



Full wwPDB EM Validation Report ⓘ

Mar 15, 2026 – 01:26 PM UTC

PDB ID : 9I1W / pdb_00009i1w
EMDB ID : EMD-52576
Title : High resolution structure of the thermophilic 60S ribosomal subunit of
Chaetomium thermophilum
Authors : Wild, K.; Klein, M.A.; Sinning, I.
Deposited on : 2025-01-17
Resolution : 2.38 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:

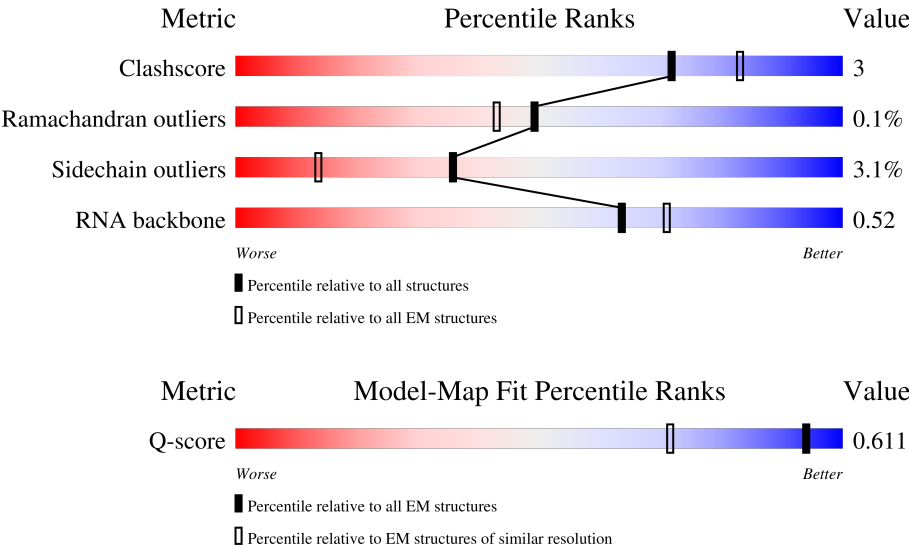
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.38 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	4811 (1.88 - 2.88)

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	1	3337	<div> <div>5%</div> <div>66%</div> <div>24%</div> <div>5%</div> <div>.</div> </div>
2	3	120	<div> <div>79%</div> <div>18%</div> <div>..</div> </div>
3	4	156	<div> <div>72%</div> <div>22%</div> <div>..</div> </div>


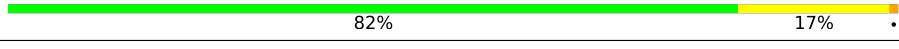
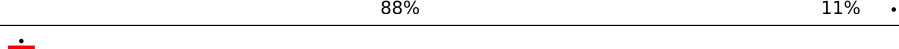
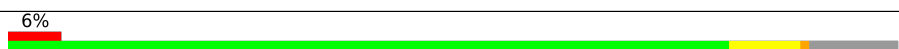


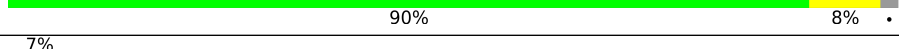
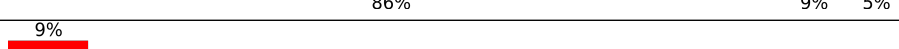





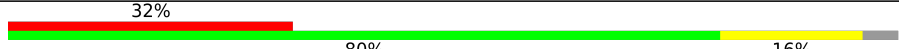
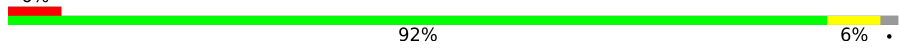








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Mol	Chain	Length	Quality of chain
4	9	3	
5	LA	254	
6	LB	392	
7	LC	365	
8	LD	304	
9	LE	200	
10	LF	249	
11	LG	262	
12	LH	192	
13	LI	219	
14	LJ	173	
15	LK	165	
16	LL	213	
17	LM	142	
18	LN	203	
19	LO	204	
20	LP	187	
21	LQ	213	
22	LR	192	
23	LS	174	
24	LT	160	
25	LU	127	
26	LV	139	
27	LW	161	
28	LX	156	

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Mol	Chain	Length	Quality of chain
29	LY	138	
30	LZ	135	
31	La	149	
32	Lb	130	
33	Lc	108	
34	Ld	120	
35	Le	131	
36	Lf	109	
37	Lg	119	
38	Lh	126	
39	Li	110	
40	Lj	95	
41	Lk	81	
42	Ll	102	
43	Lm	128	
44	Ln	25	
44	Lr	25	
45	Lo	106	
46	Lp	92	
47	Lq	147	
48	Ls	312	
49	PC	2	
50	PN	6	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	UY1	1	2277	X	-	-	-

2 Entry composition [i](#)

There are 56 unique types of molecules in this entry. The entry contains 131048 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 RNA chain called 26S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	3191	Total	C	N	O	P	0	0
			68292	30519	12333	22249	3191		

- Molecule 2 is a RNA chain called 5S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	119	Total	C	N	O	P	0	0
			2536	1132	453	832	119		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	156	Total	C	N	O	P	0	0
			3320	1485	589	1090	156		

- Molecule 4 is a RNA chain called E-site tRNA (5'-R(P*CP*CP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	9	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

- Molecule 5 is a protein called 60S ribosomal protein L2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LA	252	Total	C	N	O	S	0	0
			1925	1203	385	334	3		

- Molecule 6 is a protein called 60S ribosomal protein L3-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LB	387	Total	C	N	O	S	0	0
			3088	1964	576	535	13		

- Molecule 7 is a protein called 60S ribosomal protein L4-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LC	363	Total	C	N	O	S	0	0
			2758	1741	527	481	9		

- Molecule 8 is a protein called 60S ribosomal protein l5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LD	300	Total	C	N	O	S	0	0
			2440	1545	431	461	3		

- Molecule 9 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LE	194	Total	C	N	O	S	0	0
			1518	974	274	267	3		

- Molecule 10 is a protein called 60S ribosomal protein l7-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LF	247	Total	C	N	O	S	0	0
			2017	1294	376	344	3		

- Molecule 11 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LG	235	Total	C	N	O	S	0	0
			1900	1218	351	326	5		

- Molecule 12 is a protein called 60S ribosomal protein l9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LH	191	Total	C	N	O	S	0	0
			1505	955	269	275	6		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	PHE	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5

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Chain	Residue	Modelled	Actual	Comment	Reference
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	PHE	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	ASN	deletion	UNP G0S0E5
LH	?	-	ASP	deletion	UNP G0S0E5
LH	?	-	TYR	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	PHE	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	GLU	deletion	UNP G0S0E5
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	SER	deletion	UNP G0S0E5
LH	?	-	SER	deletion	UNP G0S0E5
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	ILE	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	GLU	deletion	UNP G0S0E5
LH	?	-	LEU	deletion	UNP G0S0E5
LH	?	-	ASP	deletion	UNP G0S0E5
LH	?	-	ILE	deletion	UNP G0S0E5
LH	?	-	ASN	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5

- Molecule 13 is a protein called 60S ribosomal protein L10-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LI	217	Total	C	N	O	S	0	0
			1760	1109	343	299	9		

- Molecule 14 is a protein called Putative ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LJ	167	Total	C	N	O	S	0	0
			1367	854	268	239	6		

- Molecule 15 is a protein called 60S ribosomal protein L12-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LK	155	Total	C	N	O	S	0	0
			762	452	155	155			

- Molecule 16 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LL	209	Total	C	N	O	S	0	0
			1666	1037	340	287	2		

- Molecule 17 is a protein called 60S ribosomal protein L14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LM	141	Total	C	N	O	S	0	0
			1125	714	216	194	1		

- Molecule 18 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LN	202	Total	C	N	O	S	0	0
			1703	1062	360	277	4		

- Molecule 19 is a protein called 60S ribosomal protein L16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LO	204	Total	C	N	O	S	0	0
			1613	1036	305	267	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LO	1	ACE	-	acetylation	UNP G0SH61

- Molecule 20 is a protein called 60S ribosomal protein l17-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LP	186	Total	C	N	O	S	0	0
			1472	912	295	262	3		

- Molecule 21 is a protein called Ribosomal protein L18-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LQ	183	Total	C	N	O	S	0	0
			1481	935	306	238	2		

- Molecule 22 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LR	150	Total	C	N	O	S	0	0
			1222	760	260	198	4		

- Molecule 23 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LS	173	Total	C	N	O	S	0	0
			1425	917	266	238	4		

- Molecule 24 is a protein called 60S ribosomal protein l21-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LT	159	Total	C	N	O	S	0	0
			1270	805	247	216	2		

- Molecule 25 is a protein called 60S ribosomal protein L22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LU	101	Total	C	N	O	S	0	0
			819	532	142	144	1		

- Molecule 26 is a protein called 60S ribosomal protein l23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LV	135	Total	C	N	O	S	0	0
			994	633	185	169	7		

- Molecule 27 is a protein called 60S ribosomal protein L24-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LW	61	Total	C	N	O	S	0	0
			528	335	106	86	1		

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LW	?	-	LYS	deletion	UNP G0S1P9
LW	?	-	VAL	deletion	UNP G0S1P9
LW	?	-	ARG	deletion	UNP G0S1P9
LW	?	-	PHE	deletion	UNP G0S1P9
LW	?	-	PRO	deletion	UNP G0S1P9
LW	?	-	ILE	deletion	UNP G0S1P9
LW	?	-	SER	deletion	UNP G0S1P9
LW	?	-	HIS	deletion	UNP G0S1P9
LW	?	-	GLU	deletion	UNP G0S1P9
LW	?	-	GLY	deletion	UNP G0S1P9
LW	?	-	ASP	deletion	UNP G0S1P9
LW	?	-	ASN	deletion	UNP G0S1P9
LW	?	-	GLY	deletion	UNP G0S1P9
LW	?	-	ASP	deletion	UNP G0S1P9
LW	?	-	ILE	deletion	UNP G0S1P9
LW	?	-	SER	deletion	UNP G0S1P9
LW	?	-	HIS	deletion	UNP G0S1P9
LW	?	-	PRO	deletion	UNP G0S1P9
LW	?	-	GLU	deletion	UNP G0S1P9
LW	?	-	GLU	deletion	UNP G0S1P9
LW	?	-	ILE	deletion	UNP G0S1P9
LW	?	-	ARG	deletion	UNP G0S1P9
LW	?	-	THR	deletion	UNP G0S1P9
LW	?	-	GLY	deletion	UNP G0S1P9
LW	?	-	ARG	deletion	UNP G0S1P9
LW	?	-	ARG	deletion	UNP G0S1P9
LW	?	-	LYS	deletion	UNP G0S1P9
LW	?	-	ILE	deletion	UNP G0S1P9
LW	?	-	ALA	deletion	UNP G0S1P9
LW	?	-	PRO	deletion	UNP G0S1P9
LW	?	-	ALA	deletion	UNP G0S1P9
LW	?	-	THR	deletion	UNP G0S1P9
LW	?	-	ARG	deletion	UNP G0S1P9
LW	?	-	GLN	deletion	UNP G0S1P9
LW	?	-	LEU	deletion	UNP G0S1P9
LW	?	-	ARG	deletion	UNP G0S1P9
LW	?	-	ALA	deletion	UNP G0S1P9

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Chain	Residue	Modelled	Actual	Comment	Reference
LW	?	-	GLU	deletion	UNP G0S1P9
LW	?	-	VAL	deletion	UNP G0S1P9
LW	?	-	GLN	deletion	UNP G0S1P9
LW	?	-	LYS	deletion	UNP G0S1P9
LW	?	-	THR	deletion	UNP G0S1P9
LW	?	-	SER	deletion	UNP G0S1P9
LW	?	-	MET	deletion	UNP G0S1P9

- Molecule 28 is a protein called 60S ribosomal protein L25-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	LX	119	Total	C	N	O	0	0
			950	609	173	168		

- Molecule 29 is a protein called 60S ribosomal protein L26-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LY	134	Total	C	N	O	S	0	0
			1065	664	215	184	2		

- Molecule 30 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LZ	135	Total	C	N	O	S	0	0
			1111	713	207	187	4		

- Molecule 31 is a protein called 60S ribosomal protein L28-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	La	148	Total	C	N	O	S	0	0
			1180	745	239	194	2		

- Molecule 32 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Lb	62	Total	C	N	O	0	0
			508	310	112	86		

- Molecule 33 is a protein called 60S ribosomal protein l30-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Lc	97	Total	C	N	O	S	0	0
			722	458	125	134	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Ld	112	Total	C	N	O	S	0	0
			911	575	178	157	1		

- Molecule 35 is a protein called 60S ribosomal protein L32-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Le	124	Total	C	N	O	S	0	0
			1001	629	205	161	6		

- Molecule 36 is a protein called 60S ribosomal protein l33-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lf	107	Total	C	N	O	S	0	0
			853	540	170	142	1		

- Molecule 37 is a protein called Ribosomal protein l34-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Lg	113	Total	C	N	O	S	0	0
			896	557	182	153	4		

- Molecule 38 is a protein called Dolichyl-diphosphooligosaccharide--protein glycotransferase.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	Lh	122	Total	C	N	O	0	0
			1003	637	198	168		

- Molecule 39 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Li	102	Total	C	N	O	S	0	0
			836	515	184	136	1		

- Molecule 40 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Lj	87	Total	C	N	O	S	0	0
			691	422	153	111	5		

- Molecule 41 is a protein called 60S ribosomal protein L38-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lk	76	Total	C	N	O	S	0	0
			632	400	121	109	2		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lk	?	-	LYS	deletion	UNP G0SG89
Lk	?	-	ILE	deletion	UNP G0SG89
Lk	?	-	LEU	deletion	UNP G0SG89
Lk	?	-	THR	deletion	UNP G0SG89
Lk	?	-	ILE	deletion	UNP G0SG89
Lk	?	-	ALA	deletion	UNP G0SG89
Lk	?	-	PHE	deletion	UNP G0SG89
Lk	?	-	PRO	deletion	UNP G0SG89
Lk	?	-	PRO	deletion	UNP G0SG89
Lk	?	-	PRO	deletion	UNP G0SG89
Lk	?	-	LEU	deletion	UNP G0SG89
Lk	?	-	THR	deletion	UNP G0SG89
Lk	?	-	ALA	deletion	UNP G0SG89

- Molecule 42 is a protein called Ribosomal protein eL39.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	Ll	50	Total	C	N	O	0	0
			435	275	97	63		

- Molecule 43 is a protein called Putative ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lm	51	Total	C	N	O	S	0	0
			410	255	85	64	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lm	1	MET	SER	conflict	UNP G0S8G4

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Chain	Residue	Modelled	Actual	Comment	Reference
Lm	2	GLN	ARG	conflict	UNP G0S8G4

- Molecule 44 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Ln	24	Total	C	N	O	S	0	0
			224	136	61	26	1		
44	Lr	24	Total	C	N	O	S	0	0
			224	136	61	26	1		

- Molecule 45 is a protein called 60S ribosomal protein L44-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lo	104	Total	C	N	O	S	0	0
			822	520	161	136	5		

- Molecule 46 is a protein called 60S ribosomal protein L43-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Lp	91	Total	C	N	O	S	0	0
			697	430	138	123	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Lq	141	Total	C	N	O		0	0
			1083	678	215	190			

- Molecule 48 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Ls	189	Total	C	N	O	S	0	0
			1449	927	250	265	7		

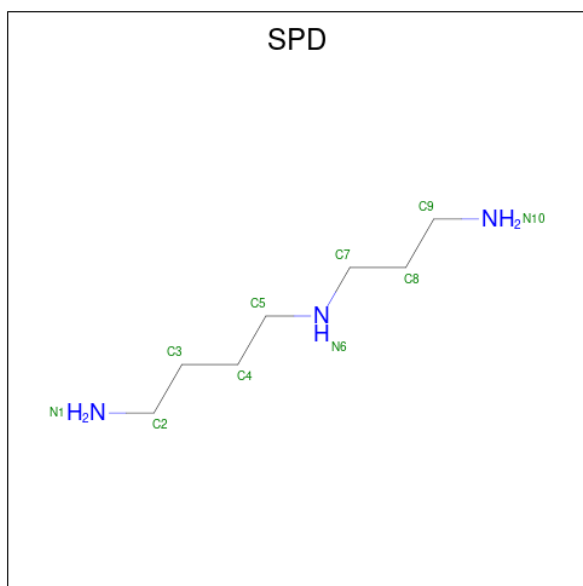
- Molecule 49 is a protein called Nascent chain C-terminus.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	PC	2	Total	C	N	O		0	0
			11	6	2	3			

- Molecule 50 is a protein called Nascent chain N-terminus.

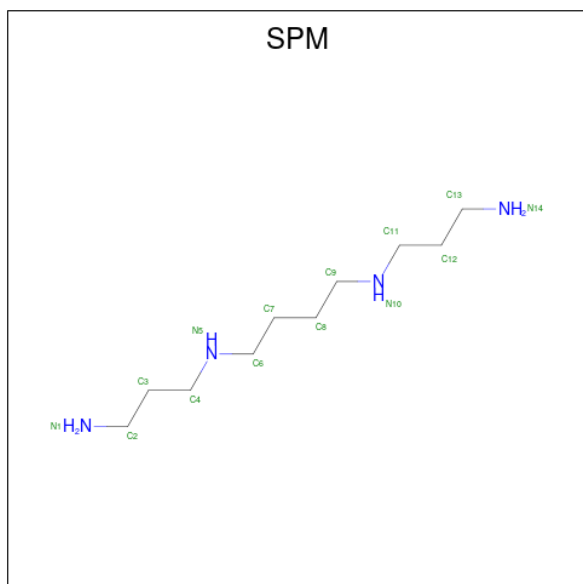
Mol	Chain	Residues	Atoms				AltConf	Trace
50	PN	6	Total	C	N	O	0	0
			30	18	6	6		

- Molecule 51 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			AltConf
51	1	1	Total	C	N	0
			10	7	3	
51	1	1	Total	C	N	0
			10	7	3	

- Molecule 52 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms			AltConf
52	1	1	Total	C	N	0
			14	10	4	
52	1	1	Total	C	N	0
			14	10	4	

- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
53	1	215	Total	Mg	0
			215	215	
53	3	3	Total	Mg	0
			3	3	
53	4	8	Total	Mg	0
			8	8	
53	LA	2	Total	Mg	0
			2	2	
53	LB	1	Total	Mg	0
			1	1	
53	LC	1	Total	Mg	0
			1	1	
53	LE	1	Total	Mg	0
			1	1	
53	LI	1	Total	Mg	0
			1	1	
53	LP	1	Total	Mg	0
			1	1	
53	LV	1	Total	Mg	0
			1	1	
53	LY	1	Total	Mg	0
			1	1	
53	Lb	1	Total	Mg	0
			1	1	
53	Le	1	Total	Mg	0
			1	1	
53	Lj	2	Total	Mg	0
			2	2	

- Molecule 54 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
54	1	177	Total	K	0
			177	177	
54	3	2	Total	K	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
54	4	1	Total 1	K 1	0
54	LA	1	Total 1	K 1	0
54	LC	2	Total 2	K 2	0
54	LI	1	Total 1	K 1	0
54	LN	1	Total 1	K 1	0
54	Lb	1	Total 1	K 1	0
54	Le	1	Total 1	K 1	0
54	Lo	1	Total 1	K 1	0

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
55	Lg	1	Total 1	Zn 1	0
55	Lj	1	Total 1	Zn 1	0
55	Lm	1	Total 1	Zn 1	0
55	Lo	1	Total 1	Zn 1	0
55	Lp	1	Total 1	Zn 1	0

- Molecule 56 is water.

Mol	Chain	Residues	Atoms		AltConf
56	1	1821	Total 1821	O 1821	0
56	3	31	Total 31	O 31	0
56	4	67	Total 67	O 67	0
56	9	1	Total 1	O 1	0

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Mol	Chain	Residues	Atoms		AltConf
56	LA	12	Total 12	O 12	0
56	LB	23	Total 23	O 23	0
56	LC	29	Total 29	O 29	0
56	LD	3	Total 3	O 3	0
56	LE	8	Total 8	O 8	0
56	LF	16	Total 16	O 16	0
56	LG	11	Total 11	O 11	0
56	LI	8	Total 8	O 8	0
56	LJ	1	Total 1	O 1	0
56	LL	18	Total 18	O 18	0
56	LM	1	Total 1	O 1	0
56	LN	19	Total 19	O 19	0
56	LO	5	Total 5	O 5	0
56	LP	12	Total 12	O 12	0
56	LQ	15	Total 15	O 15	0
56	LR	4	Total 4	O 4	0
56	LS	7	Total 7	O 7	0
56	LT	13	Total 13	O 13	0
56	LV	7	Total 7	O 7	0
56	LW	1	Total 1	O 1	0
56	LX	2	Total 2	O 2	0

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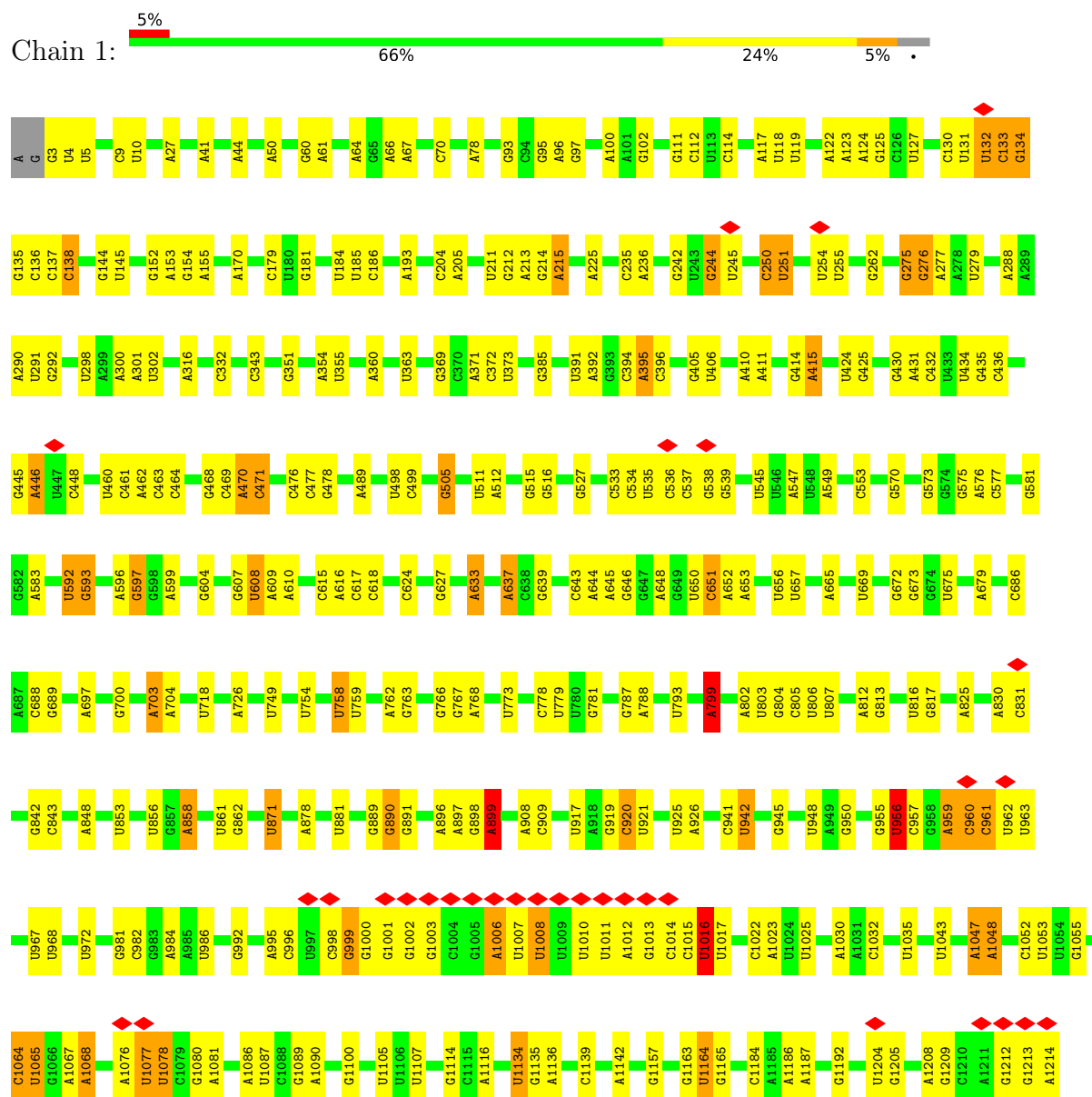
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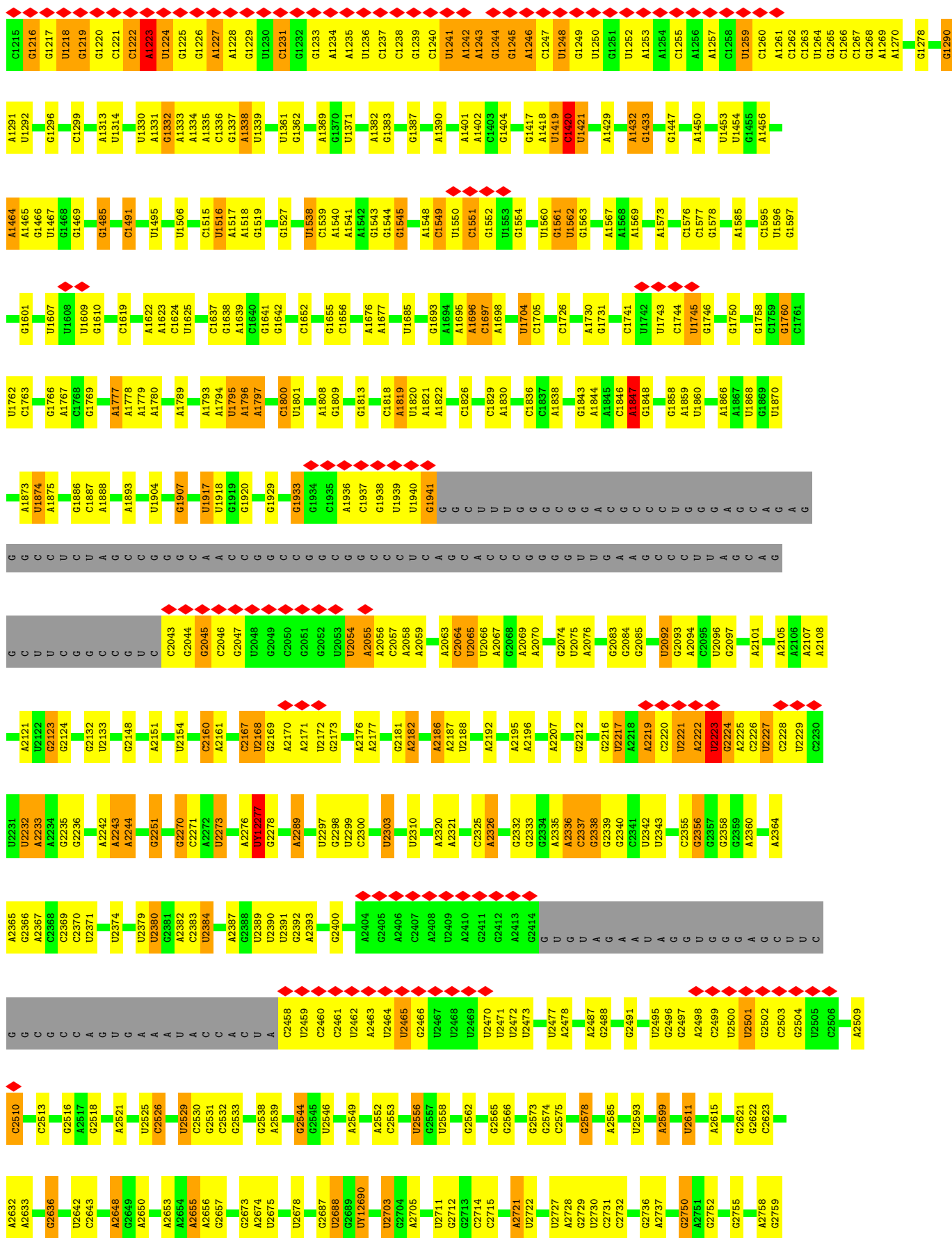
Mol	Chain	Residues	Atoms		AltConf
56	LY	6	Total 6	O 6	0
56	LZ	1	Total 1	O 1	0
56	La	19	Total 19	O 19	0
56	Lb	7	Total 7	O 7	0
56	Ld	3	Total 3	O 3	0
56	Le	20	Total 20	O 20	0
56	Lf	11	Total 11	O 11	0
56	Lg	3	Total 3	O 3	0
56	Lh	6	Total 6	O 6	0
56	Li	5	Total 5	O 5	0
56	Lj	17	Total 17	O 17	0
56	Lk	1	Total 1	O 1	0
56	Ll	2	Total 2	O 2	0
56	Lm	1	Total 1	O 1	0
56	Ln	1	Total 1	O 1	0
56	Lo	7	Total 7	O 7	0
56	Lp	2	Total 2	O 2	0
56	Lq	9	Total 9	O 9	0

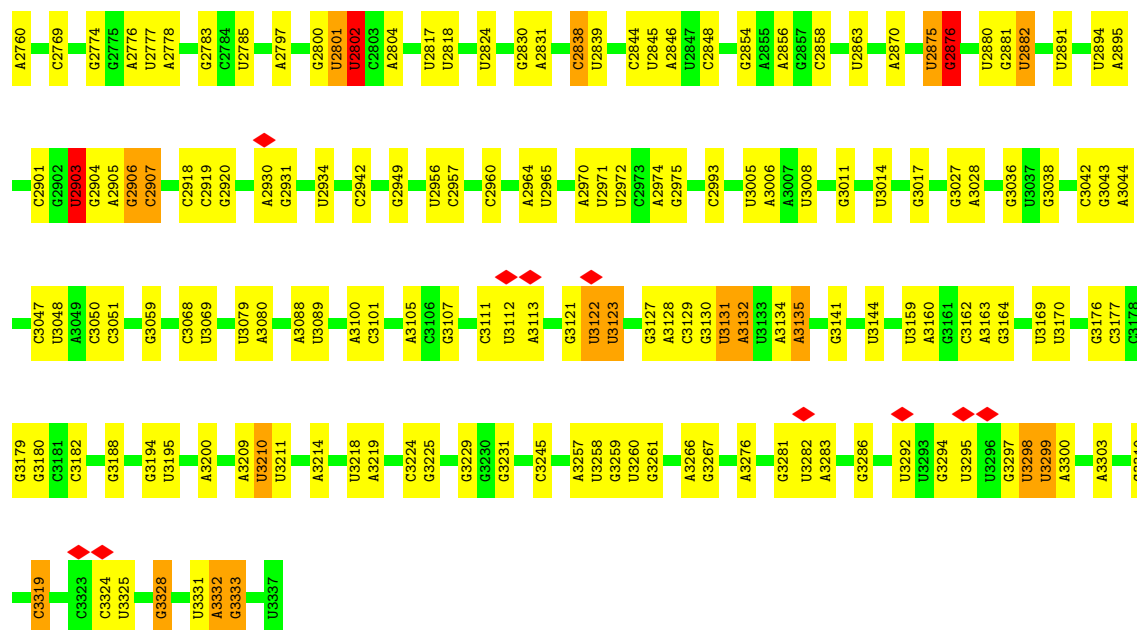
3 Residue-property plots

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: 26S rRNA







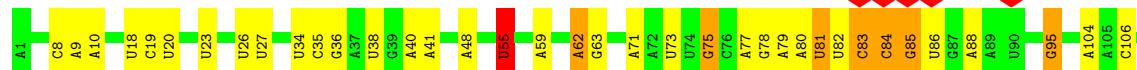
• Molecule 2: 5S RNA

Chain 3: 79% 18% ..



• Molecule 3: 5.8S RNA

Chain 4: 72% 22% ..



• Molecule 4: E-site tRNA (5'-R(P*CP*CP*A)-3')

Chain 9: 33% 67% 33%



• Molecule 5: 60S ribosomal protein L2-like protein

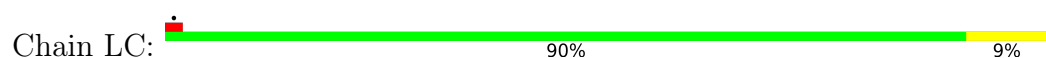
Chain LA: 91% 7% ..



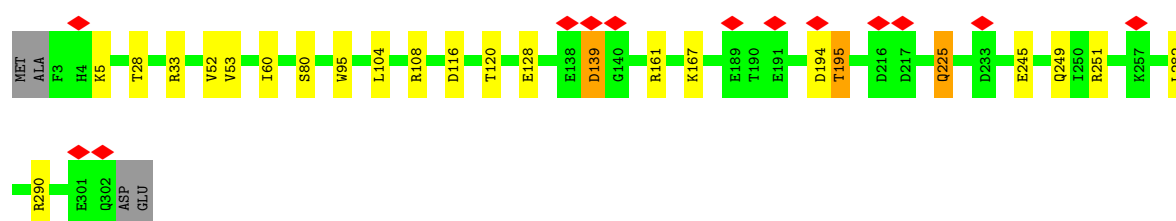
- Molecule 6: 60S ribosomal protein L3-like protein



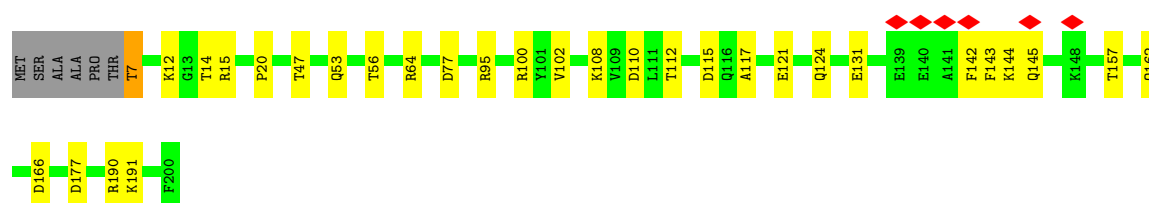
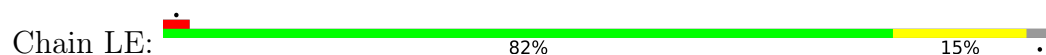
- Molecule 7: 60S ribosomal protein L4-like protein



- Molecule 8: 60S ribosomal protein l5-like protein



- Molecule 9: 60S ribosomal protein L6




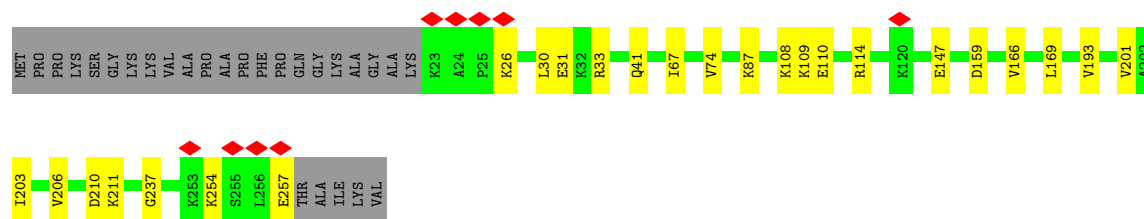
- Molecule 10: 60S ribosomal protein l7-like protein

Chain LF:  90% 9% ..



- Molecule 11: 60S ribosomal protein L8

Chain LG:  80% 10% 10%




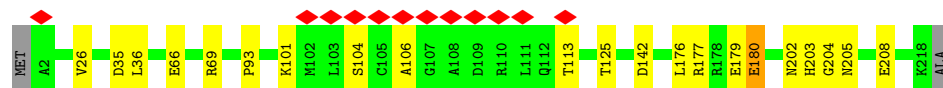
- Molecule 12: 60S ribosomal protein I9-like protein

Chain LH:  86% 12% ..




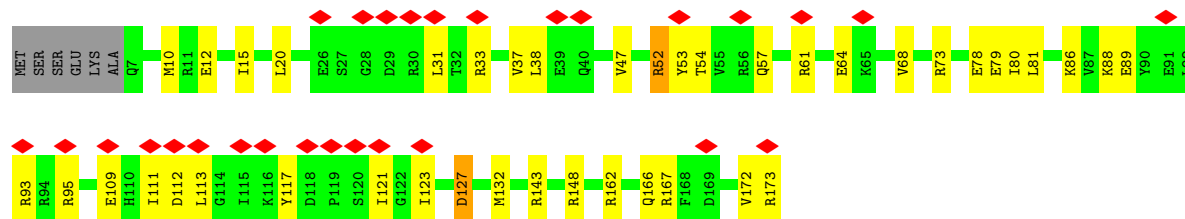
- Molecule 13: 60S ribosomal protein L10-like protein

Chain LI:  5% 89% 9% .

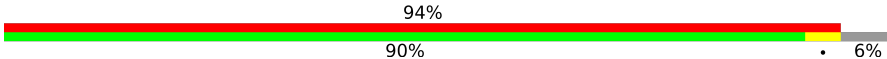


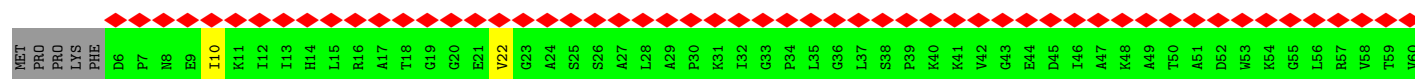
- Molecule 14: Putative ribosomal protein

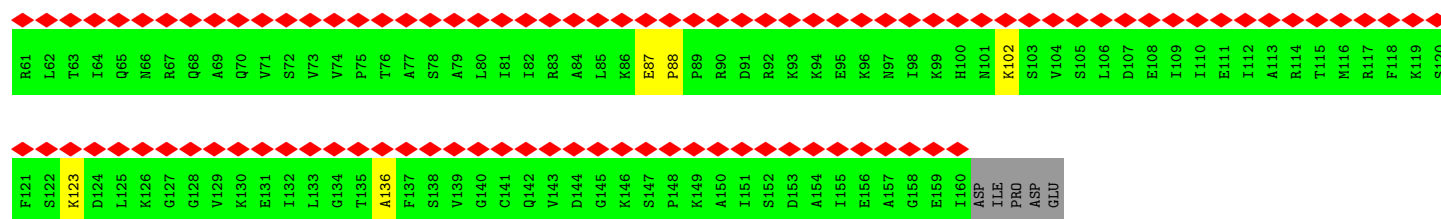
Chain LJ:  16% 72% 23% ..



- Molecule 15: 60S ribosomal protein L12-like protein

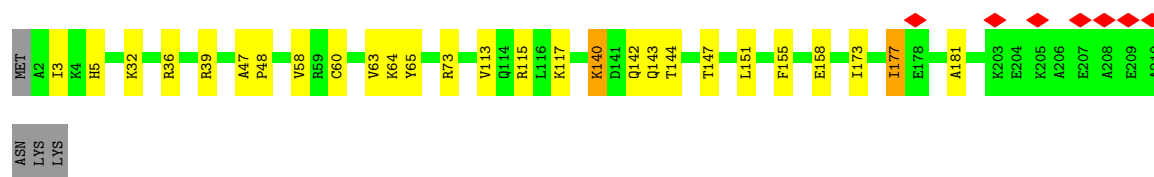
Chain LK:  94% 90% 6%





- Molecule 16: 60S ribosomal protein L13

Chain LL: 85% 12% ..



- Molecule 17: 60S ribosomal protein L14-like protein

Chain LM: 90% 9% .



- Molecule 18: Ribosomal protein L15

Chain LN: 91% 7% .



- Molecule 19: 60S ribosomal protein L16-like protein

Chain LO: 92% 7%



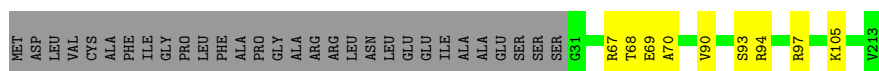
- Molecule 20: 60S ribosomal protein l17-like protein

Chain LP: 8% 90% 9% ..

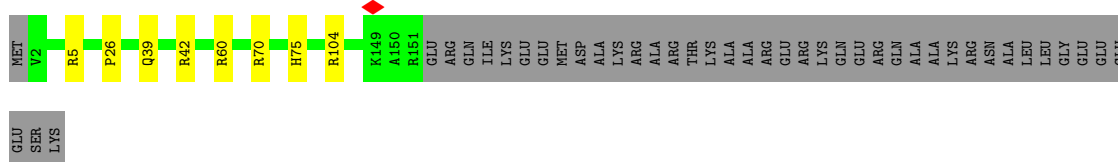
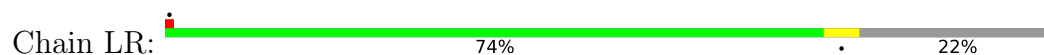


- Molecule 21: Ribosomal protein L18-like protein

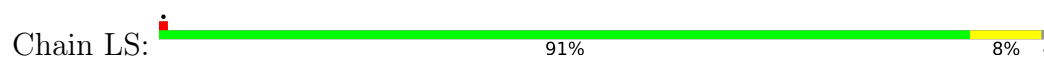
Chain LQ: 82% 14%



• Molecule 22: Ribosomal protein L19



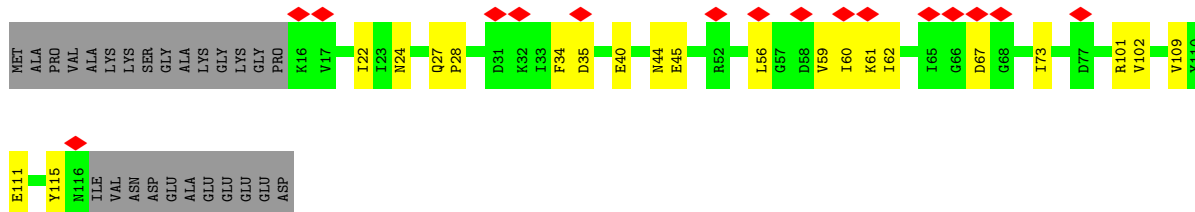
• Molecule 23: 60S ribosomal protein L20



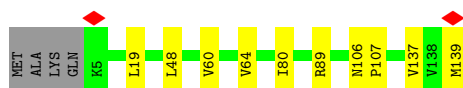
• Molecule 24: 60S ribosomal protein l21-like protein



• Molecule 25: 60S ribosomal protein L22-like protein

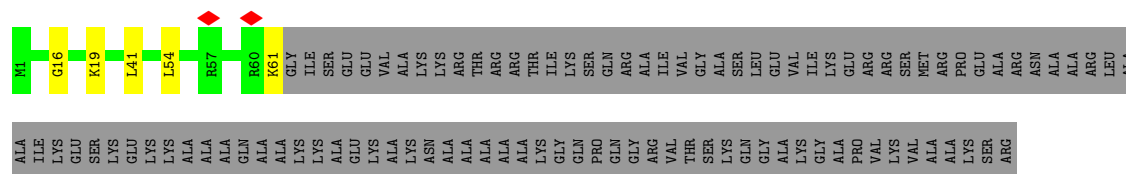


• Molecule 26: 60S ribosomal protein l23-like protein

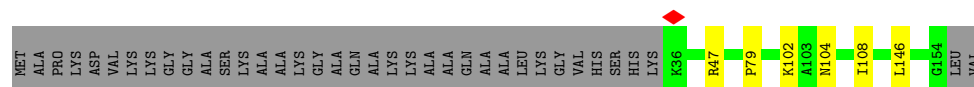


• Molecule 27: 60S ribosomal protein L24-like protein

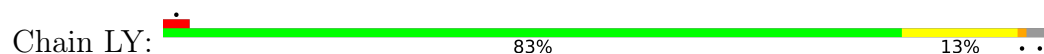




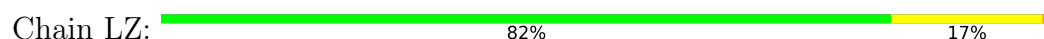
- Molecule 28: 60S ribosomal protein L25-like protein



- Molecule 29: 60S ribosomal protein L26-like protein



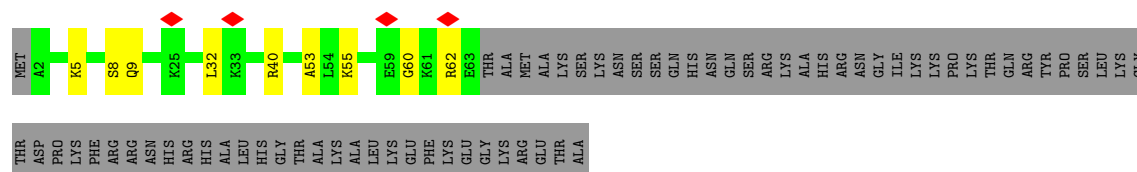
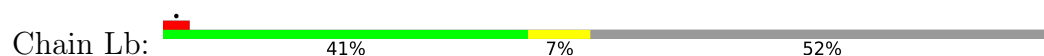
- Molecule 30: 60S ribosomal protein L27



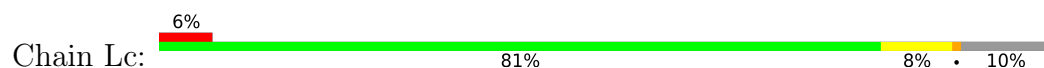
- Molecule 31: 60S ribosomal protein L28-like protein



- Molecule 32: 60S ribosomal protein L29

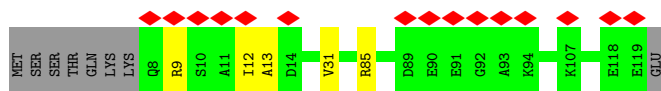
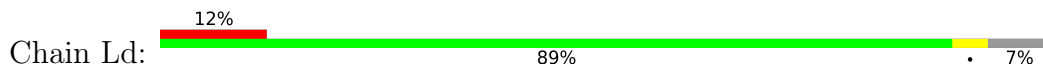


- Molecule 33: 60S ribosomal protein L30-like protein

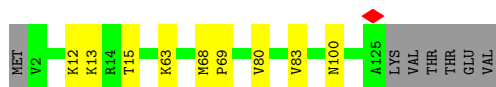
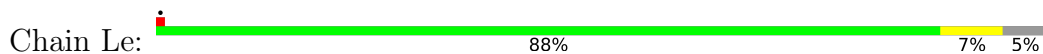




- Molecule 34: Putative 60S ribosomal protein



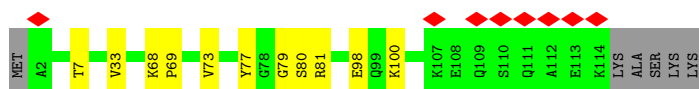
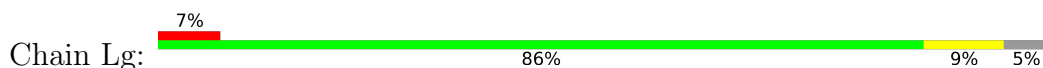
- Molecule 35: 60S ribosomal protein L32-like protein



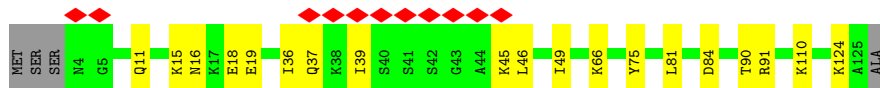
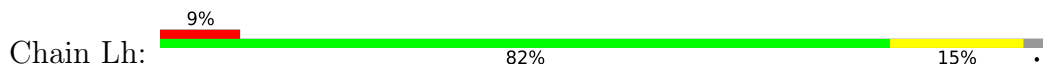
- Molecule 36: 60S ribosomal protein l33-like protein



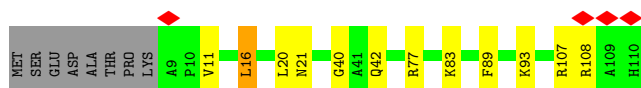
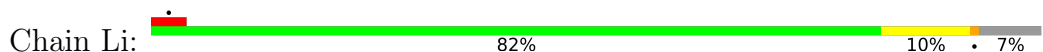
- Molecule 37: Ribosomal protein l34-like protein




- Molecule 38: Dolichyl-diphosphooligosaccharide--protein glycotransferase

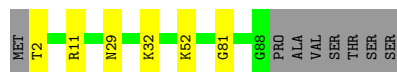


- Molecule 39: 60S ribosomal protein L36




- Molecule 40: Ribosomal protein L37

Chain Lj:  85% 6% 8%



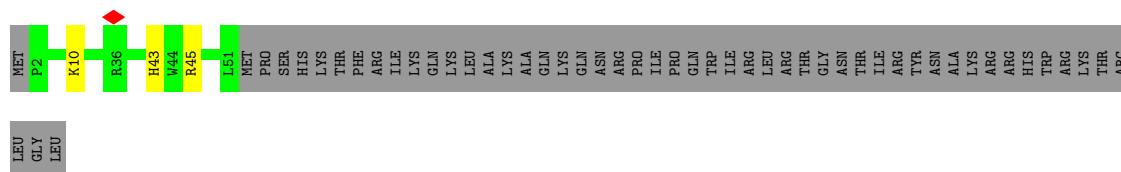
- Molecule 41: 60S ribosomal protein L38-like protein

Chain Lk:  7% 81% 10% 6%



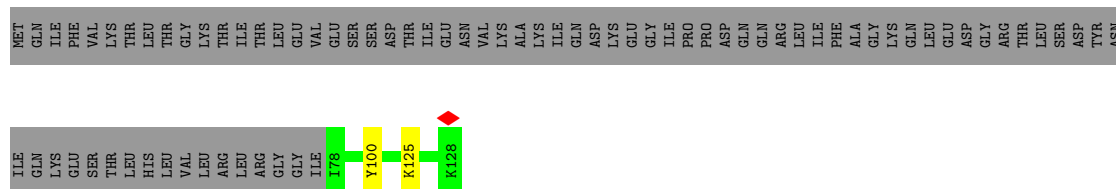
- Molecule 42: Ribosomal protein eL39

Chain Ll:  46% 51%




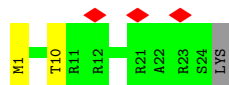
- Molecule 43: Putative ribosomal protein

Chain Lm:  38% 60%




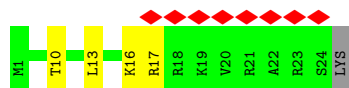
- Molecule 44: 60S ribosomal protein L41-A

Chain Ln:  12% 88% 8%



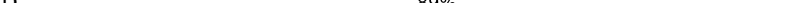
- Molecule 44: 60S ribosomal protein L41-A

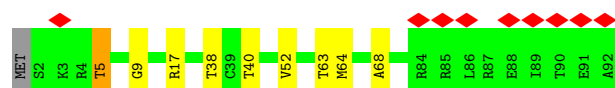
Chain Lr:  32% 80% 16%



- Molecule 45: 60S ribosomal protein L44-like protein



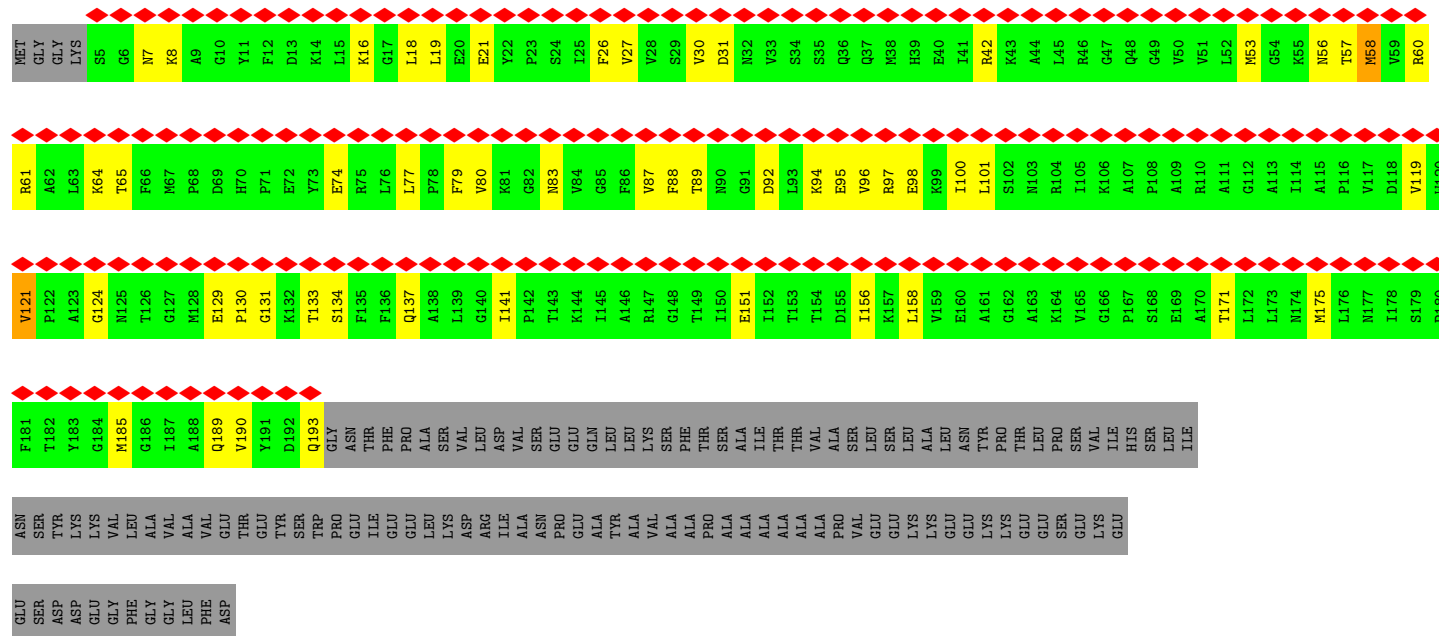
- Chain Lp:  10% 89% 9%



- Chain Lq:  87% 9% .



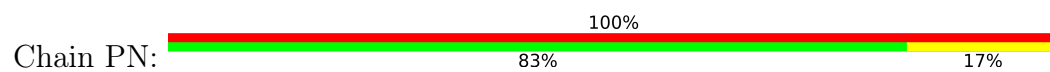
- Chain Ls: 



- Chain PC: 



- Molecule 50: Nascent chain N-terminus



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	653542	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42.7	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.254	Depositor
Minimum map value	-0.493	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.175	Depositor
Map size (Å)	694.39996, 694.39996, 694.39996	wwPDB
Map dimensions	800, 800, 800	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.868, 0.868, 0.868	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1	0.23	6/73653 (0.0%)	0.33	0/114844
2	3	0.19	0/2834	0.29	0/4415
3	4	0.22	0/3618	0.31	0/5635
4	9	0.19	0/68	0.30	0/103
5	LA	0.23	0/1964	0.39	0/2641
6	LB	0.17	0/3156	0.33	0/4238
7	LC	0.23	0/2815	0.35	1/3795 (0.0%)
8	LD	0.16	0/2487	0.28	0/3341
9	LE	0.17	0/1547	0.32	0/2081
10	LF	0.19	0/2055	0.31	0/2758
11	LG	0.18	0/1929	0.32	0/2579
12	LH	0.15	0/1525	0.27	0/2050
13	LI	0.16	0/1797	0.28	0/2413
14	LJ	0.13	0/1389	0.29	0/1856
15	LK	0.09	0/761	0.30	0/1056
16	LL	0.21	0/1695	0.37	0/2276
17	LM	0.16	0/1144	0.26	0/1539
18	LN	0.21	0/1740	0.34	0/2332
19	LO	0.18	0/1645	0.30	0/2207
20	LP	0.18	0/1495	0.31	0/2014
21	LQ	0.20	0/1507	0.33	0/2017
22	LR	0.17	0/1241	0.25	0/1655
23	LS	0.17	0/1460	0.30	0/1965
24	LT	0.18	0/1296	0.30	0/1743
25	LU	0.12	0/832	0.26	0/1112
26	LV	0.15	0/1012	0.30	0/1361
27	LW	0.16	0/540	0.26	0/718
28	LX	0.19	0/966	0.31	0/1303
29	LY	0.19	0/1079	0.31	0/1443
30	LZ	0.17	0/1134	0.28	0/1519
31	La	0.21	0/1212	0.35	0/1627
32	Lb	0.16	0/518	0.29	0/684

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Lc	0.17	0/731	0.27	0/983
34	Ld	0.18	0/925	0.28	0/1238
35	Le	0.19	0/1019	0.36	0/1358
36	Lf	0.20	0/874	0.36	0/1176
37	Lg	0.19	0/909	0.34	0/1218
38	Lh	0.19	0/1014	0.29	0/1349
39	Li	0.18	0/844	0.32	0/1115
40	Lj	0.19	0/704	0.34	0/932
41	Lk	0.15	0/640	0.27	0/850
42	Ll	0.20	0/445	0.29	0/593
43	Lm	0.14	0/416	0.29	0/550
44	Ln	0.14	0/225	0.26	0/289
44	Lr	0.11	0/225	0.22	0/289
45	Lo	0.18	0/835	0.31	0/1105
46	Lp	0.17	0/705	0.35	0/940
47	Lq	0.19	0/1101	0.32	0/1482
48	Ls	0.08	0/1477	0.23	0/1995
All	All	0.21	6/135203 (0.0%)	0.32	1/198782 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	1	0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2244	A2M	O3'-P	5.15	1.61	1.56
1	1	2219	A2M	O3'-P	5.14	1.61	1.56
1	1	1223	A2M	O3'-P	5.09	1.61	1.56
1	1	848	A2M	O3'-P	5.05	1.61	1.56
1	1	768	A2M	O3'-P	5.04	1.61	1.56
1	1	2905	A2M	O3'-P	5.00	1.61	1.56

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	LC	149	VAL	CA-C-O	-5.11	117.28	119.94

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	1	2277	UY1	C4'

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	1	68292	0	34436	417	0
2	3	2536	0	1283	10	0
3	4	3320	0	1680	24	0
4	9	62	0	34	0	0
5	LA	1925	0	1999	9	0
6	LB	3088	0	3206	23	0
7	LC	2758	0	2883	20	0
8	LD	2440	0	2431	13	0
9	LE	1518	0	1619	18	0
10	LF	2017	0	2130	13	0
11	LG	1900	0	2066	12	0
12	LH	1505	0	1581	12	0
13	LI	1760	0	1798	13	0
14	LJ	1367	0	1405	25	0
15	LK	762	0	362	3	0
16	LL	1666	0	1756	17	0
17	LM	1125	0	1198	7	0
18	LN	1703	0	1766	11	0
19	LO	1613	0	1706	8	0
20	LP	1472	0	1518	8	0
21	LQ	1481	0	1596	13	0
22	LR	1222	0	1299	6	0
23	LS	1425	0	1484	8	0
24	LT	1270	0	1331	9	0
25	LU	819	0	864	9	0
26	LV	994	0	1055	4	0
27	LW	528	0	542	3	0
28	LX	950	0	1030	4	0
29	LY	1065	0	1156	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	LZ	1111	0	1181	12	0
31	La	1180	0	1203	9	0
32	Lb	508	0	526	5	0
33	Lc	722	0	766	4	0
34	Ld	911	0	965	4	0
35	Le	1001	0	1070	5	0
36	Lf	853	0	880	4	0
37	Lg	896	0	962	5	0
38	Lh	1003	0	1116	12	0
39	Li	836	0	915	8	0
40	Lj	691	0	719	5	0
41	Lk	632	0	693	6	0
42	Ll	435	0	473	2	0
43	Lm	410	0	448	2	0
44	Ln	224	0	271	0	0
44	Lr	224	0	271	2	0
45	Lo	822	0	891	4	0
46	Lp	697	0	737	4	0
47	Lq	1083	0	1140	8	0
48	Ls	1449	0	1488	35	0
49	PC	11	0	4	0	0
50	PN	30	0	9	1	0
51	1	20	0	38	0	0
52	1	28	0	52	0	0
53	1	215	0	0	0	0
53	3	3	0	0	0	0
53	4	8	0	0	0	0
53	LA	2	0	0	0	0
53	LB	1	0	0	0	0
53	LC	1	0	0	0	0
53	LE	1	0	0	0	0
53	LI	1	0	0	0	0
53	LP	1	0	0	0	0
53	LV	1	0	0	0	0
53	LY	1	0	0	0	0
53	Lb	1	0	0	0	0
53	Le	1	0	0	0	0
53	Lj	2	0	0	0	0
54	1	177	0	0	0	0
54	3	2	0	0	0	0
54	4	1	0	0	0	0
54	LA	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	LC	2	0	0	0	0
54	LI	1	0	0	0	0
54	LN	1	0	0	0	0
54	Lb	1	0	0	0	0
54	Le	1	0	0	0	0
54	Lo	1	0	0	0	0
55	Lg	1	0	0	0	0
55	Lj	1	0	0	0	0
55	Lm	1	0	0	0	0
55	Lo	1	0	0	0	0
55	Lp	1	0	0	0	0
56	1	1821	0	0	22	0
56	3	31	0	0	0	0
56	4	67	0	0	0	0
56	9	1	0	0	0	0
56	LA	12	0	0	0	0
56	LB	23	0	0	0	0
56	LC	29	0	0	0	0
56	LD	3	0	0	1	0
56	LE	8	0	0	2	0
56	LF	16	0	0	0	0
56	LG	11	0	0	0	0
56	LI	8	0	0	0	0
56	LJ	1	0	0	0	0
56	LL	18	0	0	1	0
56	LM	1	0	0	0	0
56	LN	19	0	0	1	0
56	LO	5	0	0	0	0
56	LP	12	0	0	1	0
56	LQ	15	0	0	1	0
56	LR	4	0	0	0	0
56	LS	7	0	0	0	0
56	LT	13	0	0	0	0
56	LV	7	0	0	0	0
56	LW	1	0	0	1	0
56	LX	2	0	0	1	0
56	LY	6	0	0	0	0
56	LZ	1	0	0	0	0
56	La	19	0	0	0	0
56	Lb	7	0	0	0	0
56	Ld	3	0	0	0	0
56	Le	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	Lf	11	0	0	0	0
56	Lg	3	0	0	0	0
56	Lh	6	0	0	0	0
56	Li	5	0	0	0	0
56	Lj	17	0	0	0	0
56	Lk	1	0	0	0	0
56	Ll	2	0	0	0	0
56	Lm	1	0	0	0	0
56	Ln	1	0	0	0	0
56	Lo	7	0	0	0	0
56	Lp	2	0	0	0	0
56	Lq	9	0	0	0	0
All	All	131048	0	94032	750	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 (750) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1939:U:H3	1:1:2045:G:H1	1.22	0.83
1:1:1000:G:H1	1:1:1017:U:H3	1.28	0.81
3:4:79:A:H2'	3:4:80:A:H8	1.46	0.78
1:1:960:C:H4'	1:1:961:C:H5'	1.65	0.78
1:1:1220:G:O6	1:1:1234:A:N1	2.16	0.78
1:1:3132:A:H62	9:LE:191:LYS:HD3	1.45	0.77
48:Ls:129:GLU:HG3	48:Ls:131:GLY:H	1.51	0.76
9:LE:121:GLU:HA	9:LE:124:GLN:HG2	1.68	0.74
9:LE:12:LYS:HD3	9:LE:15:ARG:HA	1.68	0.74
1:1:2632:A:O2'	14:LJ:127:ASP:OD1	2.06	0.73
1:1:766:G:H22	21:LQ:97:ARG:HH11	1.33	0.73
1:1:1221:C:H3'	1:1:1222:C:H5''	1.70	0.72
3:4:83:C:H41	29:LY:50:ARG:HH22	1.38	0.71
38:Lh:75:TYR:HB3	38:Lh:81:LEU:HD22	1.72	0.70
1:1:1216:G:H2'	1:1:1217:G:C8	2.26	0.69
26:LV:89:ARG:NH1	26:LV:139:MET:SD	2.64	0.69
48:Ls:58:MET:SD	48:Ls:58:MET:N	2.66	0.69
1:1:1265:G:H4'	48:Ls:83:ASN:HB2	1.75	0.68
1:1:2838:OMC:H5	1:1:2906:G:H1	1.42	0.68
1:1:302:U:OP1	39:Li:93:LYS:NZ	2.27	0.68
1:1:2802:UR3:OP2	56:1:3804:HOH:O	2.11	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2705:A:N1	56:1:3839:HOH:O	2.27	0.67
1:1:2800:G:OP2	56:1:3804:HOH:O	2.12	0.67
1:1:394:C:H5''	1:1:395:A:H5''	1.75	0.67
1:1:2224:G:O2'	1:1:2226:C:N4	2.28	0.67
1:1:673:G:OP1	16:LL:39:ARG:NH2	2.27	0.66
13:LI:66:GLU:OE1	13:LI:69:ARG:NH2	2.28	0.66
23:LS:162:LYS:HG3	36:Lf:38:ASP:HB3	1.77	0.66
1:1:1332:G:H22	7:LC:294:THR:HB	1.60	0.66
1:1:2690:UY1:N3	56:1:3858:HOH:O	2.29	0.66
1:1:145:U:OP2	18:LN:49:ARG:NH2	2.27	0.66
1:1:3209:A:OP1	9:LE:64:ARG:NH2	2.27	0.65
14:LJ:78:GLU:OE2	14:LJ:167:ARG:NH1	2.29	0.65
1:1:2176:A:H2'	1:1:2177:A:C8	2.32	0.65
24:LT:51:GLY:HA3	24:LT:92:ARG:HG3	1.77	0.65
9:LE:162:GLN:NE2	9:LE:166:ASP:OD2	2.29	0.65
7:LC:55:GLU:N	7:LC:55:GLU:OE1	2.30	0.65
1:1:275:G:O2'	1:1:276:G:OP2	2.14	0.65
1:1:1695:A:H4'	1:1:1696:A:H5'	1.77	0.64
7:LC:100:MET:HE3	7:LC:103:PRO:HA	1.80	0.64
12:LH:31:ARG:NH1	12:LH:151:ASN:OD1	2.29	0.64
2:3:7:G:OP1	8:LD:33:ARG:NH1	2.30	0.64
1:1:959:A:N6	56:1:3870:HOH:O	2.31	0.64
29:LY:59:ARG:HB2	29:LY:102:ASN:HB2	1.79	0.64
23:LS:12:ARG:NH2	23:LS:57:GLU:OE2	2.29	0.64
48:Ls:26:PHE:HB3	48:Ls:87:VAL:HB	1.78	0.64
1:1:1641:G:H2'	1:1:1642:G:C8	2.32	0.64
31:La:82:VAL:O	31:La:87:ARG:NH1	2.31	0.64
1:1:1216:G:N1	1:1:1239:G:N7	2.45	0.63
1:1:1244:G:OP1	1:1:1262:C:O2'	2.16	0.63
1:1:2223:PSU:H2'	1:1:2224:G:C8	2.33	0.63
1:1:2495:U:H2'	1:1:2496:G:H8	1.62	0.63
1:1:3281:G:O2'	1:1:3283:A:OP2	2.16	0.63
1:1:360:A:N1	56:1:3867:HOH:O	2.31	0.63
48:Ls:56:ASN:O	48:Ls:60:ARG:NH2	2.30	0.63
11:LG:74:VAL:HB	11:LG:237:GLY:HA3	1.81	0.63
14:LJ:33:ARG:HD2	14:LJ:121:ILE:HA	1.80	0.63
36:Lf:105:TYR:HB2	36:Lf:106:PRO:HD3	1.80	0.63
1:1:1744:C:H3'	1:1:1745:U:H5''	1.79	0.63
41:Lk:65:ASN:N	41:Lk:65:ASN:OD1	2.31	0.63
30:LZ:32:THR:OG1	30:LZ:34:SER:O	2.17	0.63
1:1:1464:A:O2'	1:1:1838:A:H1'	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Ls:57:THR:HA	48:Ls:60:ARG:HE	1.63	0.62
7:LC:301:ARG:O	21:LQ:67:ARG:NH1	2.31	0.62
25:LU:61:LYS:HB2	25:LU:73:ILE:HB	1.81	0.62
45:Lo:25:VAL:HG22	45:Lo:72:LEU:HD22	1.80	0.62
1:1:1076:A:OP1	24:LT:120:LYS:NZ	2.31	0.62
1:1:2392:G:H2'	1:1:2393:A:H8	1.64	0.62
16:LL:177:ILE:HD11	16:LL:181:ALA:HA	1.80	0.62
48:Ls:16:LYS:HG2	48:Ls:64:LYS:HD3	1.81	0.62
1:1:1796:A:H2'	1:1:1797:A:C8	2.34	0.62
1:1:1693:G:N7	56:1:3869:HOH:O	2.31	0.62
1:1:1796:A:H2'	1:1:1797:A:H8	1.64	0.62
47:Lq:11:GLU:OE2	47:Lq:14:ARG:NH2	2.32	0.62
1:1:3107:G:O2'	6:LB:129:ALA:O	2.14	0.62
25:LU:24:ASN:HB3	25:LU:111:GLU:HG3	1.82	0.62
1:1:1779:A:H2'	1:1:1780:A:H8	1.65	0.61
18:LN:203:ARG:NH2	56:LN:401:HOH:O	2.32	0.61
13:LI:106:ALA:HB1	13:LI:113:THR:HG22	1.82	0.61
1:1:633:1MA:O2'	56:1:3807:HOH:O	2.16	0.61
1:1:1929:G:OP1	22:LR:104:ARG:NH1	2.33	0.61
1:1:2176:A:H2'	1:1:2177:A:H8	1.65	0.61
38:Lh:37:GLN:O	38:Lh:45:LYS:NZ	2.34	0.61
25:LU:28:PRO:HB2	25:LU:34:PHE:HB3	1.82	0.61
38:Lh:16:ASN:ND2	38:Lh:19:GLU:OE1	2.33	0.61
48:Ls:185:MET:SD	48:Ls:185:MET:N	2.73	0.61
1:1:124:A:OP1	11:LG:108:LYS:NZ	2.30	0.60
20:LP:16:ARG:NH1	56:LP:302:HOH:O	2.34	0.60
1:1:2332:G:H2'	1:1:2333:G:C8	2.35	0.60
13:LI:202:ASN:O	13:LI:202:ASN:ND2	2.34	0.60
31:La:126:ARG:NH1	31:La:146:GLU:OE2	2.34	0.60
40:Lj:29:ASN:O	40:Lj:32:LYS:NZ	2.28	0.60
48:Ls:121:VAL:HG13	48:Ls:158:LEU:HD11	1.82	0.60
34:Ld:9:ARG:HG2	34:Ld:13:ALA:HB2	1.83	0.60
1:1:766:G:N2	21:LQ:97:ARG:HH11	2.00	0.60
25:LU:40:GLU:O	25:LU:44:ASN:ND2	2.32	0.60
8:LD:60:ILE:HB	8:LD:80:SER:HB2	1.84	0.60
1:1:1233:G:H2'	1:1:1234:A:C8	2.36	0.60
11:LG:31:GLU:OE2	11:LG:33:ARG:NH1	2.34	0.60
25:LU:59:VAL:HG23	25:LU:60:ILE:HG12	1.82	0.60
28:LX:102:LYS:NZ	56:LX:201:HOH:O	2.35	0.60
10:LF:138:PRO:HA	10:LF:234:LEU:HD13	1.84	0.60
1:1:597:G:OP2	7:LC:317:LYS:NZ	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:608:U:OP2	47:Lq:132:LYS:NZ	2.35	0.59
1:1:1779:A:H2'	1:1:1780:A:C8	2.37	0.59
3:4:55:PSU:HN3	3:4:62:A:H2	1.48	0.59
8:LD:120:THR:O	8:LD:251:ARG:NH2	2.35	0.59
1:1:1252:U:N3	1:1:1255:C:OP2	2.35	0.59
1:1:2496:G:H2'	1:1:2497:G:H8	1.68	0.59
1:1:3113:A:N6	56:1:3900:HOH:O	2.34	0.59
1:1:1704:U:H1'	1:1:1705:C:C6	2.37	0.59
22:LR:39:GLN:OE1	22:LR:42:ARG:NH1	2.35	0.59
2:3:40:C:O2	14:LJ:73:ARG:NH1	2.35	0.59
30:LZ:83:ARG:NH1	37:Lg:98:GLU:OE1	2.36	0.59
1:1:2181:G:H2'	1:1:2182:A2M:H8	1.84	0.59
1:1:1464:A:O2'	1:1:1838:A:N3	2.31	0.58
1:1:2337:C:O2	6:LB:257:HIS:NE2	2.33	0.58
32:Lb:32:LEU:O	32:Lb:40:ARG:NH1	2.36	0.58
1:1:134:G:H2'	1:1:135:G:O4'	2.04	0.58
1:1:3122:U:O2'	1:1:3123:U:O5'	2.20	0.58
13:LI:93:PRO:HB2	13:LI:125:THR:HG22	1.85	0.58
3:4:156:U:OP2	11:LG:87:LYS:NZ	2.35	0.58
9:LE:190:ARG:NH1	56:LE:402:HOH:O	2.36	0.58
1:1:154:G:H2'	1:1:155:A:H8	1.69	0.58
30:LZ:51:LYS:O	30:LZ:64:ARG:NH1	2.36	0.58
16:LL:47:ALA:HB3	16:LL:48:PRO:HD3	1.85	0.58
1:1:2574:G:H2'	1:1:2575:C:H6	1.68	0.58
1:1:825:A:N7	56:1:3874:HOH:O	2.32	0.57
1:1:2101:A:HO2'	40:Lj:2:THR:N	2.02	0.57
1:1:2974:A:H2'	1:1:2975:G:H8	1.70	0.57
1:1:2270:G:O2'	1:1:2273:U:OP2	2.22	0.57
7:LC:60:GLN:O	40:Lj:52:LYS:NZ	2.36	0.57
48:Ls:130:PRO:O	48:Ls:133:THR:OG1	2.23	0.57
1:1:2392:G:H2'	1:1:2393:A:C8	2.39	0.57
1:1:1250:U:H3	1:1:1257:A:H61	1.52	0.57
1:1:1447:G:N2	1:1:1450:A:OP2	2.37	0.57
48:Ls:31:ASP:OD1	48:Ls:83:ASN:ND2	2.37	0.57
1:1:2045:G:H2'	1:1:2046:C:O4'	2.05	0.57
8:LD:245:GLU:OE1	8:LD:249:GLN:NE2	2.33	0.57
13:LI:101:LYS:HB3	13:LI:104:SER:HB3	1.87	0.57
1:1:1778:A:H2'	1:1:1779:A:C8	2.39	0.57
1:1:2355:C:O2'	6:LB:267:ARG:NH2	2.35	0.57
1:1:2495:U:H2'	1:1:2496:G:C8	2.39	0.57
1:1:652:A:H2'	1:1:653:A:C8	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:3144:U:OP1	19:LO:170:TYR:OH	2.22	0.57
3:4:82:U:OP1	3:4:85:G:N2	2.38	0.57
19:LO:139:THR:HG22	19:LO:141:GLY:H	1.69	0.57
1:1:1226:G:O2'	1:1:1253:A:N3	2.38	0.56
1:1:1469:G:H21	37:Lg:7:THR:HG22	1.70	0.56
1:1:1766:G:H2'	1:1:1767:A:C8	2.41	0.56
7:LC:365:ALA:HB3	23:LS:28:ARG:HD2	1.87	0.56
14:LJ:38:LEU:HD12	14:LJ:68:VAL:HG12	1.87	0.56
17:LM:32:GLU:HG2	23:LS:72:VAL:HG21	1.87	0.56
1:1:1067:A:OP1	24:LT:35:ARG:NH1	2.38	0.56
9:LE:190:ARG:NH2	56:LE:401:HOH:O	2.34	0.56
9:LE:177:ASP:OD1	9:LE:177:ASP:N	2.38	0.56
1:1:3298:U:O2'	1:1:3299:U:OP1	2.23	0.56
48:Ls:18:LEU:HA	48:Ls:21:GLU:HG2	1.88	0.56
48:Ls:57:THR:HB	48:Ls:60:ARG:HB2	1.87	0.56
1:1:675:U:OP2	16:LL:36:ARG:NH2	2.39	0.55
1:1:1745:U:H4'	1:1:1745:U:OP1	2.06	0.55
1:1:2167:C:H2'	1:1:2168:U:C6	2.41	0.55
1:1:2496:G:H2'	1:1:2497:G:C8	2.41	0.55
1:1:1222:C:H2'	1:1:1223:A2M:H8	1.88	0.55
17:LM:73:PRO:HG2	17:LM:76:ALA:HB2	1.87	0.55
6:LB:228:VAL:HG21	6:LB:271:MET:HE2	1.88	0.55
1:1:1527:G:OP1	18:LN:67:ARG:NH1	2.39	0.55
1:1:2919:C:H2'	1:1:2920:G:C8	2.42	0.55
1:1:70:C:O2'	1:1:102:G:O2'	2.23	0.55
1:1:435:G:OP1	47:Lq:126:LYS:NZ	2.35	0.55
1:1:2518:G:N2	11:LG:41:GLN:O	2.40	0.55
1:1:2549:A:N7	56:1:3885:HOH:O	2.33	0.55
8:LD:225:GLN:NE2	56:LD:401:HOH:O	2.35	0.55
1:1:1218:U:H4'	1:1:1219:G:H3'	1.88	0.55
1:1:2621:G:H2'	1:1:2622:G:H8	1.71	0.55
13:LI:205:ASN:ND2	13:LI:208:GLU:OE1	2.34	0.55
1:1:3:G:H2'	1:1:4:U:C6	2.41	0.55
1:1:1022:C:OP2	8:LD:5:LYS:NZ	2.38	0.55
7:LC:21:GLU:OE2	7:LC:263:LYS:NZ	2.39	0.55
29:LY:53:ASP:HB3	29:LY:109:HIS:H	1.72	0.55
1:1:656:U:H2'	1:1:657:U:C6	2.42	0.55
1:1:2461:C:H2'	1:1:2462:U:H6	1.72	0.55
21:LQ:67:ARG:NH2	56:LQ:304:HOH:O	2.38	0.55
48:Ls:65:THR:HG21	48:Ls:77:LEU:HD21	1.88	0.55
1:1:3194:G:H2'	1:1:3195:U:C6	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:LN:181:ASN:OD1	18:LN:184:ARG:NH2	2.40	0.54
48:Ls:19:LEU:HD11	48:Ls:64:LYS:HE2	1.89	0.54
1:1:1607:U:H2'	1:1:1794:A:N6	2.21	0.54
1:1:1638:G:H2'	1:1:1639:A:C8	2.42	0.54
1:1:1676:A:H2'	1:1:1677:A:C8	2.42	0.54
1:1:1920:G:H21	1:1:3303:A:H8	1.54	0.54
1:1:534:C:N4	1:1:535:U:O4	2.40	0.54
1:1:135:G:H2'	1:1:136:C:C6	2.43	0.54
1:1:1164:U:OP1	23:LS:161:THR:HG21	2.08	0.54
25:LU:27:GLN:OE1	25:LU:27:GLN:N	2.37	0.54
1:1:643:C:H2'	1:1:644:A:H8	1.73	0.54
1:1:644:A:H2'	1:1:645:A:C8	2.43	0.54
1:1:1260:C:H2'	1:1:1261:A:H8	1.73	0.54
1:1:766:G:N2	21:LQ:97:ARG:HD2	2.23	0.54
1:1:1220:G:C6	1:1:1234:A:N1	2.75	0.54
7:LC:8:THR:HG23	7:LC:148:GLU:OE1	2.08	0.54
23:LS:133:GLU:OE1	23:LS:133:GLU:N	2.41	0.54
1:1:292:G:C8	39:Li:40:GLY:HA3	2.43	0.54
1:1:925:U:H3'	31:La:13:GLY:HA2	1.90	0.54
1:1:959:A:N6	56:1:3813:HOH:O	2.22	0.54
1:1:1214:A:N6	1:1:1260:C:OP2	2.35	0.54
1:1:1241:U:O5'	48:Ls:42:ARG:NH2	2.41	0.54
37:Lg:79:GLY:O	37:Lg:80:SER:OG	2.25	0.54
48:Ls:19:LEU:HD21	48:Ls:64:LYS:HG3	1.89	0.54
16:LL:115:ARG:NH2	16:LL:155:PHE:O	2.38	0.53
1:1:1064:C:O2'	1:1:1065:U:O5'	2.24	0.53
1:1:3328:G:OP1	34:Ld:9:ARG:NH2	2.42	0.53
30:LZ:6:THR:O	30:LZ:6:THR:OG1	2.19	0.53
1:1:136:C:OP1	11:LG:109:LYS:NZ	2.41	0.53
1:1:2465:U:H2'	1:1:2466:G:H8	1.74	0.53
1:1:2856:A:H5''	43:Lm:125:LYS:HG3	1.91	0.53
14:LJ:61:ARG:N	14:LJ:64:GLU:OE2	2.38	0.53
13:LI:142:ASP:OD1	13:LI:142:ASP:N	2.36	0.53
1:1:2632:A:OP2	14:LJ:95:ARG:NH2	2.42	0.53
39:Li:83:LYS:HD2	39:Li:89:PHE:HD1	1.74	0.53
1:1:470:A:O2'	1:1:471:C:OP2	2.24	0.53
1:1:1223:A2M:H2	1:1:1231:C:H5	1.72	0.53
1:1:2182:A2M:OP2	39:Li:77:ARG:NH2	2.40	0.53
1:1:3294:G:H1'	1:1:3297:G:H5'	1.91	0.53
10:LF:142:TYR:CZ	10:LF:236:ASN:HB2	2.44	0.53
21:LQ:68:THR:HG22	21:LQ:70:ALA:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:119:U:O2	1:1:122:A:H5''	2.07	0.53
3:4:79:A:H2'	3:4:80:A:C8	2.35	0.53
12:LH:104:GLU:N	12:LH:104:GLU:OE1	2.42	0.53
1:1:2064:C:H2'	1:1:2065:U:C6	2.44	0.53
1:1:2499:C:H2'	1:1:2500:U:O4'	2.09	0.53
30:LZ:57:SER:O	30:LZ:61:ILE:HG12	2.09	0.53
1:1:410:A:H2'	1:1:411:A:C8	2.45	0.52
1:1:1758:G:O2'	1:1:1760:G:OP2	2.25	0.52
1:1:215:A:N6	56:1:3829:HOH:O	2.26	0.52
1:1:1419:U:H5''	1:1:1420:OMC:H5'	1.90	0.52
16:LL:142:GLN:N	16:LL:142:GLN:OE1	2.42	0.52
1:1:766:G:C8	21:LQ:93:SER:HB3	2.44	0.52
1:1:2465:U:H2'	1:1:2466:G:C8	2.45	0.52
5:LA:79:ASN:ND2	5:LA:165:MET:SD	2.83	0.52
1:1:462:A:H2'	1:1:463:C:C6	2.45	0.52
14:LJ:93:ARG:HA	14:LJ:93:ARG:HH11	1.74	0.52
1:1:2538:G:OP2	1:1:2539:A:O2'	2.23	0.52
1:1:3159:U:H1'	9:LE:190:ARG:NH1	2.24	0.52
1:1:1223:A2M:H2	1:1:1231:C:C5	2.45	0.51
1:1:726:A:OP1	21:LQ:94:ARG:NH1	2.40	0.51
1:1:2338:G:OP1	56:1:3809:HOH:O	2.19	0.51
1:1:405:G:OP1	20:LP:62:ARG:NH1	2.43	0.51
17:LM:123:LEU:HD22	19:LO:195:VAL:HG13	1.92	0.51
1:1:1219:G:H22	1:1:1227:A:P	2.33	0.51
1:1:2232:U:O2'	1:1:2233:A:O5'	2.27	0.51
1:1:615:C:H2'	1:1:616:A:C8	2.46	0.51
1:1:950:G:N7	56:1:3902:HOH:O	2.35	0.51
1:1:2623:C:OP2	14:LJ:143:ARG:NH1	2.44	0.51
14:LJ:109:GLU:HG2	14:LJ:112:ASP:HB2	1.93	0.51
33:Lc:84:CYS:SG	33:Lc:93:MET:HE1	2.51	0.51
1:1:643:C:H2'	1:1:644:A:C8	2.46	0.51
1:1:1047:A:H4'	1:1:1048:A:O5'	2.09	0.51
1:1:1795:U:O2'	1:1:1796:A:O5'	2.28	0.51
1:1:1813:G:OP1	42:Ll:10:LYS:NZ	2.43	0.51
1:1:2463:A:O2'	1:1:2465:U:O4'	2.28	0.50
1:1:2876:OMG:OP1	26:LV:48:LEU:HA	2.10	0.50
1:1:533:C:H2'	1:1:534:C:C6	2.46	0.50
1:1:806:U:H5''	5:LA:21:ARG:HD3	1.92	0.50
1:1:2854:G:O2'	43:Lm:100:TYR:O	2.29	0.50
48:Ls:65:THR:HB	48:Ls:74:GLU:HG2	1.93	0.50
48:Ls:189:GLN:OE1	48:Ls:193:GLN:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2043:C:H2'	1:1:2044:G:H4'	1.93	0.50
1:1:955:G:H2'	1:1:956:PSU:O4'	2.11	0.50
1:1:1595:C:H2'	1:1:1596:U:C6	2.47	0.50
12:LH:48:VAL:HG12	12:LH:49:LYS:HG3	1.93	0.50
1:1:1893:A:N3	1:1:2083:G:H2'	2.27	0.50
1:1:2069:A:H2'	1:1:2070:A:H8	1.76	0.50
1:1:2960:C:O2'	6:LB:181:GLU:OE2	2.22	0.50
1:1:1077:U:C4	24:LT:120:LYS:HG3	2.47	0.50
1:1:2500:U:H2'	1:1:2501:U:H4'	1.92	0.50
1:1:3332:A:O2'	1:1:3333:G:OP1	2.29	0.50
7:LC:154:ASP:OD1	7:LC:155:SER:N	2.45	0.50
28:LX:79:PRO:HD3	38:Lh:36:ILE:HG13	1.93	0.50
38:Lh:16:ASN:ND2	38:Lh:18:GLU:OE1	2.44	0.50
1:1:2123:G:H2'	1:1:2124:G:H8	1.77	0.50
2:3:107:C:OP2	13:LI:203:HIS:NE2	2.28	0.50
14:LJ:162:ARG:O	14:LJ:166:GLN:HG2	2.12	0.50
33:Lc:29:GLY:O	33:Lc:33:THR:OG1	2.25	0.50
1:1:244:G:N2	1:1:245:U:O4	2.42	0.49
6:LB:340:ARG:HH12	6:LB:343:LEU:HG	1.77	0.49
1:1:830:A:C5	1:1:831:C:H1'	2.47	0.49
1:1:1332:G:N2	7:LC:294:THR:HB	2.27	0.49
1:1:1726:C:O2'	41:Lk:4:GLU:OE2	2.29	0.49
1:1:2964:A:H2'	1:1:2965:U:O4'	2.12	0.49
11:LG:26:LYS:HE2	11:LG:30:LEU:HD12	1.94	0.49
3:4:8:C:H2'	3:4:9:A:H8	1.78	0.49
31:La:100:PRO:HG2	31:La:123:VAL:HG12	1.94	0.49
32:Lb:53:ALA:C	32:Lb:55:LYS:H	2.18	0.49
1:1:1652:C:OP1	22:LR:60:ARG:NH1	2.46	0.49
1:1:1655:G:H2'	1:1:1656:C:H6	1.78	0.49
1:1:132:U:H1'	1:1:133:C:H5''	1.94	0.49
1:1:766:G:C2	21:LQ:97:ARG:HD2	2.48	0.49
1:1:2919:C:H2'	1:1:2920:G:H8	1.77	0.49
1:1:3210:U:OP1	9:LE:95:ARG:NH1	2.45	0.49
3:4:83:C:O2'	3:4:85:G:O6	2.19	0.49
18:LN:67:ARG:NH1	18:LN:127:TYR:OH	2.45	0.49
1:1:1941:G:O4'	1:1:2044:G:N2	2.46	0.49
18:LN:124:ASP:OD1	18:LN:125:SER:N	2.46	0.49
48:Ls:134:SER:HA	48:Ls:137:GLN:HG2	1.94	0.49
1:1:1208:A:H2'	1:1:1209:G:C8	2.48	0.49
1:1:2461:C:H2'	1:1:2462:U:C6	2.48	0.49
5:LA:2:GLY:HA2	5:LA:207:VAL:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:445:G:H2'	1:1:446:A:O4'	2.13	0.49
1:1:2727:U:H2'	1:1:2728:A:H8	1.78	0.49
5:LA:52:PRO:HB2	5:LA:191:VAL:HG21	1.94	0.49
11:LG:166:VAL:HA	11:LG:169:LEU:HD23	1.94	0.49
25:LU:56:LEU:HG	25:LU:60:ILE:HB	1.94	0.49
1:1:1134:U:H3'	1:1:1135:G:C8	2.47	0.49
16:LL:60:CYS:HB2	16:LL:65:TYR:O	2.12	0.49
17:LM:131:GLU:OE1	19:LO:184:LYS:HA	2.13	0.49
22:LR:70:ARG:HE	22:LR:75:HIS:HB2	1.78	0.49
1:1:64:A:OP1	18:LN:172:ARG:NH2	2.45	0.48
1:1:135:G:H2'	1:1:136:C:H6	1.78	0.48
7:LC:301:ARG:HH21	21:LQ:69:GLU:HG3	1.78	0.48
16:LL:5:HIS:N	56:LL:302:HOH:O	2.29	0.48
41:Lk:56:GLU:O	41:Lk:60:GLN:HG2	2.13	0.48
47:Lq:128:GLU:OE1	47:Lq:128:GLU:N	2.40	0.48
47:Lq:140:ARG:O	47:Lq:140:ARG:NE	2.46	0.48
1:1:1001:G:H2'	1:1:1002:G:C8	2.48	0.48
1:1:2387:A:OP1	18:LN:90:ASN:ND2	2.46	0.48
5:LA:115:ASN:OD1	5:LA:128:ARG:HD2	2.12	0.48
30:LZ:2:LYS:HB2	30:LZ:5:LYS:HE3	1.96	0.48
1:1:1246:A:H61	15:LK:136:ALA:HA	1.78	0.48
1:1:3319:C:OP1	56:1:3810:HOH:O	2.20	0.48
3:4:19:C:H2'	3:4:20:U:C6	2.49	0.48
20:LP:64:ALA:O	20:LP:80:ARG:NH1	2.47	0.48
38:Lh:19:GLU:OE1	38:Lh:19:GLU:N	2.40	0.48
1:1:1938:G:H2'	1:1:1939:U:C6	2.49	0.48
1:1:3176:G:H2'	1:1:3177:C:C6	2.48	0.48
16:LL:64:LYS:HE2	16:LL:65:TYR:CZ	2.48	0.48
32:Lb:5:LYS:HE2	32:Lb:8:SER:HB2	1.96	0.48
1:1:1223:A2M:H2	1:1:1231:C:H41	1.79	0.48
1:1:2064:C:O2'	1:1:2065:U:OP1	2.31	0.48
1:1:1266:C:H2'	1:1:1267:C:C6	2.48	0.48
24:LT:17:ARG:NH1	24:LT:45:ASN:OD1	2.47	0.48
1:1:959:A:N6	56:1:3830:HOH:O	2.26	0.48
1:1:1517:A:H2'	1:1:1518:A:C8	2.49	0.48
1:1:1601:G:OP1	44:Lr:16:LYS:NZ	2.46	0.48
1:1:2058:A:H2'	1:1:2059:A:C8	2.49	0.48
48:Ls:98:GLU:HA	48:Ls:101:LEU:HD23	1.95	0.48
1:1:2574:G:H2'	1:1:2575:C:C6	2.47	0.48
30:LZ:75:ASN:OD1	30:LZ:76:TYR:N	2.46	0.48
3:4:9:A:H2'	3:4:10:A:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LF:13:LEU:O	10:LF:15:PRO:HD3	2.13	0.48
36:Lf:60:GLU:HG3	36:Lf:65:LYS:HE3	1.95	0.48
32:Lb:60:GLY:O	32:Lb:62:ARG:N	2.47	0.47
1:1:1938:G:H2'	1:1:1939:U:H6	1.78	0.47
20:LP:113:ILE:HG13	20:LP:153:ALA:HB2	1.96	0.47
27:LW:61:LYS:O	56:LW:201:HOH:O	2.20	0.47
1:1:1233:G:H2'	1:1:1234:A:H8	1.80	0.47
13:LI:208:GLU:OE1	13:LI:208:GLU:N	2.46	0.47
1:1:1917:OMU:HM23	1:1:1917:OMU:H1'	1.72	0.47
1:1:2356:G:H8	56:1:4060:HOH:O	1.91	0.47
3:4:83:C:H41	29:LY:50:ARG:NH2	2.07	0.47
1:1:2148:G:O2'	1:1:2277:UY1:OP2	2.30	0.47
1:1:2370:C:H2'	1:1:2371:U:H6	1.79	0.47
29:LY:50:ARG:HG2	29:LY:51:LYS:N	2.29	0.47
34:Ld:13:ALA:O	34:Ld:85:ARG:NH2	2.41	0.47
48:Ls:61:ARG:CZ	48:Ls:77:LEU:HD22	2.44	0.47
1:1:1219:G:N2	1:1:1227:A:O5'	2.47	0.47
1:1:131:U:O2'	1:1:134:G:N2	2.24	0.47
1:1:477:C:H2'	1:1:478:G:H8	1.78	0.47
18:LN:66:VAL:HG12	18:LN:67:ARG:H	1.78	0.47
29:LY:53:ASP:HB2	29:LY:107:LYS:O	2.15	0.47
1:1:2498:A:H2'	1:1:2499:C:C6	2.50	0.47
18:LN:68:ARG:HG3	18:LN:128:LYS:HG3	1.96	0.47
1:1:435:G:H2'	1:1:436:C:C6	2.49	0.47
1:1:967:U:H2'	1:1:968:U:H6	1.78	0.47
1:1:2974:A:H2'	1:1:2975:G:C8	2.49	0.47
8:LD:116:ASP:OD1	8:LD:116:ASP:N	2.40	0.47
1:1:1064:C:HO2'	1:1:1065:U:P	2.38	0.47
1:1:1544:G:O2'	1:1:1545:G:H8	1.97	0.47
3:4:71:A:N6	3:4:83:C:O2	2.48	0.47
38:Lh:84:ASP:OD1	38:Lh:84:ASP:N	2.47	0.47
1:1:956:PSU:H2'	1:1:957:C:C6	2.50	0.46
34:Ld:9:ARG:O	34:Ld:13:ALA:N	2.48	0.46
1:1:1744:C:H3'	1:1:1745:U:C5'	2.44	0.46
1:1:2389:U:H2'	1:1:2390:U:C6	2.50	0.46
1:1:2655:A:H2'	1:1:2656:A:C8	2.50	0.46
6:LB:35:ASP:OD1	6:LB:36:ASP:N	2.48	0.46
12:LH:190:VAL:HG12	12:LH:191:GLU:HG2	1.98	0.46
1:1:1638:G:H2'	1:1:1639:A:H8	1.80	0.46
25:LU:22:ILE:HB	25:LU:109:VAL:HG12	1.96	0.46
30:LZ:53:THR:HG22	30:LZ:55:ARG:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Lp:5:THR:HG21	46:Lp:9:GLY:H	1.80	0.46
1:1:2621:G:H2'	1:1:2622:G:C8	2.50	0.46
14:LJ:61:ARG:NH1	45:Lo:105:VAL:O	2.47	0.46
1:1:1022:C:H2'	1:1:1023:A:C8	2.51	0.46
1:1:1887:C:O2	6:LB:241:ARG:NH2	2.48	0.46
10:LF:91:PHE:HB2	10:LF:145:PRO:HG3	1.97	0.46
31:La:149:ALA:HB2	39:Li:16:LEU:HA	1.98	0.46
1:1:2462:U:H2'	1:1:2463:A:O4'	2.16	0.46
9:LE:56:THR:HG22	9:LE:108:LYS:HG2	1.98	0.46
31:La:75:ILE:HG12	31:La:114:GLY:HA2	1.98	0.46
1:1:1454:U:OP1	22:LR:5:ARG:NH1	2.48	0.46
1:1:1549:C:C2	1:1:1552:G:H5'	2.51	0.46
8:LD:104:LEU:HD11	8:LD:108:ARG:HH21	1.80	0.46
16:LL:147:THR:HA	38:Lh:124:LYS:HA	1.98	0.46
35:Le:80:VAL:O	35:Le:83:VAL:HG12	2.16	0.46
1:1:581:G:OP1	35:Le:63:LYS:NZ	2.46	0.46
1:1:1762:U:H2'	1:1:1763:C:C6	2.51	0.46
1:1:2727:U:H2'	1:1:2728:A:C8	2.51	0.46
1:1:371:A:H4'	29:LY:90:THR:HG22	1.97	0.46
1:1:766:G:H22	21:LQ:97:ARG:NH1	2.06	0.46
1:1:3297:G:H2'	1:1:3298:U:C6	2.51	0.46
1:1:3332:A:HO2'	1:1:3333:G:P	2.39	0.46
16:LL:158:GLU:CD	16:LL:158:GLU:H	2.24	0.46
21:LQ:90:VAL:HG13	21:LQ:94:ARG:HD2	1.98	0.46
30:LZ:89:GLU:H	30:LZ:89:GLU:CD	2.24	0.46
1:1:650:U:H2'	1:1:651:OMC:C6	2.51	0.45
1:1:1515:C:H2'	1:1:1516:U:C6	2.50	0.45
1:1:3005:U:O2'	1:1:3006:A:H5'	2.16	0.45
1:1:3042:C:H2'	1:1:3043:G:O4'	2.16	0.45
1:1:3297:G:H2'	1:1:3298:U:H6	1.81	0.45
11:LG:147:GLU:OE2	18:LN:6:TYR:OH	2.32	0.45
20:LP:10:ALA:HB3	20:LP:13:LYS:HE3	1.97	0.45
1:1:462:A:H2'	1:1:463:C:H6	1.81	0.45
1:1:1371:U:O2'	35:Le:100:ASN:O	2.33	0.45
1:1:2906:G:C2	6:LB:251:ALA:HB1	2.51	0.45
48:Ls:18:LEU:HB3	48:Ls:88:PHE:CE2	2.51	0.45
1:1:290:A:O2'	39:Li:42:GLN:HG2	2.16	0.45
9:LE:131:GLU:N	9:LE:131:GLU:OE1	2.48	0.45
1:1:78:A:N7	16:LL:73:ARG:NH2	2.64	0.45
1:1:1220:G:H2'	1:1:1221:C:C6	2.51	0.45
1:1:1330:U:H2'	1:1:1338:A:H61	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1907:OMG:HM22	1:1:1907:OMG:H1'	1.78	0.45
1:1:2525:U:H2'	1:1:2526:C:C6	2.51	0.45
1:1:2907:OMC:HM23	1:1:2907:OMC:H1'	1.76	0.45
3:4:80:A:H2'	3:4:81:U:C6	2.52	0.45
1:1:799:A2M:N3	40:Lj:11:ARG:HB3	2.32	0.45
1:1:842:G:OP1	46:Lp:17:ARG:NH2	2.39	0.45
1:1:920:C:OP2	31:La:26:ARG:NH1	2.48	0.45
1:1:1843:G:N1	1:1:1846:C:OP2	2.43	0.45
1:1:2069:A:H2'	1:1:2070:A:C8	2.51	0.45
1:1:576:A:H2'	1:1:577:C:C6	2.51	0.45
1:1:999:G:H2'	1:1:1000:G:H8	1.82	0.45
7:LC:161:ASP:HA	7:LC:164:ALA:HB3	1.98	0.45
14:LJ:173:ARG:NH1	14:LJ:173:ARG:HA	2.32	0.45
1:1:137:C:H2'	1:1:138:C:C6	2.51	0.45
1:1:1052:C:H2'	1:1:1053:U:C6	2.52	0.45
8:LD:194:ASP:O	8:LD:195:THR:HG22	2.17	0.45
10:LF:59:LYS:HE3	10:LF:59:LYS:HB2	1.77	0.45
10:LF:239:GLU:CD	10:LF:239:GLU:H	2.25	0.45
1:1:130:C:H2'	1:1:131:U:O4'	2.17	0.45
1:1:424:U:H2'	1:1:425:G:C8	2.52	0.45
1:1:703:A:H3'	31:La:115:LYS:HG3	1.98	0.45
1:1:1252:U:H1'	1:1:1255:C:H5	1.81	0.45
1:1:1548:A:H2'	1:1:1549:C:O4'	2.17	0.45
7:LC:15:LYS:HA	7:LC:15:LYS:HD3	1.77	0.45
1:1:1456:A:H4'	22:LR:26:PRO:HG3	1.99	0.45
1:1:1769:G:N7	56:1:3909:HOH:O	2.35	0.45
1:1:2195:A:H2'	1:1:2196:A:C8	2.52	0.45
1:1:2369:C:H2'	1:1:2370:C:C6	2.52	0.45
1:1:2460:C:H2'	1:1:2461:C:C6	2.52	0.45
23:LS:125:LYS:HG2	23:LS:127:VAL:HG23	1.99	0.45
29:LY:44:VAL:HG13	29:LY:121:ILE:HD13	1.99	0.45
1:1:211:U:H4'	29:LY:99:HIS:CD2	2.52	0.45
1:1:1239:G:H1'	15:LK:123:LYS:HA	1.99	0.45
3:4:36:G:N7	38:Lh:91:ARG:HD3	2.32	0.45
9:LE:142:PHE:O	9:LE:144:LYS:N	2.50	0.45
24:LT:130:ARG:O	24:LT:131:GLN:NE2	2.50	0.45
31:La:95:LYS:O	31:La:96:LYS:HG2	2.16	0.45
6:LB:117:ARG:NH2	6:LB:177:ALA:O	2.40	0.44
6:LB:160:ARG:HG2	6:LB:183:GLN:HA	2.00	0.44
7:LC:238:ASP:OD1	7:LC:238:ASP:N	2.42	0.44
17:LM:28:ALA:HB2	17:LM:52:THR:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:9:C:H2'	1:1:10:U:C6	2.53	0.44
1:1:1485:G:C5	50:PN:1:UNK:HA	2.52	0.44
1:1:2339:G:H2'	1:1:2340:G:C8	2.52	0.44
1:1:2383:C:H2'	1:1:2384:OMU:H6	2.00	0.44
1:1:2390:U:H2'	1:1:2391:U:C6	2.52	0.44
3:4:40:A:H2'	3:4:41:A:C8	2.52	0.44
35:Le:68:MET:HB2	35:Le:69:PRO:HD2	1.99	0.44
1:1:300:A:H2'	1:1:301:A:C8	2.51	0.44
1:1:448:C:N4	1:1:468:G:O2'	2.50	0.44
1:1:1015:C:H3'	1:1:1016:PSU:H5'	2.00	0.44
1:1:1265:G:H2'	1:1:1265:G:N3	2.32	0.44
1:1:1847:A2M:OP1	56:1:3811:HOH:O	2.21	0.44
3:4:84:C:O2'	3:4:85:G:O4'	2.26	0.44
1:1:1016:PSU:H2'	1:1:1017:U:C6	2.52	0.44
1:1:1223:A2M:H8	1:1:1223:A2M:O5'	2.18	0.44
1:1:1260:C:H2'	1:1:1261:A:C8	2.53	0.44
1:1:2326:A2M:H1'	1:1:2326:A2M:HM'3	1.76	0.44
1:1:2342:U:H2'	1:1:2343:U:C6	2.52	0.44
1:1:2182:A2M:HM'3	1:1:2182:A2M:H1'	1.62	0.44
6:LB:102:LEU:H	6:LB:102:LEU:HD23	1.81	0.44
12:LH:120:ILE:HD11	12:LH:179:ASP:HB2	2.00	0.44
33:Lc:44:LEU:HD23	33:Lc:69:PRO:HG2	2.00	0.44
48:Ls:8:LYS:HE3	48:Ls:8:LYS:HB3	1.83	0.44
1:1:1937:C:N4	1:1:1938:G:O6	2.50	0.44
1:1:2509:A:H4'	1:1:2510:C:OP2	2.16	0.44
10:LF:20:LYS:O	10:LF:23:LYS:HG3	2.18	0.44
26:LV:106:ASN:HB2	26:LV:107:PRO:HD2	1.99	0.44
1:1:813:G:O2'	1:1:1844:A:N3	2.47	0.44
1:1:981:G:H2'	1:1:982:C:C6	2.53	0.44
16:LL:32:LYS:O	16:LL:36:ARG:HG3	2.18	0.44
16:LL:140:LYS:HB2	16:LL:140:LYS:HE2	1.68	0.44
19:LO:190:LYS:HG2	19:LO:191:VAL:HG13	2.00	0.44
26:LV:19:LEU:HD12	26:LV:80:ILE:HD13	2.00	0.44
1:1:3131:U:O2'	1:1:3132:A:OP1	2.30	0.44
1:1:1067:A:H2'	1:1:1068:A:C8	2.53	0.44
1:1:1186:A:H2'	1:1:1187:A:C8	2.52	0.44
2:3:23:A:H2'	2:3:24:A:C8	2.53	0.44
48:Ls:119:VAL:HG13	48:Ls:158:LEU:HB2	1.99	0.44
1:1:617:C:H2'	1:1:618:C:C6	2.51	0.43
1:1:1006:A:H3'	1:1:1008:U:H5''	1.99	0.43
1:1:1541:A:HO2'	28:LX:47:ARG:HD3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2817:U:H2'	1:1:2818:U:C6	2.53	0.43
1:1:3008:U:O2'	27:LW:16:GLY:O	2.36	0.43
3:4:77:A:H2'	3:4:78:G:C8	2.53	0.43
3:4:95:G:O2'	40:Lj:81:GLY:O	2.29	0.43
16:LL:117:LYS:HE2	16:LL:117:LYS:HB3	1.80	0.43
1:1:2400:G:H1	1:1:2473:U:H3	1.66	0.43
1:1:1001:G:H2'	1:1:1002:G:H8	1.83	0.43
1:1:1223:A2M:C2	1:1:1231:C:H41	2.31	0.43
1:1:1262:C:H2'	1:1:1263:C:C6	2.53	0.43
1:1:3169:U:H2'	1:1:3170:U:O4'	2.18	0.43
3:4:85:G:O2'	3:4:86:U:H2'	2.19	0.43
6:LB:314:ARG:O	6:LB:334:LYS:HE3	2.18	0.43
1:1:1212:G:H2'	1:1:1213:G:C8	2.53	0.43
1:1:2903:PSU:H5'	1:1:2904:G:OP2	2.18	0.43
11:LG:159:ASP:N	11:LG:159:ASP:OD1	2.50	0.43
12:LH:149:SER:HB2	12:LH:189:ILE:HD11	2.01	0.43
35:Le:12:LYS:O	35:Le:13:LYS:HB2	2.17	0.43
39:Li:107:ARG:HD2	39:Li:108:ARG:HH22	1.82	0.43
1:1:250:C:H2'	1:1:251:U:H6	1.84	0.43
1:1:1212:G:H2'	1:1:1213:G:H8	1.83	0.43
1:1:1875:A:O2'	1:1:3011:G:H4'	2.18	0.43
10:LF:7:PRO:HG2	47:Lq:88:ARG:HB3	2.01	0.43
11:LG:254:LYS:O	11:LG:257:GLU:HG3	2.19	0.43
14:LJ:79:GLU:HG3	14:LJ:80:ILE:N	2.34	0.43
1:1:351:G:N2	1:1:354:A:OP2	2.45	0.43
1:1:1808:A:H2'	1:1:1809:G:C8	2.54	0.43
1:1:1940:U:H2'	1:1:2044:G:N2	2.34	0.43
1:1:2599:A2M:HM'3	32:Lb:9:GLN:OE1	2.17	0.43
1:1:3027:G:C2	1:1:3028:A:C8	3.07	0.43
1:1:3299:U:H2'	1:1:3300:A:H8	1.83	0.43
14:LJ:123:ILE:HD13	14:LJ:123:ILE:HA	1.88	0.43
16:LL:140:LYS:HA	16:LL:143:GLN:HG3	2.01	0.43
38:Lh:15:LYS:O	38:Lh:66:LYS:NZ	2.45	0.43
1:1:515:G:H2'	1:1:516:G:H8	1.83	0.43
1:1:1139:C:OP2	10:LF:100:LYS:NZ	2.52	0.43
1:1:2221:PSU:H3'	1:1:2222:A:H8	1.82	0.43
1:1:2529:U:H5''	1:1:2530:C:H5	1.83	0.43
1:1:2721:A:H2'	1:1:2722:U:H6	1.84	0.43
14:LJ:31:LEU:HD23	14:LJ:31:LEU:HA	1.85	0.43
20:LP:175:GLN:O	20:LP:179:ARG:HG2	2.19	0.43
1:1:1655:G:H2'	1:1:1656:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:LA:113:VAL:HG23	5:LA:134:VAL:HG22	2.01	0.43
8:LD:139:ASP:N	8:LD:139:ASP:OD1	2.52	0.43
1:1:802:A:H2'	1:1:803:U:C6	2.54	0.43
2:3:64:A:H3'	13:LI:204:GLY:O	2.18	0.43
7:LC:217:HIS:CE1	7:LC:264:GLN:HE21	2.36	0.43
14:LJ:57:GLN:OE1	14:LJ:57:GLN:N	2.48	0.43
47:Lq:9:ILE:HG22	47:Lq:47:VAL:HG22	2.01	0.43
1:1:651:OMC:HM23	1:1:651:OMC:H1'	1.83	0.43
1:1:1596:U:H2'	1:1:1597:G:H8	1.83	0.43
2:3:72:G:O2'	2:3:73:U:OP1	2.37	0.43
9:LE:7:THR:HB	9:LE:20:PRO:HG3	2.01	0.43
11:LG:110:GLU:OE2	11:LG:114:ARG:NE	2.40	0.43
1:1:1818:C:H5''	1:1:1819:A:H5'	2.00	0.42
1:1:2389:U:H2'	1:1:2390:U:H6	1.84	0.42
5:LA:83:TYR:HB3	46:Lp:64:MET:HG3	2.01	0.42
6:LB:37:PRO:HA	6:LB:186:GLY:O	2.19	0.42
6:LB:348:SER:C	6:LB:350:LYS:H	2.26	0.42
1:1:533:C:H2'	1:1:534:C:H6	1.83	0.42
1:1:1052:C:H2'	1:1:1053:U:H6	1.83	0.42
1:1:1077:U:H4'	1:1:1078:U:OP2	2.19	0.42
1:1:1242:A:H2'	1:1:1243:A:C8	2.54	0.42
1:1:2642:U:H2'	1:1:2643:C:C6	2.54	0.42
1:1:2993:C:H4'	12:LH:124:ILE:HD13	2.01	0.42
1:1:3047:C:H2'	1:1:3048:U:O4'	2.18	0.42
10:LF:105:PRO:HB3	10:LF:136:VAL:HG12	2.00	0.42
37:Lg:77:TYR:HB3	37:Lg:81:ARG:HG3	2.00	0.42
1:1:1208:A:H2'	1:1:1209:G:H8	1.84	0.42
1:1:3179:G:H2'	1:1:3180:G:H8	1.84	0.42
13:LI:177:ARG:HB3	13:LI:180:GLU:HG2	2.01	0.42
1:1:639:G:O2'	1:1:1418:A:OP1	2.36	0.42
1:1:898:G:H5'	1:1:899:A2M:OP1	2.19	0.42
1:1:1259:U:H2'	1:1:1260:C:O4'	2.19	0.42
1:1:2336:A:N3	1:1:2783:G:O2'	2.42	0.42
10:LF:37:GLU:O	10:LF:41:GLN:HG2	2.19	0.42
14:LJ:54:THR:HG23	14:LJ:61:ARG:HA	2.00	0.42
39:Li:20:LEU:HD12	39:Li:20:LEU:HA	1.89	0.42
1:1:804:G:H2'	1:1:805:C:H6	1.84	0.42
1:1:2186:A:H2'	1:1:2187:A:C8	2.54	0.42
9:LE:115:ASP:C	9:LE:117:ALA:H	2.27	0.42
12:LH:116:ILE:HB	12:LH:126:ARG:HB2	2.01	0.42
12:LH:163:ILE:O	12:LH:166:ILE:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:LW:19:LYS:HB3	27:LW:19:LYS:HE2	1.77	0.42
1:1:1242:A:H2	1:1:1264:U:H4'	1.84	0.42
1:1:1245:G:OP2	1:1:1245:G:H3'	2.19	0.42
29:LY:132:LYS:HE3	29:LY:132:LYS:HB3	1.88	0.42
30:LZ:2:LYS:NZ	33:Lc:39:SER:O	2.33	0.42
41:Lk:27:LYS:HE2	41:Lk:27:LYS:HB3	1.83	0.42
48:Ls:89:THR:HG21	48:Ls:96:VAL:HG11	2.01	0.42
1:1:133:C:H4'	1:1:134:G:O5'	2.19	0.42
1:1:1223:A2M:H3'	1:1:1224:U:H6	1.84	0.42
1:1:1237:C:H2'	1:1:1238:C:C6	2.55	0.42
1:1:2544:G:N3	1:1:2544:G:H2'	2.33	0.42
1:1:3105:A:O2'	6:LB:104:THR:HG22	2.20	0.42
24:LT:117:LYS:HD2	24:LT:117:LYS:HA	1.67	0.42
48:Ls:124:GLY:O	48:Ls:151:GLU:HG3	2.19	0.42
1:1:300:A:H2'	1:1:301:A:H8	1.84	0.42
1:1:1290:G:H5'	19:LO:61:LYS:HE3	2.02	0.42
1:1:2471:U:H2'	1:1:2472:U:C6	2.55	0.42
1:1:2750:OMG:H1'	1:1:2750:OMG:HM23	1.80	0.42
2:3:59:C:H2'	2:3:60:A:H8	1.85	0.42
3:4:26:U:H2'	3:4:27:U:C6	2.55	0.42
6:LB:263:TRP:CD1	6:LB:263:TRP:H	2.37	0.42
28:LX:104:ASN:O	28:LX:108:ILE:HG12	2.20	0.42
37:Lg:68:LYS:HB3	37:Lg:69:PRO:HD3	2.02	0.42
44:Lr:13:LEU:HG	44:Lr:17:ARG:HH12	1.85	0.42
14:LJ:88:LYS:C	14:LJ:89:GLU:HG3	2.45	0.42
48:Ls:92:ASP:O	48:Ls:95:GLU:HG3	2.20	0.42
48:Ls:94:LYS:HG3	48:Ls:97:ARG:HH21	1.85	0.42
48:Ls:100:ILE:H	48:Ls:100:ILE:HG12	1.68	0.42
1:1:250:C:O2'	1:1:251:U:OP1	2.30	0.42
1:1:1262:C:H2'	1:1:1263:C:H6	1.84	0.42
1:1:2066:U:H2'	1:1:2067:A:H8	1.85	0.42
1:1:2458:C:H2'	1:1:2459:U:H6	1.84	0.42
10:LF:138:PRO:HG2	10:LF:139:TRP:CZ3	2.55	0.42
20:LP:14:SER:HB3	20:LP:151:THR:HG22	2.01	0.42
23:LS:130:GLU:H	23:LS:130:GLU:CD	2.25	0.42
24:LT:70:SER:O	24:LT:70:SER:OG	2.34	0.42
1:1:4:U:H2'	1:1:5:U:O4'	2.20	0.41
1:1:405:G:H2'	1:1:406:U:C6	2.55	0.41
1:1:999:G:H2'	1:1:1000:G:C8	2.55	0.41
1:1:2956:U:H2'	1:1:2957:C:C6	2.55	0.41
7:LC:161:ASP:HA	7:LC:164:ALA:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:LD:282:LEU:HD11	8:LD:290:ARG:HH11	1.84	0.41
9:LE:110:ASP:OD1	9:LE:112:THR:HG23	2.19	0.41
14:LJ:86:LYS:HE3	14:LJ:86:LYS:HB3	1.91	0.41
36:Lf:55:TYR:CZ	36:Lf:67:ARG:HB2	2.55	0.41
1:1:415:A:N1	1:1:2325:C:O2'	2.52	0.41
1:1:1795:U:H1'	1:1:1796:A:O4'	2.20	0.41
1:1:3068:C:H2'	1:1:3069:U:C6	2.55	0.41
8:LD:128:GLU:O	8:LD:167:LYS:NZ	2.47	0.41
9:LE:77:ASP:OD1	9:LE:77:ASP:N	2.49	0.41
12:LH:29:GLY:HA3	12:LH:82:VAL:HG13	2.02	0.41
30:LZ:24:ILE:HA	30:LZ:42:VAL:HG12	2.02	0.41
45:Lo:32:LYS:HE3	45:Lo:32:LYS:HB2	1.85	0.41
1:1:592:U:H3'	1:1:593:G:O4'	2.20	0.41
1:1:858:A2M:HM'3	1:1:858:A2M:H1'	1.83	0.41
1:1:2470:U:H2'	1:1:2471:U:C6	2.55	0.41
1:1:2636:G:H2'	1:1:2636:G:N3	2.35	0.41
1:1:2656:A:H2'	1:1:2657:G:C8	2.54	0.41
3:4:84:C:H3'	3:4:85:G:C8	2.55	0.41
6:LB:102:LEU:HD21	6:LB:156:CYS:SG	2.60	0.41
6:LB:256:TRP:CD1	6:LB:256:TRP:C	2.99	0.41
13:LI:179:GLU:H	13:LI:179:GLU:CD	2.29	0.41
21:LQ:105:LYS:HB2	21:LQ:105:LYS:HE3	1.88	0.41
38:Lh:46:LEU:O	38:Lh:49:ILE:HG12	2.20	0.41
1:1:132:U:O2'	1:1:133:C:OP2	2.32	0.41
1:1:250:C:HO2'	1:1:251:U:P	2.42	0.41
1:1:1014:C:H2'	1:1:1015:C:O4'	2.21	0.41
1:1:1847:A2M:H2'	1:1:1848:G:C8	2.54	0.41
1:1:2054:U:P	1:1:2055:A:H5''	2.60	0.41
1:1:2971:U:H2'	1:1:2972:U:C6	2.56	0.41
29:LY:81:VAL:HG22	29:LY:84:VAL:HG22	2.03	0.41
38:Lh:46:LEU:HD12	38:Lh:46:LEU:HA	1.89	0.41
1:1:1221:C:H42	1:1:1233:G:H1	1.69	0.41
1:1:2648:A:H2'	1:1:2648:A:N3	2.36	0.41
14:LJ:111:ILE:HG12	14:LJ:117:TYR:HB2	2.03	0.41
15:LK:87:GLU:H	15:LK:102:LYS:HA	1.85	0.41
16:LL:113:VAL:O	16:LL:117:LYS:HG2	2.20	0.41
1:1:1624:C:OP1	1:1:1800:C:O2'	2.34	0.41
1:1:2123:G:H2'	1:1:2124:G:C8	2.54	0.41
2:3:60:A:H2'	2:3:61:C:H6	1.86	0.41
7:LC:176:ILE:HD13	7:LC:176:ILE:HA	1.89	0.41
14:LJ:15:ILE:HG12	14:LJ:132:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:476:C:H2'	1:1:477:C:C6	2.56	0.41
1:1:1260:C:C2	1:1:1261:A:C8	3.09	0.41
1:1:1933:G:O2'	1:1:2054:U:O4	2.26	0.41
3:4:8:C:H2'	3:4:9:A:C8	2.55	0.41
3:4:75:OMG:OP2	29:LY:73:TYR:OH	2.33	0.41
6:LB:234:TRP:CD1	6:LB:266:ALA:HB1	2.55	0.41
12:LH:14:GLU:HA	17:LM:2:ALA:HB2	2.03	0.41
14:LJ:52:ARG:HG2	14:LJ:53:TYR:HD1	1.86	0.41
1:1:235:C:H2'	1:1:236:A:O4'	2.21	0.41
1:1:254:U:H2'	1:1:255:U:O4'	2.21	0.41
1:1:688:C:H2'	1:1:689:G:H8	1.85	0.41
1:1:1432:A2M:HM'2	1:1:1432:A2M:H1'	1.91	0.41
1:1:1596:U:H2'	1:1:1597:G:C8	2.56	0.41
1:1:3111:C:N4	1:1:3113:A:H1'	2.36	0.41
6:LB:14:LEU:O	6:LB:17:LEU:HB2	2.20	0.41
29:LY:112:LYS:HB3	29:LY:112:LYS:HE2	1.86	0.41
1:1:498:U:H2'	1:1:499:C:C6	2.56	0.41
1:1:604:G:N7	56:1:3924:HOH:O	2.37	0.41
1:1:908:A:H2'	1:1:909:C:C6	2.56	0.41
1:1:995:A:H2'	1:1:996:C:O4'	2.20	0.41
1:1:1077:U:H2'	24:LT:120:LYS:HE2	2.03	0.41
1:1:1089:G:H2'	1:1:1090:A:C8	2.56	0.41
1:1:1387:G:N2	1:1:1390:A:OP2	2.45	0.41
1:1:2844:C:O2'	1:1:2845:U:H5'	2.20	0.41
12:LH:57:ILE:HG13	12:LH:68:LEU:HD13	2.03	0.41
14:LJ:88:LYS:O	14:LJ:89:GLU:HG3	2.21	0.41
41:Lk:18:LYS:HB3	41:Lk:18:LYS:HE2	1.78	0.41
1:1:1777:A:H2'	1:1:1778:A:C8	2.56	0.41
1:1:1789:A:OP2	30:LZ:64:ARG:NH2	2.54	0.41
1:1:2221:PSU:C4	1:1:2222:A:C8	3.09	0.41
1:1:2380:OMU:O5'	1:1:2380:OMU:H6	2.21	0.41
9:LE:100:ARG:HD3	9:LE:100:ARG:HA	1.83	0.41
45:Lo:61:LYS:HE3	45:Lo:61:LYS:HB2	1.80	0.41
48:Ls:27:VAL:HG11	48:Ls:79:PHE:CE2	2.56	0.41
1:1:1240:C:H4'	48:Ls:42:ARG:HD3	2.03	0.40
1:1:1361:U:H2'	1:1:1362:G:H8	1.86	0.40
6:LB:109:HIS:O	6:LB:110:LEU:HD23	2.22	0.40
47:Lq:35:LEU:O	47:Lq:36:THR:OG1	2.24	0.40
1:1:463:C:H2'	1:1:464:C:H6	1.86	0.40
1:1:1576:C:H2'	1:1:1577:C:C6	2.56	0.40
1:1:1697:C:H2'	1:1:1698:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2092:PSU:H2'	1:1:2093:G:C8	2.56	0.40
42:Ll:43:HIS:CE1	42:Ll:45:ARG:HB2	2.56	0.40
48:Ls:171:THR:O	48:Ls:175:MET:HG2	2.21	0.40
1:1:250:C:H2'	1:1:251:U:C6	2.57	0.40
1:1:816:U:H2'	1:1:817:G:O4'	2.21	0.40
1:1:1561:G:H4'	1:1:1562:U:H5'	2.03	0.40
1:1:2320:A:H2'	1:1:2321:A:C8	2.56	0.40
1:1:3135:A:OP2	19:LO:173:LYS:NZ	2.44	0.40
5:LA:130:SER:HB2	5:LA:171:GLY:HA3	2.03	0.40
46:Lp:52:VAL:O	46:Lp:68:ALA:HA	2.21	0.40
48:Ls:141:ILE:HG23	48:Ls:156:ILE:HG13	2.03	0.40
1:1:511:U:C4	7:LC:351:PRO:HB3	2.56	0.40
1:1:1235:A:H2'	1:1:1236:U:O4'	2.22	0.40
1:1:2729:G:O2'	1:1:2730:U:H5'	2.22	0.40
1:1:3266:A:H2'	1:1:3267:G:C8	2.56	0.40
2:3:16:U:OP1	14:LJ:148:ARG:NH1	2.54	0.40
10:LF:124:LYS:HD3	10:LF:197:VAL:HG11	2.03	0.40
13:LI:35:ASP:C	13:LI:36:LEU:HD12	2.46	0.40
17:LM:127:ARG:O	17:LM:131:GLU:HG2	2.21	0.40
20:LP:36:ILE:HG22	20:LP:39:TRP:CE3	2.56	0.40
25:LU:101:ARG:HD2	25:LU:115:TYR:CE1	2.56	0.40
1:1:95:G:H2'	1:1:96:A:C8	2.57	0.40
1:1:505:G:O2'	7:LC:343:GLU:OE1	2.26	0.40
1:1:1551:C:O2'	1:1:1552:G:N2	2.54	0.40
1:1:1578:G:H21	41:Lk:77:ARG:NH2	2.20	0.40
1:1:2674:A:OP1	56:1:3812:HOH:O	2.21	0.40
1:1:3134:A:C4	19:LO:116:LYS:HA	2.56	0.40
2:3:46:C:OP1	8:LD:161:ARG:HG3	2.21	0.40
3:4:40:A:H2'	3:4:41:A:H8	1.87	0.40
5:LA:105:SER:HB3	5:LA:160:SER:HB3	2.04	0.40
6:LB:95:THR:OG1	6:LB:98:GLY:O	2.32	0.40
48:Ls:61:ARG:O	48:Ls:65:THR:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	LA	250/254 (98%)	239 (96%)	11 (4%)	0	100	100
6	LB	385/392 (98%)	372 (97%)	13 (3%)	0	100	100
7	LC	361/365 (99%)	347 (96%)	14 (4%)	0	100	100
8	LD	298/304 (98%)	287 (96%)	11 (4%)	0	100	100
9	LE	192/200 (96%)	173 (90%)	18 (9%)	1 (0%)	24	34
10	LF	245/249 (98%)	237 (97%)	8 (3%)	0	100	100
11	LG	233/262 (89%)	228 (98%)	5 (2%)	0	100	100
12	LH	189/192 (98%)	186 (98%)	3 (2%)	0	100	100
13	LI	215/219 (98%)	205 (95%)	10 (5%)	0	100	100
14	LJ	165/173 (95%)	158 (96%)	7 (4%)	0	100	100
15	LK	153/165 (93%)	132 (86%)	18 (12%)	3 (2%)	6	6
16	LL	207/213 (97%)	199 (96%)	8 (4%)	0	100	100
17	LM	139/142 (98%)	133 (96%)	6 (4%)	0	100	100
18	LN	200/203 (98%)	188 (94%)	12 (6%)	0	100	100
19	LO	202/204 (99%)	197 (98%)	5 (2%)	0	100	100
20	LP	184/187 (98%)	176 (96%)	8 (4%)	0	100	100
21	LQ	181/213 (85%)	176 (97%)	5 (3%)	0	100	100
22	LR	148/192 (77%)	146 (99%)	2 (1%)	0	100	100
23	LS	171/174 (98%)	164 (96%)	7 (4%)	0	100	100
24	LT	157/160 (98%)	150 (96%)	7 (4%)	0	100	100
25	LU	99/127 (78%)	95 (96%)	4 (4%)	0	100	100
26	LV	133/139 (96%)	131 (98%)	2 (2%)	0	100	100
27	LW	59/161 (37%)	58 (98%)	1 (2%)	0	100	100
28	LX	117/156 (75%)	111 (95%)	6 (5%)	0	100	100
29	LY	132/138 (96%)	130 (98%)	2 (2%)	0	100	100
30	LZ	133/135 (98%)	126 (95%)	7 (5%)	0	100	100
31	La	146/149 (98%)	136 (93%)	10 (7%)	0	100	100
32	Lb	60/130 (46%)	57 (95%)	3 (5%)	0	100	100
33	Lc	95/108 (88%)	93 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	Ld	110/120 (92%)	109 (99%)	1 (1%)	0	100	100
35	Le	122/131 (93%)	118 (97%)	4 (3%)	0	100	100
36	Lf	105/109 (96%)	99 (94%)	6 (6%)	0	100	100
37	Lg	111/119 (93%)	106 (96%)	5 (4%)	0	100	100
38	Lh	120/126 (95%)	118 (98%)	2 (2%)	0	100	100
39	Li	100/110 (91%)	96 (96%)	4 (4%)	0	100	100
40	Lj	85/95 (90%)	82 (96%)	3 (4%)	0	100	100
41	Lk	74/81 (91%)	71 (96%)	3 (4%)	0	100	100
42	Ll	48/102 (47%)	47 (98%)	1 (2%)	0	100	100
43	Lm	49/128 (38%)	48 (98%)	1 (2%)	0	100	100
44	Ln	22/25 (88%)	22 (100%)	0	0	100	100
44	Lr	22/25 (88%)	22 (100%)	0	0	100	100
45	Lo	102/106 (96%)	97 (95%)	5 (5%)	0	100	100
46	Lp	89/92 (97%)	83 (93%)	6 (7%)	0	100	100
47	Lq	139/147 (95%)	130 (94%)	9 (6%)	0	100	100
48	Ls	187/312 (60%)	184 (98%)	3 (2%)	0	100	100
All	All	6734/7534 (89%)	6462 (96%)	268 (4%)	4 (0%)	49	62

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	LK	88	PRO
9	LE	143	PHE
15	LK	22	VAL
15	LK	10	ILE

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	
5	LA	196/198 (99%)	189 (96%)	7 (4%)	31	49
6	LB	327/331 (99%)	321 (98%)	6 (2%)	51	71
7	LC	284/285 (100%)	273 (96%)	11 (4%)	28	45
8	LD	250/253 (99%)	243 (97%)	7 (3%)	38	58
9	LE	162/166 (98%)	155 (96%)	7 (4%)	26	41
10	LF	213/215 (99%)	208 (98%)	5 (2%)	44	64
11	LG	203/222 (91%)	196 (97%)	7 (3%)	32	51
12	LH	168/169 (99%)	161 (96%)	7 (4%)	26	42
13	LI	182/183 (100%)	179 (98%)	3 (2%)	55	74
14	LJ	145/150 (97%)	135 (93%)	10 (7%)	14	22
16	LL	172/176 (98%)	164 (95%)	8 (5%)	23	37
17	LM	116/117 (99%)	112 (97%)	4 (3%)	32	51
18	LN	179/180 (99%)	173 (97%)	6 (3%)	32	51
19	LO	162/162 (100%)	155 (96%)	7 (4%)	26	41
20	LP	151/152 (99%)	147 (97%)	4 (3%)	40	60
21	LQ	155/178 (87%)	155 (100%)	0	100	100
22	LR	126/160 (79%)	126 (100%)	0	100	100
23	LS	153/154 (99%)	149 (97%)	4 (3%)	40	60
24	LT	134/135 (99%)	132 (98%)	2 (2%)	57	75
25	LU	89/108 (82%)	84 (94%)	5 (6%)	19	30
26	LV	99/102 (97%)	96 (97%)	3 (3%)	36	56
27	LW	55/125 (44%)	53 (96%)	2 (4%)	31	49
28	LX	106/129 (82%)	105 (99%)	1 (1%)	70	84
29	LY	117/119 (98%)	113 (97%)	4 (3%)	32	51
30	LZ	121/121 (100%)	113 (93%)	8 (7%)	15	24
31	La	121/122 (99%)	118 (98%)	3 (2%)	42	61
32	Lb	53/110 (48%)	53 (100%)	0	100	100
33	Lc	78/88 (89%)	74 (95%)	4 (5%)	21	34
34	Ld	97/105 (92%)	95 (98%)	2 (2%)	47	67
35	Le	107/114 (94%)	106 (99%)	1 (1%)	70	84
36	Lf	88/90 (98%)	86 (98%)	2 (2%)	44	64
37	Lg	97/102 (95%)	94 (97%)	3 (3%)	35	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	Lh	109/112 (97%)	105 (96%)	4 (4%)	30	47
39	Li	86/93 (92%)	83 (96%)	3 (4%)	32	50
40	Lj	71/78 (91%)	71 (100%)	0	100	100
41	Lk	73/77 (95%)	68 (93%)	5 (7%)	14	23
42	Ll	45/92 (49%)	45 (100%)	0	100	100
43	Lm	46/115 (40%)	46 (100%)	0	100	100
44	Ln	22/23 (96%)	20 (91%)	2 (9%)	9	13
44	Lr	22/23 (96%)	21 (96%)	1 (4%)	24	39
45	Lo	88/90 (98%)	87 (99%)	1 (1%)	65	81
46	Lp	73/74 (99%)	69 (94%)	4 (6%)	19	31
47	Lq	109/112 (97%)	107 (98%)	2 (2%)	51	71
48	Ls	155/255 (61%)	148 (96%)	7 (4%)	24	39
All	All	5605/6165 (91%)	5433 (97%)	172 (3%)	36	54

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	LA	47	GLU
5	LA	96	LEU
5	LA	102	LEU
5	LA	128	ARG
5	LA	129	THR
5	LA	134	VAL
5	LA	202	VAL
6	LB	105	VAL
6	LB	114	VAL
6	LB	161	VAL
6	LB	197	ARG
6	LB	257	HIS
6	LB	336	ILE
7	LC	8	THR
7	LC	13	ASP
7	LC	17	THR
7	LC	20	THR
7	LC	22	VAL
7	LC	23	LEU
7	LC	75	ILE
7	LC	158	VAL

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Mol	Chain	Res	Type
7	LC	281	ILE
7	LC	290	LEU
7	LC	354	VAL
8	LD	28	THR
8	LD	52	VAL
8	LD	53	VAL
8	LD	95	TRP
8	LD	139	ASP
8	LD	195	THR
8	LD	225	GLN
9	LE	7	THR
9	LE	14	THR
9	LE	47	THR
9	LE	53	GLN
9	LE	102	VAL
9	LE	145	GLN
9	LE	157	THR
10	LF	13	LEU
10	LF	23	LYS
10	LF	123	VAL
10	LF	125	VAL
10	LF	169	LEU
11	LG	67	ILE
11	LG	193	VAL
11	LG	201	VAL
11	LG	203	ILE
11	LG	206	VAL
11	LG	210	ASP
11	LG	211	LYS
12	LH	20	ILE
12	LH	82	VAL
12	LH	103	VAL
12	LH	120	ILE
12	LH	125	VAL
12	LH	136	VAL
12	LH	145	GLU
13	LI	26	VAL
13	LI	176	LEU
13	LI	180	GLU
14	LJ	10	MET
14	LJ	12	GLU
14	LJ	20	LEU

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Mol	Chain	Res	Type
14	LJ	37	VAL
14	LJ	47	VAL
14	LJ	52	ARG
14	LJ	81	LEU
14	LJ	113	LEU
14	LJ	127	ASP
14	LJ	172	VAL
16	LL	3	ILE
16	LL	58	VAL
16	LL	63	VAL
16	LL	140	LYS
16	LL	144	THR
16	LL	151	LEU
16	LL	173	ILE
16	LL	177	ILE
17	LM	14	VAL
17	LM	39	VAL
17	LM	102	LYS
17	LM	138	ILE
18	LN	25	VAL
18	LN	30	TYR
18	LN	60	VAL
18	LN	66	VAL
18	LN	68	ARG
18	LN	124	ASP
19	LO	2	SER
19	LO	121	VAL
19	LO	131	LEU
19	LO	162	ARG
19	LO	191	VAL
19	LO	192	ASP
19	LO	197	GLU
20	LP	2	VAL
20	LP	36	ILE
20	LP	129	THR
20	LP	172	SER
23	LS	36	VAL
23	LS	87	THR
23	LS	96	GLU
23	LS	174	SER
24	LT	3	HIS
24	LT	52	MET

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Mol	Chain	Res	Type
25	LU	35	ASP
25	LU	45	GLU
25	LU	62	ILE
25	LU	67	ASP
25	LU	102	VAL
26	LV	60	VAL
26	LV	64	VAL
26	LV	137	VAL
27	LW	41	LEU
27	LW	54	LEU
28	LX	146	LEU
29	LY	55	VAL
29	LY	81	VAL
29	LY	93	THR
29	LY	108	LEU
30	LZ	6	THR
30	LZ	7	SER
30	LZ	50	SER
30	LZ	62	GLU
30	LZ	73	VAL
30	LZ	74	ILE
30	LZ	98	ASP
30	LZ	102	GLU
31	La	16	SER
31	La	103	ASP
31	La	145	VAL
33	Lc	44	LEU
33	Lc	51	THR
33	Lc	68	THR
33	Lc	70	VAL
34	Ld	12	ILE
34	Ld	31	VAL
35	Le	15	THR
36	Lf	51	VAL
36	Lf	54	VAL
37	Lg	33	VAL
37	Lg	73	VAL
37	Lg	100	LYS
38	Lh	11	GLN
38	Lh	39	ILE
38	Lh	90	THR
38	Lh	110	LYS

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Mol	Chain	Res	Type
39	Li	11	VAL
39	Li	16	LEU
39	Li	21	ASN
41	Lk	4	GLU
41	Lk	31	THR
41	Lk	62	LEU
41	Lk	65	ASN
41	Lk	66	LEU
44	Ln	1	MET
44	Ln	10	THR
45	Lo	93	LEU
46	Lp	5	THR
46	Lp	38	THR
46	Lp	40	THR
46	Lp	63	THR
47	Lq	4	VAL
47	Lq	12	VAL
44	Lr	10	THR
48	Ls	7	ASN
48	Ls	30	VAL
48	Ls	53	MET
48	Ls	58	MET
48	Ls	80	VAL
48	Ls	121	VAL
48	Ls	190	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
5	LA	19	HIS
5	LA	187	HIS
5	LA	216	HIS
6	LB	183	GLN
6	LB	346	HIS
7	LC	141	HIS
7	LC	217	HIS
7	LC	324	GLN
7	LC	330	ASN
8	LD	57	ASN
8	LD	302	GLN
10	LF	192	HIS
10	LF	206	ASN

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Mol	Chain	Res	Type
11	LG	62	GLN
11	LG	194	HIS
13	LI	73	ASN
16	LL	5	HIS
19	LO	56	HIS
20	LP	97	ASN
24	LT	139	HIS
25	LU	24	ASN
27	LW	59	HIS
28	LX	73	HIS
28	LX	92	GLN
29	LY	18	HIS
29	LY	102	ASN
29	LY	116	ASN
30	LZ	35	HIS
31	La	60	HIS
31	La	89	GLN
32	Lb	17	HIS
32	Lb	19	ASN
39	Li	100	GLN
39	Li	110	HIS
40	Lj	76	ASN
41	Lk	28	ASN
42	Ll	4	HIS
48	Ls	83	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3186/3337 (95%)	518 (16%)	34 (1%)
2	3	118/120 (98%)	13 (11%)	1 (0%)
3	4	155/156 (99%)	22 (14%)	0
4	9	2/3 (66%)	1 (50%)	0
All	All	3461/3616 (95%)	554 (16%)	35 (1%)

All (554) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	27	A
1	1	41	A
1	1	44	A

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Mol	Chain	Res	Type
1	1	50	A
1	1	60	G
1	1	61	A
1	1	66	A
1	1	67	A
1	1	93	G
1	1	97	G
1	1	100	A
1	1	111	G
1	1	112	C
1	1	114	C
1	1	117	A
1	1	118	U
1	1	123	A
1	1	125	G
1	1	132	U
1	1	133	C
1	1	134	G
1	1	138	C
1	1	144	G
1	1	152	G
1	1	153	A
1	1	170	A
1	1	179	C
1	1	181	G
1	1	184	U
1	1	185	U
1	1	186	C
1	1	204	C
1	1	205	A
1	1	212	G
1	1	213	A
1	1	214	G
1	1	215	A
1	1	225	A
1	1	242	G
1	1	244	G
1	1	251	U
1	1	262	G
1	1	276	G
1	1	277	A
1	1	279	U

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Mol	Chain	Res	Type
1	1	288	A
1	1	291	U
1	1	298	U
1	1	316	A
1	1	332	C
1	1	343	C
1	1	363	U
1	1	369	G
1	1	372	C
1	1	391	U
1	1	392	A
1	1	395	A
1	1	396	C
1	1	414	G
1	1	415	A
1	1	430	G
1	1	432	C
1	1	434	U
1	1	446	A
1	1	460	U
1	1	461	C
1	1	469	C
1	1	470	A
1	1	471	C
1	1	489	A
1	1	505	G
1	1	512	A
1	1	527	G
1	1	536	C
1	1	537	C
1	1	538	G
1	1	539	G
1	1	545	U
1	1	547	A
1	1	549	A
1	1	553	C
1	1	570	G
1	1	573	G
1	1	575	G
1	1	583	A
1	1	592	U
1	1	593	G

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Mol	Chain	Res	Type
1	1	596	A
1	1	597	G
1	1	599	A
1	1	607	G
1	1	608	U
1	1	609	A
1	1	610	A
1	1	624	C
1	1	637	A2M
1	1	648	A
1	1	665	A
1	1	669	U
1	1	672	G
1	1	679	A
1	1	686	C
1	1	697	A
1	1	700	G
1	1	703	A
1	1	704	A
1	1	749	U
1	1	758	PSU
1	1	759	U
1	1	762	A
1	1	763	G
1	1	767	G
1	1	781	G
1	1	788	A
1	1	799	A2M
1	1	812	A
1	1	843	C
1	1	853	U
1	1	856	U
1	1	861	U
1	1	862	G
1	1	871	PSU
1	1	878	A
1	1	889	G
1	1	890	OMG
1	1	891	G
1	1	896	A
1	1	899	A2M
1	1	919	G

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Mol	Chain	Res	Type
1	1	920	C
1	1	921	U
1	1	926	A
1	1	941	C
1	1	942	PSU
1	1	945	G
1	1	956	PSU
1	1	959	A
1	1	960	C
1	1	961	C
1	1	962	U
1	1	963	U
1	1	984	A
1	1	992	G
1	1	998	C
1	1	999	G
1	1	1003	G
1	1	1006	A
1	1	1007	U
1	1	1008	U
1	1	1010	U
1	1	1011	U
1	1	1012	A
1	1	1013	G
1	1	1016	PSU
1	1	1030	A
1	1	1032	C
1	1	1047	A
1	1	1048	A
1	1	1055	G
1	1	1064	C
1	1	1065	U
1	1	1068	A
1	1	1077	U
1	1	1078	U
1	1	1080	G
1	1	1081	A
1	1	1086	A
1	1	1087	U
1	1	1100	G
1	1	1114	G
1	1	1134	U

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Mol	Chain	Res	Type
1	1	1136	A
1	1	1142	A
1	1	1157	G
1	1	1163	G
1	1	1164	U
1	1	1165	G
1	1	1184	C
1	1	1192	G
1	1	1204	U
1	1	1205	G
1	1	1216	G
1	1	1218	U
1	1	1219	G
1	1	1222	C
1	1	1223	A2M
1	1	1224	U
1	1	1225	G
1	1	1227	A
1	1	1228	A
1	1	1229	G
1	1	1231	C
1	1	1241	U
1	1	1242	A
1	1	1243	A
1	1	1244	G
1	1	1245	G
1	1	1246	A
1	1	1247	C
1	1	1248	PSU
1	1	1249	G
1	1	1259	U
1	1	1268	G
1	1	1269	A
1	1	1270	A
1	1	1278	G
1	1	1290	G
1	1	1291	A
1	1	1292	U
1	1	1296	G
1	1	1299	C
1	1	1313	A
1	1	1314	U

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Mol	Chain	Res	Type
1	1	1331	A
1	1	1332	G
1	1	1333	A
1	1	1334	A
1	1	1335	A
1	1	1336	C
1	1	1337	G
1	1	1339	U
1	1	1369	A
1	1	1382	A
1	1	1383	G
1	1	1401	A
1	1	1402	A
1	1	1404	G
1	1	1417	G
1	1	1419	U
1	1	1420	OMC
1	1	1421	PSU
1	1	1429	A
1	1	1433	OMG
1	1	1464	A
1	1	1465	A
1	1	1466	G
1	1	1467	U
1	1	1485	G
1	1	1491	OMC
1	1	1495	U
1	1	1506	U
1	1	1516	U
1	1	1519	G
1	1	1538	PSU
1	1	1539	C
1	1	1540	A
1	1	1543	G
1	1	1545	G
1	1	1549	C
1	1	1550	U
1	1	1551	C
1	1	1554	G
1	1	1560	U
1	1	1561	G
1	1	1562	U

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Mol	Chain	Res	Type
1	1	1563	G
1	1	1567	A
1	1	1569	A
1	1	1573	A
1	1	1585	A
1	1	1609	U
1	1	1610	G
1	1	1619	C
1	1	1622	A
1	1	1623	A
1	1	1625	U
1	1	1637	C
1	1	1685	U
1	1	1696	A
1	1	1697	C
1	1	1704	U
1	1	1730	A
1	1	1731	G
1	1	1741	C
1	1	1743	U
1	1	1745	U
1	1	1746	G
1	1	1750	G
1	1	1760	G
1	1	1777	A
1	1	1793	A
1	1	1795	U
1	1	1796	A
1	1	1797	A
1	1	1800	C
1	1	1801	U
1	1	1819	A
1	1	1820	U
1	1	1821	A
1	1	1822	A
1	1	1826	C
1	1	1829	C
1	1	1830	A
1	1	1847	A2M
1	1	1858	G
1	1	1859	A
1	1	1860	U

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Mol	Chain	Res	Type
1	1	1866	A
1	1	1873	A
1	1	1874	PSU
1	1	1886	G
1	1	1888	A
1	1	1933	G
1	1	1936	A
1	1	1941	G
1	1	2045	G
1	1	2047	G
1	1	2054	U
1	1	2055	A
1	1	2056	A
1	1	2057	C
1	1	2063	A
1	1	2065	U
1	1	2074	G
1	1	2076	A
1	1	2084	G
1	1	2085	G
1	1	2094	A
1	1	2097	G
1	1	2107	A
1	1	2108	A
1	1	2121	A
1	1	2123	G
1	1	2132	G
1	1	2133	U
1	1	2151	A
1	1	2160	OMC
1	1	2161	A
1	1	2168	U
1	1	2169	G
1	1	2170	A
1	1	2171	A
1	1	2172	U
1	1	2173	G
1	1	2186	A
1	1	2188	U
1	1	2192	A
1	1	2207	A
1	1	2212	G

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Mol	Chain	Res	Type
1	1	2216	G
1	1	2217	PSU
1	1	2219	A2M
1	1	2220	C
1	1	2222	A
1	1	2223	PSU
1	1	2224	G
1	1	2225	A
1	1	2227	PSU
1	1	2228	C
1	1	2233	A
1	1	2235	G
1	1	2236	G
1	1	2242	A
1	1	2244	A2M
1	1	2251	OMG
1	1	2270	G
1	1	2271	C
1	1	2273	U
1	1	2276	A
1	1	2277	UY1
1	1	2278	G
1	1	2289	A2M
1	1	2297	U
1	1	2298	G
1	1	2299	U
1	1	2303	PSU
1	1	2335	A
1	1	2336	A
1	1	2337	C
1	1	2338	G
1	1	2356	G
1	1	2360	A
1	1	2364	A
1	1	2365	A
1	1	2366	G
1	1	2367	A
1	1	2374	U
1	1	2382	A
1	1	2464	U
1	1	2465	U
1	1	2477	U

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Mol	Chain	Res	Type
1	1	2478	A
1	1	2487	A
1	1	2488	G
1	1	2501	U
1	1	2502	G
1	1	2503	C
1	1	2504	G
1	1	2510	C
1	1	2513	C
1	1	2516	G
1	1	2521	A
1	1	2526	C
1	1	2529	U
1	1	2531	G
1	1	2532	C
1	1	2533	G
1	1	2544	G
1	1	2552	A
1	1	2553	C
1	1	2556	PSU
1	1	2562	G
1	1	2565	G
1	1	2566	G
1	1	2573	G
1	1	2578	OMG
1	1	2585	A
1	1	2611	PSU
1	1	2615	A
1	1	2633	A
1	1	2636	G
1	1	2648	A
1	1	2650	A
1	1	2653	A
1	1	2655	A
1	1	2673	G
1	1	2678	U
1	1	2687	G
1	1	2688	OMU
1	1	2703	PSU
1	1	2711	U
1	1	2712	G
1	1	2714	C

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Mol	Chain	Res	Type
1	1	2721	A
1	1	2731	C
1	1	2732	C
1	1	2736	G
1	1	2737	A
1	1	2755	G
1	1	2758	A
1	1	2759	G
1	1	2760	A
1	1	2769	C
1	1	2776	A
1	1	2777	U
1	1	2778	A
1	1	2797	A
1	1	2801	PSU
1	1	2802	UR3
1	1	2804	A
1	1	2830	G
1	1	2831	A
1	1	2846	A
1	1	2848	C
1	1	2858	C
1	1	2870	A
1	1	2875	PSU
1	1	2876	OMG
1	1	2882	PSU
1	1	2894	U
1	1	2895	A
1	1	2901	C
1	1	2903	PSU
1	1	2906	G
1	1	2930	A
1	1	2931	G
1	1	2942	C
1	1	2949	G
1	1	2970	A
1	1	3014	U
1	1	3017	G
1	1	3036	G
1	1	3038	G
1	1	3044	A
1	1	3050	C

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Mol	Chain	Res	Type
1	1	3051	C
1	1	3059	G
1	1	3080	A
1	1	3088	A
1	1	3089	U
1	1	3100	A
1	1	3101	C
1	1	3112	U
1	1	3121	G
1	1	3122	U
1	1	3123	U
1	1	3127	G
1	1	3128	A
1	1	3129	C
1	1	3130	G
1	1	3131	U
1	1	3132	A
1	1	3135	A
1	1	3141	G
1	1	3160	A
1	1	3162	C
1	1	3163	A
1	1	3164	G
1	1	3182	C
1	1	3188	G
1	1	3200	A
1	1	3211	U
1	1	3214	A
1	1	3218	U
1	1	3219	A
1	1	3225	G
1	1	3229	G
1	1	3231	G
1	1	3245	C
1	1	3257	A
1	1	3258	U
1	1	3259	G
1	1	3260	U
1	1	3261	G
1	1	3276	A
1	1	3282	U
1	1	3286	G

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Mol	Chain	Res	Type
1	1	3292	U
1	1	3295	U
1	1	3299	U
1	1	3310	G
1	1	3319	C
1	1	3324	C
1	1	3325	U
1	1	3328	G
1	1	3331	U
1	1	3332	A
1	1	3333	G
2	3	7	G
2	3	29	G
2	3	42	C
2	3	54	U
2	3	55	A
2	3	65	G
2	3	73	U
2	3	90	G
2	3	92	C
2	3	93	G
2	3	101	A
2	3	111	G
2	3	118	G
3	4	23	U
3	4	34	U
3	4	35	C
3	4	38	U
3	4	48	A
3	4	55	PSU
3	4	59	A
3	4	62	A
3	4	63	G
3	4	81	U
3	4	83	C
3	4	84	C
3	4	85	G
3	4	88	A
3	4	95	G
3	4	104	A
3	4	106	C
3	4	111	A

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Mol	Chain	Res	Type
3	4	113	U
3	4	125	U
3	4	138	A
3	4	152	G
4	9	76	A

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	133	C
1	1	193	A
1	1	250	C
1	1	275	G
1	1	431	A
1	1	703	A
1	1	897	A
1	1	960	C
1	1	1047	A
1	1	1064	C
1	1	1248	PSU
1	1	1290	G
1	1	1338	A
1	1	1796	A
1	1	2064	C
1	1	2075	U
1	1	2160	OMC
1	1	2167	C
1	1	2227	PSU
1	1	2232	U
1	1	2243	A2M
1	1	2503	C
1	1	2532	C
1	1	2715	C
1	1	2731	C
1	1	2875	PSU
1	1	3079	U
1	1	3122	U
1	1	3163	A
1	1	3210	U
1	1	3224	C
1	1	3258	U
1	1	3298	U

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Mol	Chain	Res	Type
1	1	3332	A
2	3	72	G

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

121 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$
1	OMC	1	2838	1	19,22,23	1.14	3 (15%)	25,31,34	1.26	3 (12%)
1	5MC	1	2241	53,1	19,22,23	0.58	0	26,32,35	0.63	0
1	OMG	1	2358	53,1	23,26,27	2.38	9 (39%)	32,38,41	2.07	9 (28%)
1	OMG	1	2752	1	23,26,27	2.39	9 (39%)	32,38,41	2.32	10 (31%)
1	PSU	1	2891	1	18,21,22	1.62	5 (27%)	21,30,33	1.91	4 (19%)
1	PSU	1	1421	1	18,21,22	2.65	9 (50%)	21,30,33	2.13	6 (28%)
1	A2M	1	2244	1	22,25,26	3.87	8 (36%)	30,36,39	2.53	12 (40%)
1	PSU	1	1453	1	18,21,22	1.66	5 (27%)	21,30,33	1.88	5 (23%)
1	OMG	1	2876	1	23,26,27	2.42	9 (39%)	32,38,41	2.31	10 (31%)
1	PSU	1	2092	1	18,21,22	1.63	5 (27%)	21,30,33	1.90	4 (19%)
1	A2M	1	2219	1	22,25,26	0.24	0	30,36,39	0.40	0
1	A2M	1	1116	53,54,1	22,25,26	3.93	8 (36%)	30,36,39	2.39	10 (33%)
1	OMC	1	1836	1	19,22,23	0.98	2 (10%)	25,31,34	0.90	1 (4%)
3	PSU	4	18	3,1	18,21,22	1.72	5 (27%)	21,30,33	1.85	4 (19%)
1	PSU	1	373	1	18,21,22	2.59	10 (55%)	21,30,33	2.21	6 (28%)
1	OMG	1	2750	1	23,26,27	2.40	9 (39%)	32,38,41	2.37	11 (34%)
1	PSU	1	2154	1	18,21,22	1.65	5 (27%)	21,30,33	1.92	4 (19%)
1	OMG	1	890	54,1	23,26,27	2.42	9 (39%)	32,38,41	2.49	10 (31%)
1	PSU	1	2546	1	18,21,22	2.61	10 (55%)	21,30,33	2.18	7 (33%)
1	OMC	1	2907	1	19,22,23	1.06	3 (15%)	25,31,34	0.91	1 (4%)
1	PSU	1	758	1	18,21,22	1.63	5 (27%)	21,30,33	1.86	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	1	2229	1	18,21,22	1.53	5 (27%)	21,30,33	1.78	4 (19%)
1	PSU	1	1016	1	18,21,22	2.52	10 (55%)	21,30,33	1.95	5 (23%)
1	OMG	1	2881	1	23,26,27	2.42	9 (39%)	32,38,41	2.33	10 (31%)
1	PSU	1	793	54,1	18,21,22	1.73	5 (27%)	21,30,33	2.03	5 (23%)
1	PSU	1	2785	1	18,21,22	1.67	6 (33%)	21,30,33	1.91	5 (23%)
1	A2M	1	799	53,1	22,25,26	3.98	8 (36%)	30,36,39	2.33	9 (30%)
1	PSU	1	718	1	18,21,22	2.56	10 (55%)	21,30,33	2.15	6 (28%)
1	PSU	1	2675	1	18,21,22	2.60	10 (55%)	21,30,33	2.02	5 (23%)
1	OMG	1	787	1	23,26,27	2.39	9 (39%)	32,38,41	2.28	11 (34%)
1	PSU	1	871	1	18,21,22	2.62	10 (55%)	21,30,33	2.05	6 (28%)
1	PSU	1	2556	1	18,21,22	1.63	5 (27%)	21,30,33	1.86	4 (19%)
1	PSU	1	2379	53,1	18,21,22	1.64	5 (27%)	21,30,33	1.94	4 (19%)
1	PSU	1	917	1	18,21,22	2.55	9 (50%)	21,30,33	2.20	5 (23%)
1	PSU	1	2558	1	18,21,22	2.57	9 (50%)	21,30,33	2.34	7 (33%)
1	PSU	1	1248	1	18,21,22	2.47	9 (50%)	21,30,33	2.43	7 (33%)
1	PSU	1	1035	54,1	18,21,22	2.58	10 (55%)	21,30,33	2.15	5 (23%)
1	PSU	1	2227	1	18,21,22	2.61	10 (55%)	21,30,33	1.98	5 (23%)
1	A2M	1	2905	53,1	22,25,26	3.92	7 (31%)	30,36,39	2.40	10 (33%)
1	OMC	1	1420	1	19,22,23	1.06	3 (15%)	25,31,34	1.14	2 (8%)
1	PSU	1	986	54,1	18,21,22	1.63	5 (27%)	21,30,33	1.91	5 (23%)
1	OMG	1	627	1	23,26,27	2.37	8 (34%)	32,38,41	2.34	10 (31%)
1	A2M	1	2326	1	22,25,26	3.96	8 (36%)	30,36,39	2.25	11 (36%)
1	OMG	1	385	1	23,26,27	2.40	9 (39%)	32,38,41	2.28	11 (34%)
1	PSU	1	948	54,1	18,21,22	2.64	10 (55%)	21,30,33	2.10	6 (28%)
1	PSU	1	956	1	18,21,22	2.51	10 (55%)	21,30,33	2.33	6 (28%)
1	A2M	1	2289	1	22,25,26	3.94	7 (31%)	30,36,39	2.37	9 (30%)
3	OMG	4	75	3	23,26,27	2.42	9 (39%)	32,38,41	2.30	10 (31%)
1	A2M	1	768	1	22,25,26	3.95	8 (36%)	30,36,39	2.51	12 (40%)
1	A2M	1	637	1	22,25,26	3.93	7 (31%)	30,36,39	2.35	8 (26%)
1	UR3	1	2593	1	19,22,23	2.65	4 (21%)	26,32,35	1.68	3 (11%)
1	A2M	1	1847	54,1	22,25,26	3.93	7 (31%)	30,36,39	2.37	9 (30%)
1	PSU	1	1025	1	18,21,22	2.56	9 (50%)	21,30,33	2.13	6 (28%)
1	A2M	1	848	54,1	22,25,26	3.92	7 (31%)	30,36,39	2.45	10 (33%)
1	A2M	1	2182	1	22,25,26	3.94	7 (31%)	30,36,39	2.36	9 (30%)
1	OMU	1	2880	54,1	19,22,23	2.07	6 (31%)	25,31,34	1.85	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMU	1	1868	54,1	19,22,23	2.06	6 (31%)	25,31,34	1.90	5 (20%)
1	PSU	1	2863	1	18,21,22	2.56	10 (55%)	21,30,33	2.13	5 (23%)
1	OMU	1	2384	1	19,22,23	2.09	6 (31%)	25,31,34	1.82	4 (16%)
1	PSU	1	807	54,1	18,21,22	2.63	9 (50%)	21,30,33	2.17	6 (28%)
1	1MA	1	2105	53,54,1	21,25,26	0.51	0	30,37,40	0.78	1 (3%)
1	UY1	1	2277	54,1	19,22,23	2.80	8 (42%)	21,31,34	1.91	6 (28%)
1	PSU	1	773	54,1	18,21,22	2.59	10 (55%)	21,30,33	2.23	6 (28%)
1	PSU	1	1870	1	18,21,22	1.68	5 (27%)	21,30,33	2.01	5 (23%)
1	OMC	1	2918	1	19,22,23	1.03	3 (15%)	25,31,34	0.87	0
1	OMC	1	2160	54,1	19,22,23	1.07	3 (15%)	25,31,34	0.82	0
1	PSU	1	2303	1	18,21,22	2.63	9 (50%)	21,30,33	2.06	7 (33%)
1	PSU	1	1105	1	18,21,22	1.64	5 (27%)	21,30,33	1.92	4 (19%)
1	OMU	1	2688	1	19,22,23	2.06	6 (31%)	25,31,34	1.82	4 (16%)
1	OMG	1	646	1	23,26,27	2.39	9 (39%)	32,38,41	2.29	11 (34%)
1	OMG	1	2251	1	23,26,27	2.43	9 (39%)	32,38,41	2.41	11 (34%)
1	PSU	1	1874	1	18,21,22	1.67	5 (27%)	21,30,33	1.94	4 (19%)
1	A2M	1	2599	1	22,25,26	3.93	7 (31%)	30,36,39	2.44	10 (33%)
1	A2M	1	858	1	22,25,26	3.92	7 (31%)	30,36,39	2.42	9 (30%)
1	PSU	1	754	1	18,21,22	2.58	9 (50%)	21,30,33	2.24	6 (28%)
1	A2M	1	1432	53,1	22,25,26	3.94	9 (40%)	30,36,39	2.56	12 (40%)
1	PSU	1	2221	1	18,21,22	2.53	10 (55%)	21,30,33	1.93	5 (23%)
1	PSU	1	881	1	18,21,22	2.59	9 (50%)	21,30,33	2.18	6 (28%)
1	A2M	1	2243	54,1	22,25,26	3.99	7 (31%)	30,36,39	2.49	13 (43%)
1	OMG	1	2491	1	23,26,27	2.41	9 (39%)	32,38,41	2.35	11 (34%)
1	PSU	1	355	1	18,21,22	2.63	10 (55%)	21,30,33	2.07	5 (23%)
1	PSU	1	2882	1	18,21,22	1.62	5 (27%)	21,30,33	1.98	5 (23%)
1	PSU	1	2611	54,1	18,21,22	0.96	1 (5%)	21,30,33	0.91	1 (4%)
1	PSU	1	1904	1	18,21,22	2.56	10 (55%)	21,30,33	2.26	6 (28%)
1	OMC	1	651	1	19,22,23	0.94	2 (10%)	25,31,34	0.79	0
1	PSU	1	2839	1	18,21,22	1.65	5 (27%)	21,30,33	1.86	5 (23%)
1	PSU	1	2223	1	18,21,22	2.45	10 (55%)	21,30,33	2.31	7 (33%)
1	PSU	1	127	1	18,21,22	2.60	9 (50%)	21,30,33	2.03	6 (28%)
1	PSU	1	1538	1	18,21,22	1.62	5 (27%)	21,30,33	1.81	4 (19%)
1	PSU	1	2903	53,54,1	18,21,22	1.63	5 (27%)	21,30,33	1.90	4 (19%)
1	OMG	1	1907	1	23,26,27	2.40	9 (39%)	32,38,41	2.43	11 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	1MA	1	633	1	21,25,26	0.53	0	30,37,40	0.75	1 (3%)
1	PSU	1	942	54,1	18,21,22	1.79	6 (33%)	21,30,33	2.05	5 (23%)
1	OMC	1	1491	53,1	19,22,23	1.01	3 (15%)	25,31,34	0.83	0
1	UR3	1	2802	1	19,22,23	2.80	4 (21%)	26,32,35	1.79	4 (15%)
1	PSU	1	1918	54,1	18,21,22	1.66	5 (27%)	21,30,33	1.99	5 (23%)
1	A2M	1	1223	1	22,25,26	3.94	7 (31%)	30,36,39	2.43	11 (36%)
1	PSU	1	972	54,1	18,21,22	1.65	5 (27%)	21,30,33	2.00	5 (23%)
1	PSU	1	2703	54,1	18,21,22	2.67	10 (55%)	21,30,33	2.23	8 (38%)
1	A2M	1	899	1	22,25,26	3.94	8 (36%)	30,36,39	2.33	8 (26%)
3	PSU	4	55	3	18,21,22	2.65	10 (55%)	21,30,33	1.99	5 (23%)
1	PSU	1	2875	54,1	18,21,22	2.67	9 (50%)	21,30,33	1.99	6 (28%)
1	OMU	1	1917	1	19,22,23	2.11	6 (31%)	25,31,34	1.84	5 (20%)
3	PSU	4	73	3	18,21,22	1.62	5 (27%)	21,30,33	1.83	4 (19%)
1	PSU	1	779	1	18,21,22	2.66	9 (50%)	21,30,33	2.14	6 (28%)
1	OMG	1	2578	54,1	23,26,27	2.42	9 (39%)	32,38,41	2.35	11 (34%)
1	PSU	1	2310	54,1	18,21,22	0.92	1 (5%)	21,30,33	0.81	0
1	PSU	1	1043	1	18,21,22	1.68	5 (27%)	21,30,33	1.93	5 (23%)
1	PSU	1	2096	54,1	18,21,22	1.69	5 (27%)	21,30,33	1.95	5 (23%)
1	OMC	1	778	1	19,22,23	0.96	2 (10%)	25,31,34	0.90	0
1	PSU	1	2824	1	18,21,22	1.68	6 (33%)	21,30,33	1.98	5 (23%)
1	PSU	1	1107	1	18,21,22	1.62	5 (27%)	21,30,33	1.96	4 (19%)
1	PSU	1	2801	1	18,21,22	2.49	9 (50%)	21,30,33	2.32	6 (28%)
1	OMU	1	2380	1	19,22,23	2.07	6 (31%)	25,31,34	1.81	5 (20%)
1	OMG	1	2774	1	23,26,27	2.40	9 (39%)	32,38,41	2.33	10 (31%)
1	OMC	1	2300	1	19,22,23	1.06	3 (15%)	25,31,34	0.89	1 (4%)
1	PSU	1	2934	1	18,21,22	1.64	5 (27%)	21,30,33	2.01	5 (23%)
1	UY1	1	2690	54,1	19,22,23	2.62	6 (31%)	21,31,34	2.01	5 (23%)
1	5MC	1	2829	54,1	19,22,23	0.70	0	26,32,35	0.63	0
1	PSU	1	2217	1	18,21,22	2.56	10 (55%)	21,30,33	2.04	6 (28%)
1	OMG	1	1433	53,1	23,26,27	2.37	9 (39%)	32,38,41	2.31	12 (37%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	1	2838	1	-	2/9/27/28	0/2/2/2
1	5MC	1	2241	53,1	-	0/7/25/26	0/2/2/2
1	OMG	1	2358	53,1	-	1/9/27/28	0/3/3/3
1	OMG	1	2752	1	-	0/9/27/28	0/3/3/3
1	PSU	1	2891	1	-	2/7/25/26	0/2/2/2
1	PSU	1	1421	1	-	2/7/25/26	0/2/2/2
1	A2M	1	2244	1	-	4/9/27/28	0/3/3/3
1	PSU	1	1453	1	-	0/7/25/26	0/2/2/2
1	OMG	1	2876	1	-	1/9/27/28	0/3/3/3
1	PSU	1	2092	1	-	0/7/25/26	0/2/2/2
1	A2M	1	2219	1	-	4/9/27/28	0/3/3/3
1	A2M	1	1116	53,54,1	-	0/9/27/28	0/3/3/3
1	OMC	1	1836	1	-	0/9/27/28	0/2/2/2
3	PSU	4	18	3,1	-	0/7/25/26	0/2/2/2
1	PSU	1	373	1	-	0/7/25/26	0/2/2/2
1	OMG	1	2750	1	-	1/9/27/28	0/3/3/3
1	PSU	1	2154	1	-	2/7/25/26	0/2/2/2
1	OMG	1	890	54,1	-	2/9/27/28	0/3/3/3
1	PSU	1	2546	1	-	0/7/25/26	0/2/2/2
1	OMC	1	2907	1	-	1/9/27/28	0/2/2/2
1	PSU	1	758	1	-	2/7/25/26	0/2/2/2
1	PSU	1	2229	1	-	0/7/25/26	0/2/2/2
1	PSU	1	1016	1	-	3/7/25/26	0/2/2/2
1	OMG	1	2881	1	-	0/9/27/28	0/3/3/3
1	PSU	1	793	54,1	-	0/7/25/26	0/2/2/2
1	PSU	1	2785	1	-	0/7/25/26	0/2/2/2
1	A2M	1	799	53,1	-	2/9/27/28	0/3/3/3
1	PSU	1	718	1	-	0/7/25/26	0/2/2/2
1	PSU	1	2675	1	-	2/7/25/26	0/2/2/2
1	OMG	1	787	1	-	0/9/27/28	0/3/3/3
1	PSU	1	871	1	-	2/7/25/26	0/2/2/2
1	PSU	1	2556	1	-	2/7/25/26	0/2/2/2
1	PSU	1	2379	53,1	-	0/7/25/26	0/2/2/2
1	PSU	1	917	1	-	0/7/25/26	0/2/2/2
1	PSU	1	2558	1	-	1/7/25/26	0/2/2/2
1	PSU	1	1248	1	-	3/7/25/26	0/2/2/2
1	PSU	1	1035	54,1	-	0/7/25/26	0/2/2/2
1	PSU	1	2227	1	-	0/7/25/26	0/2/2/2
1	A2M	1	2905	53,1	-	0/9/27/28	0/3/3/3
1	OMC	1	1420	1	-	3/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1	986	54,1	-	0/7/25/26	0/2/2/2
1	OMG	1	627	1	-	0/9/27/28	0/3/3/3
1	A2M	1	2326	1	-	5/9/27/28	0/3/3/3
1	OMG	1	385	1	-	0/9/27/28	0/3/3/3
1	PSU	1	948	54,1	-	0/7/25/26	0/2/2/2
1	PSU	1	956	1	-	2/7/25/26	0/2/2/2
1	A2M	1	2289	1	-	2/9/27/28	0/3/3/3
3	OMG	4	75	3	-	0/9/27/28	0/3/3/3
1	A2M	1	768	1	-	3/9/27/28	0/3/3/3
1	A2M	1	637	1	-	3/9/27/28	0/3/3/3
1	UR3	1	2593	1	-	0/7/25/26	0/2/2/2
1	A2M	1	1847	54,1	-	2/9/27/28	0/3/3/3
1	PSU	1	1025	1	-	0/7/25/26	0/2/2/2
1	A2M	1	848	54,1	-	1/9/27/28	0/3/3/3
1	A2M	1	2182	1	-	1/9/27/28	0/3/3/3
1	OMU	1	2880	54,1	-	0/9/27/28	0/2/2/2
1	OMU	1	1868	54,1	-	0/9/27/28	0/2/2/2
1	PSU	1	2863	1	-	0/7/25/26	0/2/2/2
1	OMU	1	2384	1	-	0/9/27/28	0/2/2/2
1	UY1	1	2277	54,1	1/1/5/5	0/9/27/28	0/2/2/2
1	PSU	1	807	54,1	-	0/7/25/26	0/2/2/2
1	1MA	1	2105	53,54,1	-	0/7/25/26	0/3/3/3
1	PSU	1	773	54,1	-	0/7/25/26	0/2/2/2
1	PSU	1	1870	1	-	0/7/25/26	0/2/2/2
1	OMC	1	2918	1	-	0/9/27/28	0/2/2/2
1	OMC	1	2160	54,1	-	5/9/27/28	0/2/2/2
1	PSU	1	2303	1	-	3/7/25/26	0/2/2/2
1	PSU	1	1105	1	-	0/7/25/26	0/2/2/2
1	OMU	1	2688	1	-	0/9/27/28	0/2/2/2
1	OMG	1	646	1	-	1/9/27/28	0/3/3/3
1	OMG	1	2251	1	-	2/9/27/28	0/3/3/3
1	PSU	1	1874	1	-	2/7/25/26	0/2/2/2
1	A2M	1	2599	1	-	0/9/27/28	0/3/3/3
1	A2M	1	858	1	-	0/9/27/28	0/3/3/3
1	PSU	1	754	1	-	0/7/25/26	0/2/2/2
1	A2M	1	1432	53,1	-	1/9/27/28	0/3/3/3
1	PSU	1	2221	1	-	0/7/25/26	0/2/2/2
1	PSU	1	881	1	-	0/7/25/26	0/2/2/2
1	A2M	1	2243	54,1	-	0/9/27/28	0/3/3/3
1	OMG	1	2491	1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1	355	1	-	0/7/25/26	0/2/2/2
1	PSU	1	2882	1	-	5/7/25/26	0/2/2/2
1	PSU	1	2611	54,1	-	0/7/25/26	0/2/2/2
1	PSU	1	1904	1	-	0/7/25/26	0/2/2/2
1	OMC	1	651	1	-	0/9/27/28	0/2/2/2
1	PSU	1	2839	1	-	0/7/25/26	0/2/2/2
1	PSU	1	2223	1	-	3/7/25/26	0/2/2/2
1	PSU	1	127	1	-	0/7/25/26	0/2/2/2
1	PSU	1	1538	1	-	3/7/25/26	0/2/2/2
1	PSU	1	2903	53,54,1	-	2/7/25/26	0/2/2/2
1	OMG	1	1907	1	-	1/9/27/28	0/3/3/3
1	1MA	1	633	1	-	2/7/25/26	0/3/3/3
1	PSU	1	942	54,1	-	0/7/25/26	0/2/2/2
1	OMC	1	1491	53,1	-	0/9/27/28	0/2/2/2
1	UR3	1	2802	1	-	5/7/25/26	0/2/2/2
1	PSU	1	1918	54,1	-	1/7/25/26	0/2/2/2
1	A2M	1	1223	1	-	3/9/27/28	0/3/3/3
1	PSU	1	972	54,1	-	0/7/25/26	0/2/2/2
1	PSU	1	2703	54,1	-	2/7/25/26	0/2/2/2
1	A2M	1	899	1	-	2/9/27/28	0/3/3/3
3	PSU	4	55	3	-	2/7/25/26	0/2/2/2
1	PSU	1	2875	54,1	-	2/7/25/26	0/2/2/2
1	OMU	1	1917	1	-	1/9/27/28	0/2/2/2
3	PSU	4	73	3	-	0/7/25/26	0/2/2/2
1	PSU	1	779	1	-	0/7/25/26	0/2/2/2
1	OMG	1	2578	54,1	-	2/9/27/28	0/3/3/3
1	PSU	1	2310	54,1	-	2/7/25/26	0/2/2/2
1	PSU	1	1043	1	-	0/7/25/26	0/2/2/2
1	PSU	1	2096	54,1	-	0/7/25/26	0/2/2/2
1	OMC	1	778	1	-	0/9/27/28	0/2/2/2
1	PSU	1	2824	1	-	0/7/25/26	0/2/2/2
1	PSU	1	1107	1	-	2/7/25/26	0/2/2/2
1	PSU	1	2801	1	-	3/7/25/26	0/2/2/2
1	OMU	1	2380	1	-	0/9/27/28	0/2/2/2
1	OMG	1	2774	1	-	0/9/27/28	0/3/3/3
1	OMC	1	2300	1	-	2/9/27/28	0/2/2/2
1	PSU	1	2934	1	-	0/7/25/26	0/2/2/2
1	UY1	1	2690	54,1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	1	2829	54,1	-	4/7/25/26	0/2/2/2
1	PSU	1	2217	1	-	2/7/25/26	0/2/2/2
1	OMG	1	1433	53,1	-	2/9/27/28	0/3/3/3

All (816) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	768	A2M	C2'-C1'	-10.55	1.27	1.53
1	1	637	A2M	C2'-C1'	-10.41	1.27	1.53
1	1	1116	A2M	C2'-C1'	-10.40	1.27	1.53
1	1	2244	A2M	C2'-C1'	-10.40	1.27	1.53
1	1	858	A2M	C2'-C1'	-10.36	1.27	1.53
1	1	799	A2M	C2'-C1'	-10.35	1.27	1.53
1	1	1432	A2M	C2'-C1'	-10.34	1.27	1.53
1	1	2182	A2M	C2'-C1'	-10.33	1.27	1.53
1	1	899	A2M	C2'-C1'	-10.33	1.27	1.53
1	1	2326	A2M	C2'-C1'	-10.31	1.27	1.53
1	1	2599	A2M	C2'-C1'	-10.26	1.27	1.53
1	1	2289	A2M	C2'-C1'	-10.25	1.27	1.53
1	1	848	A2M	C2'-C1'	-10.23	1.27	1.53
1	1	2243	A2M	C2'-C1'	-10.22	1.27	1.53
1	1	1847	A2M	C2'-C1'	-10.19	1.28	1.53
1	1	2802	UR3	C2-N1	10.13	1.52	1.38
1	1	1223	A2M	C2'-C1'	-10.05	1.28	1.53
1	1	2905	A2M	C2'-C1'	-10.04	1.28	1.53
1	1	2289	A2M	C3'-C4'	-9.53	1.28	1.53
1	1	2243	A2M	C3'-C4'	-9.47	1.29	1.53
1	1	799	A2M	C3'-C4'	-9.45	1.29	1.53
1	1	1116	A2M	C3'-C4'	-9.45	1.29	1.53
1	1	2593	UR3	C2-N1	9.45	1.51	1.38
1	1	2326	A2M	C3'-C4'	-9.38	1.29	1.53
1	1	2905	A2M	C3'-C4'	-9.37	1.29	1.53
1	1	899	A2M	C3'-C4'	-9.35	1.29	1.53
1	1	858	A2M	C3'-C4'	-9.31	1.29	1.53
1	1	2182	A2M	C3'-C4'	-9.30	1.29	1.53
1	1	848	A2M	C3'-C4'	-9.29	1.29	1.53
1	1	1847	A2M	C3'-C4'	-9.26	1.29	1.53
1	1	2599	A2M	C3'-C4'	-9.25	1.29	1.53
1	1	637	A2M	C3'-C4'	-9.24	1.29	1.53
1	1	1432	A2M	C3'-C4'	-9.19	1.29	1.53
1	1	1223	A2M	C3'-C4'	-9.14	1.29	1.53
1	1	768	A2M	C3'-C4'	-9.06	1.30	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2244	A2M	C3'-C4'	-8.91	1.30	1.53
1	1	2690	UY1	C6-N1	7.29	1.48	1.36
1	1	2277	UY1	C6-N1	7.00	1.47	1.36
1	1	2243	A2M	O4'-C1'	6.61	1.57	1.42
1	1	2690	UY1	C2-N1	6.61	1.45	1.36
1	1	2251	OMG	C4-N3	6.54	1.49	1.34
1	1	2876	OMG	C4-N3	6.52	1.49	1.34
1	1	890	OMG	C4-N3	6.48	1.49	1.34
1	1	2774	OMG	C4-N3	6.48	1.49	1.34
1	1	2578	OMG	C4-N3	6.47	1.49	1.34
1	1	2881	OMG	C4-N3	6.47	1.49	1.34
1	1	2752	OMG	C4-N3	6.45	1.49	1.34
3	4	75	OMG	C4-N3	6.44	1.49	1.34
1	1	2750	OMG	C4-N3	6.43	1.49	1.34
1	1	1907	OMG	C4-N3	6.43	1.49	1.34
1	1	385	OMG	C4-N3	6.42	1.48	1.34
1	1	2491	OMG	C4-N3	6.42	1.48	1.34
1	1	787	OMG	C4-N3	6.42	1.48	1.34
1	1	799	A2M	O4'-C1'	6.41	1.56	1.42
1	1	848	A2M	O4'-C1'	6.37	1.56	1.42
1	1	2289	A2M	O4'-C1'	6.35	1.56	1.42
1	1	627	OMG	C4-N3	6.35	1.48	1.34
1	1	2182	A2M	O4'-C1'	6.34	1.56	1.42
1	1	1223	A2M	O4'-C1'	6.33	1.56	1.42
1	1	646	OMG	C4-N3	6.33	1.48	1.34
1	1	2358	OMG	C4-N3	6.32	1.48	1.34
1	1	2905	A2M	O4'-C1'	6.31	1.56	1.42
1	1	1847	A2M	O4'-C1'	6.29	1.56	1.42
1	1	899	A2M	O4'-C1'	6.28	1.56	1.42
1	1	2326	A2M	O4'-C1'	6.28	1.56	1.42
1	1	1433	OMG	C4-N3	6.26	1.48	1.34
1	1	1116	A2M	O4'-C1'	6.26	1.56	1.42
1	1	1223	A2M	C6-N6	6.24	1.50	1.34
1	1	858	A2M	O4'-C1'	6.24	1.56	1.42
1	1	637	A2M	O4'-C1'	6.24	1.56	1.42
1	1	2599	A2M	O4'-C1'	6.21	1.56	1.42
1	1	2182	A2M	C6-N6	6.15	1.49	1.34
1	1	2243	A2M	C6-N6	6.14	1.49	1.34
1	1	1847	A2M	C6-N6	6.13	1.49	1.34
1	1	2289	A2M	C6-N6	6.13	1.49	1.34
1	1	2599	A2M	C6-N6	6.13	1.49	1.34
1	1	2905	A2M	C6-N6	6.12	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	799	A2M	C6-N6	6.12	1.49	1.34
1	1	2227	PSU	O4'-C1'	6.10	1.52	1.43
1	1	1432	A2M	O4'-C1'	6.10	1.56	1.42
1	1	848	A2M	C6-N6	6.09	1.49	1.34
1	1	768	A2M	O4'-C1'	6.08	1.56	1.42
1	1	2277	UY1	C2-N1	6.08	1.44	1.36
1	1	768	A2M	C6-N6	6.06	1.49	1.34
1	1	899	A2M	C6-N6	6.05	1.49	1.34
1	1	1432	A2M	C6-N6	6.05	1.49	1.34
1	1	858	A2M	C6-N6	6.04	1.49	1.34
1	1	2326	A2M	C6-N6	6.02	1.49	1.34
1	1	637	A2M	C6-N6	6.02	1.49	1.34
1	1	2875	PSU	O4'-C1'	6.00	1.52	1.43
1	1	1116	A2M	C6-N6	6.00	1.49	1.34
1	1	2244	A2M	C6-N6	5.99	1.49	1.34
1	1	2244	A2M	O4'-C1'	5.84	1.55	1.42
3	4	55	PSU	O4'-C1'	5.80	1.51	1.43
1	1	871	PSU	O4'-C1'	5.80	1.51	1.43
1	1	2221	PSU	O4'-C1'	5.79	1.51	1.43
1	1	1223	A2M	C3'-C2'	5.78	1.65	1.53
1	1	2703	PSU	O4'-C1'	5.78	1.51	1.43
1	1	2217	PSU	O4'-C1'	5.72	1.51	1.43
1	1	2675	PSU	O4'-C1'	5.63	1.51	1.43
1	1	1421	PSU	O4'-C1'	5.60	1.51	1.43
1	1	1432	A2M	C3'-C2'	5.60	1.65	1.53
1	1	1248	PSU	O4'-C1'	5.58	1.51	1.43
1	1	2303	PSU	O4'-C1'	5.57	1.51	1.43
1	1	754	PSU	O4'-C1'	5.55	1.51	1.43
1	1	1035	PSU	O4'-C1'	5.55	1.51	1.43
1	1	2546	PSU	O4'-C1'	5.53	1.51	1.43
1	1	2243	A2M	C3'-C2'	5.52	1.65	1.53
1	1	948	PSU	O4'-C1'	5.51	1.51	1.43
1	1	1904	PSU	O4'-C1'	5.51	1.51	1.43
1	1	799	A2M	C3'-C2'	5.50	1.65	1.53
1	1	1025	PSU	O4'-C1'	5.50	1.51	1.43
1	1	373	PSU	O4'-C1'	5.49	1.51	1.43
1	1	2863	PSU	O4'-C1'	5.49	1.51	1.43
1	1	2223	PSU	O4'-C1'	5.49	1.51	1.43
1	1	1847	A2M	C3'-C2'	5.48	1.65	1.53
1	1	2599	A2M	C3'-C2'	5.46	1.64	1.53
1	1	2801	PSU	O4'-C1'	5.45	1.51	1.43
1	1	773	PSU	O4'-C1'	5.43	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2326	A2M	C3'-C2'	5.43	1.64	1.53
1	1	2905	A2M	C3'-C2'	5.43	1.64	1.53
1	1	355	PSU	O4'-C1'	5.42	1.51	1.43
1	1	768	A2M	C3'-C2'	5.42	1.64	1.53
1	1	881	PSU	O4'-C1'	5.41	1.51	1.43
1	1	1016	PSU	O4'-C1'	5.40	1.51	1.43
1	1	718	PSU	O4'-C1'	5.40	1.51	1.43
1	1	2182	A2M	C3'-C2'	5.39	1.64	1.53
1	1	127	PSU	O4'-C1'	5.37	1.51	1.43
1	1	917	PSU	O4'-C1'	5.36	1.51	1.43
1	1	899	A2M	C3'-C2'	5.35	1.64	1.53
1	1	807	PSU	O4'-C1'	5.34	1.51	1.43
1	1	890	OMG	C2-N3	5.33	1.46	1.33
1	1	2558	PSU	O4'-C1'	5.32	1.51	1.43
1	1	779	PSU	O4'-C1'	5.32	1.51	1.43
1	1	2251	OMG	C2-N3	5.32	1.46	1.33
1	1	637	A2M	C3'-C2'	5.31	1.64	1.53
1	1	1907	OMG	C2-N3	5.28	1.46	1.33
1	1	858	A2M	C3'-C2'	5.27	1.64	1.53
1	1	848	A2M	C3'-C2'	5.27	1.64	1.53
3	4	75	OMG	C2-N3	5.25	1.45	1.33
1	1	2881	OMG	C2-N3	5.24	1.45	1.33
1	1	2244	A2M	C3'-C2'	5.24	1.64	1.53
1	1	2876	OMG	C2-N3	5.23	1.45	1.33
1	1	2750	OMG	C2-N3	5.22	1.45	1.33
1	1	2491	OMG	C2-N3	5.21	1.45	1.33
1	1	2578	OMG	C2-N3	5.18	1.45	1.33
1	1	2752	OMG	C2-N3	5.17	1.45	1.33
1	1	2774	OMG	C2-N3	5.16	1.45	1.33
1	1	2289	A2M	C3'-C2'	5.15	1.64	1.53
1	1	787	OMG	C2-N3	5.12	1.45	1.33
1	1	385	OMG	C2-N3	5.10	1.45	1.33
1	1	646	OMG	C2-N3	5.09	1.45	1.33
1	1	1116	A2M	C3'-C2'	5.07	1.64	1.53
1	1	627	OMG	C2-N3	5.05	1.45	1.33
1	1	2358	OMG	C2-N3	4.98	1.45	1.33
1	1	1433	OMG	C2-N3	4.96	1.45	1.33
1	1	2881	OMG	C2-N2	4.73	1.45	1.34
1	1	2491	OMG	C2-N2	4.73	1.45	1.34
1	1	779	PSU	C2'-C1'	-4.68	1.47	1.53
3	4	75	OMG	C2-N2	4.68	1.45	1.34
1	1	385	OMG	C2-N2	4.68	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	890	OMG	C2-N2	4.66	1.45	1.34
1	1	2876	OMG	C2-N2	4.66	1.45	1.34
1	1	2251	OMG	C2-N2	4.66	1.45	1.34
1	1	1917	OMU	C2-N1	4.65	1.45	1.38
1	1	2578	OMG	C2-N2	4.64	1.45	1.34
1	1	956	PSU	O4'-C1'	4.64	1.50	1.43
1	1	2358	OMG	C2-N2	4.64	1.45	1.34
1	1	646	OMG	C2-N2	4.61	1.45	1.34
1	1	1907	OMG	C2-N2	4.61	1.45	1.34
1	1	2750	OMG	C2-N2	4.61	1.45	1.34
1	1	2752	OMG	C2-N2	4.60	1.44	1.34
1	1	1421	PSU	C2'-C1'	-4.60	1.47	1.53
1	1	1433	OMG	C2-N2	4.59	1.44	1.34
1	1	2384	OMU	C2-N1	4.57	1.45	1.38
1	1	2774	OMG	C2-N2	4.57	1.44	1.34
1	1	787	OMG	C2-N2	4.56	1.44	1.34
1	1	627	OMG	C2-N2	4.54	1.44	1.34
1	1	2380	OMU	C6-N1	4.52	1.48	1.38
1	1	2688	OMU	C2-N1	4.50	1.45	1.38
1	1	1917	OMU	C6-N1	4.49	1.48	1.38
1	1	2384	OMU	C6-N1	4.46	1.48	1.38
1	1	1223	A2M	O4'-C4'	4.45	1.54	1.45
1	1	2880	OMU	C6-N1	4.42	1.48	1.38
1	1	355	PSU	C2'-C1'	-4.40	1.47	1.53
1	1	2703	PSU	C2'-C1'	-4.40	1.47	1.53
1	1	1868	OMU	C6-N1	4.40	1.48	1.38
1	1	948	PSU	C2'-C1'	-4.39	1.47	1.53
1	1	1868	OMU	C2-N1	4.37	1.45	1.38
1	1	2688	OMU	C6-N1	4.36	1.48	1.38
1	1	2244	A2M	O4'-C4'	4.33	1.54	1.45
1	1	2880	OMU	C2-N1	4.32	1.45	1.38
1	1	127	PSU	C2'-C1'	-4.31	1.47	1.53
1	1	807	PSU	C2'-C1'	-4.31	1.47	1.53
1	1	2380	OMU	C2-N1	4.30	1.45	1.38
1	1	2875	PSU	C2'-C1'	-4.27	1.47	1.53
1	1	1035	PSU	C2'-C1'	-4.26	1.48	1.53
1	1	2289	A2M	O4'-C4'	4.24	1.54	1.45
1	1	2243	A2M	O4'-C4'	4.22	1.54	1.45
1	1	2905	A2M	O4'-C4'	4.22	1.54	1.45
1	1	373	PSU	C2'-C1'	-4.20	1.48	1.53
1	1	2546	PSU	C2'-C1'	-4.20	1.48	1.53
1	1	799	A2M	O4'-C4'	4.19	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2303	PSU	C2'-C1'	-4.14	1.48	1.53
1	1	1868	OMU	C5-C4	4.14	1.52	1.43
1	1	773	PSU	C2'-C1'	-4.13	1.48	1.53
1	1	956	PSU	C2'-C1'	-4.12	1.48	1.53
1	1	2599	A2M	O4'-C4'	4.11	1.54	1.45
1	1	1904	PSU	C2'-C1'	-4.11	1.48	1.53
1	1	1847	A2M	O4'-C4'	4.10	1.54	1.45
1	1	2801	PSU	C2'-C1'	-4.10	1.48	1.53
1	1	848	A2M	O4'-C4'	4.10	1.54	1.45
1	1	2182	A2M	O4'-C4'	4.09	1.54	1.45
1	1	2384	OMU	C5-C4	4.09	1.52	1.43
1	1	2880	OMU	C5-C4	4.08	1.52	1.43
1	1	754	PSU	C2'-C1'	-4.08	1.48	1.53
1	1	718	PSU	C2'-C1'	-4.08	1.48	1.53
1	1	1432	A2M	O4'-C4'	4.08	1.54	1.45
1	1	637	A2M	O4'-C4'	4.08	1.54	1.45
1	1	881	PSU	C2'-C1'	-4.07	1.48	1.53
1	1	1917	OMU	C5-C4	4.07	1.52	1.43
1	1	2863	PSU	C2'-C1'	-4.07	1.48	1.53
3	4	55	PSU	C2'-C1'	-4.05	1.48	1.53
1	1	2326	A2M	O4'-C4'	4.03	1.54	1.45
1	1	768	A2M	O4'-C4'	4.02	1.53	1.45
1	1	1116	A2M	O4'-C4'	4.02	1.53	1.45
1	1	2558	PSU	C2'-C1'	-4.02	1.48	1.53
1	1	1025	PSU	C2'-C1'	-4.00	1.48	1.53
1	1	1016	PSU	C2'-C1'	-4.00	1.48	1.53
1	1	2380	OMU	C5-C4	3.99	1.52	1.43
1	1	2217	PSU	C2'-C1'	-3.97	1.48	1.53
1	1	858	A2M	O4'-C4'	3.95	1.53	1.45
1	1	2675	PSU	C2'-C1'	-3.95	1.48	1.53
1	1	917	PSU	C2'-C1'	-3.95	1.48	1.53
1	1	899	A2M	O4'-C4'	3.95	1.53	1.45
1	1	2802	UR3	C5-C4	3.94	1.53	1.43
1	1	871	PSU	C2'-C1'	-3.93	1.48	1.53
1	1	2688	OMU	C5-C4	3.92	1.52	1.43
1	1	2221	PSU	C2'-C1'	-3.87	1.48	1.53
1	1	2227	PSU	C2'-C1'	-3.86	1.48	1.53
1	1	2593	UR3	C5-C4	3.86	1.53	1.43
1	1	2802	UR3	C6-N1	3.85	1.47	1.38
1	1	355	PSU	C4-N3	-3.84	1.31	1.38
1	1	779	PSU	C4-N3	-3.84	1.31	1.38
3	4	18	PSU	C4-N3	-3.84	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2303	PSU	C4-N3	-3.83	1.31	1.38
1	1	807	PSU	C4-N3	-3.82	1.31	1.38
1	1	2096	PSU	C4-N3	-3.81	1.31	1.38
1	1	881	PSU	C4-N3	-3.80	1.31	1.38
1	1	2558	PSU	C4-N3	-3.80	1.31	1.38
1	1	793	PSU	C4-N3	-3.79	1.31	1.38
3	4	55	PSU	C4-N3	-3.78	1.31	1.38
1	1	948	PSU	C4-N3	-3.78	1.31	1.38
1	1	1248	PSU	C2'-C1'	-3.77	1.48	1.53
1	1	956	PSU	C4-N3	-3.76	1.31	1.38
1	1	1874	PSU	C4-N3	-3.75	1.31	1.38
1	1	773	PSU	C4-N3	-3.75	1.31	1.38
1	1	942	PSU	C4-N3	-3.74	1.31	1.38
1	1	2546	PSU	C4-N3	-3.74	1.31	1.38
1	1	1918	PSU	C4-N3	-3.73	1.31	1.38
1	1	127	PSU	C4-N3	-3.73	1.31	1.38
1	1	1870	PSU	C4-N3	-3.72	1.31	1.38
1	1	917	PSU	C4-N3	-3.72	1.31	1.38
1	1	2703	PSU	C4-N3	-3.71	1.31	1.38
1	1	1043	PSU	C4-N3	-3.70	1.31	1.38
1	1	2903	PSU	C4-N3	-3.70	1.31	1.38
1	1	2675	PSU	C4-N3	-3.69	1.32	1.38
1	1	2875	PSU	C4-N3	-3.67	1.32	1.38
1	1	1421	PSU	C4-N3	-3.67	1.32	1.38
1	1	2934	PSU	C4-N3	-3.67	1.32	1.38
1	1	2223	PSU	C2'-C1'	-3.65	1.48	1.53
1	1	2593	UR3	C6-N1	3.65	1.46	1.38
1	1	754	PSU	C4-N3	-3.65	1.32	1.38
1	1	2839	PSU	C4-N3	-3.64	1.32	1.38
1	1	1105	PSU	C4-N3	-3.64	1.32	1.38
1	1	2092	PSU	C4-N3	-3.64	1.32	1.38
1	1	986	PSU	C4-N3	-3.63	1.32	1.38
1	1	1025	PSU	C4-N3	-3.63	1.32	1.38
1	1	2863	PSU	C4-N3	-3.62	1.32	1.38
1	1	373	PSU	C4-N3	-3.62	1.32	1.38
1	1	2824	PSU	C4-N3	-3.62	1.32	1.38
3	4	73	PSU	C4-N3	-3.61	1.32	1.38
1	1	718	PSU	C4-N3	-3.61	1.32	1.38
1	1	1904	PSU	C4-N3	-3.60	1.32	1.38
1	1	1035	PSU	C4-N3	-3.60	1.32	1.38
1	1	1453	PSU	C4-N3	-3.60	1.32	1.38
1	1	2379	PSU	C4-N3	-3.60	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	871	PSU	C4-N3	-3.60	1.32	1.38
1	1	972	PSU	C4-N3	-3.59	1.32	1.38
1	1	2556	PSU	C4-N3	-3.59	1.32	1.38
1	1	2154	PSU	C4-N3	-3.57	1.32	1.38
1	1	758	PSU	C4-N3	-3.56	1.32	1.38
1	1	2882	PSU	C4-N3	-3.56	1.32	1.38
1	1	2785	PSU	C4-N3	-3.55	1.32	1.38
1	1	1107	PSU	C4-N3	-3.53	1.32	1.38
1	1	2891	PSU	C4-N3	-3.53	1.32	1.38
1	1	2611	PSU	C6-C5	3.52	1.39	1.35
1	1	1538	PSU	C4-N3	-3.48	1.32	1.38
1	1	2227	PSU	C4-N3	-3.47	1.32	1.38
1	1	2277	UY1	O4-C4	-3.46	1.17	1.23
1	1	2593	UR3	O2-C2	-3.44	1.16	1.22
1	1	2229	PSU	C4-N3	-3.40	1.32	1.38
1	1	2223	PSU	C4-N3	-3.40	1.32	1.38
1	1	1016	PSU	C4-N3	-3.39	1.32	1.38
1	1	2802	UR3	O2-C2	-3.39	1.16	1.22
1	1	2221	PSU	C4-N3	-3.39	1.32	1.38
1	1	2217	PSU	C4-N3	-3.38	1.32	1.38
1	1	2801	PSU	C4-N3	-3.36	1.32	1.38
1	1	779	PSU	C4-C5	-3.34	1.35	1.44
1	1	807	PSU	C4-C5	-3.32	1.35	1.44
1	1	1248	PSU	C4-N3	-3.32	1.32	1.38
1	1	2310	PSU	C6-C5	3.31	1.39	1.35
1	1	956	PSU	C4-C5	-3.31	1.35	1.44
1	1	779	PSU	C3'-C2'	-3.28	1.44	1.53
3	4	55	PSU	C3'-C2'	-3.22	1.44	1.53
1	1	718	PSU	C4-C5	-3.21	1.35	1.44
1	1	127	PSU	C4-C5	-3.20	1.35	1.44
1	1	2303	PSU	C3'-C2'	-3.19	1.44	1.53
1	1	1421	PSU	C3'-C2'	-3.18	1.44	1.53
1	1	2558	PSU	C4-C5	-3.18	1.35	1.44
1	1	2380	OMU	O4-C4	-3.18	1.18	1.24
1	1	1043	PSU	C4-C5	-3.16	1.35	1.44
1	1	948	PSU	C3'-C2'	-3.16	1.44	1.53
1	1	1918	PSU	C4-C5	-3.16	1.35	1.44
1	1	2675	PSU	C3'-C2'	-3.16	1.44	1.53
1	1	948	PSU	C4-C5	-3.16	1.35	1.44
1	1	2546	PSU	C3'-C2'	-3.16	1.44	1.53
1	1	793	PSU	C4-C5	-3.16	1.35	1.44
1	1	754	PSU	C4-C5	-3.15	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2703	PSU	C4-C5	-3.15	1.35	1.44
1	1	942	PSU	O4'-C1'	-3.15	1.39	1.43
1	1	1025	PSU	C4-C5	-3.15	1.35	1.44
1	1	2688	OMU	O4-C4	-3.14	1.18	1.24
1	1	942	PSU	C4-C5	-3.14	1.35	1.44
1	1	373	PSU	C4-C5	-3.13	1.35	1.44
1	1	1035	PSU	C3'-C2'	-3.13	1.44	1.53
1	1	1868	OMU	O4-C4	-3.13	1.18	1.24
1	1	2227	PSU	O4'-C4'	3.12	1.51	1.45
1	1	754	PSU	C3'-C2'	-3.12	1.44	1.53
1	1	1421	PSU	C4-C5	-3.12	1.35	1.44
1	1	2703	PSU	C3'-C2'	-3.11	1.44	1.53
1	1	773	PSU	C4-C5	-3.11	1.35	1.44
1	1	2379	PSU	C4-C5	-3.11	1.35	1.44
1	1	373	PSU	C3'-C2'	-3.11	1.44	1.53
1	1	1016	PSU	C3'-C2'	-3.10	1.45	1.53
1	1	986	PSU	C4-C5	-3.10	1.35	1.44
1	1	2546	PSU	C4-C5	-3.10	1.35	1.44
1	1	2875	PSU	O4'-C4'	3.10	1.51	1.45
1	1	127	PSU	C3'-C2'	-3.10	1.45	1.53
1	1	2839	PSU	C4-C5	-3.10	1.35	1.44
1	1	890	OMG	C5-N7	-3.10	1.32	1.39
1	1	1917	OMU	O4-C4	-3.09	1.18	1.24
1	1	2863	PSU	C3'-C2'	-3.09	1.45	1.53
1	1	2221	PSU	C3'-C2'	-3.09	1.45	1.53
1	1	2558	PSU	C3'-C2'	-3.09	1.45	1.53
1	1	2882	PSU	C4-C5	-3.09	1.35	1.44
1	1	1538	PSU	C4-C5	-3.09	1.35	1.44
1	1	2303	PSU	C4-C5	-3.09	1.35	1.44
1	1	956	PSU	C3'-C2'	-3.09	1.45	1.53
1	1	2891	PSU	C4-C5	-3.08	1.35	1.44
1	1	871	PSU	C4-C5	-3.08	1.35	1.44
1	1	881	PSU	C3'-C2'	-3.08	1.45	1.53
1	1	355	PSU	C4-C5	-3.08	1.35	1.44
1	1	2154	PSU	C4-C5	-3.08	1.35	1.44
1	1	1870	PSU	C4-C5	-3.08	1.35	1.44
1	1	972	PSU	C4-C5	-3.08	1.35	1.44
1	1	2875	PSU	C3'-C2'	-3.08	1.45	1.53
1	1	1105	PSU	C4-C5	-3.07	1.35	1.44
1	1	871	PSU	C3'-C2'	-3.07	1.45	1.53
1	1	2880	OMU	O4-C4	-3.07	1.18	1.24
1	1	1025	PSU	C3'-C2'	-3.06	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1904	PSU	C4-C5	-3.06	1.35	1.44
3	4	18	PSU	C4-C5	-3.06	1.35	1.44
1	1	2217	PSU	C3'-C2'	-3.05	1.45	1.53
1	1	1453	PSU	C4-C5	-3.05	1.35	1.44
1	1	2384	OMU	O4-C4	-3.05	1.18	1.24
1	1	718	PSU	C3'-C2'	-3.04	1.45	1.53
1	1	355	PSU	C3'-C2'	-3.03	1.45	1.53
1	1	917	PSU	C4-C5	-3.03	1.35	1.44
1	1	2785	PSU	C4-C5	-3.03	1.35	1.44
1	1	2096	PSU	C4-C5	-3.03	1.35	1.44
1	1	881	PSU	C4-C5	-3.02	1.36	1.44
1	1	1016	PSU	C4-C5	-3.02	1.36	1.44
1	1	773	PSU	C3'-C2'	-3.01	1.45	1.53
1	1	2824	PSU	C4-C5	-3.01	1.36	1.44
1	1	1035	PSU	C4-C5	-3.01	1.36	1.44
1	1	2801	PSU	C3'-C2'	-3.00	1.45	1.53
1	1	2092	PSU	C4-C5	-3.00	1.36	1.44
1	1	2556	PSU	C4-C5	-3.00	1.36	1.44
1	1	1874	PSU	C4-C5	-2.99	1.36	1.44
3	4	55	PSU	C4-C5	-2.99	1.36	1.44
1	1	2903	PSU	C4-C5	-2.97	1.36	1.44
1	1	1248	PSU	C4-C5	-2.96	1.36	1.44
1	1	2303	PSU	O4'-C4'	2.96	1.51	1.45
3	4	73	PSU	C4-C5	-2.96	1.36	1.44
1	1	2838	OMC	C2-N1	2.95	1.46	1.40
1	1	2934	PSU	C4-C5	-2.95	1.36	1.44
1	1	2221	PSU	O4'-C4'	2.94	1.51	1.45
1	1	2217	PSU	C4-C5	-2.94	1.36	1.44
1	1	807	PSU	C3'-C2'	-2.94	1.45	1.53
1	1	1904	PSU	C3'-C2'	-2.93	1.45	1.53
1	1	2801	PSU	C4-C5	-2.93	1.36	1.44
1	1	2223	PSU	C3'-C2'	-2.93	1.45	1.53
1	1	2863	PSU	C4-C5	-2.92	1.36	1.44
1	1	917	PSU	C3'-C2'	-2.91	1.45	1.53
1	1	1016	PSU	O4'-C4'	2.91	1.51	1.45
1	1	627	OMG	C5-N7	-2.91	1.33	1.39
1	1	2227	PSU	C3'-C2'	-2.89	1.45	1.53
1	1	1907	OMG	C5-N7	-2.89	1.33	1.39
1	1	1248	PSU	O4'-C4'	2.89	1.51	1.45
1	1	2217	PSU	O4'-C4'	2.89	1.51	1.45
1	1	646	OMG	C5-N7	-2.88	1.33	1.39
3	4	75	OMG	C5-N7	-2.88	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2223	PSU	C4-C5	-2.88	1.36	1.44
1	1	2774	OMG	C5-N7	-2.87	1.33	1.39
1	1	2251	OMG	C5-N7	-2.86	1.33	1.39
1	1	2675	PSU	C4-C5	-2.86	1.36	1.44
1	1	646	OMG	O6-C6	-2.86	1.18	1.23
1	1	2277	UY1	C2'-C1'	-2.85	1.48	1.53
1	1	2227	PSU	C4-C5	-2.85	1.36	1.44
1	1	787	OMG	C5-N7	-2.85	1.33	1.39
1	1	1433	OMG	C5-N7	-2.85	1.33	1.39
1	1	1107	PSU	C4-C5	-2.85	1.36	1.44
1	1	385	OMG	C5-N7	-2.85	1.33	1.39
1	1	2875	PSU	C4-C5	-2.84	1.36	1.44
3	4	18	PSU	O4-C4	-2.84	1.18	1.23
1	1	917	PSU	O4'-C4'	2.83	1.51	1.45
1	1	807	PSU	O4-C4	-2.83	1.18	1.23
1	1	2675	PSU	O4'-C4'	2.83	1.51	1.45
1	1	2750	OMG	C5-N7	-2.83	1.33	1.39
1	1	2690	UY1	C4-C5	2.82	1.52	1.44
1	1	1248	PSU	C3'-C2'	-2.81	1.45	1.53
1	1	2491	OMG	C5-N7	-2.80	1.33	1.39
1	1	2881	OMG	C2-N1	2.80	1.44	1.37
1	1	2358	OMG	O6-C6	-2.80	1.18	1.23
1	1	2752	OMG	C5-N7	-2.80	1.33	1.39
1	1	2876	OMG	C5-N7	-2.80	1.33	1.39
1	1	758	PSU	C4-C5	-2.80	1.36	1.44
1	1	871	PSU	O4'-C4'	2.79	1.51	1.45
1	1	2863	PSU	O4'-C4'	2.79	1.51	1.45
1	1	754	PSU	O4'-C4'	2.79	1.51	1.45
1	1	1421	PSU	C6-N1	-2.79	1.31	1.36
1	1	779	PSU	O4-C4	-2.78	1.18	1.23
1	1	1035	PSU	O4'-C4'	2.78	1.51	1.45
3	4	55	PSU	O4'-C4'	2.78	1.51	1.45
1	1	2578	OMG	C5-N7	-2.78	1.33	1.39
1	1	2881	OMG	C5-N7	-2.77	1.33	1.39
1	1	948	PSU	O4-C4	-2.77	1.18	1.23
1	1	127	PSU	O4'-C4'	2.77	1.51	1.45
1	1	2774	OMG	O6-C6	-2.77	1.18	1.23
1	1	2750	OMG	O6-C6	-2.77	1.18	1.23
1	1	2277	UY1	C3'-C2'	-2.77	1.46	1.53
1	1	881	PSU	O4'-C4'	2.76	1.51	1.45
1	1	2303	PSU	O4-C4	-2.76	1.18	1.23
1	1	627	OMG	O6-C6	-2.76	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	956	PSU	O4-C4	-2.75	1.18	1.23
1	1	1025	PSU	O4'-C4'	2.75	1.51	1.45
1	1	2839	PSU	O4-C4	-2.75	1.18	1.23
1	1	1870	PSU	C6-N1	-2.75	1.31	1.36
1	1	2801	PSU	O4'-C4'	2.75	1.51	1.45
1	1	2221	PSU	C4-C5	-2.75	1.36	1.44
1	1	881	PSU	C6-N1	-2.74	1.31	1.36
1	1	2785	PSU	O4-C4	-2.73	1.18	1.23
1	1	2903	PSU	O4-C4	-2.73	1.18	1.23
1	1	355	PSU	O4-C4	-2.73	1.18	1.23
1	1	793	PSU	O4-C4	-2.72	1.18	1.23
1	1	1918	PSU	O4-C4	-2.72	1.18	1.23
1	1	2690	UY1	O4-C4	-2.72	1.18	1.23
1	1	2558	PSU	O4-C4	-2.72	1.18	1.23
1	1	2229	PSU	C4-C5	-2.72	1.36	1.44
1	1	890	OMG	O6-C6	-2.72	1.18	1.23
1	1	127	PSU	O4-C4	-2.71	1.18	1.23
1	1	718	PSU	O4-C4	-2.71	1.18	1.23
1	1	2876	OMG	O6-C6	-2.71	1.18	1.23
1	1	1043	PSU	O4-C4	-2.71	1.18	1.23
1	1	2251	OMG	C2-N1	2.70	1.44	1.37
1	1	2703	PSU	C6-N1	-2.70	1.31	1.36
1	1	2752	OMG	O6-C6	-2.70	1.18	1.23
1	1	773	PSU	O4'-C4'	2.70	1.51	1.45
1	1	355	PSU	O4'-C4'	2.70	1.51	1.45
1	1	871	PSU	O4-C4	-2.70	1.18	1.23
1	1	2223	PSU	O4'-C4'	2.70	1.51	1.45
1	1	917	PSU	O4-C4	-2.70	1.18	1.23
1	1	2491	OMG	O6-C6	-2.69	1.18	1.23
1	1	1874	PSU	O4-C4	-2.69	1.18	1.23
1	1	2154	PSU	O4-C4	-2.69	1.18	1.23
1	1	2092	PSU	O4-C4	-2.69	1.18	1.23
1	1	948	PSU	C6-N1	-2.69	1.31	1.36
1	1	2876	OMG	C2-N1	2.69	1.44	1.37
1	1	1904	PSU	C6-N1	-2.68	1.31	1.36
1	1	2688	OMU	O2-C2	-2.68	1.18	1.23
1	1	956	PSU	C6-N1	-2.68	1.31	1.36
3	4	55	PSU	O4-C4	-2.68	1.18	1.23
1	1	793	PSU	C6-N1	-2.68	1.31	1.36
1	1	2546	PSU	O4-C4	-2.67	1.18	1.23
1	1	355	PSU	C6-N1	-2.67	1.31	1.36
1	1	718	PSU	O4'-C4'	2.67	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2558	PSU	O4'-C4'	2.67	1.50	1.45
1	1	2546	PSU	O4'-C4'	2.67	1.50	1.45
1	1	787	OMG	O6-C6	-2.67	1.18	1.23
3	4	75	OMG	C2-N1	2.67	1.44	1.37
1	1	807	PSU	O4'-C4'	2.67	1.50	1.45
1	1	2578	OMG	C2-N1	2.67	1.44	1.37
1	1	2880	OMU	O2-C2	-2.67	1.18	1.23
3	4	75	OMG	O6-C6	-2.66	1.18	1.23
1	1	2380	OMU	O2-C2	-2.66	1.18	1.23
1	1	1107	PSU	C6-N1	-2.66	1.32	1.36
1	1	385	OMG	C2-N1	2.66	1.44	1.37
1	1	1907	OMG	O6-C6	-2.65	1.18	1.23
1	1	2703	PSU	O4-C4	-2.65	1.18	1.23
1	1	773	PSU	O4-C4	-2.65	1.18	1.23
1	1	2578	OMG	O6-C6	-2.65	1.18	1.23
1	1	373	PSU	O4'-C4'	2.65	1.50	1.45
1	1	373	PSU	C6-N1	-2.64	1.32	1.36
1	1	948	PSU	O4'-C4'	2.64	1.50	1.45
1	1	773	PSU	C6-N1	-2.64	1.32	1.36
1	1	1904	PSU	O4'-C4'	2.64	1.50	1.45
1	1	917	PSU	C6-N1	-2.64	1.32	1.36
1	1	2217	PSU	C6-N1	-2.64	1.32	1.36
1	1	1453	PSU	O4-C4	-2.64	1.18	1.23
1	1	2882	PSU	O4-C4	-2.64	1.18	1.23
1	1	2934	PSU	C6-N1	-2.64	1.32	1.36
1	1	2675	PSU	C6-N1	-2.64	1.32	1.36
1	1	1025	PSU	O4-C4	-2.64	1.18	1.23
1	1	2096	PSU	O4-C4	-2.64	1.18	1.23
1	1	385	OMG	O6-C6	-2.64	1.18	1.23
1	1	2824	PSU	O4-C4	-2.64	1.18	1.23
1	1	972	PSU	C6-N1	-2.63	1.32	1.36
1	1	1105	PSU	O4-C4	-2.63	1.18	1.23
1	1	1421	PSU	O4-C4	-2.63	1.18	1.23
3	4	73	PSU	O4-C4	-2.63	1.18	1.23
1	1	768	A2M	C5-N7	-2.63	1.34	1.39
1	1	1907	OMG	C2-N1	2.62	1.44	1.37
1	1	881	PSU	O4-C4	-2.62	1.18	1.23
1	1	373	PSU	O4-C4	-2.62	1.18	1.23
1	1	2875	PSU	O4-C4	-2.62	1.18	1.23
1	1	1433	OMG	O6-C6	-2.62	1.18	1.23
3	4	18	PSU	C6-N1	-2.62	1.32	1.36
1	1	2096	PSU	C6-N1	-2.62	1.32	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	758	PSU	C6-N1	-2.62	1.32	1.36
1	1	2358	OMG	C4-N9	-2.62	1.31	1.38
1	1	787	OMG	C2-N1	2.62	1.44	1.37
1	1	1917	OMU	O2-C2	-2.61	1.18	1.23
1	1	2251	OMG	O6-C6	-2.61	1.18	1.23
1	1	2690	UY1	C2-N3	2.61	1.41	1.37
1	1	2556	PSU	O4-C4	-2.61	1.18	1.23
1	1	1868	OMU	O2-C2	-2.61	1.18	1.23
1	1	1035	PSU	O4-C4	-2.61	1.18	1.23
1	1	807	PSU	C6-N1	-2.61	1.32	1.36
1	1	2358	OMG	C2-N1	2.61	1.44	1.37
1	1	758	PSU	O4-C4	-2.60	1.18	1.23
1	1	2750	OMG	C2-N1	2.60	1.43	1.37
1	1	986	PSU	O4-C4	-2.60	1.18	1.23
1	1	972	PSU	O4-C4	-2.59	1.18	1.23
1	1	2277	UY1	C4-C5	2.59	1.51	1.44
1	1	1107	PSU	O4-C4	-2.59	1.18	1.23
1	1	942	PSU	O4-C4	-2.59	1.18	1.23
1	1	1421	PSU	O4'-C4'	2.59	1.50	1.45
1	1	1453	PSU	C6-N1	-2.59	1.32	1.36
1	1	1433	OMG	C2-N1	2.59	1.43	1.37
1	1	2891	PSU	O4-C4	-2.59	1.18	1.23
1	1	2752	OMG	C2-N1	2.59	1.43	1.37
1	1	2785	PSU	C6-N1	-2.58	1.32	1.36
1	1	1538	PSU	O4-C4	-2.58	1.18	1.23
1	1	2277	UY1	O2-C2	-2.58	1.17	1.23
1	1	942	PSU	C6-N1	-2.58	1.32	1.36
1	1	2379	PSU	O4-C4	-2.58	1.18	1.23
3	4	55	PSU	C6-N1	-2.57	1.32	1.36
1	1	2491	OMG	C2-N1	2.57	1.43	1.37
1	1	1016	PSU	O4-C4	-2.57	1.18	1.23
1	1	1043	PSU	C6-N1	-2.57	1.32	1.36
1	1	2303	PSU	C6-N1	-2.57	1.32	1.36
1	1	779	PSU	O4'-C4'	2.57	1.50	1.45
1	1	2774	OMG	C2-N1	2.57	1.43	1.37
1	1	2384	OMU	O2-C2	-2.56	1.18	1.23
1	1	1870	PSU	O4-C4	-2.56	1.18	1.23
1	1	754	PSU	O4-C4	-2.56	1.18	1.23
1	1	2546	PSU	C6-N1	-2.56	1.32	1.36
1	1	2863	PSU	C6-N1	-2.55	1.32	1.36
1	1	2934	PSU	O4-C4	-2.55	1.18	1.23
1	1	1904	PSU	O4-C4	-2.55	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	890	OMG	C2-N1	2.55	1.43	1.37
1	1	2881	OMG	O6-C6	-2.55	1.18	1.23
1	1	2558	PSU	C6-N1	-2.55	1.32	1.36
1	1	2675	PSU	O4-C4	-2.55	1.18	1.23
1	1	1035	PSU	C6-N1	-2.55	1.32	1.36
1	1	986	PSU	C6-N1	-2.54	1.32	1.36
1	1	768	A2M	C4-N9	-2.54	1.32	1.37
1	1	646	OMG	C4-N9	-2.54	1.31	1.38
1	1	127	PSU	C6-N1	-2.54	1.32	1.36
1	1	1420	OMC	C2-N1	2.53	1.45	1.40
1	1	2824	PSU	C6-N1	-2.53	1.32	1.36
1	1	2801	PSU	O4-C4	-2.52	1.18	1.23
1	1	2882	PSU	C6-N1	-2.52	1.32	1.36
1	1	1025	PSU	C6-N1	-2.52	1.32	1.36
1	1	2379	PSU	C6-N1	-2.52	1.32	1.36
1	1	2227	PSU	O4-C4	-2.52	1.18	1.23
1	1	2217	PSU	O4-C4	-2.52	1.18	1.23
1	1	2154	PSU	C6-N1	-2.52	1.32	1.36
1	1	2223	PSU	O4-C4	-2.52	1.18	1.23
1	1	779	PSU	C6-N1	-2.51	1.32	1.36
1	1	718	PSU	C6-N1	-2.51	1.32	1.36
1	1	2326	A2M	C5-N7	-2.51	1.34	1.39
1	1	1874	PSU	C6-N1	-2.51	1.32	1.36
1	1	899	A2M	C5-N7	-2.51	1.34	1.39
1	1	2556	PSU	C6-N1	-2.51	1.32	1.36
1	1	2277	UY1	O4'-C1'	2.51	1.47	1.43
1	1	871	PSU	C6-N1	-2.51	1.32	1.36
1	1	2839	PSU	C6-N1	-2.50	1.32	1.36
1	1	2838	OMC	C4-N4	2.50	1.40	1.33
1	1	2863	PSU	O4-C4	-2.49	1.18	1.23
1	1	1105	PSU	C6-N1	-2.49	1.32	1.36
1	1	2229	PSU	C6-N1	-2.49	1.32	1.36
1	1	956	PSU	O4'-C4'	2.49	1.50	1.45
1	1	1432	A2M	C5-N7	-2.49	1.34	1.39
1	1	646	OMG	C2-N1	2.48	1.43	1.37
1	1	2907	OMC	C2-N3	2.48	1.41	1.36
1	1	2358	OMG	C5-C6	2.48	1.53	1.44
1	1	2891	PSU	C6-N1	-2.47	1.32	1.36
1	1	627	OMG	C2-N1	2.47	1.43	1.37
1	1	2599	A2M	C5-N7	-2.47	1.34	1.39
1	1	2774	OMG	C5-C6	2.47	1.53	1.44
1	1	2801	PSU	C6-N1	-2.47	1.32	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	754	PSU	C6-N1	-2.47	1.32	1.36
1	1	2160	OMC	C4-N4	2.47	1.39	1.33
1	1	385	OMG	C4-N9	-2.47	1.31	1.38
1	1	1918	PSU	C6-N1	-2.46	1.32	1.36
1	1	2881	OMG	C5-C6	2.46	1.53	1.44
1	1	2907	OMC	C4-N4	2.46	1.39	1.33
1	1	2221	PSU	C6-N1	-2.46	1.32	1.36
1	1	2358	OMG	C5-N7	-2.46	1.34	1.39
1	1	1248	PSU	C6-N1	-2.46	1.32	1.36
1	1	2918	OMC	C4-N4	2.46	1.39	1.33
1	1	2227	PSU	C6-N1	-2.45	1.32	1.36
1	1	2229	PSU	O4-C4	-2.45	1.18	1.23
1	1	2578	OMG	C5-C6	2.45	1.53	1.44
1	1	2300	OMC	C4-N4	2.45	1.39	1.33
1	1	2221	PSU	O4-C4	-2.44	1.18	1.23
1	1	2876	OMG	C5-C6	2.44	1.53	1.44
1	1	651	OMC	C4-N4	2.43	1.39	1.33
1	1	793	PSU	O2-C2	-2.43	1.18	1.23
1	1	2092	PSU	C6-N1	-2.42	1.32	1.36
1	1	773	PSU	O2-C2	-2.42	1.18	1.23
3	4	73	PSU	C6-N1	-2.42	1.32	1.36
1	1	2326	A2M	C4-N9	-2.42	1.32	1.37
1	1	1491	OMC	C4-N4	2.42	1.39	1.33
1	1	2703	PSU	O4'-C4'	2.42	1.50	1.45
1	1	1836	OMC	C4-N4	2.42	1.39	1.33
1	1	858	A2M	C5-N7	-2.42	1.34	1.39
1	1	807	PSU	O2-C2	-2.42	1.18	1.23
1	1	2675	PSU	O2-C2	-2.42	1.18	1.23
1	1	799	A2M	C5-N7	-2.42	1.34	1.39
1	1	948	PSU	O2-C2	-2.41	1.18	1.23
1	1	627	OMG	C5-C6	2.41	1.53	1.44
1	1	1433	OMG	C5-C6	2.41	1.53	1.44
1	1	637	A2M	C5-N7	-2.41	1.34	1.39
1	1	1420	OMC	C4-N4	2.41	1.39	1.33
1	1	1433	OMG	C4-N9	-2.41	1.31	1.38
1	1	2875	PSU	C6-N1	-2.41	1.32	1.36
1	1	2903	PSU	C6-N1	-2.41	1.32	1.36
1	1	1248	PSU	O4-C4	-2.40	1.19	1.23
3	4	18	PSU	O2-C2	-2.40	1.18	1.23
1	1	2300	OMC	C2-N3	2.40	1.41	1.36
3	4	75	OMG	C5-C6	2.40	1.53	1.44
1	1	355	PSU	O2-C2	-2.40	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2750	OMG	C5-C6	2.40	1.53	1.44
1	1	1016	PSU	C6-N1	-2.39	1.32	1.36
1	1	2703	PSU	C3'-C4'	-2.39	1.46	1.53
1	1	881	PSU	O2-C2	-2.39	1.18	1.23
1	1	2251	OMG	C5-C6	2.39	1.53	1.44
1	1	2223	PSU	C6-N1	-2.39	1.32	1.36
1	1	385	OMG	C5-C6	2.39	1.53	1.44
1	1	778	OMC	C4-N4	2.38	1.39	1.33
1	1	2096	PSU	O2-C2	-2.38	1.18	1.23
1	1	1907	OMG	C5-C6	2.38	1.53	1.44
1	1	848	A2M	C5-N7	-2.38	1.34	1.39
1	1	2558	PSU	O2-C2	-2.38	1.18	1.23
1	1	1116	A2M	C5-N7	-2.38	1.34	1.39
1	1	2491	OMG	C5-C6	2.37	1.53	1.44
1	1	2244	A2M	C5-N7	-2.37	1.34	1.39
1	1	1538	PSU	C6-N1	-2.37	1.32	1.36
1	1	2934	PSU	O2-C2	-2.37	1.18	1.23
1	1	2881	OMG	C6-N1	2.37	1.43	1.38
1	1	627	OMG	C4-N9	-2.37	1.32	1.38
1	1	2300	OMC	C2-N1	2.37	1.45	1.40
1	1	1870	PSU	O2-C2	-2.37	1.18	1.23
1	1	2154	PSU	O2-C2	-2.37	1.18	1.23
1	1	1847	A2M	C5-N7	-2.37	1.34	1.39
1	1	2578	OMG	C4-N9	-2.36	1.32	1.38
1	1	890	OMG	C5-C6	2.35	1.53	1.44
1	1	779	PSU	O2-C2	-2.35	1.18	1.23
1	1	2703	PSU	O2-C2	-2.35	1.18	1.23
3	4	55	PSU	O2-C2	-2.35	1.18	1.23
1	1	2243	A2M	C5-N7	-2.35	1.34	1.39
1	1	2578	OMG	C6-N1	2.35	1.43	1.38
1	1	1874	PSU	O2-C2	-2.35	1.18	1.23
1	1	2752	OMG	C5-C6	2.35	1.53	1.44
1	1	2824	PSU	O4'-C1'	-2.34	1.40	1.43
1	1	787	OMG	C4-N9	-2.34	1.32	1.38
1	1	787	OMG	C5-C6	2.34	1.53	1.44
1	1	917	PSU	O2-C2	-2.34	1.18	1.23
1	1	2905	A2M	C5-N7	-2.33	1.34	1.39
1	1	2690	UY1	O2-C2	-2.33	1.18	1.23
1	1	1433	OMG	C6-N1	2.33	1.43	1.38
1	1	2303	PSU	O2-C2	-2.33	1.18	1.23
1	1	2182	A2M	C5-N7	-2.33	1.34	1.39
1	1	2379	PSU	O2-C2	-2.33	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	646	OMG	C5-C6	2.32	1.53	1.44
1	1	1105	PSU	O2-C2	-2.32	1.18	1.23
1	1	2092	PSU	O2-C2	-2.31	1.18	1.23
1	1	972	PSU	O2-C2	-2.31	1.18	1.23
1	1	127	PSU	O2-C2	-2.30	1.18	1.23
1	1	1907	OMG	C6-N1	2.30	1.43	1.38
1	1	2491	OMG	C6-N1	2.30	1.43	1.38
1	1	2824	PSU	O2-C2	-2.30	1.18	1.23
1	1	1043	PSU	O2-C2	-2.30	1.18	1.23
1	1	2160	OMC	C2-N3	2.30	1.40	1.36
1	1	2251	OMG	C6-N1	2.29	1.43	1.38
1	1	373	PSU	O2-C2	-2.29	1.18	1.23
1	1	1453	PSU	O2-C2	-2.29	1.18	1.23
1	1	2546	PSU	O2-C2	-2.29	1.18	1.23
1	1	942	PSU	O2-C2	-2.29	1.18	1.23
1	1	2491	OMG	C4-N9	-2.29	1.32	1.38
3	4	73	PSU	O2-C2	-2.29	1.18	1.23
1	1	1107	PSU	O2-C2	-2.28	1.18	1.23
1	1	1904	PSU	O2-C2	-2.28	1.18	1.23
1	1	1421	PSU	O2-C2	-2.28	1.18	1.23
1	1	2380	OMU	C2-N3	2.28	1.41	1.38
1	1	2876	OMG	C6-N1	2.28	1.43	1.38
1	1	2752	OMG	C4-N9	-2.28	1.32	1.38
1	1	956	PSU	O2-C2	-2.28	1.18	1.23
3	4	75	OMG	C6-N1	2.27	1.43	1.38
1	1	2907	OMC	C2-N1	2.27	1.44	1.40
1	1	2839	PSU	O2-C2	-2.27	1.18	1.23
1	1	2891	PSU	O2-C2	-2.27	1.18	1.23
1	1	1918	PSU	O2-C2	-2.27	1.18	1.23
1	1	871	PSU	C3'-C4'	-2.27	1.47	1.53
3	4	75	OMG	C4-N9	-2.27	1.32	1.38
1	1	2876	OMG	C4-N9	-2.26	1.32	1.38
1	1	2289	A2M	C5-N7	-2.26	1.35	1.39
1	1	754	PSU	O2-C2	-2.26	1.18	1.23
1	1	758	PSU	O2-C2	-2.26	1.18	1.23
1	1	2880	OMU	C2-N3	2.26	1.41	1.38
1	1	2752	OMG	C6-N1	2.26	1.43	1.38
1	1	2556	PSU	O2-C2	-2.26	1.18	1.23
1	1	2875	PSU	O2-C2	-2.25	1.18	1.23
1	1	1917	OMU	C2-N3	2.25	1.41	1.38
1	1	1432	A2M	O2'-C2'	2.25	1.48	1.42
1	1	2863	PSU	O2-C2	-2.25	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	718	PSU	O2-C2	-2.25	1.18	1.23
1	1	2785	PSU	O2-C2	-2.24	1.18	1.23
1	1	1538	PSU	O2-C2	-2.24	1.18	1.23
1	1	2384	OMU	C2-N3	2.23	1.41	1.38
1	1	2774	OMG	C4-N9	-2.23	1.32	1.38
1	1	2251	OMG	C4-N9	-2.23	1.32	1.38
1	1	1035	PSU	O2-C2	-2.23	1.18	1.23
1	1	986	PSU	O2-C2	-2.23	1.18	1.23
1	1	2881	OMG	C4-N9	-2.22	1.32	1.38
3	4	55	PSU	C3'-C4'	-2.22	1.47	1.53
1	1	2918	OMC	C2-N3	2.21	1.40	1.36
1	1	2750	OMG	C4-N9	-2.21	1.32	1.38
1	1	871	PSU	O2-C2	-2.21	1.18	1.23
1	1	1907	OMG	C4-N9	-2.21	1.32	1.38
1	1	2160	OMC	C2-N1	2.20	1.44	1.40
1	1	1025	PSU	O2-C2	-2.20	1.18	1.23
1	1	2918	OMC	C2-N1	2.20	1.44	1.40
1	1	1491	OMC	C2-N3	2.20	1.40	1.36
1	1	2358	OMG	C6-N1	2.20	1.43	1.38
1	1	2217	PSU	O2-C2	-2.19	1.18	1.23
1	1	385	OMG	C6-N1	2.18	1.42	1.38
1	1	2750	OMG	C6-N1	2.17	1.42	1.38
1	1	2688	OMU	C2-N3	2.17	1.41	1.38
1	1	2903	PSU	O2-C2	-2.17	1.18	1.23
1	1	2244	A2M	C4-N9	-2.16	1.33	1.37
1	1	787	OMG	C6-N1	2.15	1.42	1.38
1	1	2882	PSU	O2-C2	-2.15	1.18	1.23
1	1	890	OMG	C6-N1	2.14	1.42	1.38
1	1	2774	OMG	C6-N1	2.14	1.42	1.38
1	1	1868	OMU	C2-N3	2.14	1.41	1.38
1	1	2227	PSU	O2-C2	-2.14	1.18	1.23
1	1	1904	PSU	C3'-C4'	-2.14	1.47	1.53
1	1	1116	A2M	C4-N9	-2.14	1.33	1.37
1	1	1016	PSU	O2-C2	-2.14	1.18	1.23
1	1	2546	PSU	C3'-C4'	-2.13	1.47	1.53
1	1	2675	PSU	C3'-C4'	-2.12	1.47	1.53
1	1	2229	PSU	O2-C2	-2.12	1.18	1.23
1	1	1223	A2M	C5-N7	-2.12	1.35	1.39
1	1	1836	OMC	C2-N3	2.12	1.40	1.36
1	1	2801	PSU	O2-C2	-2.11	1.18	1.23
1	1	2221	PSU	O2-C2	-2.11	1.18	1.23
1	1	2785	PSU	O4'-C1'	-2.11	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	890	OMG	C4-N9	-2.11	1.32	1.38
1	1	1248	PSU	O2-C2	-2.10	1.18	1.23
1	1	899	A2M	C4-N9	-2.10	1.33	1.37
1	1	2838	OMC	C2-N3	2.10	1.40	1.36
1	1	1420	OMC	C2-N3	2.09	1.40	1.36
1	1	2223	PSU	O2-C2	-2.09	1.18	1.23
1	1	1016	PSU	C3'-C4'	-2.08	1.47	1.53
1	1	373	PSU	C3'-C4'	-2.07	1.47	1.53
1	1	1432	A2M	C4-N9	-2.07	1.33	1.37
1	1	355	PSU	C3'-C4'	-2.07	1.47	1.53
1	1	2221	PSU	C3'-C4'	-2.06	1.47	1.53
1	1	718	PSU	C3'-C4'	-2.05	1.47	1.53
1	1	1491	OMC	C2-N1	2.05	1.44	1.40
1	1	2863	PSU	C3'-C4'	-2.05	1.47	1.53
1	1	651	OMC	C2-N3	2.04	1.40	1.36
1	1	2223	PSU	C3'-C4'	-2.03	1.47	1.53
1	1	2217	PSU	C3'-C4'	-2.03	1.47	1.53
1	1	956	PSU	C3'-C4'	-2.02	1.47	1.53
1	1	799	A2M	C4-N9	-2.02	1.33	1.37
1	1	1035	PSU	C3'-C4'	-2.01	1.47	1.53
1	1	646	OMG	C6-N1	2.01	1.42	1.38
1	1	773	PSU	C3'-C4'	-2.01	1.47	1.53
1	1	948	PSU	C3'-C4'	-2.01	1.47	1.53
1	1	2227	PSU	C3'-C4'	-2.01	1.47	1.53
1	1	778	OMC	C2-N3	2.00	1.40	1.36

All (724) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	890	OMG	C1'-N9-C8	-6.96	106.95	126.73
1	1	858	A2M	C5-C4-N3	-6.93	117.18	126.72
1	1	2243	A2M	C5-C4-N3	-6.81	117.35	126.72
1	1	2599	A2M	C5-C4-N3	-6.77	117.39	126.72
1	1	1847	A2M	C5-C4-N3	-6.74	117.43	126.72
1	1	799	A2M	C5-C4-N3	-6.72	117.46	126.72
1	1	1907	OMG	C1'-N9-C8	-6.69	107.73	126.73
1	1	2905	A2M	C5-C4-N3	-6.67	117.53	126.72
1	1	848	A2M	C5-C4-N3	-6.66	117.55	126.72
1	1	2289	A2M	C5-C4-N3	-6.64	117.57	126.72
1	1	899	A2M	C5-C4-N3	-6.64	117.58	126.72
1	1	2182	A2M	C5-C4-N3	-6.62	117.60	126.72
1	1	637	A2M	C5-C4-N3	-6.62	117.61	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2251	OMG	C1'-N9-C8	-6.60	107.97	126.73
1	1	1432	A2M	C5-C4-N3	-6.57	117.68	126.72
1	1	2244	A2M	C5-C4-N3	-6.51	117.75	126.72
1	1	1223	A2M	C5-C4-N3	-6.44	117.85	126.72
1	1	1116	A2M	C5-C4-N3	-6.34	117.98	126.72
1	1	2750	OMG	C1'-N9-C8	-6.19	109.16	126.73
1	1	1433	OMG	C1'-N9-C8	-6.13	109.31	126.73
1	1	2881	OMG	C1'-N9-C8	-6.11	109.36	126.73
1	1	2326	A2M	C5-C4-N3	-6.10	118.31	126.72
1	1	2578	OMG	C1'-N9-C8	-6.10	109.41	126.73
1	1	385	OMG	C1'-N9-C8	-6.08	109.47	126.73
1	1	646	OMG	C1'-N9-C8	-6.06	109.50	126.73
1	1	2774	OMG	C1'-N9-C8	-6.04	109.57	126.73
3	4	75	OMG	C1'-N9-C8	-6.03	109.61	126.73
1	1	2876	OMG	C1'-N9-C8	-5.99	109.72	126.73
1	1	2491	OMG	C1'-N9-C8	-5.98	109.74	126.73
1	1	2593	UR3	C4-N3-C2	-5.93	119.81	124.58
1	1	2752	OMG	C1'-N9-C8	-5.91	109.95	126.73
1	1	627	OMG	C1'-N9-C8	-5.90	109.96	126.73
1	1	768	A2M	C5-C4-N3	-5.84	118.68	126.72
1	1	890	OMG	C1'-N9-C4	5.77	143.53	126.49
1	1	1248	PSU	C3'-C2'-C1'	5.75	108.48	101.69
1	1	787	OMG	C1'-N9-C8	-5.71	110.51	126.73
1	1	1868	OMU	C4-N3-C2	-5.64	119.61	126.61
1	1	2801	PSU	C3'-C2'-C1'	5.64	108.34	101.69
1	1	2880	OMU	C4-N3-C2	-5.61	119.65	126.61
1	1	2223	PSU	C3'-C2'-C1'	5.60	108.29	101.69
1	1	1907	OMG	C1'-N9-C4	5.45	142.58	126.49
1	1	2802	UR3	C4-N3-C2	-5.44	120.20	124.58
1	1	858	A2M	N3-C4-N9	5.44	136.42	127.17
1	1	1917	OMU	C4-N3-C2	-5.37	119.94	126.61
1	1	2384	OMU	C4-N3-C2	-5.35	119.97	126.61
1	1	2380	OMU	C4-N3-C2	-5.33	120.00	126.61
1	1	2251	OMG	C1'-N9-C4	5.31	142.16	126.49
1	1	848	A2M	N3-C4-N9	5.30	136.19	127.17
1	1	2688	OMU	C4-N3-C2	-5.29	120.04	126.61
1	1	2182	A2M	N3-C4-N9	5.27	136.13	127.17
1	1	890	OMG	C5-C4-N3	-5.26	120.01	128.39
1	1	1847	A2M	N3-C4-N9	5.25	136.10	127.17
1	1	2599	A2M	N3-C4-N9	5.25	136.10	127.17
1	1	637	A2M	N3-C4-N9	5.21	136.03	127.17
1	1	956	PSU	C3'-C2'-C1'	5.19	107.82	101.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2289	A2M	N3-C4-N9	5.18	135.98	127.17
1	1	2243	A2M	N3-C4-N9	5.14	135.91	127.17
1	1	2905	A2M	N3-C4-N9	5.14	135.91	127.17
1	1	773	PSU	N1-C2-N3	5.11	120.56	115.17
1	1	2934	PSU	N1-C2-N3	5.09	120.53	115.17
1	1	1116	A2M	N3-C4-N9	5.08	135.81	127.17
1	1	2244	A2M	N3-C4-N9	5.07	135.79	127.17
1	1	899	A2M	N3-C4-N9	5.07	135.79	127.17
1	1	799	A2M	N3-C4-N9	5.06	135.77	127.17
1	1	1223	A2M	N3-C4-N9	5.04	135.73	127.17
1	1	1904	PSU	N1-C2-N3	5.03	120.48	115.17
1	1	1432	A2M	N3-C4-N9	5.02	135.70	127.17
1	1	942	PSU	N1-C2-N3	5.00	120.45	115.17
1	1	948	PSU	N1-C2-N3	5.00	120.45	115.17
1	1	881	PSU	N1-C2-N3	4.99	120.44	115.17
1	1	793	PSU	N1-C2-N3	4.98	120.42	115.17
1	1	2277	UY1	C4-N3-C2	-4.98	119.52	126.37
1	1	1107	PSU	N1-C2-N3	4.94	120.38	115.17
1	1	972	PSU	N1-C2-N3	4.94	120.37	115.17
1	1	2774	OMG	C1'-N9-C4	4.93	141.04	126.49
1	1	2251	OMG	C5-C4-N3	-4.92	120.55	128.39
1	1	917	PSU	N1-C2-N3	4.91	120.35	115.17
1	1	2096	PSU	N1-C2-N3	4.91	120.34	115.17
1	1	2750	OMG	C1'-N9-C4	4.91	140.98	126.49
1	1	1918	PSU	N1-C2-N3	4.90	120.34	115.17
1	1	2881	OMG	C1'-N9-C4	4.89	140.92	126.49
1	1	355	PSU	N1-C2-N3	4.88	120.32	115.17
1	1	942	PSU	C4-N3-C2	-4.87	119.66	126.37
1	1	1870	PSU	N1-C2-N3	4.87	120.30	115.17
1	1	2703	PSU	N1-C2-N3	4.87	120.30	115.17
1	1	2558	PSU	N1-C2-N3	4.87	120.30	115.17
1	1	2558	PSU	C3'-C2'-C1'	4.86	107.42	101.69
1	1	2750	OMG	C5-C4-N3	-4.85	120.67	128.39
1	1	2690	UY1	C4-N3-C2	-4.85	119.69	126.37
1	1	1874	PSU	N1-C2-N3	4.85	120.28	115.17
1	1	373	PSU	N1-C2-N3	4.84	120.28	115.17
1	1	1907	OMG	C5-C4-N3	-4.83	120.71	128.39
3	4	75	OMG	C1'-N9-C4	4.83	140.75	126.49
1	1	956	PSU	N1-C2-N3	4.83	120.26	115.17
1	1	793	PSU	C4-N3-C2	-4.82	119.73	126.37
1	1	1433	OMG	C1'-N9-C4	4.82	140.72	126.49
1	1	2774	OMG	C5-C4-N3	-4.81	120.73	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1918	PSU	C4-N3-C2	-4.81	119.75	126.37
1	1	2578	OMG	C1'-N9-C4	4.80	140.67	126.49
1	1	2546	PSU	C4-N3-C2	-4.80	119.76	126.37
1	1	768	A2M	N3-C4-N9	4.80	135.33	127.17
1	1	627	OMG	C5-C4-N3	-4.80	120.76	128.39
1	1	2882	PSU	N1-C2-N3	4.79	120.22	115.17
1	1	2358	OMG	C1'-N9-C8	-4.78	113.14	126.73
1	1	2824	PSU	N1-C2-N3	4.77	120.20	115.17
1	1	2690	UY1	N1-C2-N3	4.77	120.20	115.17
1	1	2491	OMG	C5-C4-N3	-4.76	120.81	128.39
1	1	2154	PSU	N1-C2-N3	4.76	120.19	115.17
1	1	2546	PSU	N1-C2-N3	4.76	120.19	115.17
1	1	2876	OMG	C1'-N9-C4	4.75	140.53	126.49
1	1	2379	PSU	N1-C2-N3	4.74	120.17	115.17
1	1	385	OMG	C1'-N9-C4	4.74	140.49	126.49
1	1	2752	OMG	C5-C4-N3	-4.74	120.85	128.39
1	1	2881	OMG	C5-C4-N3	-4.73	120.86	128.39
1	1	779	PSU	N1-C2-N3	4.73	120.15	115.17
1	1	2092	PSU	N1-C2-N3	4.73	120.15	115.17
1	1	1421	PSU	N1-C2-N3	4.73	120.15	115.17
1	1	807	PSU	N1-C2-N3	4.72	120.15	115.17
1	1	1105	PSU	N1-C2-N3	4.72	120.15	115.17
1	1	1043	PSU	C4-N3-C2	-4.72	119.87	126.37
1	1	2703	PSU	C4-N3-C2	-4.72	119.87	126.37
1	1	948	PSU	C4-N3-C2	-4.71	119.89	126.37
1	1	1035	PSU	N1-C2-N3	4.71	120.13	115.17
3	4	75	OMG	C5-C4-N3	-4.71	120.90	128.39
1	1	718	PSU	C4-N3-C2	-4.70	119.89	126.37
1	1	1870	PSU	C4-N3-C2	-4.70	119.90	126.37
1	1	2876	OMG	C5-C4-N3	-4.70	120.91	128.39
1	1	754	PSU	C4-N3-C2	-4.69	119.91	126.37
1	1	758	PSU	N1-C2-N3	4.69	120.12	115.17
1	1	754	PSU	N1-C2-N3	4.69	120.12	115.17
1	1	373	PSU	C4-N3-C2	-4.69	119.91	126.37
1	1	2326	A2M	N3-C4-N9	4.69	135.14	127.17
1	1	972	PSU	C4-N3-C2	-4.69	119.91	126.37
1	1	627	OMG	C1'-N9-C4	4.69	140.33	126.49
1	1	2217	PSU	N1-C2-N3	4.68	120.11	115.17
1	1	2578	OMG	C5-C4-N3	-4.68	120.94	128.39
1	1	2303	PSU	N1-C2-N3	4.68	120.11	115.17
1	1	355	PSU	C4-N3-C2	-4.68	119.93	126.37
1	1	807	PSU	C4-N3-C2	-4.68	119.93	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	637	A2M	N3-C2-N1	-4.68	121.50	128.58
1	1	2491	OMG	C1'-N9-C4	4.67	140.28	126.49
1	1	1223	A2M	N3-C2-N1	-4.67	121.51	128.58
1	1	646	OMG	C1'-N9-C4	4.67	140.28	126.49
1	1	773	PSU	C4-N3-C2	-4.67	119.94	126.37
1	1	2903	PSU	C4-N3-C2	-4.67	119.94	126.37
1	1	881	PSU	C4-N3-C2	-4.67	119.94	126.37
1	1	917	PSU	C4-N3-C2	-4.66	119.95	126.37
1	1	2096	PSU	C4-N3-C2	-4.66	119.95	126.37
1	1	1904	PSU	C4-N3-C2	-4.65	119.96	126.37
1	1	1025	PSU	C4-N3-C2	-4.65	119.96	126.37
1	1	1043	PSU	N1-C2-N3	4.65	120.07	115.17
1	1	2891	PSU	N1-C2-N3	4.65	120.07	115.17
1	1	2752	OMG	C1'-N9-C4	4.65	140.23	126.49
1	1	787	OMG	C5-C4-N3	-4.65	120.99	128.39
1	1	2675	PSU	N1-C2-N3	4.65	120.07	115.17
1	1	779	PSU	C4-N3-C2	-4.65	119.97	126.37
1	1	2558	PSU	C4-N3-C2	-4.65	119.97	126.37
1	1	1025	PSU	N1-C2-N3	4.64	120.06	115.17
1	1	2863	PSU	N1-C2-N3	4.64	120.06	115.17
1	1	2905	A2M	N3-C2-N1	-4.64	121.56	128.58
1	1	1421	PSU	C4-N3-C2	-4.63	119.99	126.37
1	1	2934	PSU	C4-N3-C2	-4.63	120.00	126.37
1	1	1847	A2M	N3-C2-N1	-4.62	121.59	128.58
1	1	1874	PSU	C4-N3-C2	-4.62	120.01	126.37
1	1	2289	A2M	N3-C2-N1	-4.62	121.59	128.58
1	1	1105	PSU	C4-N3-C2	-4.62	120.01	126.37
1	1	871	PSU	C4-N3-C2	-4.61	120.02	126.37
1	1	2774	OMG	C2-N3-C4	4.61	120.25	112.30
1	1	1035	PSU	C4-N3-C2	-4.61	120.02	126.37
1	1	2227	PSU	N1-C2-N3	4.61	120.03	115.17
1	1	2891	PSU	C4-N3-C2	-4.61	120.02	126.37
1	1	2556	PSU	N1-C2-N3	4.61	120.03	115.17
1	1	718	PSU	N1-C2-N3	4.59	120.01	115.17
3	4	55	PSU	N1-C2-N3	4.59	120.01	115.17
1	1	2882	PSU	C4-N3-C2	-4.59	120.05	126.37
1	1	1453	PSU	N1-C2-N3	4.59	120.01	115.17
1	1	1432	A2M	N3-C2-N1	-4.58	121.66	128.58
1	1	2903	PSU	N1-C2-N3	4.57	119.99	115.17
3	4	18	PSU	N1-C2-N3	4.57	119.99	115.17
1	1	2839	PSU	C4-N3-C2	-4.57	120.08	126.37
1	1	1116	A2M	N3-C2-N1	-4.57	121.67	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	956	PSU	C4-N3-C2	-4.57	120.08	126.37
1	1	127	PSU	N1-C2-N3	4.57	119.99	115.17
1	1	848	A2M	N3-C2-N1	-4.57	121.67	128.58
1	1	871	PSU	N1-C2-N3	4.56	119.98	115.17
1	1	2379	PSU	C4-N3-C2	-4.56	120.09	126.37
1	1	2154	PSU	C4-N3-C2	-4.56	120.09	126.37
1	1	2578	OMG	C2-N3-C4	4.55	120.14	112.30
1	1	1538	PSU	C4-N3-C2	-4.55	120.10	126.37
1	1	986	PSU	N1-C2-N3	4.55	119.97	115.17
1	1	986	PSU	C4-N3-C2	-4.55	120.11	126.37
1	1	627	OMG	C2-N3-C4	4.54	120.12	112.30
1	1	1248	PSU	N1-C2-N3	4.54	119.95	115.17
3	4	73	PSU	N1-C2-N3	4.53	119.95	115.17
1	1	2244	A2M	N3-C2-N1	-4.53	121.72	128.58
1	1	2303	PSU	C4-N3-C2	-4.53	120.13	126.37
1	1	2875	PSU	N1-C2-N3	4.53	119.94	115.17
1	1	2785	PSU	N1-C2-N3	4.52	119.93	115.17
1	1	2491	OMG	C2-N3-C4	4.51	120.06	112.30
1	1	2824	PSU	C4-N3-C2	-4.50	120.17	126.37
3	4	18	PSU	C4-N3-C2	-4.50	120.17	126.37
1	1	1538	PSU	N1-C2-N3	4.50	119.91	115.17
1	1	2752	OMG	C2-N3-C4	4.49	120.03	112.30
3	4	73	PSU	C4-N3-C2	-4.49	120.19	126.37
1	1	890	OMG	C2-N3-C4	4.48	120.02	112.30
1	1	1433	OMG	C5-C4-N3	-4.47	121.27	128.39
1	1	127	PSU	C4-N3-C2	-4.47	120.21	126.37
1	1	2801	PSU	N1-C2-N3	4.47	119.88	115.17
1	1	799	A2M	N3-C2-N1	-4.47	121.82	128.58
1	1	2881	OMG	C2-N3-C4	4.46	119.99	112.30
1	1	2182	A2M	N3-C2-N1	-4.46	121.83	128.58
1	1	787	OMG	C1'-N9-C4	4.46	139.67	126.49
1	1	2839	PSU	N1-C2-N3	4.46	119.88	115.17
1	1	2785	PSU	C4-N3-C2	-4.46	120.23	126.37
1	1	917	PSU	C3'-C2'-C1'	4.46	106.95	101.69
1	1	2092	PSU	C4-N3-C2	-4.46	120.23	126.37
1	1	1107	PSU	C4-N3-C2	-4.45	120.24	126.37
1	1	2750	OMG	C2-N3-C4	4.45	119.96	112.30
1	1	1433	OMG	C2-N3-C4	4.44	119.95	112.30
1	1	2599	A2M	N3-C2-N1	-4.42	121.88	128.58
1	1	646	OMG	C5-C4-N3	-4.42	121.35	128.39
1	1	2217	PSU	C4-N3-C2	-4.42	120.28	126.37
1	1	1016	PSU	N1-C2-N3	4.42	119.83	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	858	A2M	N3-C2-N1	-4.41	121.91	128.58
1	1	385	OMG	C5-C4-N3	-4.40	121.38	128.39
1	1	2221	PSU	N1-C2-N3	4.40	119.81	115.17
1	1	2229	PSU	N1-C2-N3	4.40	119.81	115.17
1	1	2243	A2M	N3-C2-N1	-4.39	121.94	128.58
1	1	768	A2M	O4'-C1'-C2'	-4.38	99.05	106.59
1	1	2876	OMG	C2-N3-C4	4.38	119.84	112.30
1	1	2326	A2M	N3-C2-N1	-4.37	121.96	128.58
1	1	1016	PSU	C4-N3-C2	-4.36	120.36	126.37
1	1	2863	PSU	C4-N3-C2	-4.36	120.37	126.37
1	1	2556	PSU	C4-N3-C2	-4.35	120.37	126.37
1	1	787	OMG	C2-N3-C4	4.35	119.80	112.30
1	1	1453	PSU	C4-N3-C2	-4.35	120.38	126.37
1	1	2251	OMG	C2-N3-C4	4.35	119.78	112.30
1	1	2875	PSU	C4-N3-C2	-4.34	120.39	126.37
1	1	2675	PSU	C4-N3-C2	-4.34	120.40	126.37
1	1	1248	PSU	C4-N3-C2	-4.34	120.40	126.37
1	1	2223	PSU	N1-C2-N3	4.33	119.73	115.17
1	1	1907	OMG	C2-N3-C4	4.32	119.74	112.30
3	4	75	OMG	C2-N3-C4	4.31	119.73	112.30
1	1	2384	OMU	N3-C2-N1	4.31	120.50	114.89
1	1	899	A2M	N3-C2-N1	-4.31	122.06	128.58
1	1	1868	OMU	N3-C2-N1	4.28	120.47	114.89
1	1	2863	PSU	C3'-C2'-C1'	4.28	106.74	101.69
1	1	768	A2M	N3-C2-N1	-4.27	122.11	128.58
1	1	754	PSU	C3'-C2'-C1'	4.25	106.71	101.69
3	4	55	PSU	C4-N3-C2	-4.25	120.52	126.37
1	1	758	PSU	C4-N3-C2	-4.25	120.52	126.37
1	1	2880	OMU	N3-C2-N1	4.24	120.42	114.89
1	1	2221	PSU	C4-N3-C2	-4.24	120.53	126.37
1	1	646	OMG	C2-N3-C4	4.24	119.60	112.30
1	1	2358	OMG	C2-N3-C4	4.23	119.58	112.30
1	1	2227	PSU	C4-N3-C2	-4.22	120.56	126.37
1	1	2229	PSU	C4-N3-C2	-4.19	120.59	126.37
1	1	768	A2M	C4'-O4'-C1'	-4.19	100.21	109.47
1	1	1847	A2M	C2-N3-C4	4.18	122.03	111.83
1	1	2688	OMU	N3-C2-N1	4.15	120.30	114.89
1	1	385	OMG	C2-N3-C4	4.15	119.45	112.30
1	1	2223	PSU	C4-N3-C2	-4.14	120.66	126.37
1	1	799	A2M	C2-N3-C4	4.13	121.92	111.83
1	1	2905	A2M	C2-N3-C4	4.13	121.92	111.83
1	1	858	A2M	C2-N3-C4	4.12	121.90	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	637	A2M	C2-N3-C4	4.12	121.89	111.83
1	1	1432	A2M	C2-N3-C4	4.10	121.86	111.83
1	1	2380	OMU	N3-C2-N1	4.10	120.23	114.89
1	1	848	A2M	C2-N3-C4	4.09	121.83	111.83
1	1	2289	A2M	C2-N3-C4	4.08	121.78	111.83
1	1	2243	A2M	C2-N3-C4	4.07	121.78	111.83
1	1	2801	PSU	C4-N3-C2	-4.07	120.77	126.37
1	1	2599	A2M	C2-N3-C4	4.05	121.73	111.83
1	1	2182	A2M	C2-N3-C4	4.03	121.67	111.83
1	1	2244	A2M	C2-N3-C4	4.03	121.66	111.83
1	1	373	PSU	C3'-C2'-C1'	4.01	106.42	101.69
1	1	2358	OMG	C5-C4-N3	-4.00	122.02	128.39
1	1	899	A2M	C2-N3-C4	3.99	121.57	111.83
1	1	1223	A2M	C2-N3-C4	3.97	121.54	111.83
1	1	768	A2M	C2'-C1'-N9	3.97	120.28	113.75
1	1	1116	A2M	C2-N3-C4	3.96	121.51	111.83
1	1	1035	PSU	C3'-C2'-C1'	3.93	106.33	101.69
1	1	1917	OMU	N3-C2-N1	3.92	120.00	114.89
1	1	1025	PSU	C3'-C2'-C1'	3.91	106.30	101.69
1	1	1904	PSU	C3'-C2'-C1'	3.88	106.27	101.69
1	1	773	PSU	C3'-C2'-C1'	3.88	106.26	101.69
1	1	1917	OMU	C5-C4-N3	3.88	120.23	114.80
1	1	807	PSU	C3'-C2'-C1'	3.87	106.25	101.69
1	1	2277	UY1	N1-C2-N3	3.85	119.23	115.17
1	1	2491	OMG	N9-C8-N7	-3.83	106.29	113.40
1	1	385	OMG	N9-C8-N7	-3.83	106.31	113.40
1	1	646	OMG	N9-C8-N7	-3.82	106.32	113.40
1	1	2593	UR3	C5-C4-N3	3.80	120.04	115.04
1	1	2880	OMU	C5-C4-N3	3.80	120.12	114.80
1	1	1433	OMG	N9-C8-N7	-3.80	106.36	113.40
1	1	2675	PSU	C3'-C2'-C1'	3.79	106.16	101.69
1	1	2380	OMU	C5-C4-N3	3.76	120.07	114.80
1	1	2578	OMG	N9-C8-N7	-3.76	106.42	113.40
1	1	2326	A2M	C2-N3-C4	3.74	120.96	111.83
1	1	1868	OMU	C5-C4-N3	3.74	120.03	114.80
1	1	2750	OMG	N9-C8-N7	-3.73	106.48	113.40
1	1	718	PSU	C3'-C2'-C1'	3.73	106.09	101.69
1	1	2244	A2M	O4'-C1'-N9	3.73	115.25	108.09
1	1	2802	UR3	C1'-N1-C2	3.72	123.14	117.04
1	1	2358	OMG	C1'-N9-C4	3.69	137.40	126.49
1	1	2752	OMG	N9-C8-N7	-3.69	106.55	113.40
1	1	881	PSU	C3'-C2'-C1'	3.69	106.04	101.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2546	PSU	C3'-C2'-C1'	3.69	106.04	101.69
1	1	627	OMG	N9-C8-N7	-3.68	106.57	113.40
1	1	2881	OMG	N9-C8-N7	-3.68	106.58	113.40
1	1	2876	OMG	N9-C8-N7	-3.64	106.64	113.40
1	1	890	OMG	N9-C4-N3	3.63	133.22	125.95
1	1	2688	OMU	C5-C4-N3	3.63	119.88	114.80
1	1	2802	UR3	C5-C4-N3	3.62	119.81	115.04
1	1	2251	OMG	N9-C8-N7	-3.62	106.68	113.40
1	1	1432	A2M	N9-C8-N7	-3.61	108.81	113.94
1	1	787	OMG	N9-C8-N7	-3.60	106.72	113.40
3	4	75	OMG	N9-C8-N7	-3.58	106.76	113.40
1	1	1116	A2M	N9-C8-N7	-3.57	108.87	113.94
1	1	2384	OMU	C5-C4-N3	3.56	119.79	114.80
1	1	848	A2M	N9-C8-N7	-3.54	108.91	113.94
1	1	1907	OMG	N9-C8-N7	-3.54	106.84	113.40
1	1	2838	OMC	C1'-N1-C2	3.52	126.22	118.44
1	1	1432	A2M	C5-N7-C8	3.50	108.95	103.45
1	1	2801	PSU	C6-N1-C2	-3.50	119.45	122.69
1	1	768	A2M	C2-N3-C4	3.50	120.37	111.83
1	1	2774	OMG	N9-C8-N7	-3.49	106.92	113.40
1	1	1432	A2M	C2'-C1'-N9	-3.47	108.05	113.75
1	1	890	OMG	N9-C8-N7	-3.43	107.05	113.40
1	1	2182	A2M	N9-C8-N7	-3.43	109.08	113.94
1	1	127	PSU	C3'-C2'-C1'	3.40	105.70	101.69
1	1	2217	PSU	O2-C2-N1	-3.37	119.32	122.79
1	1	858	A2M	N9-C8-N7	-3.36	109.17	113.94
1	1	848	A2M	C5-N7-C8	3.36	108.72	103.45
1	1	773	PSU	C6-N1-C2	-3.36	119.58	122.69
1	1	899	A2M	N9-C8-N7	-3.35	109.18	113.94
1	1	1107	PSU	C6-N1-C2	-3.33	119.60	122.69
1	1	2358	OMG	N9-C8-N7	-3.32	107.24	113.40
1	1	2244	A2M	N9-C8-N7	-3.32	109.23	113.94
1	1	858	A2M	C5-N7-C8	3.30	108.64	103.45
1	1	758	PSU	C6-N1-C2	-3.30	119.63	122.69
1	1	899	A2M	C5-N7-C8	3.29	108.63	103.45
1	1	1420	OMC	C1'-N1-C2	3.29	125.71	118.44
1	1	779	PSU	C3'-C2'-C1'	3.29	105.57	101.69
1	1	1107	PSU	O2-C2-N1	-3.29	119.40	122.79
1	1	1116	A2M	C5-N7-C8	3.29	108.62	103.45
1	1	2326	A2M	C4'-O4'-C1'	-3.29	102.21	109.47
1	1	2599	A2M	C5-N7-C8	3.28	108.60	103.45
1	1	2251	OMG	N9-C4-N3	3.28	132.51	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2289	A2M	N9-C8-N7	-3.27	109.29	113.94
1	1	637	A2M	N9-C8-N7	-3.27	109.30	113.94
1	1	2244	A2M	C4'-O4'-C1'	-3.27	102.25	109.47
1	1	2217	PSU	C6-N1-C2	-3.27	119.66	122.69
1	1	2182	A2M	C5-N7-C8	3.27	108.58	103.45
1	1	2802	UR3	C6-N1-C2	-3.24	119.15	121.80
1	1	2599	A2M	N9-C8-N7	-3.24	109.33	113.94
1	1	2227	PSU	C6-N1-C2	-3.24	119.69	122.69
1	1	1847	A2M	C5-N7-C8	3.23	108.53	103.45
1	1	2934	PSU	C6-N1-C2	-3.23	119.69	122.69
1	1	1248	PSU	C6-N1-C2	-3.22	119.70	122.69
1	1	1432	A2M	C4-C5-N7	-3.22	106.90	110.58
1	1	1907	OMG	N9-C4-N3	3.20	132.36	125.95
1	1	1904	PSU	C6-N1-C2	-3.20	119.72	122.69
1	1	2289	A2M	C5-N7-C8	3.20	108.47	103.45
1	1	1847	A2M	N9-C8-N7	-3.19	109.41	113.94
1	1	773	PSU	O2-C2-N1	-3.19	119.50	122.79
1	1	637	A2M	C5-N7-C8	3.19	108.46	103.45
1	1	2905	A2M	C5-N7-C8	3.19	108.46	103.45
1	1	1432	A2M	C3'-C2'-C1'	3.18	108.90	102.81
1	1	890	OMG	C2-N1-C6	-3.18	119.35	125.11
1	1	956	PSU	C6-N1-C2	-3.17	119.75	122.69
1	1	1907	OMG	C2-N1-C6	-3.16	119.37	125.11
1	1	2243	A2M	C5-N7-C8	3.16	108.42	103.45
1	1	2905	A2M	N9-C8-N7	-3.16	109.45	113.94
1	1	1870	PSU	O2-C2-N1	-3.16	119.53	122.79
1	1	2882	PSU	C6-N1-C2	-3.15	119.77	122.69
3	4	55	PSU	C6-N1-C2	-3.14	119.78	122.69
1	1	2824	PSU	C6-N1-C2	-3.14	119.78	122.69
1	1	2750	OMG	N9-C4-N3	3.13	132.22	125.95
1	1	355	PSU	C3'-C2'-C1'	3.13	105.38	101.69
1	1	2243	A2M	O3'-C3'-C4'	3.13	120.06	111.08
1	1	1116	A2M	C4-N9-C8	3.13	109.02	105.74
1	1	948	PSU	C6-N1-C2	-3.12	119.79	122.69
1	1	1223	A2M	N9-C8-N7	-3.12	109.51	113.94
1	1	2221	PSU	C3'-C2'-C1'	3.12	105.37	101.69
1	1	2092	PSU	C6-N1-C2	-3.12	119.80	122.69
1	1	2223	PSU	C6-N1-C2	-3.11	119.80	122.69
1	1	2229	PSU	C6-N1-C2	-3.11	119.80	122.69
1	1	2243	A2M	N9-C8-N7	-3.09	109.56	113.94
1	1	917	PSU	C6-N1-C2	-3.09	119.83	122.69
1	1	2750	OMG	C2-N1-C6	-3.07	119.53	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2556	PSU	C6-N1-C2	-3.07	119.84	122.69
1	1	1223	A2M	C5-N7-C8	3.07	108.27	103.45
1	1	2244	A2M	C5-N7-C8	3.07	108.27	103.45
1	1	972	PSU	C6-N1-C2	-3.07	119.85	122.69
1	1	2934	PSU	O2-C2-N1	-3.06	119.63	122.79
1	1	799	A2M	C5-N7-C8	3.06	108.26	103.45
1	1	2154	PSU	C6-N1-C2	-3.06	119.85	122.69
1	1	899	A2M	C4-C5-N7	-3.06	107.09	110.58
1	1	2599	A2M	C4-C5-N7	-3.06	107.09	110.58
1	1	2558	PSU	C6-N1-C2	-3.05	119.86	122.69
1	1	1453	PSU	C6-N1-C2	-3.05	119.86	122.69
1	1	2703	PSU	C6-N1-C2	-3.04	119.87	122.69
1	1	2491	OMG	N9-C4-N3	3.04	132.03	125.95
1	1	1904	PSU	O2-C2-N1	-3.04	119.65	122.79
1	1	1421	PSU	C3'-C2'-C1'	3.04	105.27	101.69
1	1	1016	PSU	C6-N1-C2	-3.04	119.87	122.69
1	1	2675	PSU	C6-N1-C2	-3.03	119.88	122.69
1	1	799	A2M	C4-C5-N7	-3.03	107.12	110.58
1	1	1248	PSU	C2'-C3'-C4'	3.03	108.46	102.61
1	1	2379	PSU	C6-N1-C2	-3.03	119.88	122.69
1	1	2491	OMG	C2-N1-C6	-3.02	119.63	125.11
1	1	2243	A2M	O4'-C4'-C3'	-3.02	99.15	105.15
1	1	2752	OMG	N9-C4-N3	3.02	132.00	125.95
1	1	2303	PSU	C3'-C2'-C1'	3.02	105.25	101.69
1	1	2882	PSU	O2-C2-N1	-3.01	119.68	122.79
1	1	793	PSU	C6-N1-C2	-3.01	119.90	122.69
1	1	2703	PSU	O2-C2-N1	-3.01	119.69	122.79
1	1	2752	OMG	C2-N1-C6	-3.00	119.66	125.11
1	1	2863	PSU	C6-N1-C2	-3.00	119.91	122.69
1	1	858	A2M	C4-C5-N7	-3.00	107.16	110.58
1	1	2243	A2M	C4-C5-N7	-3.00	107.16	110.58
1	1	627	OMG	N9-C4-N3	2.99	131.94	125.95
1	1	848	A2M	C4-N9-C8	2.99	108.88	105.74
1	1	2891	PSU	C6-N1-C2	-2.98	119.92	122.69
1	1	2251	OMG	C2-N1-C6	-2.98	119.71	125.11
1	1	1421	PSU	O2-C2-N1	-2.97	119.72	122.79
1	1	2380	OMU	O4-C4-C5	-2.97	120.04	125.16
3	4	75	OMG	N9-C4-N3	2.97	131.89	125.95
1	1	1874	PSU	C6-N1-C2	-2.97	119.94	122.69
1	1	768	A2M	C3'-C2'-C1'	-2.97	97.13	102.81
1	1	355	PSU	C6-N1-C2	-2.97	119.94	122.69
1	1	1105	PSU	C6-N1-C2	-2.96	119.94	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	373	PSU	C6-N1-C2	-2.96	119.94	122.69
1	1	2774	OMG	N9-C4-N3	2.96	131.87	125.95
1	1	799	A2M	N9-C8-N7	-2.96	109.74	113.94
1	1	1917	OMU	O4-C4-C5	-2.96	120.06	125.16
1	1	2876	OMG	N9-C4-N3	2.96	131.86	125.95
1	1	2905	A2M	C4-C5-N7	-2.95	107.20	110.58
1	1	1918	PSU	C6-N1-C2	-2.95	119.95	122.69
1	1	2578	OMG	C2-N1-C6	-2.95	119.76	125.11
1	1	972	PSU	O2-C2-N1	-2.95	119.75	122.79
1	1	881	PSU	C6-N1-C2	-2.95	119.96	122.69
1	1	2876	OMG	C2-N1-C6	-2.94	119.77	125.11
1	1	627	OMG	C2-N1-C6	-2.94	119.77	125.11
1	1	793	PSU	O2-C2-N1	-2.94	119.75	122.79
1	1	787	OMG	C2-N1-C6	-2.94	119.78	125.11
1	1	942	PSU	C6-N1-C2	-2.94	119.97	122.69
1	1	2690	UY1	C6-N1-C2	-2.94	119.97	122.69
1	1	848	A2M	C4-C5-N7	-2.94	107.23	110.58
1	1	2881	OMG	N9-C4-N3	2.93	131.82	125.95
1	1	2578	OMG	N9-C4-N3	2.93	131.82	125.95
1	1	2289	A2M	C4-C5-N7	-2.93	107.23	110.58
1	1	127	PSU	C6-N1-C2	-2.93	119.97	122.69
1	1	779	PSU	C6-N1-C2	-2.92	119.98	122.69
1	1	787	OMG	N9-C4-N3	2.92	131.80	125.95
1	1	1847	A2M	C4-C5-N7	-2.92	107.24	110.58
1	1	1870	PSU	C6-N1-C2	-2.91	119.99	122.69
1	1	848	A2M	C2'-C1'-N9	-2.91	108.95	113.75
3	4	75	OMG	C2-N1-C6	-2.91	119.84	125.11
1	1	2774	OMG	C2-N1-C6	-2.90	119.84	125.11
1	1	1433	OMG	C2-N1-C6	-2.90	119.85	125.11
1	1	2785	PSU	C6-N1-C2	-2.90	120.00	122.69
1	1	2182	A2M	C4-N9-C8	2.90	108.78	105.74
1	1	986	PSU	O2-C2-N1	-2.89	119.81	122.79
1	1	2875	PSU	C6-N1-C2	-2.89	120.01	122.69
1	1	1116	A2M	C4-C5-N7	-2.89	107.28	110.58
1	1	986	PSU	C6-N1-C2	-2.88	120.02	122.69
1	1	2881	OMG	C2-N1-C6	-2.88	119.89	125.11
1	1	2182	A2M	C4-C5-N7	-2.88	107.29	110.58
1	1	2096	PSU	C6-N1-C2	-2.88	120.02	122.69
1	1	2229	PSU	O2-C2-N1	-2.87	119.83	122.79
1	1	1538	PSU	C6-N1-C2	-2.87	120.03	122.69
1	1	1223	A2M	C4-C5-N7	-2.87	107.31	110.58
1	1	2303	PSU	C6-N1-C2	-2.86	120.04	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4	18	PSU	C6-N1-C2	-2.86	120.04	122.69
1	1	646	OMG	C2-N1-C6	-2.86	119.92	125.11
1	1	2801	PSU	C2'-C3'-C4'	2.86	108.13	102.61
1	1	871	PSU	C3'-C2'-C1'	2.85	105.05	101.69
1	1	1223	A2M	C2'-C3'-C4'	2.85	108.12	101.99
1	1	1432	A2M	C4-N9-C8	2.84	108.72	105.74
1	1	2227	PSU	O2-C2-N1	-2.84	119.86	122.79
1	1	1035	PSU	C6-N1-C2	-2.84	120.06	122.69
1	1	2880	OMU	O4-C4-C5	-2.84	120.27	125.16
1	1	637	A2M	C4-C5-N7	-2.84	107.34	110.58
1	1	1025	PSU	C6-N1-C2	-2.84	120.06	122.69
1	1	1116	A2M	C2'-C1'-N9	-2.84	109.08	113.75
3	4	73	PSU	C6-N1-C2	-2.83	120.06	122.69
1	1	1918	PSU	O2-C2-N1	-2.83	119.87	122.79
1	1	2839	PSU	C6-N1-C2	-2.83	120.07	122.69
1	1	646	OMG	N9-C4-N3	2.82	131.59	125.95
1	1	2221	PSU	C6-N1-C2	-2.82	120.08	122.69
1	1	1453	PSU	O2-C2-N1	-2.81	119.89	122.79
1	1	385	OMG	C2-N1-C6	-2.81	120.02	125.11
1	1	2688	OMU	O4-C4-C5	-2.80	120.33	125.16
1	1	2154	PSU	O2-C2-N1	-2.80	119.90	122.79
1	1	373	PSU	O2-C2-N1	-2.80	119.90	122.79
1	1	754	PSU	C6-N1-C2	-2.80	120.10	122.69
1	1	2358	OMG	C2-N1-C6	-2.79	120.05	125.11
1	1	2358	OMG	C5-C6-N1	2.79	120.35	113.25
1	1	1433	OMG	N9-C4-N3	2.79	131.53	125.95
3	4	55	PSU	C3'-C2'-C1'	2.78	104.97	101.69
1	1	2801	PSU	O2-C2-N1	-2.78	119.92	122.79
1	1	2752	OMG	C5-C6-N1	2.78	120.32	113.25
1	1	807	PSU	C6-N1-C2	-2.77	120.12	122.69
1	1	2244	A2M	C4-C5-N7	-2.77	107.41	110.58
1	1	2750	OMG	C5-C6-N1	2.77	120.30	113.25
1	1	2824	PSU	O2-C2-N1	-2.77	119.93	122.79
1	1	942	PSU	C6-C5-C4	2.77	120.04	118.17
1	1	2774	OMG	C5-C6-N1	2.77	120.30	113.25
1	1	2785	PSU	O2-C2-N1	-2.76	119.94	122.79
1	1	2491	OMG	C5-C6-N1	2.76	120.28	113.25
1	1	858	A2M	C4-N9-C8	2.76	108.64	105.74
1	1	718	PSU	C6-N1-C2	-2.75	120.14	122.69
1	1	2244	A2M	C4-N9-C8	2.75	108.63	105.74
1	1	758	PSU	O2-C2-N1	-2.75	119.95	122.79
1	1	2578	OMG	C5-C6-N1	2.75	120.25	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	881	PSU	C6-C5-C4	2.75	120.03	118.17
1	1	627	OMG	C5-C6-N1	2.75	120.24	113.25
1	1	385	OMG	N9-C4-N3	2.75	131.44	125.95
1	1	1016	PSU	O2-C2-N1	-2.75	119.96	122.79
1	1	2891	PSU	O2-C2-N1	-2.74	119.96	122.79
1	1	1907	OMG	C5-C6-N1	2.74	120.23	113.25
1	1	2379	PSU	O2-C2-N1	-2.74	119.96	122.79
1	1	871	PSU	C6-N1-C2	-2.73	120.15	122.69
1	1	2599	A2M	O2'-C2'-C1'	-2.73	103.80	108.99
1	1	1043	PSU	C6-N1-C2	-2.73	120.16	122.69
1	1	2326	A2M	N9-C8-N7	-2.73	110.06	113.94
1	1	1248	PSU	O2-C2-N1	-2.73	119.97	122.79
1	1	1868	OMU	O4-C4-C5	-2.73	120.46	125.16
1	1	1421	PSU	C6-N1-C2	-2.73	120.16	122.69
1	1	646	OMG	C5-C6-N1	2.72	120.18	113.25
1	1	787	OMG	C5-C6-N1	2.71	120.15	113.25
1	1	890	OMG	C5-C6-N1	2.71	120.14	113.25
1	1	718	PSU	O2-C2-N1	-2.71	120.00	122.79
1	1	2556	PSU	O2-C2-N1	-2.71	120.00	122.79
1	1	871	PSU	O2-C2-N1	-2.70	120.00	122.79
1	1	2876	OMG	C5-C6-N1	2.69	120.11	113.25
1	1	1016	PSU	C3'-C2'-C1'	2.69	104.87	101.69
1	1	2384	OMU	O4-C4-C5	-2.69	120.53	125.16
1	1	2690	UY1	C6-C5-C4	2.69	119.99	118.17
1	1	956	PSU	C6-C5-C4	2.68	119.98	118.17
1	1	2289	A2M	C4-N9-C8	2.67	108.55	105.74
1	1	881	PSU	O2-C2-N1	-2.67	120.03	122.79
1	1	2221	PSU	O2-C2-N1	-2.67	120.03	122.79
1	1	637	A2M	C4-N9-C8	2.67	108.54	105.74
1	1	956	PSU	O2-C2-N1	-2.65	120.05	122.79
1	1	1433	OMG	C5-C6-N1	2.65	120.01	113.25
1	1	2546	PSU	C6-N1-C2	-2.65	120.23	122.69
1	1	2903	PSU	C6-N1-C2	-2.64	120.24	122.69
1	1	1223	A2M	C4-N9-C8	2.63	108.50	105.74
1	1	2863	PSU	O2-C2-N1	-2.63	120.07	122.79
1	1	2251	OMG	C5-C6-N1	2.62	119.93	113.25
1	1	2881	OMG	C5-C6-N1	2.62	119.93	113.25
3	4	75	OMG	C5-C6-N1	2.62	119.92	113.25
1	1	2903	PSU	O2-C2-N1	-2.61	120.09	122.79
1	1	948	PSU	C3'-C2'-C1'	2.61	104.77	101.69
1	1	1223	A2M	C3'-C2'-C1'	2.61	107.80	102.81
1	1	899	A2M	C4-N9-C8	2.61	108.48	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	754	PSU	O2-C2-N1	-2.60	120.10	122.79
1	1	2599	A2M	C4-N9-C8	2.59	108.46	105.74
1	1	1918	PSU	C6-C5-C4	2.59	119.92	118.17
1	1	385	OMG	C5-C6-N1	2.59	119.85	113.25
1	1	1035	PSU	O2-C2-N1	-2.59	120.12	122.79
1	1	2326	A2M	C5-N7-C8	2.58	107.50	103.45
1	1	917	PSU	O2-C2-N1	-2.57	120.13	122.79
1	1	942	PSU	O2-C2-N1	-2.57	120.13	122.79
1	1	1538	PSU	O2-C2-N1	-2.57	120.13	122.79
1	1	2703	PSU	C3'-C2'-C1'	2.57	104.72	101.69
1	1	2838	OMC	O2-C2-N3	-2.57	118.28	122.33
1	1	948	PSU	O2-C2-N1	-2.57	120.14	122.79
1	1	2277	UY1	C5-C4-N3	2.56	122.19	116.55
1	1	1105	PSU	O2-C2-N1	-2.56	120.15	122.79
1	1	2223	PSU	O2-C2-N1	-2.55	120.15	122.79
1	1	1904	PSU	C6-C5-C4	2.55	119.90	118.17
1	1	1025	PSU	O2-C2-N1	-2.55	120.16	122.79
1	1	355	PSU	O2-C2-N1	-2.55	120.16	122.79
1	1	2593	UR3	C6-N1-C2	-2.54	119.72	121.80
1	1	807	PSU	C6-C5-C4	2.54	119.89	118.17
1	1	2092	PSU	O2-C2-N1	-2.53	120.17	122.79
1	1	2839	PSU	O2-C2-N1	-2.53	120.18	122.79
1	1	127	PSU	O2-C2-N1	-2.52	120.19	122.79
1	1	1043	PSU	O2-C2-N1	-2.52	120.19	122.79
1	1	2244	A2M	C2'-C1'-N9	-2.51	109.62	113.75
1	1	807	PSU	O2-C2-N1	-2.51	120.20	122.79
1	1	2558	PSU	O2-C2-N1	-2.50	120.21	122.79
1	1	2491	OMG	O6-C6-C5	-2.50	119.93	126.53
3	4	55	PSU	O2-C2-N1	-2.50	120.21	122.79
1	1	1847	A2M	C4-N9-C8	2.50	108.36	105.74
1	1	787	OMG	O6-C6-C5	-2.50	119.95	126.53
1	1	890	OMG	O6-C6-C5	-2.49	119.97	126.53
1	1	2227	PSU	O3'-C3'-C2'	2.49	119.79	111.82
1	1	2752	OMG	O6-C6-C5	-2.47	120.01	126.53
1	1	2905	A2M	C4-N9-C8	2.47	108.33	105.74
1	1	1917	OMU	C1'-N1-C2	2.46	122.02	117.59
1	1	2303	PSU	O2-C2-N1	-2.46	120.25	122.79
1	1	1421	PSU	C6-C5-C4	2.46	119.83	118.17
1	1	2578	OMG	O6-C6-C5	-2.46	120.05	126.53
1	1	768	A2M	O3'-C3'-C2'	-2.46	104.31	111.19
3	4	18	PSU	O2-C2-N1	-2.45	120.26	122.79
1	1	2750	OMG	C8-N7-C5	2.45	108.62	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2881	OMG	C8-N7-C5	2.45	108.62	104.26
1	1	2690	UY1	O2-C2-N1	-2.44	120.27	122.79
1	1	2326	A2M	C4-C5-N7	-2.44	107.79	110.58
1	1	1907	OMG	O6-C6-C5	-2.44	120.10	126.53
1	1	2251	OMG	O6-C6-C5	-2.44	120.10	126.53
1	1	768	A2M	N9-C8-N7	-2.43	110.49	113.94
1	1	2491	OMG	C8-N7-C5	2.42	108.58	104.26
1	1	2096	PSU	O2-C2-N1	-2.41	120.30	122.79
1	1	2578	OMG	C8-N7-C5	2.41	108.56	104.26
1	1	1874	PSU	O2-C2-N1	-2.41	120.31	122.79
1	1	2277	UY1	C6-N1-C2	-2.40	120.46	122.69
1	1	2824	PSU	O4'-C1'-C2'	2.40	108.47	105.15
1	1	627	OMG	C8-N7-C5	2.40	108.53	104.26
1	1	2905	A2M	C4'-O4'-C1'	-2.39	104.18	109.47
1	1	2675	PSU	O2-C2-N1	-2.39	120.32	122.79
1	1	385	OMG	C8-N7-C5	2.39	108.52	104.26
1	1	2223	PSU	C2'-C3'-C4'	2.39	107.22	102.61
1	1	1870	PSU	C6-C5-C4	2.39	119.79	118.17
1	1	2876	OMG	O6-C6-C5	-2.39	120.23	126.53
1	1	373	PSU	C6-C5-C4	2.39	119.78	118.17
1	1	779	PSU	C6-C5-C4	2.38	119.78	118.17
1	1	2905	A2M	C2'-C1'-N9	-2.38	109.83	113.75
1	1	2875	PSU	O2-C2-N1	-2.38	120.33	122.79
1	1	385	OMG	O6-C6-C5	-2.38	120.26	126.53
1	1	2785	PSU	O4'-C1'-C2'	2.37	108.43	105.15
1	1	2907	OMC	C1'-N1-C2	2.37	123.68	118.44
1	1	2251	OMG	C8-N7-C5	2.37	108.48	104.26
1	1	1432	A2M	C2'-C3'-C4'	2.36	107.08	101.99
1	1	1433	OMG	C8-N7-C5	2.36	108.47	104.26
1	1	754	PSU	C6-C5-C4	2.36	119.77	118.17
1	1	779	PSU	O2-C2-N1	-2.36	120.36	122.79
1	1	2881	OMG	O6-C6-C5	-2.35	120.32	126.53
3	4	73	PSU	O2-C2-N1	-2.35	120.36	122.79
1	1	2750	OMG	O6-C6-C5	-2.35	120.33	126.53
1	1	2243	A2M	C4'-O4'-C1'	-2.35	104.28	109.47
1	1	2876	OMG	C8-N7-C5	2.35	108.44	104.26
1	1	2223	PSU	O4'-C1'-C2'	2.35	108.40	105.15
1	1	646	OMG	C8-N7-C5	2.35	108.44	104.26
1	1	2380	OMU	O2-C2-N1	-2.34	119.74	122.80
1	1	2774	OMG	O6-C6-C5	-2.32	120.40	126.53
3	4	75	OMG	C8-N7-C5	2.32	108.39	104.26
3	4	75	OMG	O6-C6-C5	-2.31	120.43	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2277	UY1	C2'-C3'-C4'	2.31	106.96	101.99
1	1	2703	PSU	C6-C5-C4	2.31	119.73	118.17
1	1	2752	OMG	C8-N7-C5	2.30	108.36	104.26
1	1	2546	PSU	C6-C5-C4	2.30	119.73	118.17
1	1	2546	PSU	C4'-O4'-C1'	-2.30	102.68	108.44
1	1	2277	UY1	C3'-C2'-C1'	2.30	107.62	103.42
1	1	1433	OMG	O6-C6-C5	-2.30	120.47	126.53
1	1	768	A2M	C4-N9-C8	2.29	108.15	105.74
1	1	773	PSU	C6-C5-C4	2.28	119.72	118.17
1	1	2880	OMU	O2-C2-N1	-2.28	119.82	122.80
1	1	2217	PSU	C5'-C4'-C3'	-2.28	106.99	115.21
1	1	2326	A2M	C3'-C2'-C1'	2.28	107.17	102.81
1	1	1907	OMG	C8-N7-C5	2.28	108.32	104.26
1	1	2774	OMG	C8-N7-C5	2.28	108.32	104.26
1	1	2599	A2M	C2'-C1'-N9	2.28	117.50	113.75
1	1	890	OMG	C8-N7-C5	2.27	108.31	104.26
1	1	2243	A2M	C4-N9-C8	2.27	108.12	105.74
1	1	627	OMG	O6-C6-C5	-2.27	120.55	126.53
1	1	1116	A2M	C4'-O4'-C1'	-2.26	104.47	109.47
1	1	1248	PSU	O4'-C1'-C2'	2.26	108.27	105.15
1	1	2882	PSU	C6-C5-C4	2.26	119.70	118.17
1	1	799	A2M	C4-N9-C8	2.25	108.11	105.74
1	1	2326	A2M	C4-N9-C8	2.24	108.09	105.74
1	1	2875	PSU	O3'-C3'-C2'	2.24	119.00	111.82
1	1	2326	A2M	O4'-C1'-N9	2.24	112.39	108.09
1	1	1847	A2M	C3'-C2'-C1'	2.24	107.09	102.81
1	1	646	OMG	C8-N9-C4	2.23	110.21	106.03
1	1	787	OMG	C8-N7-C5	2.23	108.24	104.26
1	1	2611	PSU	C3'-C2'-C1'	2.23	104.32	101.69
1	1	972	PSU	C6-C5-C4	2.23	119.68	118.17
1	1	2546	PSU	O2-C2-N1	-2.23	120.49	122.79
1	1	793	PSU	C6-C5-C4	2.23	119.68	118.17
1	1	2217	PSU	C3'-C2'-C1'	2.22	104.31	101.69
1	1	2838	OMC	C1'-N1-C6	-2.22	116.03	120.78
1	1	1420	OMC	C1'-N1-C6	-2.22	116.04	120.78
1	1	2875	PSU	O3'-C3'-C4'	2.21	117.44	111.08
1	1	1836	OMC	C1'-N1-C2	2.20	123.30	118.44
1	1	2558	PSU	O4'-C1'-C2'	2.19	108.19	105.15
1	1	768	A2M	C5-N7-C8	2.19	106.89	103.45
1	1	1223	A2M	C2'-C1'-N9	-2.19	110.15	113.75
1	1	2703	PSU	C5'-C4'-C3'	-2.19	107.34	115.21
1	1	1907	OMG	CM2-O2'-C2'	2.18	120.08	114.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	718	PSU	C6-C5-C4	2.17	119.64	118.17
1	1	646	OMG	O6-C6-C5	-2.17	120.81	126.53
1	1	1432	A2M	O2'-C2'-C1'	2.15	113.07	108.99
1	1	385	OMG	C8-N9-C4	2.14	110.04	106.03
1	1	1025	PSU	C6-C5-C4	2.14	119.62	118.17
1	1	2358	OMG	O6-C6-C5	-2.14	120.88	126.53
1	1	2303	PSU	C4'-O4'-C1'	-2.14	103.08	108.44
1	1	127	PSU	C6-C5-C4	2.14	119.62	118.17
1	1	2358	OMG	N9-C4-N3	2.13	130.21	125.95
1	1	799	A2M	C4'-O4'-C1'	-2.13	104.77	109.47
1	1	858	A2M	C3'-C2'-C1'	2.13	106.88	102.81
1	1	2491	OMG	C8-N9-C4	2.11	109.98	106.03
1	1	871	PSU	C5'-C4'-C3'	-2.11	107.63	115.21
1	1	2243	A2M	O4'-C1'-N9	2.10	112.13	108.09
1	1	948	PSU	C6-C5-C4	2.10	119.59	118.17
1	1	2558	PSU	C6-C5-C4	2.10	119.59	118.17
1	1	2300	OMC	C1'-N1-C2	2.09	123.06	118.44
1	1	2703	PSU	O4'-C1'-C2'	2.09	108.05	105.15
1	1	1433	OMG	C8-N9-C4	2.09	109.95	106.03
1	1	787	OMG	C2'-C1'-N9	-2.08	110.29	114.24
1	1	2578	OMG	C8-N9-C4	2.08	109.92	106.03
1	1	1043	PSU	C6-C5-C4	2.07	119.57	118.17
1	1	848	A2M	C4'-O4'-C1'	-2.07	104.90	109.47
1	1	2243	A2M	C2'-C1'-N9	-2.05	110.38	113.75
1	1	2251	OMG	C8-N9-C4	2.05	109.87	106.03
1	1	2750	OMG	C8-N9-C4	2.05	109.86	106.03
1	1	2934	PSU	C6-C5-C4	2.04	119.55	118.17
1	1	2289	A2M	C4'-O4'-C1'	-2.04	104.96	109.47
1	1	986	PSU	C6-C5-C4	2.04	119.55	118.17
1	1	2182	A2M	C4'-O4'-C1'	-2.03	104.99	109.47
1	1	1868	OMU	O2-C2-N1	-2.03	120.16	122.80
1	1	1433	OMG	N2-C2-N1	2.02	121.03	116.76
1	1	2096	PSU	C6-C5-C4	2.02	119.54	118.17
1	1	2105	1MA	N1-C6-N6	2.02	124.77	119.71
1	1	1453	PSU	O4'-C1'-C2'	2.02	107.94	105.15
1	1	2839	PSU	O4'-C1'-C2'	2.01	107.94	105.15
1	1	633	1MA	N1-C6-N6	2.01	124.76	119.71
1	1	2244	A2M	O4'-C1'-C2'	-2.00	103.14	106.59
1	1	2303	PSU	C6-C5-C4	2.00	119.52	118.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	1	2277	UY1	C4'

All (128) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	637	A2M	O4'-C4'-C5'-O5'
1	1	871	PSU	O4'-C4'-C5'-O5'
1	1	890	OMG	O4'-C4'-C5'-O5'
1	1	890	OMG	C3'-C4'-C5'-O5'
1	1	956	PSU	C3'-C4'-C5'-O5'
1	1	1016	PSU	C4'-C5'-O5'-P
1	1	1223	A2M	O4'-C4'-C5'-O5'
1	1	1248	PSU	O4'-C4'-C5'-O5'
1	1	1432	A2M	C1'-C2'-O2'-CM'
1	1	1433	OMG	O4'-C4'-C5'-O5'
1	1	1433	OMG	C3'-C4'-C5'-O5'
1	1	1874	PSU	C3'-C4'-C5'-O5'
1	1	1874	PSU	O4'-C4'-C5'-O5'
1	1	1907	OMG	C1'-C2'-O2'-CM2
1	1	1917	OMU	C1'-C2'-O2'-CM2
1	1	2160	OMC	C2'-C1'-N1-C2
1	1	2160	OMC	C2'-C1'-N1-C6
1	1	2182	A2M	C1'-C2'-O2'-CM'
1	1	2223	PSU	C4'-C5'-O5'-P
1	1	2244	A2M	O4'-C4'-C5'-O5'
1	1	2244	A2M	C3'-C4'-C5'-O5'
1	1	2251	OMG	O4'-C4'-C5'-O5'
1	1	2251	OMG	C3'-C4'-C5'-O5'
1	1	2326	A2M	C1'-C2'-O2'-CM'
1	1	2326	A2M	O4'-C1'-N9-C8
1	1	2326	A2M	O4'-C1'-N9-C4
1	1	2556	PSU	O4'-C4'-C5'-O5'
1	1	2578	OMG	O4'-C4'-C5'-O5'
1	1	2578	OMG	C3'-C4'-C5'-O5'
1	1	2703	PSU	O4'-C4'-C5'-O5'
1	1	2801	PSU	O4'-C1'-C5-C4
1	1	2801	PSU	O4'-C1'-C5-C6
1	1	2802	UR3	O4'-C1'-N1-C6
1	1	2802	UR3	O4'-C1'-N1-C2
1	1	2838	OMC	O4'-C1'-N1-C2
1	1	2838	OMC	O4'-C1'-N1-C6
1	1	2882	PSU	C3'-C4'-C5'-O5'
1	1	2882	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	1	2903	PSU	C3'-C4'-C5'-O5'
1	1	2903	PSU	O4'-C4'-C5'-O5'
1	1	2907	OMC	C1'-C2'-O2'-CM2
3	4	55	PSU	C3'-C4'-C5'-O5'
3	4	55	PSU	O4'-C4'-C5'-O5'
1	1	871	PSU	C3'-C4'-C5'-O5'
1	1	1016	PSU	C3'-C4'-C5'-O5'
1	1	1223	A2M	C3'-C4'-C5'-O5'
1	1	1248	PSU	C3'-C4'-C5'-O5'
1	1	1538	PSU	C3'-C4'-C5'-O5'
1	1	2217	PSU	C3'-C4'-C5'-O5'
1	1	2223	PSU	C3'-C4'-C5'-O5'
1	1	2556	PSU	C3'-C4'-C5'-O5'
1	1	2675	PSU	O4'-C4'-C5'-O5'
1	1	2703	PSU	C3'-C4'-C5'-O5'
1	1	2875	PSU	C3'-C4'-C5'-O5'
1	1	2875	PSU	O4'-C4'-C5'-O5'
1	1	637	A2M	C3'-C4'-C5'-O5'
1	1	758	PSU	C3'-C4'-C5'-O5'
1	1	899	A2M	C3'-C4'-C5'-O5'
1	1	956	PSU	O4'-C4'-C5'-O5'
1	1	1016	PSU	O4'-C4'-C5'-O5'
1	1	1421	PSU	O4'-C4'-C5'-O5'
1	1	2217	PSU	O4'-C4'-C5'-O5'
1	1	2289	A2M	O4'-C4'-C5'-O5'
1	1	2303	PSU	O4'-C4'-C5'-O5'
1	1	768	A2M	C3'-C2'-O2'-CM'
1	1	848	A2M	O4'-C4'-C5'-O5'
1	1	2300	OMC	O4'-C4'-C5'-O5'
1	1	2829	5MC	C2'-C1'-N1-C6
1	1	2310	PSU	C3'-C4'-C5'-O5'
1	1	758	PSU	O4'-C4'-C5'-O5'
1	1	1847	A2M	O4'-C4'-C5'-O5'
1	1	2223	PSU	O4'-C4'-C5'-O5'
1	1	899	A2M	O4'-C4'-C5'-O5'
1	1	1538	PSU	O4'-C4'-C5'-O5'
1	1	1847	A2M	C3'-C4'-C5'-O5'
1	1	2802	UR3	C3'-C4'-C5'-O5'
1	1	2219	A2M	C2'-C1'-N9-C8
1	1	1223	A2M	C4'-C5'-O5'-P
1	1	2303	PSU	C3'-C4'-C5'-O5'
1	1	2675	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	1	799	A2M	C4'-C5'-O5'-P
1	1	2829	5MC	O4'-C1'-N1-C6
1	1	2829	5MC	C2'-C1'-N1-C2
1	1	2244	A2M	C3'-C2'-O2'-CM'
1	1	2310	PSU	O4'-C4'-C5'-O5'
1	1	2829	5MC	O4'-C1'-N1-C2
1	1	1107	PSU	C3'-C4'-C5'-O5'
1	1	2303	PSU	C4'-C5'-O5'-P
1	1	2154	PSU	O4'-C1'-C5-C4
1	1	2558	PSU	O4'-C1'-C5-C4
1	1	2882	PSU	O4'-C1'-C5-C4
1	1	2891	PSU	O4'-C1'-C5-C4
1	1	2219	A2M	C2'-C1'-N9-C4
1	1	2326	A2M	C3'-C4'-C5'-O5'
1	1	1248	PSU	C4'-C5'-O5'-P
1	1	2882	PSU	C4'-C5'-O5'-P
1	1	2160	OMC	O4'-C1'-N1-C6
1	1	2802	UR3	O4'-C4'-C5'-O5'
1	1	2876	OMG	C3'-C2'-O2'-CM2
1	1	646	OMG	O4'-C4'-C5'-O5'
1	1	2289	A2M	C3'-C4'-C5'-O5'
1	1	2300	OMC	C3'-C4'-C5'-O5'
1	1	633	1MA	C2'-C1'-N9-C8
1	1	637	A2M	C4'-C5'-O5'-P
1	1	2160	OMC	O4'-C1'-N1-C2
1	1	2219	A2M	C1'-C2'-O2'-CM'
1	1	2750	OMG	C1'-C2'-O2'-CM2
1	1	633	1MA	C2'-C1'-N9-C4
1	1	1918	PSU	O4'-C1'-C5-C6
1	1	2154	PSU	O4'-C1'-C5-C6
1	1	2882	PSU	O4'-C1'-C5-C6
1	1	2891	PSU	O4'-C1'-C5-C6
1	1	2244	A2M	C2'-C1'-N9-C8
1	1	1421	PSU	C3'-C4'-C5'-O5'
1	1	1420	OMC	C2'-C1'-N1-C6
1	1	2802	UR3	C2'-C1'-N1-C6
1	1	768	A2M	O4'-C1'-N9-C8
1	1	2219	A2M	O4'-C1'-N9-C8
1	1	2358	OMG	O4'-C4'-C5'-O5'
1	1	1538	PSU	C2'-C1'-C5-C6
1	1	2801	PSU	C2'-C1'-C5-C6
1	1	2160	OMC	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
1	1	799	A2M	C3'-C2'-O2'-CM'
1	1	1420	OMC	C3'-C2'-O2'-CM2
1	1	768	A2M	C2'-C1'-N9-C8
1	1	2326	A2M	O4'-C4'-C5'-O5'
1	1	1420	OMC	C2'-C1'-N1-C2
1	1	1107	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

31 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	2838	OMC	1	0
1	1	2876	OMG	1	0
1	1	2092	PSU	1	0
1	1	2750	OMG	1	0
1	1	2907	OMC	1	0
1	1	1016	PSU	2	0
1	1	799	A2M	1	0
1	1	1420	OMC	1	0
1	1	2326	A2M	1	0
1	1	956	PSU	2	0
3	4	75	OMG	1	0
1	1	1847	A2M	2	0
1	1	2182	A2M	3	0
1	1	2384	OMU	1	0
1	1	2277	UY1	1	0
1	1	2599	A2M	1	0
1	1	858	A2M	1	0
1	1	1432	A2M	1	0
1	1	2221	PSU	2	0
1	1	651	OMC	2	0
1	1	2223	PSU	1	0
1	1	2903	PSU	1	0
1	1	1907	OMG	1	0
1	1	633	1MA	1	0
1	1	2802	UR3	1	0
1	1	1223	A2M	7	0
1	1	899	A2M	1	0
3	4	55	PSU	1	0
1	1	1917	OMU	1	0
1	1	2380	OMU	1	0
1	1	2690	UY1	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 436 ligands modelled in this entry, 432 are monoatomic - leaving 4 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	$\# Z > 2$
52	SPM	1	3403	-	13,13,13	0.35	0	12,12,12	0.95	0
51	SPD	1	3401	-	9,9,9	0.27	0	8,8,8	0.26	0
52	SPM	1	3404	-	13,13,13	0.34	0	12,12,12	0.89	0
51	SPD	1	3402	-	9,9,9	0.27	0	8,8,8	0.25	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	SPM	1	3403	-	-	2/11/11/11	-
51	SPD	1	3401	-	-	0/7/7/7	-
52	SPM	1	3404	-	-	1/11/11/11	-
51	SPD	1	3402	-	-	2/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	1	3403	SPM	N10-C11-C12-C13
51	1	3402	SPD	C3-C4-C5-N6

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Mol	Chain	Res	Type	Atoms
52	1	3404	SPM	N1-C2-C3-C4
51	1	3402	SPD	C8-C7-N6-C5
52	1	3403	SPM	C12-C11-N10-C9

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

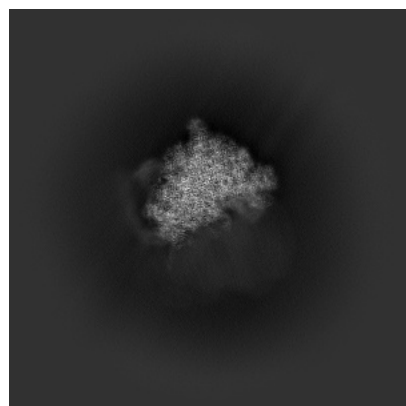
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52576. These allow visual inspection of the internal detail of the map and identification of artifacts.

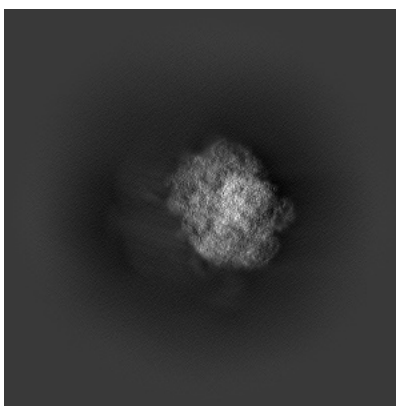
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

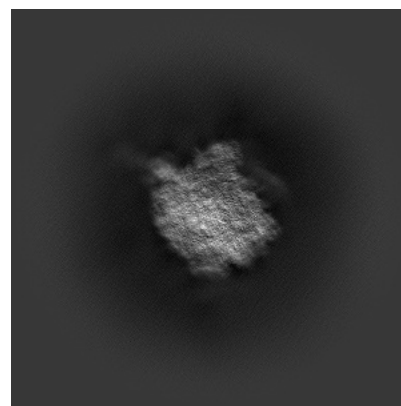
6.1.1 Primary map



X

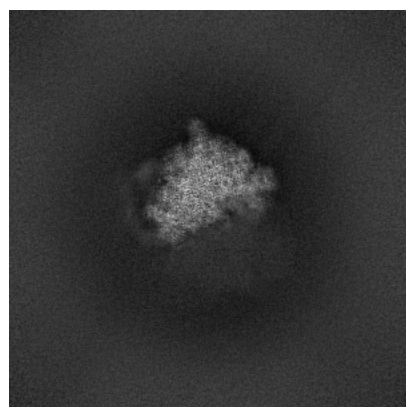


Y

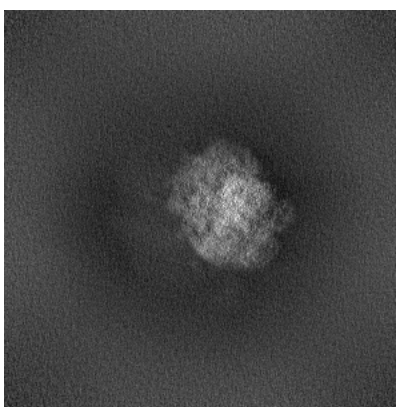


Z

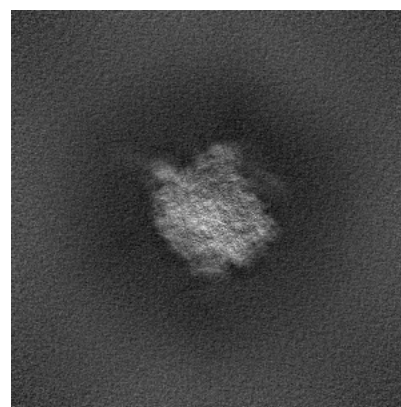
6.1.2 Raw map



X



Y

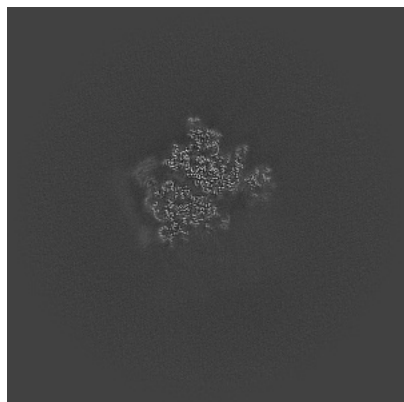


Z

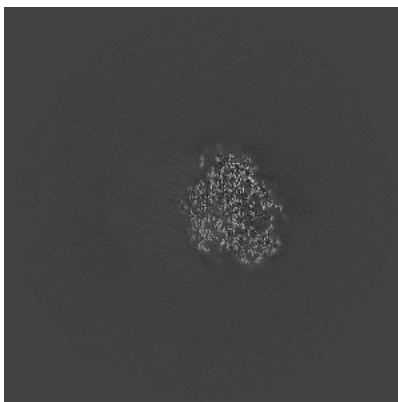
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

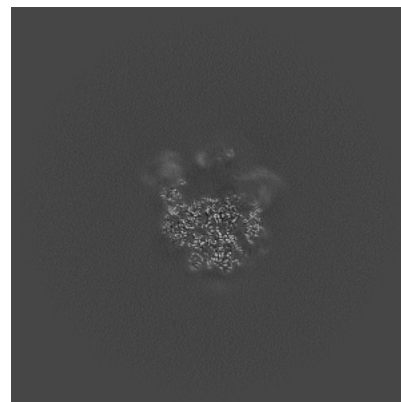
6.2.1 Primary map



X Index: 400

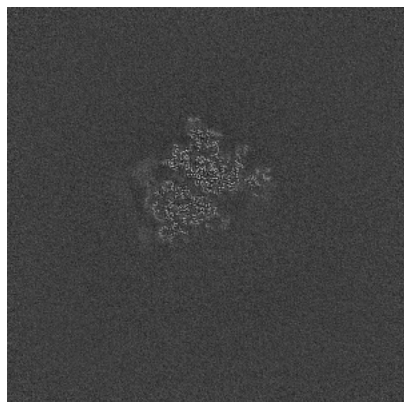


Y Index: 400

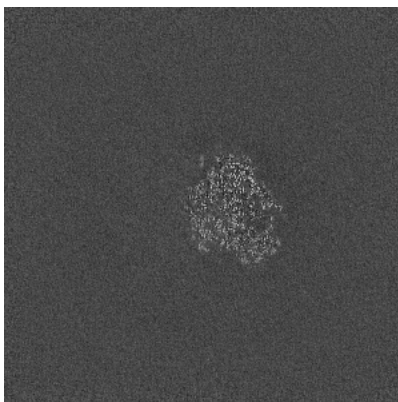


Z Index: 400

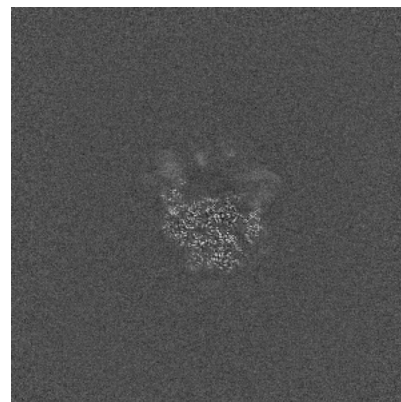
6.2.2 Raw map



X Index: 400



Y Index: 400

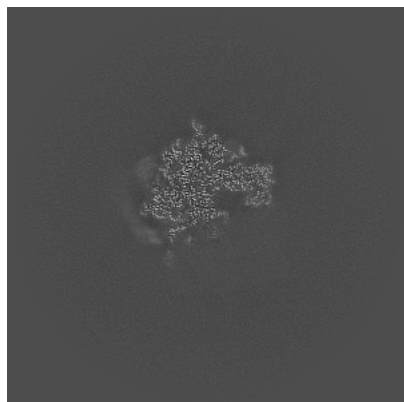


Z Index: 400

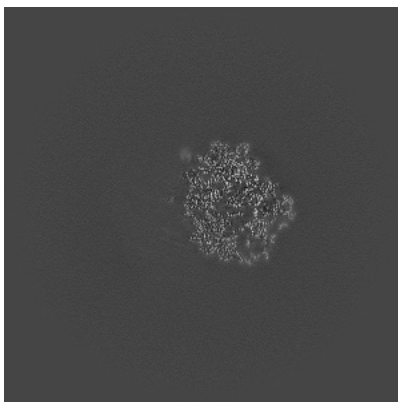
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

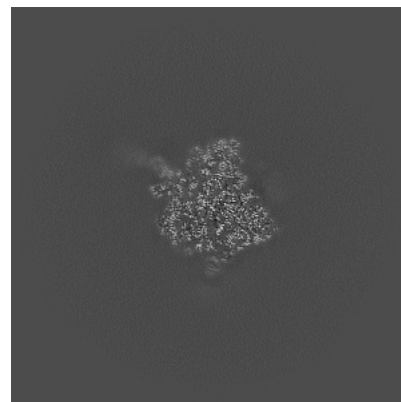
6.3.1 Primary map



X Index: 419

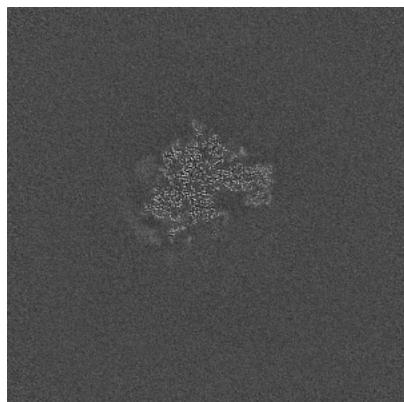


Y Index: 374

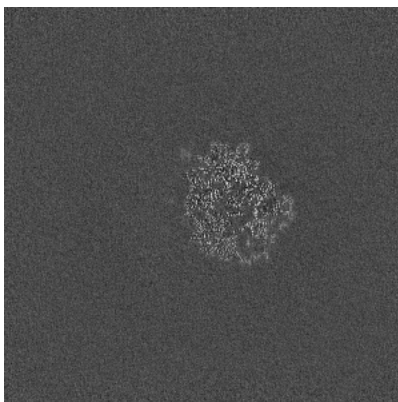


Z Index: 449

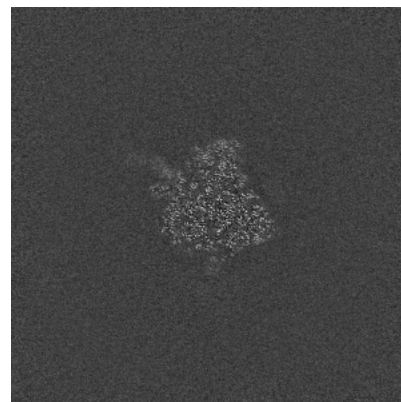
6.3.2 Raw map



X Index: 419



Y Index: 374

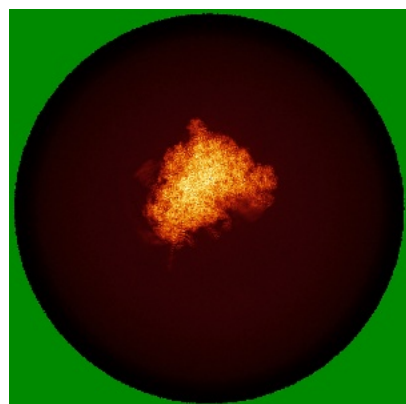


Z Index: 450

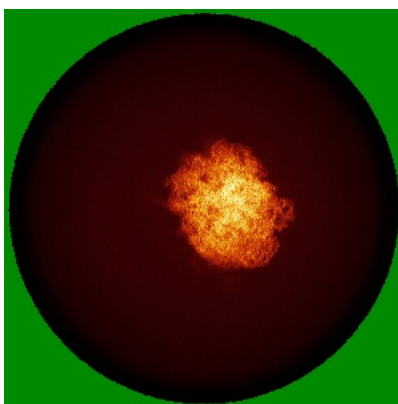
The images above show the largest variance slices of the map in three orthogonal directions.

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

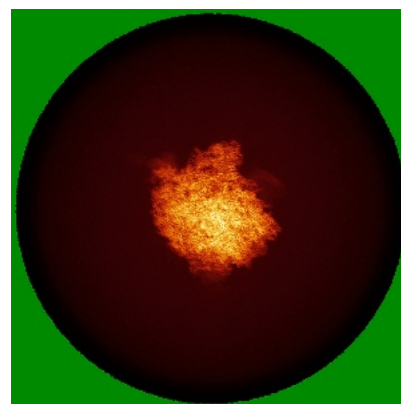
6.4.1 Primary map



X

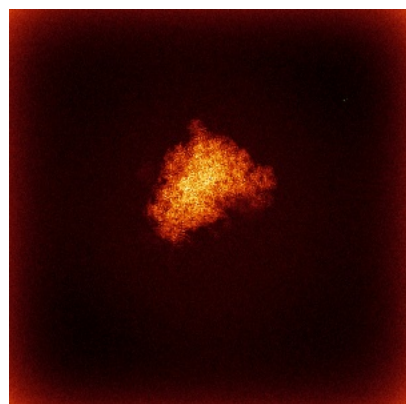


Y

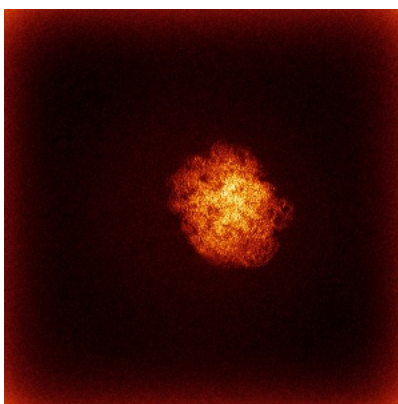


Z

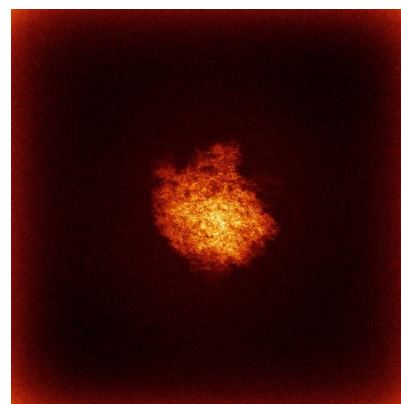
6.4.2 Raw map



X



Y

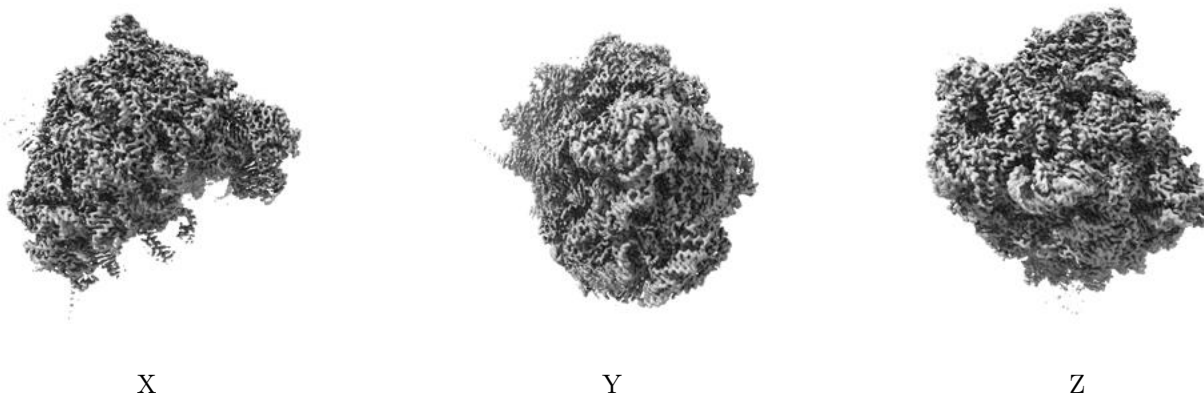


Z

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

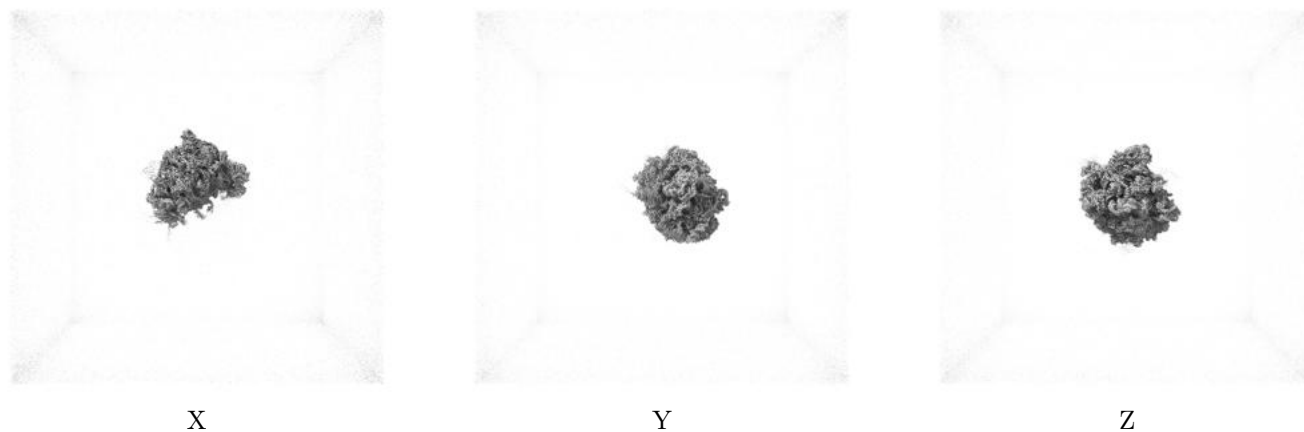
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.175. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

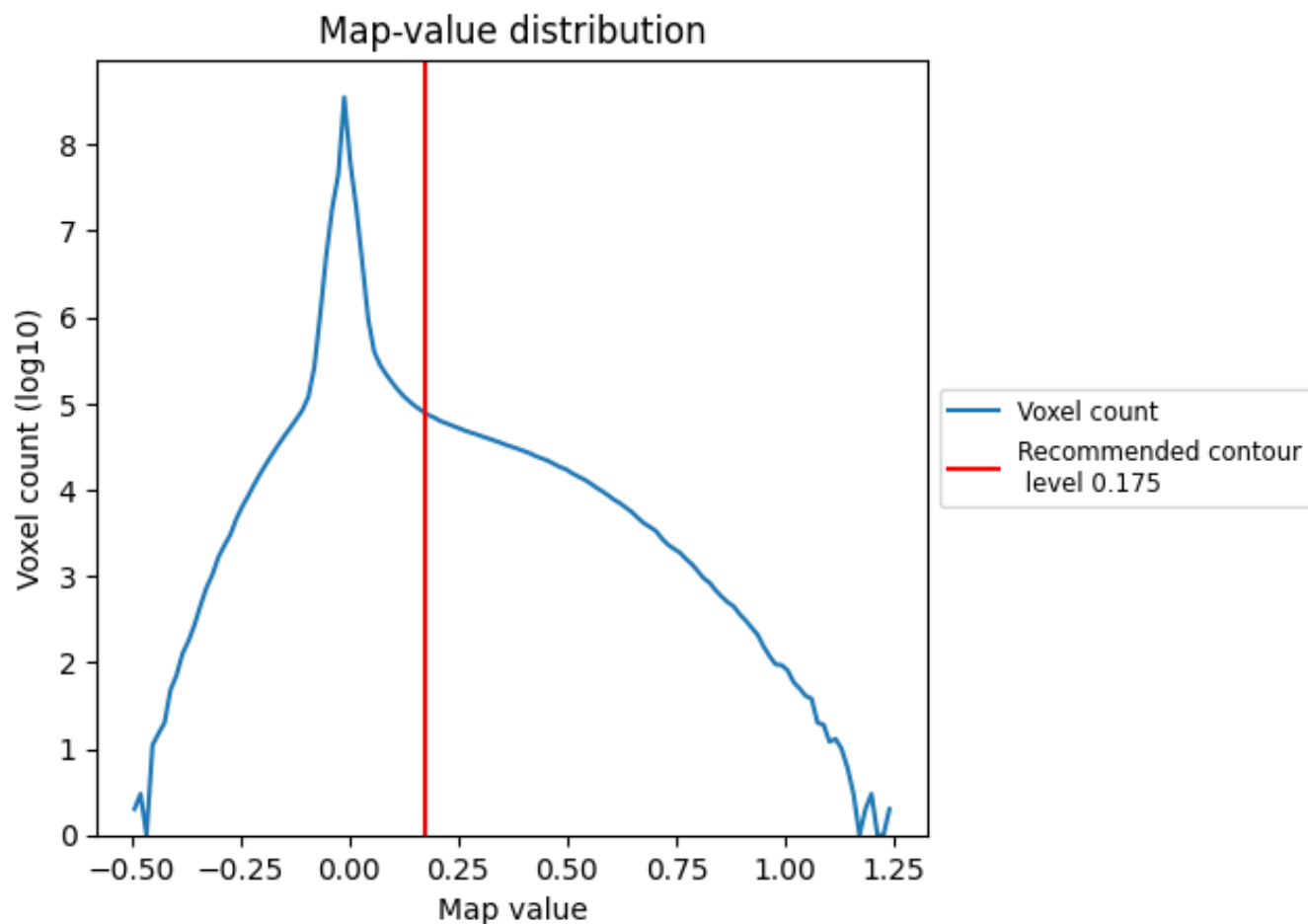
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

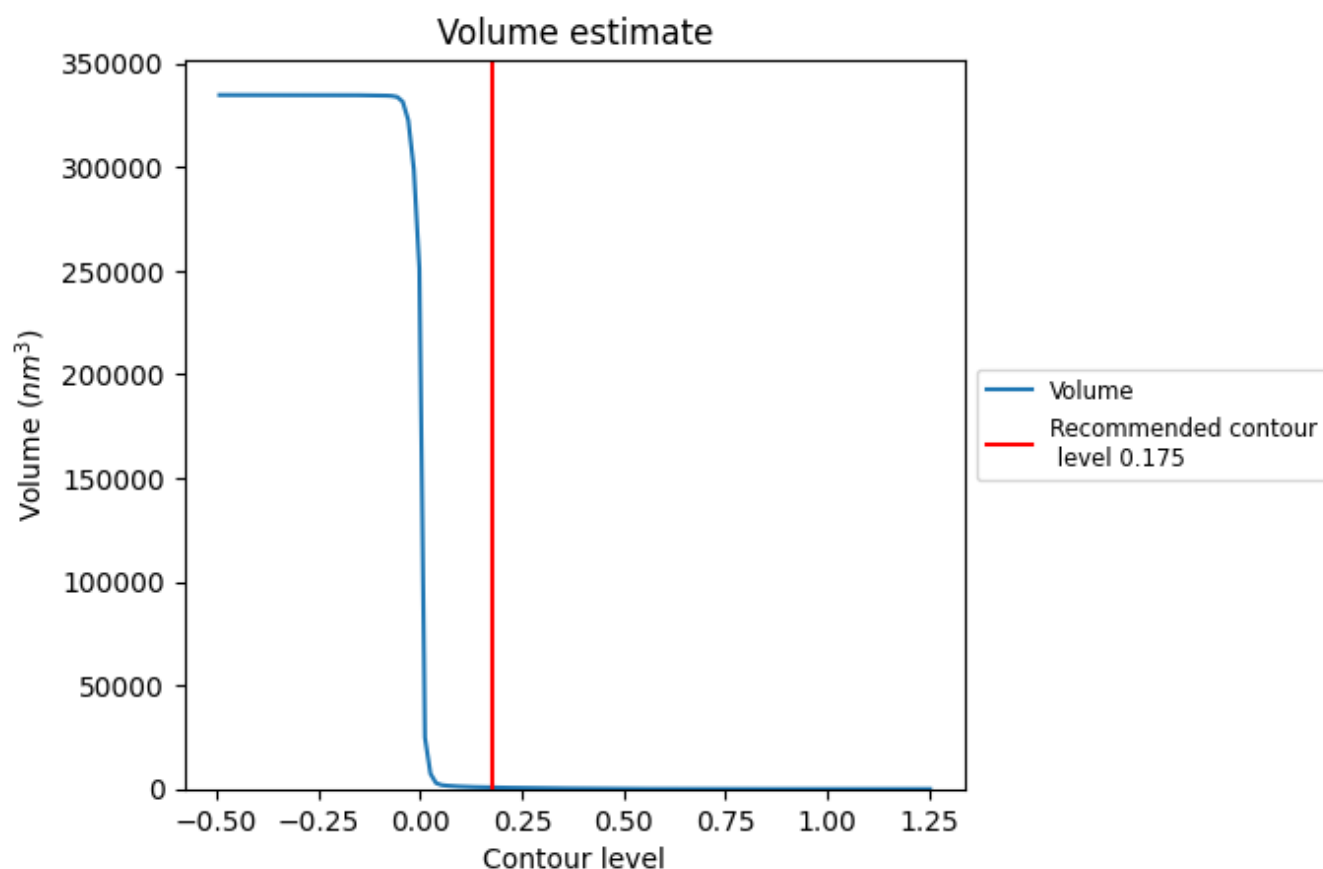
This section contains the results of statistical analysis of the map.

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.

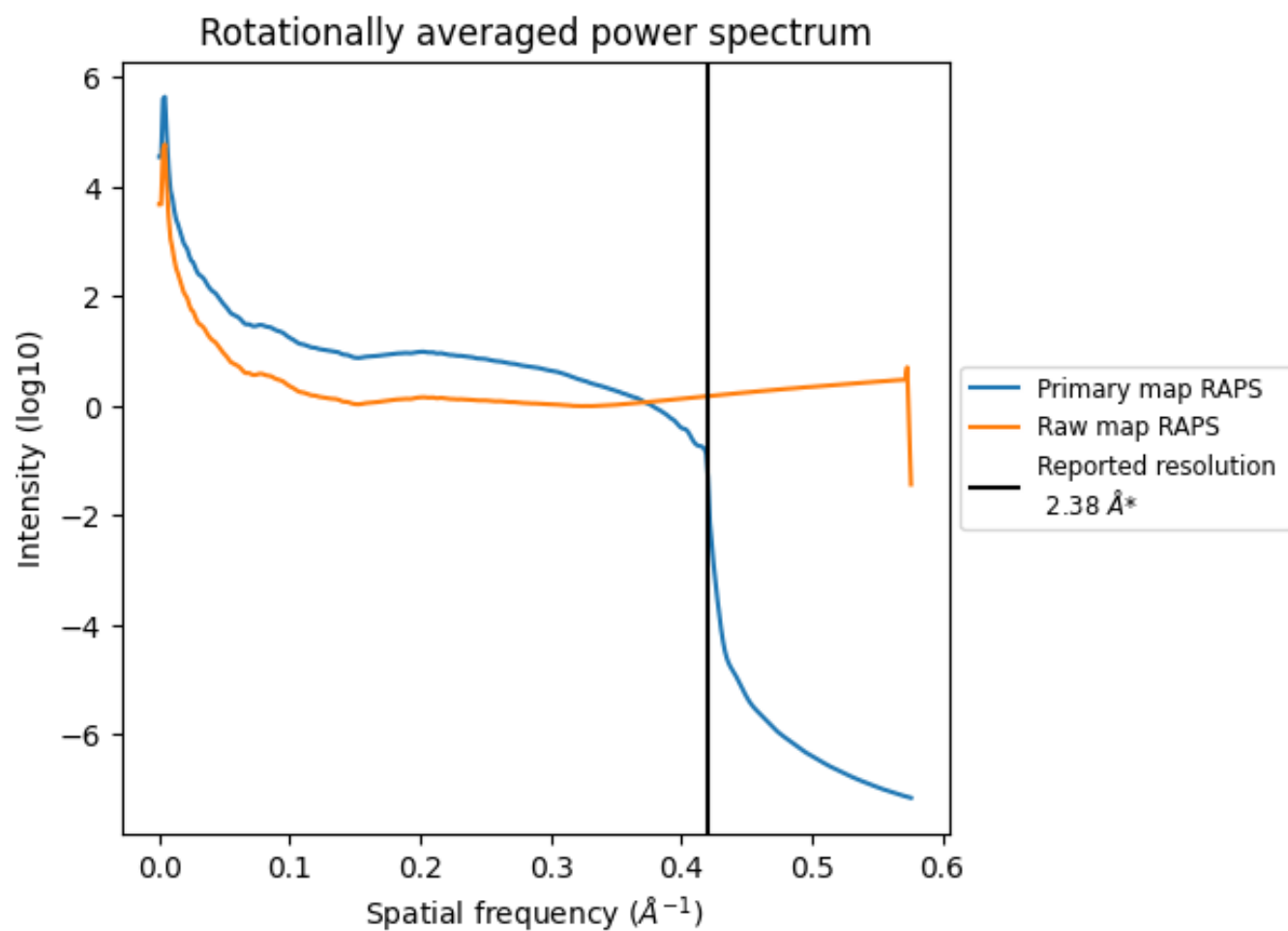
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 731 nm^3 ; this corresponds to an approximate mass of 660 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 ⓘ

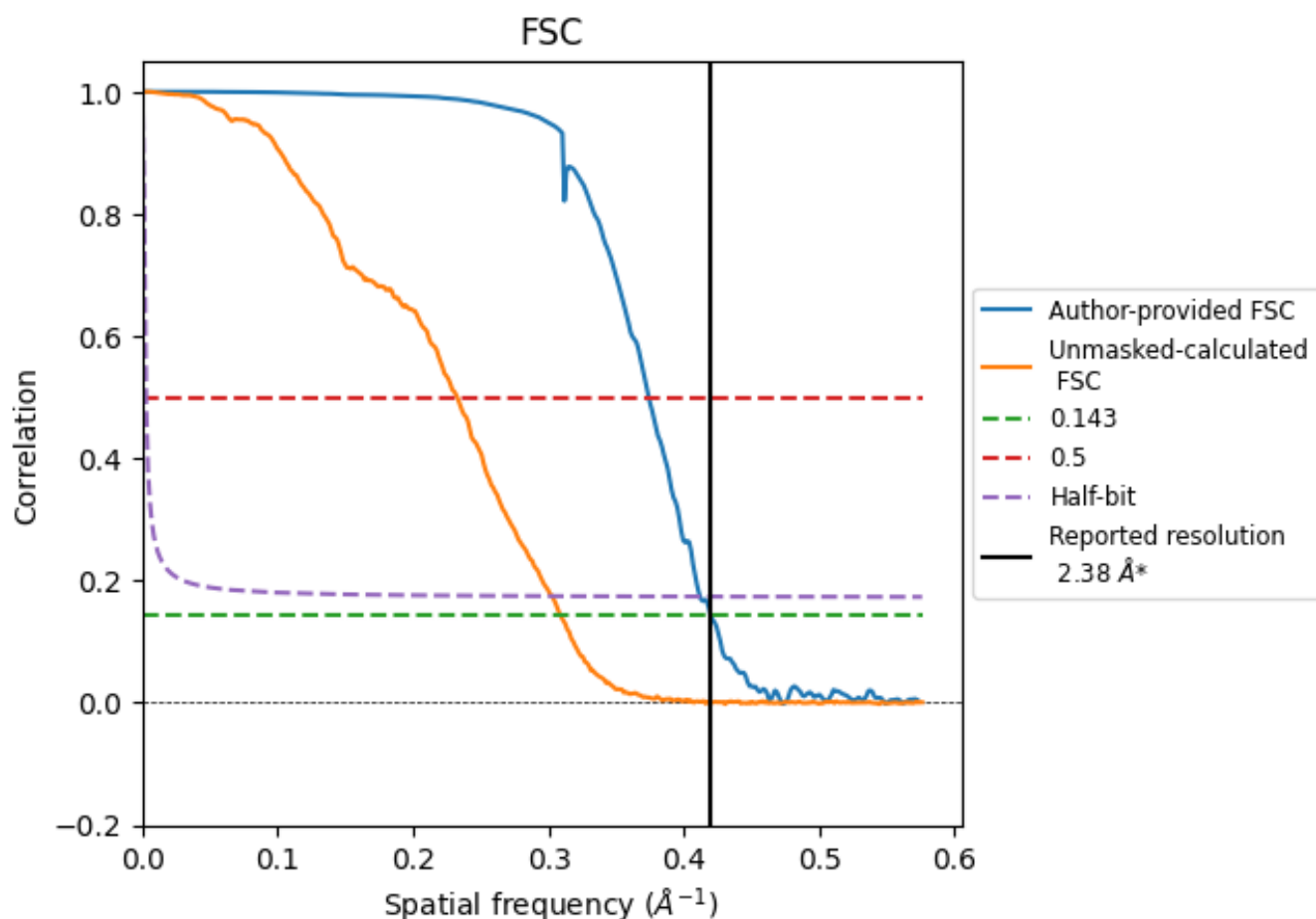


*Reported resolution corresponds to spatial frequency of 0.420 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.420 \AA^{-1}

8.2 Resolution estimates [i](#)

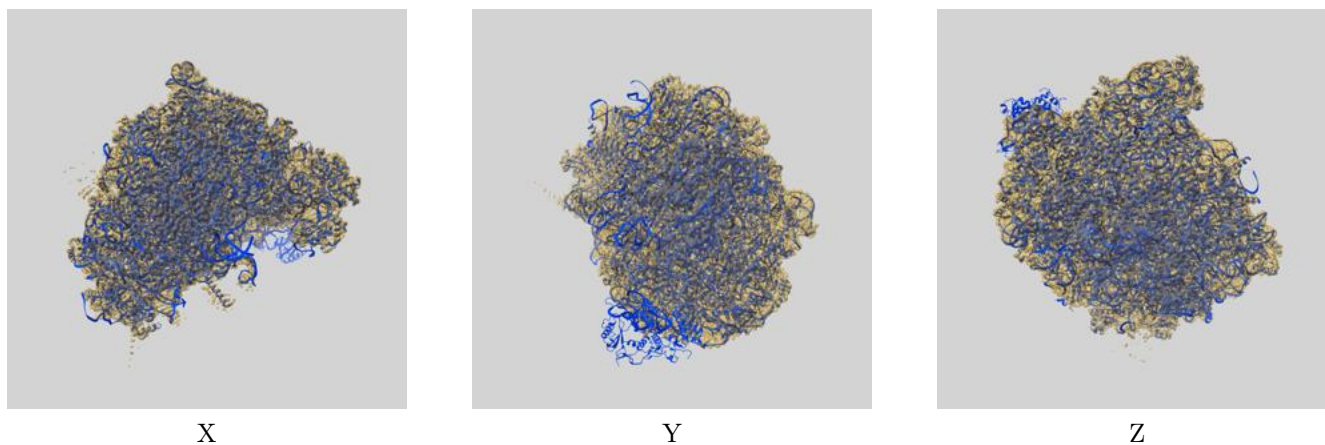
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.38	-	-
Author-provided FSC curve	2.38	2.67	2.43
Unmasked-calculated*	3.24	4.30	3.30

*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 3.24 differs from the reported value 2.38 by more than 10 %

9 Map-model fit [i](#)

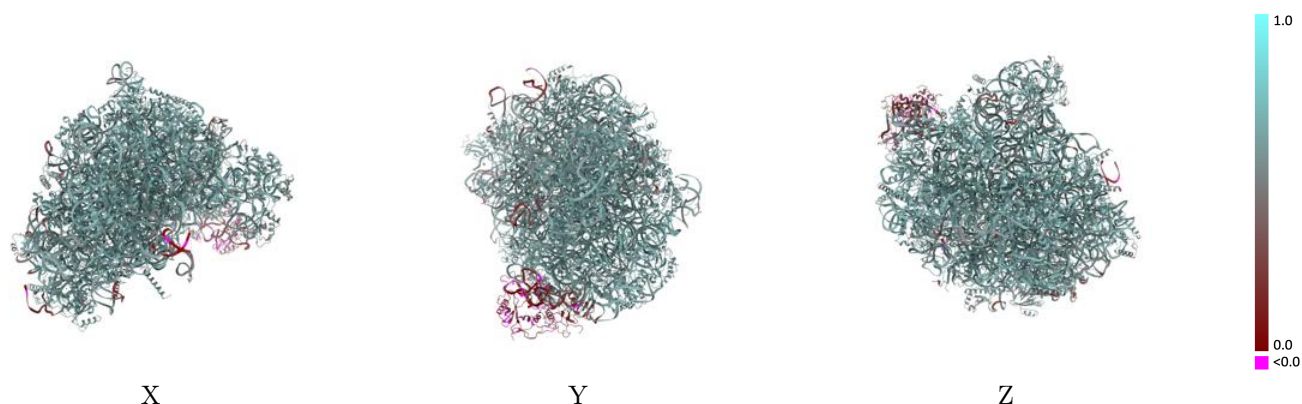
This section contains information regarding the fit between EMDB map EMD-52576 and PDB model 9I1W. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



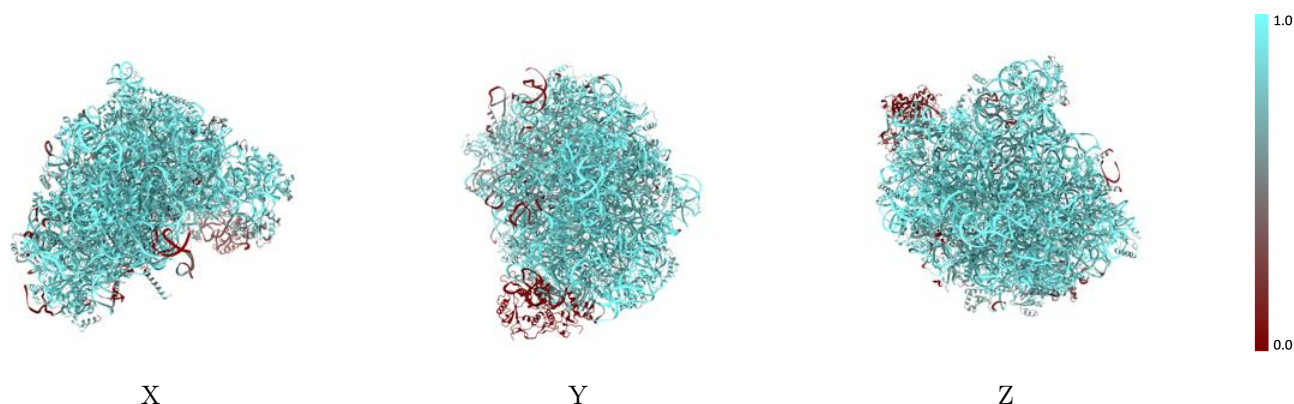
The images above show the 3D surface view of the map at the recommended contour level 0.175 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



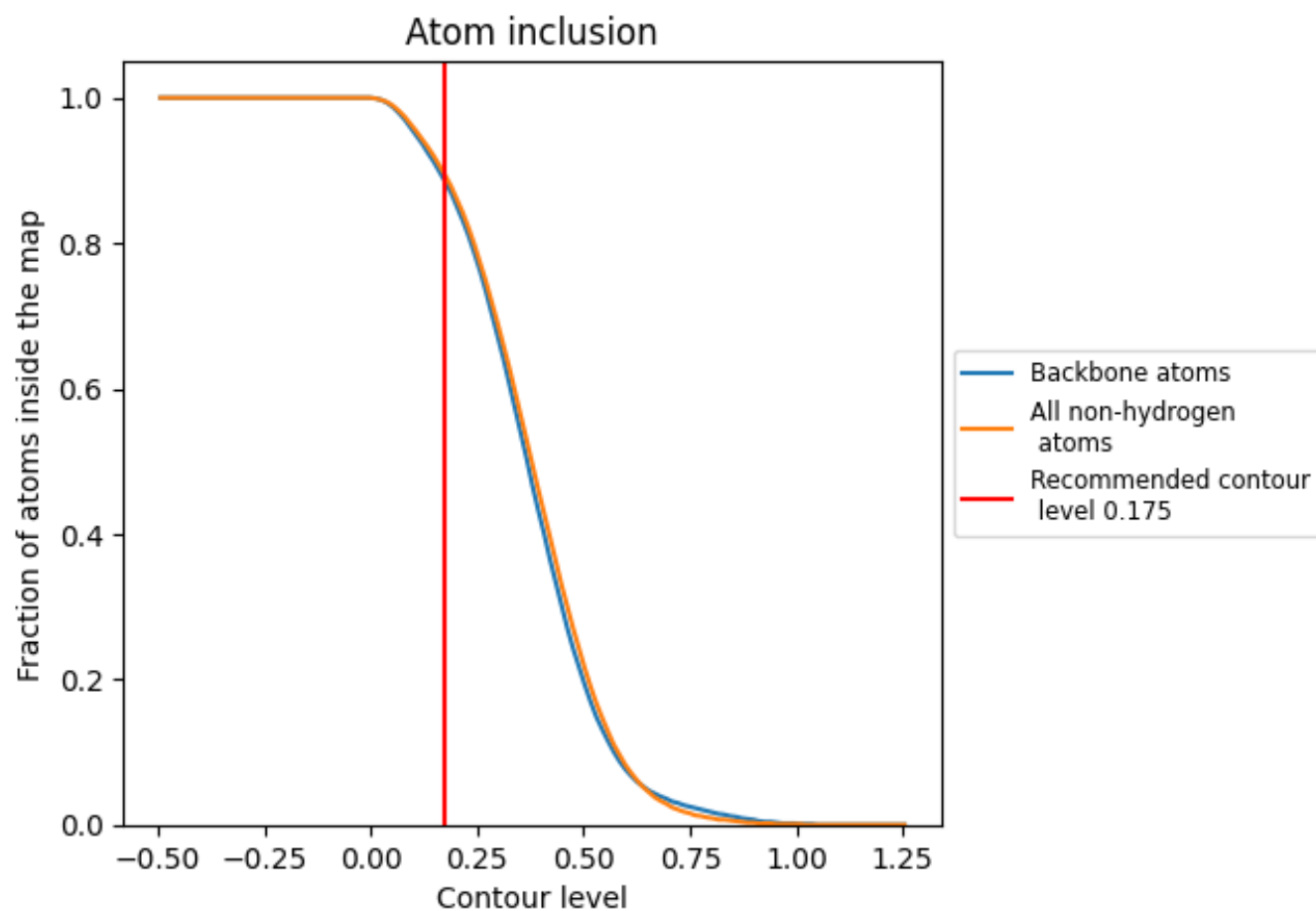
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.175).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 89% 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 (0.175) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8940	 0.6110
1	 0.9270	 0.6110
3	 0.9890	 0.6280
4	 0.9490	 0.6210
9	 0.5160	 0.5940
LA	 0.9000	 0.6420
LB	 0.9160	 0.6440
LC	 0.9310	 0.6460
LD	 0.8350	 0.6020
LE	 0.8500	 0.6060
LF	 0.9300	 0.6500
LG	 0.8610	 0.6120
LH	 0.8460	 0.6140
LI	 0.8670	 0.6190
LJ	 0.6840	 0.5600
LK	 0.0000	 0.1500
LL	 0.9000	 0.6350
LM	 0.8960	 0.6310
LN	 0.9750	 0.6610
LO	 0.9400	 0.6440
LP	 0.8590	 0.6110
LQ	 0.9660	 0.6590
LR	 0.9200	 0.6400
LS	 0.9380	 0.6440
LT	 0.8920	 0.6270
LU	 0.6360	 0.5530
LV	 0.8840	 0.6410
LW	 0.8770	 0.6380
LX	 0.8690	 0.6230
LY	 0.8920	 0.6350
LZ	 0.8790	 0.6120
La	 0.9450	 0.6520
Lb	 0.8490	 0.6030
Lc	 0.8100	 0.6060
Ld	 0.8350	 0.6100



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Chain	Atom inclusion	Q-score
Le	 0.9500	 0.6560
Lf	 0.9660	 0.6600
Lg	 0.8780	 0.6270
Lh	 0.8440	 0.6110
Li	 0.8380	 0.5940
Lj	 0.9640	 0.6590
Lk	 0.7360	 0.5900
Ll	 0.8860	 0.6280
Lm	 0.8970	 0.6350
Ln	 0.6700	 0.5950
Lo	 0.8680	 0.6280
Lp	 0.8050	 0.6050
Lq	 0.9200	 0.6380
Lr	 0.5620	 0.5610
Ls	 0.0020	 0.1970
PC	 0.0000	 0.5420
PN	 0.0000	 0.4720