



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 04:01 AM UTC

PDB ID : 8FL2 / pdb_00008fl2
EMDB ID : EMD-29265
Title : Human nuclear pre-60S ribosomal subunit (State I1)
Authors : Vanden Broeck, A.; Klinge, S.
Deposited on : 2022-12-21
Resolution : 2.67 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:

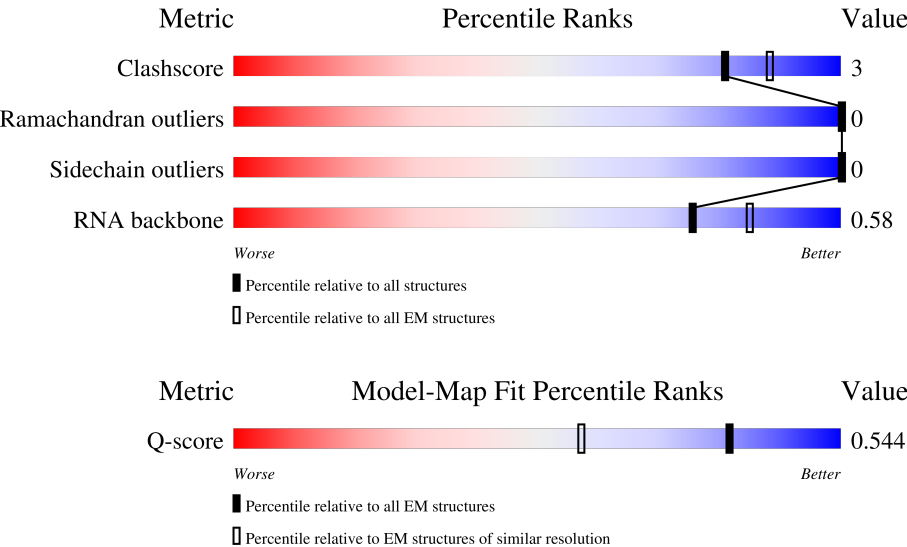
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.67 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.



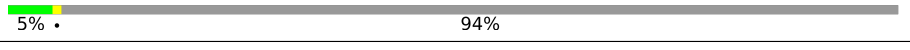
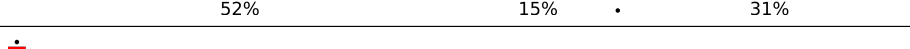
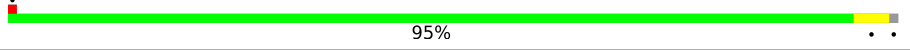
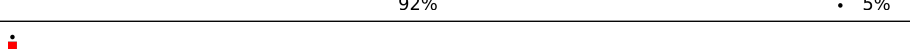
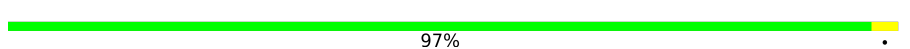
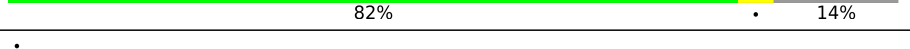
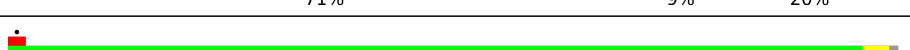
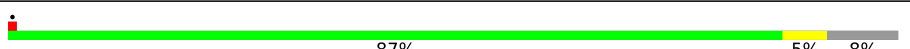
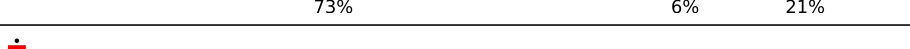
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	9182 (2.17 - 3.17)

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	28% 90% 7% .
2	BB	217	85% 15%
3	BD	734	97%

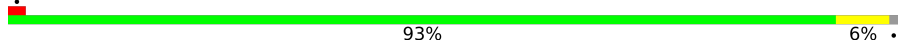
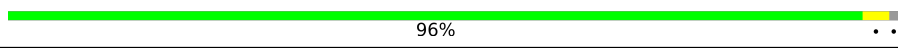
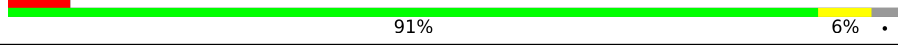
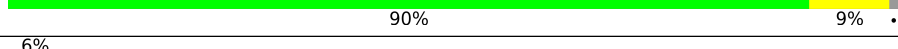
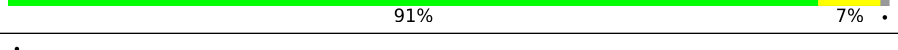
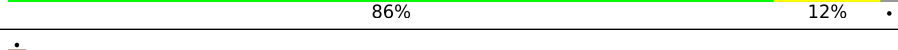
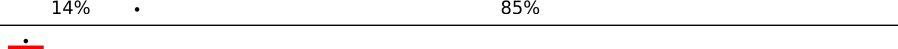
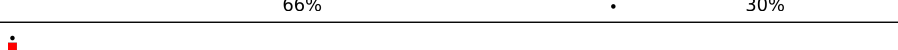
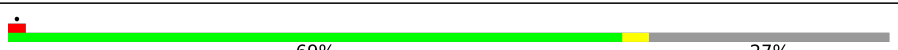
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Mol	Chain	Length	Quality of chain
4	L1	157	
5	L2	1167	
6	L3	5070	
7	L4	121	
8	L5	178	
9	L6	211	
10	L7	203	
11	L8	215	
12	L9	204	
13	LA	184	
14	LB	188	
15	LC	176	
16	LD	196	
17	LE	160	
18	LF	128	
19	LG	140	
20	LH	156	
21	LI	145	
22	LJ	136	
23	LK	148	
24	LL	137	
25	LN	403	
26	LO	115	
27	LP	125	
28	LQ	135	

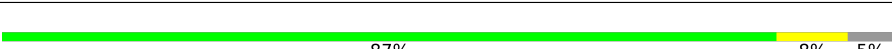
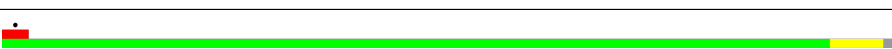
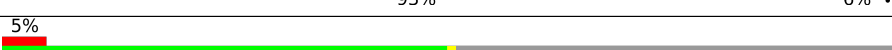
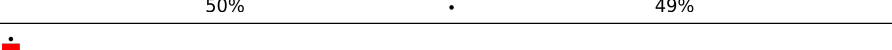
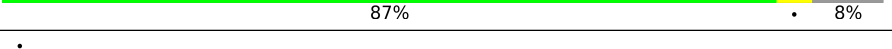
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Mol	Chain	Length	Quality of chain
29	LR	117	
30	LS	123	
31	LT	110	
32	LU	105	
33	LW	97	
34	LX	92	
35	LY	70	
36	LZ	51	
37	NB	549	
38	NC	731	
39	NF	260	
40	NJ	485	
41	NK	129	
42	NL	478	
43	NP	134	
44	NT	687	
45	NU	929	
46	NV	432	
46	NW	432	
47	NX	1130	
47	NY	1130	
48	NZ	360	
49	SA	427	
50	SB	297	
51	SC	288	

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Mol	Chain	Length	Quality of chain
52	SD	248	
53	SE	266	
54	SF	257	
55	SG	192	
56	SH	293	
57	SI	255	
58	SK	245	
59	SL	490	
60	SM	588	
61	SQ	239	
62	SR	634	
63	SV	163	

2 Entry composition

There are 68 unique types of molecules in this entry. The entry contains 189616 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 ITS2 rRNA.

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

- Molecule 6 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L3	3495	Total	C	N	O	P	0	0
			75027	33448	13734	24350	3495		

- Molecule 7 is a RNA chain called 5S rRNA.

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

- Molecule 8 is a protein called 60S ribosomal protein L11.

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

- Molecule 9 is a protein called 60S ribosomal protein L13.

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

- Molecule 10 is a protein called 60S ribosomal protein L13a.

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

- Molecule 11 is a protein called 60S ribosomal protein L14.

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

- Molecule 12 is a protein called 60S ribosomal protein L15.

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

- Molecule 13 is a protein called 60S ribosomal protein L17.

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

- Molecule 14 is a protein called 60S ribosomal protein L18.

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

- Molecule 15 is a protein called 60S ribosomal protein L18a.

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

- Molecule 16 is a protein called 60S ribosomal protein L19.

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

- Molecule 17 is a protein called 60S ribosomal protein L21.

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

- Molecule 18 is a protein called 60S ribosomal protein L22.

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

- Molecule 19 is a protein called 60S ribosomal protein L23.

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

- Molecule 20 is a protein called 60S ribosomal protein L23a.

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

- Molecule 21 is a protein called 60S ribosomal protein L26.

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

- Molecule 22 is a protein called 60S ribosomal protein L27.

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

- Molecule 23 is a protein called 60S ribosomal protein L27a.

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

- Molecule 24 is a protein called 60S ribosomal protein L28.

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

- Molecule 25 is a protein called 60S ribosomal protein L3.

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

- Molecule 26 is a protein called 60S ribosomal protein L30.

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

- Molecule 27 is a protein called 60S ribosomal protein L31.

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

- Molecule 28 is a protein called 60S ribosomal protein L32.

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

- Molecule 29 is a protein called 60S ribosomal protein L34.

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

- Molecule 30 is a protein called 60S ribosomal protein L35.

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

- Molecule 31 is a protein called 60S ribosomal protein L35a.

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

- Molecule 32 is a protein called 60S ribosomal protein L36.

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

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

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

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

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

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

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

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

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

- Molecule 37 is a protein called Guanine nucleotide-binding protein-like 3.

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

- Molecule 38 is a protein called Nucleolar GTP-binding protein 2.

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

- Molecule 39 is a protein called Ribosome biogenesis protein NSA2 homolog.

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

- Molecule 40 is a protein called Notchless protein homolog 1.

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

- Molecule 41 is a protein called Protein LLP homolog.

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

- Molecule 42 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	NL	360	Total	C	N	O	S	0	0
			2980	1852	593	533	2		

- Molecule 43 is a protein called Zinc finger protein 593.

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

- Molecule 44 is a protein called Protein SDA1 homolog.

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

- Molecule 45 is a protein called Testis-expressed protein 10.

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

- Molecule 46 is a protein called WD repeat-containing protein 18.

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

- Molecule 47 is a protein called Proline-, glutamic acid- and leucine-rich protein 1.

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

- Molecule 48 is a protein called Coiled-coil domain-containing protein 86.

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

- Molecule 49 is a protein called 60S ribosomal protein L4.

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

- Molecule 50 is a protein called 60S ribosomal protein L5.

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

- Molecule 51 is a protein called 60S ribosomal protein L6.

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

- Molecule 52 is a protein called 60S ribosomal protein L7.

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

- Molecule 53 is a protein called 60S ribosomal protein L7a.

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

- Molecule 54 is a protein called 60S ribosomal protein L8.

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

- Molecule 55 is a protein called 60S ribosomal protein L9.

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

- Molecule 56 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SH	150	Total	C	N	O	S	1	0
			1275	824	227	220	4		

- Molecule 57 is a protein called 60S ribosomal protein L7-like 1.

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

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

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

- Molecule 59 is a protein called Ribosomal L1 domain-containing protein 1.

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

- Molecule 60 is a protein called Pescadillo homolog.

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

- Molecule 61 is a protein called mRNA turnover protein 4 homolog.

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

- Molecule 62 is a protein called GTP-binding protein 4.

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

- Molecule 63 is a protein called Probable ribosome biogenesis protein RLP24.

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

- Molecule 64 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
64	L1	5	Total	Mg	0
			5	5	
64	L3	84	Total	Mg	0
			84	84	
64	L4	1	Total	Mg	0
			1	1	
64	L6	1	Total	Mg	0
			1	1	
64	L9	1	Total	Mg	0
			1	1	
64	LQ	1	Total	Mg	0
			1	1	
64	LR	1	Total	Mg	0
			1	1	
64	LT	1	Total	Mg	0
			1	1	
64	LW	1	Total	Mg	0
			1	1	
64	NC	1	Total	Mg	0
			1	1	
64	SA	1	Total	Mg	0
			1	1	
64	SF	1	Total	Mg	0
			1	1	
64	SR	1	Total	Mg	0
			1	1	

- Molecule 65 is ZINC ION (CCD ID: ZN) (formula: Zn).

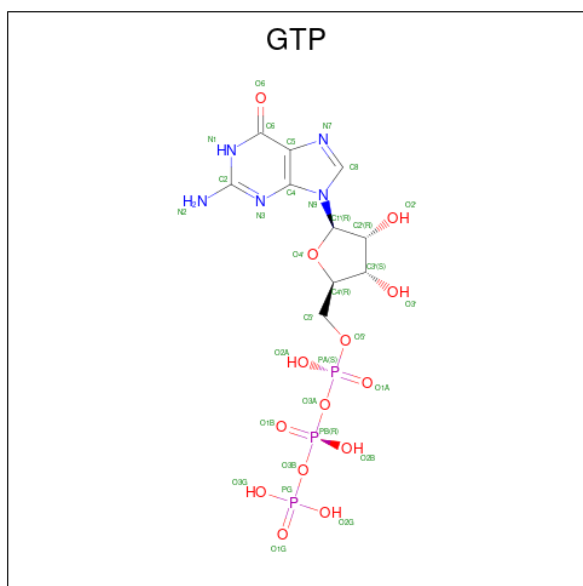
Mol	Chain	Residues	Atoms		AltConf
65	LR	1	Total	Zn	0
			1	1	
65	LW	1	Total	Zn	0
			1	1	
65	LX	1	Total	Zn	0
			1	1	
65	NP	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
65	SV	1	Total	Zn	0
			1	1	

- Molecule 66 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

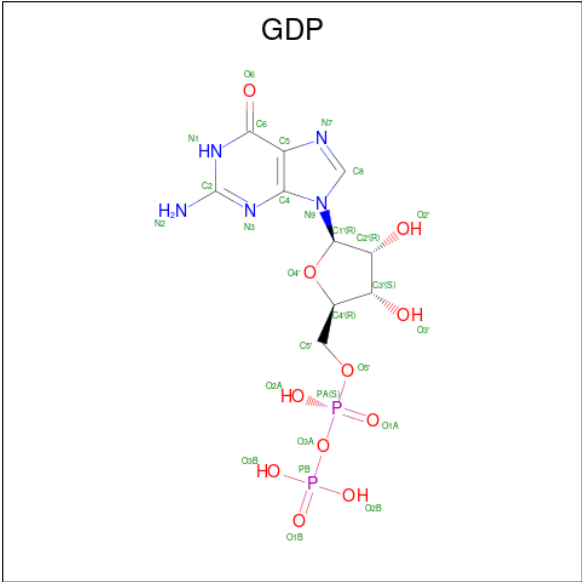


Mol	Chain	Residues	Atoms					AltConf
66	NC	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 67 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
67	NC	1	Total	K	0
			1	1	
67	SR	1	Total	K	0
			1	1	

- Molecule 68 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

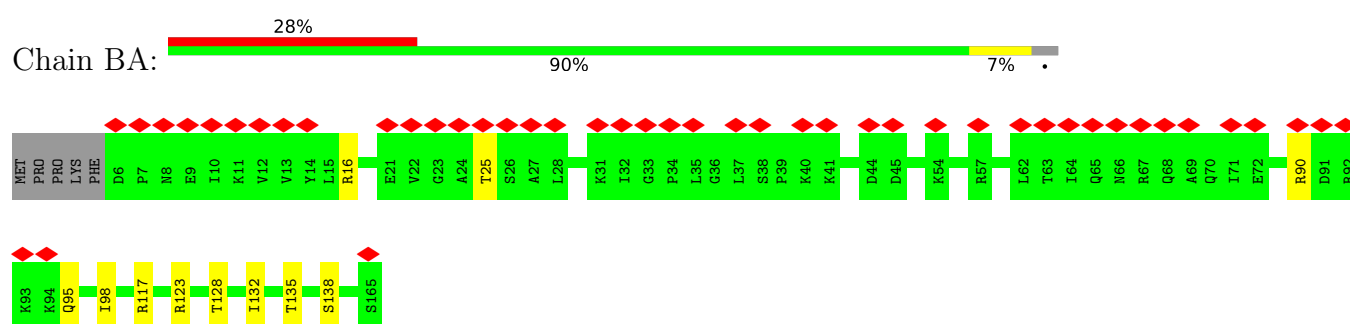


Mol	Chain	Residues	Atoms					AltConf
68	SR	1	Total	C	N	O	P	0
			28	10	5	11	2	

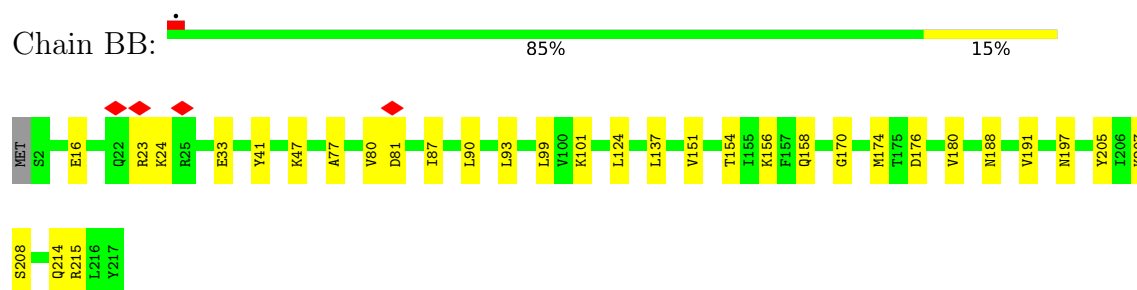
3 Residue-property plots [i](#)

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

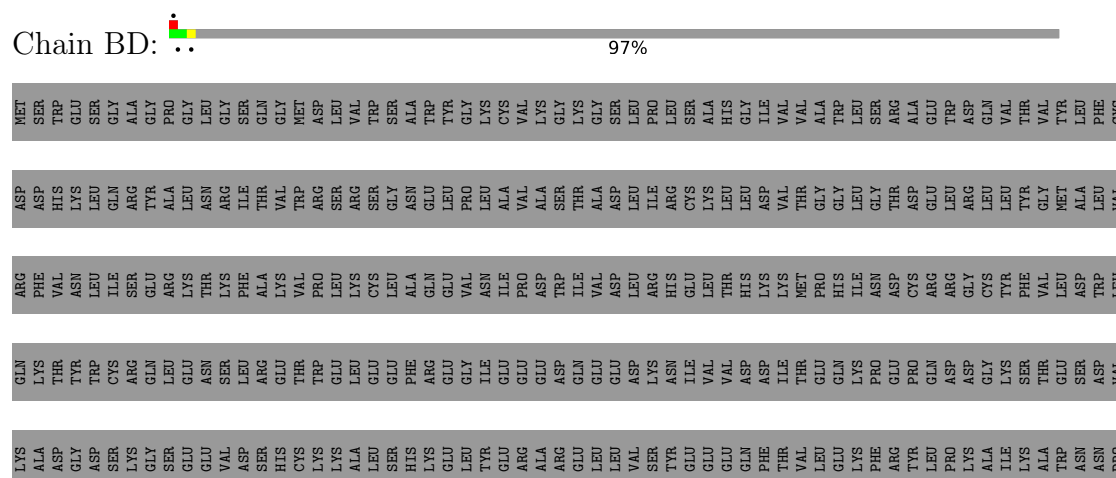
- Molecule 1: 60S ribosomal protein L12

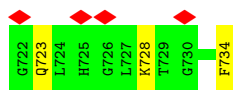


- Molecule 2: 60S ribosomal protein L10a



- Molecule 3: Ribosomal biogenesis protein LAS1L

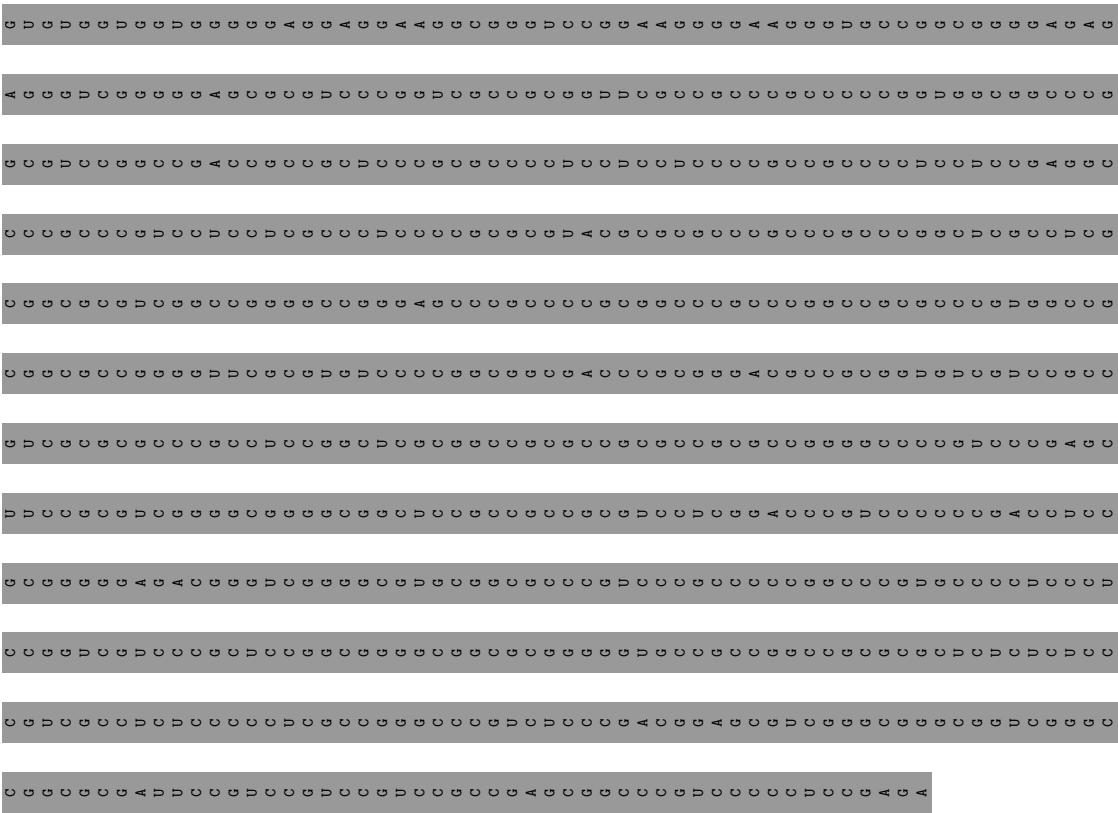




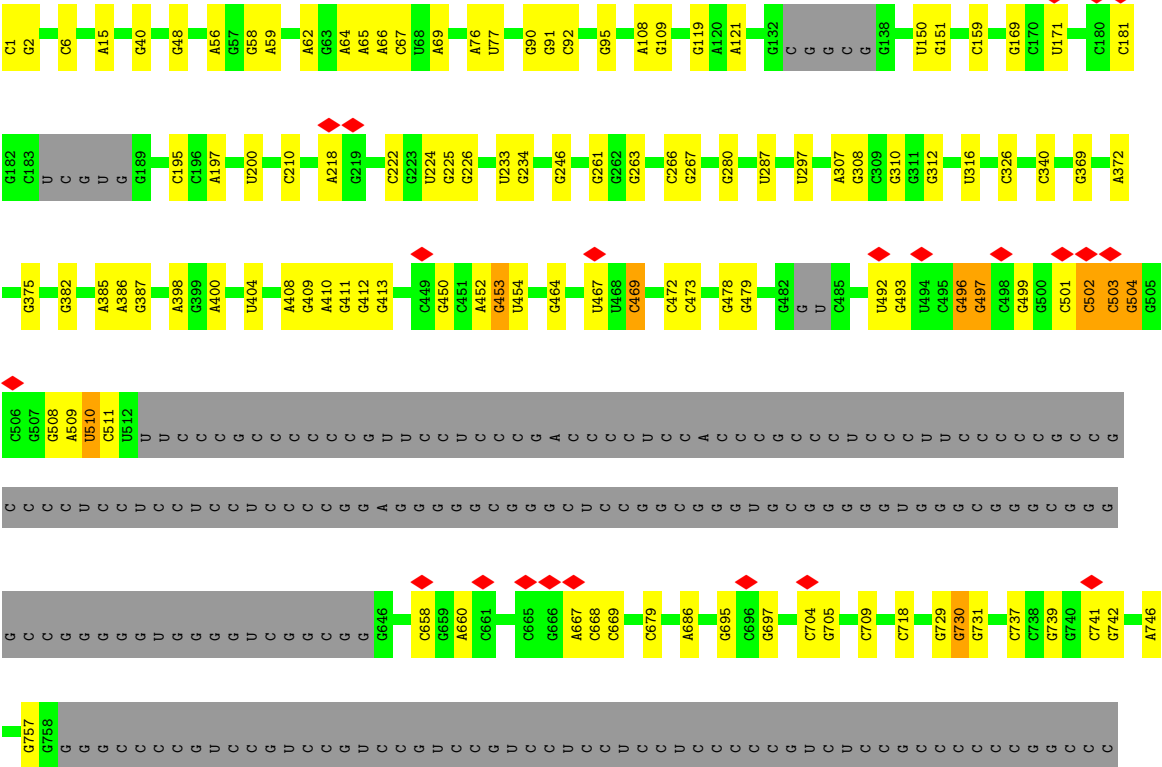
Chain L1:

Chain L2: 5% . 94%



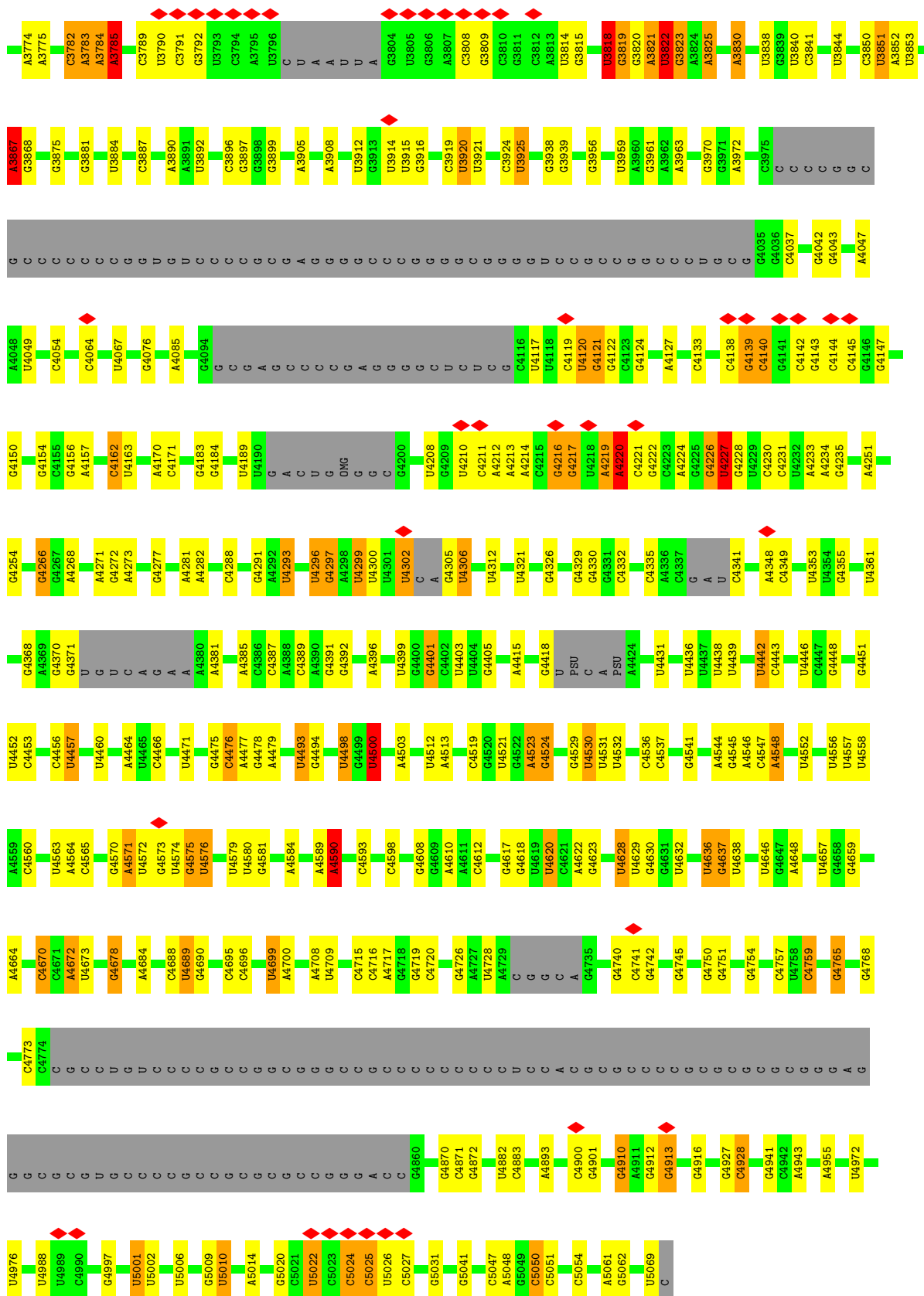


● Molecule 6: 28S rRNA



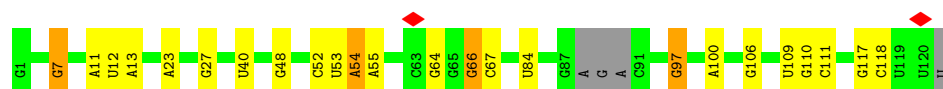






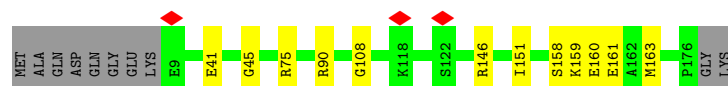
• Molecule 7: 5S rRNA

Chain L4:  77% 17% . .

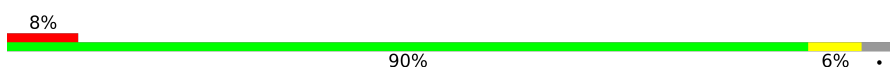


- Molecule 8: 60S ribosomal protein L11

Chain L5:  88% 7% 6%

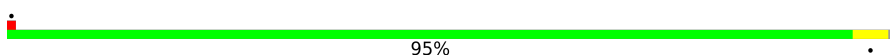


- Molecule 9: 60S ribosomal protein L13

Chain L6:  8% 90% 6% .



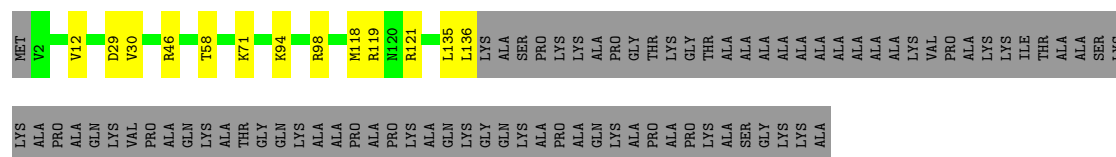
- Molecule 10: 60S ribosomal protein L13a

Chain L7:  95% . .

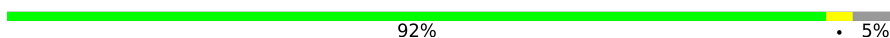


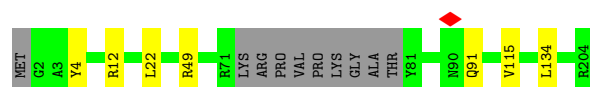
- Molecule 11: 60S ribosomal protein L14

Chain L8:  57% 6% 37%



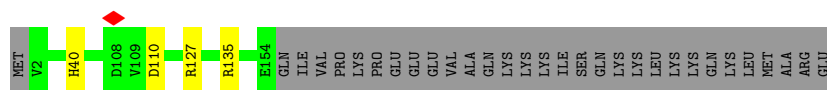
- Molecule 12: 60S ribosomal protein L15

Chain L9:  92% . 5%

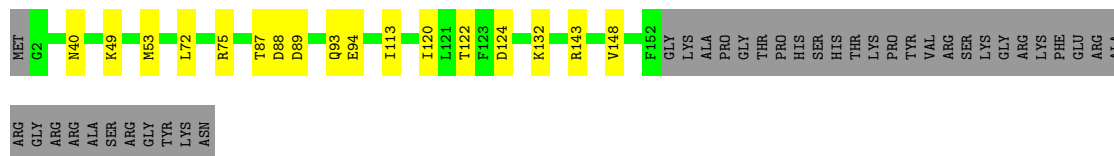


- Molecule 13: 60S ribosomal protein L17

Chain LA:  81% . 17%



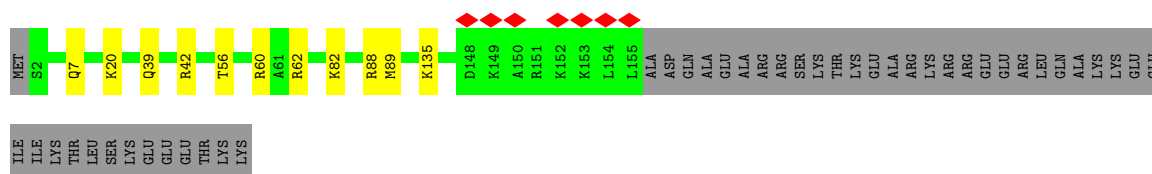
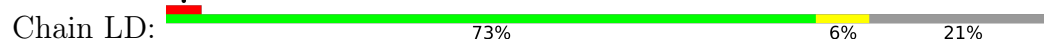
- Molecule 14: 60S ribosomal protein L18



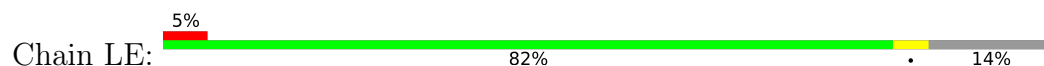
- Molecule 15: 60S ribosomal protein L18a



- Molecule 16: 60S ribosomal protein L19



- Molecule 17: 60S ribosomal protein L21



- Molecule 18: 60S ribosomal protein L22

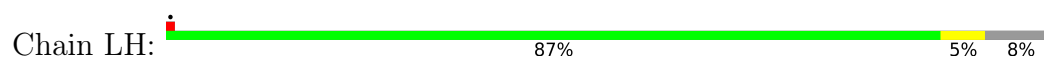


- Molecule 19: 60S ribosomal protein L23

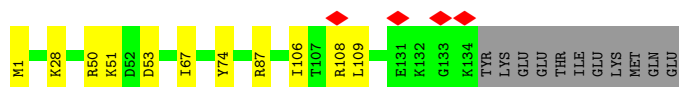
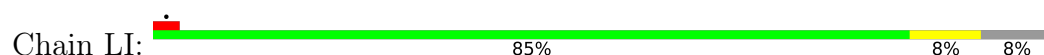




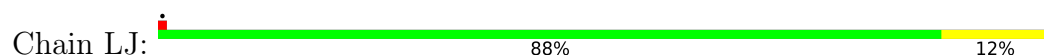
- Molecule 20: 60S ribosomal protein L23a



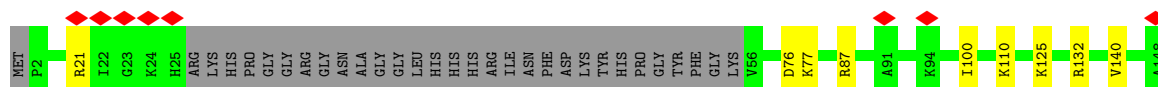
- Molecule 21: 60S ribosomal protein L26



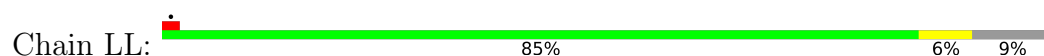
- Molecule 22: 60S ribosomal protein L27



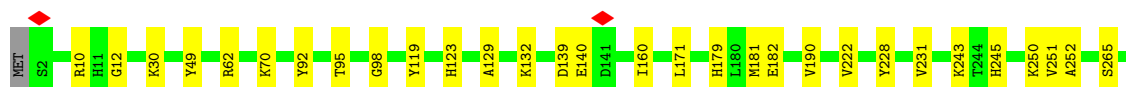
- Molecule 23: 60S ribosomal protein L27a

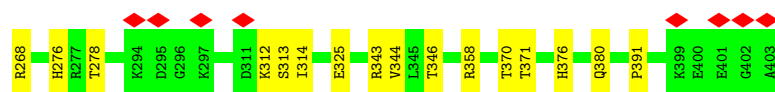


- Molecule 24: 60S ribosomal protein L28

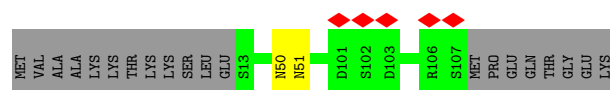
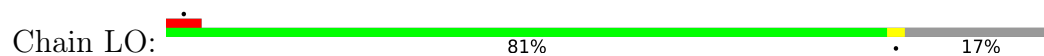


- Molecule 25: 60S ribosomal protein L3

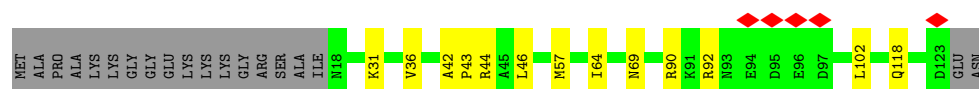
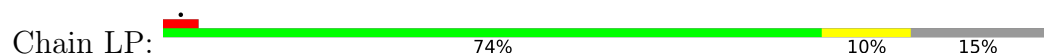




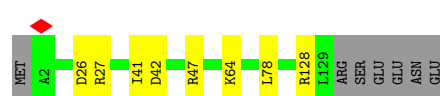
- Molecule 26: 60S ribosomal protein L30



- Molecule 27: 60S ribosomal protein L31



- Molecule 28: 60S ribosomal protein L32



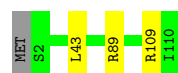
- Molecule 29: 60S ribosomal protein L34



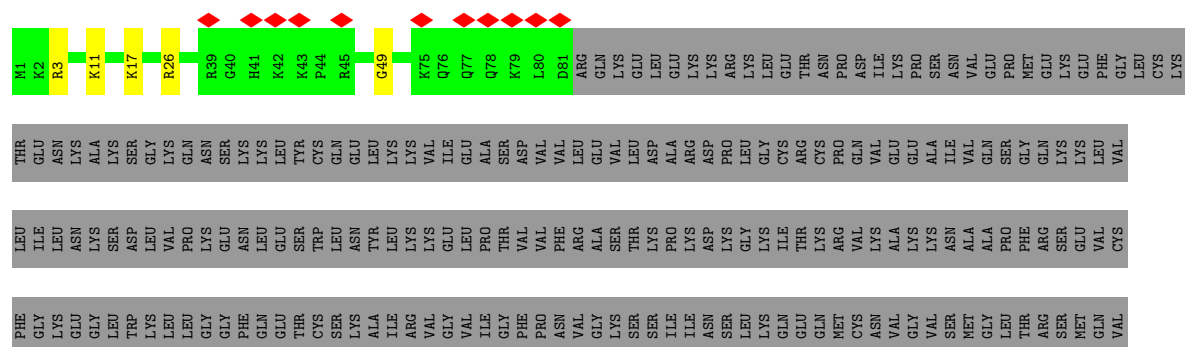
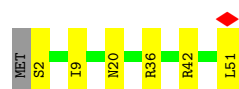
- Molecule 30: 60S ribosomal protein L35



- Molecule 31: 60S ribosomal protein L35a

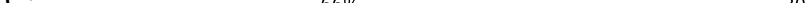


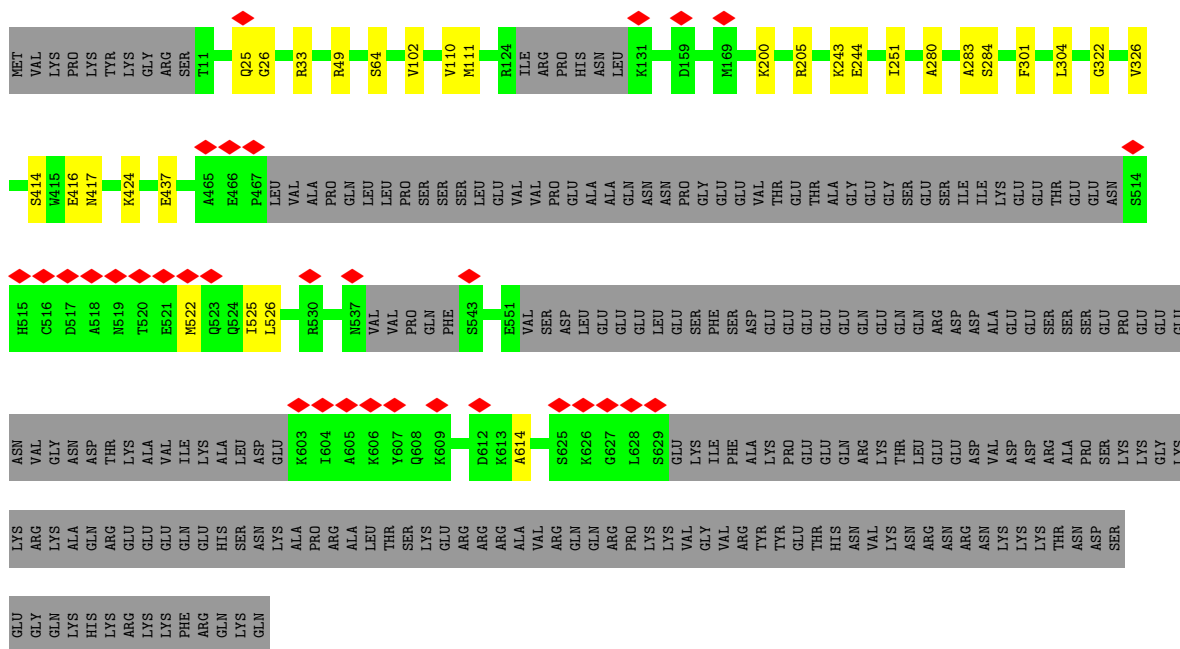
- Molecule 32: 60S ribosomal protein L36



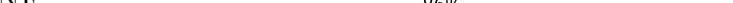
ILE	LYS	PHE	VAL	VAL
ILE	ARG	ASN	PRO	PRO
GLU	LYS	GLU	GLY	GLU
GLU	GLU	SER	TYR	ASP
ASP	ARG	ILE	ARG	LYS
ASP	LYS	VAL	ASN	GLN
ALA	GLN	VAL	ASN	ILE
TYR	GLU	ASP	LEU	THR
ASP	GLU	MET	GLU	THR
ASP	ARG	LYS	PHE	ILE
PHE	GLU	SER	PHE	ASP
SER	GLU	GLY	THR	SER
THR	ASP	GLY	THR	SER
ASP	ASP	PHE	VAL	PRO
ASP	LYS	ASN	LEU	SER
TYR	ASP	LEU	ALA	PHE
VAL	SER	GLU	GLN	ILE
	ASP	GLU	ARG	VAL
	GLN	LEU	ARG	SER
	GLU	LYS	GLY	PRO
	THR	GLU	MET	LEU
	VAL	ASN	HIS	ASN
	ASP	ASN	GLN	SER
	GLU	ALA	LYS	SER
	GLU	GLN	GLY	SER
	VAL	SER	GLY	ALA
	ASP	ILE	ILE	LEU
	GLU	ARG	PRO	ALA
	ASN	ALA	ASN	LEU
	SER	ILE	VAL	ARG
	SER	LYS	GLU	SER
	GLY	GLY	GLY	PRO
	MET	PRO	ALA	ALA
	PHE	HIS	ALA	SER
	ALA	LEU	LYS	ILE
	ALA	ALA	LEU	GLU
	GLU	ASN	LEU	VAL
	GLU	SER	TRP	VAL
	THR	ILE	SER	LYS
	GLY	THR	GLU	PRO
	GLU	PHE	TRP	MET
	ALA	GLN	THR	GLU
	LEU	SER	GLY	ALA
	SER	SER	ALA	ALA
	GLU	GLY	SER	ALA
	GLU	LEU	LEU	ALA
	THR	THR	ALA	ILE
	THR	ASN	TYR	LEU
	ALA	GLY	TYR	SER
	GLY	ILE	CYS	GLN
	GLU	ILE	HIS	ALA
	GLN	GLU	PRO	ASP
	SER	GLU	PRO	ALA
	THR	LYS	THR	ARG
	ARG	ILE	SER	GLN
	PHE	HIS	TRP	VAL
	ILE	THR	PRO	VAL
	LEU	GLU	PRO	LYS
	ASP	LEU	PRO	TYR

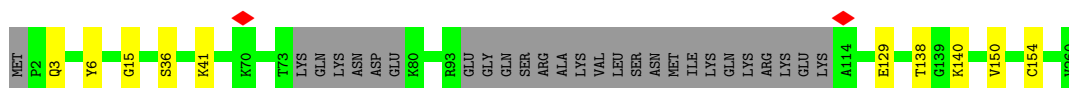
- Molecule 38: Nucleolar GTP-binding protein 2

Chain NC:  66% 30%



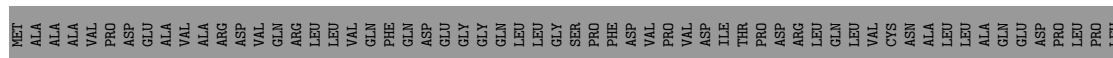
- Molecule 39: Ribosome biogenesis protein NSA2 homolog

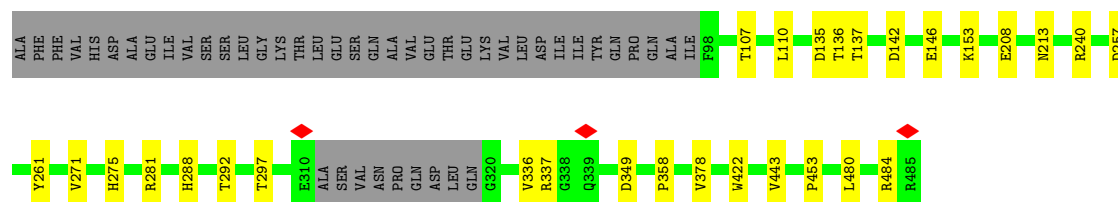
Chain NF:  86% 10%



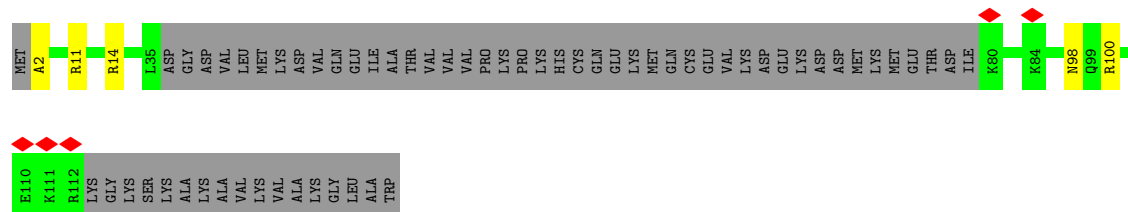
- Molecule 40: Notchless protein homolog 1

Chain NJ:  72% 6% 22%

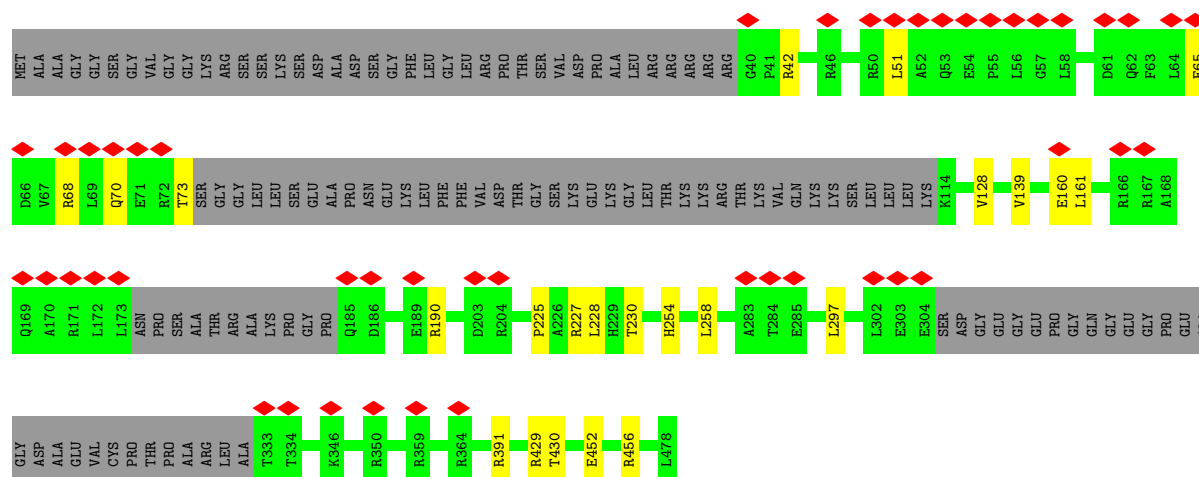
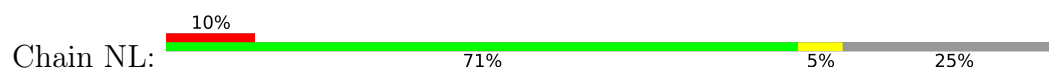




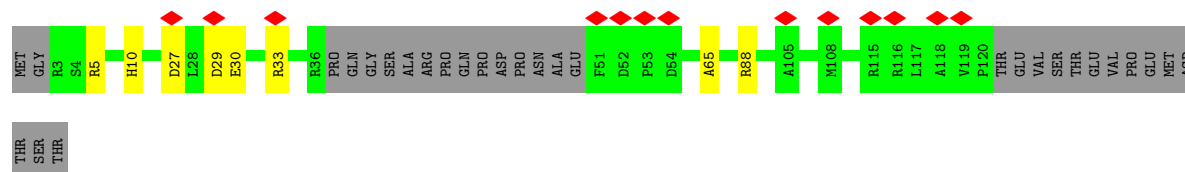
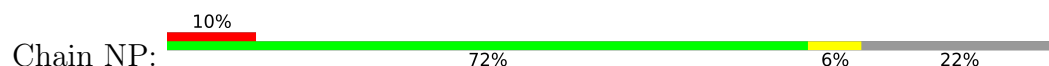
• Molecule 41: Protein LLP homolog



• Molecule 42: Ribosome biogenesis protein NOP53

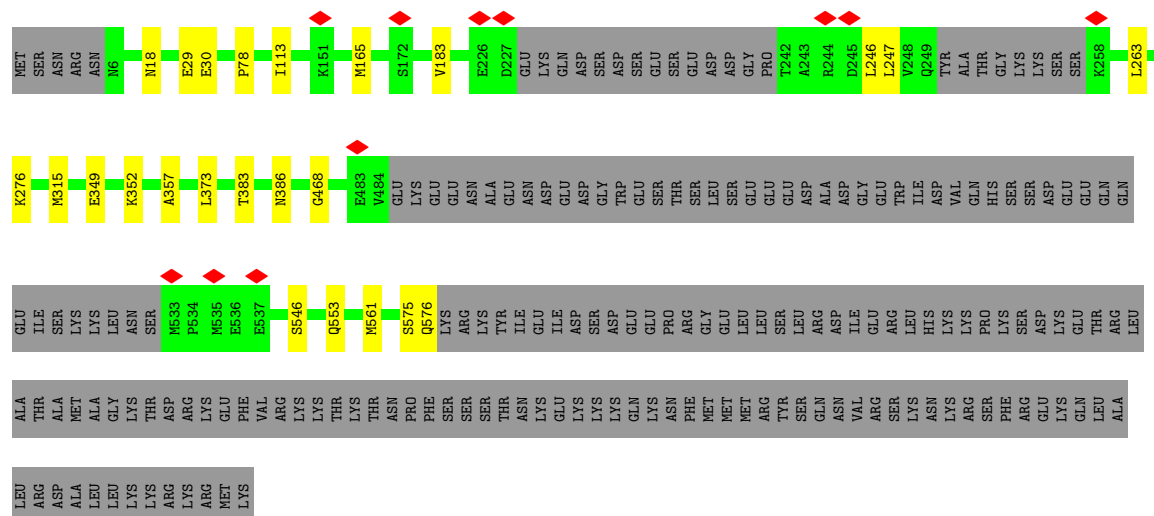


• Molecule 43: Zinc finger protein 593

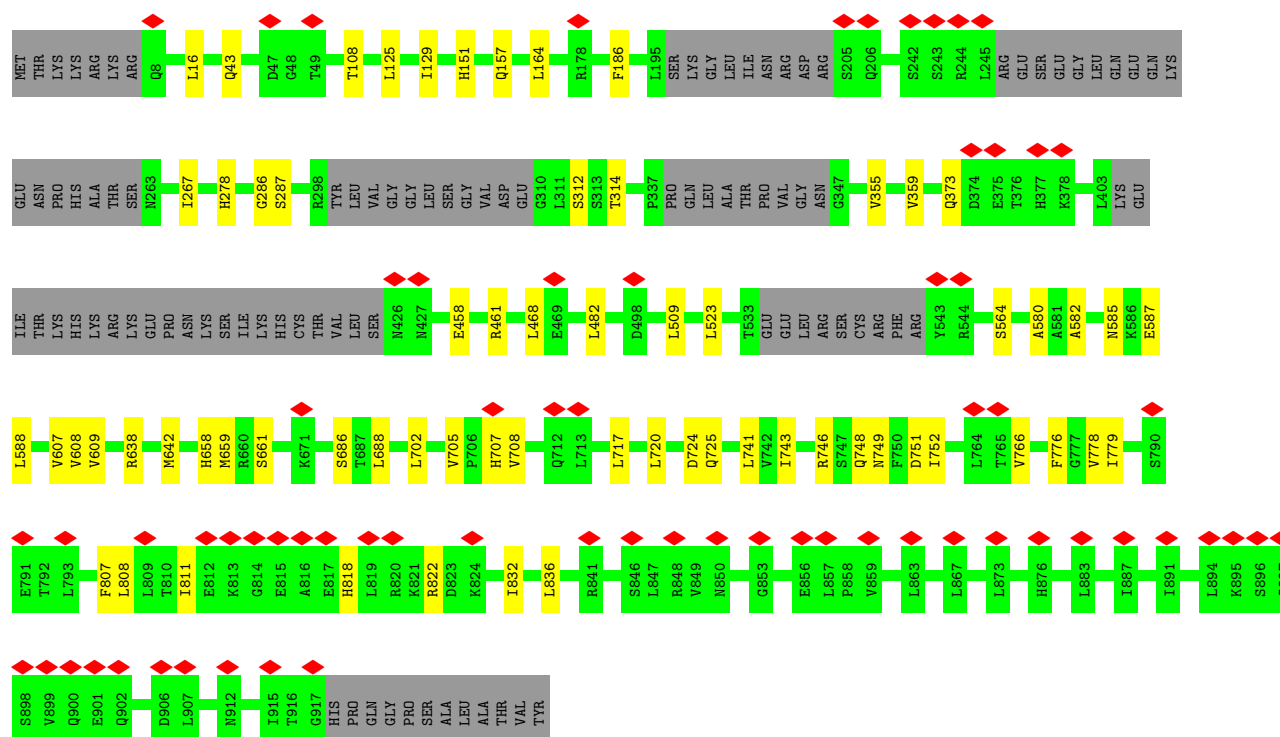
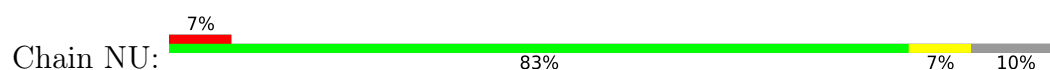


• Molecule 44: Protein SDA1 homolog

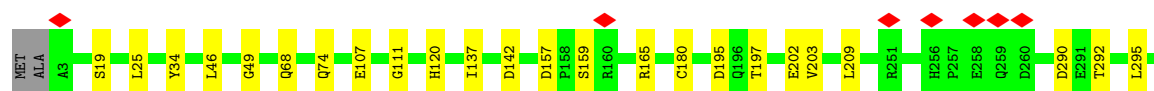
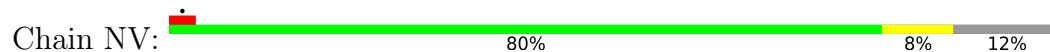


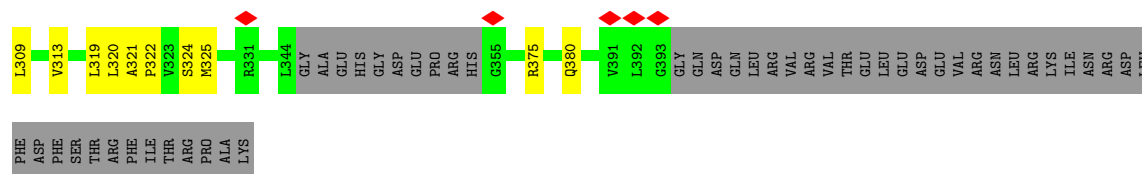


• Molecule 45: Testis-expressed protein 10



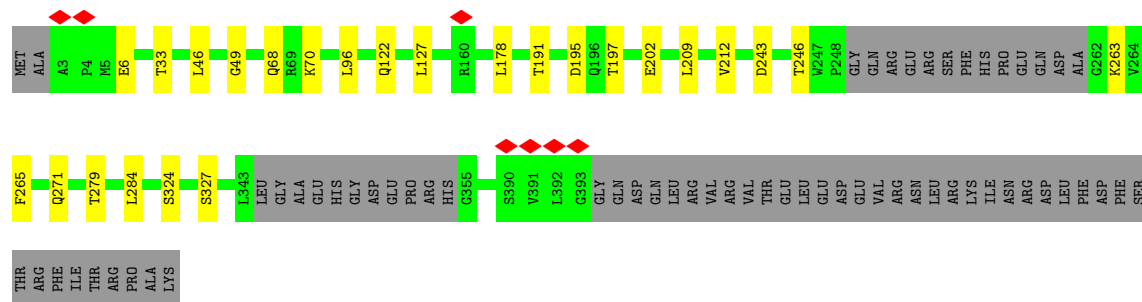
• Molecule 46: WD repeat-containing protein 18





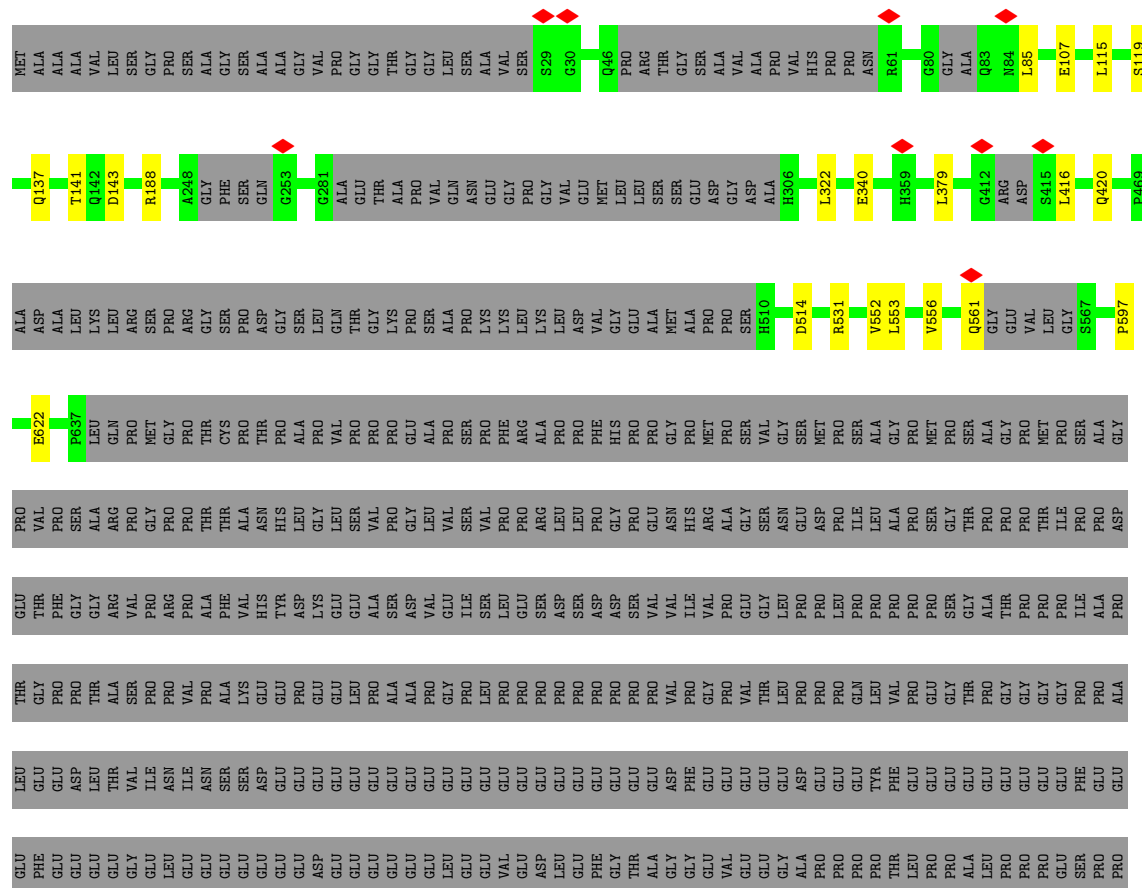
- Molecule 46: WD repeat-containing protein 18

Chain NW: 79% 6% 15%

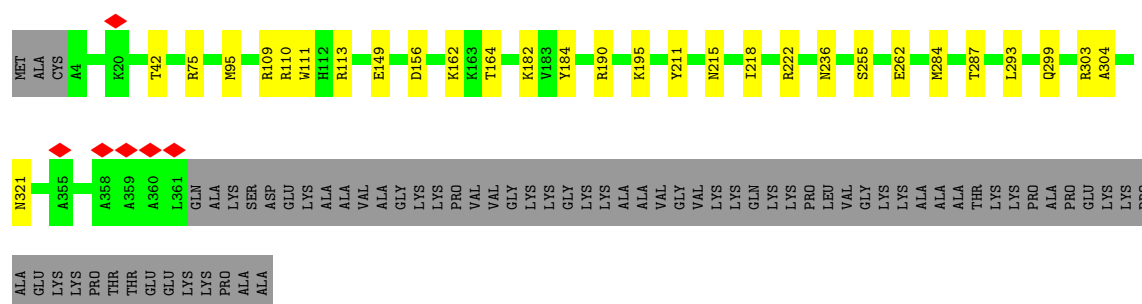
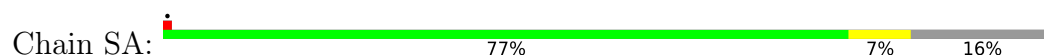


- Molecule 47: Proline-, glutamic acid- and leucine-rich protein 1

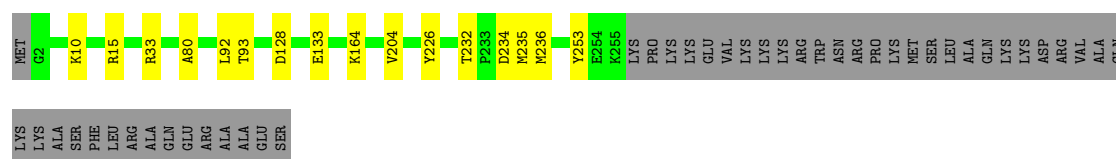
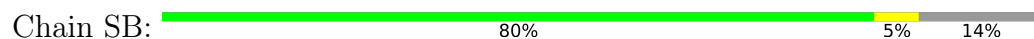
Chain NX: 44% 54%



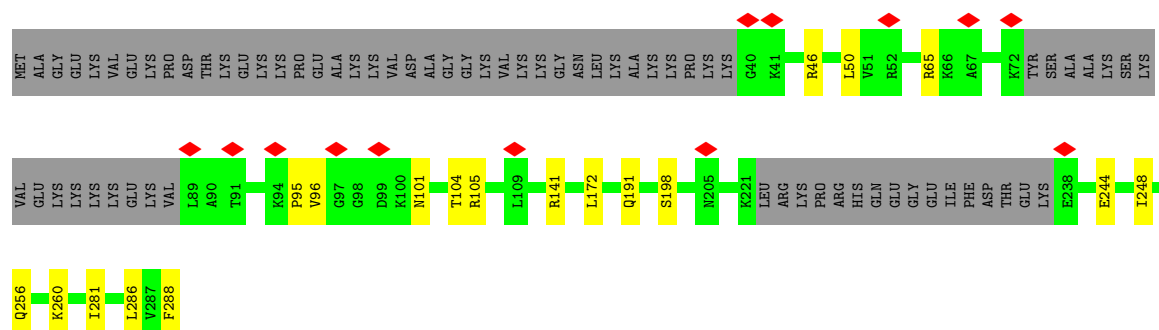
- Molecule 49: 60S ribosomal protein L4



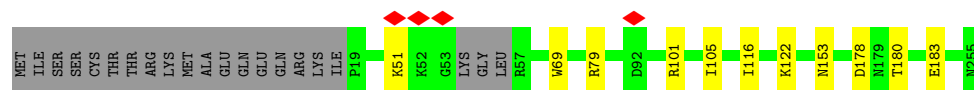
- Molecule 50: 60S ribosomal protein L5



- Molecule 51: 60S ribosomal protein L6

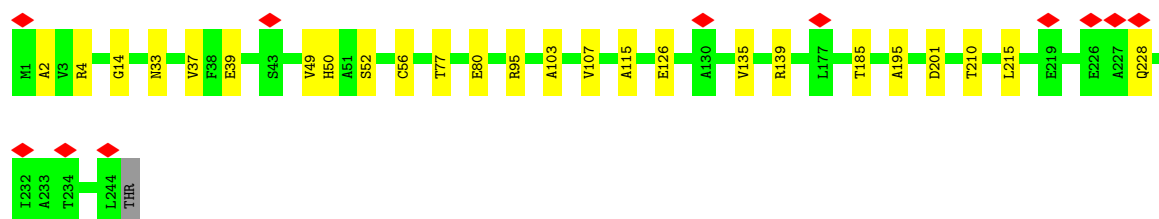


- Molecule 52: 60S ribosomal protein L7



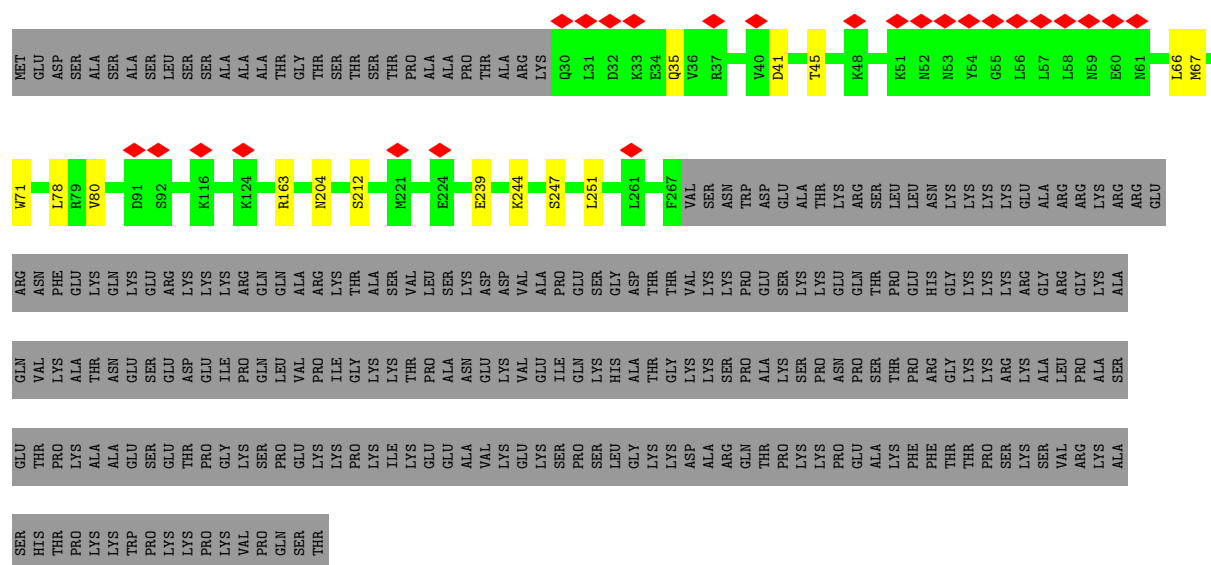
- Molecule 58: Eukaryotic translation initiation factor 6

Chain SK: 89% 10%



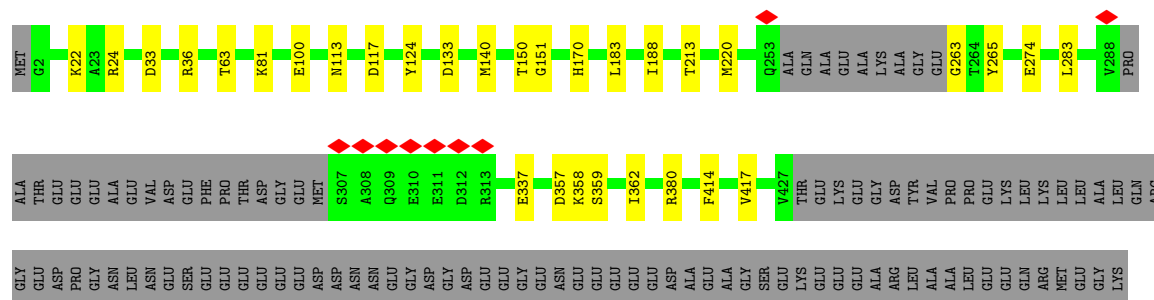
- Molecule 59: Ribosomal L1 domain-containing protein 1

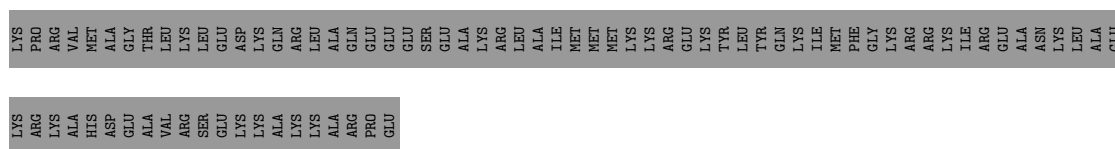
Chain SL: 5% 46% 51%



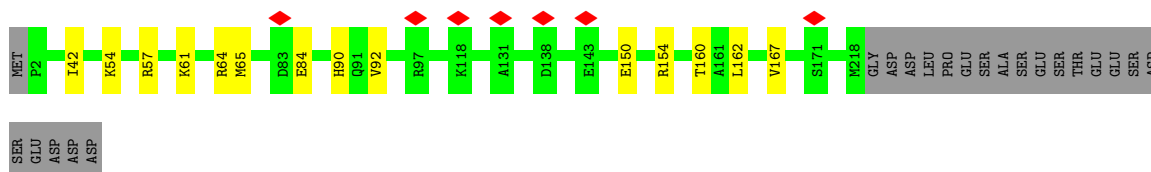
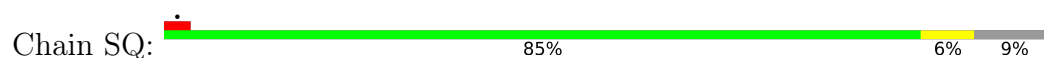
- Molecule 60: Pescadillo homolog

Chain SM: 63% 5% 32%

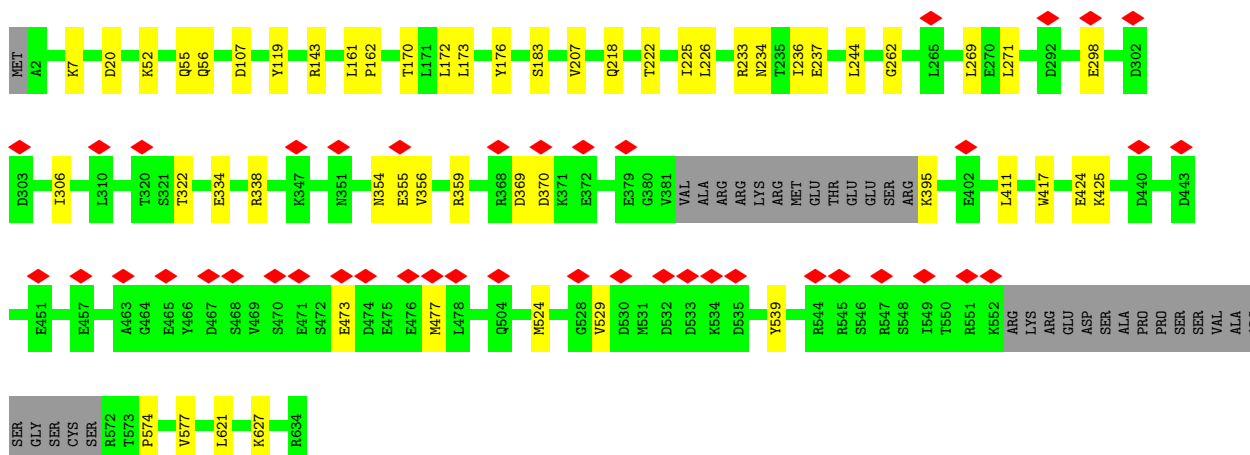
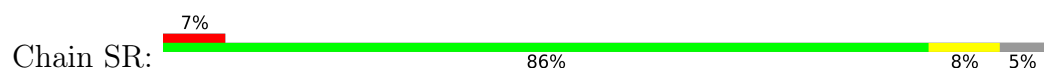




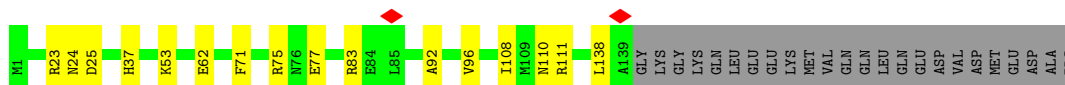
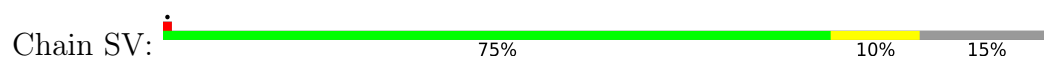
- Molecule 61: mRNA turnover protein 4 homolog



- Molecule 62: GTP-binding protein 4



- Molecule 63: Probable ribosome biogenesis protein RLP24



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	70162	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	8.539	Depositor
Minimum map value	-0.211	Depositor
Average map value	0.053	Depositor
Map value standard deviation	0.188	Depositor
Recommended contour level	0.8	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: OMC, OMG, HIC, ZN, MG, PSU, OMU, 6MZ, UR3, A2M, GTP, K, GDP, 5MC, 1MA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	BA	0.12	0/1224	0.27	0/1651
2	BB	0.12	0/1764	0.29	0/2365
3	BD	0.11	0/152	0.27	0/202
4	L1	0.10	0/3589	0.24	0/5589
5	L2	0.10	0/1709	0.27	0/2653
6	L3	0.13	1/80944 (0.0%)	0.26	0/126242
7	L4	0.10	0/2784	0.25	0/4336
8	L5	0.10	0/1372	0.26	0/1836
9	L6	0.10	0/1682	0.26	0/2248
10	L7	0.10	0/1682	0.25	0/2250
11	L8	0.09	0/1133	0.23	0/1516
12	L9	0.10	0/1677	0.27	0/2243
13	LA	0.09	0/1279	0.28	0/1716
14	LB	0.10	0/1239	0.28	0/1658
15	LC	0.11	0/1501	0.26	0/2013
16	LD	0.10	0/1305	0.26	0/1727
17	LE	0.11	0/1146	0.28	0/1533
18	LF	0.09	0/856	0.29	0/1149
19	LG	0.11	0/1048	0.28	0/1402
20	LH	0.11	0/1175	0.26	0/1572
21	LI	0.12	0/1132	0.26	0/1504
22	LJ	0.11	0/1130	0.26	0/1507
23	LK	0.11	0/935	0.25	0/1249
24	LL	0.10	0/1017	0.26	0/1364
25	LN	0.11	0/3294	0.29	0/4406
26	LO	0.09	0/748	0.22	0/1004
27	LP	0.12	0/894	0.27	0/1204
28	LQ	0.09	0/1071	0.25	0/1429
29	LR	0.10	0/898	0.27	0/1197
30	LS	0.09	0/1023	0.24	0/1351
31	LT	0.10	0/895	0.26	0/1198
32	LU	0.11	0/843	0.27	0/1115

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	LW	0.11	0/720	0.33	0/952
34	LX	0.09	0/718	0.25	0/953
35	LY	0.09	0/575	0.24	0/761
36	LZ	0.10	0/454	0.28	0/599
37	NB	0.13	0/701	0.26	0/920
38	NC	0.10	0/4175	0.26	0/5621
39	NF	0.11	0/1929	0.27	0/2579
40	NJ	0.16	0/3024	0.32	0/4099
41	NK	0.10	0/587	0.26	0/767
42	NL	0.13	0/3023	0.26	0/4049
43	NP	0.11	0/864	0.26	0/1154
44	NT	0.10	0/4144	0.24	0/5575
45	NU	0.10	0/6590	0.25	0/8941
46	NV	0.10	0/2987	0.27	0/4065
46	NW	0.12	0/2853	0.29	0/3883
47	NX	0.10	0/3993	0.24	0/5410
47	NY	0.10	0/4054	0.25	0/5496
48	NZ	0.10	0/1020	0.25	0/1343
49	SA	0.12	0/2907	0.28	0/3905
50	SB	0.12	0/2098	0.27	0/2817
51	SC	0.11	0/1776	0.27	0/2381
52	SD	0.10	0/1905	0.27	0/2539
53	SE	0.14	0/1919	0.31	0/2580
54	SF	0.12	0/1914	0.30	0/2567
55	SG	0.11	0/1537	0.24	0/2066
56	SH	0.11	0/1309	0.27	0/1756
57	SI	0.12	0/1980	0.29	0/2656
58	SK	0.11	0/1877	0.28	0/2554
59	SL	0.11	0/1949	0.30	0/2621
60	SM	0.11	0/3357	0.26	0/4529
61	SQ	0.10	0/1817	0.26	0/2435
62	SR	0.11	0/5025	0.26	0/6742
63	SV	0.11	0/1207	0.27	0/1600
All	All	0.12	1/198129 (0.0%)	0.26	0/285344

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L3	2415	OMU	O3'-P	5.12	1.61	1.56

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	11	0
2	BB	1736	0	1847	21	0
3	BD	149	0	152	4	0
4	L1	3278	0	1665	13	0
5	L2	1535	0	789	7	0
6	L3	75027	0	38014	402	0
7	L4	2494	0	1263	12	0
8	L5	1349	0	1383	8	0
9	L6	1652	0	1770	12	0
10	L7	1650	0	1794	8	0
11	L8	1111	0	1174	11	0
12	L9	1635	0	1671	6	0
13	LA	1249	0	1276	3	0
14	LB	1223	0	1330	11	0
15	LC	1461	0	1502	5	0
16	LD	1289	0	1429	12	0
17	LE	1119	0	1177	5	0
18	LF	842	0	864	7	0
19	LG	1034	0	1097	5	0
20	LH	1156	0	1268	7	0
21	LI	1115	0	1205	10	0
22	LJ	1107	0	1182	11	0
23	LK	918	0	985	7	0
24	LL	1002	0	1068	7	0
25	LN	3239	0	3377	38	0
26	LO	738	0	774	1	0
27	LP	879	0	924	10	0
28	LQ	1053	0	1147	7	0
29	LR	888	0	977	5	0
30	LS	1015	0	1148	6	0
31	LT	876	0	912	2	0
32	LU	832	0	917	5	0
33	LW	705	0	737	6	0
34	LX	708	0	756	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	LY	569	0	637	4	0
36	LZ	444	0	483	4	0
37	NB	691	0	770	6	0
38	NC	4097	0	4176	21	0
39	NF	1891	0	2015	9	0
40	NJ	2951	0	2895	18	0
41	NK	581	0	656	5	0
42	NL	2980	0	3089	19	0
43	NP	847	0	854	6	0
44	NT	4072	0	4225	18	0
45	NU	6469	0	6478	46	0
46	NV	2915	0	2896	20	0
46	NW	2789	0	2781	16	0
47	NX	3926	0	4073	14	0
47	NY	3983	0	4129	20	0
48	NZ	1010	0	1106	9	0
49	SA	2853	0	3028	22	0
50	SB	2057	0	2050	12	0
51	SC	1743	0	1899	12	0
52	SD	1870	0	1996	7	0
53	SE	1885	0	2036	13	0
54	SF	1876	0	1970	16	0
55	SG	1518	0	1601	7	0
56	SH	1275	0	1304	3	0
57	SI	1937	0	2070	8	0
58	SK	1852	0	1828	17	0
59	SL	1917	0	2018	9	0
60	SM	3278	0	3332	21	0
61	SQ	1778	0	1817	10	0
62	SR	4939	0	5079	37	0
63	SV	1184	0	1248	13	0
64	L1	5	0	0	0	0
64	L3	84	0	0	0	0
64	L4	1	0	0	0	0
64	L6	1	0	0	0	0
64	L9	1	0	0	0	0
64	LQ	1	0	0	0	0
64	LR	1	0	0	0	0
64	LT	1	0	0	0	0
64	LW	1	0	0	0	0
64	NC	1	0	0	0	0
64	SA	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	SF	1	0	0	0	0
64	SR	1	0	0	0	0
65	LR	1	0	0	0	0
65	LW	1	0	0	0	0
65	LX	1	0	0	0	0
65	NP	1	0	0	0	0
65	SV	1	0	0	0	0
66	NC	32	0	12	0	0
67	NC	1	0	0	0	0
67	SR	1	0	0	0	0
68	SR	28	0	12	0	0
All	All	189616	0	153394	870	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 3.

All (870) 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)
19:LG:97:TYR:HH	63:SV:37:HIS:HE2	1.21	0.87
47:NY:322:LEU:HD22	47:NY:379:LEU:HD11	1.58	0.86
6:L3:4648:A:OP1	16:LD:62:ARG:NH1	2.10	0.85
6:L3:3896:C:O2'	25:LN:268:ARG:NH2	2.10	0.85
61:SQ:150:GLU:OE2	61:SQ:154:ARG:NH1	2.10	0.84
6:L3:62:A:N3	6:L3:77:U:O2'	2.10	0.83
6:L3:3961:G:O2'	6:L3:4043:G:N2	2.10	0.83
6:L3:4226:G:O2'	6:L3:4227:OMU:OP1	1.97	0.82
6:L3:2520:C:O2	6:L3:2640:G:N2	2.11	0.82
2:BB:207:LYS:NZ	2:BB:208:SER:O	2.13	0.81
6:L3:4927:G:OP2	6:L3:4927:G:N2	2.13	0.81
6:L3:1670:G:N2	6:L3:1670:G:OP2	2.13	0.81
47:NX:115:LEU:O	47:NX:119:SER:OG	1.97	0.81
1:BA:25:THR:OG1	62:SR:262:GLY:O	2.00	0.80
6:L3:1480:C:O2'	6:L3:1482:G:OP2	1.99	0.79
6:L3:151:G:OP1	12:L9:49:ARG:NH2	2.14	0.79
6:L3:308:G:OP2	6:L3:308:G:N2	2.14	0.78
6:L3:4598:C:O2	6:L3:4612:C:N4	2.16	0.78
6:L3:4617:G:OP2	25:LN:358:ARG:NH2	2.16	0.78
42:NL:429:ARG:NH1	57:SI:183:GLU:OE2	2.16	0.78
8:L5:158:SER:OG	8:L5:161:GLU:OE1	2.01	0.78
2:BB:156:LYS:NZ	2:BB:158:GLN:OE1	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:NZ:317:GLU:OE1	48:NZ:342:ARG:NH2	2.16	0.78
1:BA:16:ARG:NH1	6:L3:1975:G:O2'	2.18	0.77
6:L3:1319:U:OP2	23:LK:21:ARG:NH2	2.18	0.77
4:L1:156:U:OP2	53:SE:89:ARG:NH2	2.18	0.77
6:L3:2848:G:O2'	6:L3:3838:U:O4	2.01	0.77
6:L3:4670:C:O2'	6:L3:4672:A:OP2	2.02	0.77
24:LL:71:ARG:NH1	49:SA:149:GLU:OE2	2.17	0.77
47:NY:188:ARG:NH1	47:NY:190:GLU:OE2	2.18	0.77
6:L3:1293:G:OP2	6:L3:1293:G:N2	2.18	0.76
6:L3:1420:A:O2'	6:L3:1500:A:O2'	2.02	0.76
6:L3:4646:U:OP2	16:LD:62:ARG:NH2	2.19	0.76
6:L3:413:G:OP2	36:LZ:36:ARG:NH2	2.19	0.75
6:L3:2695:A:OP1	35:LY:35:LYS:NZ	2.20	0.75
7:L4:40:U:O2	8:L5:75:ARG:NH1	2.20	0.75
6:L3:3717:A:OP2	6:L3:3735:G:N2	2.18	0.75
46:NV:321:ALA:O	47:NX:561:GLN:NE2	2.19	0.75
62:SR:417:TRP:O	62:SR:425:LYS:NZ	2.20	0.75
6:L3:2079:G:OP2	28:LQ:64:LYS:NZ	2.20	0.74
6:L3:4768:G:OP1	10:L7:168:TYR:OH	2.05	0.74
59:SL:204:ASN:O	59:SL:212:SER:OG	2.04	0.74
6:L3:3770:PSU:H2'	6:L3:3771:C:C6	2.22	0.74
6:L3:1818:G:O2'	6:L3:1820:C:OP2	2.05	0.74
6:L3:2414:G:O2'	6:L3:2415:OMU:O5'	2.01	0.74
7:L4:23:A:N3	7:L4:118:C:O2'	2.21	0.74
6:L3:67:C:OP2	6:L3:312:G:N2	2.21	0.74
60:SM:357:ASP:OD2	60:SM:359:SER:OG	2.04	0.74
6:L3:2262:G:OP2	24:LL:98:ARG:NH1	2.21	0.74
6:L3:4717:A:OP2	25:LN:30:LYS:NZ	2.20	0.74
47:NY:200:LYS:NZ	47:NY:238:GLU:OE1	2.21	0.74
48:NZ:340:GLU:OE2	48:NZ:342:ARG:NH2	2.21	0.73
5:L2:53:G:OP2	56:SH:81:ARG:NH1	2.22	0.73
6:L3:502:C:O2'	6:L3:503:C:OP1	2.04	0.73
6:L3:375:G:OP2	33:LW:52:LYS:NZ	2.21	0.73
6:L3:4389:C:OP2	62:SR:627:LYS:NZ	2.21	0.73
6:L3:1508:A:OP1	49:SA:110:ARG:NH2	2.22	0.73
6:L3:1373:A:O2'	49:SA:236:ASN:OD1	2.03	0.73
43:NP:27:ASP:OD2	63:SV:23:ARG:NH2	2.22	0.73
2:BB:101:LYS:NZ	6:L3:4047:A:OP1	2.20	0.73
6:L3:4696:C:OP1	48:NZ:242:SER:OG	2.06	0.73
6:L3:4620:OMU:OP2	6:L3:4670:C:N4	2.21	0.72
21:LI:50:ARG:NH1	21:LI:51:LYS:O	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L3:4688:C:O2'	55:SG:155:SER:OG	2.07	0.72
6:L3:1548:G:O2'	6:L3:2812:A:N3	2.22	0.71
6:L3:3709:U:OP2	44:NT:18:ASN:ND2	2.23	0.71
5:L2:1165:A:O2'	5:L2:1167:A:OP1	2.08	0.71
2:BB:23:ARG:NH1	2:BB:24:LYS:O	2.23	0.71
6:L3:4226:G:O2'	6:L3:4227:OMU:H5''	1.90	0.71
22:LJ:21:ARG:NH1	22:LJ:47:ASP:OD1	2.23	0.71
34:LX:26:VAL:HG21	54:SF:180:LEU:HD11	1.70	0.71
40:NJ:288:HIS:HD1	40:NJ:349:ASP:HB2	1.55	0.71
6:L3:4124:G:N2	53:SE:43:GLN:O	2.24	0.71
6:L3:2753:G:OP1	22:LJ:133:LYS:NZ	2.24	0.71
6:L3:4689:PSU:N3	6:L3:4699:U:O4	2.20	0.71
6:L3:151:G:OP2	12:L9:4:TYR:OH	2.08	0.70
6:L3:4460:U:OP1	25:LN:10:ARG:NH1	2.22	0.70
6:L3:1883:G:OP1	28:LQ:47:ARG:NH1	2.23	0.70
6:L3:408:A:O2'	6:L3:411:G:OP2	2.09	0.70
6:L3:695:G:O2'	6:L3:697:G:OP2	2.08	0.70
6:L3:1364:U:OP2	9:L6:36:ARG:NH2	2.25	0.70
32:LU:50:PHE:O	32:LU:55:ARG:NH1	2.25	0.70
25:LN:70:LYS:NZ	58:SK:80:GLU:OE2	2.23	0.70
6:L3:4401:G:O4'	37:NB:17:LYS:NZ	2.23	0.69
61:SQ:42:ILE:HD11	61:SQ:92:VAL:HG13	1.74	0.69
2:BB:41:TYR:OH	2:BB:47:LYS:O	2.11	0.69
59:SL:239:GLU:O	59:SL:244:LYS:NZ	2.25	0.69
1:BA:123:ARG:NH1	61:SQ:61:LYS:O	2.25	0.69
6:L3:2555:G:O2'	22:LJ:108:ARG:NH2	2.26	0.69
6:L3:5047:C:O2'	6:L3:5050:C:OP2	2.10	0.69
17:LE:115:LYS:NZ	17:LE:127:GLN:O	2.26	0.69
43:NP:33:ARG:NH1	63:SV:25:ASP:OD2	2.25	0.69
57:SI:153:ASN:ND2	60:SM:263:GLY:O	2.25	0.69
4:L1:66:A:OP1	30:LS:7:ARG:NH1	2.26	0.69
6:L3:2763:U:O2'	42:NL:391:ARG:NH2	2.26	0.69
6:L3:4299:PSU:H2'	6:L3:4300:U:C6	2.28	0.69
6:L3:1255:A:OP1	6:L3:1257:A:N6	2.26	0.68
47:NY:143:ASP:O	47:NY:188:ARG:NH2	2.26	0.68
6:L3:2545:U:O2'	6:L3:2547:G:N7	2.24	0.68
7:L4:7:G:OP1	50:SB:33:ARG:NH1	2.27	0.68
6:L3:169:G:O2'	9:L6:136:LYS:NZ	2.27	0.68
6:L3:1280:C:O2'	49:SA:321:ASN:OD1	2.10	0.67
6:L3:5024:C:OP2	6:L3:5025:C:N4	2.27	0.67
6:L3:4678:G:OP1	41:NK:14:ARG:NH1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L4:66:G:OP1	50:SB:10:LYS:NZ	2.26	0.67
60:SM:265:TYR:OH	60:SM:358:LYS:O	2.08	0.67
6:L3:76:A:N7	9:L6:74:ARG:NH2	2.43	0.67
6:L3:2483:G:O6	60:SM:24:ARG:NH1	2.28	0.67
53:SE:105:GLU:OE2	53:SE:113:ARG:NH2	2.27	0.67
55:SG:41:ILE:HG21	55:SG:73:ILE:HD11	1.76	0.67
6:L3:3867:A2M:H2'	6:L3:3868:G:C8	2.29	0.66
33:LW:54:LYS:O	33:LW:58:THR:HG23	1.94	0.66
6:L3:1369:C:OP2	6:L3:1370:G:O2'	2.06	0.66
2:BB:16:GLU:OE1	2:BB:214:GLN:NE2	2.29	0.66
15:LC:92:ASN:ND2	37:NB:49:GLY:O	2.27	0.66
46:NV:157:ASP:OD2	46:NV:159:SER:OG	2.09	0.66
6:L3:3785:A2M:H8	6:L3:3785:A2M:H5''	1.76	0.66
6:L3:121:A:OP1	53:SE:110:LYS:NZ	2.27	0.66
6:L3:4548:A:OP2	39:NF:138:THR:OG1	2.08	0.66
62:SR:52:LYS:O	62:SR:56:GLN:NE2	2.29	0.66
6:L3:4457:PSU:OP1	19:LG:50:ASN:ND2	2.29	0.66
3:BD:728:LYS:NZ	45:NU:751:ASP:O	2.29	0.66
6:L3:4156:G:OP2	6:L3:4157:A:O2'	2.11	0.66
42:NL:190:ARG:NH2	60:SM:117:ASP:OD1	2.28	0.65
6:L3:2378:G:N2	6:L3:2381:A:OP2	2.27	0.65
38:NC:25:GLN:NE2	38:NC:26:GLY:O	2.29	0.65
6:L3:76:A:OP2	9:L6:74:ARG:NE	2.29	0.65
6:L3:2363:A2M:H2'	6:L3:2364:OMG:O4'	1.97	0.65
6:L3:2876:OMG:HM22	6:L3:2877:G:H5'	1.77	0.65
6:L3:2922:G:O2'	6:L3:3275:A:N6	2.29	0.65
52:SD:154:ILE:HG22	52:SD:187:MET:HE1	1.79	0.65
63:SV:71:PHE:O	63:SV:75:ARG:NH2	2.30	0.65
60:SM:124:TYR:OH	60:SM:133:ASP:OD2	2.14	0.65
6:L3:2306:G:OP1	28:LQ:128:ARG:NH1	2.30	0.64
6:L3:937:U:OP1	11:L8:46:ARG:NH1	2.30	0.64
6:L3:4664:A:OP1	25:LN:376:HIS:NE2	2.31	0.64
6:L3:3912:U:OP1	38:NC:49:ARG:NH2	2.31	0.64
22:LJ:22:LYS:NZ	22:LJ:132:GLN:O	2.26	0.64
46:NW:202:GLU:OE2	46:NW:209:LEU:HD21	1.98	0.64
6:L3:4477:A:OP1	39:NF:6:TYR:OH	2.15	0.64
60:SM:33:ASP:OD1	60:SM:36:ARG:NH2	2.31	0.64
60:SM:337:GLU:OE2	60:SM:380:ARG:NE	2.30	0.64
62:SR:172:LEU:HD23	62:SR:244:LEU:HD23	1.79	0.64
6:L3:4216:G:N2	6:L3:4219:A:OP2	2.30	0.64
6:L3:1676:C:O2'	6:L3:1677:PSU:H5'	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:NJ:257:ASP:OD1	40:NJ:337:ARG:NH1	2.32	0.64
60:SM:414:PHE:O	60:SM:417:VAL:HG22	1.98	0.64
60:SM:81:LYS:NZ	60:SM:113:ASN:O	2.30	0.63
2:BB:33:GLU:OE2	6:L3:3970:G:O2'	2.08	0.63
6:L3:4524:G:C2	25:LN:252:ALA:HB1	2.32	0.63
6:L3:3734:PSU:H2'	6:L3:3735:G:O4'	1.99	0.63
25:LN:222:VAL:O	25:LN:343:ARG:NH1	2.31	0.63
6:L3:4370:OMG:H2'	6:L3:4371:G:C8	2.33	0.63
6:L3:4618:OMG:H5''	19:LG:15:ARG:HB2	1.80	0.63
20:LH:16:GLU:N	20:LH:16:GLU:OE1	2.31	0.63
46:NV:120:HIS:ND1	46:NV:142:ASP:OD2	2.31	0.63
6:L3:4997:G:O2'	27:LP:118:GLN:OE1	2.09	0.63
7:L4:55:A:O2'	8:L5:151:ILE:O	2.13	0.63
6:L3:1783:C:OP1	48:NZ:329:LYS:NZ	2.25	0.62
13:LA:135:ARG:NH2	62:SR:621:LEU:HD13	2.15	0.62
48:NZ:256:GLN:O	48:NZ:264:ARG:NH2	2.32	0.62
6:L3:1318:C:N4	28:LQ:42:ASP:OD1	2.32	0.62
55:SG:47:LEU:HD22	55:SG:53:LYS:NZ	2.14	0.62
58:SK:39:GLU:O	62:SR:395:LYS:NZ	2.33	0.62
6:L3:150:U:OP2	53:SE:200:THR:OG1	2.12	0.62
6:L3:2415:OMU:OP2	6:L3:2415:OMU:H6	2.00	0.62
6:L3:3821:A:N6	38:NC:283:ALA:O	2.31	0.62
1:BA:90:ARG:NE	1:BA:98:ILE:HD11	2.13	0.62
6:L3:226:G:N7	49:SA:184:TYR:OH	2.31	0.62
6:L3:1683:PSU:H2'	6:L3:1684:A:H8	1.65	0.62
18:LF:47:ILE:HD12	18:LF:63:ILE:HD11	1.80	0.62
46:NW:33:THR:OG1	46:NW:70:LYS:NZ	2.32	0.62
6:L3:4637:OMG:H2'	6:L3:4638:U:C6	2.35	0.62
6:L3:5022:U:O2'	6:L3:5025:C:N4	2.32	0.62
8:L5:90:ARG:NH2	8:L5:108:GLY:O	2.33	0.62
16:LD:39:GLN:OE1	16:LD:42:ARG:NH1	2.33	0.62
47:NX:531:ARG:NH1	47:NY:622:GLU:OE2	2.34	0.61
47:NY:34:ARG:NH1	47:NY:81:GLY:O	2.32	0.61
63:SV:53:LYS:NZ	63:SV:62:GLU:OE2	2.32	0.61
24:LL:32:LEU:HD12	24:LL:106:LEU:HD22	1.82	0.61
6:L3:4042:OMG:H2'	6:L3:4043:G:H8	1.65	0.61
6:L3:4385:A:N1	39:NF:140:LYS:NZ	2.42	0.61
6:L3:2616:C:OP1	16:LD:60:ARG:NH1	2.33	0.61
6:L3:709:C:OP1	31:LT:89:ARG:NH2	2.34	0.61
6:L3:4910:G:N2	10:L7:106:ASP:O	2.34	0.61
6:L3:2487:G:O6	57:SI:51:LYS:NZ	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:SR:55:GLN:NE2	62:SR:107:ASP:OD1	2.33	0.61
6:L3:90:G:OP2	6:L3:92:C:N4	2.33	0.60
6:L3:4580:U:O2'	25:LN:182:GLU:OE2	2.18	0.60
5:L2:4:G:HO2'	57:SI:69:TRP:CD1	2.19	0.60
6:L3:404:U:O2'	21:LI:87:ARG:NH2	2.34	0.60
6:L3:4299:PSU:H2'	6:L3:4300:U:H6	1.67	0.60
17:LE:68:THR:HG22	17:LE:69:GLN:H	1.66	0.60
40:NJ:240:ARG:NH2	40:NJ:275:HIS:O	2.34	0.60
6:L3:737:C:OP2	11:L8:71:LYS:NZ	2.33	0.60
6:L3:1322:1MA:H2'	6:L3:1323:A:O4'	2.02	0.60
6:L3:3759:A:C6	6:L3:4220:6MZ:H9	2.37	0.60
5:L2:1167:A:O3'	6:L3:1:C:OP2	2.16	0.60
42:NL:452:GLU:OE1	60:SM:63:THR:OG1	2.20	0.60
6:L3:369:G:N2	6:L3:372:A:OP2	2.30	0.59
6:L3:4216:G:N3	6:L3:4217:G:O2'	2.33	0.59
6:L3:5001:PSU:H2'	6:L3:5002:U:O4'	2.02	0.59
6:L3:3938:G:N2	6:L3:4171:C:OP2	2.35	0.59
6:L3:4042:OMG:H2'	6:L3:4043:G:C8	2.37	0.59
6:L3:4457:PSU:O4	25:LN:252:ALA:HB3	2.02	0.59
6:L3:3605:C:O2'	16:LD:89:MET:HE1	2.02	0.59
6:L3:4726:G:OP2	41:NK:100:ARG:NH2	2.35	0.59
6:L3:4765:G:OP1	55:SG:23:ARG:NE	2.36	0.59
6:L3:4476:C:O2'	6:L3:4478:G:OP2	2.21	0.59
6:L3:4622:A:O2'	6:L3:4623:OMG:H5'	2.02	0.59
6:L3:2373:C:H5'	27:LP:46:LEU:HD21	1.85	0.58
7:L4:27:G:OP1	8:L5:146:ARG:NH2	2.35	0.58
38:NC:437:GLU:OE1	38:NC:437:GLU:N	2.36	0.58
27:LP:36:VAL:HG21	27:LP:44:ARG:HD3	1.85	0.58
47:NY:322:LEU:CD2	47:NY:379:LEU:HD11	2.32	0.58
47:NY:165:LEU:HD12	47:NY:168:LEU:HD12	1.86	0.58
18:LF:117:ILE:HD11	62:SR:539:TYR:O	2.03	0.58
46:NV:290:ASP:OD1	46:NV:292:THR:HG22	2.04	0.58
6:L3:2480:G:OP1	60:SM:22:LYS:NZ	2.37	0.58
25:LN:10:ARG:NH2	25:LN:265:SER:O	2.36	0.58
49:SA:156:ASP:OD2	49:SA:255:SER:OG	2.22	0.58
6:L3:4541:G:N2	6:L3:4544:A:OP2	2.24	0.58
6:L3:1693:U:OP2	14:LB:49:LYS:NZ	2.28	0.58
6:L3:1772:C:O2'	6:L3:1773:OMU:H5''	2.04	0.58
6:L3:2299:G:OP1	49:SA:182:LYS:NZ	2.32	0.58
6:L3:2601:A:N6	6:L3:2744:A:OP2	2.34	0.58
6:L3:3681:G:OP2	54:SF:128:ARG:NH2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SB:80:ALA:O	50:SB:92:LEU:HD12	2.04	0.58
6:L3:935:A:O2'	11:L8:46:ARG:NH1	2.37	0.57
6:L3:3658:C:OP1	54:SF:242:ARG:NH1	2.36	0.57
6:L3:3924:C:O2'	6:L3:3925:OMU:H5''	2.03	0.57
29:LR:100:GLN:NE2	38:NC:614:ALA:O	2.37	0.57
49:SA:303:ARG:NH1	49:SA:304:ALA:O	2.37	0.57
1:BA:128:THR:O	1:BA:132:ILE:HD12	2.03	0.57
6:L3:66:A:O2'	6:L3:326:C:O2	2.23	0.57
45:NU:724:ASP:OD1	45:NU:725:GLN:N	2.38	0.57
44:NT:357:ALA:HB1	44:NT:373:LEU:HD21	1.86	0.57
6:L3:3648:A:N6	6:L3:3830:A2M:O4'	2.38	0.57
6:L3:4529:G:O2'	6:L3:4530:UR3:H5'	2.04	0.57
6:L3:2590:G:O2'	6:L3:2755:A:N6	2.38	0.57
6:L3:4728:U:OP1	25:LN:132:LYS:NZ	2.37	0.57
19:LG:97:TYR:OH	63:SV:37:HIS:NE2	2.27	0.57
4:L1:75:OMG:OP2	21:LI:74:TYR:OH	2.23	0.57
61:SQ:64:ARG:NH1	61:SQ:65:MET:O	2.38	0.57
62:SR:524:MET:HE2	62:SR:524:MET:HA	1.87	0.57
6:L3:934:C:O2'	6:L3:935:A:O5'	2.17	0.57
50:SB:234:ASP:OD1	50:SB:235:MET:N	2.38	0.57
6:L3:3867:A2M:HM'2	6:L3:3867:A2M:N3	2.20	0.56
40:NJ:422:TRP:CZ3	40:NJ:443:VAL:HG21	2.40	0.56
46:NW:68:GLN:NE2	46:NW:324:SER:O	2.38	0.56
2:BB:77:ALA:O	2:BB:81:ASP:N	2.38	0.56
6:L3:4266:G:OP2	50:SB:15:ARG:NE	2.38	0.56
40:NJ:261:TYR:HE1	40:NJ:271:VAL:HG13	1.70	0.56
54:SF:29:LEU:O	54:SF:123:ARG:NE	2.36	0.56
5:L2:48:G:O2'	57:SI:79:ARG:NH1	2.38	0.56
6:L3:4696:C:OP2	48:NZ:244:ARG:NH2	2.37	0.56
7:L4:48:G:OP1	50:SB:226:TYR:OH	2.21	0.56
14:LB:122:THR:OG1	14:LB:124:ASP:OD1	2.08	0.56
54:SF:102:LEU:HB2	54:SF:107:MET:HE3	1.88	0.56
6:L3:4536:OMC:H2'	6:L3:4537:C:H6	1.71	0.56
16:LD:7:GLN:N	16:LD:7:GLN:OE1	2.38	0.56
24:LL:20:ARG:NH1	28:LQ:78:LEU:O	2.38	0.56
49:SA:211:TYR:OH	49:SA:218:ILE:HD11	2.06	0.56
62:SR:176:TYR:HE1	62:SR:271:LEU:HD22	1.70	0.56
6:L3:3695:PSU:H2'	6:L3:3696:C:C6	2.41	0.56
6:L3:4565:C:O2	25:LN:268:ARG:NH1	2.38	0.56
42:NL:456:ARG:NH2	60:SM:213:THR:O	2.39	0.56
45:NU:748:GLN:O	45:NU:752:ILE:HD12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SB:204:VAL:HG11	50:SB:236:MET:HE1	1.87	0.56
6:L3:2000:G:O6	61:SQ:54:LYS:NZ	2.32	0.56
38:NC:416:GLU:OE1	38:NC:417:ASN:ND2	2.39	0.56
6:L3:1564:A:N3	6:L3:3789:C:O2'	2.39	0.56
6:L3:4436:U:O2	62:SR:143:ARG:NH1	2.39	0.56
38:NC:522:MET:SD	45:NU:702:LEU:HD12	2.46	0.56
44:NT:383:THR:OG1	44:NT:386:ASN:OD1	2.23	0.56
57:SI:105:ILE:HD13	57:SI:116:ILE:HD13	1.88	0.56
45:NU:688:LEU:HD21	45:NU:778:VAL:HG11	1.88	0.56
2:BB:205:TYR:OH	2:BB:215:ARG:NH2	2.39	0.55
62:SR:173:LEU:O	62:SR:222:THR:OG1	2.22	0.55
6:L3:1625:OMG:H4'	6:L3:1626:G:O5'	2.07	0.55
6:L3:3715:PSU:H2'	6:L3:3716:C:O4'	2.07	0.55
18:LF:48:LYS:NZ	18:LF:51:GLY:O	2.39	0.55
6:L3:1378:C:N3	9:L6:158:ARG:NH1	2.53	0.55
45:NU:832:ILE:HD11	45:NU:836:LEU:HD12	1.88	0.55
47:NX:340:GLU:OE1	47:NX:340:GLU:N	2.39	0.55
58:SK:185:THR:HG23	62:SR:359:ARG:HH22	1.71	0.55
6:L3:4305:G:O2'	6:L3:4306:OMU:H5''	2.06	0.55
44:NT:246:LEU:N	44:NT:561:MET:HE1	2.22	0.55
58:SK:185:THR:HG23	62:SR:359:ARG:NH2	2.22	0.55
6:L3:2578:G:N7	22:LJ:17:ARG:NH1	2.54	0.55
6:L3:3654:G:O2'	6:L3:3693:U:OP1	2.17	0.55
6:L3:4120:U:O2'	6:L3:4121:G:OP1	2.25	0.55
6:L3:4912:G:N7	6:L3:4913:G:N2	2.55	0.55
25:LN:181:MET:HE1	25:LN:346:THR:HG23	1.88	0.55
32:LU:46:GLU:OE1	42:NL:68:ARG:NE	2.39	0.55
42:NL:65:GLU:OE2	53:SE:234:ARG:NH1	2.36	0.55
6:L3:1754:U:O2'	6:L3:1755:C:O5'	2.21	0.55
25:LN:370:THR:O	25:LN:370:THR:HG22	2.06	0.55
6:L3:2407:G:O6	36:LZ:2:SER:N	2.39	0.55
6:L3:4678:G:N7	41:NK:11:ARG:NH2	2.55	0.55
46:NV:322:PRO:HD2	46:NV:325:MET:HE3	1.89	0.55
6:L3:1892:A:OP2	6:L3:3875:G:N1	2.37	0.55
45:NU:808:LEU:O	45:NU:822:ARG:NH1	2.40	0.55
62:SR:161:LEU:HD12	62:SR:162:PRO:HD2	1.89	0.55
19:LG:99:GLU:OE1	63:SV:24:ASN:ND2	2.38	0.55
60:SM:183:LEU:HD23	60:SM:188:ILE:HG12	1.89	0.55
33:LW:63:ARG:O	33:LW:68:LYS:NZ	2.39	0.54
2:BB:197:ASN:O	44:NT:553:GLN:NE2	2.39	0.54
6:L3:3782:5MC:H4'	6:L3:3783:A:O5'	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:NL:70:GLN:O	42:NL:73:THR:HG23	2.06	0.54
6:L3:934:C:HO2'	6:L3:935:A:P	2.30	0.54
6:L3:2380:G:N2	6:L3:2425:U:OP1	2.37	0.54
25:LN:391:PRO:HD2	63:SV:108:ILE:HD11	1.88	0.54
6:L3:2580:U:O2'	22:LJ:79:HIS:ND1	2.36	0.54
6:L3:2822:G:N7	16:LD:20:LYS:NZ	2.48	0.54
6:L3:1433:A:N6	6:L3:1451:G:O2'	2.40	0.54
6:L3:2366:A:N3	6:L3:3850:C:O2'	2.39	0.54
42:NL:227:ARG:O	42:NL:230:THR:HG22	2.08	0.54
6:L3:1818:G:OP2	6:L3:1818:G:N2	2.29	0.54
6:L3:4928:C:O4'	11:L8:121:ARG:NH1	2.40	0.54
7:L4:97:G:OP1	52:SD:134:ARG:NH1	2.41	0.54
17:LE:115:LYS:NZ	17:LE:128:LEU:HD23	2.23	0.54
25:LN:312:LYS:NZ	25:LN:380:GLN:OE1	2.35	0.54
40:NJ:292:THR:HG23	40:NJ:378:VAL:HG12	1.91	0.53
6:L3:4306:OMU:HM22	6:L3:4306:OMU:O2	2.07	0.53
20:LH:82:THR:O	20:LH:82:THR:HG22	2.08	0.53
6:L3:4546:A:N7	54:SF:215:ASN:ND2	2.56	0.53
23:LK:100:ILE:HD11	23:LK:125:LYS:HD2	1.91	0.53
6:L3:3623:C:O2	16:LD:82:LYS:NZ	2.41	0.53
6:L3:4536:OMC:H2'	6:L3:4537:C:C6	2.43	0.53
6:L3:5009:G:O2'	6:L3:5010:PSU:H5''	2.08	0.53
6:L3:4296:PSU:H2'	6:L3:4297:G:C8	2.44	0.53
46:NV:46:LEU:HD21	46:NV:49:GLY:HA2	1.91	0.53
46:NV:137:ILE:HD13	46:NV:180:CYS:SG	2.49	0.53
58:SK:33:ASN:O	58:SK:37:VAL:HG23	2.09	0.53
60:SM:265:TYR:HB3	60:SM:362:ILE:HD11	1.91	0.53
6:L3:2580:U:OP1	22:LJ:36:ARG:NH1	2.41	0.53
7:L4:12:U:OP2	7:L4:67:C:O2'	2.27	0.53
63:SV:110:ASN:OD1	63:SV:111:ARG:N	2.41	0.53
6:L3:4219:A:O3'	6:L3:4220:6MZ:H4'	2.09	0.52
6:L3:4695:C:OP1	48:NZ:247:LYS:NZ	2.36	0.52
58:SK:201:ASP:N	58:SK:201:ASP:OD1	2.42	0.52
6:L3:1601:A:OP1	33:LW:5:THR:OG1	2.26	0.52
6:L3:2373:C:O4'	27:LP:69:ASN:ND2	2.41	0.52
20:LH:64:SER:OG	30:LS:82:ASP:OD1	2.24	0.52
42:NL:128:VAL:O	53:SE:150:LYS:NZ	2.33	0.52
20:LH:149:VAL:O	20:LH:153:ILE:HD12	2.10	0.52
34:LX:26:VAL:HG22	54:SF:178:PRO:HD2	1.91	0.52
58:SK:126:GLU:OE1	58:SK:139:ARG:NH2	2.41	0.52
59:SL:66:LEU:HD11	59:SL:251:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L3:2562:G:O2'	6:L3:2565:A:N6	2.43	0.52
6:L3:4478:G:O6	62:SR:7:LYS:NZ	2.30	0.52
40:NJ:135:ASP:O	40:NJ:136:THR:OG1	2.23	0.52
2:BB:191:VAL:O	2:BB:197:ASN:ND2	2.40	0.52
6:L3:3705:G:H21	54:SF:224:THR:HG21	1.75	0.52
6:L3:3723:A:H2'	6:L3:3724:A2M:H8	1.91	0.52
11:L8:12:VAL:O	11:L8:58:THR:OG1	2.15	0.52
44:NT:575:SER:OG	44:NT:576:GLN:OE1	2.27	0.52
6:L3:3760:A2M:O5'	6:L3:3760:A2M:H8	2.09	0.52
14:LB:93:GLN:OE1	23:LK:87:ARG:NH2	2.43	0.52
45:NU:585:ASN:ND2	45:NU:587:GLU:OE1	2.40	0.52
4:L1:69:PSU:H2'	4:L1:70:G:O4'	2.09	0.52
4:L1:102:G:OP2	4:L1:104:A:O2'	2.23	0.52
40:NJ:107:THR:HG21	40:NJ:484:ARG:HD3	1.92	0.52
14:LB:94:GLU:OE1	14:LB:94:GLU:N	2.42	0.52
6:L3:2837:OMU:H4'	25:LN:250:LYS:NZ	2.25	0.51
32:LU:59:GLU:OE2	42:NL:51:LEU:HD22	2.10	0.51
42:NL:452:GLU:OE2	60:SM:63:THR:HG23	2.09	0.51
44:NT:315:MET:HE1	44:NT:352:LYS:HB2	1.93	0.51
38:NC:251:ILE:HD11	38:NC:301:PHE:CE2	2.45	0.51
38:NC:280:ALA:O	45:NU:43:GLN:NE2	2.42	0.51
6:L3:4593:C:OP2	41:NK:2:ALA:N	2.43	0.51
24:LL:27:THR:HG22	24:LL:27:THR:O	2.10	0.51
38:NC:526:LEU:HD21	45:NU:707:HIS:NE2	2.25	0.51
45:NU:458:GLU:OE1	45:NU:461:ARG:NH2	2.43	0.51
45:NU:314:THR:HG22	45:NU:373:GLN:OE1	2.11	0.51
51:SC:281:ILE:CG2	51:SC:286:LEU:HD11	2.41	0.51
62:SR:170:THR:HG23	62:SR:218:GLN:HG3	1.93	0.51
2:BB:176:ASP:O	2:BB:180:VAL:HG23	2.10	0.51
6:L3:3808:OMC:H2'	6:L3:3809:G:C8	2.46	0.51
10:L7:190:ASP:OD1	10:L7:191:LYS:N	2.44	0.51
14:LB:40:ASN:OD1	14:LB:132:LYS:NZ	2.44	0.51
47:NX:137:GLN:O	47:NX:141:THR:HG23	2.11	0.51
6:L3:1325:C:H3'	6:L3:1326:A2M:H8	1.93	0.51
9:L6:129:ARG:NH1	30:LS:116:LEU:O	2.43	0.51
6:L3:1683:PSU:H2'	6:L3:1684:A:C8	2.45	0.51
36:LZ:9:ILE:HG23	36:LZ:51:LEU:HD21	1.93	0.51
45:NU:286:GLY:O	45:NU:287:SER:OG	2.20	0.51
62:SR:225:ILE:HG23	62:SR:271:LEU:HD21	1.93	0.51
26:LO:50:ASN:OD1	26:LO:51:ASN:N	2.43	0.50
45:NU:705:VAL:HG21	45:NU:707:HIS:NE2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L5:160:GLU:N	8:L5:160:GLU:OE1	2.43	0.50
47:NY:172:ILE:HD13	47:NY:176:HIS:HD2	1.74	0.50
58:SK:103:ALA:O	58:SK:107:VAL:HG23	2.11	0.50
44:NT:247:LEU:HD22	44:NT:263:LEU:HD11	1.93	0.50
55:SG:187:VAL:HG12	55:SG:188:GLN:HG3	1.93	0.50
61:SQ:84:GLU:OE1	61:SQ:90:HIS:ND1	2.44	0.50
61:SQ:154:ARG:NH1	61:SQ:160:THR:OG1	2.45	0.50
6:L3:3708:C:O2'	6:L3:3710:G:OP2	2.26	0.50
42:NL:430:THR:O	42:NL:430:THR:HG22	2.12	0.50
45:NU:807:PHE:CZ	45:NU:811:ILE:HD11	2.47	0.50
11:L8:29:ASP:OD1	11:L8:30:VAL:N	2.42	0.50
45:NU:564:SER:HB3	45:NU:609:VAL:HG12	1.94	0.50
4:L1:46:G:O2'	4:L1:61:A:N1	2.45	0.50
6:L3:307:A:N3	6:L3:310:G:O2'	2.44	0.50
6:L3:3770:PSU:H2'	6:L3:3771:C:H6	1.70	0.50
6:L3:4493:PSU:O2'	6:L3:4494:OMG:H5'	2.12	0.50
2:BB:170:GLY:HA3	2:BB:174:MET:HE2	1.94	0.50
17:LE:115:LYS:HZ1	17:LE:128:LEU:HD23	1.76	0.50
47:NY:132:LEU:CD2	47:NY:172:ILE:HD12	2.42	0.50
6:L3:1744:PSU:H2'	6:L3:1745:G:C8	2.47	0.50
6:L3:2572:C:O2'	22:LJ:112:ARG:NH2	2.45	0.50
6:L3:4117:U:O4'	53:SE:43:GLN:NE2	2.42	0.50
22:LJ:95:VAL:HG13	22:LJ:96:VAL:HG23	1.94	0.50
38:NC:243:LYS:NZ	38:NC:244:GLU:OE2	2.44	0.50
46:NV:309:LEU:HD12	46:NV:313:VAL:HG22	1.94	0.50
6:L3:4657:U:O2'	6:L3:4659:G:OP2	2.30	0.49
39:NF:150:VAL:HG11	39:NF:154:CYS:SG	2.52	0.49
46:NV:375:ARG:NH2	47:NX:514:ASP:OD2	2.45	0.49
6:L3:287:U:O2'	12:L9:91:GLN:OE1	2.30	0.49
6:L3:1740:C:N4	6:L3:1741:G:O6	2.45	0.49
6:L3:2725:A:N6	16:LD:88:ARG:O	2.45	0.49
6:L3:4405:G:N2	62:SR:20:ASP:OD1	2.34	0.49
34:LX:22:LEU:O	34:LX:26:VAL:HG23	2.13	0.49
6:L3:4217:G:O4'	6:L3:4222:G:N2	2.46	0.49
10:L7:182:GLU:OE2	11:L8:119:ARG:NH2	2.45	0.49
6:L3:2820:C:O3'	16:LD:56:THR:OG1	2.30	0.49
9:L6:208:GLU:N	9:L6:208:GLU:OE1	2.45	0.49
62:SR:411:LEU:HD12	62:SR:411:LEU:O	2.12	0.49
6:L3:1271:G:O2'	52:SD:34:ARG:NH2	2.45	0.49
6:L3:1744:PSU:H2'	6:L3:1745:G:H8	1.77	0.49
6:L3:2694:G:OP2	6:L3:2696:A:N6	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:LQ:26:ASP:OD1	28:LQ:27:ARG:N	2.45	0.49
56:SH:183:TYR:OH	59:SL:35:GLN:OE1	2.09	0.49
62:SR:529:VAL:HG22	63:SV:138:LEU:HD21	1.95	0.49
6:L3:4479:A:OP1	6:L3:4610:A:O2'	2.31	0.49
30:LS:37:THR:O	30:LS:37:THR:HG22	2.13	0.49
62:SR:226:LEU:O	62:SR:233:ARG:NH1	2.45	0.49
62:SR:269:LEU:HD22	62:SR:306:ILE:HG23	1.94	0.49
6:L3:1946:G:O2'	39:NF:36:SER:OG	2.30	0.49
46:NW:6:GLU:OE2	46:NW:279:THR:HG22	2.13	0.49
46:NW:178:LEU:HD23	46:NW:191:THR:HG22	1.94	0.49
6:L3:679:C:OP1	24:LL:84:LYS:NZ	2.35	0.49
6:L3:4293:PSU:OP2	6:L3:4329:G:O2'	2.25	0.49
18:LF:67:LYS:O	18:LF:68:SER:OG	2.28	0.49
9:L6:62:PRO:O	9:L6:63:THR:OG1	2.30	0.48
45:NU:638:ARG:HE	45:NU:642:MET:HE3	1.78	0.48
50:SB:128:ASP:O	50:SB:164:LYS:NZ	2.42	0.48
6:L3:3606:U:H4'	16:LD:89:MET:HE3	1.95	0.48
6:L3:1997:U:O3'	61:SQ:57:ARG:NH2	2.47	0.48
6:L3:2632:PSU:H2'	6:L3:2633:U:C6	2.48	0.48
40:NJ:110:LEU:N	40:NJ:480:LEU:O	2.46	0.48
44:NT:29:GLU:OE1	54:SF:155:LYS:NZ	2.44	0.48
6:L3:4067:U:OP2	42:NL:42:ARG:NH1	2.43	0.48
23:LK:76:ASP:OD1	23:LK:77:LYS:N	2.47	0.48
25:LN:371:THR:HG23	25:LN:380:GLN:HE21	1.78	0.48
46:NV:165:ARG:NH2	46:NV:203:VAL:O	2.45	0.48
47:NY:279:TYR:CE2	47:NY:351:VAL:HG21	2.48	0.48
47:NY:466:ILE:CD1	47:NY:529:LEU:HD12	2.43	0.48
53:SE:195:HIS:ND1	60:SM:100:GLU:OE2	2.34	0.48
4:L1:60:G:O6	4:L1:96:C:O2'	2.26	0.48
6:L3:4715:C:H5''	25:LN:278:THR:HG21	1.94	0.48
6:L3:453:G:O2'	6:L3:705:G:OP1	2.31	0.48
6:L3:1655:C:O2'	6:L3:4391:G:O2'	2.30	0.48
6:L3:4228:OMG:HM22	6:L3:4228:OMG:H1'	1.55	0.48
24:LL:32:LEU:O	24:LL:113:ARG:NH1	2.46	0.48
40:NJ:281:ARG:NE	40:NJ:358:PRO:O	2.45	0.48
58:SK:2:ALA:HB3	58:SK:215:LEU:HD11	1.96	0.48
6:L3:3822:PSU:O2	38:NC:284:SER:OG	2.32	0.48
47:NX:322:LEU:HD23	47:NX:379:LEU:HD21	1.95	0.48
58:SK:115:ALA:HB2	58:SK:135:VAL:HG21	1.94	0.48
13:LA:40:HIS:NE2	13:LA:110:ASP:O	2.46	0.48
40:NJ:208:GLU:OE1	40:NJ:213:ASN:ND2	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L3:40:G:H21	6:L3:4189:U:H4'	1.79	0.48
6:L3:730:G:OP2	52:SD:76:ARG:NE	2.44	0.48
6:L3:1326:A2M:H2'	6:L3:1327:C:H6	1.79	0.48
6:L3:4227:OMU:H2'	6:L3:4228:OMG:O4'	2.14	0.48
38:NC:64:SER:OG	39:NF:129:GLU:OE1	2.17	0.48
44:NT:315:MET:HE2	44:NT:349:GLU:OE1	2.14	0.48
6:L3:1524:A2M:HM'3	6:L3:3916:G:H1'	1.95	0.47
6:L3:4341:C:H42	6:L3:4371:G:H1	1.62	0.47
6:L3:4442:PSU:H2'	6:L3:4443:C:O2	2.14	0.47
25:LN:313:SER:OG	25:LN:314:ILE:N	2.45	0.47
58:SK:14:GLY:N	58:SK:195:ALA:O	2.45	0.47
45:NU:151:HIS:O	45:NU:157:GLN:NE2	2.47	0.47
54:SF:133:TYR:HB3	54:SF:168:VAL:HG12	1.96	0.47
12:L9:115:VAL:HG22	12:L9:134:LEU:CD2	2.44	0.47
20:LH:14:LYS:N	20:LH:16:GLU:OE1	2.47	0.47
50:SB:232:THR:OG1	50:SB:234:ASP:OD1	2.31	0.47
6:L3:2672:C:OP1	34:LX:44:LYS:NZ	2.37	0.47
10:L7:189:ILE:HG22	10:L7:189:ILE:O	2.13	0.47
54:SF:47:ASP:OD1	54:SF:48:ILE:N	2.47	0.47
6:L3:4689:PSU:H2'	6:L3:4690:G:O4'	2.14	0.47
46:NV:322:PRO:CD	46:NV:325:MET:HE3	2.45	0.47
4:L1:152:U:OP1	6:L3:4162:C:N4	2.47	0.47
6:L3:3757:G:O2'	6:L3:3758:PSU:H5''	2.14	0.47
6:L3:3808:OMC:HM23	6:L3:3808:OMC:H1'	1.50	0.47
35:LY:29:LYS:O	35:LY:50:LYS:NZ	2.45	0.47
6:L3:404:U:O3'	21:LI:87:ARG:NH2	2.44	0.47
6:L3:2340:C:H4'	49:SA:42:THR:HG23	1.96	0.47
6:L3:2837:OMU:HM23	6:L3:2837:OMU:H1'	1.67	0.47
6:L3:2923:A:O2'	35:LY:52:LYS:NZ	2.42	0.47
6:L3:3717:A:H2'	6:L3:3718:A2M:H8	1.96	0.47
6:L3:3851:PSU:H2'	6:L3:3852:A:O4'	2.15	0.47
6:L3:4500:PSU:H2'	38:NC:205:ARG:HD3	1.96	0.47
25:LN:49:TYR:CE1	25:LN:344:VAL:HG12	2.48	0.47
45:NU:108:THR:O	45:NU:108:THR:HG22	2.14	0.47
53:SE:58:PRO:HD2	53:SE:61:ILE:HD12	1.94	0.47
53:SE:153:GLN:N	53:SE:204:PHE:O	2.45	0.47
62:SR:234:ASN:ND2	62:SR:237:GLU:OE2	2.47	0.47
6:L3:2517:A:N3	6:L3:2539:C:O2'	2.48	0.47
6:L3:3890:A:N6	6:L3:4570:G:O2'	2.45	0.47
12:L9:22:LEU:HD13	53:SE:165:GLU:OE2	2.15	0.47
21:LI:67:ILE:HD13	21:LI:108:ARG:HH12	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:LP:42:ALA:HB3	27:LP:43:PRO:HD3	1.96	0.47
57:SI:101:ARG:NH1	57:SI:122:LYS:O	2.48	0.47
6:L3:1522:OMG:HM22	6:L3:1523:A:H5''	1.97	0.47
6:L3:2422:OMC:H1'	6:L3:2422:OMC:HM23	1.50	0.47
6:L3:3956:G:OP1	47:NY:170:ARG:NH2	2.45	0.47
14:LB:72:LEU:HD12	14:LB:75:ARG:NH1	2.30	0.47
25:LN:119:TYR:OH	25:LN:129:ALA:N	2.47	0.47
50:SB:133:GLU:N	50:SB:133:GLU:OE1	2.47	0.47
60:SM:140:MET:HE1	60:SM:220:MET:HE3	1.97	0.47
7:L4:11:A:O2'	7:L4:13:A:OP2	2.25	0.46
25:LN:160:ILE:HD11	25:LN:190:VAL:HG13	1.96	0.46
6:L3:3759:A:N6	6:L3:4220:6MZ:H9	2.30	0.46
46:NV:380:GLN:OE1	47:NY:74:ARG:NH1	2.48	0.46
51:SC:46:ARG:O	51:SC:65:ARG:NH2	2.49	0.46
62:SR:355:GLU:CD	62:SR:356:VAL:HG13	2.40	0.46
45:NU:312:SER:O	45:NU:373:GLN:NE2	2.49	0.46
45:NU:582:ALA:O	46:NW:122:GLN:NE2	2.49	0.46
49:SA:109:ARG:HG2	49:SA:111:TRP:CE2	2.50	0.46
3:BD:734:PHE:N	45:NU:686:SER:OG	2.48	0.46
6:L3:1320:U:O4	6:L3:4392:OMG:H5''	2.15	0.46
6:L3:2588:C:OP1	6:L3:2768:C:O2'	2.25	0.46
6:L3:4590:A2M:HM'3	6:L3:4590:A2M:H1'	1.71	0.46
6:L3:5022:U:C2'	6:L3:5025:C:H42	2.28	0.46
45:NU:720:LEU:HD11	45:NU:818:HIS:CE1	2.50	0.46
46:NV:25:LEU:HD22	46:NV:295:LEU:HD21	1.98	0.46
6:L3:4745:G:H22	6:L3:4955:A:H2	1.62	0.46
53:SE:164:ILE:O	53:SE:168:VAL:HG13	2.15	0.46
6:L3:2861:OMC:H2'	6:L3:2862:G:O4'	2.16	0.46
11:L8:118:MET:HE2	11:L8:118:MET:HA	1.98	0.46
25:LN:95:THR:OG1	25:LN:98:GLY:O	2.30	0.46
42:NL:139:VAL:O	42:NL:139:VAL:HG13	2.16	0.46
1:BA:135:THR:HG22	6:L3:1974:U:O4	2.16	0.46
6:L3:2424:OMG:HM23	6:L3:2424:OMG:H1'	1.55	0.46
35:LY:66:VAL:HG13	35:LY:66:VAL:O	2.16	0.46
50:SB:93:THR:HG22	50:SB:93:THR:O	2.16	0.46
51:SC:256:GLN:O	51:SC:260:LYS:NZ	2.46	0.46
58:SK:228:GLN:OE1	58:SK:228:GLN:N	2.48	0.46
6:L3:2362:U:H2'	6:L3:2363:A2M:H8	1.98	0.46
44:NT:30:GLU:OE1	54:SF:155:LYS:NZ	2.39	0.46
45:NU:705:VAL:HG21	45:NU:707:HIS:CE1	2.51	0.46
58:SK:49:VAL:HG12	58:SK:50:HIS:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L3:1322:1MA:H5'	6:L3:1880:G:O2'	2.16	0.46
6:L3:1927:U:OP1	6:L3:1949:U:O2'	2.34	0.46
45:NU:355:VAL:O	45:NU:359:VAL:HG23	2.15	0.46
49:SA:162:LYS:NZ	49:SA:215:ASN:O	2.35	0.46
21:LI:53:ASP:OD2	21:LI:106:ILE:HG23	2.16	0.46
25:LN:49:TYR:CE2	25:LN:171:LEU:HD13	2.51	0.46
2:BB:151:VAL:O	2:BB:154:THR:HG22	2.16	0.45
6:L3:508:G:O2'	6:L3:510:U:OP2	2.31	0.45
40:NJ:261:TYR:CE1	40:NJ:271:VAL:HG13	2.49	0.45
40:NJ:288:HIS:ND1	40:NJ:349:ASP:HB2	2.28	0.45
46:NW:178:LEU:CD2	46:NW:191:THR:HG22	2.46	0.45
6:L3:1522:OMG:H4'	49:SA:75:ARG:O	2.16	0.45
6:L3:4500:PSU:OP1	38:NC:200:LYS:NZ	2.28	0.45
6:L3:4620:OMU:HM23	6:L3:4620:OMU:H1'	1.73	0.45
38:NC:525:ILE:HG21	45:NU:702:LEU:HD13	1.97	0.45
39:NF:15:GLY:HA3	61:SQ:162:LEU:HD12	1.97	0.45
40:NJ:453:PRO:HB3	48:NZ:348:LEU:HD12	1.96	0.45
44:NT:78:PRO:HB3	44:NT:113:ILE:HD11	1.97	0.45
46:NW:96:LEU:HB3	46:NW:127:LEU:HD21	1.98	0.45
2:BB:80:VAL:HG12	2:BB:80:VAL:O	2.16	0.45
25:LN:371:THR:HG23	25:LN:380:GLN:NE2	2.30	0.45
6:L3:195:C:OP2	21:LI:28:LYS:NZ	2.49	0.45
6:L3:469:C:O2	51:SC:105:ARG:NH1	2.50	0.45
6:L3:2373:C:O2'	27:LP:64:ILE:O	2.33	0.45
6:L3:3720:G:H22	6:L3:3733:A:H2	1.63	0.45
37:NB:3:ARG:NH1	39:NF:41:LYS:O	2.48	0.45
51:SC:244:GLU:OE2	51:SC:248:ILE:HD11	2.16	0.45
6:L3:4872:G:OP2	11:L8:94:LYS:NZ	2.43	0.45
38:NC:414:SER:O	38:NC:424:LYS:NZ	2.47	0.45
6:L3:2351:OMC:HM23	49:SA:95:MET:HG3	1.98	0.45
6:L3:4277:G:O2'	6:L3:4282:A:N1	2.39	0.45
14:LB:53:MET:SD	14:LB:143:ARG:NH2	2.90	0.45
42:NL:225:PRO:HD2	42:NL:228:LEU:HD12	1.97	0.45
2:BB:188:ASN:ND2	44:NT:546:SER:O	2.50	0.45
6:L3:1279:A:O2'	6:L3:1281:G:N7	2.41	0.45
6:L3:1396:G:N7	23:LK:110:LYS:NZ	2.63	0.45
6:L3:2843:U:O2'	6:L3:4632:U:OP1	2.31	0.45
6:L3:3899:OMG:HM23	6:L3:3899:OMG:H1'	1.61	0.45
6:L3:4893:A:OP1	10:L7:188:LYS:NZ	2.47	0.45
45:NU:743:ILE:HD12	45:NU:749:ASN:ND2	2.31	0.45
60:SM:274:GLU:HB3	60:SM:362:ILE:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L3:1859:C:OP1	37:NB:26:ARG:NH1	2.50	0.45
45:NU:164:LEU:HD21	45:NU:186:PHE:HZ	1.81	0.45
6:L3:4139:G:H21	6:L3:4140:C:N4	2.14	0.45
23:LK:140:VAL:HG22	23:LK:140:VAL:O	2.17	0.45
29:LR:15:THR:HG22	29:LR:16:ALA:N	2.32	0.45
51:SC:95:PRO:HA	51:SC:104:THR:HG22	1.99	0.45
62:SR:236:ILE:H	62:SR:236:ILE:HD12	1.81	0.45
6:L3:718:C:OP1	52:SD:217:ARG:NH1	2.50	0.45
6:L3:4227:OMU:HM22	6:L3:4227:OMU:H1'	1.75	0.45
45:NU:720:LEU:HD11	45:NU:818:HIS:HE1	1.81	0.45
46:NW:265:PHE:HE2	46:NW:284:LEU:HD22	1.82	0.45
47:NY:70:MET:HE1	47:NY:111:LEU:HD23	1.99	0.45
6:L3:3841:OMC:HM23	6:L3:3841:OMC:H1'	1.51	0.44
6:L3:4622:A:OP1	25:LN:12:GLY:N	2.49	0.44
20:LH:143:ASP:N	20:LH:143:ASP:OD1	2.50	0.44
27:LP:57:MET:SD	27:LP:90:ARG:NH1	2.91	0.44
6:L3:2422:OMC:OP1	13:LA:127:ARG:NH1	2.45	0.44
6:L3:2533:C:OP1	20:LH:139:ARG:NH1	2.41	0.44
9:L6:100:PRO:O	32:LU:25:ARG:NH2	2.50	0.44
25:LN:139:ASP:OD1	25:LN:140:GLU:N	2.51	0.44
40:NJ:422:TRP:HZ3	40:NJ:443:VAL:HG21	1.81	0.44
58:SK:77:THR:HG23	58:SK:80:GLU:H	1.82	0.44
6:L3:2787:A2M:HM'3	6:L3:2790:U:OP2	2.17	0.44
6:L3:2835:A:O2'	25:LN:228:TYR:O	2.34	0.44
6:L3:4401:G:O5'	37:NB:17:LYS:NZ	2.50	0.44
6:L3:4759:C:O2	10:L7:165:LYS:NZ	2.32	0.44
8:L5:159:LYS:HG2	8:L5:163:MET:HE2	1.98	0.44
45:NU:16:LEU:HD23	45:NU:16:LEU:H	1.81	0.44
46:NW:243:ASP:OD2	46:NW:263:LYS:NZ	2.50	0.44
6:L3:1390:G:N2	6:L3:1393:G:OP2	2.43	0.44
6:L3:2674:A:N6	34:LX:41:PHE:O	2.51	0.44
45:NU:659:MET:HE1	46:NW:271:GLN:NE2	2.32	0.44
45:NU:741:LEU:HD23	45:NU:746:ARG:HH12	1.80	0.44
46:NW:195:ASP:O	46:NW:197:THR:N	2.48	0.44
3:BD:717:LEU:HD22	45:NU:748:GLN:HE21	1.82	0.44
6:L3:1950:U:O2'	15:LC:116:ARG:NH1	2.50	0.44
6:L3:2840:A:OP2	25:LN:243:LYS:NZ	2.49	0.44
6:L3:3919:C:O2'	6:L3:3920:PSU:H5''	2.17	0.44
6:L3:4042:OMG:H1'	6:L3:4042:OMG:HM23	1.76	0.44
42:NL:254:HIS:CE1	42:NL:258:LEU:HD11	2.52	0.44
46:NV:74:GLN:OE1	46:NV:74:GLN:N	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:90:ARG:CZ	1:BA:98:ILE:HD11	2.48	0.44
1:BA:117:ARG:HD2	1:BA:128:THR:HG21	1.99	0.44
6:L3:2373:C:C5'	27:LP:46:LEU:HD21	2.48	0.44
6:L3:2515:G:OP1	29:LR:37:LYS:NZ	2.42	0.44
6:L3:3920:PSU:H2'	6:L3:3921:U:C6	2.53	0.44
6:L3:4456:OMC:HM23	6:L3:4456:OMC:H1'	1.56	0.44
45:NU:580:ALA:HB3	45:NU:588:LEU:CD2	2.47	0.44
58:SK:4:ARG:NH1	58:SK:210:THR:O	2.50	0.44
6:L3:1646:A:O2'	33:LW:49:TRP:O	2.33	0.44
6:L3:4226:G:C2'	6:L3:4227:OMU:H5''	2.48	0.44
11:L8:135:LEU:HD12	11:L8:136:LEU:HD22	2.00	0.44
42:NL:160:GLU:C	42:NL:161:LEU:HD12	2.43	0.44
43:NP:29:ASP:OD1	43:NP:30:GLU:N	2.50	0.44
62:SR:334:GLU:OE2	62:SR:338:ARG:NE	2.51	0.44
3:BD:720:SER:OG	3:BD:723:GLN:OE1	2.07	0.44
5:L2:5:A:N6	5:L2:95:A:O2'	2.50	0.44
14:LB:113:ILE:HG21	14:LB:120:ILE:HD11	2.00	0.44
40:NJ:142:ASP:O	40:NJ:146:GLU:N	2.47	0.44
44:NT:246:LEU:CA	44:NT:561:MET:HE1	2.47	0.44
49:SA:293:LEU:O	49:SA:299:GLN:NE2	2.51	0.44
59:SL:67:MET:SD	59:SL:67:MET:N	2.91	0.44
6:L3:1088:C:O2	52:SD:74:MET:HE1	2.17	0.44
6:L3:1754:U:H4'	6:L3:1755:C:OP1	2.17	0.44
6:L3:2415:OMU:H4'	6:L3:2416:G:OP1	2.18	0.44
30:LS:27:GLU:OE2	30:LS:46:LYS:NZ	2.41	0.44
2:BB:87:ILE:HD12	2:BB:87:ILE:H	1.82	0.43
6:L3:3784:A:HO2'	6:L3:3785:A2M:P	2.41	0.43
6:L3:4216:G:O3'	6:L3:4217:G:H4'	2.18	0.43
6:L3:4759:C:OP1	10:L7:116:LYS:NZ	2.51	0.43
46:NV:319:LEU:HD23	46:NV:320:LEU:O	2.18	0.43
47:NX:143:ASP:O	47:NX:188:ARG:NH2	2.51	0.43
2:BB:47:LYS:NZ	44:NT:276:LYS:O	2.35	0.43
6:L3:2483:G:O2'	6:L3:2485:U:OP2	2.33	0.43
6:L3:3908:A:O2'	6:L3:4531:U:OP1	2.31	0.43
22:LJ:33:THR:HG22	22:LJ:34:SER:N	2.34	0.43
45:NU:278:HIS:ND1	46:NW:246:THR:HG23	2.33	0.43
2:BB:93:LEU:HD22	2:BB:99:LEU:HB3	2.00	0.43
6:L3:2424:OMG:H8	6:L3:2424:OMG:OP2	2.01	0.43
6:L3:3744:OMG:HM23	6:L3:3744:OMG:H1'	1.74	0.43
6:L3:4637:OMG:H1'	6:L3:4637:OMG:HM23	1.44	0.43
6:L3:4988:U:OP2	25:LN:123:HIS:ND1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:LC:81:TRP:NE1	15:LC:92:ASN:OD1	2.47	0.43
56:SH:106:MET:HE3	56:SH:116:LEU:HD23	2.00	0.43
58:SK:52:SER:OG	58:SK:56:CYS:O	2.33	0.43
6:L3:1934:A:OP2	37:NB:11:LYS:NZ	2.44	0.43
6:L3:2334:C:OP2	49:SA:195:LYS:NZ	2.48	0.43
6:L3:4530:UR3:H6	6:L3:4530:UR3:O5'	2.18	0.43
18:LF:37:ALA:O	18:LF:41:GLN:NE2	2.51	0.43
21:LI:106:ILE:HG21	21:LI:109:LEU:CD2	2.49	0.43
27:LP:92:ARG:HA	27:LP:102:LEU:HD23	2.01	0.43
40:NJ:137:THR:HG22	40:NJ:153:LYS:HG2	1.99	0.43
45:NU:580:ALA:HB3	45:NU:588:LEU:HD22	2.01	0.43
45:NU:808:LEU:HA	45:NU:811:ILE:HD12	1.99	0.43
51:SC:198:SER:N	51:SC:288:PHE:O	2.51	0.43
6:L3:4872:G:O6	11:L8:98:ARG:NH1	2.51	0.43
25:LN:179:HIS:CE1	25:LN:344:VAL:HG11	2.54	0.43
45:NU:125:LEU:O	45:NU:129:ILE:HD12	2.18	0.43
45:NU:267:ILE:HD11	46:NW:212:VAL:HG22	2.01	0.43
45:NU:607:VAL:HG13	45:NU:608:VAL:HG13	2.01	0.43
54:SF:129:ALA:O	54:SF:169:VAL:HG11	2.19	0.43
1:BA:132:ILE:O	1:BA:135:THR:OG1	2.30	0.43
6:L3:1532:G:OP2	33:LW:31:LYS:NZ	2.48	0.43
6:L3:2364:OMG:HM23	6:L3:2364:OMG:H1'	1.60	0.43
6:L3:3920:PSU:H2'	6:L3:3921:U:H6	1.84	0.43
6:L3:4571:A2M:H2'	6:L3:4572:U:O4'	2.18	0.43
46:NV:202:GLU:HG3	46:NV:209:LEU:HD21	2.00	0.43
47:NX:416:LEU:HD11	47:NX:420:GLN:CD	2.44	0.43
62:SR:183:SER:OG	62:SR:322:THR:HG21	2.19	0.43
62:SR:574:PRO:HG2	62:SR:577:VAL:HG22	2.00	0.43
4:L1:75:OMG:HM23	4:L1:75:OMG:H1'	1.49	0.43
6:L3:1562:G:N2	6:L3:1565:A:OP2	2.32	0.43
38:NC:102:VAL:HG11	38:NC:110:VAL:HG23	2.01	0.43
6:L3:1590:C:O2'	43:NP:5:ARG:NH2	2.52	0.43
6:L3:1773:OMU:H2'	6:L3:1774:C:C6	2.54	0.43
6:L3:2630:U:H2'	6:L3:2632:PSU:H1'	2.01	0.43
22:LJ:68:ILE:O	22:LJ:115:LYS:NZ	2.46	0.43
4:L1:68:G:O2'	4:L1:69:PSU:H5''	2.18	0.43
6:L3:382:G:N1	6:L3:385:A:OP2	2.43	0.43
6:L3:2815:A2M:H2'	6:L3:2816:G:C8	2.54	0.43
6:L3:3818:OMU:H5'	6:L3:3819:G:H5''	2.01	0.43
6:L3:4618:OMG:H1'	6:L3:4618:OMG:HM23	1.54	0.43
6:L3:4726:G:OP2	41:NK:98:ASN:ND2	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:LX:69:TRP:NE1	54:SF:173:GLY:O	2.51	0.43
49:SA:284:MET:HE3	49:SA:287:THR:HA	2.01	0.43
59:SL:41:ASP:O	59:SL:45:THR:OG1	2.34	0.43
6:L3:2651:C:O2	29:LR:54:ARG:NH2	2.52	0.42
6:L3:3792:OMG:HM23	6:L3:3792:OMG:H1'	1.88	0.42
6:L3:4575:G:O2'	6:L3:4576:PSU:H5''	2.18	0.42
51:SC:50:LEU:HD23	51:SC:50:LEU:H	1.83	0.42
57:SI:178:ASP:HB3	57:SI:180:THR:HG22	2.00	0.42
6:L3:4581:G:O2'	25:LN:92:TYR:OH	2.30	0.42
14:LB:88:ASP:OD1	14:LB:89:ASP:N	2.52	0.42
45:NU:468:LEU:HG	45:NU:482:LEU:HD21	2.01	0.42
6:L3:1387:A:N6	6:L3:1397:A:OP2	2.41	0.42
62:SR:424:GLU:OE2	63:SV:83:ARG:NH2	2.53	0.42
4:L1:83:C:N4	21:LI:50:ARG:HE	2.16	0.42
6:L3:3712:A:HO2'	6:L3:3713:U:P	2.42	0.42
39:NF:3:GLN:NE2	62:SR:207:VAL:O	2.52	0.42
1:BA:90:ARG:NH2	1:BA:95:GLN:O	2.52	0.42
4:L1:7:U:O2'	6:L3:1305:C:OP1	2.33	0.42
6:L3:1577:G:C2	6:L3:3637:PSU:H1'	2.55	0.42
6:L3:3784:A:O2'	6:L3:3785:A2M:P	2.78	0.42
6:L3:3822:PSU:H1'	6:L3:3823:G:P	2.58	0.42
6:L3:4589:A:N3	6:L3:4590:A2M:HM'3	2.35	0.42
6:L3:5051:C:O2'	25:LN:325:GLU:OE2	2.38	0.42
45:NU:658:HIS:O	45:NU:661:SER:OG	2.32	0.42
6:L3:496:G:O2'	6:L3:497:G:OP1	2.30	0.42
6:L3:4541:G:O2'	38:NC:33:ARG:NH2	2.52	0.42
47:NY:172:ILE:HD13	47:NY:176:HIS:CD2	2.54	0.42
63:SV:92:ALA:O	63:SV:96:VAL:HG23	2.20	0.42
6:L3:1326:A2M:H2'	6:L3:1327:C:C6	2.55	0.42
6:L3:1340:OMC:HM23	6:L3:1340:OMC:H1'	1.51	0.42
6:L3:4054:OMC:HM23	6:L3:4054:OMC:H1'	1.56	0.42
6:L3:4448:G:OP2	62:SR:119:TYR:OH	2.35	0.42
47:NX:85:LEU:H	47:NX:85:LEU:HD23	1.85	0.42
47:NX:622:GLU:OE2	47:NY:531:ARG:NH1	2.52	0.42
61:SQ:150:GLU:HG2	61:SQ:167:VAL:HG13	2.02	0.42
6:L3:1727:U:OP1	52:SD:131:ASN:ND2	2.53	0.42
6:L3:1831:G:O2'	6:L3:1832:C:OP1	2.28	0.42
6:L3:3825:A2M:H1'	6:L3:3825:A2M:HM'3	1.77	0.42
6:L3:4716:C:OP1	25:LN:276:HIS:ND1	2.53	0.42
7:L4:52:C:O2'	7:L4:54:A:N7	2.52	0.42
15:LC:99:ASP:OD1	15:LC:100:LEU:N	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:NY:542:GLU:OE1	47:NY:593:ARG:NH2	2.53	0.42
6:L3:1780:A:H3'	6:L3:1781:PSU:H5'	2.02	0.42
6:L3:2841:G:OP1	43:NP:10:HIS:NE2	2.52	0.42
6:L3:3661:G:N7	54:SF:152:SER:OG	2.43	0.42
9:L6:125:ILE:HD12	9:L6:143:GLU:HG2	2.02	0.42
45:NU:509:LEU:HD22	45:NU:523:LEU:HD11	2.02	0.42
6:L3:1346:C:OP1	14:LB:148:VAL:HG12	2.19	0.41
6:L3:3768:PSU:H2'	6:L3:3769:C:C6	2.55	0.41
6:L3:5048:A:OP1	27:LP:31:LYS:NZ	2.43	0.41
8:L5:41:GLU:O	8:L5:45:GLY:N	2.48	0.41
9:L6:201:GLU:O	9:L6:205:GLN:N	2.49	0.41
38:NC:322:GLY:O	38:NC:326:VAL:HG23	2.20	0.41
59:SL:71:TRP:N	59:SL:247:SER:O	2.47	0.41
1:BA:138:SER:OG	6:L3:2002:A:N6	2.54	0.41
2:BB:90:LEU:HD23	2:BB:124:LEU:HD23	2.03	0.41
6:L3:4571:A2M:HM'2	6:L3:4571:A2M:H1'	1.64	0.41
6:L3:4617:G:OP1	25:LN:62:ARG:NH1	2.52	0.41
46:NV:19:SER:N	46:NV:34:TYR:O	2.52	0.41
62:SR:354:ASN:OD1	62:SR:355:GLU:N	2.54	0.41
6:L3:225:G:OP1	49:SA:222:ARG:NE	2.43	0.41
6:L3:1468:C:H4'	23:LK:132:ARG:HH22	1.84	0.41
6:L3:1503:A:N6	14:LB:87:THR:HG21	2.35	0.41
6:L3:1577:G:O2'	6:L3:1612:G:H4'	2.19	0.41
6:L3:1854:G:O2'	6:L3:1855:G:P	2.78	0.41
6:L3:3784:A:H2'	6:L3:3785:A2M:H8	2.03	0.41
6:L3:4302:U:O2	6:L3:4306:OMU:H5	2.20	0.41
4:L1:83:C:O2'	4:L1:84:A:N7	2.49	0.41
6:L3:3925:OMU:HM23	6:L3:3925:OMU:H1'	1.55	0.41
46:NW:68:GLN:NE2	46:NW:327:SER:O	2.53	0.41
49:SA:262:GLU:OE1	49:SA:262:GLU:N	2.53	0.41
6:L3:4628:PSU:C4	6:L3:4629:U:C5	3.09	0.41
31:LT:43:LEU:O	31:LT:109:ARG:NH1	2.53	0.41
46:NV:107:GLU:O	46:NV:111:GLY:N	2.43	0.41
51:SC:141:ARG:NH1	51:SC:191:GLN:O	2.47	0.41
6:L3:2519:U:C2	6:L3:2520:C:C5	3.07	0.41
6:L3:2898:G:OP2	16:LD:135:LYS:NZ	2.34	0.41
6:L3:3768:PSU:H2'	6:L3:3769:C:H6	1.83	0.41
46:NV:68:GLN:NE2	46:NV:324:SER:O	2.49	0.41
47:NY:279:TYR:O	47:NY:365:ARG:NH1	2.54	0.41
55:SG:92:MET:HE2	55:SG:179:ILE:HG22	2.01	0.41
6:L3:2691:U:C2	6:L3:2692:U:C5	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L3:3785:A2M:HM'3	6:L3:3785:A2M:H1'	1.70	0.41
6:L3:4370:OMG:HM23	6:L3:4370:OMG:H1'	1.69	0.41
6:L3:4571:A2M:H8	6:L3:4571:A2M:O5'	2.21	0.41
6:L3:4629:U:C2	6:L3:4630:G:C8	3.08	0.41
45:NU:717:LEU:HD22	45:NU:766:VAL:HG13	2.03	0.41
51:SC:96:VAL:HG11	51:SC:101:ASN:HB2	2.01	0.41
2:BB:137:LEU:N	44:NT:468:GLY:O	2.47	0.41
6:L3:1368:A:N3	21:LI:1:MET:HE2	2.35	0.41
38:NC:111:MET:SD	38:NC:304:LEU:HD22	2.61	0.41
47:NX:107:GLU:OE1	47:NX:107:GLU:N	2.50	0.41
62:SR:473:GLU:OE1	62:SR:477:MET:HE3	2.21	0.41
5:L2:10:U:OP2	59:SL:163:ARG:NH1	2.53	0.41
6:L3:224:U:OP2	49:SA:164:THR:N	2.46	0.41
6:L3:469:C:N3	51:SC:105:ARG:NH2	2.64	0.41
6:L3:1077:C:OP1	6:L3:1215:C:O2'	2.35	0.41
6:L3:1760:OMG:HM23	6:L3:1760:OMG:H1'	1.54	0.41
6:L3:2296:G:OP2	49:SA:190:ARG:NH1	2.45	0.41
6:L3:3721:U:OP1	32:LU:68:ARG:NH2	2.54	0.41
6:L3:4941:G:C8	51:SC:172:LEU:HD21	2.56	0.41
34:LX:52:VAL:O	34:LX:52:VAL:HG13	2.20	0.41
45:NU:776:PHE:HA	45:NU:779:ILE:HG22	2.02	0.41
46:NV:195:ASP:O	46:NV:197:THR:N	2.50	0.41
46:NW:46:LEU:HD21	46:NW:49:GLY:HA2	2.02	0.41
54:SF:116:LEU:HD12	54:SF:164:ALA:HB2	2.03	0.41
6:L3:1269:G:O2'	6:L3:1270:A:N3	2.53	0.41
6:L3:1922:G:OP1	15:LC:160:ARG:NH2	2.53	0.41
6:L3:2804:OMC:H2'	6:L3:2805:C:C6	2.56	0.41
60:SM:170:HIS:HB3	60:SM:283:LEU:HD11	2.02	0.41
6:L3:1316:OMG:HM23	6:L3:1316:OMG:H1'	1.51	0.40
6:L3:3627:OMG:H1'	6:L3:3627:OMG:HM23	1.76	0.40
6:L3:3808:OMC:H2'	6:L3:3809:G:H8	1.85	0.40
29:LR:102:ILE:HG23	42:NL:297:LEU:HD11	2.03	0.40
44:NT:78:PRO:CB	44:NT:113:ILE:HD11	2.51	0.40
47:NY:177:LEU:HD23	47:NY:209:ALA:HB3	2.01	0.40
48:NZ:239:LYS:HD3	48:NZ:245:VAL:HG12	2.03	0.40
6:L3:197:A:N3	6:L3:222:C:O2'	2.51	0.40
6:L3:308:G:O6	12:L9:12:ARG:NH1	2.54	0.40
6:L3:4306:OMU:HM22	6:L3:4306:OMU:C2	2.51	0.40
7:L4:117:G:OP1	50:SB:253:TYR:OH	2.31	0.40
9:L6:143:GLU:OE2	30:LS:122:LYS:NZ	2.53	0.40
18:LF:76:VAL:HG22	18:LF:77:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:LQ:41:ILE:HG23	28:LQ:42:ASP:OD1	2.22	0.40
34:LX:8:VAL:O	34:LX:11:VAL:HG22	2.21	0.40
44:NT:165:MET:HE2	44:NT:183:VAL:HG11	2.02	0.40
59:SL:78:LEU:HD21	59:SL:80:VAL:HG12	2.03	0.40
6:L3:2351:OMC:HM22	6:L3:2352:U:H5'	2.02	0.40
6:L3:3641:U:OP2	6:L3:3646:A:N6	2.39	0.40
36:LZ:20:ASN:ND2	36:LZ:42:ARG:O	2.55	0.40
45:NU:708:VAL:HG13	45:NU:717:LEU:HD21	2.02	0.40
6:L3:503:C:O2'	6:L3:504:G:O5'	2.35	0.40
6:L3:1831:G:H3'	6:L3:1832:C:H5''	2.03	0.40
6:L3:3695:PSU:H2'	6:L3:3696:C:H6	1.84	0.40
6:L3:4288:C:O2'	6:L3:4321:U:OP1	2.38	0.40
6:L3:4563:U:C2	6:L3:4564:A:C8	3.09	0.40
18:LF:44:GLN:HG2	18:LF:63:ILE:HD12	2.04	0.40
40:NJ:297:THR:HG22	40:NJ:336:VAL:HG13	2.03	0.40
47:NX:553:LEU:HD11	47:NX:597:PRO:HG2	2.03	0.40
55:SG:103:VAL:HG11	55:SG:144:LEU:HD21	2.04	0.40
62:SR:369:ASP:OD1	62:SR:370:ASP:N	2.54	0.40
6:L3:1426:G:N1	6:L3:1458:C:OP2	2.44	0.40
6:L3:1733:G:OP1	17:LE:43:LYS:NZ	2.54	0.40
6:L3:3867:A2M:HM'3	6:L3:3867:A2M:H1'	1.54	0.40
25:LN:231:VAL:HG21	25:LN:251:VAL:HG23	2.02	0.40
43:NP:65:ALA:O	43:NP:88:ARG:NH1	2.52	0.40
47:NX:552:VAL:O	47:NX:556:VAL:HG23	2.21	0.40
49:SA:110:ARG:O	49:SA:113:ARG:NH1	2.54	0.40
58:SK:95:ARG:NH2	63:SV:77:GLU:OE1	2.54	0.40
60:SM:150:THR:HG22	60:SM:151:GLY:N	2.37	0.40
62:SR:298:GLU:OE1	62:SR:298:GLU:N	2.52	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%)	155 (98%)	3 (2%)	0	100	100
2	BB	214/217 (99%)	208 (97%)	6 (3%)	0	100	100
3	BD	17/734 (2%)	17 (100%)	0	0	100	100
8	L5	166/178 (93%)	165 (99%)	1 (1%)	0	100	100
9	L6	201/211 (95%)	197 (98%)	4 (2%)	0	100	100
10	L7	199/203 (98%)	198 (100%)	1 (0%)	0	100	100
11	L8	133/215 (62%)	131 (98%)	2 (2%)	0	100	100
12	L9	190/204 (93%)	189 (100%)	1 (0%)	0	100	100
13	LA	152/184 (83%)	148 (97%)	4 (3%)	0	100	100
14	LB	149/188 (79%)	148 (99%)	1 (1%)	0	100	100
15	LC	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
16	LD	152/196 (78%)	151 (99%)	1 (1%)	0	100	100
17	LE	134/160 (84%)	131 (98%)	3 (2%)	0	100	100
18	LF	101/128 (79%)	99 (98%)	2 (2%)	0	100	100
19	LG	137/140 (98%)	133 (97%)	4 (3%)	0	100	100
20	LH	141/156 (90%)	140 (99%)	1 (1%)	0	100	100
21	LI	132/145 (91%)	132 (100%)	0	0	100	100
22	LJ	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
23	LK	113/148 (76%)	113 (100%)	0	0	100	100
24	LL	123/137 (90%)	120 (98%)	3 (2%)	0	100	100
25	LN	399/403 (99%)	394 (99%)	5 (1%)	0	100	100
26	LO	93/115 (81%)	93 (100%)	0	0	100	100
27	LP	104/125 (83%)	104 (100%)	0	0	100	100
28	LQ	126/135 (93%)	126 (100%)	0	0	100	100
29	LR	110/117 (94%)	109 (99%)	1 (1%)	0	100	100
30	LS	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
31	LT	107/110 (97%)	107 (100%)	0	0	100	100
32	LU	100/105 (95%)	100 (100%)	0	0	100	100
33	LW	84/97 (87%)	84 (100%)	0	0	100	100
34	LX	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
35	LY	67/70 (96%)	67 (100%)	0	0	100	100
36	LZ	48/51 (94%)	48 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	NB	79/549 (14%)	79 (100%)	0	0	100	100
38	NC	501/731 (68%)	496 (99%)	5 (1%)	0	100	100
39	NF	227/260 (87%)	224 (99%)	3 (1%)	0	100	100
40	NJ	375/485 (77%)	365 (97%)	10 (3%)	0	100	100
41	NK	63/129 (49%)	63 (100%)	0	0	100	100
42	NL	352/478 (74%)	350 (99%)	2 (1%)	0	100	100
43	NP	100/134 (75%)	100 (100%)	0	0	100	100
44	NT	493/687 (72%)	491 (100%)	2 (0%)	0	100	100
45	NU	819/929 (88%)	809 (99%)	10 (1%)	0	100	100
46	NV	378/432 (88%)	373 (99%)	5 (1%)	0	100	100
46	NW	361/432 (84%)	352 (98%)	9 (2%)	0	100	100
47	NX	502/1130 (44%)	498 (99%)	4 (1%)	0	100	100
47	NY	514/1130 (46%)	511 (99%)	3 (1%)	0	100	100
48	NZ	115/360 (32%)	115 (100%)	0	0	100	100
49	SA	356/427 (83%)	351 (99%)	5 (1%)	0	100	100
50	SB	252/297 (85%)	248 (98%)	4 (2%)	0	100	100
51	SC	211/288 (73%)	206 (98%)	5 (2%)	0	100	100
52	SD	223/248 (90%)	219 (98%)	4 (2%)	0	100	100
53	SE	230/266 (86%)	228 (99%)	2 (1%)	0	100	100
54	SF	243/257 (95%)	235 (97%)	8 (3%)	0	100	100
55	SG	188/192 (98%)	187 (100%)	1 (0%)	0	100	100
56	SH	149/293 (51%)	145 (97%)	4 (3%)	0	100	100
57	SI	231/255 (91%)	229 (99%)	2 (1%)	0	100	100
58	SK	242/245 (99%)	234 (97%)	8 (3%)	0	100	100
59	SL	236/490 (48%)	226 (96%)	10 (4%)	0	100	100
60	SM	393/588 (67%)	389 (99%)	4 (1%)	0	100	100
61	SQ	216/239 (90%)	216 (100%)	0	0	100	100
62	SR	596/634 (94%)	588 (99%)	8 (1%)	0	100	100
63	SV	137/163 (84%)	136 (99%)	1 (1%)	0	100	100
All	All	13148/18312 (72%)	12979 (99%)	169 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BA	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
8	L5	142/149 (95%)	142 (100%)	0	100	100
9	L6	171/177 (97%)	171 (100%)	0	100	100
10	L7	173/174 (99%)	173 (100%)	0	100	100
11	L8	115/161 (71%)	115 (100%)	0	100	100
12	L9	164/172 (95%)	164 (100%)	0	100	100
13	LA	135/163 (83%)	135 (100%)	0	100	100
14	LB	136/165 (82%)	136 (100%)	0	100	100
15	LC	157/157 (100%)	157 (100%)	0	100	100
16	LD	138/175 (79%)	138 (100%)	0	100	100
17	LE	121/140 (86%)	121 (100%)	0	100	100
18	LF	93/115 (81%)	93 (100%)	0	100	100
19	LG	106/107 (99%)	106 (100%)	0	100	100
20	LH	124/133 (93%)	124 (100%)	0	100	100
21	LI	124/135 (92%)	124 (100%)	0	100	100
22	LJ	117/118 (99%)	117 (100%)	0	100	100
23	LK	98/121 (81%)	98 (100%)	0	100	100
24	LL	109/121 (90%)	109 (100%)	0	100	100
25	LN	347/348 (100%)	347 (100%)	0	100	100
26	LO	80/97 (82%)	80 (100%)	0	100	100
27	LP	97/110 (88%)	97 (100%)	0	100	100
28	LQ	114/121 (94%)	114 (100%)	0	100	100
29	LR	96/100 (96%)	96 (100%)	0	100	100
30	LS	109/110 (99%)	109 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	LT	88/89 (99%)	88 (100%)	0	100	100
32	LU	86/89 (97%)	86 (100%)	0	100	100
33	LW	73/80 (91%)	73 (100%)	0	100	100
34	LX	74/75 (99%)	74 (100%)	0	100	100
35	LY	64/65 (98%)	64 (100%)	0	100	100
36	LZ	47/48 (98%)	47 (100%)	0	100	100
37	NB	74/485 (15%)	74 (100%)	0	100	100
38	NC	455/654 (70%)	455 (100%)	0	100	100
39	NF	203/228 (89%)	203 (100%)	0	100	100
40	NJ	314/404 (78%)	314 (100%)	0	100	100
41	NK	61/115 (53%)	61 (100%)	0	100	100
42	NL	313/402 (78%)	313 (100%)	0	100	100
43	NP	88/114 (77%)	88 (100%)	0	100	100
44	NT	457/629 (73%)	457 (100%)	0	100	100
45	NU	694/843 (82%)	694 (100%)	0	100	100
46	NV	324/368 (88%)	324 (100%)	0	100	100
46	NW	311/368 (84%)	311 (100%)	0	100	100
47	NX	440/944 (47%)	440 (100%)	0	100	100
47	NY	445/944 (47%)	445 (100%)	0	100	100
48	NZ	108/312 (35%)	108 (100%)	0	100	100
49	SA	298/348 (86%)	298 (100%)	0	100	100
50	SB	213/250 (85%)	213 (100%)	0	100	100
51	SC	192/252 (76%)	192 (100%)	0	100	100
52	SD	194/215 (90%)	194 (100%)	0	100	100
53	SE	200/223 (90%)	200 (100%)	0	100	100
54	SF	188/199 (94%)	188 (100%)	0	100	100
55	SG	169/171 (99%)	169 (100%)	0	100	100
56	SH	141/274 (52%)	141 (100%)	0	100	100
57	SI	210/228 (92%)	210 (100%)	0	100	100
58	SK	212/213 (100%)	212 (100%)	0	100	100
59	SL	221/437 (51%)	221 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
60	SM	354/509 (70%)	354 (100%)	0	100	100
61	SQ	195/214 (91%)	195 (100%)	0	100	100
62	SR	546/574 (95%)	546 (100%)	0	100	100
63	SV	128/149 (86%)	128 (100%)	0	100	100
All	All	11588/15855 (73%)	11588 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	BA	65	GLN
2	BB	19	HIS
8	L5	71	HIS
10	L7	167	HIS
10	L7	180	GLN
10	L7	199	HIS
11	L8	34	ASN
11	L8	56	GLN
12	L9	15	GLN
12	L9	109	HIS
12	L9	158	HIS
13	LA	97	ASN
16	LD	40	GLN
16	LD	141	HIS
20	LH	35	HIS
20	LH	125	ASN
21	LI	14	ASN
24	LL	4	HIS
24	LL	21	ASN
24	LL	100	ASN
25	LN	145	GLN
25	LN	179	HIS
28	LQ	23	HIS
30	LS	20	GLN
30	LS	65	GLN
31	LT	99	HIS
38	NC	31	ASN
38	NC	89	GLN
38	NC	133	HIS

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Mol	Chain	Res	Type
38	NC	222	GLN
38	NC	523	GLN
39	NF	247	ASN
40	NJ	323	GLN
40	NJ	372	GLN
41	NK	92	GLN
43	NP	91	GLN
44	NT	48	GLN
44	NT	89	HIS
44	NT	114	ASN
44	NT	291	HIS
44	NT	319	ASN
45	NU	357	GLN
45	NU	361	ASN
45	NU	532	GLN
45	NU	558	GLN
45	NU	658	HIS
45	NU	712	GLN
45	NU	738	HIS
45	NU	845	GLN
46	NV	179	HIS
46	NV	241	GLN
46	NV	256	HIS
46	NV	259	GLN
46	NV	342	HIS
46	NW	68	GLN
46	NW	166	HIS
46	NW	179	HIS
46	NW	229	HIS
46	NW	315	ASN
47	NX	65	HIS
47	NX	84	ASN
47	NX	561	GLN
47	NX	603	GLN
47	NY	65	HIS
47	NY	175	ASN
47	NY	176	HIS
47	NY	310	GLN
47	NY	313	GLN
47	NY	560	GLN
47	NY	561	GLN
47	NY	632	HIS

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Mol	Chain	Res	Type
49	SA	38	ASN
49	SA	347	HIS
50	SB	45	ASN
51	SC	135	GLN
51	SC	136	HIS
51	SC	157	HIS
51	SC	190	HIS
51	SC	245	GLN
52	SD	235	ASN
53	SE	149	ASN
53	SE	153	GLN
54	SF	22	HIS
54	SF	139	HIS
56	SH	119	HIS
57	SI	225	HIS
58	SK	50	HIS
58	SK	82	GLN
59	SL	128	GLN
59	SL	133	GLN
60	SM	159	GLN
60	SM	245	HIS
60	SM	253	GLN
62	SR	3	HIS
62	SR	37	HIS
62	SR	59	HIS
62	SR	91	HIS
62	SR	100	ASN
62	SR	482	GLN
62	SR	612	HIS
63	SV	17	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	L1	152/157 (96%)	16 (10%)	0
5	L2	67/1167 (5%)	9 (13%)	0
6	L3	3464/5070 (68%)	481 (13%)	12 (0%)
7	L4	115/121 (95%)	11 (9%)	1 (0%)
All	All	3798/6515 (58%)	517 (13%)	13 (0%)

All (517) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	L1	34	U
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	111	U
4	L1	151	G
4	L1	153	C
4	L1	156	U
5	L2	11	C
5	L2	48	G
5	L2	49	G
5	L2	51	U
5	L2	62	U
5	L2	96	A
5	L2	101	A
5	L2	1165	A
5	L2	1166	G
6	L3	2	G
6	L3	6	C
6	L3	15	A
6	L3	48	G
6	L3	56	A
6	L3	58	G
6	L3	59	A
6	L3	64	A
6	L3	65	A
6	L3	69	A
6	L3	91	G
6	L3	95	G
6	L3	108	A
6	L3	109	G
6	L3	119	G
6	L3	159	C
6	L3	171	U
6	L3	181	C

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Mol	Chain	Res	Type
6	L3	200	U
6	L3	210	C
6	L3	218	A
6	L3	233	U
6	L3	234	G
6	L3	246	G
6	L3	261	G
6	L3	263	G
6	L3	266	C
6	L3	267	G
6	L3	280	G
6	L3	297	U
6	L3	316	U
6	L3	340	C
6	L3	386	A
6	L3	387	G
6	L3	409	G
6	L3	410	A
6	L3	412	G
6	L3	450	G
6	L3	452	A
6	L3	453	G
6	L3	454	U
6	L3	464	G
6	L3	467	U
6	L3	469	C
6	L3	472	C
6	L3	473	C
6	L3	478	G
6	L3	479	G
6	L3	492	U
6	L3	493	G
6	L3	496	G
6	L3	497	G
6	L3	499	G
6	L3	501	C
6	L3	502	C
6	L3	503	C
6	L3	504	G
6	L3	509	A
6	L3	510	U
6	L3	511	C

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Mol	Chain	Res	Type
6	L3	658	C
6	L3	660	A
6	L3	667	A
6	L3	668	C
6	L3	669	C
6	L3	686	A
6	L3	704	C
6	L3	729	G
6	L3	730	G
6	L3	731	G
6	L3	739	G
6	L3	741	C
6	L3	742	G
6	L3	746	A
6	L3	757	G
6	L3	913	U
6	L3	915	A
6	L3	916	C
6	L3	917	A
6	L3	926	G
6	L3	932	A
6	L3	933	G
6	L3	935	A
6	L3	943	A
6	L3	944	A
6	L3	945	U
6	L3	956	A
6	L3	960	A
6	L3	1066	G
6	L3	1070	G
6	L3	1072	C
6	L3	1080	C
6	L3	1211	G
6	L3	1253	G
6	L3	1254	A
6	L3	1255	A
6	L3	1256	G
6	L3	1266	G
6	L3	1269	G
6	L3	1270	A
6	L3	1272	C
6	L3	1273	G

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Mol	Chain	Res	Type
6	L3	1280	C
6	L3	1284	G
6	L3	1287	G
6	L3	1294	A
6	L3	1295	C
6	L3	1301	C
6	L3	1313	C
6	L3	1314	C
6	L3	1315	C
6	L3	1319	U
6	L3	1320	U
6	L3	1322	1MA
6	L3	1337	A
6	L3	1354	A
6	L3	1358	G
6	L3	1359	G
6	L3	1365	C
6	L3	1366	G
6	L3	1367	C
6	L3	1379	C
6	L3	1397	A
6	L3	1399	G
6	L3	1420	A
6	L3	1457	G
6	L3	1497	A
6	L3	1498	G
6	L3	1502	G
6	L3	1523	A
6	L3	1534	A2M
6	L3	1547	A
6	L3	1578	U
6	L3	1592	G
6	L3	1596	U
6	L3	1597	G
6	L3	1613	A
6	L3	1624	G
6	L3	1625	OMG
6	L3	1631	A
6	L3	1633	G
6	L3	1634	A
6	L3	1640	C
6	L3	1654	G

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Mol	Chain	Res	Type
6	L3	1661	C
6	L3	1671	U
6	L3	1676	C
6	L3	1677	PSU
6	L3	1678	C
6	L3	1680	G
6	L3	1684	A
6	L3	1691	G
6	L3	1726	U
6	L3	1734	G
6	L3	1735	U
6	L3	1736	A
6	L3	1737	A
6	L3	1739	G
6	L3	1743	A
6	L3	1744	PSU
6	L3	1747	U
6	L3	1749	A
6	L3	1750	G
6	L3	1753	G
6	L3	1754	U
6	L3	1755	C
6	L3	1756	U
6	L3	1758	G
6	L3	1775	A
6	L3	1781	PSU
6	L3	1804	A
6	L3	1806	G
6	L3	1811	G
6	L3	1813	U
6	L3	1815	G
6	L3	1825	A
6	L3	1827	C
6	L3	1829	G
6	L3	1832	C
6	L3	1833	G
6	L3	1835	G
6	L3	1836	G
6	L3	1837	A
6	L3	1842	G
6	L3	1852	U
6	L3	1854	G

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Mol	Chain	Res	Type
6	L3	1855	G
6	L3	1870	C
6	L3	1881	C
6	L3	1883	G
6	L3	1891	A
6	L3	1897	A
6	L3	1910	G
6	L3	1919	G
6	L3	1921	C
6	L3	1922	G
6	L3	1925	G
6	L3	1931	C
6	L3	1935	C
6	L3	1941	A
6	L3	1943	A
6	L3	1969	G
6	L3	1974	U
6	L3	1983	A
6	L3	1984	A
6	L3	2002	A
6	L3	2004	U
6	L3	2025	A
6	L3	2026	A
6	L3	2041	A
6	L3	2042	A
6	L3	2044	U
6	L3	2046	G
6	L3	2055	G
6	L3	2056	G
6	L3	2069	A
6	L3	2084	C
6	L3	2289	C
6	L3	2300	A
6	L3	2301	G
6	L3	2313	A
6	L3	2316	G
6	L3	2331	G
6	L3	2348	G
6	L3	2351	OMC
6	L3	2395	A
6	L3	2415	OMU
6	L3	2416	G

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Mol	Chain	Res	Type
6	L3	2417	A
6	L3	2422	OMC
6	L3	2424	OMG
6	L3	2425	U
6	L3	2434	G
6	L3	2450	G
6	L3	2453	A
6	L3	2470	C
6	L3	2471	G
6	L3	2475	G
6	L3	2476	G
6	L3	2477	A
6	L3	2478	C
6	L3	2480	G
6	L3	2486	G
6	L3	2487	G
6	L3	2488	C
6	L3	2489	C
6	L3	2492	C
6	L3	2507	A
6	L3	2512	A
6	L3	2513	A
6	L3	2519	U
6	L3	2529	A
6	L3	2544	G
6	L3	2545	U
6	L3	2548	C
6	L3	2554	U
6	L3	2567	G
6	L3	2587	A
6	L3	2601	A
6	L3	2627	C
6	L3	2638	G
6	L3	2653	C
6	L3	2669	C
6	L3	2687	U
6	L3	2694	G
6	L3	2695	A
6	L3	2696	A
6	L3	2710	C
6	L3	2711	G
6	L3	2724	G

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Mol	Chain	Res	Type
6	L3	2743	A
6	L3	2760	G
6	L3	2764	A
6	L3	2769	U
6	L3	2771	G
6	L3	2787	A2M
6	L3	2788	U
6	L3	2790	U
6	L3	2814	C
6	L3	2826	U
6	L3	2827	G
6	L3	2829	U
6	L3	2850	A
6	L3	2855	G
6	L3	2877	G
6	L3	2896	G
6	L3	2902	G
6	L3	2917	G
6	L3	2918	G
6	L3	3271	G
6	L3	3593	C
6	L3	3595	U
6	L3	3597	G
6	L3	3626	G
6	L3	3635	A
6	L3	3644	U
6	L3	3653	A
6	L3	3662	A
6	L3	3702	A
6	L3	3709	U
6	L3	3710	G
6	L3	3713	U
6	L3	3753	G
6	L3	3760	A2M
6	L3	3774	A
6	L3	3775	A
6	L3	3782	5MC
6	L3	3783	A
6	L3	3784	A
6	L3	3785	A2M
6	L3	3790	U
6	L3	3791	C

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Mol	Chain	Res	Type
6	L3	3814	U
6	L3	3815	G
6	L3	3818	OMU
6	L3	3820	G
6	L3	3821	A
6	L3	3822	PSU
6	L3	3823	G
6	L3	3840	U
6	L3	3867	A2M
6	L3	3881	G
6	L3	3887	OMC
6	L3	3892	U
6	L3	3897	G
6	L3	3905	A
6	L3	3914	U
6	L3	3915	U
6	L3	3939	G
6	L3	3963	A
6	L3	3972	A
6	L3	4037	C
6	L3	4049	U
6	L3	4064	C
6	L3	4076	G
6	L3	4085	A
6	L3	4119	C
6	L3	4120	U
6	L3	4121	G
6	L3	4122	G
6	L3	4127	A
6	L3	4133	C
6	L3	4138	C
6	L3	4139	G
6	L3	4140	C
6	L3	4142	C
6	L3	4143	G
6	L3	4144	C
6	L3	4145	C
6	L3	4147	G
6	L3	4150	G
6	L3	4154	G
6	L3	4162	C
6	L3	4163	U

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Mol	Chain	Res	Type
6	L3	4170	A
6	L3	4183	G
6	L3	4184	G
6	L3	4208	U
6	L3	4210	U
6	L3	4211	C
6	L3	4212	A
6	L3	4213	A
6	L3	4214	A
6	L3	4216	G
6	L3	4217	G
6	L3	4219	A
6	L3	4220	6MZ
6	L3	4221	C
6	L3	4224	A
6	L3	4226	G
6	L3	4227	OMU
6	L3	4230	C
6	L3	4231	C
6	L3	4233	A
6	L3	4234	A
6	L3	4235	G
6	L3	4251	A
6	L3	4254	G
6	L3	4266	G
6	L3	4268	A
6	L3	4271	A
6	L3	4272	G
6	L3	4273	A
6	L3	4281	A
6	L3	4291	G
6	L3	4297	G
6	L3	4302	U
6	L3	4326	G
6	L3	4330	G
6	L3	4332	C
6	L3	4335	C
6	L3	4348	A
6	L3	4349	C
6	L3	4355	G
6	L3	4368	G
6	L3	4381	A

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Mol	Chain	Res	Type
6	L3	4387	C
6	L3	4396	A
6	L3	4399	U
6	L3	4401	G
6	L3	4415	A
6	L3	4418	G
6	L3	4438	U
6	L3	4439	U
6	L3	4446	U
6	L3	4451	G
6	L3	4452	U
6	L3	4453	C
6	L3	4464	A
6	L3	4466	C
6	L3	4475	G
6	L3	4476	C
6	L3	4498	OMU
6	L3	4500	PSU
6	L3	4503	A
6	L3	4512	U
6	L3	4513	A
6	L3	4519	C
6	L3	4523	A2M
6	L3	4524	G
6	L3	4545	G
6	L3	4547	C
6	L3	4548	A
6	L3	4556	U
6	L3	4557	U
6	L3	4558	U
6	L3	4560	C
6	L3	4573	G
6	L3	4574	U
6	L3	4575	G
6	L3	4584	A
6	L3	4590	A2M
6	L3	4608	G
6	L3	4636	PSU
6	L3	4637	OMG
6	L3	4670	C
6	L3	4672	A
6	L3	4678	G

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Mol	Chain	Res	Type
6	L3	4684	A
6	L3	4700	A
6	L3	4708	A
6	L3	4709	U
6	L3	4719	G
6	L3	4720	C
6	L3	4740	G
6	L3	4741	C
6	L3	4742	G
6	L3	4750	G
6	L3	4751	G
6	L3	4754	G
6	L3	4757	C
6	L3	4759	C
6	L3	4765	G
6	L3	4773	C
6	L3	4870	G
6	L3	4871	C
6	L3	4882	U
6	L3	4883	C
6	L3	4900	C
6	L3	4901	G
6	L3	4910	G
6	L3	4913	G
6	L3	4916	G
6	L3	4928	C
6	L3	4943	A
6	L3	4976	U
6	L3	5006	U
6	L3	5014	A
6	L3	5020	G
6	L3	5022	U
6	L3	5024	C
6	L3	5025	C
6	L3	5026	U
6	L3	5027	C
6	L3	5031	G
6	L3	5041	G
6	L3	5050	C
6	L3	5054	C
6	L3	5061	A
6	L3	5062	G

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Mol	Chain	Res	Type
6	L3	5069	U
7	L4	7	G
7	L4	53	U
7	L4	54	A
7	L4	64	G
7	L4	66	G
7	L4	84	U
7	L4	97	G
7	L4	100	A
7	L4	106	G
7	L4	110	G
7	L4	111	C

All (13) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	L3	496	G
6	L3	502	C
6	L3	503	C
6	L3	934	C
6	L3	1742	A
6	L3	1754	U
6	L3	1831	G
6	L3	3712	A
6	L3	3819	G
6	L3	3822	PSU
6	L3	4213	A
6	L3	4699	U
7	L4	109	U

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

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
6	A2M	L3	1534	6,64	22,25,26	0.83	0	30,36,39	2.11	7 (23%)
25	HIC	LN	245	25	10,11,12	1.53	1 (10%)	9,14,16	1.34	2 (22%)
6	PSU	L3	4403	6	18,21,22	1.11	1 (5%)	21,30,33	1.94	6 (28%)
6	A2M	L3	2815	6	22,25,26	0.84	0	30,36,39	2.09	8 (26%)
6	PSU	L3	3851	6	18,21,22	1.12	1 (5%)	21,30,33	1.95	6 (28%)
6	OMC	L3	2422	6,64	19,22,23	0.49	0	25,31,34	0.68	0
6	OMU	L3	3818	6	19,22,23	2.10	7 (36%)	25,31,34	1.80	5 (20%)
6	PSU	L3	3853	6	18,21,22	1.08	1 (5%)	21,30,33	1.90	5 (23%)
6	A2M	L3	2787	6	22,25,26	0.84	0	30,36,39	2.11	7 (23%)
6	PSU	L3	4293	6	18,21,22	1.11	1 (5%)	21,30,33	1.93	5 (23%)
6	PSU	L3	4361	6	18,21,22	1.11	1 (5%)	21,30,33	1.99	5 (23%)
6	PSU	L3	1677	6	18,21,22	1.12	1 (5%)	21,30,33	1.90	5 (23%)
6	OMC	L3	1340	6	19,22,23	0.49	0	25,31,34	0.68	0
6	OMG	L3	1760	6	23,26,27	0.44	0	32,38,41	0.53	0
6	OMG	L3	4494	6	23,26,27	0.46	0	32,38,41	0.46	0
6	OMG	L3	3792	6	23,26,27	0.46	0	32,38,41	0.45	0
6	5MC	L3	3782	6	19,22,23	0.47	0	26,32,35	0.64	0
6	OMG	L3	2364	6	23,26,27	0.46	0	32,38,41	0.45	0
6	A2M	L3	3830	6	22,25,26	0.85	0	30,36,39	2.09	7 (23%)
6	PSU	L3	1582	6	18,21,22	1.08	1 (5%)	21,30,33	1.94	5 (23%)
6	PSU	L3	4576	6	18,21,22	1.13	1 (5%)	21,30,33	1.94	6 (28%)
6	PSU	L3	4579	6	18,21,22	1.08	1 (5%)	21,30,33	1.87	4 (19%)
6	PSU	L3	3695	6	18,21,22	1.10	1 (5%)	21,30,33	1.99	6 (28%)
6	PSU	L3	1744	6	18,21,22	1.12	1 (5%)	21,30,33	1.92	5 (23%)
6	OMG	L3	1625	6	23,26,27	0.45	0	32,38,41	0.48	0
6	OMG	L3	4623	6	23,26,27	0.47	0	32,38,41	0.51	0
6	OMC	L3	2824	6	19,22,23	0.49	0	25,31,34	0.65	0
6	A2M	L3	400	6	22,25,26	0.85	0	30,36,39	2.13	8 (26%)
6	PSU	L3	3637	6	18,21,22	1.09	1 (5%)	21,30,33	2.06	5 (23%)
6	PSU	L3	3730	6	18,21,22	1.12	1 (5%)	21,30,33	1.96	5 (23%)
6	A2M	L3	398	6	22,25,26	0.84	0	30,36,39	2.14	8 (26%)
6	OMC	L3	2804	6	19,22,23	0.50	0	25,31,34	0.71	0
6	OMG	L3	3899	6	23,26,27	0.46	0	32,38,41	0.54	0
6	PSU	L3	1779	6	18,21,22	1.11	1 (5%)	21,30,33	1.96	5 (23%)
6	PSU	L3	4431	6	18,21,22	1.10	1 (5%)	21,30,33	1.95	5 (23%)
6	PSU	L3	3734	6	18,21,22	1.13	1 (5%)	21,30,33	1.93	6 (28%)
6	PSU	L3	3959	6	18,21,22	1.11	1 (5%)	21,30,33	1.98	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	OMC	L3	2351	6,64	19,22,23	0.51	0	25,31,34	0.79	1 (4%)
6	A2M	L3	3724	6	22,25,26	0.87	0	30,36,39	2.00	7 (23%)
6	UR3	L3	4530	6	19,22,23	1.08	3 (15%)	26,32,35	1.53	2 (7%)
6	PSU	L3	4457	6	18,21,22	1.11	1 (5%)	21,30,33	1.95	6 (28%)
6	PSU	L3	4500	6	18,21,22	1.11	1 (5%)	21,30,33	1.91	5 (23%)
6	PSU	L3	1862	6	18,21,22	1.09	1 (5%)	21,30,33	1.93	5 (23%)
6	OMC	L3	3808	6	19,22,23	0.47	0	25,31,34	0.71	0
6	OMC	L3	4456	6	19,22,23	0.52	0	25,31,34	0.69	0
6	A2M	L3	2363	6,64	22,25,26	0.86	0	30,36,39	2.06	7 (23%)
6	OMG	L3	4499	6	23,26,27	0.46	0	32,38,41	0.52	0
4	OMG	L1	75	4	23,26,27	0.47	0	32,38,41	0.46	0
6	PSU	L3	4628	6	18,21,22	1.05	2 (11%)	21,30,33	1.80	5 (23%)
6	PSU	L3	5001	6	18,21,22	1.10	1 (5%)	21,30,33	1.93	5 (23%)
6	PSU	L3	1782	6	18,21,22	1.09	1 (5%)	21,30,33	1.95	5 (23%)
6	OMG	L3	2876	6	23,26,27	0.45	0	32,38,41	0.48	0
6	OMC	L3	3869	6	19,22,23	0.50	0	25,31,34	0.68	0
6	PSU	L3	4442	6	18,21,22	1.12	1 (5%)	21,30,33	1.91	5 (23%)
6	A2M	L3	3825	6	22,25,26	0.84	0	30,36,39	2.07	7 (23%)
6	PSU	L3	4552	6	18,21,22	1.08	1 (5%)	21,30,33	1.96	5 (23%)
6	OMG	L3	4370	6	23,26,27	0.46	0	32,38,41	0.45	0
6	PSU	L3	3762	6	18,21,22	1.09	1 (5%)	21,30,33	1.93	6 (28%)
6	5MC	L3	4447	6	19,22,23	0.48	0	26,32,35	0.67	0
6	PSU	L3	4532	6	18,21,22	1.11	1 (5%)	21,30,33	1.98	5 (23%)
6	PSU	L3	3715	6	18,21,22	1.12	1 (5%)	21,30,33	1.98	6 (28%)
6	PSU	L3	2508	6	18,21,22	1.11	1 (5%)	21,30,33	1.91	5 (23%)
6	OMG	L3	4637	6	23,26,27	0.48	0	32,38,41	0.47	0
6	PSU	L3	3822	6	18,21,22	1.07	1 (5%)	21,30,33	1.74	4 (19%)
6	OMC	L3	3841	6	19,22,23	0.49	0	25,31,34	0.63	0
6	PSU	L3	3884	6	18,21,22	1.11	1 (5%)	21,30,33	1.93	5 (23%)
6	PSU	L3	3639	6	18,21,22	1.10	1 (5%)	21,30,33	2.01	5 (23%)
6	PSU	L3	4673	6	18,21,22	1.10	1 (5%)	21,30,33	1.91	5 (23%)
6	PSU	L3	1781	6	18,21,22	1.19	1 (5%)	21,30,33	1.93	5 (23%)
6	A2M	L3	4523	6	22,25,26	0.85	0	30,36,39	2.12	8 (26%)
6	6MZ	L3	4220	6	22,25,26	1.10	1 (4%)	29,36,39	2.19	9 (31%)
6	A2M	L3	3867	6	22,25,26	0.88	0	30,36,39	2.09	7 (23%)
6	OMC	L3	2365	6	19,22,23	0.49	0	25,31,34	0.69	0
6	PSU	L3	1683	6	18,21,22	1.12	1 (5%)	21,30,33	1.96	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PSU	L3	4299	6	18,21,22	1.12	1 (5%)	21,30,33	1.99	6 (28%)
6	A2M	L3	3718	6	22,25,26	0.86	0	30,36,39	2.13	8 (26%)
6	OMU	L3	1773	6	19,22,23	2.10	7 (36%)	25,31,34	1.81	5 (20%)
6	OMG	L3	3627	6	23,26,27	0.46	0	32,38,41	0.57	0
6	OMU	L3	4227	6	19,22,23	2.11	7 (36%)	25,31,34	1.79	5 (20%)
6	PSU	L3	4493	6	18,21,22	1.11	1 (5%)	21,30,33	1.95	5 (23%)
6	PSU	L3	4471	6	18,21,22	1.10	1 (5%)	21,30,33	1.98	5 (23%)
6	PSU	L3	3764	6	18,21,22	1.13	1 (5%)	21,30,33	1.93	5 (23%)
6	OMU	L3	4620	6	19,22,23	2.05	7 (36%)	25,31,34	1.74	5 (20%)
6	OMC	L3	3701	6	19,22,23	0.50	0	25,31,34	0.67	0
6	OMG	L3	4228	6	23,26,27	0.45	0	32,38,41	0.50	0
6	OMG	L3	4042	6	23,26,27	0.46	0	32,38,41	0.49	0
6	A2M	L3	1326	6	22,25,26	0.88	0	30,36,39	2.02	7 (23%)
6	OMG	L3	1316	6	23,26,27	0.47	0	32,38,41	0.50	0
6	PSU	L3	4353	6	18,21,22	1.11	1 (5%)	21,30,33	1.96	5 (23%)
6	OMU	L3	3925	6	19,22,23	2.08	7 (36%)	25,31,34	1.76	5 (20%)
6	PSU	L3	4521	6	18,21,22	1.11	1 (5%)	21,30,33	1.95	5 (23%)
6	OMC	L3	4536	6	19,22,23	0.50	0	25,31,34	0.68	0
6	PSU	L3	4296	6	18,21,22	1.11	1 (5%)	21,30,33	1.95	5 (23%)
6	OMU	L3	4498	6	19,22,23	2.09	7 (36%)	25,31,34	1.78	5 (20%)
6	A2M	L3	1871	6	22,25,26	0.84	0	30,36,39	2.14	8 (26%)
6	PSU	L3	2839	6	18,21,22	1.08	1 (5%)	21,30,33	1.95	5 (23%)
6	PSU	L3	3768	6	18,21,22	1.07	1 (5%)	21,30,33	1.92	5 (23%)
6	A2M	L3	1524	6	22,25,26	0.89	0	30,36,39	2.10	8 (26%)
6	A2M	L3	3760	6	22,25,26	0.85	0	30,36,39	2.11	8 (26%)
6	OMU	L3	2837	6	19,22,23	2.07	7 (36%)	25,31,34	1.81	5 (20%)
6	OMC	L3	2861	6	19,22,23	0.51	0	25,31,34	0.76	1 (4%)
4	PSU	L1	55	4	18,21,22	1.11	1 (5%)	21,30,33	1.99	5 (23%)
6	PSU	L3	2632	6	18,21,22	1.11	1 (5%)	21,30,33	1.82	4 (19%)
6	OMC	L3	4054	6	19,22,23	0.50	0	25,31,34	0.75	0
6	OMG	L3	1522	6	23,26,27	0.45	0	32,38,41	0.47	0
6	PSU	L3	1860	6	18,21,22	1.10	1 (5%)	21,30,33	1.94	5 (23%)
6	OMG	L3	4392	6	23,26,27	0.47	0	32,38,41	0.50	0
6	A2M	L3	4590	6	22,25,26	0.85	0	30,36,39	2.07	7 (23%)
6	PSU	L3	3770	6	18,21,22	1.12	1 (5%)	21,30,33	1.93	5 (23%)
6	OMG	L3	4618	6	23,26,27	0.46	0	32,38,41	0.55	0
6	PSU	L3	1536	6	18,21,22	1.10	1 (5%)	21,30,33	1.97	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	OMG	L3	2424	6	23,26,27	0.48	0	32,38,41	0.47	0
6	A2M	L3	4571	6	22,25,26	0.86	0	30,36,39	2.04	7 (23%)
6	PSU	L3	5010	6	18,21,22	1.12	1 (5%)	21,30,33	1.93	5 (23%)
6	PSU	L3	4972	6	18,21,22	1.08	1 (5%)	21,30,33	1.95	5 (23%)
6	PSU	L3	3758	6	18,21,22	1.09	1 (5%)	21,30,33	1.97	5 (23%)
6	OMG	L3	3744	6	23,26,27	0.46	0	32,38,41	0.48	0
6	PSU	L3	4312	6	18,21,22	1.12	1 (5%)	21,30,33	1.95	5 (23%)
6	OMC	L3	3887	6	19,22,23	0.48	0	25,31,34	0.69	0
6	PSU	L3	3844	6	18,21,22	1.13	1 (5%)	21,30,33	1.94	5 (23%)
6	A2M	L3	2401	6	22,25,26	0.85	0	30,36,39	2.14	8 (26%)
6	OMU	L3	2415	6	19,22,23	2.10	7 (36%)	25,31,34	1.80	5 (20%)
6	OMU	L3	4306	6	19,22,23	2.09	7 (36%)	25,31,34	1.82	5 (20%)
4	PSU	L1	69	4	18,21,22	1.12	1 (5%)	21,30,33	2.01	6 (28%)
6	1MA	L3	1322	6	21,25,26	0.40	0	30,37,40	0.74	1 (3%)
6	PSU	L3	4636	6	18,21,22	1.10	1 (5%)	21,30,33	1.96	6 (28%)
6	A2M	L3	3785	6	22,25,26	0.84	0	30,36,39	2.08	7 (23%)
6	PSU	L3	4689	6,64	18,21,22	1.09	1 (5%)	21,30,33	1.96	5 (23%)
6	PSU	L3	3920	6,64	18,21,22	1.10	1 (5%)	21,30,33	1.98	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
6	A2M	L3	1534	6,64	-	2/9/27/28	0/3/3/3
25	HIC	LN	245	25	-	2/5/6/8	0/1/1/1
6	PSU	L3	4403	6	-	0/7/25/26	0/2/2/2
6	A2M	L3	2815	6	-	0/9/27/28	0/3/3/3
6	PSU	L3	3851	6	-	0/7/25/26	0/2/2/2
6	OMC	L3	2422	6,64	-	2/9/27/28	0/2/2/2
6	OMU	L3	3818	6	-	2/9/27/28	0/2/2/2
6	PSU	L3	3853	6	-	0/7/25/26	0/2/2/2
6	A2M	L3	2787	6	-	5/9/27/28	0/3/3/3
6	PSU	L3	4293	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	4361	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	1677	6	-	2/7/25/26	0/2/2/2
6	OMC	L3	1340	6	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	OMG	L3	1760	6	-	1/9/27/28	0/3/3/3
6	OMG	L3	4494	6	-	0/9/27/28	0/3/3/3
6	OMG	L3	3792	6	-	0/9/27/28	0/3/3/3
6	5MC	L3	3782	6	-	2/7/25/26	0/2/2/2
6	OMG	L3	2364	6	-	2/9/27/28	0/3/3/3
6	A2M	L3	3830	6	-	0/9/27/28	0/3/3/3
6	PSU	L3	1582	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	4576	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	4579	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	3695	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	1744	6	-	2/7/25/26	0/2/2/2
6	OMG	L3	1625	6	-	1/9/27/28	0/3/3/3
6	OMG	L3	4623	6	-	1/9/27/28	0/3/3/3
6	OMC	L3	2824	6	-	0/9/27/28	0/2/2/2
6	A2M	L3	400	6	-	1/9/27/28	0/3/3/3
6	PSU	L3	3637	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	3730	6	-	0/7/25/26	0/2/2/2
6	A2M	L3	398	6	-	1/9/27/28	0/3/3/3
6	OMC	L3	2804	6	-	0/9/27/28	0/2/2/2
6	OMG	L3	3899	6	-	1/9/27/28	0/3/3/3
6	PSU	L3	1779	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	4431	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	3734	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	3959	6	-	0/7/25/26	0/2/2/2
6	OMC	L3	2351	6,64	-	3/9/27/28	0/2/2/2
6	A2M	L3	3724	6	-	1/9/27/28	0/3/3/3
6	UR3	L3	4530	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	4457	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	4500	6	-	3/7/25/26	0/2/2/2
6	PSU	L3	1862	6	-	0/7/25/26	0/2/2/2
6	OMC	L3	3808	6	-	1/9/27/28	0/2/2/2
6	OMC	L3	4456	6	-	1/9/27/28	0/2/2/2
6	A2M	L3	2363	6,64	-	1/9/27/28	0/3/3/3
6	OMG	L3	4499	6	-	0/9/27/28	0/3/3/3
4	OMG	L1	75	4	-	1/9/27/28	0/3/3/3
6	PSU	L3	4628	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	5001	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	1782	6	-	0/7/25/26	0/2/2/2
6	OMG	L3	2876	6	-	1/9/27/28	0/3/3/3
6	OMC	L3	3869	6	-	0/9/27/28	0/2/2/2
6	PSU	L3	4442	6	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	A2M	L3	3825	6	-	1/9/27/28	0/3/3/3
6	PSU	L3	4552	6	-	0/7/25/26	0/2/2/2
6	OMG	L3	4370	6	-	1/9/27/28	0/3/3/3
6	PSU	L3	3762	6	-	0/7/25/26	0/2/2/2
6	5MC	L3	4447	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	4532	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	3715	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	2508	6	-	0/7/25/26	0/2/2/2
6	OMG	L3	4637	6	-	3/9/27/28	0/3/3/3
6	PSU	L3	3822	6	-	0/7/25/26	0/2/2/2
6	OMC	L3	3841	6	-	1/9/27/28	0/2/2/2
6	PSU	L3	3884	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	3639	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	4673	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	1781	6	-	2/7/25/26	0/2/2/2
6	A2M	L3	4523	6	-	2/9/27/28	0/3/3/3
6	6MZ	L3	4220	6	-	5/9/27/28	0/3/3/3
6	A2M	L3	3867	6	-	4/9/27/28	0/3/3/3
6	OMC	L3	2365	6	-	0/9/27/28	0/2/2/2
6	PSU	L3	1683	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	4299	6	-	0/7/25/26	0/2/2/2
6	A2M	L3	3718	6	-	1/9/27/28	0/3/3/3
6	OMU	L3	1773	6	-	2/9/27/28	0/2/2/2
6	OMG	L3	3627	6	-	1/9/27/28	0/3/3/3
6	OMU	L3	4227	6	-	4/9/27/28	0/2/2/2
6	PSU	L3	4493	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	4471	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	3764	6	-	0/7/25/26	0/2/2/2
6	OMU	L3	4620	6	-	1/9/27/28	0/2/2/2
6	OMC	L3	3701	6	-	4/9/27/28	0/2/2/2
6	OMG	L3	4228	6	-	2/9/27/28	0/3/3/3
6	OMG	L3	4042	6	-	1/9/27/28	0/3/3/3
6	A2M	L3	1326	6	-	1/9/27/28	0/3/3/3
6	OMG	L3	1316	6	-	1/9/27/28	0/3/3/3
6	PSU	L3	4353	6	-	0/7/25/26	0/2/2/2
6	OMU	L3	3925	6	-	1/9/27/28	0/2/2/2
6	PSU	L3	4521	6	-	0/7/25/26	0/2/2/2
6	OMC	L3	4536	6	-	0/9/27/28	0/2/2/2
6	PSU	L3	4296	6	-	0/7/25/26	0/2/2/2
6	OMU	L3	4498	6	-	6/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	A2M	L3	1871	6	-	0/9/27/28	0/3/3/3
6	PSU	L3	2839	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	3768	6	-	0/7/25/26	0/2/2/2
6	A2M	L3	1524	6	-	2/9/27/28	0/3/3/3
6	A2M	L3	3760	6	-	3/9/27/28	0/3/3/3
6	OMU	L3	2837	6	-	1/9/27/28	0/2/2/2
6	OMC	L3	2861	6	-	1/9/27/28	0/2/2/2
4	PSU	L1	55	4	-	0/7/25/26	0/2/2/2
6	PSU	L3	2632	6	-	0/7/25/26	0/2/2/2
6	OMC	L3	4054	6	-	1/9/27/28	0/2/2/2
6	OMG	L3	1522	6	-	0/9/27/28	0/3/3/3
6	PSU	L3	1860	6	-	0/7/25/26	0/2/2/2
6	OMG	L3	4392	6	-	1/9/27/28	0/3/3/3
6	A2M	L3	4590	6	-	2/9/27/28	0/3/3/3
6	PSU	L3	3770	6	-	0/7/25/26	0/2/2/2
6	OMG	L3	4618	6	-	2/9/27/28	0/3/3/3
6	PSU	L3	1536	6	-	0/7/25/26	0/2/2/2
6	OMG	L3	2424	6	-	3/9/27/28	0/3/3/3
6	A2M	L3	4571	6	-	1/9/27/28	0/3/3/3
6	PSU	L3	5010	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	4972	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	3758	6	-	0/7/25/26	0/2/2/2
6	OMG	L3	3744	6	-	1/9/27/28	0/3/3/3
6	PSU	L3	4312	6	-	0/7/25/26	0/2/2/2
6	OMC	L3	3887	6	-	2/9/27/28	0/2/2/2
6	PSU	L3	3844	6	-	1/7/25/26	0/2/2/2
6	A2M	L3	2401	6	-	2/9/27/28	0/3/3/3
6	OMU	L3	2415	6	-	3/9/27/28	0/2/2/2
6	OMU	L3	4306	6	-	1/9/27/28	0/2/2/2
4	PSU	L1	69	4	-	0/7/25/26	0/2/2/2
6	1MA	L3	1322	6	-	2/7/25/26	0/3/3/3
6	PSU	L3	4636	6	-	3/7/25/26	0/2/2/2
6	A2M	L3	3785	6	-	3/9/27/28	0/3/3/3
6	PSU	L3	4689	6,64	-	0/7/25/26	0/2/2/2
6	PSU	L3	3920	6,64	-	0/7/25/26	0/2/2/2

All (127) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L3	1773	OMU	C6-N1	4.84	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L3	3818	OMU	C6-N1	4.82	1.49	1.38
6	L3	4227	OMU	C6-N1	4.82	1.49	1.38
6	L3	4498	OMU	C6-N1	4.81	1.49	1.38
6	L3	4306	OMU	C6-N1	4.79	1.49	1.38
6	L3	3925	OMU	C6-N1	4.77	1.49	1.38
6	L3	4620	OMU	C6-N1	4.74	1.49	1.38
6	L3	2415	OMU	C6-N1	4.73	1.49	1.38
6	L3	2837	OMU	C6-N1	4.72	1.49	1.38
6	L3	4227	OMU	C2-N1	4.39	1.45	1.38
6	L3	2415	OMU	C2-N1	4.37	1.45	1.38
6	L3	4306	OMU	C2-N1	4.36	1.45	1.38
6	L3	3818	OMU	C2-N1	4.33	1.45	1.38
6	L3	2837	OMU	C2-N1	4.31	1.45	1.38
6	L3	4498	OMU	C2-N1	4.31	1.45	1.38
6	L3	1773	OMU	C2-N1	4.31	1.45	1.38
6	L3	3925	OMU	C2-N1	4.25	1.45	1.38
6	L3	3818	OMU	C5-C4	4.16	1.52	1.43
6	L3	4498	OMU	C5-C4	4.16	1.52	1.43
6	L3	4227	OMU	C5-C4	4.15	1.52	1.43
6	L3	4620	OMU	C2-N1	4.15	1.45	1.38
6	L3	1773	OMU	C5-C4	4.13	1.52	1.43
6	L3	4306	OMU	C5-C4	4.13	1.52	1.43
6	L3	2415	OMU	C5-C4	4.06	1.52	1.43
6	L3	2837	OMU	C5-C4	4.04	1.52	1.43
6	L3	4620	OMU	C5-C4	4.03	1.52	1.43
6	L3	3925	OMU	C5-C4	4.03	1.52	1.43
6	L3	4220	6MZ	C6-N6	3.93	1.38	1.34
6	L3	1781	PSU	C6-C5	3.77	1.39	1.35
6	L3	2632	PSU	C6-C5	3.74	1.39	1.35
6	L3	1677	PSU	C6-C5	3.73	1.39	1.35
6	L3	3764	PSU	C6-C5	3.70	1.39	1.35
6	L3	1744	PSU	C6-C5	3.69	1.39	1.35
6	L3	4576	PSU	C6-C5	3.68	1.39	1.35
6	L3	4312	PSU	C6-C5	3.68	1.39	1.35
6	L3	4442	PSU	C6-C5	3.68	1.39	1.35
6	L3	4500	PSU	C6-C5	3.67	1.39	1.35
6	L3	3730	PSU	C6-C5	3.67	1.39	1.35
6	L3	3770	PSU	C6-C5	3.66	1.39	1.35
6	L3	4296	PSU	C6-C5	3.66	1.39	1.35
6	L3	2508	PSU	C6-C5	3.66	1.39	1.35
6	L3	3822	PSU	C6-C5	3.64	1.39	1.35
6	L3	3884	PSU	C6-C5	3.64	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L3	3844	PSU	C6-C5	3.64	1.39	1.35
6	L3	1862	PSU	C6-C5	3.63	1.39	1.35
6	L3	3715	PSU	C6-C5	3.63	1.39	1.35
6	L3	4293	PSU	C6-C5	3.63	1.39	1.35
6	L3	4403	PSU	C6-C5	3.63	1.39	1.35
6	L3	3851	PSU	C6-C5	3.62	1.39	1.35
6	L3	1779	PSU	C6-C5	3.62	1.39	1.35
6	L3	5010	PSU	C6-C5	3.62	1.39	1.35
6	L3	1683	PSU	C6-C5	3.62	1.39	1.35
6	L3	4299	PSU	C6-C5	3.62	1.39	1.35
6	L3	4521	PSU	C6-C5	3.62	1.39	1.35
6	L3	3734	PSU	C6-C5	3.61	1.39	1.35
6	L3	4532	PSU	C6-C5	3.60	1.39	1.35
6	L3	5001	PSU	C6-C5	3.60	1.39	1.35
6	L3	4636	PSU	C6-C5	3.60	1.39	1.35
6	L3	4673	PSU	C6-C5	3.60	1.39	1.35
6	L3	4353	PSU	C6-C5	3.59	1.39	1.35
6	L3	4431	PSU	C6-C5	3.58	1.39	1.35
6	L3	3959	PSU	C6-C5	3.57	1.39	1.35
6	L3	1860	PSU	C6-C5	3.57	1.39	1.35
6	L3	4493	PSU	C6-C5	3.57	1.39	1.35
6	L3	1782	PSU	C6-C5	3.56	1.39	1.35
6	L3	4361	PSU	C6-C5	3.56	1.39	1.35
6	L3	4471	PSU	C6-C5	3.56	1.39	1.35
6	L3	3695	PSU	C6-C5	3.56	1.39	1.35
4	L1	55	PSU	C6-C5	3.56	1.39	1.35
6	L3	3853	PSU	C6-C5	3.56	1.39	1.35
6	L3	4457	PSU	C6-C5	3.55	1.39	1.35
6	L3	1582	PSU	C6-C5	3.54	1.39	1.35
6	L3	4689	PSU	C6-C5	3.54	1.39	1.35
4	L1	69	PSU	C6-C5	3.54	1.39	1.35
6	L3	1536	PSU	C6-C5	3.54	1.39	1.35
6	L3	3920	PSU	C6-C5	3.53	1.39	1.35
6	L3	3758	PSU	C6-C5	3.53	1.39	1.35
6	L3	4972	PSU	C6-C5	3.52	1.39	1.35
6	L3	3637	PSU	C6-C5	3.52	1.39	1.35
6	L3	4552	PSU	C6-C5	3.51	1.39	1.35
6	L3	3639	PSU	C6-C5	3.50	1.39	1.35
6	L3	2839	PSU	C6-C5	3.49	1.39	1.35
6	L3	4579	PSU	C6-C5	3.48	1.39	1.35
6	L3	3762	PSU	C6-C5	3.48	1.39	1.35
6	L3	3768	PSU	C6-C5	3.36	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L3	4628	PSU	C6-C5	3.25	1.38	1.35
25	LN	245	HIC	CD2-CG	3.06	1.41	1.36
6	L3	4530	UR3	C2-N1	-2.80	1.34	1.38
6	L3	2837	OMU	O4-C4	-2.74	1.19	1.24
6	L3	3925	OMU	O4-C4	-2.74	1.19	1.24
6	L3	4530	UR3	C4-N3	-2.73	1.35	1.40
6	L3	4227	OMU	C2-N3	2.72	1.42	1.38
6	L3	4620	OMU	O4-C4	-2.70	1.19	1.24
6	L3	4498	OMU	O4-C4	-2.69	1.19	1.24
6	L3	4227	OMU	O4-C4	-2.69	1.19	1.24
6	L3	4306	OMU	O4-C4	-2.68	1.19	1.24
6	L3	3818	OMU	O4-C4	-2.68	1.19	1.24
6	L3	2415	OMU	O4-C4	-2.67	1.19	1.24
6	L3	1773	OMU	C2-N3	2.67	1.42	1.38
6	L3	1773	OMU	O4-C4	-2.65	1.19	1.24
6	L3	3818	OMU	C2-N3	2.65	1.42	1.38
6	L3	4498	OMU	C2-N3	2.64	1.42	1.38
6	L3	3925	OMU	C2-N3	2.64	1.42	1.38
6	L3	2837	OMU	C2-N3	2.62	1.42	1.38
6	L3	2415	OMU	C2-N3	2.61	1.42	1.38
6	L3	4306	OMU	C2-N3	2.60	1.42	1.38
6	L3	4620	OMU	C2-N3	2.55	1.42	1.38
6	L3	1773	OMU	C4-N3	2.24	1.42	1.38
6	L3	4498	OMU	C4-N3	2.23	1.42	1.38
6	L3	3818	OMU	C4-N3	2.22	1.42	1.38
6	L3	3925	OMU	O2-C2	-2.22	1.19	1.23
6	L3	2415	OMU	O2-C2	-2.20	1.19	1.23
6	L3	4306	OMU	C4-N3	2.19	1.42	1.38
6	L3	4620	OMU	O2-C2	-2.18	1.19	1.23
6	L3	2415	OMU	C4-N3	2.18	1.42	1.38
6	L3	4227	OMU	C4-N3	2.17	1.42	1.38
6	L3	2837	OMU	O2-C2	-2.16	1.19	1.23
6	L3	4306	OMU	O2-C2	-2.15	1.19	1.23
6	L3	2837	OMU	C4-N3	2.14	1.42	1.38
6	L3	3925	OMU	C4-N3	2.14	1.42	1.38
6	L3	3818	OMU	O2-C2	-2.14	1.19	1.23
6	L3	1773	OMU	O2-C2	-2.12	1.19	1.23
6	L3	4530	UR3	C2-N3	-2.11	1.34	1.39
6	L3	4227	OMU	O2-C2	-2.10	1.19	1.23
6	L3	4498	OMU	O2-C2	-2.09	1.19	1.23
6	L3	4620	OMU	C4-N3	2.06	1.42	1.38
6	L3	4628	PSU	C4-C5	-2.02	1.38	1.44

All (510) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L3	3867	A2M	C5-C4-N3	-5.74	118.82	126.72
6	L3	4220	6MZ	C5-C4-N3	-5.62	118.98	126.72
6	L3	3825	A2M	C5-C4-N3	-5.60	119.01	126.72
6	L3	2787	A2M	C5-C4-N3	-5.58	119.04	126.72
6	L3	3718	A2M	C5-C4-N3	-5.57	119.05	126.72
6	L3	398	A2M	C5-C4-N3	-5.56	119.06	126.72
6	L3	3760	A2M	C5-C4-N3	-5.56	119.06	126.72
6	L3	3785	A2M	C5-C4-N3	-5.56	119.06	126.72
6	L3	4523	A2M	C5-C4-N3	-5.55	119.08	126.72
6	L3	4571	A2M	C5-C4-N3	-5.53	119.10	126.72
6	L3	2363	A2M	C5-C4-N3	-5.53	119.11	126.72
6	L3	1534	A2M	C5-C4-N3	-5.52	119.11	126.72
6	L3	1524	A2M	C5-C4-N3	-5.51	119.13	126.72
6	L3	3830	A2M	C5-C4-N3	-5.50	119.14	126.72
6	L3	2401	A2M	C5-C4-N3	-5.49	119.16	126.72
6	L3	4306	OMU	C4-N3-C2	-5.46	119.83	126.61
6	L3	4530	UR3	C4-N3-C2	-5.45	120.19	124.58
6	L3	2815	A2M	C5-C4-N3	-5.41	119.27	126.72
6	L3	1773	OMU	C4-N3-C2	-5.39	119.92	126.61
6	L3	1871	A2M	C5-C4-N3	-5.38	119.31	126.72
6	L3	1326	A2M	C5-C4-N3	-5.38	119.31	126.72
6	L3	3818	OMU	C4-N3-C2	-5.35	119.97	126.61
6	L3	400	A2M	C5-C4-N3	-5.35	119.35	126.72
6	L3	2837	OMU	C4-N3-C2	-5.35	119.97	126.61
6	L3	3724	A2M	C5-C4-N3	-5.32	119.39	126.72
6	L3	4498	OMU	C4-N3-C2	-5.32	120.01	126.61
6	L3	4227	OMU	C4-N3-C2	-5.28	120.06	126.61
6	L3	2415	OMU	C4-N3-C2	-5.25	120.09	126.61
6	L3	3637	PSU	N1-C2-N3	5.22	120.67	115.17
6	L3	3925	OMU	C4-N3-C2	-5.20	120.16	126.61
6	L3	4590	A2M	C5-C4-N3	-5.19	119.56	126.72
6	L3	4620	OMU	C4-N3-C2	-5.02	120.38	126.61
6	L3	3637	PSU	C4-N3-C2	-4.98	119.51	126.37
6	L3	3639	PSU	N1-C2-N3	4.96	120.40	115.17
6	L3	4471	PSU	N1-C2-N3	4.93	120.36	115.17
6	L3	4532	PSU	C4-N3-C2	-4.91	119.60	126.37
6	L3	4636	PSU	C4-N3-C2	-4.91	119.61	126.37
6	L3	1536	PSU	N1-C2-N3	4.90	120.34	115.17
6	L3	3959	PSU	N1-C2-N3	4.89	120.32	115.17
6	L3	1582	PSU	C4-N3-C2	-4.88	119.64	126.37
6	L3	3695	PSU	N1-C2-N3	4.88	120.32	115.17
6	L3	4361	PSU	N1-C2-N3	4.88	120.32	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L3	4521	PSU	N1-C2-N3	4.88	120.32	115.17
6	L3	3920	PSU	N1-C2-N3	4.88	120.31	115.17
6	L3	4689	PSU	N1-C2-N3	4.88	120.31	115.17
4	L1	55	PSU	N1-C2-N3	4.88	120.31	115.17
4	L1	55	PSU	C4-N3-C2	-4.87	119.66	126.37
4	L1	69	PSU	N1-C2-N3	4.87	120.31	115.17
6	L3	4532	PSU	N1-C2-N3	4.87	120.31	115.17
6	L3	4299	PSU	N1-C2-N3	4.87	120.31	115.17
6	L3	3920	PSU	C4-N3-C2	-4.87	119.67	126.37
6	L3	3639	PSU	C4-N3-C2	-4.86	119.68	126.37
6	L3	1683	PSU	N1-C2-N3	4.86	120.29	115.17
6	L3	1779	PSU	C4-N3-C2	-4.86	119.68	126.37
6	L3	4431	PSU	C4-N3-C2	-4.85	119.69	126.37
6	L3	3715	PSU	N1-C2-N3	4.85	120.29	115.17
6	L3	3758	PSU	C4-N3-C2	-4.85	119.69	126.37
6	L3	1862	PSU	C4-N3-C2	-4.85	119.69	126.37
6	L3	3730	PSU	C4-N3-C2	-4.85	119.69	126.37
6	L3	4500	PSU	C4-N3-C2	-4.85	119.69	126.37
6	L3	4457	PSU	N1-C2-N3	4.85	120.28	115.17
6	L3	3695	PSU	C4-N3-C2	-4.85	119.70	126.37
6	L3	4552	PSU	C4-N3-C2	-4.84	119.70	126.37
6	L3	4361	PSU	C4-N3-C2	-4.84	119.70	126.37
6	L3	3758	PSU	N1-C2-N3	4.84	120.27	115.17
6	L3	4972	PSU	C4-N3-C2	-4.84	119.71	126.37
6	L3	4431	PSU	N1-C2-N3	4.84	120.27	115.17
6	L3	1683	PSU	C4-N3-C2	-4.83	119.71	126.37
6	L3	4552	PSU	N1-C2-N3	4.83	120.27	115.17
6	L3	4353	PSU	C4-N3-C2	-4.83	119.71	126.37
6	L3	4353	PSU	N1-C2-N3	4.83	120.27	115.17
6	L3	3959	PSU	C4-N3-C2	-4.83	119.72	126.37
6	L3	4312	PSU	N1-C2-N3	4.83	120.26	115.17
6	L3	2839	PSU	N1-C2-N3	4.83	120.26	115.17
6	L3	1779	PSU	N1-C2-N3	4.83	120.26	115.17
6	L3	1536	PSU	C4-N3-C2	-4.83	119.72	126.37
6	L3	1782	PSU	N1-C2-N3	4.83	120.26	115.17
6	L3	4403	PSU	N1-C2-N3	4.83	120.26	115.17
6	L3	3730	PSU	N1-C2-N3	4.82	120.26	115.17
6	L3	4296	PSU	C4-N3-C2	-4.82	119.73	126.37
6	L3	4299	PSU	C4-N3-C2	-4.82	119.73	126.37
6	L3	4500	PSU	N1-C2-N3	4.82	120.25	115.17
6	L3	4293	PSU	N1-C2-N3	4.82	120.25	115.17
6	L3	3851	PSU	C4-N3-C2	-4.82	119.73	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L3	3844	PSU	N1-C2-N3	4.82	120.25	115.17
6	L3	4296	PSU	N1-C2-N3	4.82	120.25	115.17
6	L3	3715	PSU	C4-N3-C2	-4.82	119.74	126.37
6	L3	4312	PSU	C4-N3-C2	-4.82	119.74	126.37
6	L3	3851	PSU	N1-C2-N3	4.82	120.25	115.17
6	L3	1781	PSU	N1-C2-N3	4.81	120.25	115.17
6	L3	4972	PSU	N1-C2-N3	4.81	120.24	115.17
6	L3	4636	PSU	N1-C2-N3	4.81	120.24	115.17
6	L3	4471	PSU	C4-N3-C2	-4.81	119.75	126.37
6	L3	4493	PSU	C4-N3-C2	-4.81	119.75	126.37
6	L3	3770	PSU	C4-N3-C2	-4.80	119.75	126.37
4	L1	69	PSU	C4-N3-C2	-4.80	119.76	126.37
6	L3	1782	PSU	C4-N3-C2	-4.80	119.76	126.37
6	L3	2508	PSU	C4-N3-C2	-4.80	119.76	126.37
6	L3	1860	PSU	C4-N3-C2	-4.80	119.76	126.37
6	L3	3764	PSU	N1-C2-N3	4.80	120.23	115.17
6	L3	4403	PSU	C4-N3-C2	-4.80	119.77	126.37
6	L3	5001	PSU	N1-C2-N3	4.79	120.22	115.17
6	L3	1677	PSU	C4-N3-C2	-4.79	119.78	126.37
6	L3	1582	PSU	N1-C2-N3	4.79	120.22	115.17
6	L3	4576	PSU	N1-C2-N3	4.78	120.21	115.17
6	L3	3770	PSU	N1-C2-N3	4.78	120.21	115.17
6	L3	4673	PSU	C4-N3-C2	-4.78	119.79	126.37
6	L3	1677	PSU	N1-C2-N3	4.78	120.21	115.17
6	L3	3884	PSU	C4-N3-C2	-4.78	119.79	126.37
6	L3	3764	PSU	C4-N3-C2	-4.78	119.79	126.37
6	L3	1744	PSU	N1-C2-N3	4.78	120.21	115.17
6	L3	3884	PSU	N1-C2-N3	4.78	120.20	115.17
6	L3	2839	PSU	C4-N3-C2	-4.78	119.79	126.37
6	L3	4442	PSU	C4-N3-C2	-4.77	119.80	126.37
6	L3	4521	PSU	C4-N3-C2	-4.77	119.80	126.37
6	L3	5010	PSU	N1-C2-N3	4.77	120.20	115.17
6	L3	1862	PSU	N1-C2-N3	4.77	120.19	115.17
6	L3	4493	PSU	N1-C2-N3	4.76	120.19	115.17
6	L3	4457	PSU	C4-N3-C2	-4.76	119.81	126.37
6	L3	1860	PSU	N1-C2-N3	4.76	120.19	115.17
6	L3	5001	PSU	C4-N3-C2	-4.75	119.82	126.37
6	L3	3867	A2M	N3-C4-N9	4.74	135.24	127.17
6	L3	4576	PSU	C4-N3-C2	-4.74	119.83	126.37
6	L3	3762	PSU	N1-C2-N3	4.74	120.17	115.17
6	L3	4293	PSU	C4-N3-C2	-4.74	119.84	126.37
6	L3	3844	PSU	C4-N3-C2	-4.73	119.85	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L3	2508	PSU	N1-C2-N3	4.73	120.16	115.17
6	L3	3768	PSU	N1-C2-N3	4.73	120.15	115.17
6	L3	3853	PSU	N1-C2-N3	4.72	120.15	115.17
6	L3	4442	PSU	N1-C2-N3	4.72	120.15	115.17
6	L3	3734	PSU	N1-C2-N3	4.72	120.15	115.17
6	L3	5010	PSU	C4-N3-C2	-4.71	119.88	126.37
6	L3	3762	PSU	C4-N3-C2	-4.71	119.89	126.37
6	L3	3768	PSU	C4-N3-C2	-4.70	119.89	126.37
6	L3	4689	PSU	C4-N3-C2	-4.70	119.90	126.37
6	L3	3734	PSU	C4-N3-C2	-4.69	119.91	126.37
6	L3	4673	PSU	N1-C2-N3	4.69	120.11	115.17
6	L3	1744	PSU	C4-N3-C2	-4.68	119.92	126.37
6	L3	3830	A2M	N3-C4-N9	4.66	135.09	127.17
6	L3	2632	PSU	C4-N3-C2	-4.65	119.96	126.37
6	L3	3760	A2M	N3-C4-N9	4.65	135.08	127.17
6	L3	4220	6MZ	N3-C4-N9	4.65	135.07	127.17
6	L3	4523	A2M	N3-C4-N9	4.65	135.07	127.17
6	L3	3853	PSU	C4-N3-C2	-4.64	119.97	126.37
6	L3	1534	A2M	N3-C4-N9	4.63	135.05	127.17
6	L3	4579	PSU	C4-N3-C2	-4.62	120.01	126.37
6	L3	1781	PSU	C4-N3-C2	-4.61	120.02	126.37
6	L3	2787	A2M	N3-C4-N9	4.61	135.01	127.17
6	L3	2632	PSU	N1-C2-N3	4.60	120.02	115.17
6	L3	398	A2M	N3-C4-N9	4.60	134.99	127.17
6	L3	3825	A2M	N3-C4-N9	4.59	134.97	127.17
6	L3	3785	A2M	N3-C4-N9	4.59	134.97	127.17
6	L3	2401	A2M	N3-C4-N9	4.57	134.95	127.17
6	L3	4579	PSU	N1-C2-N3	4.57	119.99	115.17
6	L3	1524	A2M	N3-C4-N9	4.56	134.92	127.17
6	L3	4571	A2M	N3-C4-N9	4.54	134.90	127.17
6	L3	3718	A2M	N3-C4-N9	4.52	134.86	127.17
6	L3	3822	PSU	C4-N3-C2	-4.51	120.16	126.37
6	L3	3822	PSU	N1-C2-N3	4.50	119.92	115.17
6	L3	4628	PSU	C4-N3-C2	-4.50	120.17	126.37
6	L3	2815	A2M	N3-C4-N9	4.47	134.76	127.17
6	L3	2363	A2M	N3-C4-N9	4.46	134.76	127.17
6	L3	400	A2M	N3-C4-N9	4.45	134.73	127.17
6	L3	1871	A2M	N3-C4-N9	4.43	134.69	127.17
6	L3	3724	A2M	N3-C4-N9	4.42	134.69	127.17
6	L3	4628	PSU	N1-C2-N3	4.33	119.74	115.17
6	L3	400	A2M	N3-C2-N1	-4.28	122.11	128.58
6	L3	4590	A2M	N3-C2-N1	-4.27	122.11	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L3	1326	A2M	N3-C4-N9	4.24	134.38	127.17
6	L3	4590	A2M	N3-C4-N9	4.24	134.37	127.17
6	L3	3724	A2M	N3-C2-N1	-4.22	122.19	128.58
6	L3	1326	A2M	N3-C2-N1	-4.22	122.20	128.58
6	L3	2815	A2M	N3-C2-N1	-4.21	122.21	128.58
6	L3	1871	A2M	N3-C2-N1	-4.19	122.24	128.58
6	L3	2401	A2M	N3-C2-N1	-4.17	122.27	128.58
6	L3	3830	A2M	N3-C2-N1	-4.16	122.28	128.58
6	L3	2363	A2M	N3-C2-N1	-4.15	122.29	128.58
6	L3	398	A2M	N3-C2-N1	-4.13	122.32	128.58
6	L3	3760	A2M	N3-C2-N1	-4.12	122.34	128.58
6	L3	1534	A2M	N3-C2-N1	-4.10	122.38	128.58
6	L3	4523	A2M	N3-C2-N1	-4.10	122.38	128.58
6	L3	4571	A2M	N3-C2-N1	-4.08	122.40	128.58
6	L3	3825	A2M	N3-C2-N1	-4.07	122.42	128.58
6	L3	2787	A2M	N3-C2-N1	-4.06	122.43	128.58
6	L3	4220	6MZ	N1-C2-N3	-4.05	122.45	128.58
6	L3	4306	OMU	N3-C2-N1	4.05	120.16	114.89
6	L3	1773	OMU	N3-C2-N1	4.05	120.16	114.89
6	L3	1524	A2M	N3-C2-N1	-4.05	122.46	128.58
6	L3	3785	A2M	N3-C2-N1	-4.05	122.46	128.58
6	L3	3718	A2M	N3-C2-N1	-4.03	122.48	128.58
6	L3	2415	OMU	N3-C2-N1	4.01	120.11	114.89
6	L3	3867	A2M	N3-C2-N1	-3.99	122.55	128.58
6	L3	3925	OMU	N3-C2-N1	3.96	120.05	114.89
6	L3	4227	OMU	N3-C2-N1	3.96	120.04	114.89
6	L3	4620	OMU	N3-C2-N1	3.89	119.96	114.89
6	L3	3818	OMU	N3-C2-N1	3.89	119.95	114.89
6	L3	4498	OMU	N3-C2-N1	3.87	119.93	114.89
6	L3	2837	OMU	N3-C2-N1	3.85	119.90	114.89
6	L3	4220	6MZ	C5-N7-C8	3.79	109.41	103.45
6	L3	2815	A2M	C5-N7-C8	3.79	109.40	103.45
6	L3	2787	A2M	C5-N7-C8	3.78	109.39	103.45
6	L3	1534	A2M	C5-N7-C8	3.78	109.39	103.45
6	L3	398	A2M	C5-N7-C8	3.78	109.39	103.45
6	L3	4523	A2M	C5-N7-C8	3.78	109.39	103.45
6	L3	3825	A2M	C5-N7-C8	3.77	109.37	103.45
6	L3	3785	A2M	C5-N7-C8	3.76	109.36	103.45
6	L3	2837	OMU	C5-C4-N3	3.76	120.06	114.80
6	L3	4590	A2M	C5-N7-C8	3.76	109.35	103.45
6	L3	400	A2M	C5-N7-C8	3.75	109.35	103.45
6	L3	2401	A2M	C5-N7-C8	3.75	109.34	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L3	3760	A2M	C5-N7-C8	3.75	109.34	103.45
6	L3	2363	A2M	C5-N7-C8	3.74	109.32	103.45
6	L3	3718	A2M	C5-N7-C8	3.73	109.31	103.45
6	L3	4498	OMU	C5-C4-N3	3.72	120.01	114.80
6	L3	3818	OMU	C5-C4-N3	3.72	120.00	114.80
6	L3	3830	A2M	C5-N7-C8	3.71	109.28	103.45
6	L3	4306	OMU	C5-C4-N3	3.71	119.99	114.80
6	L3	1773	OMU	C5-C4-N3	3.70	119.99	114.80
6	L3	3867	A2M	C5-N7-C8	3.70	109.26	103.45
6	L3	4571	A2M	C5-N7-C8	3.70	109.26	103.45
6	L3	1871	A2M	C5-N7-C8	3.68	109.24	103.45
6	L3	2401	A2M	C2-N3-C4	3.65	120.76	111.83
6	L3	3825	A2M	C2-N3-C4	3.65	120.75	111.83
6	L3	398	A2M	C2-N3-C4	3.65	120.75	111.83
6	L3	2363	A2M	C2-N3-C4	3.65	120.74	111.83
6	L3	3867	A2M	C2-N3-C4	3.65	120.74	111.83
6	L3	4227	OMU	C5-C4-N3	3.64	119.90	114.80
6	L3	3760	A2M	C2-N3-C4	3.64	120.72	111.83
6	L3	2815	A2M	C2-N3-C4	3.64	120.72	111.83
6	L3	4220	6MZ	C2-N3-C4	3.63	120.71	111.83
6	L3	4571	A2M	C2-N3-C4	3.63	120.70	111.83
6	L3	2787	A2M	C2-N3-C4	3.63	120.69	111.83
6	L3	1326	A2M	C5-N7-C8	3.63	109.15	103.45
6	L3	1534	A2M	C2-N3-C4	3.63	120.69	111.83
6	L3	2415	OMU	C5-C4-N3	3.62	119.88	114.80
6	L3	3785	A2M	C2-N3-C4	3.62	120.67	111.83
6	L3	4523	A2M	C2-N3-C4	3.62	120.67	111.83
6	L3	1326	A2M	C2-N3-C4	3.61	120.65	111.83
6	L3	1871	A2M	C2-N3-C4	3.61	120.65	111.83
6	L3	400	A2M	C2-N3-C4	3.61	120.64	111.83
6	L3	3724	A2M	C5-N7-C8	3.61	109.12	103.45
6	L3	3718	A2M	C2-N3-C4	3.60	120.63	111.83
6	L3	1524	A2M	C2-N3-C4	3.59	120.60	111.83
6	L3	3830	A2M	C2-N3-C4	3.59	120.59	111.83
6	L3	3925	OMU	C5-C4-N3	3.57	119.80	114.80
6	L3	4590	A2M	C2-N3-C4	3.57	120.54	111.83
6	L3	3724	A2M	C2-N3-C4	3.53	120.44	111.83
6	L3	4620	OMU	C5-C4-N3	3.52	119.73	114.80
6	L3	1524	A2M	C5-N7-C8	3.51	108.97	103.45
6	L3	4530	UR3	C5-C4-N3	3.33	119.43	115.04
6	L3	4689	PSU	O2-C2-N1	-3.16	119.53	122.79
6	L3	3718	A2M	C2'-C1'-N9	-3.10	108.64	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L3	4220	6MZ	C9-N6-C6	-3.09	119.98	122.85
6	L3	2363	A2M	C4-C5-N7	-3.08	107.06	110.58
25	LN	245	HIC	NE2-CE1-ND1	-3.07	111.49	112.66
6	L3	1326	A2M	C4-C5-N7	-3.06	107.08	110.58
6	L3	2415	OMU	O4-C4-C5	-3.04	119.92	125.16
6	L3	4590	A2M	C4-C5-N7	-3.03	107.11	110.58
6	L3	3825	A2M	C4-C5-N7	-3.03	107.12	110.58
6	L3	2837	OMU	O4-C4-C5	-3.03	119.94	125.16
6	L3	4498	OMU	O4-C4-C5	-3.03	119.94	125.16
6	L3	3785	A2M	C4-C5-N7	-3.01	107.14	110.58
6	L3	3818	OMU	O4-C4-C5	-3.01	119.97	125.16
6	L3	2815	A2M	C4-C5-N7	-3.00	107.15	110.58
6	L3	3639	PSU	O2-C2-N1	-3.00	119.69	122.79
6	L3	3718	A2M	C4-C5-N7	-3.00	107.15	110.58
6	L3	4306	OMU	O4-C4-C5	-2.99	120.00	125.16
6	L3	4571	A2M	C4-C5-N7	-2.99	107.16	110.58
6	L3	3637	PSU	C6-C5-C4	2.98	120.18	118.17
6	L3	398	A2M	C4-C5-N7	-2.98	107.18	110.58
6	L3	2787	A2M	C4-C5-N7	-2.97	107.18	110.58
6	L3	4220	6MZ	C4-C5-N7	-2.96	107.19	110.58
6	L3	4227	OMU	O4-C4-C5	-2.96	120.05	125.16
6	L3	5001	PSU	O2-C2-N1	-2.95	119.75	122.79
6	L3	4523	A2M	C4-C5-N7	-2.94	107.22	110.58
6	L3	3695	PSU	O2-C2-N1	-2.94	119.75	122.79
6	L3	1773	OMU	O4-C4-C5	-2.94	120.09	125.16
4	L1	69	PSU	O2-C2-N1	-2.94	119.76	122.79
6	L3	1536	PSU	O2-C2-N1	-2.93	119.76	122.79
6	L3	5010	PSU	O2-C2-N1	-2.92	119.77	122.79
6	L3	400	A2M	C4-C5-N7	-2.92	107.24	110.58
6	L3	1534	A2M	C4-C5-N7	-2.92	107.24	110.58
6	L3	1871	A2M	C4-C5-N7	-2.92	107.25	110.58
6	L3	3867	A2M	C4-C5-N7	-2.92	107.25	110.58
6	L3	3830	A2M	C4-C5-N7	-2.91	107.25	110.58
6	L3	1781	PSU	O2-C2-N1	-2.91	119.78	122.79
6	L3	2401	A2M	C4-C5-N7	-2.91	107.26	110.58
6	L3	3853	PSU	O2-C2-N1	-2.90	119.80	122.79
6	L3	3760	A2M	C4-C5-N7	-2.89	107.27	110.58
6	L3	3920	PSU	O2-C2-N1	-2.89	119.80	122.79
6	L3	2839	PSU	O2-C2-N1	-2.89	119.81	122.79
6	L3	3925	OMU	O4-C4-C5	-2.89	120.18	125.16
6	L3	4590	A2M	N9-C8-N7	-2.89	109.84	113.94
6	L3	1744	PSU	O2-C2-N1	-2.89	119.81	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L3	3734	PSU	O2-C2-N1	-2.88	119.82	122.79
6	L3	3768	PSU	O2-C2-N1	-2.88	119.82	122.79
6	L3	4299	PSU	O2-C2-N1	-2.87	119.83	122.79
6	L3	3715	PSU	O2-C2-N1	-2.87	119.83	122.79
6	L3	3724	A2M	C4-C5-N7	-2.87	107.30	110.58
6	L3	4471	PSU	O2-C2-N1	-2.87	119.83	122.79
6	L3	4521	PSU	O2-C2-N1	-2.87	119.83	122.79
6	L3	400	A2M	N9-C8-N7	-2.87	109.87	113.94
6	L3	4620	OMU	O4-C4-C5	-2.87	120.22	125.16
6	L3	3959	PSU	O2-C2-N1	-2.87	119.83	122.79
6	L3	1871	A2M	C2'-C1'-N9	-2.86	109.04	113.75
6	L3	400	A2M	C2'-C1'-N9	-2.86	109.05	113.75
6	L3	3758	PSU	O2-C2-N1	-2.84	119.86	122.79
6	L3	4361	PSU	O2-C2-N1	-2.84	119.86	122.79
6	L3	4552	PSU	O2-C2-N1	-2.84	119.86	122.79
6	L3	4457	PSU	O2-C2-N1	-2.84	119.86	122.79
4	L1	55	PSU	O2-C2-N1	-2.83	119.86	122.79
6	L3	1683	PSU	O2-C2-N1	-2.83	119.86	122.79
6	L3	3730	PSU	O2-C2-N1	-2.83	119.87	122.79
6	L3	4442	PSU	O2-C2-N1	-2.83	119.87	122.79
6	L3	4579	PSU	O2-C2-N1	-2.82	119.88	122.79
6	L3	4296	PSU	O2-C2-N1	-2.82	119.88	122.79
6	L3	2401	A2M	N9-C8-N7	-2.82	109.94	113.94
6	L3	4500	PSU	O2-C2-N1	-2.81	119.89	122.79
6	L3	2815	A2M	N9-C8-N7	-2.81	109.95	113.94
6	L3	3770	PSU	O2-C2-N1	-2.81	119.89	122.79
6	L3	1781	PSU	C6-N1-C2	-2.81	120.09	122.69
6	L3	1677	PSU	O2-C2-N1	-2.81	119.89	122.79
6	L3	4293	PSU	O2-C2-N1	-2.80	119.90	122.79
6	L3	4523	A2M	N9-C8-N7	-2.79	109.97	113.94
6	L3	4576	PSU	O2-C2-N1	-2.79	119.91	122.79
6	L3	4689	PSU	C6-N1-C2	-2.78	120.11	122.69
6	L3	3762	PSU	O2-C2-N1	-2.78	119.92	122.79
6	L3	3884	PSU	O2-C2-N1	-2.78	119.92	122.79
6	L3	1534	A2M	N9-C8-N7	-2.77	110.00	113.94
6	L3	4532	PSU	O2-C2-N1	-2.77	119.93	122.79
6	L3	4220	6MZ	N9-C8-N7	-2.77	110.00	113.94
6	L3	3764	PSU	O2-C2-N1	-2.77	119.94	122.79
6	L3	398	A2M	N9-C8-N7	-2.77	110.01	113.94
6	L3	4493	PSU	O2-C2-N1	-2.76	119.94	122.79
6	L3	1524	A2M	C4-C5-N7	-2.76	107.42	110.58
6	L3	4312	PSU	O2-C2-N1	-2.76	119.94	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L3	2787	A2M	N9-C8-N7	-2.76	110.03	113.94
6	L3	3822	PSU	O2-C2-N1	-2.76	119.95	122.79
6	L3	4353	PSU	O2-C2-N1	-2.75	119.95	122.79
6	L3	4403	PSU	O2-C2-N1	-2.75	119.95	122.79
6	L3	3760	A2M	N9-C8-N7	-2.75	110.04	113.94
6	L3	4636	PSU	O2-C2-N1	-2.74	119.96	122.79
6	L3	1860	PSU	O2-C2-N1	-2.74	119.97	122.79
6	L3	3825	A2M	N9-C8-N7	-2.73	110.06	113.94
6	L3	1779	PSU	O2-C2-N1	-2.72	119.98	122.79
6	L3	1782	PSU	O2-C2-N1	-2.72	119.99	122.79
6	L3	4972	PSU	O2-C2-N1	-2.72	119.99	122.79
6	L3	1871	A2M	N9-C8-N7	-2.72	110.08	113.94
6	L3	3844	PSU	O2-C2-N1	-2.71	120.00	122.79
6	L3	3830	A2M	N9-C8-N7	-2.71	110.09	113.94
6	L3	4431	PSU	O2-C2-N1	-2.71	120.00	122.79
6	L3	3851	PSU	O2-C2-N1	-2.70	120.00	122.79
6	L3	3785	A2M	N9-C8-N7	-2.69	110.12	113.94
6	L3	1744	PSU	C6-N1-C2	-2.67	120.21	122.69
6	L3	3768	PSU	C6-N1-C2	-2.64	120.24	122.69
6	L3	4299	PSU	C6-C5-C4	2.64	119.96	118.17
6	L3	1862	PSU	O2-C2-N1	-2.63	120.07	122.79
6	L3	2839	PSU	C6-N1-C2	-2.62	120.26	122.69
6	L3	3762	PSU	C6-N1-C2	-2.62	120.26	122.69
6	L3	3639	PSU	C6-C5-C4	2.61	119.94	118.17
6	L3	4457	PSU	C6-N1-C2	-2.61	120.27	122.69
4	L1	69	PSU	C6-N1-C2	-2.61	120.27	122.69
6	L3	3718	A2M	N9-C8-N7	-2.61	110.24	113.94
6	L3	3867	A2M	N9-C8-N7	-2.59	110.26	113.94
6	L3	4673	PSU	O2-C2-N1	-2.59	120.12	122.79
6	L3	4521	PSU	C6-N1-C2	-2.59	120.29	122.69
6	L3	2401	A2M	C2'-C1'-N9	-2.58	109.50	113.75
6	L3	4571	A2M	N9-C8-N7	-2.58	110.27	113.94
6	L3	4471	PSU	C6-C5-C4	2.58	119.92	118.17
6	L3	2508	PSU	O2-C2-N1	-2.57	120.13	122.79
6	L3	4628	PSU	O2-C2-N1	-2.57	120.13	122.79
6	L3	5010	PSU	C6-N1-C2	-2.57	120.31	122.69
6	L3	3853	PSU	C6-N1-C2	-2.57	120.31	122.69
6	L3	2363	A2M	N9-C8-N7	-2.56	110.30	113.94
6	L3	3637	PSU	C6-N1-C2	-2.56	120.31	122.69
6	L3	3639	PSU	C6-N1-C2	-2.56	120.31	122.69
6	L3	3734	PSU	C6-N1-C2	-2.56	120.32	122.69
6	L3	4579	PSU	C6-N1-C2	-2.56	120.32	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L3	5001	PSU	C6-N1-C2	-2.56	120.32	122.69
6	L3	4293	PSU	C6-N1-C2	-2.56	120.32	122.69
6	L3	1536	PSU	C6-N1-C2	-2.56	120.32	122.69
6	L3	398	A2M	C2'-C1'-N9	-2.55	109.55	113.75
4	L1	55	PSU	C6-C5-C4	2.55	119.89	118.17
6	L3	4361	PSU	C6-C5-C4	2.54	119.89	118.17
6	L3	4471	PSU	C6-N1-C2	-2.54	120.33	122.69
6	L3	3724	A2M	N9-C8-N7	-2.54	110.33	113.94
6	L3	4361	PSU	C6-N1-C2	-2.54	120.33	122.69
6	L3	3844	PSU	C6-C5-C4	2.53	119.88	118.17
6	L3	4532	PSU	C6-C5-C4	2.53	119.88	118.17
6	L3	3822	PSU	C6-N1-C2	-2.53	120.34	122.69
6	L3	3844	PSU	C6-N1-C2	-2.53	120.34	122.69
6	L3	1779	PSU	C6-N1-C2	-2.53	120.34	122.69
6	L3	3920	PSU	C6-N1-C2	-2.53	120.35	122.69
6	L3	4576	PSU	C6-N1-C2	-2.53	120.35	122.69
6	L3	1326	A2M	N9-C8-N7	-2.52	110.36	113.94
6	L3	4628	PSU	C6-N1-C2	-2.52	120.35	122.69
6	L3	1582	PSU	O2-C2-N1	-2.52	120.19	122.79
6	L3	4353	PSU	C6-C5-C4	2.52	119.87	118.17
6	L3	3770	PSU	C6-N1-C2	-2.51	120.36	122.69
6	L3	3715	PSU	C6-C5-C4	2.51	119.87	118.17
6	L3	3959	PSU	C6-N1-C2	-2.51	120.36	122.69
6	L3	1683	PSU	C6-N1-C2	-2.50	120.37	122.69
6	L3	3884	PSU	C6-N1-C2	-2.49	120.38	122.69
6	L3	4493	PSU	C6-C5-C4	2.49	119.86	118.17
6	L3	1677	PSU	C6-C5-C4	2.49	119.85	118.17
6	L3	4312	PSU	C6-N1-C2	-2.49	120.38	122.69
6	L3	2632	PSU	O2-C2-N1	-2.48	120.23	122.79
4	L1	69	PSU	C6-C5-C4	2.47	119.84	118.17
4	L1	55	PSU	C6-N1-C2	-2.47	120.40	122.69
6	L3	3695	PSU	C6-C5-C4	2.47	119.84	118.17
6	L3	3695	PSU	C6-N1-C2	-2.46	120.40	122.69
6	L3	4403	PSU	C6-N1-C2	-2.46	120.40	122.69
6	L3	3758	PSU	C6-N1-C2	-2.46	120.41	122.69
6	L3	3764	PSU	C6-N1-C2	-2.46	120.41	122.69
6	L3	4296	PSU	C6-C5-C4	2.46	119.83	118.17
6	L3	3715	PSU	C6-N1-C2	-2.45	120.41	122.69
6	L3	1582	PSU	C6-C5-C4	2.45	119.83	118.17
6	L3	3758	PSU	C6-C5-C4	2.44	119.82	118.17
6	L3	3730	PSU	C6-N1-C2	-2.44	120.42	122.69
6	L3	3851	PSU	C6-N1-C2	-2.44	120.42	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L3	1677	PSU	C6-N1-C2	-2.44	120.43	122.69
6	L3	4972	PSU	C6-N1-C2	-2.44	120.43	122.69
6	L3	1782	PSU	C6-C5-C4	2.43	119.81	118.17
6	L3	4552	PSU	C6-C5-C4	2.42	119.81	118.17
6	L3	4500	PSU	C6-C5-C4	2.42	119.81	118.17
6	L3	4500	PSU	C6-N1-C2	-2.42	120.44	122.69
6	L3	4431	PSU	C6-N1-C2	-2.42	120.45	122.69
6	L3	1782	PSU	C6-N1-C2	-2.42	120.45	122.69
6	L3	4353	PSU	C6-N1-C2	-2.41	120.45	122.69
6	L3	4442	PSU	C6-N1-C2	-2.41	120.45	122.69
6	L3	4552	PSU	C6-N1-C2	-2.41	120.45	122.69
6	L3	4299	PSU	C6-N1-C2	-2.40	120.46	122.69
6	L3	3959	PSU	C6-C5-C4	2.40	119.80	118.17
6	L3	4493	PSU	C6-N1-C2	-2.40	120.46	122.69
6	L3	4296	PSU	C6-N1-C2	-2.40	120.47	122.69
6	L3	4636	PSU	C6-C5-C4	2.39	119.79	118.17
6	L3	3637	PSU	O2-C2-N1	-2.39	120.32	122.79
6	L3	2632	PSU	C6-N1-C2	-2.38	120.48	122.69
6	L3	1683	PSU	C6-C5-C4	2.38	119.78	118.17
6	L3	1860	PSU	C6-N1-C2	-2.38	120.49	122.69
6	L3	3762	PSU	C6-C5-C4	2.38	119.78	118.17
6	L3	4532	PSU	C6-N1-C2	-2.37	120.49	122.69
4	L1	69	PSU	O4'-C1'-C2'	2.37	108.42	105.15
6	L3	1524	A2M	N9-C8-N7	-2.36	110.58	113.94
6	L3	4431	PSU	C6-C5-C4	2.35	119.76	118.17
6	L3	3920	PSU	C6-C5-C4	2.35	119.76	118.17
6	L3	1860	PSU	C6-C5-C4	2.34	119.76	118.17
6	L3	3730	PSU	C6-C5-C4	2.34	119.75	118.17
6	L3	2508	PSU	C6-N1-C2	-2.34	120.52	122.69
6	L3	4972	PSU	C6-C5-C4	2.34	119.75	118.17
6	L3	4673	PSU	C6-N1-C2	-2.34	120.52	122.69
6	L3	4403	PSU	C6-C5-C4	2.30	119.72	118.17
6	L3	1536	PSU	C6-C5-C4	2.29	119.72	118.17
6	L3	4521	PSU	C6-C5-C4	2.29	119.72	118.17
6	L3	1862	PSU	C6-N1-C2	-2.28	120.57	122.69
6	L3	2351	OMC	C1'-N1-C2	2.28	123.47	118.44
6	L3	4636	PSU	C6-N1-C2	-2.28	120.58	122.69
6	L3	1781	PSU	C6-C5-C4	2.28	119.71	118.17
6	L3	4312	PSU	C6-C5-C4	2.28	119.71	118.17
6	L3	3764	PSU	C6-C5-C4	2.27	119.70	118.17
6	L3	5010	PSU	C6-C5-C4	2.25	119.69	118.17
6	L3	1779	PSU	C6-C5-C4	2.25	119.69	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L3	4306	OMU	O2-C2-N1	-2.24	119.88	122.80
6	L3	1322	1MA	N1-C6-N6	2.24	125.33	119.71
6	L3	4293	PSU	C6-C5-C4	2.23	119.68	118.17
6	L3	2508	PSU	C6-C5-C4	2.22	119.67	118.17
6	L3	3851	PSU	C6-C5-C4	2.22	119.67	118.17
6	L3	4576	PSU	C6-C5-C4	2.22	119.67	118.17
6	L3	3734	PSU	O4'-C1'-C2'	2.21	108.21	105.15
6	L3	1862	PSU	C6-C5-C4	2.21	119.66	118.17
6	L3	3760	A2M	C2'-C1'-N9	-2.20	110.14	113.75
6	L3	3768	PSU	C6-C5-C4	2.19	119.65	118.17
6	L3	3925	OMU	O2-C2-N1	-2.19	119.94	122.80
6	L3	3734	PSU	C6-C5-C4	2.19	119.65	118.17
6	L3	1582	PSU	C6-N1-C2	-2.19	120.66	122.69
6	L3	2839	PSU	C6-C5-C4	2.18	119.65	118.17
6	L3	2861	OMC	C1'-N1-C2	2.18	123.25	118.44
6	L3	4523	A2M	C2'-C1'-N9	-2.17	110.17	113.75
6	L3	3715	PSU	O4'-C1'-C2'	2.17	108.15	105.15
6	L3	4673	PSU	C6-C5-C4	2.16	119.63	118.17
6	L3	4442	PSU	C6-C5-C4	2.15	119.62	118.17
6	L3	3851	PSU	O4'-C1'-C2'	2.14	108.11	105.15
6	L3	3818	OMU	O2-C2-N1	-2.13	120.02	122.80
6	L3	4576	PSU	O4'-C1'-C2'	2.13	108.10	105.15
6	L3	2415	OMU	O2-C2-N1	-2.13	120.02	122.80
6	L3	1773	OMU	O2-C2-N1	-2.13	120.03	122.80
6	L3	4299	PSU	O4'-C1'-C2'	2.13	108.09	105.15
25	LN	245	HIC	CB-CG-CD2	-2.12	124.85	129.96
6	L3	4227	OMU	O2-C2-N1	-2.12	120.04	122.80
6	L3	4457	PSU	C6-C5-C4	2.11	119.60	118.17
6	L3	4620	OMU	O2-C2-N1	-2.11	120.05	122.80
6	L3	3884	PSU	C6-C5-C4	2.11	119.60	118.17
6	L3	4457	PSU	O4'-C1'-C2'	2.10	108.06	105.15
6	L3	5001	PSU	C6-C5-C4	2.10	119.59	118.17
6	L3	3695	PSU	O4'-C1'-C2'	2.08	108.03	105.15
6	L3	4498	OMU	O2-C2-N1	-2.08	120.08	122.80
6	L3	3853	PSU	O4'-C1'-C2'	2.08	108.03	105.15
6	L3	4689	PSU	C6-C5-C4	2.08	119.58	118.17
6	L3	3920	PSU	O4'-C1'-C2'	2.07	108.01	105.15
6	L3	2815	A2M	C2'-C1'-N9	-2.06	110.36	113.75
6	L3	1524	A2M	O4'-C1'-N9	2.06	112.04	108.09
6	L3	4628	PSU	O4'-C1'-C2'	2.05	107.99	105.15
6	L3	2837	OMU	O2-C2-N1	-2.04	120.14	122.80
6	L3	3762	PSU	O4'-C1'-C2'	2.04	107.97	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L3	4636	PSU	O4'-C1'-C2'	2.04	107.97	105.15
6	L3	3959	PSU	O4'-C1'-C2'	2.03	107.96	105.15
6	L3	1744	PSU	O4'-C1'-C2'	2.02	107.94	105.15
6	L3	3770	PSU	C6-C5-C4	2.02	119.54	118.17
6	L3	4220	6MZ	C6-C5-N7	2.02	134.63	132.43
6	L3	4403	PSU	O4'-C1'-C2'	2.01	107.93	105.15

There are no chirality outliers.

All (119) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L1	75	OMG	C1'-C2'-O2'-CM2
6	L3	398	A2M	C1'-C2'-O2'-CM'
6	L3	400	A2M	C1'-C2'-O2'-CM'
6	L3	1316	OMG	C1'-C2'-O2'-CM2
6	L3	1322	1MA	O4'-C4'-C5'-O5'
6	L3	1326	A2M	C1'-C2'-O2'-CM'
6	L3	1340	OMC	C1'-C2'-O2'-CM2
6	L3	1625	OMG	C3'-C2'-O2'-CM2
6	L3	1760	OMG	C1'-C2'-O2'-CM2
6	L3	1773	OMU	C1'-C2'-O2'-CM2
6	L3	2363	A2M	C1'-C2'-O2'-CM'
6	L3	2364	OMG	C1'-C2'-O2'-CM2
6	L3	2422	OMC	C1'-C2'-O2'-CM2
6	L3	2424	OMG	O4'-C4'-C5'-O5'
6	L3	2424	OMG	C1'-C2'-O2'-CM2
6	L3	2837	OMU	C1'-C2'-O2'-CM2
6	L3	2861	OMC	C1'-C2'-O2'-CM2
6	L3	3627	OMG	C1'-C2'-O2'-CM2
6	L3	3701	OMC	C2'-C1'-N1-C6
6	L3	3718	A2M	C1'-C2'-O2'-CM'
6	L3	3724	A2M	C1'-C2'-O2'-CM'
6	L3	3744	OMG	C1'-C2'-O2'-CM2
6	L3	3782	5MC	O4'-C4'-C5'-O5'
6	L3	3785	A2M	C1'-C2'-O2'-CM'
6	L3	3808	OMC	C1'-C2'-O2'-CM2
6	L3	3818	OMU	O4'-C4'-C5'-O5'
6	L3	3825	A2M	C1'-C2'-O2'-CM'
6	L3	3841	OMC	C1'-C2'-O2'-CM2
6	L3	3867	A2M	O4'-C4'-C5'-O5'
6	L3	3867	A2M	C3'-C4'-C5'-O5'
6	L3	3867	A2M	C1'-C2'-O2'-CM'

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Mol	Chain	Res	Type	Atoms
6	L3	3887	OMC	O4'-C4'-C5'-O5'
6	L3	3899	OMG	C1'-C2'-O2'-CM2
6	L3	3925	OMU	C1'-C2'-O2'-CM2
6	L3	4042	OMG	C1'-C2'-O2'-CM2
6	L3	4054	OMC	C1'-C2'-O2'-CM2
6	L3	4220	6MZ	C4'-C5'-O5'-P
6	L3	4227	OMU	C1'-C2'-O2'-CM2
6	L3	4228	OMG	C1'-C2'-O2'-CM2
6	L3	4306	OMU	C1'-C2'-O2'-CM2
6	L3	4370	OMG	C1'-C2'-O2'-CM2
6	L3	4392	OMG	C1'-C2'-O2'-CM2
6	L3	4456	OMC	C1'-C2'-O2'-CM2
6	L3	4571	A2M	C1'-C2'-O2'-CM'
6	L3	4590	A2M	C4'-C5'-O5'-P
6	L3	4590	A2M	C1'-C2'-O2'-CM'
6	L3	4618	OMG	C1'-C2'-O2'-CM2
6	L3	4620	OMU	C1'-C2'-O2'-CM2
6	L3	4637	OMG	O4'-C4'-C5'-O5'
6	L3	4637	OMG	C1'-C2'-O2'-CM2
6	L3	1744	PSU	O4'-C4'-C5'-O5'
6	L3	2424	OMG	C3'-C4'-C5'-O5'
6	L3	2787	A2M	C3'-C4'-C5'-O5'
6	L3	3782	5MC	C3'-C4'-C5'-O5'
6	L3	3887	OMC	C3'-C4'-C5'-O5'
6	L3	4220	6MZ	C3'-C4'-C5'-O5'
6	L3	4227	OMU	C3'-C4'-C5'-O5'
6	L3	1744	PSU	C3'-C4'-C5'-O5'
6	L3	1781	PSU	O4'-C4'-C5'-O5'
6	L3	2401	A2M	O4'-C4'-C5'-O5'
6	L3	2401	A2M	C3'-C4'-C5'-O5'
6	L3	2415	OMU	O4'-C4'-C5'-O5'
6	L3	3760	A2M	O4'-C4'-C5'-O5'
6	L3	4227	OMU	O4'-C4'-C5'-O5'
6	L3	4523	A2M	O4'-C4'-C5'-O5'
6	L3	4523	A2M	C3'-C4'-C5'-O5'
25	LN	245	HIC	CA-CB-CG-ND1
6	L3	4498	OMU	C2'-C1'-N1-C6
6	L3	3701	OMC	C2'-C1'-N1-C2
6	L3	1322	1MA	C3'-C4'-C5'-O5'
6	L3	1781	PSU	C3'-C4'-C5'-O5'
6	L3	3818	OMU	C3'-C4'-C5'-O5'
6	L3	4637	OMG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
6	L3	1677	PSU	O4'-C4'-C5'-O5'
6	L3	3785	A2M	C3'-C4'-C5'-O5'
6	L3	2787	A2M	C2'-C1'-N9-C8
6	L3	4498	OMU	C2'-C1'-N1-C2
25	LN	245	HIC	CA-CB-CG-CD2
6	L3	2787	A2M	O4'-C4'-C5'-O5'
6	L3	4220	6MZ	O4'-C4'-C5'-O5'
6	L3	4498	OMU	O4'-C4'-C5'-O5'
6	L3	1677	PSU	C4'-C5'-O5'-P
6	L3	4500	PSU	O4'-C4'-C5'-O5'
6	L3	2415	OMU	C4'-C5'-O5'-P
6	L3	2415	OMU	C3'-C4'-C5'-O5'
6	L3	3760	A2M	C3'-C4'-C5'-O5'
6	L3	2787	A2M	C2'-C1'-N9-C4
6	L3	2364	OMG	O4'-C4'-C5'-O5'
6	L3	1534	A2M	C3'-C2'-O2'-CM'
6	L3	4220	6MZ	N1-C6-N6-C9
6	L3	4228	OMG	O4'-C4'-C5'-O5'
6	L3	4498	OMU	O4'-C1'-N1-C2
6	L3	4498	OMU	O4'-C1'-N1-C6
6	L3	3701	OMC	O4'-C1'-N1-C6
6	L3	2351	OMC	C3'-C2'-O2'-CM2
6	L3	4500	PSU	O4'-C1'-C5-C4
6	L3	4636	PSU	O4'-C1'-C5-C4
6	L3	3701	OMC	O4'-C1'-N1-C2
6	L3	1534	A2M	C4'-C5'-O5'-P
6	L3	4623	OMG	C3'-C2'-O2'-CM2
6	L3	4498	OMU	C4'-C5'-O5'-P
6	L3	2876	OMG	C3'-C4'-C5'-O5'
6	L3	3844	PSU	C4'-C5'-O5'-P
6	L3	3867	A2M	C4'-C5'-O5'-P
6	L3	2351	OMC	C2'-C1'-N1-C6
6	L3	2422	OMC	O4'-C4'-C5'-O5'
6	L3	4618	OMG	O4'-C4'-C5'-O5'
6	L3	4500	PSU	O4'-C1'-C5-C6
6	L3	1773	OMU	C3'-C2'-O2'-CM2
6	L3	3760	A2M	C3'-C2'-O2'-CM'
6	L3	4227	OMU	C3'-C2'-O2'-CM2
6	L3	2351	OMC	C2'-C1'-N1-C2
6	L3	1524	A2M	O4'-C1'-N9-C8
6	L3	2787	A2M	O4'-C1'-N9-C8
6	L3	3785	A2M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
6	L3	4636	PSU	O4'-C4'-C5'-O5'
6	L3	1524	A2M	O4'-C1'-N9-C4
6	L3	4220	6MZ	C5-C6-N6-C9
6	L3	4636	PSU	C4'-C5'-O5'-P

There are no ring outliers.

84 monomers are involved in 139 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L3	2815	A2M	1	0
6	L3	3851	PSU	1	0
6	L3	2422	OMC	2	0
6	L3	3818	OMU	1	0
6	L3	2787	A2M	1	0
6	L3	4293	PSU	1	0
6	L3	1677	PSU	1	0
6	L3	1340	OMC	1	0
6	L3	1760	OMG	1	0
6	L3	4494	OMG	1	0
6	L3	3792	OMG	1	0
6	L3	3782	5MC	1	0
6	L3	2364	OMG	2	0
6	L3	3830	A2M	1	0
6	L3	4576	PSU	1	0
6	L3	3695	PSU	2	0
6	L3	1744	PSU	2	0
6	L3	1625	OMG	1	0
6	L3	4623	OMG	1	0
6	L3	3637	PSU	1	0
6	L3	2804	OMC	1	0
6	L3	3899	OMG	1	0
6	L3	3734	PSU	1	0
6	L3	2351	OMC	2	0
6	L3	3724	A2M	1	0
6	L3	4530	UR3	2	0
6	L3	4457	PSU	2	0
6	L3	4500	PSU	2	0
6	L3	3808	OMC	3	0
6	L3	4456	OMC	1	0
6	L3	2363	A2M	2	0
4	L1	75	OMG	2	0
6	L3	4628	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L3	5001	PSU	1	0
6	L3	2876	OMG	1	0
6	L3	4442	PSU	1	0
6	L3	3825	A2M	1	0
6	L3	4370	OMG	2	0
6	L3	3715	PSU	1	0
6	L3	4637	OMG	2	0
6	L3	3822	PSU	2	0
6	L3	3841	OMC	1	0
6	L3	1781	PSU	1	0
6	L3	4220	6MZ	3	0
6	L3	3867	A2M	3	0
6	L3	1683	PSU	2	0
6	L3	4299	PSU	2	0
6	L3	3718	A2M	1	0
6	L3	1773	OMU	2	0
6	L3	3627	OMG	1	0
6	L3	4227	OMU	5	0
6	L3	4493	PSU	1	0
6	L3	4620	OMU	2	0
6	L3	4228	OMG	2	0
6	L3	4042	OMG	3	0
6	L3	1326	A2M	3	0
6	L3	1316	OMG	1	0
6	L3	3925	OMU	2	0
6	L3	4536	OMC	2	0
6	L3	4296	PSU	1	0
6	L3	3768	PSU	2	0
6	L3	1524	A2M	1	0
6	L3	3760	A2M	1	0
6	L3	2837	OMU	2	0
6	L3	2861	OMC	1	0
6	L3	2632	PSU	2	0
6	L3	4054	OMC	1	0
6	L3	1522	OMG	2	0
6	L3	4392	OMG	1	0
6	L3	4590	A2M	2	0
6	L3	3770	PSU	2	0
6	L3	4618	OMG	2	0
6	L3	2424	OMG	2	0
6	L3	4571	A2M	3	0
6	L3	5010	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L3	3758	PSU	1	0
6	L3	3744	OMG	1	0
6	L3	2415	OMU	3	0
6	L3	4306	OMU	4	0
4	L1	69	PSU	2	0
6	L3	1322	1MA	2	0
6	L3	3785	A2M	5	0
6	L3	4689	PSU	2	0
6	L3	3920	PSU	3	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	$\# Z > 2$
68	GDP	SR	1001	64,67	29,30,30	3.05	12 (41%)	45,47,47	2.66	17 (37%)
66	GTP	NC	1000	67,64	33,34,34	3.25	15 (45%)	50,54,54	1.77	14 (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
68	GDP	SR	1001	64,67	-	0/16/32/32	0/3/3/3
66	GTP	NC	1000	67,64	-	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)
68	SR	1001	GDP	O6-C6	8.86	1.40	1.23
66	NC	1000	GTP	O6-C6	8.83	1.40	1.23
66	NC	1000	GTP	C5-N7	6.62	1.52	1.39
68	SR	1001	GDP	C5-N7	6.55	1.52	1.39
68	SR	1001	GDP	PA-O3A	5.24	1.65	1.59
66	NC	1000	GTP	PB-O3B	5.12	1.65	1.59
66	NC	1000	GTP	PA-O3A	5.09	1.65	1.59
66	NC	1000	GTP	PB-O3A	5.01	1.64	1.59
66	NC	1000	GTP	C2-N2	4.85	1.45	1.34
68	SR	1001	GDP	C2-N2	4.82	1.45	1.34
66	NC	1000	GTP	C2-N1	4.69	1.49	1.37
66	NC	1000	GTP	C2-N3	4.38	1.43	1.33
66	NC	1000	GTP	C8-N9	-4.08	1.28	1.37
68	SR	1001	GDP	C8-N9	-3.97	1.28	1.37
68	SR	1001	GDP	C4-N9	-3.84	1.28	1.38
68	SR	1001	GDP	C5-C4	3.81	1.49	1.38
66	NC	1000	GTP	C4-N9	-3.58	1.28	1.38
68	SR	1001	GDP	C4-N3	2.79	1.40	1.34
66	NC	1000	GTP	O4'-C1'	2.61	1.48	1.42
66	NC	1000	GTP	C4-N3	2.40	1.39	1.34
66	NC	1000	GTP	C2'-C3'	-2.36	1.47	1.53
68	SR	1001	GDP	PB-O2B	-2.31	1.46	1.54
68	SR	1001	GDP	PB-O3B	-2.27	1.46	1.54
68	SR	1001	GDP	O4'-C1'	2.27	1.47	1.42
66	NC	1000	GTP	PG-O3G	-2.26	1.46	1.54
66	NC	1000	GTP	PG-O2G	-2.23	1.46	1.54
68	SR	1001	GDP	C2'-C3'	-2.13	1.47	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	SR	1001	GDP	C8-N9-C4	7.81	120.67	106.03
66	NC	1000	GTP	C8-N9-C4	6.82	118.81	106.03
68	SR	1001	GDP	C5-C4-N3	-6.68	117.76	128.39
68	SR	1001	GDP	N9-C4-N3	6.63	139.20	125.95
68	SR	1001	GDP	C2-N3-C4	5.35	121.52	112.30
68	SR	1001	GDP	C6-C5-N7	4.85	139.12	130.29
68	SR	1001	GDP	C4-C5-N7	-4.67	103.27	110.67
66	NC	1000	GTP	C2-N1-C6	-3.34	119.06	125.11
68	SR	1001	GDP	N9-C8-N7	-3.09	107.67	113.40
68	SR	1001	GDP	C2-N1-C6	-2.97	119.73	125.11
66	NC	1000	GTP	O2G-PG-O3B	2.87	114.27	104.64
68	SR	1001	GDP	O2B-PB-O3A	2.84	114.17	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	NC	1000	GTP	O3G-PG-O3B	2.83	114.13	104.64
68	SR	1001	GDP	O3B-PB-O3A	2.81	114.06	104.64
68	SR	1001	GDP	C1'-N9-C4	-2.62	118.75	126.49
68	SR	1001	GDP	C5-C6-N1	2.57	119.78	113.25
66	NC	1000	GTP	N9-C4-N3	2.52	131.00	125.95
66	NC	1000	GTP	C5-C6-N1	2.47	119.55	113.25
66	NC	1000	GTP	O6-C6-C5	-2.47	120.02	126.53
68	SR	1001	GDP	O6-C6-C5	-2.41	120.16	126.53
66	NC	1000	GTP	O2B-PB-O1B	-2.40	101.30	112.44
66	NC	1000	GTP	O2A-PA-O1A	-2.35	101.49	112.44
68	SR	1001	GDP	C3'-C2'-C1'	2.32	105.86	101.46
68	SR	1001	GDP	O2A-PA-O1A	-2.29	101.80	112.44
68	SR	1001	GDP	C2'-C3'-C4'	2.19	106.84	102.61
68	SR	1001	GDP	C1'-N9-C8	-2.17	120.56	126.73
66	NC	1000	GTP	C3'-C2'-C1'	2.14	105.51	101.46
66	NC	1000	GTP	C1'-N9-C8	-2.12	120.72	126.73
66	NC	1000	GTP	C1'-N9-C4	-2.04	120.45	126.49
66	NC	1000	GTP	C5-C4-N9	-2.03	102.02	105.66
66	NC	1000	GTP	C8-N7-C5	-2.02	100.66	104.26

There are no chirality outliers.

All (3) torsion outliers are listed below:

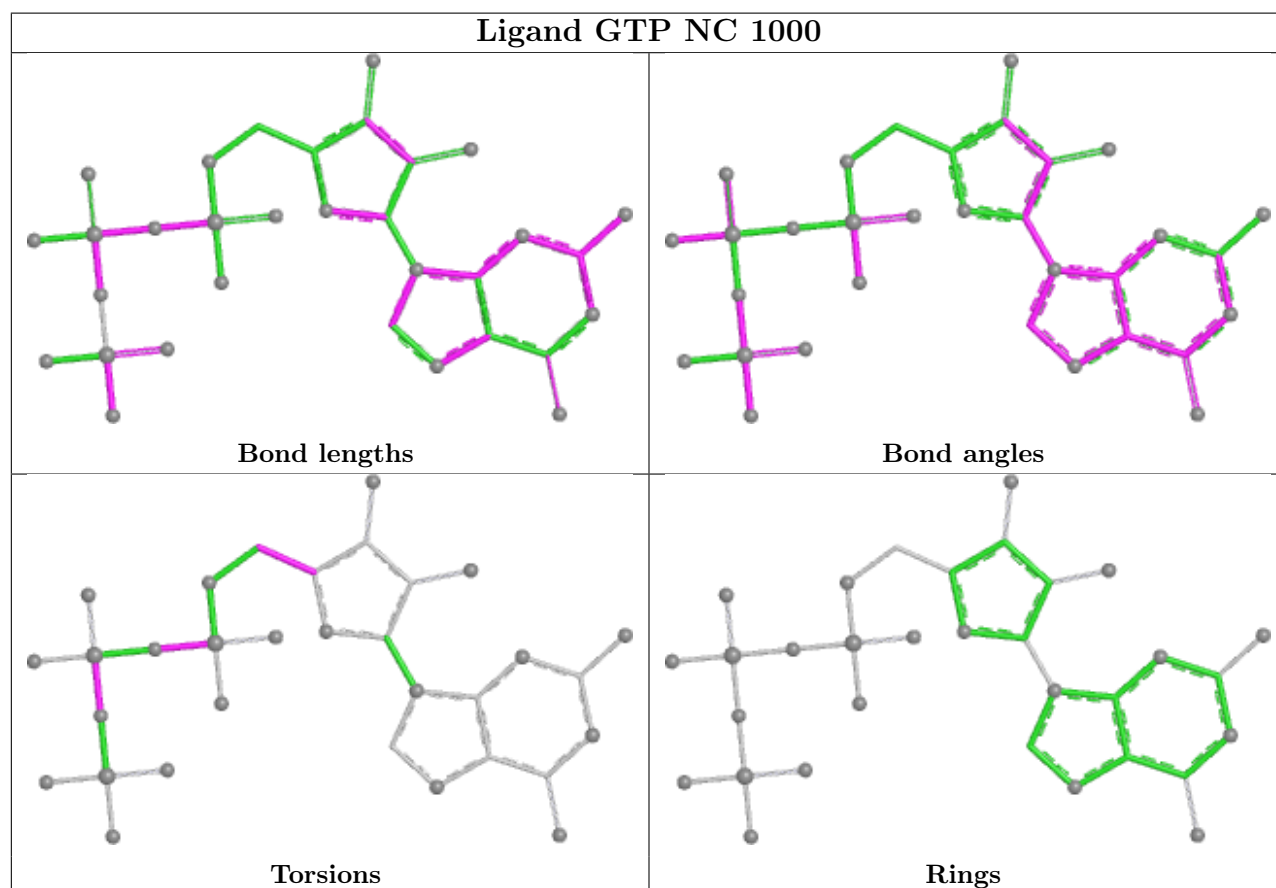
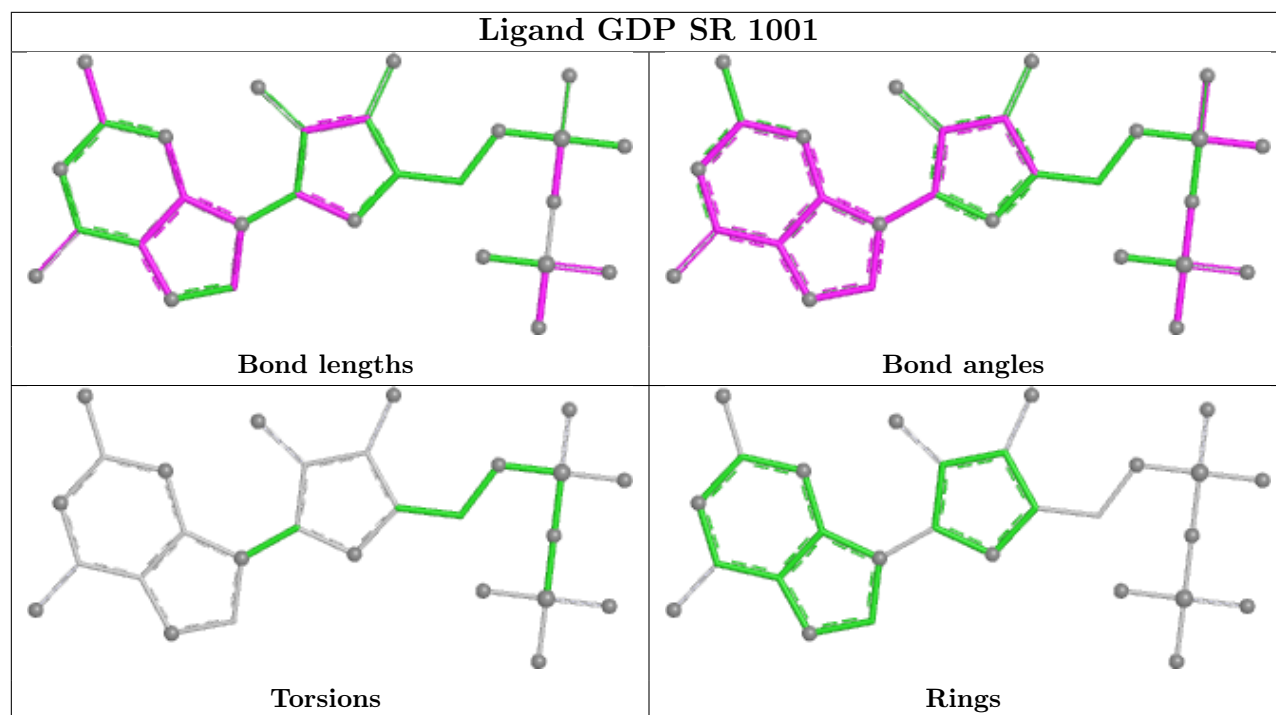
Mol	Chain	Res	Type	Atoms
66	NC	1000	GTP	PB-O3A-PA-O1A
66	NC	1000	GTP	PG-O3B-PB-O2B
66	NC	1000	GTP	O4'-C4'-C5'-O5'

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

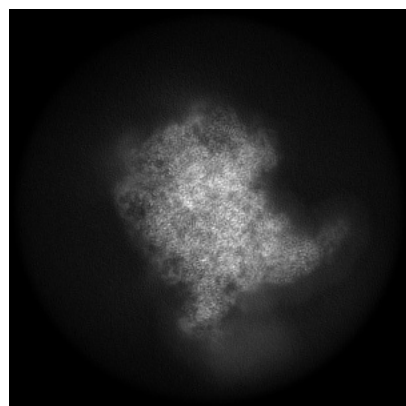
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29265. These allow visual inspection of the internal detail of the map and identification of artifacts.

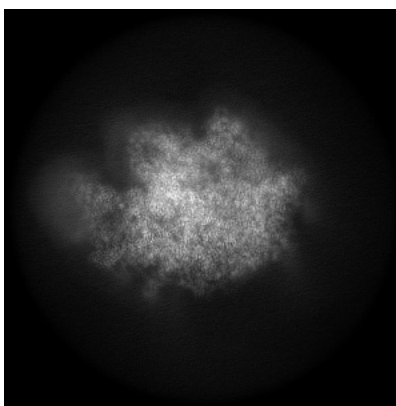
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

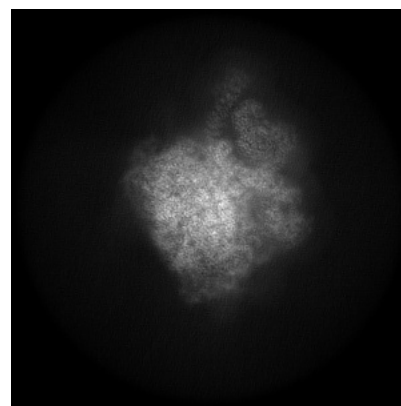
6.1.1 Primary map



X

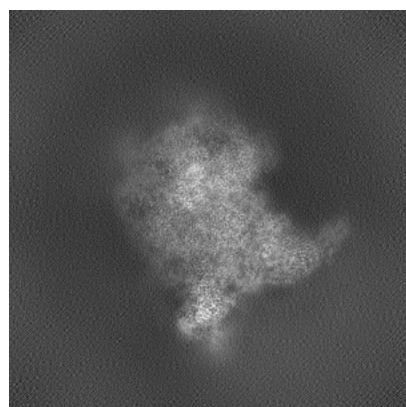


Y

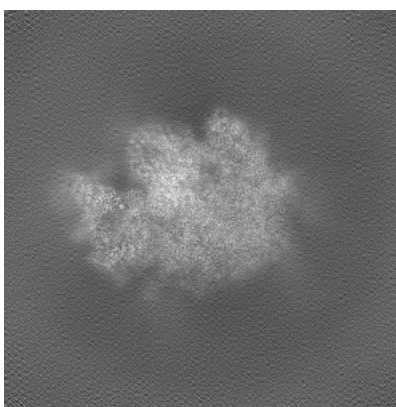


Z

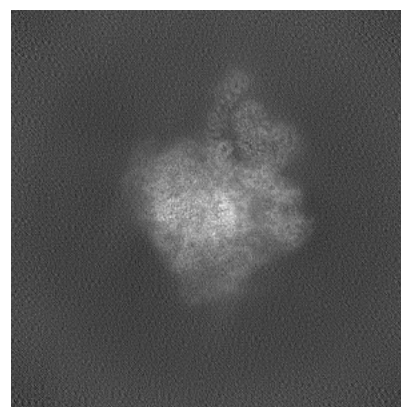
6.1.2 Raw map



X



Y

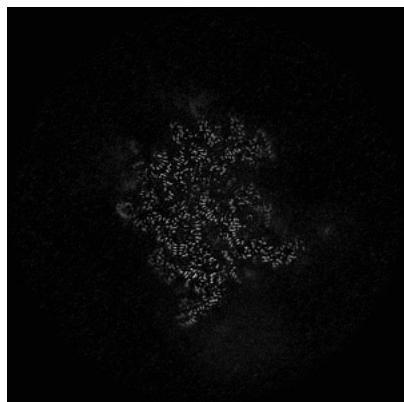


Z

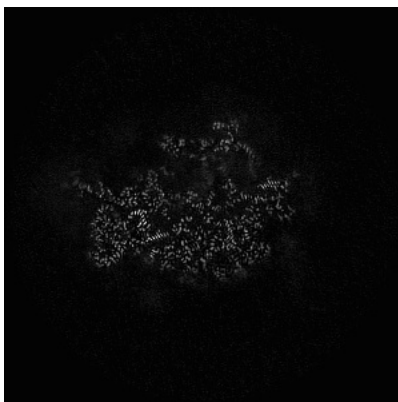
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

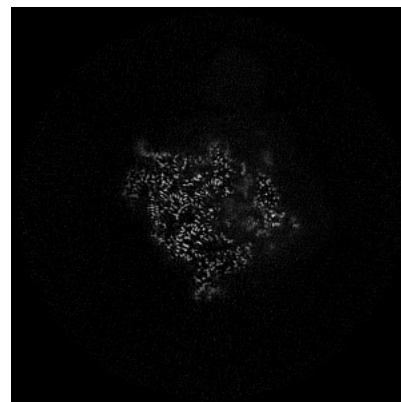
6.2.1 Primary map



X Index: 240

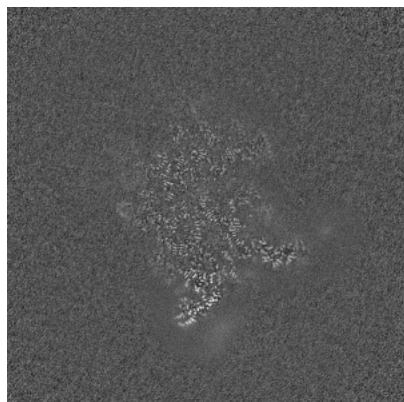


Y Index: 240

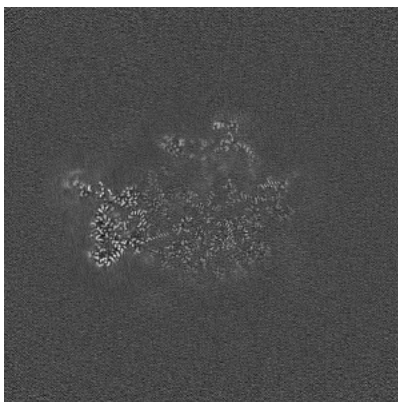


Z Index: 240

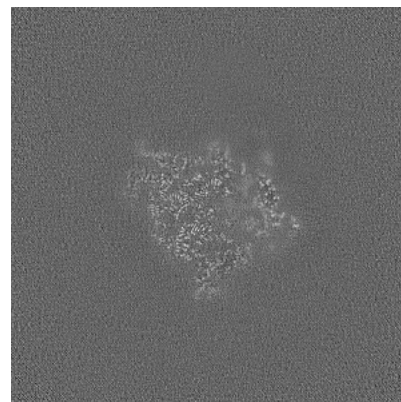
6.2.2 Raw map



X Index: 240



Y Index: 240

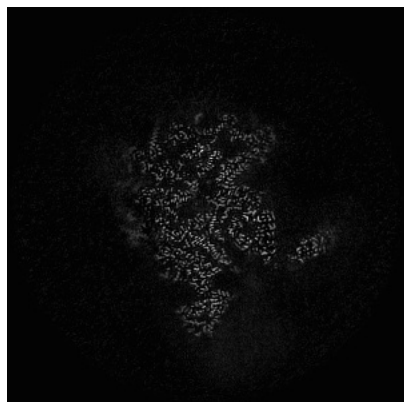


Z Index: 240

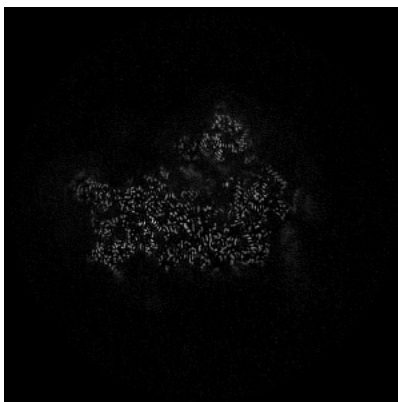
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

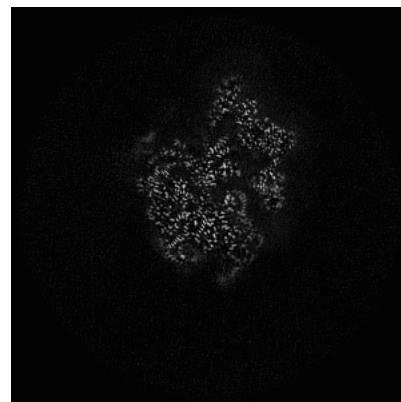
6.3.1 Primary map



X Index: 254

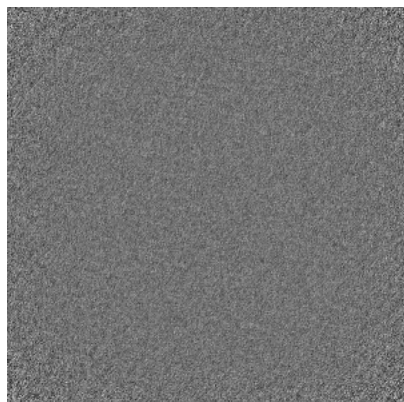


Y Index: 231

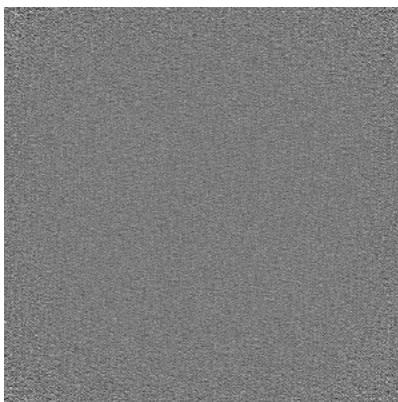


Z Index: 196

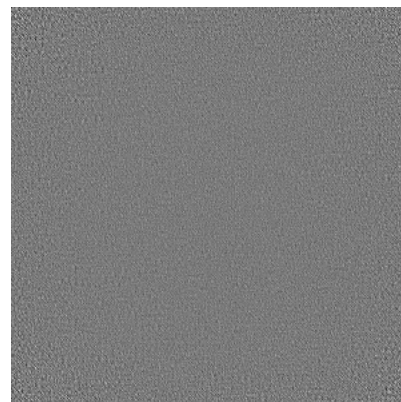
6.3.2 Raw map



X Index: 0



Y Index: 0

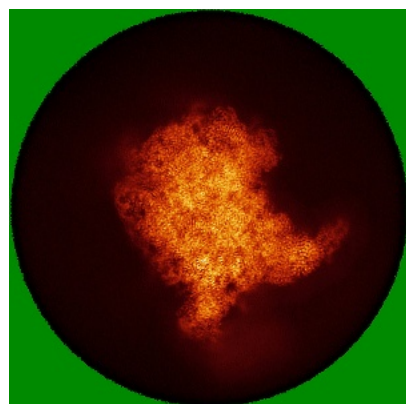


Z Index: 0

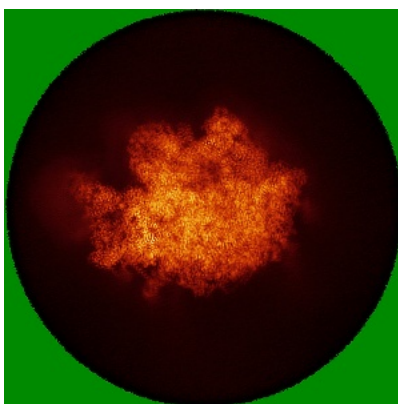
The images above show the largest variance slices of the map in three orthogonal directions.

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

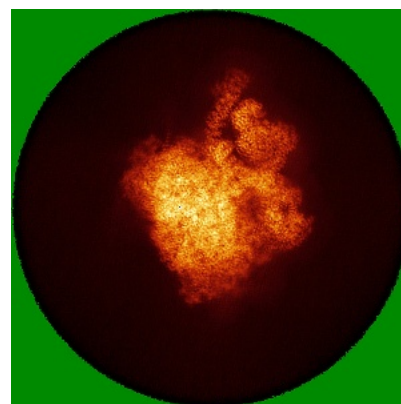
6.4.1 Primary map



X

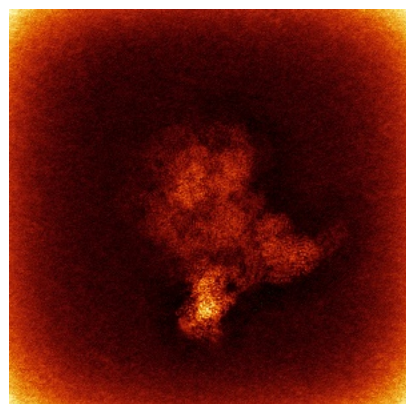


Y

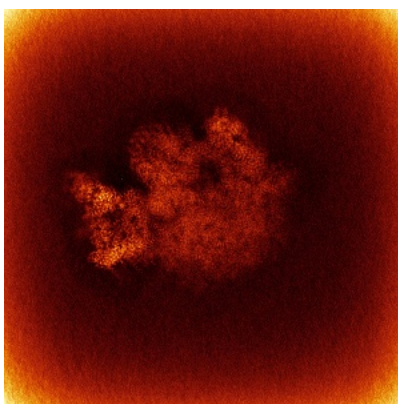


Z

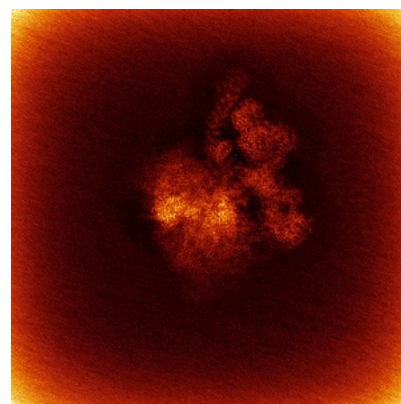
6.4.2 Raw map



X



Y



Z

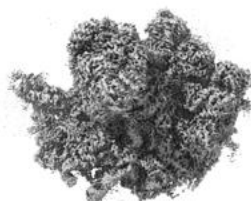
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



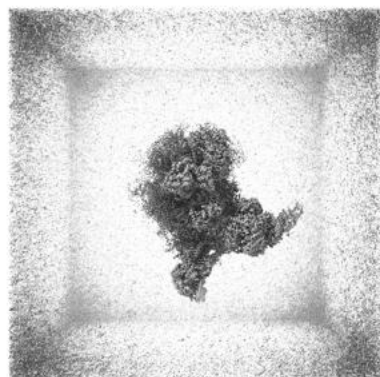
Y



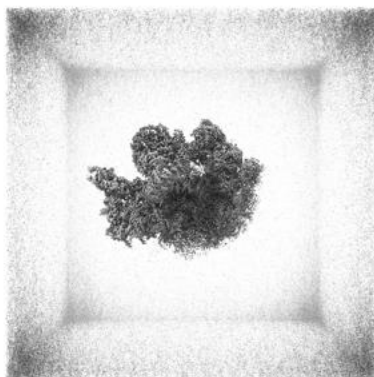
Z

The images above show the 3D surface view of the map at the recommended contour level 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

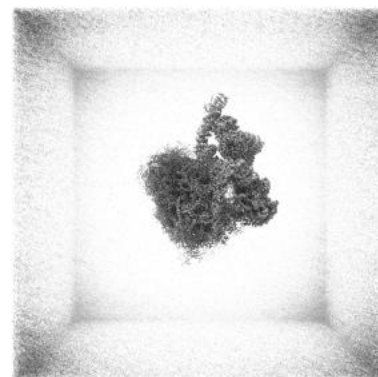
6.5.2 Raw map



X



Y



Z

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

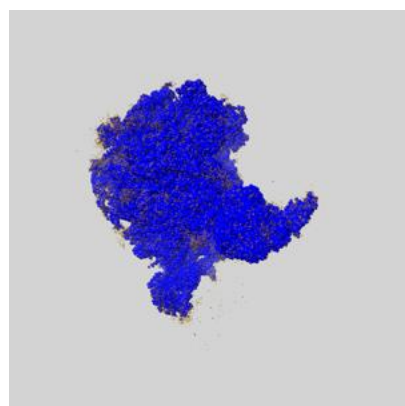
6.6 Mask visualisation [i](#)

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

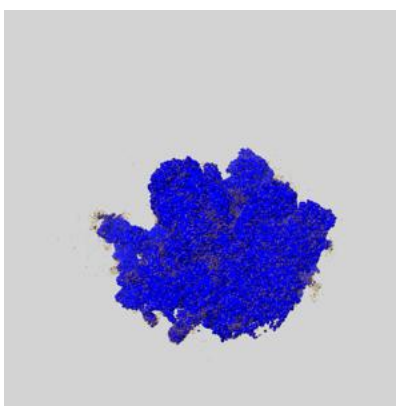
A mask typically either:

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

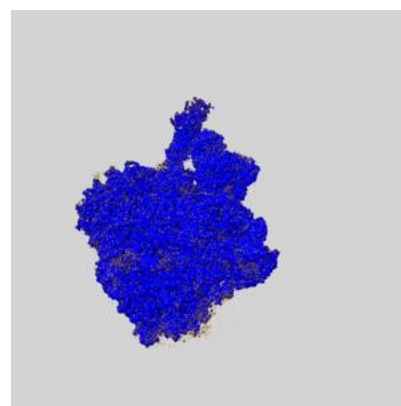
6.6.1 emd_29265_msk_1.map [i](#)



X



Y

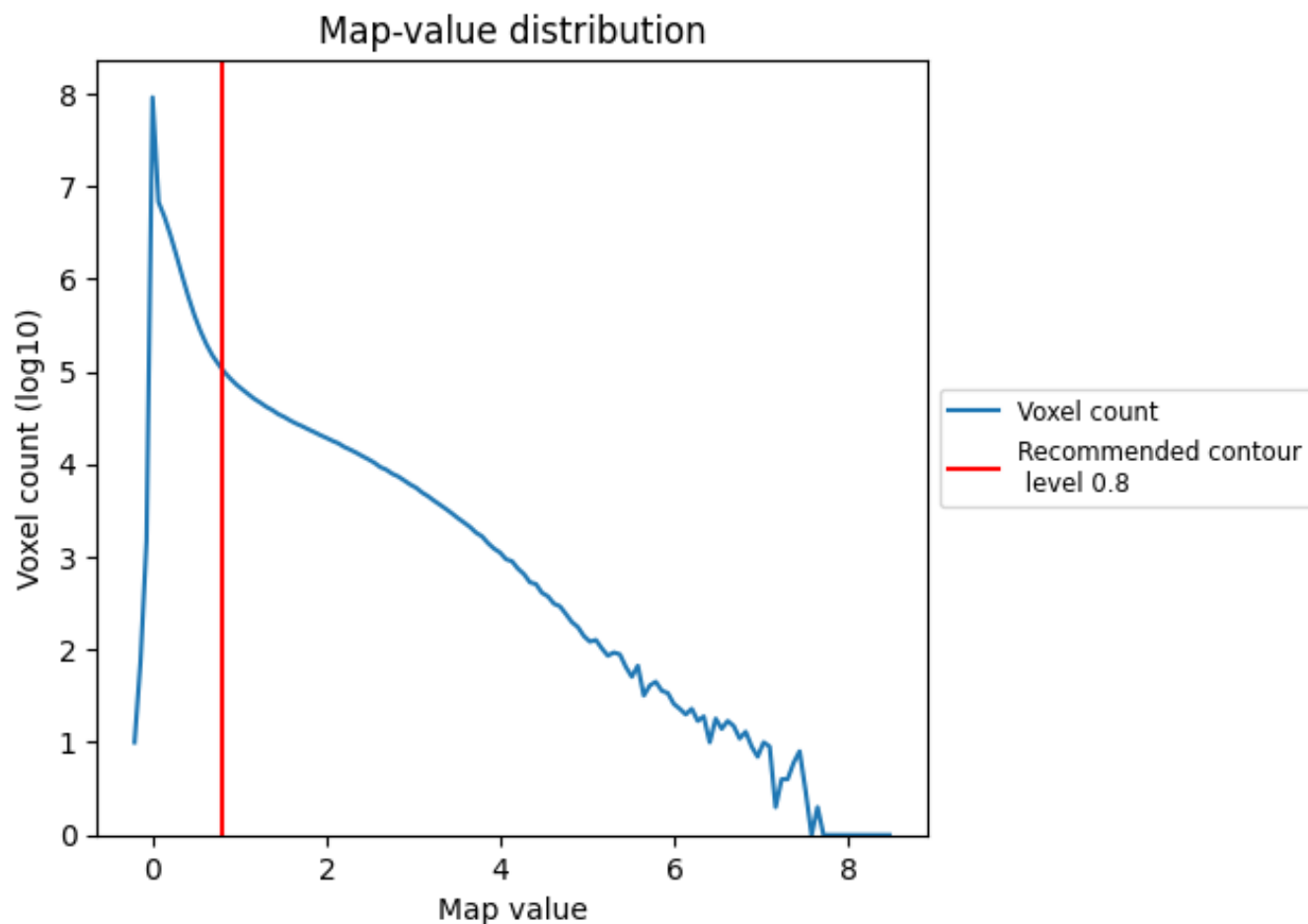


Z

7 Map analysis [i](#)

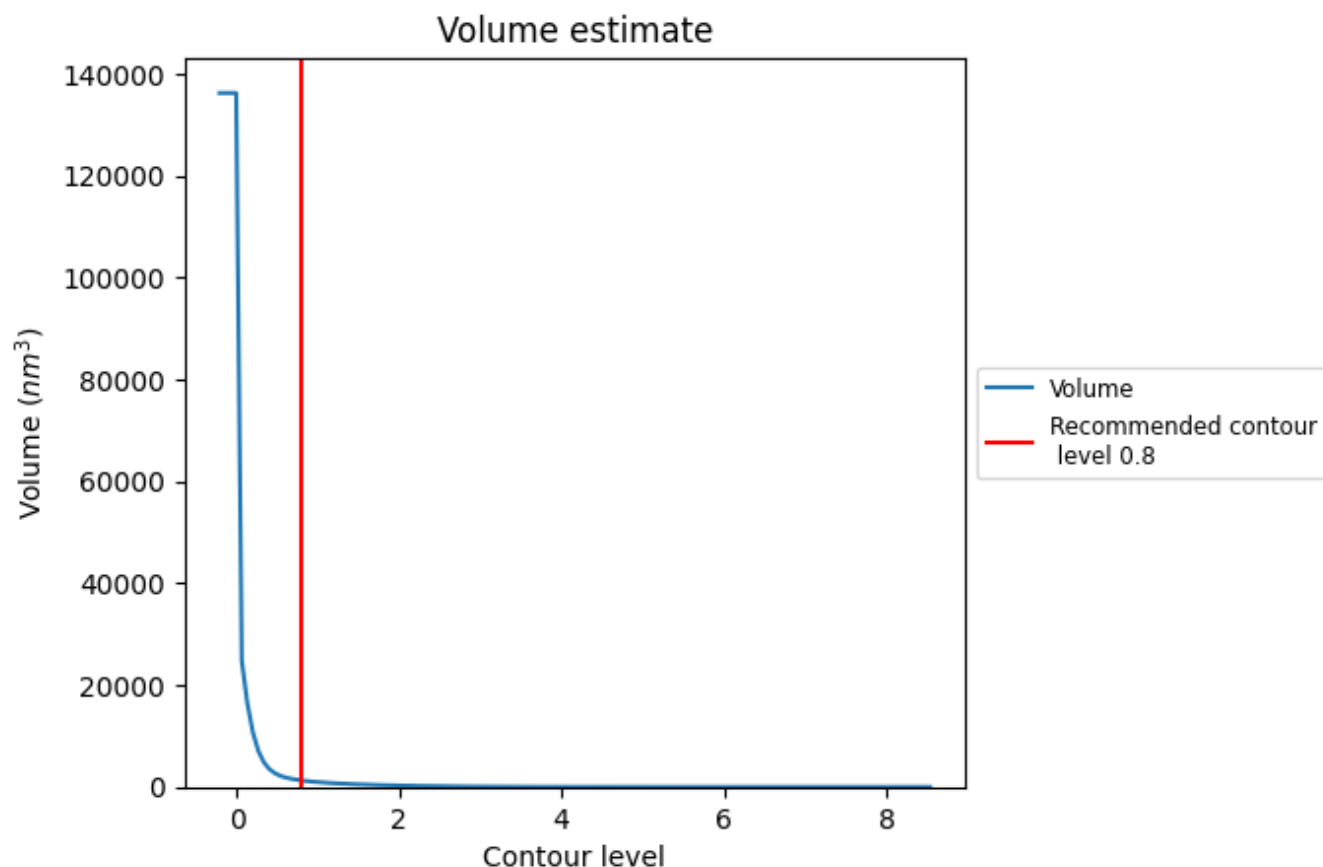
This section contains the results of statistical analysis of the map.

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.

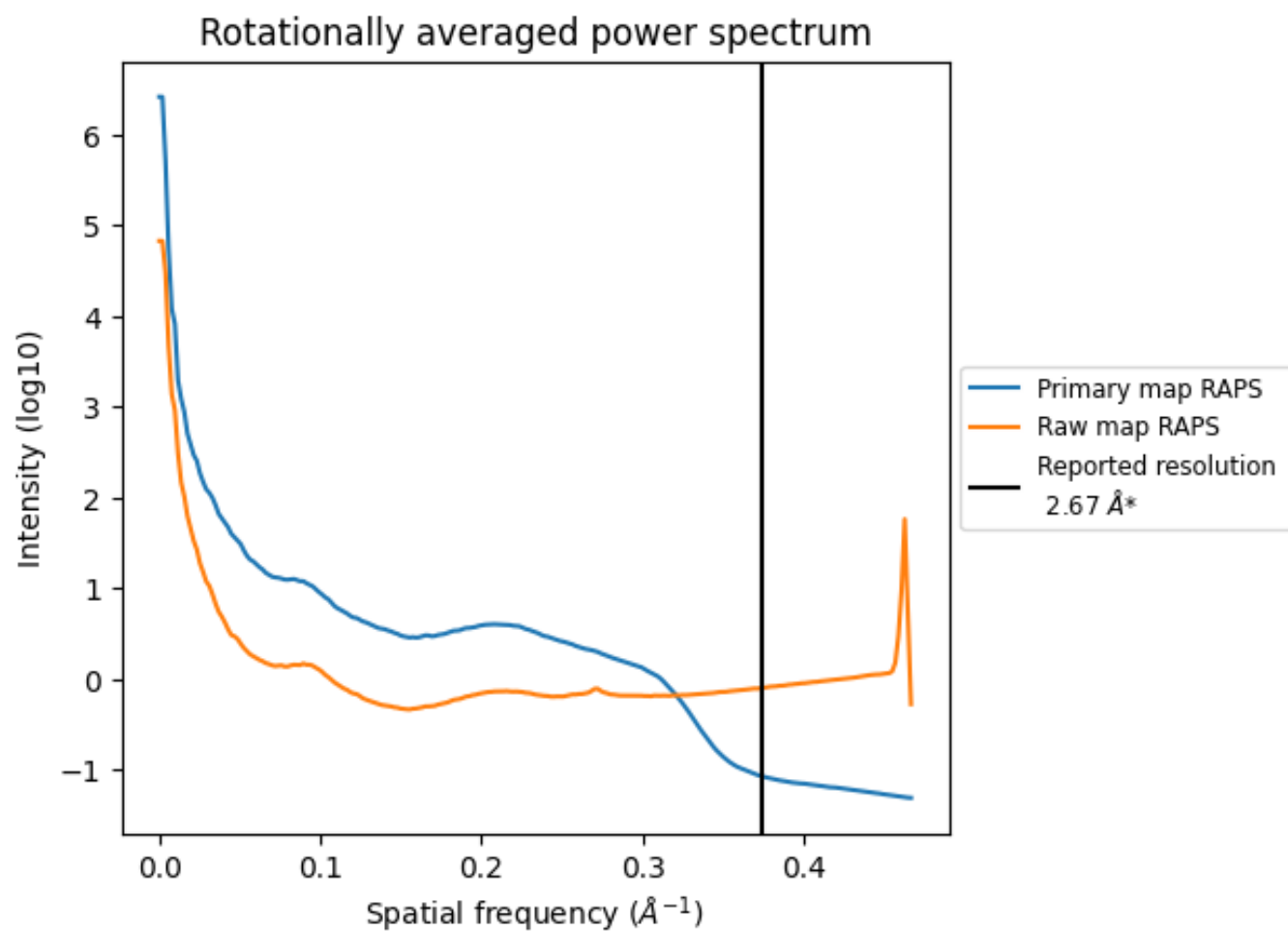
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1274 nm^3 ; this corresponds to an approximate mass of 1151 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 ⓘ

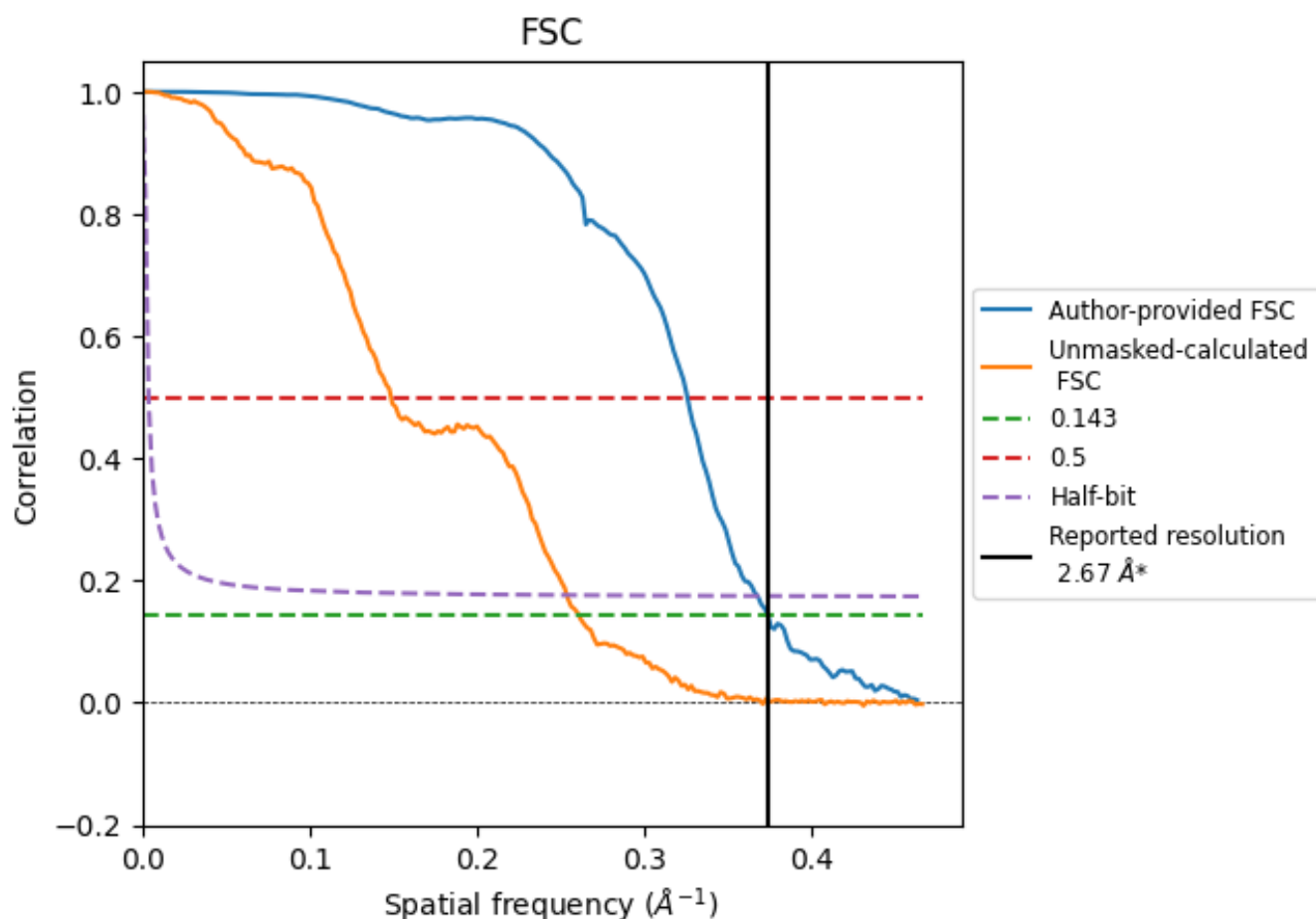


*Reported resolution corresponds to spatial frequency of 0.375 Å⁻¹

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 0.375 Å⁻¹

8.2 Resolution estimates [i](#)

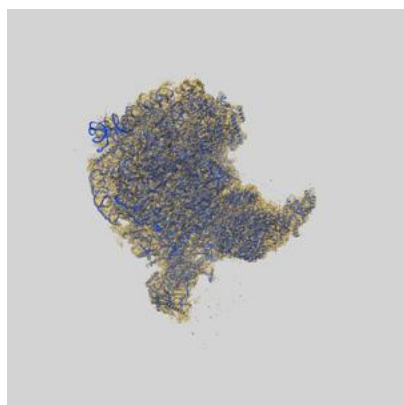
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.67	-	-
Author-provided FSC curve	2.67	3.07	2.72
Unmasked-calculated*	3.83	6.72	3.94

*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 3.83 differs from the reported value 2.67 by more than 10 %

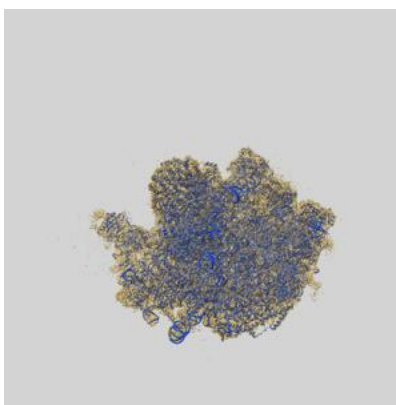
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29265 and PDB model 8FL2. Per-residue inclusion information can be found in section [3](#) on page [18](#).

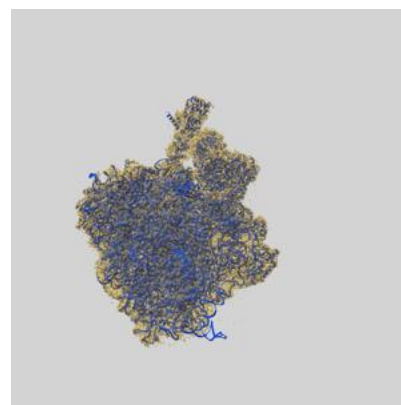
9.1 Map-model overlay [i](#)



X



Y



Z

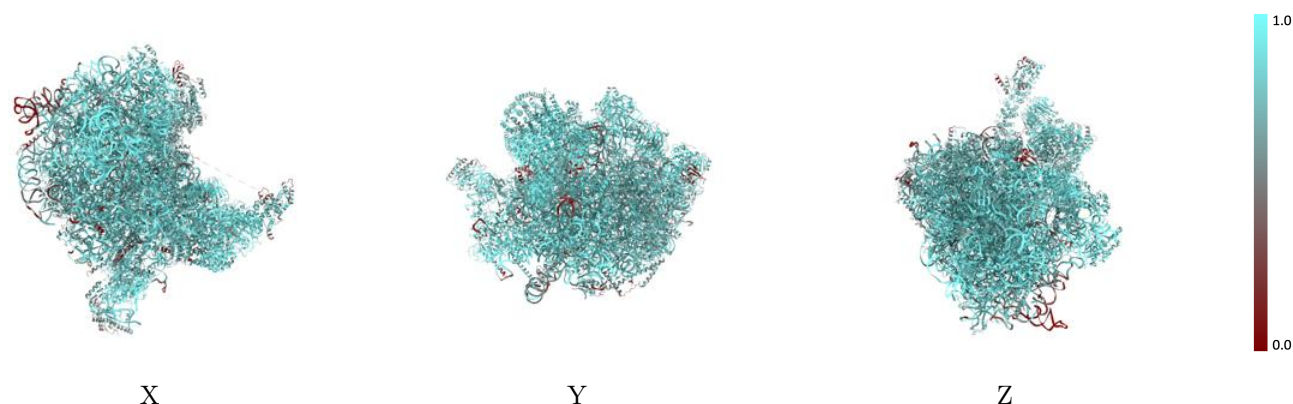
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



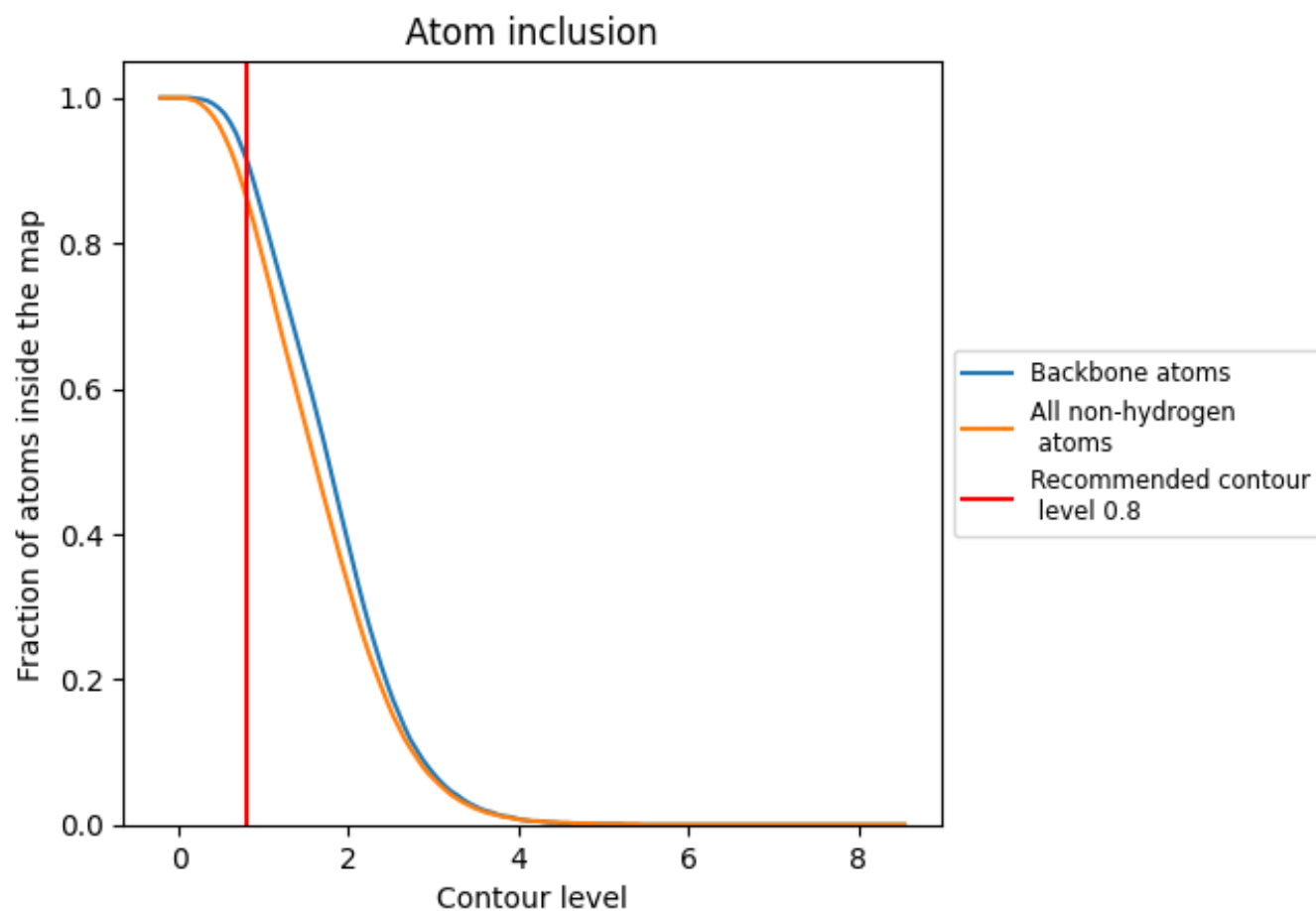
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8630	 0.5440
BA	 0.5980	 0.4080
BB	 0.8100	 0.5330
BD	 0.4390	 0.3460
L1	 0.9590	 0.5980
L2	 0.8970	 0.5310
L3	 0.8960	 0.5360
L4	 0.9680	 0.5810
L5	 0.8650	 0.5570
L6	 0.7450	 0.5000
L7	 0.8830	 0.5810
L8	 0.8810	 0.5710
L9	 0.9340	 0.6150
LA	 0.8860	 0.5870
LB	 0.8240	 0.5540
LC	 0.9300	 0.6320
LD	 0.8090	 0.5310
LE	 0.8170	 0.5520
LF	 0.7050	 0.4750
LG	 0.8120	 0.5350
LH	 0.8700	 0.5940
LI	 0.8230	 0.5530
LJ	 0.9050	 0.5980
LK	 0.7840	 0.5300
LL	 0.8470	 0.5530
LN	 0.8320	 0.5450
LO	 0.7930	 0.5230
LP	 0.8240	 0.5380
LQ	 0.8860	 0.5930
LR	 0.8790	 0.5810
LS	 0.8440	 0.5680
LT	 0.9150	 0.6160
LU	 0.7720	 0.5110
LW	 0.9390	 0.6060
LX	 0.8870	 0.5610



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Chain	Atom inclusion	Q-score
LY	 0.7160	 0.5160
LZ	 0.9270	 0.6050
NB	 0.7110	 0.5320
NC	 0.8040	 0.5370
NF	 0.9150	 0.6160
NJ	 0.9050	 0.5960
NK	 0.7140	 0.4740
NL	 0.7450	 0.5290
NP	 0.7340	 0.4930
NT	 0.8650	 0.5520
NU	 0.8130	 0.4930
NV	 0.8570	 0.5560
NW	 0.9180	 0.5630
NX	 0.8650	 0.5480
NY	 0.8680	 0.5570
NZ	 0.7700	 0.5360
SA	 0.8570	 0.5640
SB	 0.8990	 0.5890
SC	 0.7730	 0.5230
SD	 0.8450	 0.5750
SE	 0.8760	 0.5800
SF	 0.9440	 0.6120
SG	 0.8090	 0.5480
SH	 0.7780	 0.5120
SI	 0.8800	 0.5780
SK	 0.7140	 0.4490
SL	 0.6940	 0.4640
SM	 0.9190	 0.6170
SQ	 0.7790	 0.5240
SR	 0.7600	 0.5020
SV	 0.7720	 0.4840