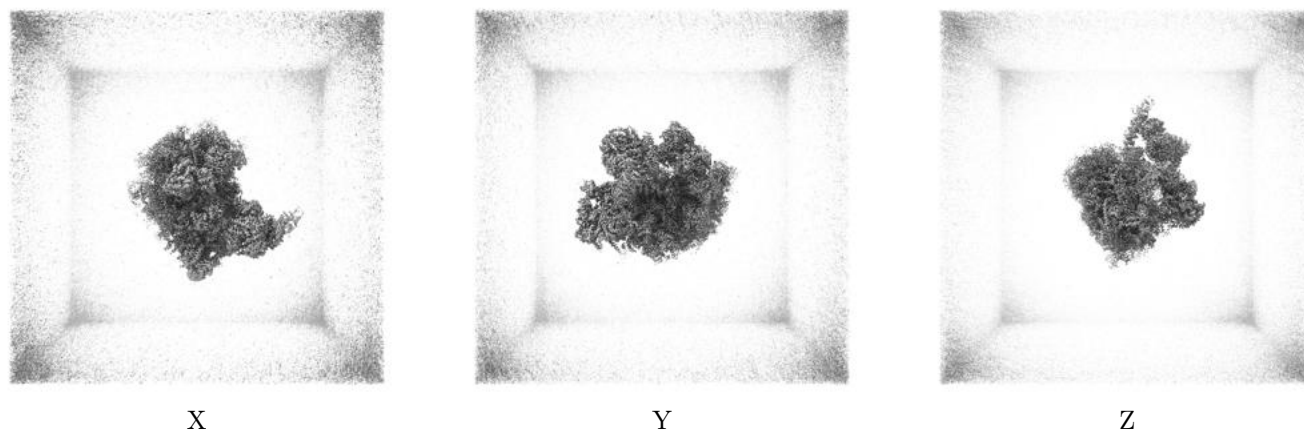
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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.

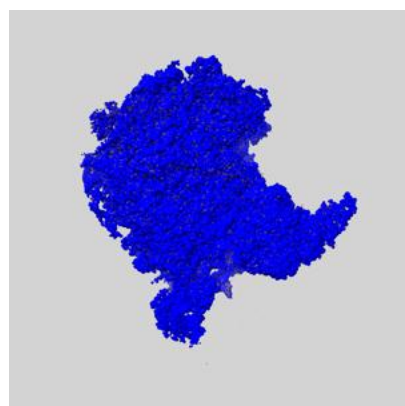
6.6 Mask visualisation [i](#)

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

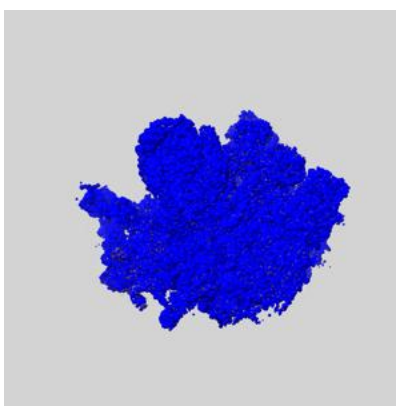
A mask typically either:

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

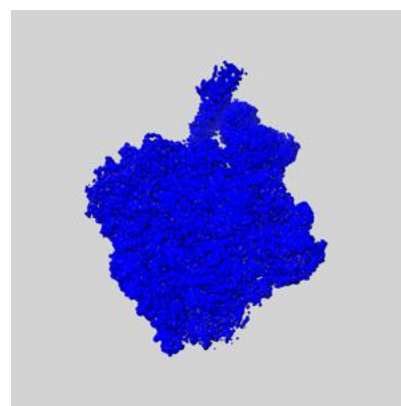
6.6.1 emd_29266_msk_1.map [i](#)



X



Y

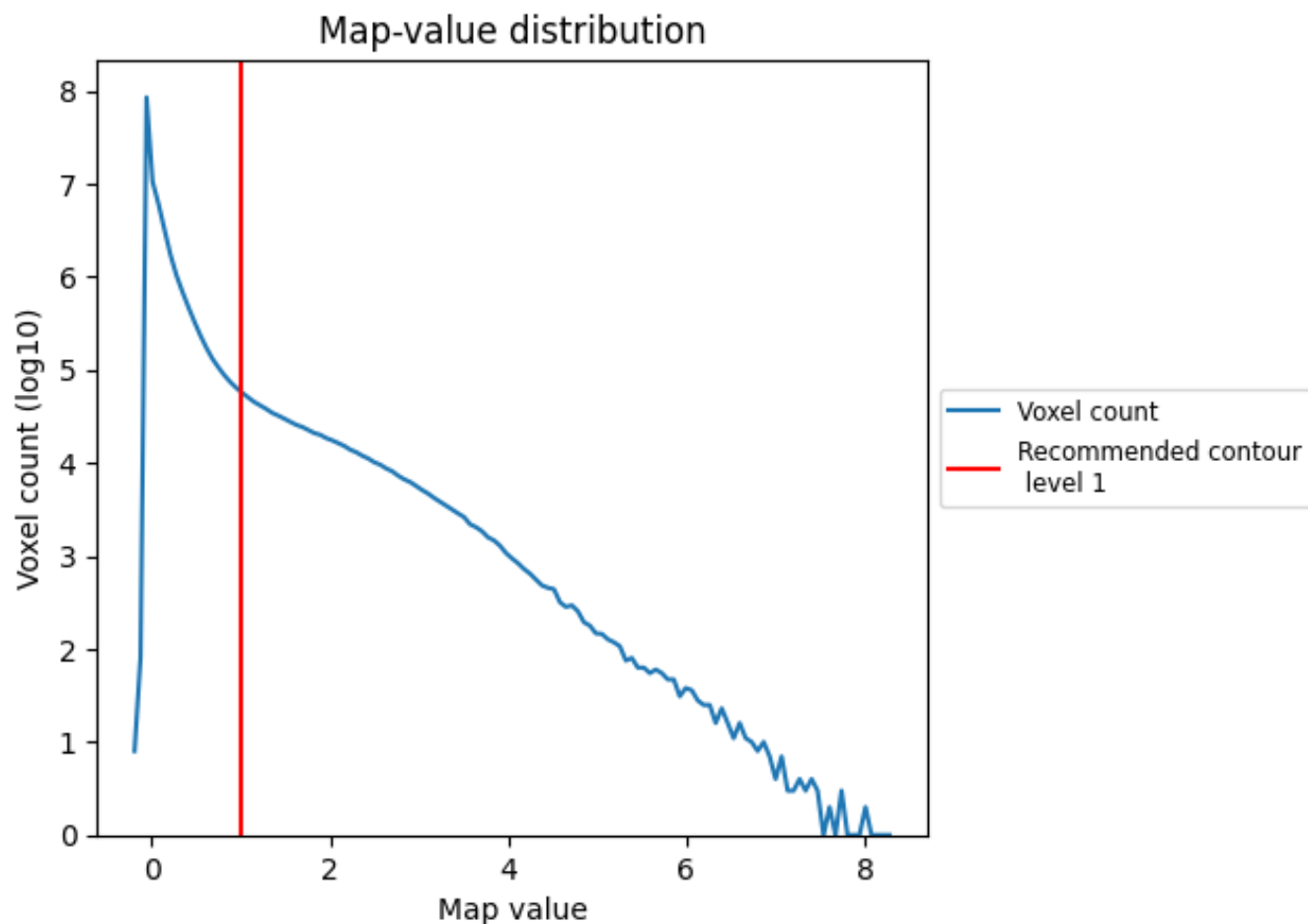


Z

7 Map analysis [i](#)

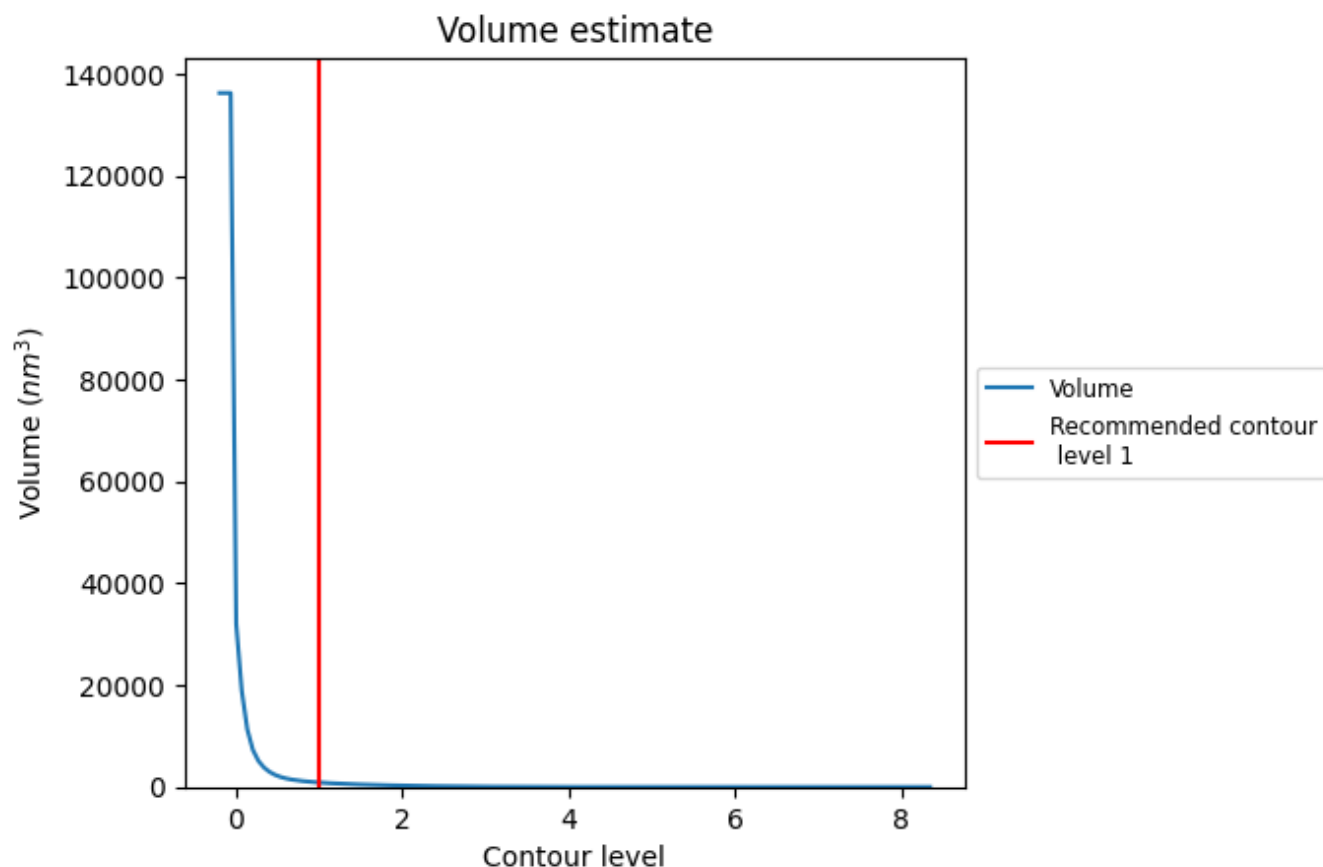
This section contains the results of statistical analysis of the map.

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.

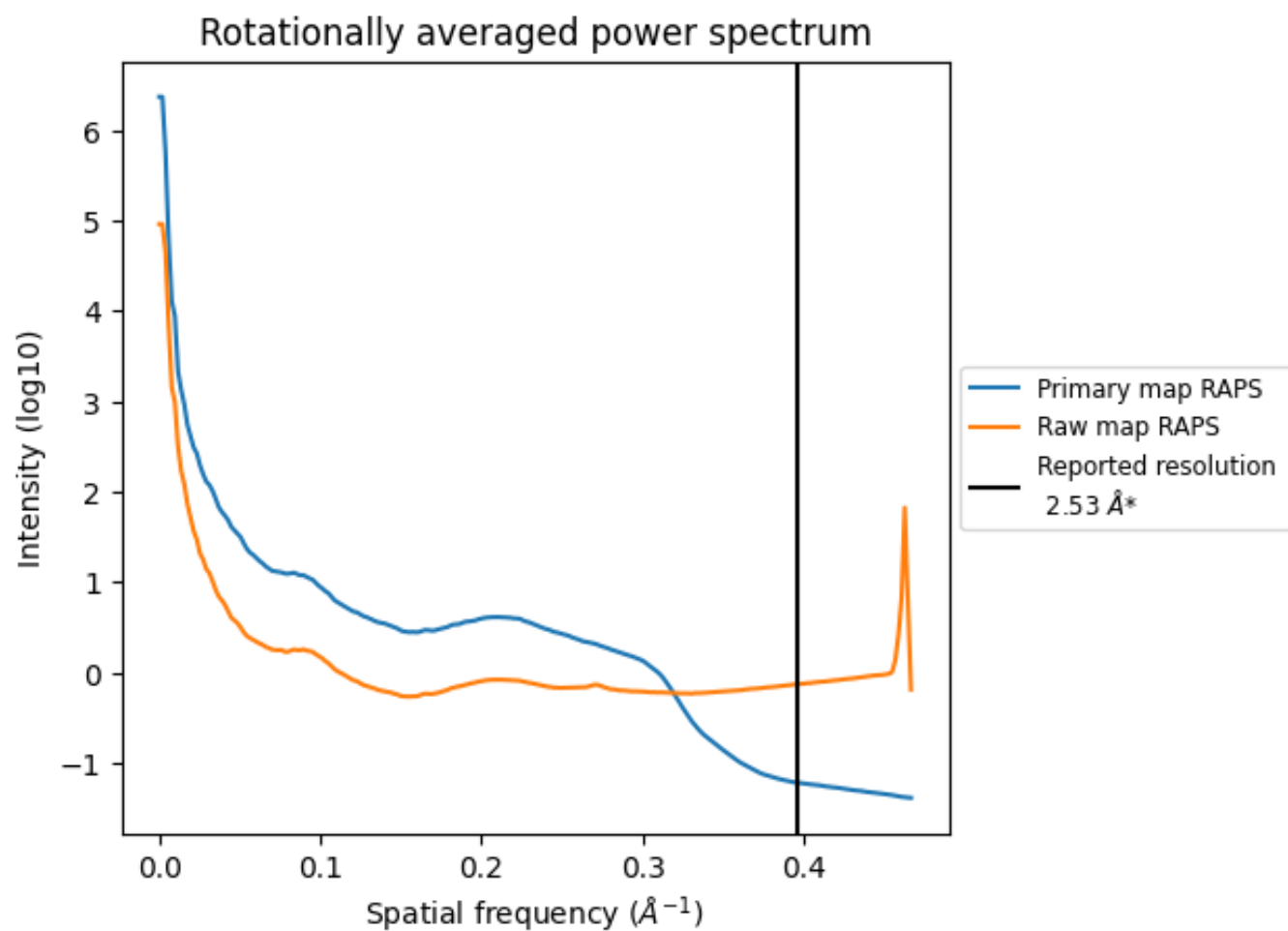
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 879 nm³; this corresponds to an approximate mass of 794 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 ⓘ

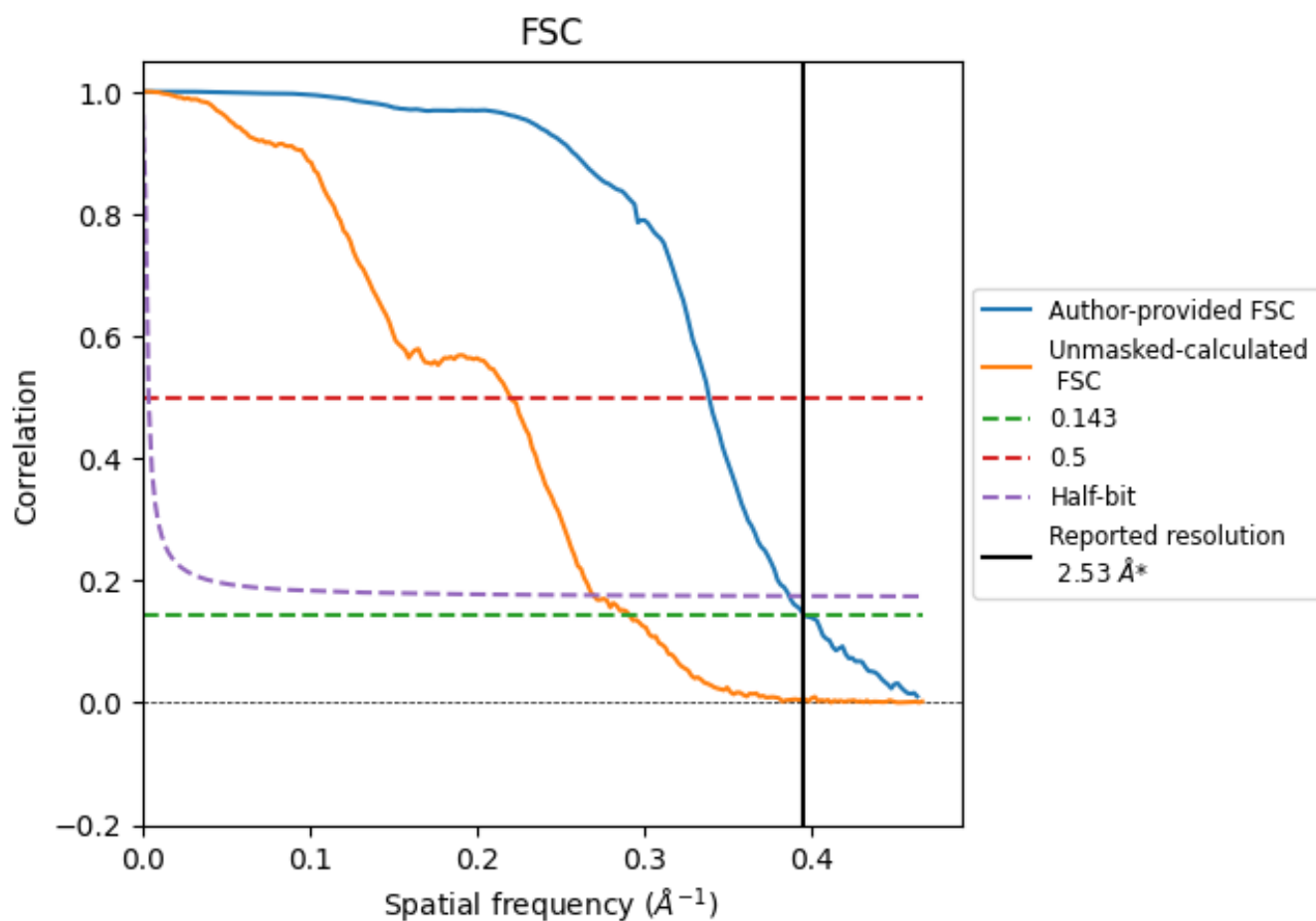


*Reported resolution corresponds to spatial frequency of 0.395 Å⁻¹

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 0.395 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

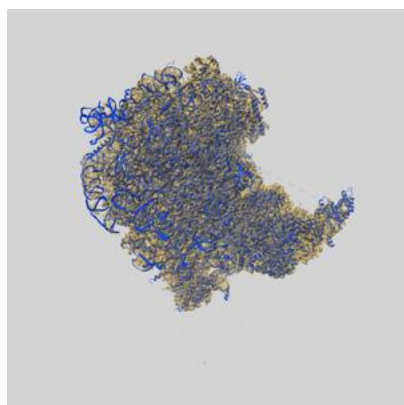
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.53	-	-
Author-provided FSC curve	2.53	2.95	2.59
Unmasked-calculated*	3.43	4.54	3.71

*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 3.43 differs from the reported value 2.53 by more than 10 %

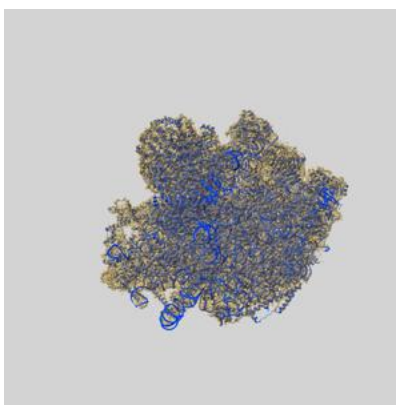
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29266 and PDB model 8FL3. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

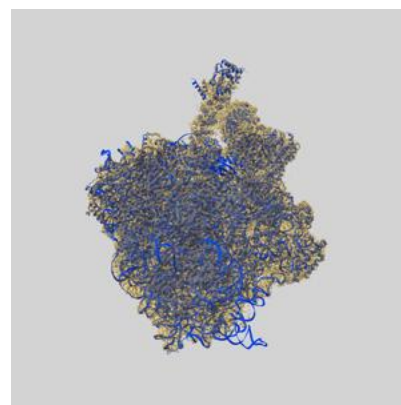
9.1 Map-model overlay [i](#)



X



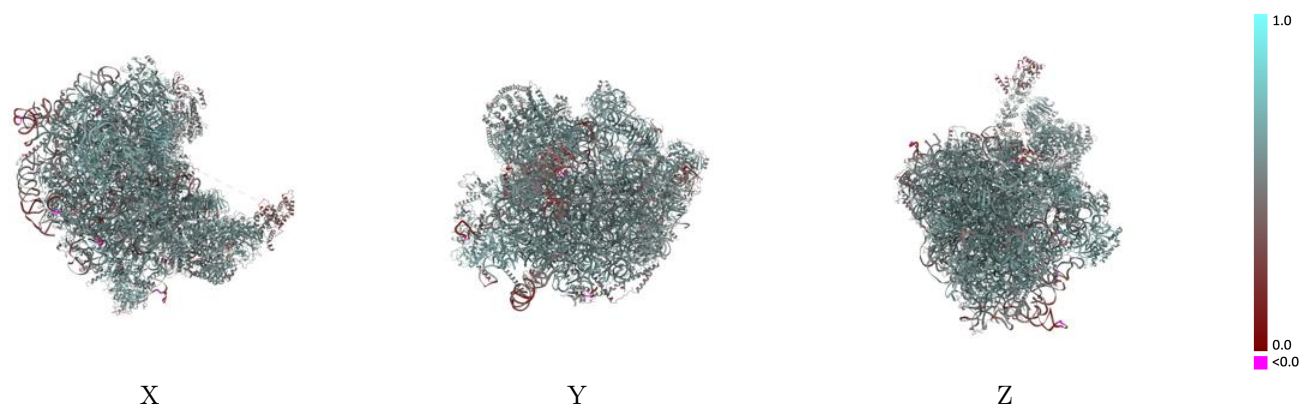
Y



Z

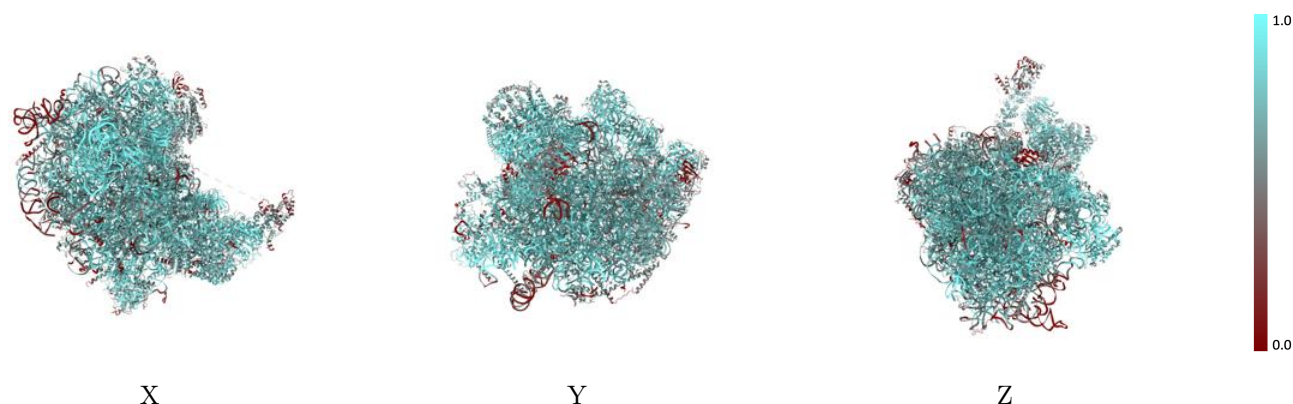
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



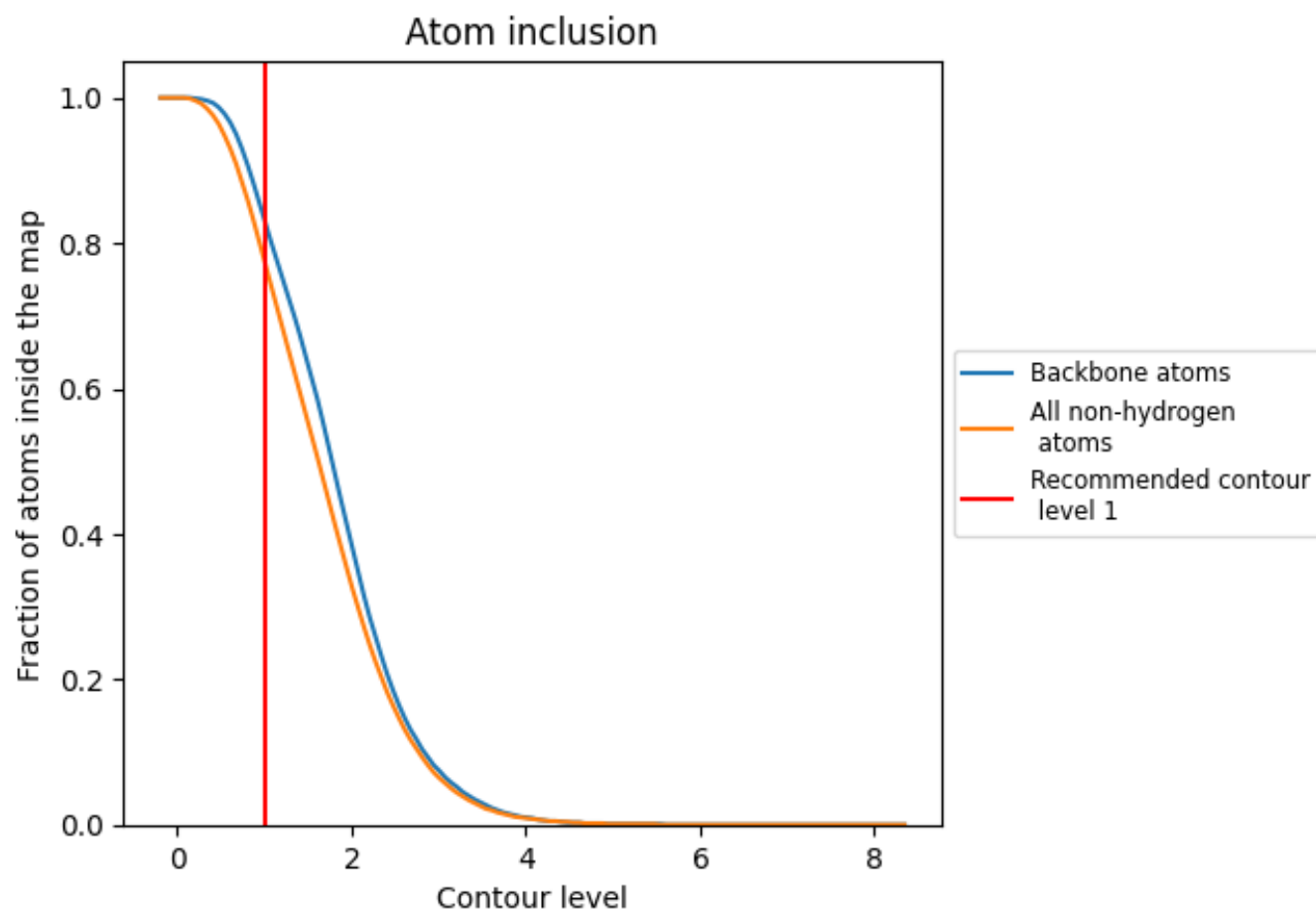
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 83% of all backbone atoms, 78% 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	 0.7750	 0.5630
BA	 0.4480	 0.4420
BB	 0.6860	 0.5360
BD	 0.2570	 0.3780
L1	 0.9200	 0.6070
L3	 0.8110	 0.5550
L4	 0.9310	 0.6020
L5	 0.7940	 0.5710
L6	 0.6370	 0.5340
L7	 0.7780	 0.5940
L8	 0.7660	 0.5860
L9	 0.8560	 0.6300
LA	 0.7720	 0.5950
LB	 0.7390	 0.5850
LC	 0.8740	 0.6420
LD	 0.7170	 0.5630
LE	 0.7330	 0.5680
LF	 0.6060	 0.5420
LG	 0.7060	 0.5740
LH	 0.7800	 0.6080
LI	 0.7390	 0.5780
LJ	 0.8940	 0.6240
LK	 0.6620	 0.5770
LL	 0.7660	 0.5900
LN	 0.7660	 0.5800
LO	 0.6730	 0.5490
LP	 0.7040	 0.5730
LQ	 0.7910	 0.6050
LR	 0.8100	 0.5980
LS	 0.7620	 0.5960
LT	 0.8390	 0.6180
LU	 0.6270	 0.5410
LW	 0.8380	 0.6090
LX	 0.7550	 0.5660
LY	 0.5780	 0.5540



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Chain	Atom inclusion	Q-score
LZ	 0.8270	 0.6040
NB	 0.5970	 0.5220
NC	 0.6970	 0.5490
NF	 0.8680	 0.6310
NJ	 0.8540	 0.6030
NK	 0.5580	 0.5060
NL	 0.6590	 0.5540
NP	 0.6140	 0.5470
NT	 0.7840	 0.5610
NU	 0.6910	 0.4980
NV	 0.7540	 0.5620
NW	 0.8470	 0.5680
NX	 0.7530	 0.5520
NY	 0.7590	 0.5570
NZ	 0.6390	 0.5460
SA	 0.7640	 0.5900
SB	 0.8400	 0.6010
SC	 0.6320	 0.5540
SD	 0.7740	 0.5940
SE	 0.8330	 0.5980
SF	 0.8670	 0.6140
SG	 0.6690	 0.5680
SH	 0.6240	 0.5150
SI	 0.7080	 0.5450
SK	 0.6210	 0.5240
SM	 0.8900	 0.6250
SQ	 0.6360	 0.5510
SR	 0.6420	 0.5320
SV	 0.6890	 0.5530