Full wwPDB EM Validation Report ⓘ

Apr 17, 2024 – 07:28 pm BST

PDB ID	:	6SKG
EMDB ID	:	EMD-10224
Title	:	Cryo-EM Structure of T. kodakarensis 70S ribosome in TkNat10 deleted strain
Authors	:	Matzov, D.; Sas-Chen, A.; Thomas, J.M.; Santangelo, T.; Meier, J.L.; Schwartz, S.; Shalev-Benami, M.
Deposited on	:	2019-08-15
Resolution	:	2.65 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:

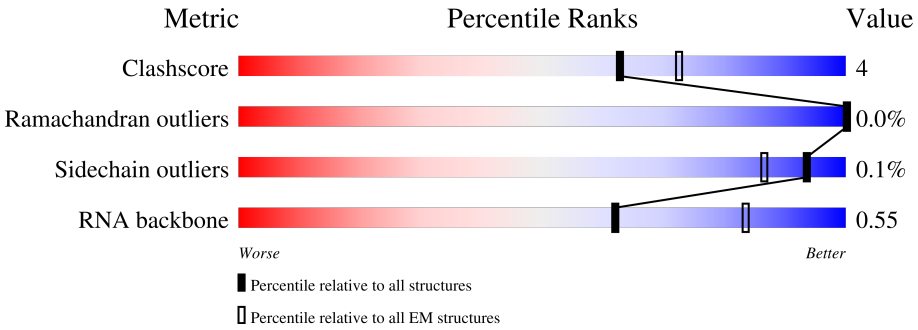
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.65 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	Aa	1498	8% 78% 18%
2	Ab	201	20% 98%
3	Ac	209	71% 93% 7%
4	Ad	200	25% 95% 5%
5	Ae	180	13% 97%
6	Af	243	12% 100%
7	Ag	235	10% 95% 5%

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Mol	Chain	Length	Quality of chain
8	Ah	125	49% 98%
9	Ai	215	35% 100%
10	Aj	130	5% 99%
11	Ak	130	11% 96%
12	Al	135	30% 99%
13	Am	102	70% 98%
14	An	140	17% 88% 9%
15	Ao	147	11% 97%
16	Ap	149	32% 91% 9%
17	Aq	151	13% 99%
18	Ar	56	38% 96%
19	As	114	11% 95% 5%
20	At	67	64% 96%
20	Bm	67	33% 94% 6%
21	Au	133	30% 87% 13%
22	Av	150	27% 99%
23	Aw	98	20% 97%
23	Bn	98	33% 94% 6%
24	Ax	65	28% 94% 6%
25	Ay	70	53% 91% 9%
26	Az	62	11% 89% 11%
27	BA	3037	9% 66% 24% 6%
28	BB	126	17% 72% 23%
29	BC	239	5% 92% 8%
30	BD	346	6% 90% 10%

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Mol	Chain	Length	Quality of chain
31	BE	255	87% 13%
32	BF	183	83% 67% 23% 9%
33	BG	184	10% 91% 8%
34	BH	123	26% 89% 10%
34	BI	123	96% 83% 15%
35	BJ	182	10% 86% 8% 6%
36	BK	142	94% 6%
37	BL	141	11% 94% 6%
38	BM	83	29% 78% 19%
38	BN	83	31% 82% 16%
39	BO	148	25% 88% 12%
40	BP	194	95% 5%
41	BQ	201	32% 66% 15% 18%
42	BR	121	85% 14%
43	BS	150	5% 88% 9%
44	BT	77	13% 96%
45	BU	98	89% 9%
46	BV	156	92% 6%
47	BW	86	12% 85% 14%
48	BX	121	89% 10%
49	BY	67	15% 84% 9% 7%
50	BZ	66	26% 89% 9%
51	Ba	155	6% 99%
52	Bb	102	18% 94% 6%
53	Bc	90	10% 99%

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Mol	Chain	Length	Quality of chain
54	Bd	125	99%
55	Be	90	98%
56	Bf	101	6% 85% 15%
57	Bg	86	6% 98%
58	Bh	63	98%
59	Bi	51	96%
60	Bj	51	8% 92% 8%
61	Bk	37	5% 97%
62	Bl	94	9% 99%
63	Bo	47	91% 9%
64	Bp	236	98% 98%
65	Bq	34	100% 100%

2 Entry composition

There are 67 unique types of molecules in this entry. The entry contains 167402 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	Aa	1463	31531	14063	5836	10169	1463	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	Ab	196	1580	1021	272	284	3	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	Ac	195	1536	979	283	271	3	0	0

- Molecule 4 is a protein called 30S ribosomal protein S3Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	Ad	190	1550	997	277	273	3	0	0

- Molecule 5 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	Ae	174	1454	912	287	253	2	0	0

- Molecule 6 is a protein called 30S ribosomal protein S4e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	Af	242	1952	1261	349	337	5	0	0

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Ag	223	Total	C	N	O	S	0	0
			1753	1107	327	312	7		

- Molecule 8 is a protein called 30S ribosomal protein S6e.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Ah	123	Total	C	N	O	S	0	0
			952	599	179	172	2		

- Molecule 9 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Ai	214	Total	C	N	O	S	0	0
			1715	1087	317	303	8		

- Molecule 10 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Aj	129	Total	C	N	O	S	0	0
			1020	662	176	180	2		

- Molecule 11 is a protein called 30S ribosomal protein S8e.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	Ak	125	Total	C	N	O	0	0
			982	615	198	169		

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Al	133	Total	C	N	O	S	0	0
			1054	656	205	188	5		

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Am	100	Total	C	N	O	S	0	0
			803	498	154	148	3		

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	An	127	Total 953	C 587	N 190	O 173	S 3	0	0

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ao	143	Total 1122	C 712	N 216	O 192	S 2	0	0

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Ap	135	Total 1090	C 691	N 214	O 181	S 4	0	0

- Molecule 17 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Aq	149	Total 1217	C 776	N 233	O 206	S 2	0	0

- Molecule 18 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Ar	54	Total 447	C 284	N 92	O 65	S 6	0	0

- Molecule 19 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	As	108	Total 879	C 560	N 164	O 152	S 3	0	0

- Molecule 20 is a protein called 30S ribosomal protein S17e.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	At	64	Total 538	C 338	N 103	O 95	S 2	0	0
20	Bm	63	Total 534	C 336	N 102	O 94	S 2	0	0

- Molecule 21 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Au	116	Total	C	N	O	S	0	0
			952	608	175	163	6		

- Molecule 22 is a protein called 30S ribosomal protein S19e.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	Av	149	Total	C	N	O	0	0
			1216	788	215	213		

- Molecule 23 is a protein called 30S ribosomal protein S24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Aw	95	Total	C	N	O	S	0	0
			777	497	131	146	3		
23	Bn	92	Total	C	N	O	S	0	0
			752	481	126	142	3		

- Molecule 24 is a protein called 30S ribosomal protein S27e.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Ax	61	Total	C	N	O	S	0	0
			461	294	83	79	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ax	64	GLU	LEU	conflict	UNP Q5JE50

- Molecule 25 is a protein called 30S ribosomal protein S28e.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Ay	64	Total	C	N	O	0	0
			499	307	99	93		

- Molecule 26 is a protein called Predicted zinc-ribbon RNA-binding protein involved in translation.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Az	55	Total	C	N	O	S	0	0
			426	269	74	75	8		

- Molecule 27 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	BA	2934	Total	C	N	O	P	S	0	0
			63209	28168	11754	20351	2934	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BB	125	Total	C	N	O	P	0	0
			2678	1191	492	870	125		

- Molecule 29 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BC	237	Total	C	N	O	S	0	0
			1820	1150	356	311	3		

- Molecule 30 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BD	344	Total	C	N	O	S	0	0
			2746	1765	505	469	7		

- Molecule 31 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BE	255	Total	C	N	O	S	0	0
			2026	1286	389	347	4		

- Molecule 32 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BF	166	Total	C	N	O	S	0	0
			1339	839	258	235	7		

- Molecule 33 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BG	183	Total	C	N	O	S	0	0
			1463	942	253	266	2		

- Molecule 34 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BH	121	Total	C	N	O	S	0	0
			928	591	154	180	3		
34	BI	121	Total	C	N	O	S	0	0
			928	591	154	180	3		

- Molecule 35 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BJ	171	Total	C	N	O	S	0	0
			1399	891	261	240	7		

- Molecule 36 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BK	142	Total	C	N	O	S	0	0
			1146	731	213	198	4		

- Molecule 37 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BL	140	Total	C	N	O	S	0	0
			1055	658	214	180	3		

- Molecule 38 is a protein called 50S ribosomal protein L14e.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BM	81	Total	C	N	O	S	0	0
			610	382	119	108	1		
38	BN	81	Total	C	N	O	S	0	0
			610	382	119	108	1		

- Molecule 39 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BO	148	Total	C	N	O	S	0	0
			1166	743	222	198	3		

- Molecule 40 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BP	193	Total	C	N	O	S	0	0
			1582	1010	316	250	6		

- Molecule 41 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BQ	164	Total	C	N	O	S	0	0
			1314	841	243	228	2		

- Molecule 42 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BR	120	Total	C	N	O	S	0	0
			959	601	187	169	2		

- Molecule 43 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BS	146	Total	C	N	O	S	0	0
			1200	753	246	194	7		

- Molecule 44 is a protein called 50S ribosomal protein L18Ae.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	BT	74	Total	C	N	O	0	0
			624	399	113	112		

- Molecule 45 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BU	96	Total	C	N	O	S	0	0
			784	502	158	123	1		

- Molecule 46 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BV	154	Total	C	N	O	S	0	0
			1234	777	242	211	4		

- Molecule 47 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BW	85	Total	C	N	O	S	0	0
			683	438	119	123	3		

- Molecule 48 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BX	120	Total	C	N	O	S	0	0
			991	628	188	170	5		

- Molecule 49 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BY	62	Total	C	N	O	S	0	0
			524	334	99	85	6		

- Molecule 50 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BZ	60	Total	C	N	O	S	0	0
			506	314	98	90	4		

- Molecule 51 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Ba	154	Total	C	N	O	S	0	0
			1242	788	235	214	5		

- Molecule 52 is a protein called 50S ribosomal protein L30e.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Bb	96	Total	C	N	O	S	0	0
			730	473	123	133	1		

- Molecule 53 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	Bc	89	Total	C	N	O	0	0
			721	463	140	118		

- Molecule 54 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Bd	124	Total	C	N	O	S	0	0
			1022	650	208	162	2		

- Molecule 55 is a protein called 50S ribosomal protein L34e.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Be	89	Total	C	N	O	S	0	0
			728	454	155	110	9		

- Molecule 56 is a protein called Ribosomal protein eL35A.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	Bf	86	Total	C	N	O	0	0
			669	424	133	112		

- Molecule 57 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Bg	84	Total	C	N	O	S	0	0
			630	392	132	101	5		

- Molecule 58 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Bh	62	Total	C	N	O	S	0	0
			512	314	118	75	5		

- Molecule 59 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms				AltConf	Trace
59	Bi	50	Total	C	N	O	0	0
			432	276	97	59		

- Molecule 60 is a protein called 50S ribosomal protein L40e.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Bj	47	Total	C	N	O	S	0	0
			373	233	79	56	5		

- Molecule 61 is a protein called LSU ribosomal protein L41E.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Bk	36	Total	C	N	O	S	0	0
			345	218	86	39	2		

- Molecule 62 is a protein called 50S ribosomal protein L44e.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Bl	93	Total	C	N	O	S	0	0
			778	494	160	119	5		

- Molecule 63 is a protein called Nucleic acid-binding protein, containing C2H2 zinc-finger.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Bo	43	Total	C	N	O	S	0	0
			349	222	69	55	3		

- Molecule 64 is a protein called Predicted exosome subunit, UPF0023 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Bp	232	Total	C	N	O	S	0	0
			1862	1193	323	342	4		

- Molecule 65 is a protein called Unknown ribosomal protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
65	Bq	34	Total	C	N	O	0	0
			170	102	34	34		

- Molecule 66 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
66	Ag	1	Total	Zn	0
			1	1	
66	Ar	1	Total	Zn	0
			1	1	
66	As	1	Total	Zn	0
			1	1	
66	Ax	1	Total	Zn	0
			1	1	
66	Az	2	Total	Zn	0
			2	2	
66	BY	1	Total	Zn	0
			1	1	
66	Be	2	Total	Zn	0
			2	2	
66	Bg	1	Total	Zn	0
			1	1	
66	Bh	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms	AltConf
66	Bj	1	Total Zn 1 1	0
66	Bl	1	Total Zn 1 1	0
66	Bo	1	Total Zn 1 1	0

- Molecule 67 is water.

Mol	Chain	Residues	Atoms	AltConf
67	Aa	266	Total O 266 266	0
67	Ad	1	Total O 1 1	0
67	Af	4	Total O 4 4	0
67	Ag	1	Total O 1 1	0
67	Ai	1	Total O 1 1	0
67	Aj	2	Total O 2 2	0
67	Ak	6	Total O 6 6	0
67	Al	2	Total O 2 2	0
67	Am	2	Total O 2 2	0
67	An	2	Total O 2 2	0
67	Ao	1	Total O 1 1	0
67	Ap	3	Total O 3 3	0
67	Aq	5	Total O 5 5	0
67	As	2	Total O 2 2	0
67	Au	1	Total O 1 1	0
67	Av	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
67	Az	1	Total O 1 1	0
67	BA	2715	Total O 2715 2715	0
67	BB	23	Total O 23 23	0
67	BC	51	Total O 51 51	0
67	BD	59	Total O 59 59	0
67	BE	41	Total O 41 41	0
67	BF	2	Total O 2 2	0
67	BG	1	Total O 1 1	0
67	BH	1	Total O 1 1	0
67	BJ	13	Total O 13 13	0
67	BK	18	Total O 18 18	0
67	BL	15	Total O 15 15	0
67	BM	3	Total O 3 3	0
67	BN	3	Total O 3 3	0
67	BO	30	Total O 30 30	0
67	BP	36	Total O 36 36	0
67	BQ	6	Total O 6 6	0
67	BR	14	Total O 14 14	0
67	BS	17	Total O 17 17	0
67	BT	2	Total O 2 2	0
67	BU	13	Total O 13 13	0

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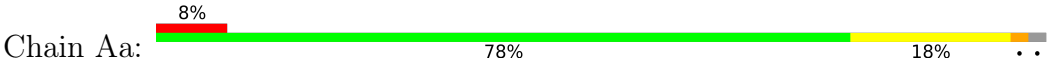
Mol	Chain	Residues	Atoms	AltConf
67	BV	22	Total O 22 22	0
67	BW	3	Total O 3 3	0
67	BX	10	Total O 10 10	0
67	BY	12	Total O 12 12	0
67	BZ	7	Total O 7 7	0
67	Ba	14	Total O 14 14	0
67	Bb	8	Total O 8 8	0
67	Bc	10	Total O 10 10	0
67	Bd	23	Total O 23 23	0
67	Be	8	Total O 8 8	0
67	Bf	7	Total O 7 7	0
67	Bg	15	Total O 15 15	0
67	Bh	23	Total O 23 23	0
67	Bi	10	Total O 10 10	0
67	Bj	3	Total O 3 3	0
67	Bk	3	Total O 3 3	0
67	Bl	8	Total O 8 8	0
67	Bm	1	Total O 1 1	0
67	Bn	1	Total O 1 1	0
67	Bo	4	Total O 4 4	0

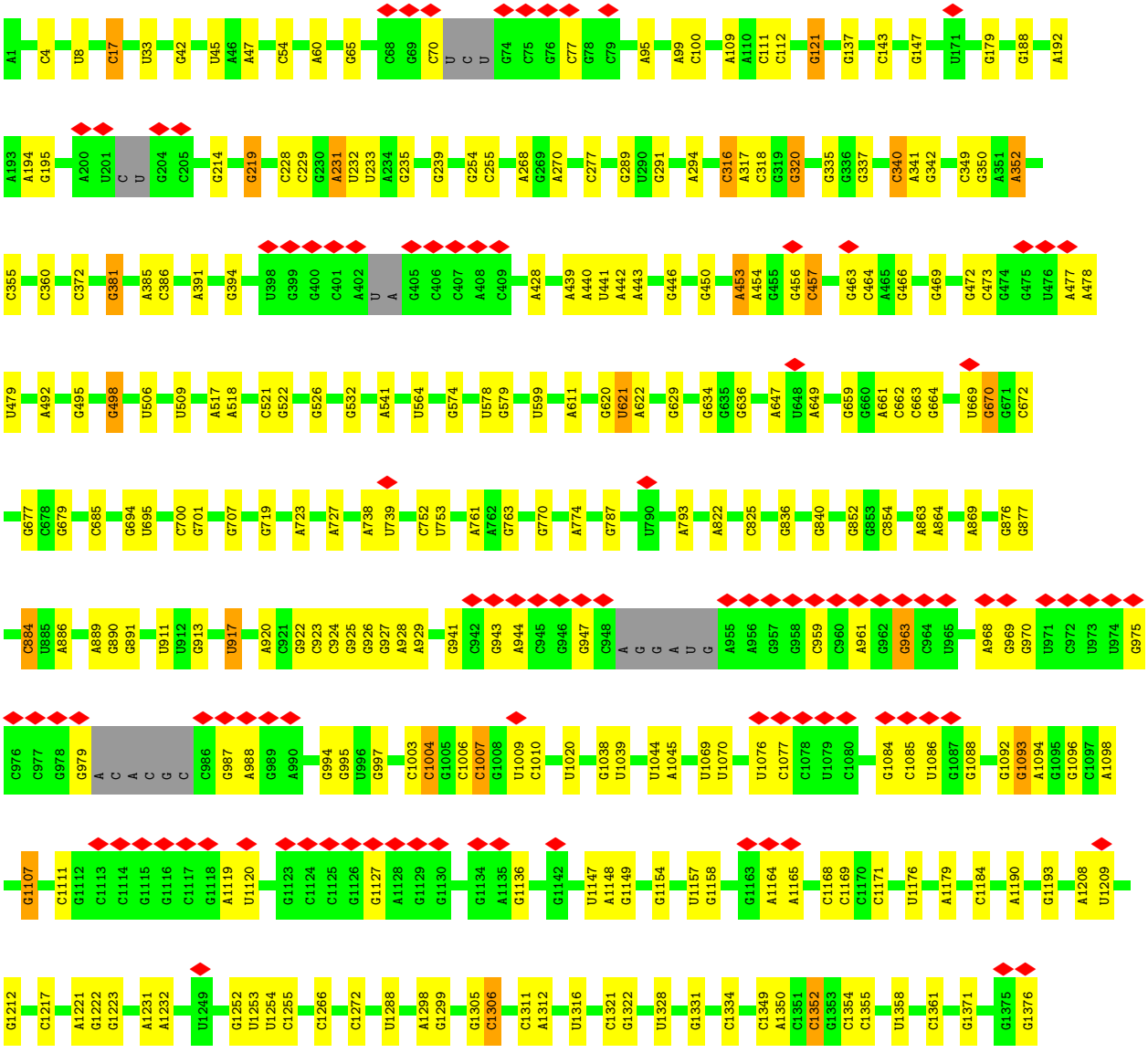
3 Residue-property plots (i)

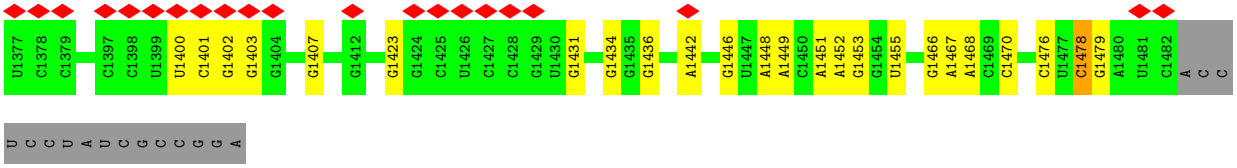
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 16S ribosomal RNA

Chain Aa:

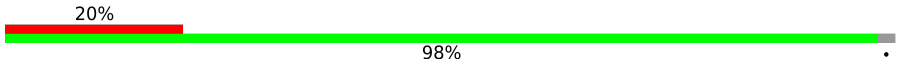


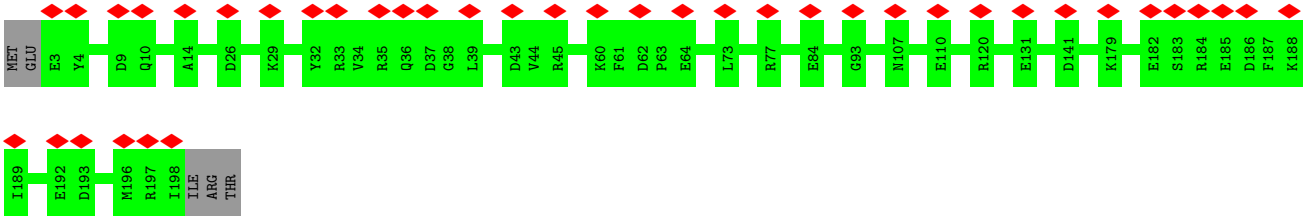




• Molecule 2: 30S ribosomal protein S2

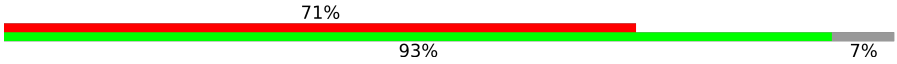
Chain Ab:

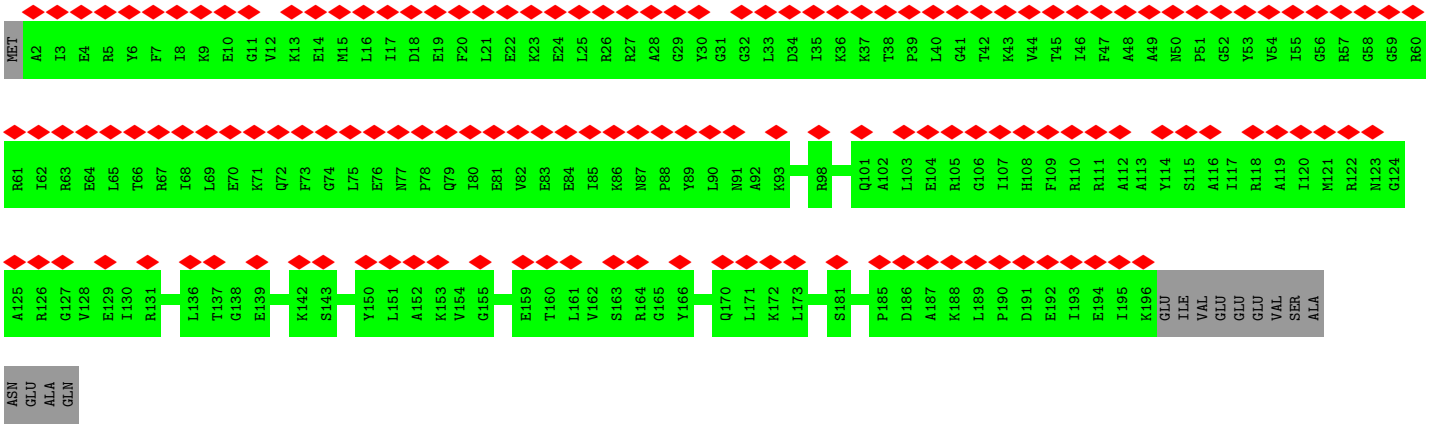




• Molecule 3: 30S ribosomal protein S3

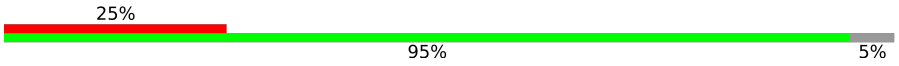
Chain Ac:

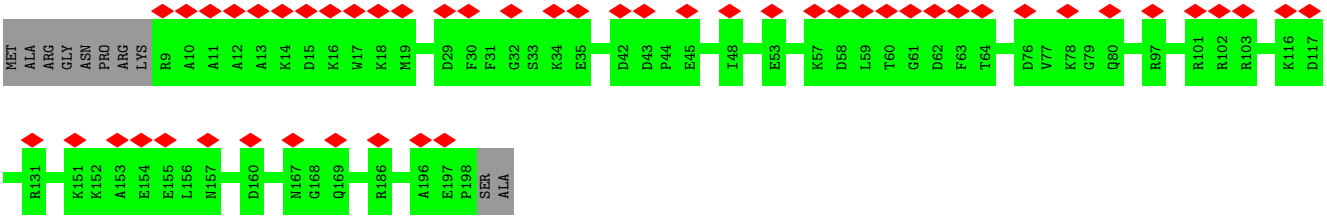




• Molecule 4: 30S ribosomal protein S3Ae

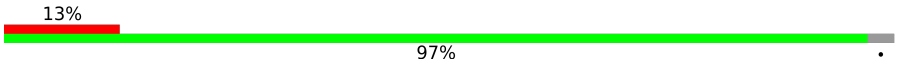
Chain Ad:

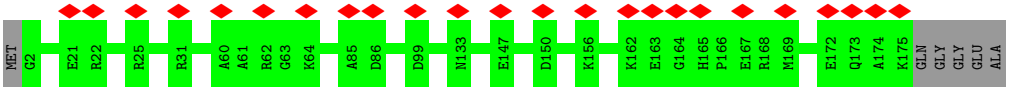




• Molecule 5: 30S ribosomal protein S4

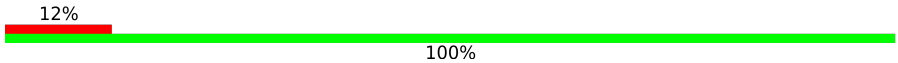
Chain Ae:

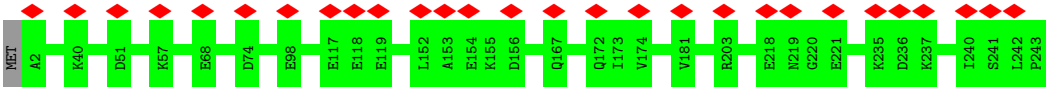




• Molecule 6: 30S ribosomal protein S4e

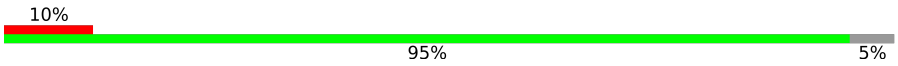
Chain Af:

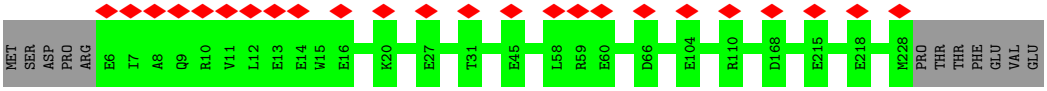




• Molecule 7: 30S ribosomal protein S5

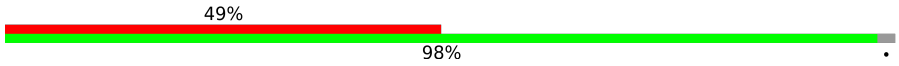
Chain Ag:





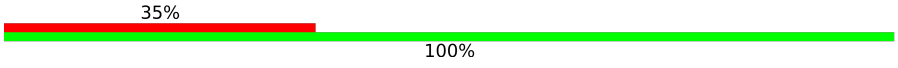
• Molecule 8: 30S ribosomal protein S6e

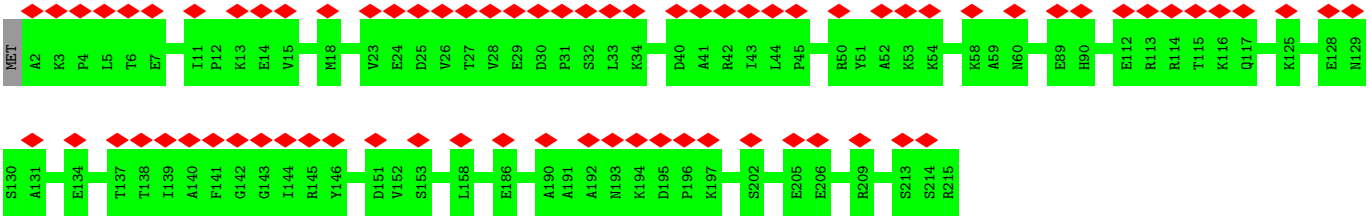
Chain Ah:



• Molecule 9: 30S ribosomal protein S7

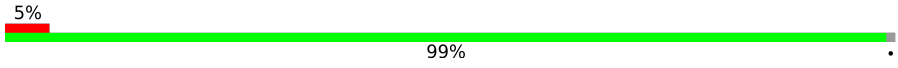
Chain Ai:

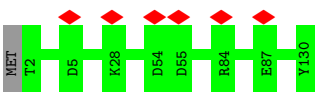




• Molecule 10: 30S ribosomal protein S8

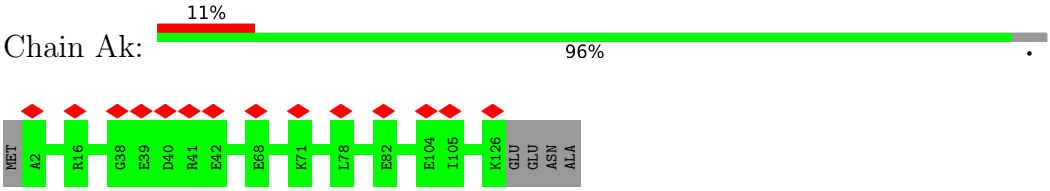
Chain Aj:





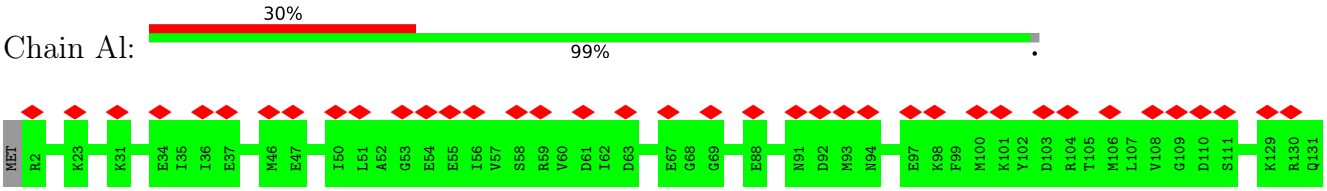
• Molecule 11: 30S ribosomal protein S8e

Chain Ak:



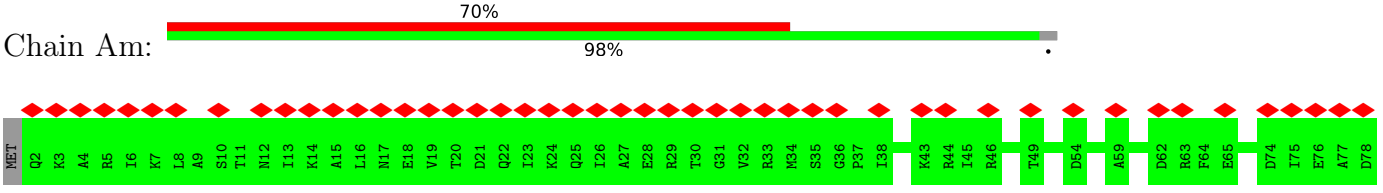
• Molecule 12: 30S ribosomal protein S9

Chain Al:



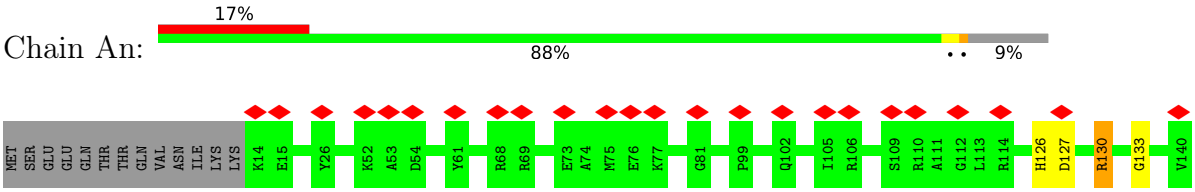
• Molecule 13: 30S ribosomal protein S10

Chain Am:



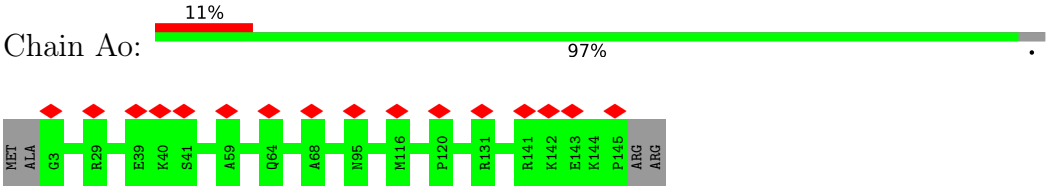
• Molecule 14: 30S ribosomal protein S11

Chain An:



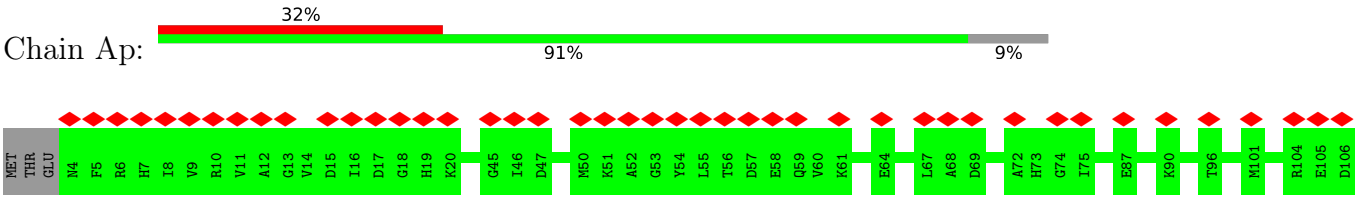
• Molecule 15: 30S ribosomal protein S12

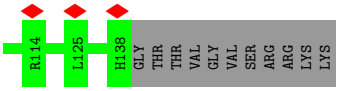
Chain Ao:



• Molecule 16: 30S ribosomal protein S13

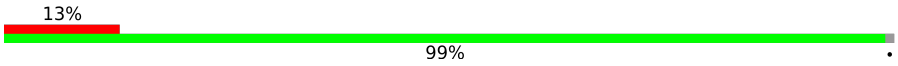
Chain Ap:

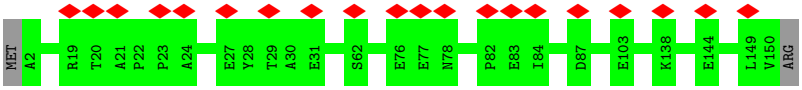




• Molecule 17: 30S ribosomal protein S15

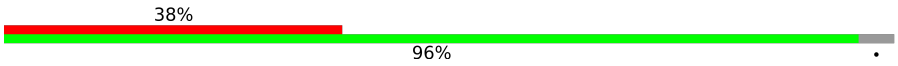
Chain Aq:

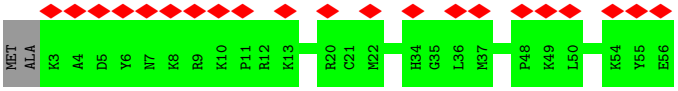




• Molecule 18: 30S ribosomal protein S14 type Z

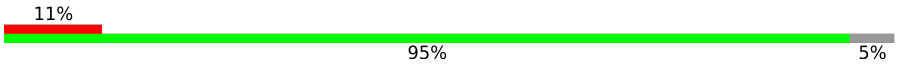
Chain Ar:

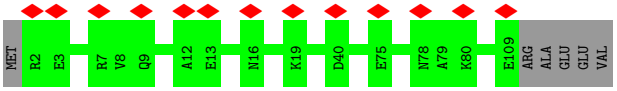




• Molecule 19: 30S ribosomal protein S17

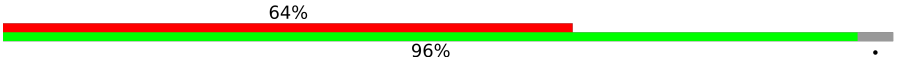
Chain As:

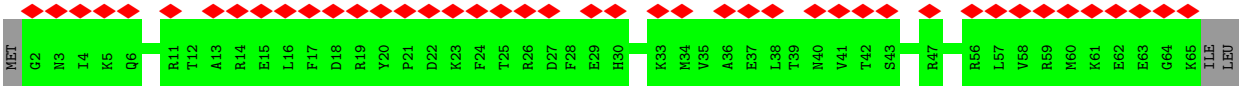




• Molecule 20: 30S ribosomal protein S17e

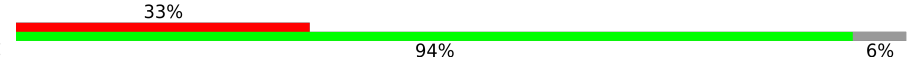
Chain At:

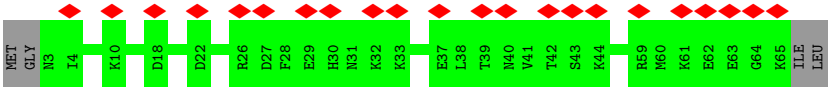




• Molecule 20: 30S ribosomal protein S17e

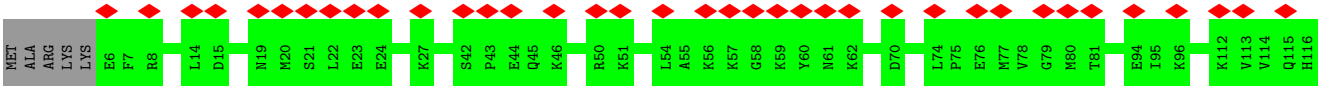
Chain Bm:

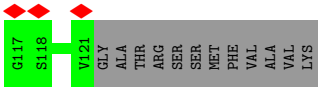




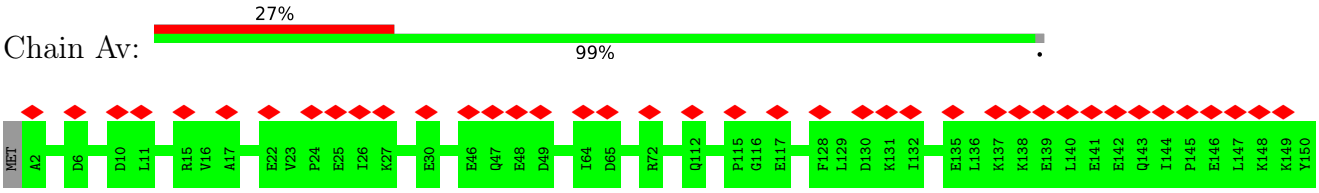
• Molecule 21: 30S ribosomal protein S19

Chain Au:

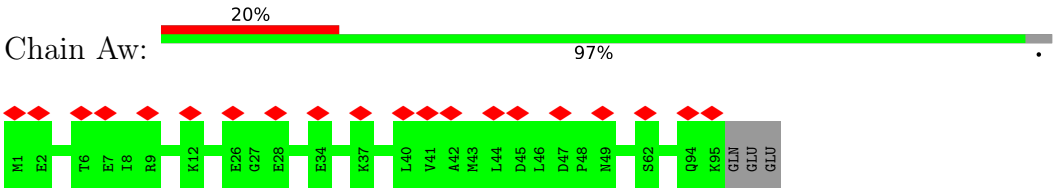




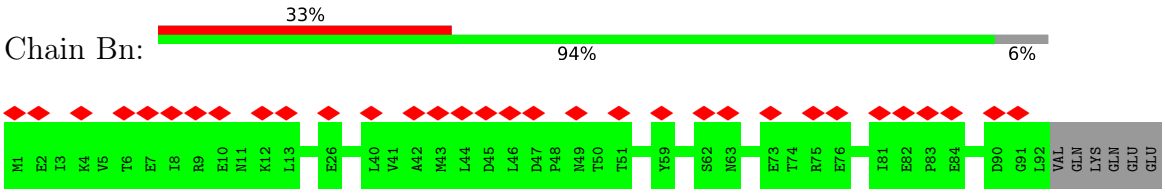
• Molecule 22: 30S ribosomal protein S19e



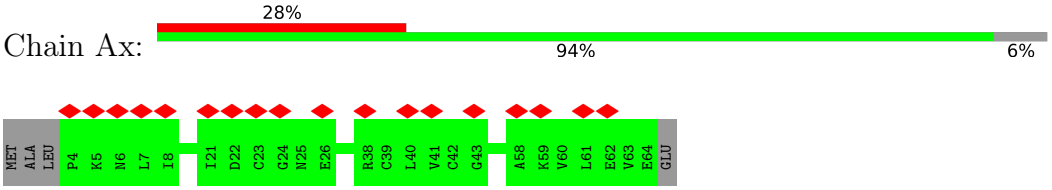
• Molecule 23: 30S ribosomal protein S24e



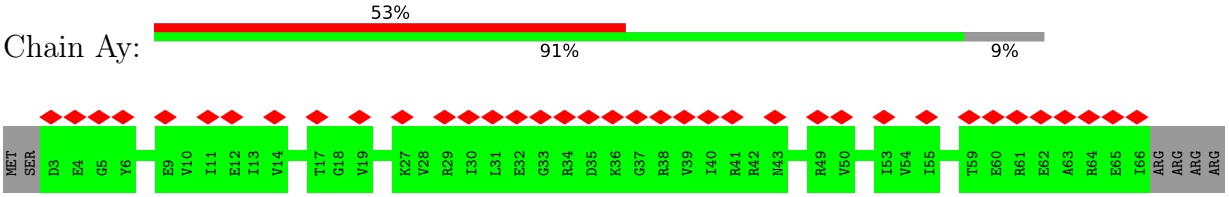
• Molecule 23: 30S ribosomal protein S24e



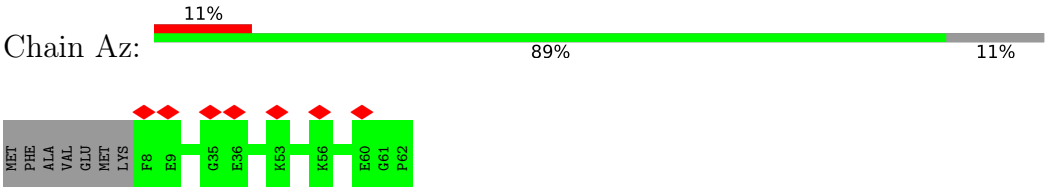
• Molecule 24: 30S ribosomal protein S27e



• Molecule 25: 30S ribosomal protein S28e

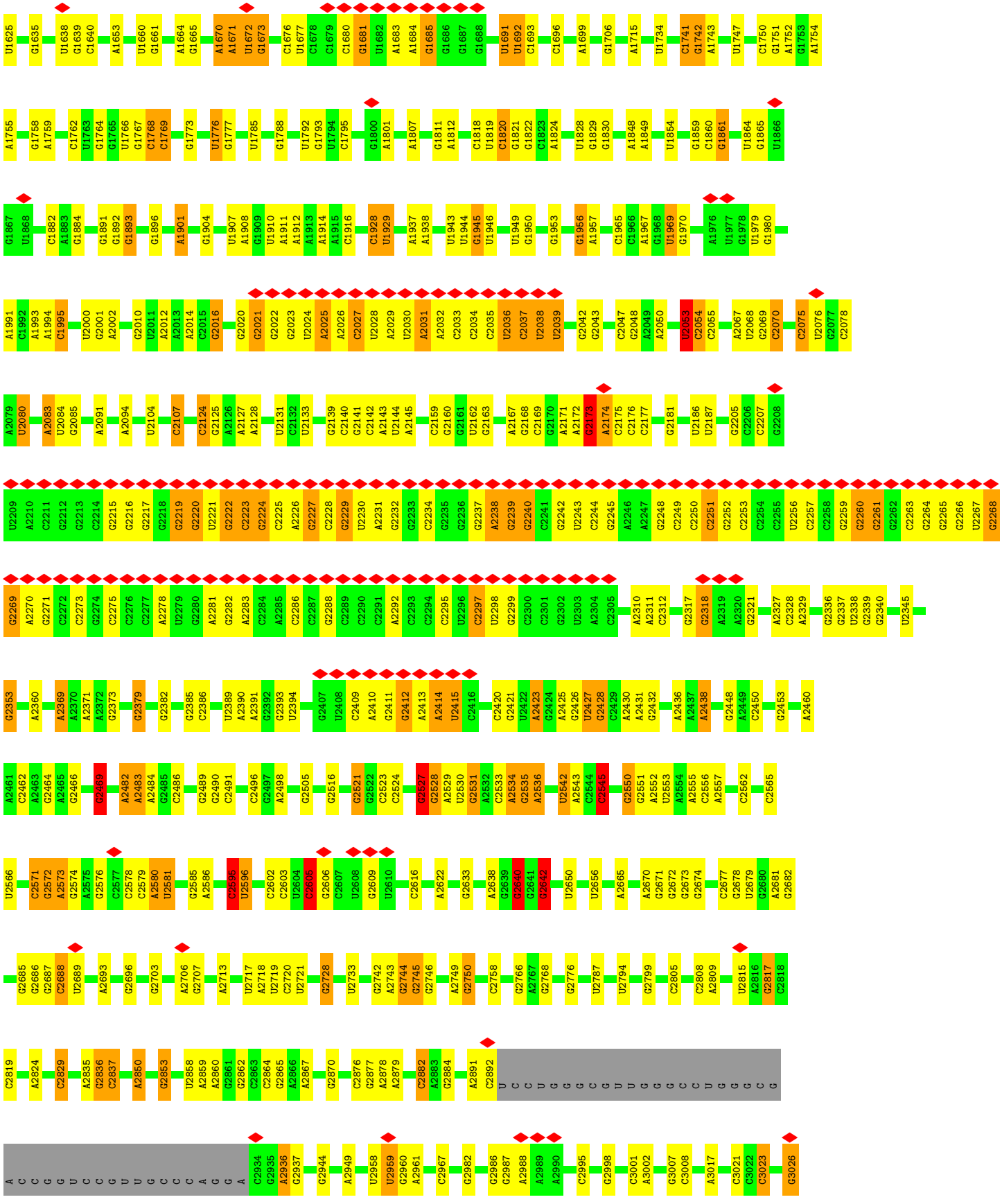


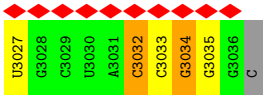
• Molecule 26: Predicted zinc-ribbon RNA-binding protein involved in translation



• Molecule 27: 23S ribosomal RNA

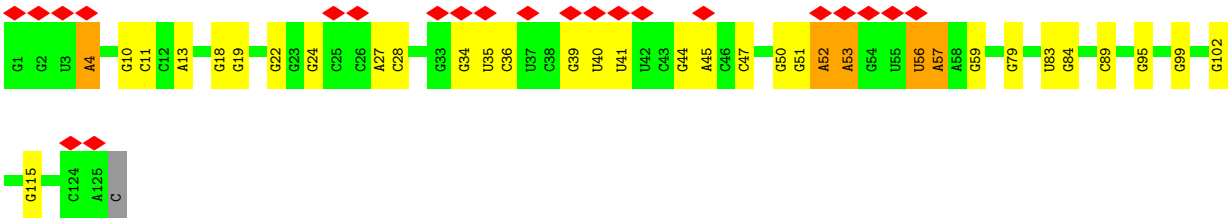
Chain BA:





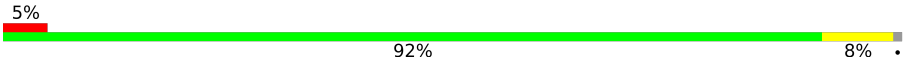
• Molecule 28: 5S ribosomal RNA

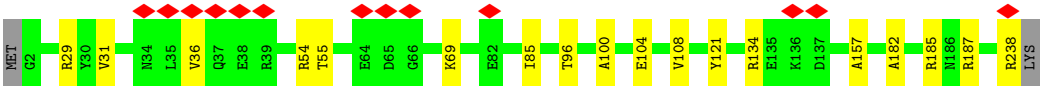
Chain BB:



• Molecule 29: 50S ribosomal protein L2

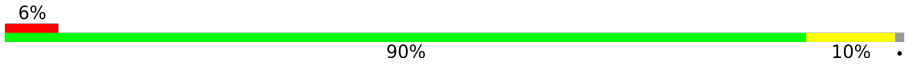
Chain BC:

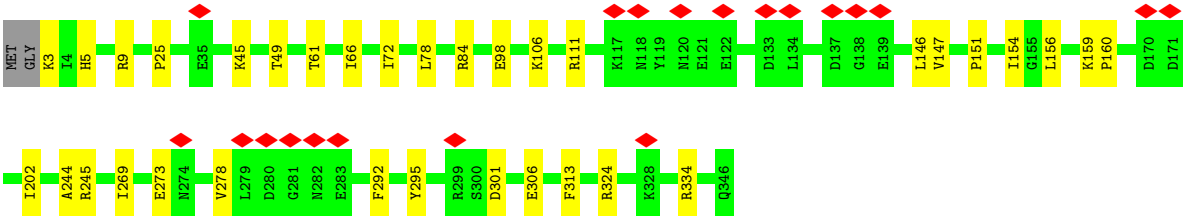




• Molecule 30: 50S ribosomal protein L3

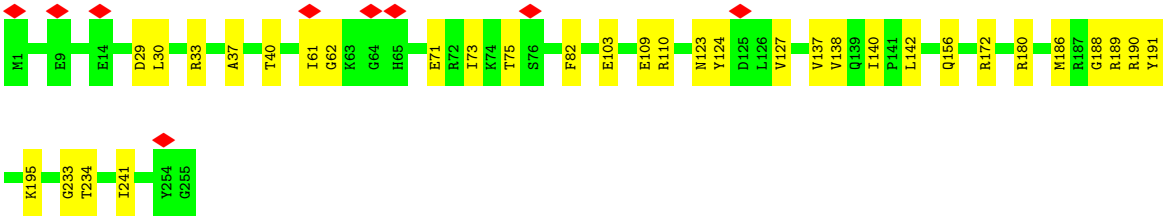
Chain BD:





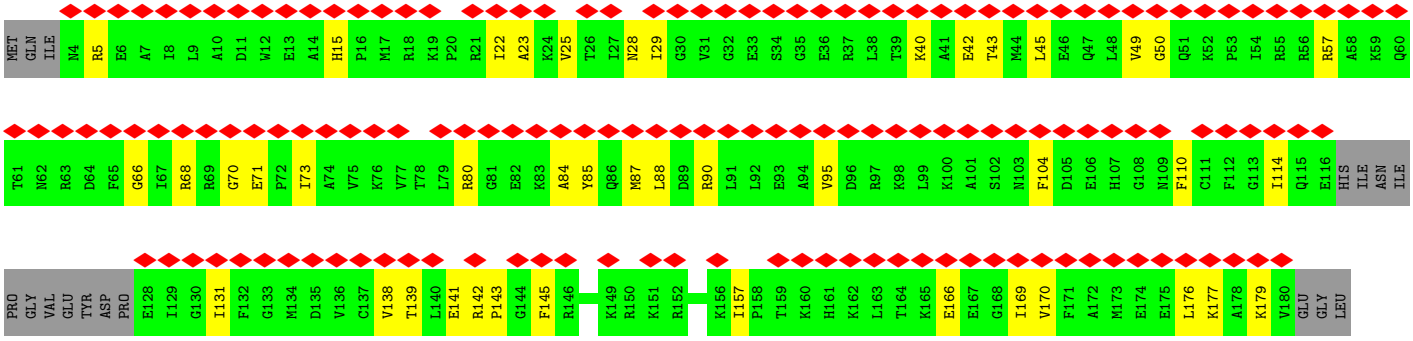
• Molecule 31: 50S ribosomal protein L4

Chain BE:

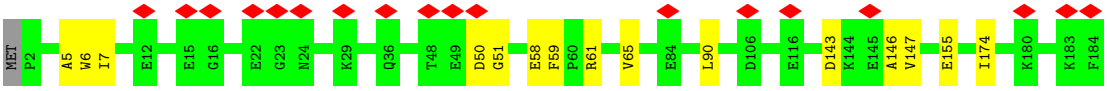


• Molecule 32: 50S ribosomal protein L5

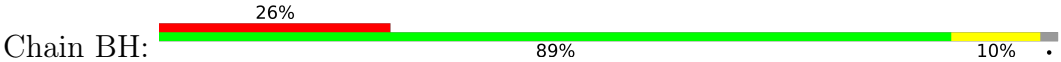
Chain BF:

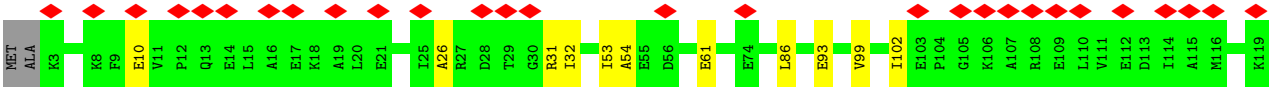


• Molecule 33: 50S ribosomal protein L6

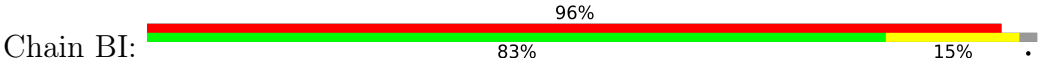


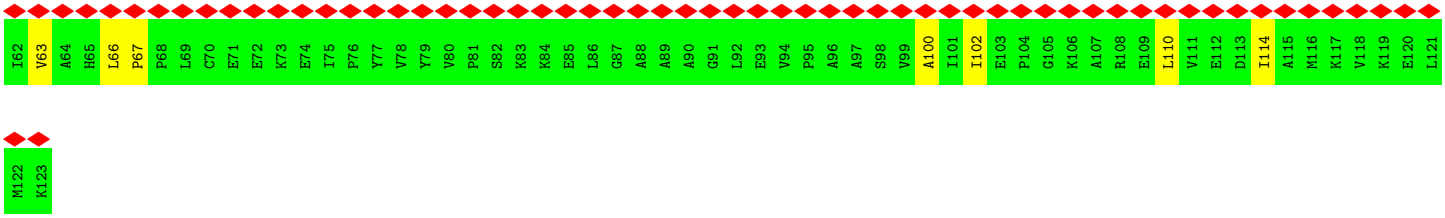
• Molecule 34: 50S ribosomal protein L7Ae



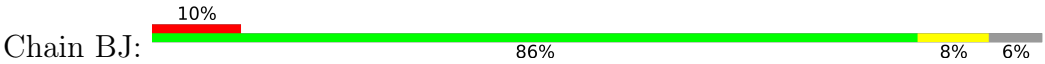


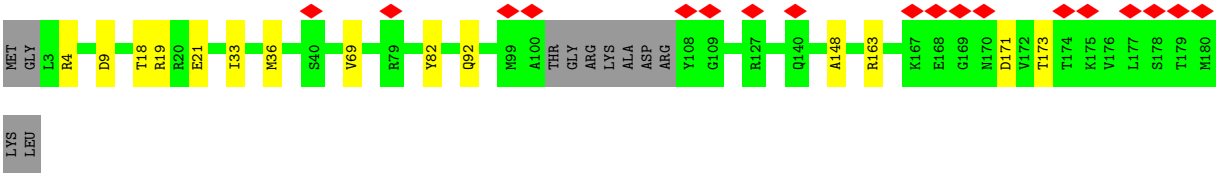
• Molecule 34: 50S ribosomal protein L7Ae



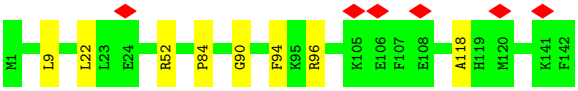


• Molecule 35: 50S ribosomal protein L10e

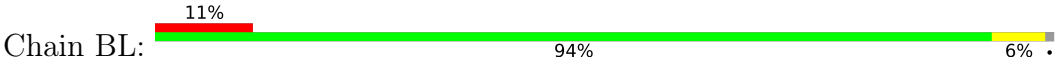


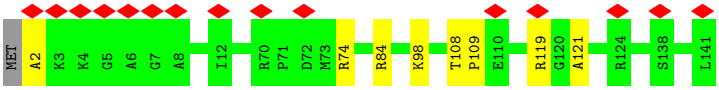


• Molecule 36: 50S ribosomal protein L13

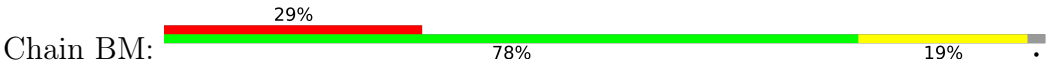


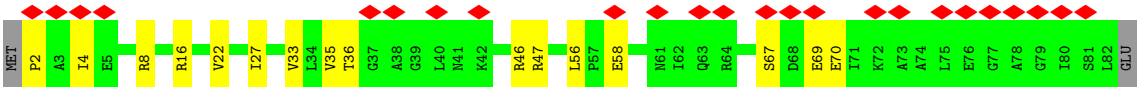
• Molecule 37: 50S ribosomal protein L14



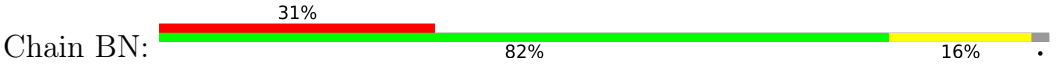


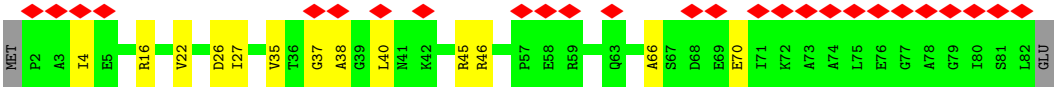
• Molecule 38: 50S ribosomal protein L14e



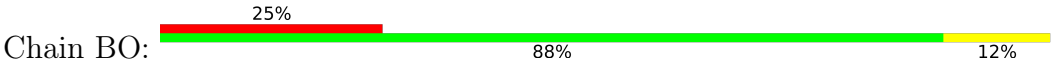


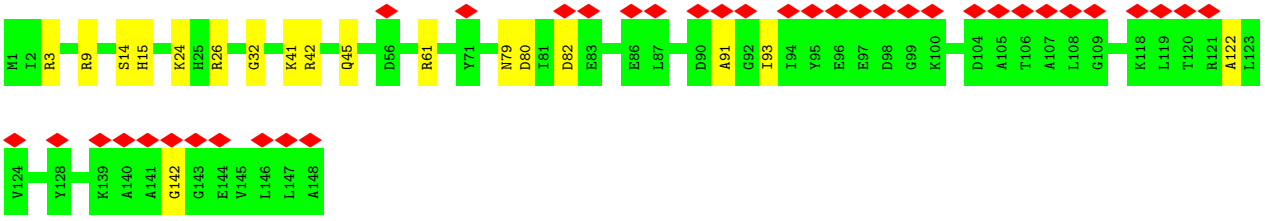
• Molecule 38: 50S ribosomal protein L14e





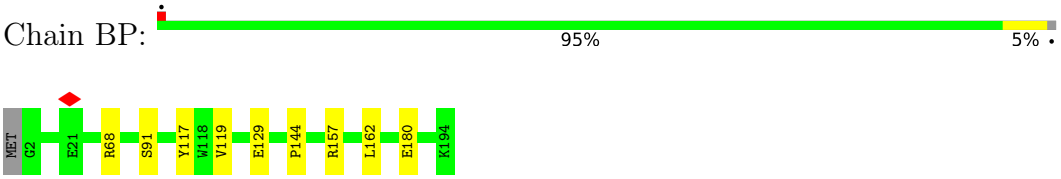
• Molecule 39: 50S ribosomal protein L15





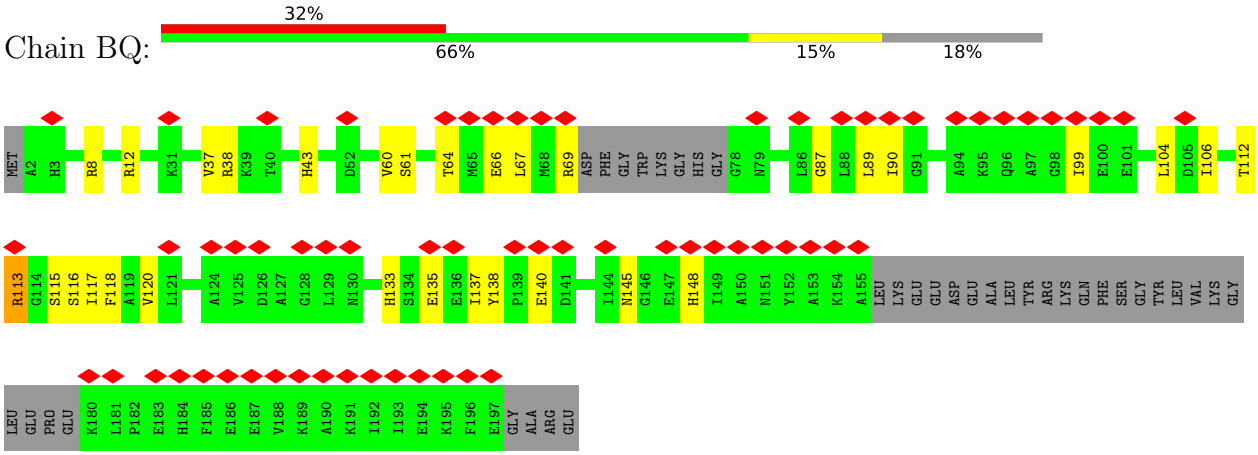
• Molecule 40: 50S ribosomal protein L15e

Chain BP:



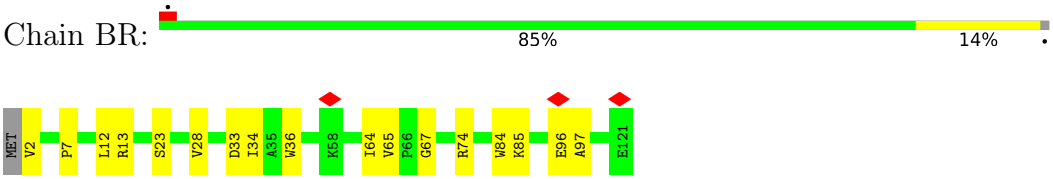
• Molecule 41: 50S ribosomal protein L18

Chain BQ:



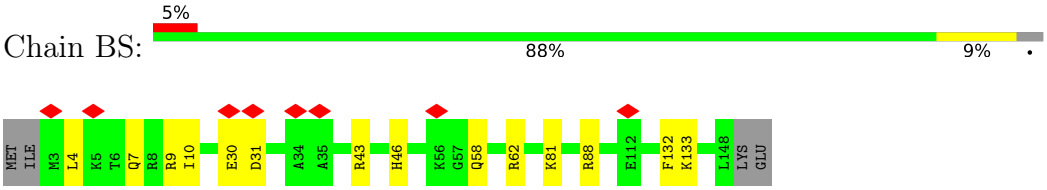
• Molecule 42: 50S ribosomal protein L18e

Chain BR:



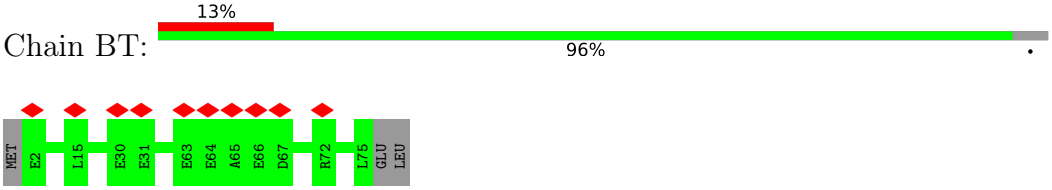
• Molecule 43: 50S ribosomal protein L19e

Chain BS:



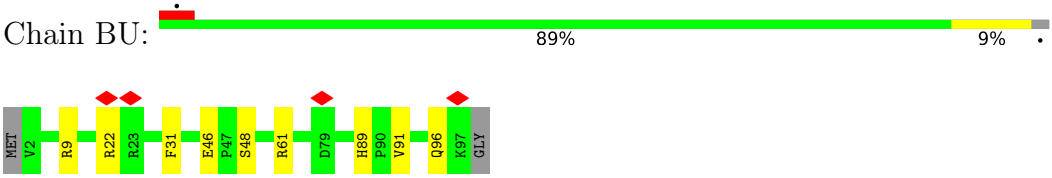
• Molecule 44: 50S ribosomal protein L18Ae

Chain BT:



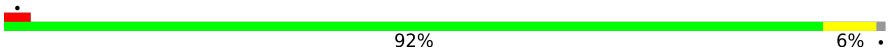
• Molecule 45: 50S ribosomal protein L21e

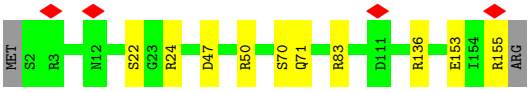
Chain BU:



• Molecule 46: 50S ribosomal protein L22

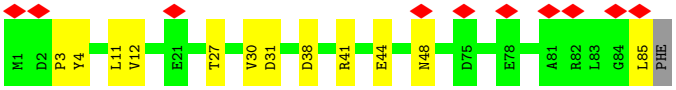
Chain BV:





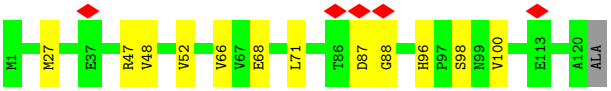
• Molecule 47: 50S ribosomal protein L23

Chain BW:



• Molecule 48: 50S ribosomal protein L24

Chain BX:

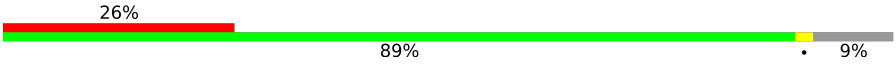


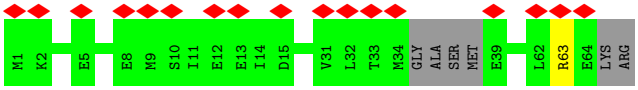
• Molecule 49: 50S ribosomal protein L24e

Chain BY:

• Molecule 50: 50S ribosomal protein L29

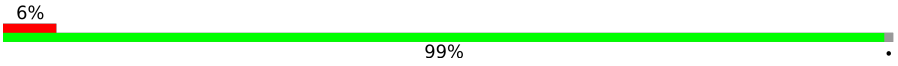
Chain BZ:

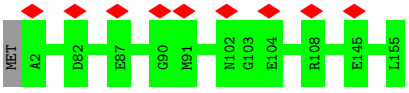




• Molecule 51: 50S ribosomal protein L30

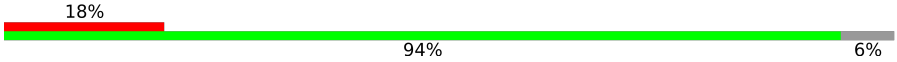
Chain Ba:

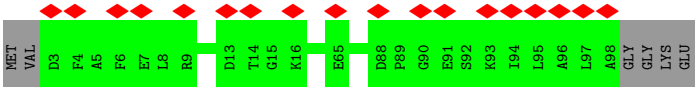




• Molecule 52: 50S ribosomal protein L30e

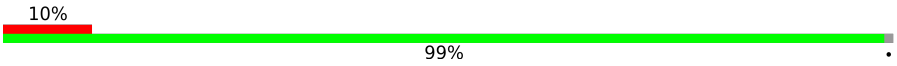
Chain Bb:

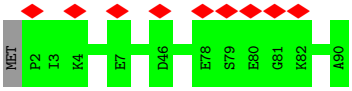




• Molecule 53: 50S ribosomal protein L31e

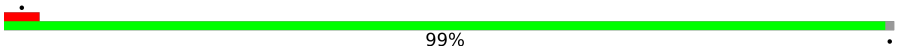
Chain Bc:

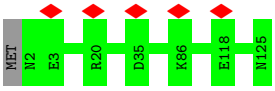




• Molecule 54: 50S ribosomal protein L32e

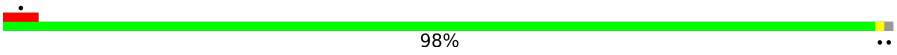
Chain Bd:

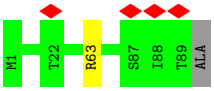




• Molecule 55: 50S ribosomal protein L34e

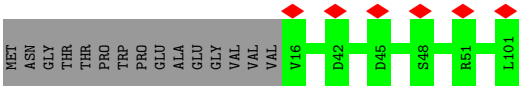
Chain Be:





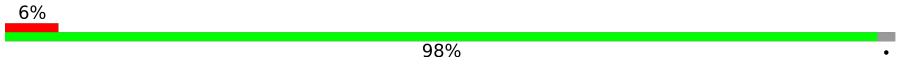
• Molecule 56: Ribosomal protein eL35A

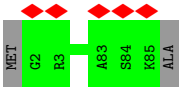
Chain Bf:



• Molecule 57: 50S ribosomal protein L37Ae

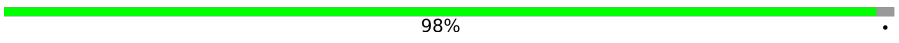
Chain Bg:





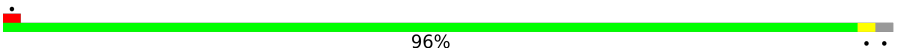
• Molecule 58: 50S ribosomal protein L37e

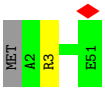
Chain Bh:



• Molecule 59: 50S ribosomal protein L39e

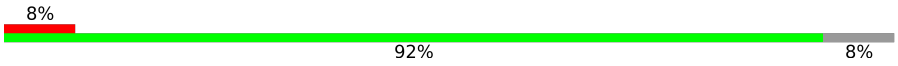
Chain Bi:

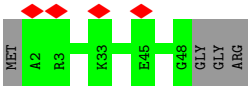




• Molecule 60: 50S ribosomal protein L40e

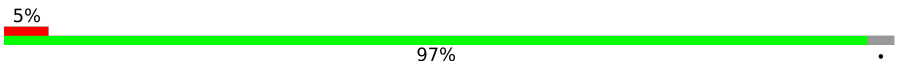
Chain Bj:

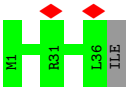




• Molecule 61: LSU ribosomal protein L41E

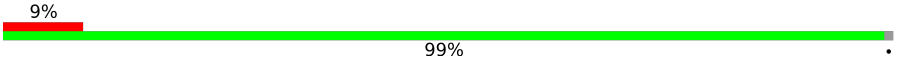
Chain Bk:

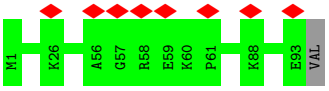




• Molecule 62: 50S ribosomal protein L44e

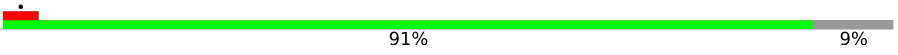
Chain Bl:

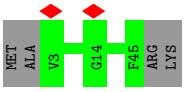




• Molecule 63: Nucleic acid-binding protein, containing C2H2 zinc-finger

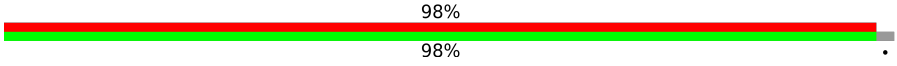
Chain Bo:

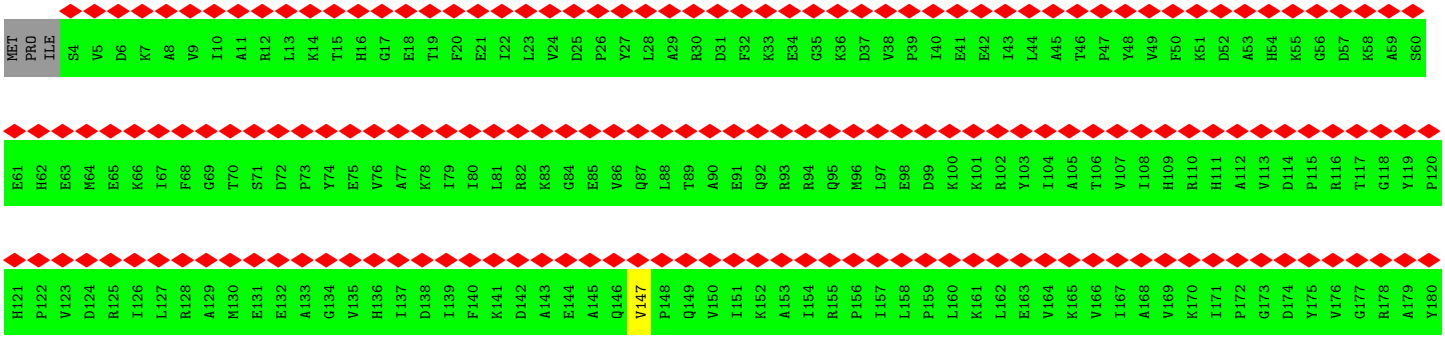


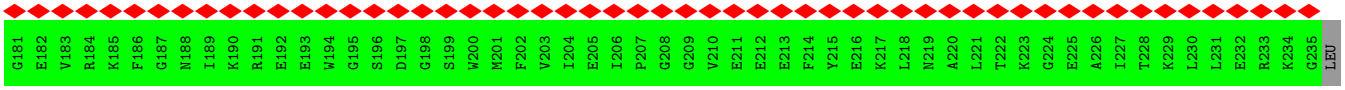


• Molecule 64: Predicted exosome subunit, UPF0023 family

Chain Bp:

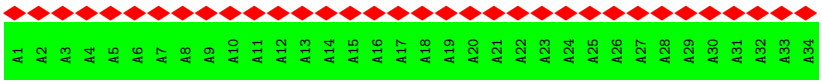






• Molecule 65: Unknown ribosomal protein

Chain Bq:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	116585	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	34	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	29000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.497	Depositor
Minimum map value	-0.266	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	408.0, 408.0, 408.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, OMU, MA6, 2MG, OMC, 5MU, LV2, 6MZ, OMG, A2M, 4SU, ZN

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	Aa	0.38	0/33690	0.81	17/52572 (0.0%)
2	Ab	0.28	0/1611	0.45	0/2179
3	Ac	0.28	0/1558	0.44	0/2089
4	Ad	0.28	0/1578	0.48	0/2119
5	Ae	0.29	0/1477	0.48	0/1980
6	Af	0.30	0/1999	0.48	0/2700
7	Ag	0.29	0/1779	0.48	0/2396
8	Ah	0.31	0/968	0.49	0/1300
9	Ai	0.27	0/1748	0.45	0/2347
10	Aj	0.30	0/1039	0.48	0/1397
11	Ak	0.30	0/991	0.53	0/1322
12	Al	0.25	0/1068	0.50	0/1430
13	Am	0.25	0/810	0.45	0/1087
14	An	0.43	1/971 (0.1%)	0.53	0/1308
15	Ao	0.29	0/1139	0.46	0/1518
16	Ap	0.28	0/1113	0.48	0/1500
17	Aq	0.30	0/1241	0.45	0/1667
18	Ar	0.27	0/457	0.45	0/602
19	As	0.30	0/899	0.47	0/1214
20	At	0.26	0/545	0.42	0/725
20	Bm	0.28	0/541	0.45	0/720
21	Au	0.28	0/970	0.44	0/1295
22	Av	0.28	0/1249	0.43	0/1687
23	Aw	0.30	0/790	0.46	0/1063
23	Bn	0.29	0/765	0.46	0/1030
24	Ax	0.27	0/469	0.45	0/633
25	Ay	0.26	0/501	0.48	0/672
26	Az	0.30	0/440	0.45	0/599
27	BA	0.49	1/68729 (0.0%)	0.85	15/107278 (0.0%)
28	BB	0.33	0/2993	0.79	0/4668
29	BC	0.35	0/1860	0.53	0/2511
30	BD	0.33	0/2815	0.51	0/3795

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	BE	0.32	0/2066	0.49	0/2785
32	BF	0.27	0/1356	0.52	0/1806
33	BG	0.30	0/1490	0.48	0/2006
34	BH	0.28	0/941	0.44	0/1272
34	BI	0.26	0/941	0.44	0/1272
35	BJ	0.32	0/1429	0.48	0/1921
36	BK	0.32	0/1165	0.54	0/1558
37	BL	0.30	0/1067	0.52	0/1435
38	BM	0.33	0/614	0.52	0/824
38	BN	0.28	0/614	0.53	0/824
39	BO	0.29	0/1188	0.52	0/1585
40	BP	0.36	0/1621	0.52	0/2163
41	BQ	0.29	0/1342	0.48	0/1804
42	BR	0.30	0/971	0.52	0/1301
43	BS	0.31	0/1216	0.53	0/1607
44	BT	0.29	0/636	0.46	0/852
45	BU	0.33	0/806	0.48	0/1080
46	BV	0.31	0/1259	0.49	0/1688
47	BW	0.30	0/690	0.48	0/925
48	BX	0.33	0/1007	0.50	0/1344
49	BY	0.36	0/538	0.47	0/716
50	BZ	0.28	0/506	0.49	0/668
51	Ba	0.30	0/1259	0.52	0/1680
52	Bb	0.28	0/742	0.45	0/1001
53	Bc	0.30	0/736	0.48	0/990
54	Bd	0.31	0/1044	0.49	0/1394
55	Be	0.32	0/746	0.50	0/997
56	Bf	0.33	0/681	0.55	0/919
57	Bg	0.35	0/640	0.53	0/855
58	Bh	0.38	0/524	0.53	0/692
59	Bi	0.31	0/441	0.51	0/588
60	Bj	0.34	0/381	0.56	0/505
61	Bk	0.49	0/351	0.63	0/454
62	Bl	0.33	0/796	0.53	0/1056
63	Bo	0.32	0/356	0.48	0/474
64	Bp	0.28	0/1900	0.50	1/2559 (0.0%)
65	Bq	0.30	0/169	0.44	0/235
All	All	0.40	2/173032 (0.0%)	0.73	33/255238 (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
14	An	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	An	130	ARG	C-N	8.62	1.50	1.34
27	BA	2173	G	O3'-P	6.46	1.69	1.61

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BA	2173	G	P-O3'-C3'	9.17	130.70	119.70
1	Aa	1298	A	C2'-C3'-O3'	7.62	126.26	109.50
27	BA	2251	C	N3-C2-O2	-7.20	116.86	121.90
27	BA	549	G	O4'-C1'-N9	7.13	113.90	108.20
1	Aa	622	A	N9-C1'-C2'	-7.12	104.17	112.00
1	Aa	1470	C	N1-C2-O2	6.92	123.05	118.90
27	BA	1741	C	C2'-C3'-O3'	6.82	124.62	113.70
1	Aa	453	A	C2'-C3'-O3'	6.55	124.18	113.70
1	Aa	884	C	C2-N1-C1'	6.39	125.83	118.80
1	Aa	316	C	C2-N1-C1'	6.32	125.75	118.80
1	Aa	700	C	C2-N1-C1'	6.32	125.75	118.80
1	Aa	1093	G	C2'-C3'-O3'	6.29	123.77	113.70
27	BA	1449	U	C2-N1-C1'	6.17	125.10	117.70
64	Bp	147	VAL	CG1-CB-CG2	6.16	120.76	110.90
27	BA	2038	U	C2-N1-C1'	6.14	125.07	117.70
27	BA	1450	C	C2-N1-C1'	5.97	125.37	118.80
27	BA	2027	C	C2-N1-C1'	5.79	125.17	118.80
1	Aa	231	A	C2'-C3'-O3'	5.69	122.81	113.70
27	BA	2523	C	N3-C2-O2	-5.69	117.92	121.90
1	Aa	622	A	C4'-C3'-O3'	5.54	124.09	113.00
1	Aa	316	C	P-O3'-C3'	5.53	126.33	119.70
27	BA	2297	C	N3-C2-O2	-5.49	118.05	121.90
27	BA	128	U	C2'-C3'-O3'	5.43	122.39	113.70
27	BA	2273	C	N1-C2-O2	5.37	122.12	118.90
1	Aa	661	A	N9-C1'-C2'	-5.35	106.11	112.00
1	Aa	621	U	C4'-C3'-O3'	5.32	123.63	113.00
27	BA	1742	G	C2'-C3'-O3'	5.30	122.18	113.70
27	BA	2742	G	O4'-C1'-N9	5.27	112.42	108.20
1	Aa	700	C	C6-N1-C1'	-5.17	114.60	120.80
1	Aa	863	A	P-O3'-C3'	5.13	125.86	119.70
1	Aa	439	A	C4'-C3'-O3'	5.08	123.17	113.00
1	Aa	884	C	N1-C2-O2	5.07	121.94	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BA	2053	U	P-O3'-C3'	5.00	125.70	119.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	An	126	HIS	Peptide
14	An	127	ASP	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Aa	31531	0	16007	0	0
2	Ab	1580	0	1634	0	0
3	Ac	1536	0	1621	0	0
4	Ad	1550	0	1618	0	0
5	Ae	1454	0	1521	0	0
6	Af	1952	0	2035	0	0
7	Ag	1753	0	1822	0	0
8	Ah	952	0	997	0	0
9	Ai	1715	0	1779	0	0
10	Aj	1020	0	1066	0	0
11	Ak	982	0	1071	0	0
12	Al	1054	0	1105	0	0
13	Am	803	0	854	0	0
14	An	953	0	973	0	0
15	Ao	1122	0	1212	0	0
16	Ap	1090	0	1121	0	0
17	Aq	1217	0	1302	0	0
18	Ar	447	0	469	0	0
19	As	879	0	907	0	0
20	At	538	0	560	0	0
20	Bm	534	0	557	0	0
21	Au	952	0	1000	0	0
22	Av	1216	0	1236	0	0
23	Aw	777	0	797	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	Bn	752	0	767	0	0
24	Ax	461	0	492	0	0
25	Ay	499	0	528	0	0
26	Az	426	0	402	0	0
27	BA	63209	0	32023	474	0
28	BB	2678	0	1361	18	0
29	BC	1820	0	1902	14	0
30	BD	2746	0	2840	27	0
31	BE	2026	0	2128	26	0
32	BF	1339	0	1403	31	0
33	BG	1463	0	1520	12	0
34	BH	928	0	970	7	0
34	BI	928	0	970	12	0
35	BJ	1399	0	1426	11	0
36	BK	1146	0	1213	5	0
37	BL	1055	0	1134	6	0
38	BM	610	0	660	16	0
38	BN	610	0	660	11	0
39	BO	1166	0	1229	12	0
40	BP	1582	0	1677	8	0
41	BQ	1314	0	1359	20	0
42	BR	959	0	1018	11	0
43	BS	1200	0	1298	10	0
44	BT	624	0	647	0	0
45	BU	784	0	821	9	0
46	BV	1234	0	1274	7	0
47	BW	683	0	743	8	0
48	BX	991	0	1053	7	0
49	BY	524	0	512	5	0
50	BZ	506	0	559	1	0
51	Ba	1242	0	1332	0	0
52	Bb	730	0	768	0	0
53	Bc	721	0	776	0	0
54	Bd	1022	0	1106	0	0
55	Be	728	0	786	0	0
56	Bf	669	0	714	0	0
57	Bg	630	0	675	0	0
58	Bh	512	0	527	0	0
59	Bi	432	0	488	0	0
60	Bj	373	0	390	0	0
61	Bk	345	0	407	0	0
62	Bl	778	0	831	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	Bo	349	0	358	0	0
64	Bp	1862	0	1900	0	0
65	Bq	170	0	172	0	0
66	Ag	1	0	0	0	0
66	Ar	1	0	0	0	0
66	As	1	0	0	0	0
66	Ax	1	0	0	0	0
66	Az	2	0	0	0	0
66	BY	1	0	0	0	0
66	Be	2	0	0	0	0
66	Bg	1	0	0	0	0
66	Bh	1	0	0	0	0
66	Bj	1	0	0	0	0
66	Bl	1	0	0	0	0
66	Bo	1	0	0	0	0
67	Aa	266	0	0	0	0
67	Ad	1	0	0	0	0
67	Af	4	0	0	0	0
67	Ag	1	0	0	0	0
67	Ai	1	0	0	0	0
67	Aj	2	0	0	0	0
67	Ak	6	0	0	0	0
67	Al	2	0	0	0	0
67	Am	2	0	0	0	0
67	An	2	0	0	0	0
67	Ao	1	0	0	0	0
67	Ap	3	0	0	0	0
67	Aq	5	0	0	0	0
67	As	2	0	0	0	0
67	Au	1	0	0	0	0
67	Av	1	0	0	0	0
67	Az	1	0	0	0	0
67	BA	2715	0	0	170	0
67	BB	23	0	0	3	0
67	BC	51	0	0	1	0
67	BD	59	0	0	1	0
67	BE	41	0	0	7	0
67	BF	2	0	0	1	0
67	BG	1	0	0	0	0
67	BH	1	0	0	0	0
67	BJ	13	0	0	0	0
67	BK	18	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
67	BL	15	0	0	1	0
67	BM	3	0	0	2	0
67	BN	3	0	0	1	0
67	BO	30	0	0	1	0
67	BP	36	0	0	1	0
67	BQ	6	0	0	1	0
67	BR	14	0	0	0	0
67	BS	17	0	0	0	0
67	BT	2	0	0	0	0
67	BU	13	0	0	3	0
67	BV	22	0	0	0	0
67	BW	3	0	0	0	0
67	BX	10	0	0	1	0
67	BY	12	0	0	1	0
67	BZ	7	0	0	0	0
67	Ba	14	0	0	0	0
67	Bb	8	0	0	0	0
67	Bc	10	0	0	0	0
67	Bd	23	0	0	0	0
67	Be	8	0	0	0	0
67	Bf	7	0	0	0	0
67	Bg	15	0	0	0	0
67	Bh	23	0	0	0	0
67	Bi	10	0	0	0	0
67	Bj	3	0	0	0	0
67	Bk	3	0	0	0	0
67	Bl	8	0	0	0	0
67	Bm	1	0	0	0	0
67	Bn	1	0	0	0	0
67	Bo	4	0	0	0	0
All	All	167402	0	119083	723	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (723) 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)
27:BA:2678:G:OP1	67:BA:3101:HOH:O	1.68	1.09
27:BA:1478:A:OP2	67:BA:3102:HOH:O	1.75	1.04
27:BA:1137:A:OP2	67:BA:3104:HOH:O	1.83	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:1463:C:OP2	67:BA:3103:HOH:O	1.81	0.96
27:BA:168:G:N7	67:BA:3120:HOH:O	2.00	0.93
27:BA:1030:U:O2'	27:BA:1031:C:OP1	1.84	0.93
27:BA:1635:G:N2	27:BA:1653:A:N7	2.16	0.92
27:BA:341:C:H6	27:BA:341:C:H5'	1.34	0.92
27:BA:2318:G:OP1	27:BA:2318:G:N2	2.03	0.90
27:BA:489:G:OP2	67:BA:3105:HOH:O	1.90	0.88
29:BC:100:ALA:O	29:BC:134:ARG:NH2	2.06	0.88
27:BA:3023:C:H5"	27:BA:3023:C:H6	1.38	0.87
27:BA:1041:C:OP1	35:BJ:19:ARG:NH2	2.08	0.87
41:BQ:145:ASN:OD1	67:BQ:301:HOH:O	1.91	0.87
27:BA:2125:G:OP2	67:BA:3106:HOH:O	1.91	0.87
27:BA:2531:G:N7	67:BA:3161:HOH:O	2.07	0.86
27:BA:2744:G:N7	67:BA:3131:HOH:O	2.10	0.85
32:BF:87:MET:SD	32:BF:90:ARG:NH2	2.50	0.85
27:BA:1681:G:O6	27:BA:1685:G:N2	2.11	0.84
27:BA:1759:A:OP1	67:BA:3108:HOH:O	1.94	0.84
27:BA:348:A:N1	67:BA:3178:HOH:O	2.11	0.83
27:BA:2536:A:OP2	67:BA:3109:HOH:O	1.94	0.83
27:BA:2836:G:O2'	27:BA:2837:C:O5'	1.96	0.83
27:BA:1624:A:O2'	27:BA:1625:U:O5'	1.96	0.83
27:BA:189:C:OP2	67:BA:3110:HOH:O	1.96	0.83
27:BA:1178:A:O2'	27:BA:1179:G:O5'	1.96	0.82
31:BE:172:ARG:NH1	31:BE:195:LYS:O	2.12	0.82
27:BA:2556:C:N3	67:BA:3185:HOH:O	2.12	0.82
27:BA:2616:C:OP1	30:BD:9:ARG:NH1	2.12	0.82
27:BA:2835:A:O2'	27:BA:2836:G:O4'	1.96	0.82
27:BA:671:G:N7	67:BA:3186:HOH:O	2.13	0.81
27:BA:3033:C:N4	27:BA:3034:G:O6	2.12	0.81
28:BB:28:C:O2	28:BB:59:G:N2	2.13	0.81
27:BA:1008:U:O2'	27:BA:1009:U:O4'	1.99	0.81
27:BA:2586:A:OP2	67:BA:3112:HOH:O	1.98	0.81
27:BA:1390:U:OP1	67:BA:3111:HOH:O	1.97	0.81
27:BA:2987:G:O6	67:BA:3115:HOH:O	1.99	0.80
27:BA:1861:G:N7	67:BA:3191:HOH:O	2.14	0.80
27:BA:317:G:H8	27:BA:317:G:H5"	1.47	0.80
39:BO:82:ASP:OD2	42:BR:74:ARG:NH2	2.15	0.80
27:BA:1384:U:OP1	67:BA:3113:HOH:O	1.99	0.80
27:BA:857:C:OP2	67:BA:3114:HOH:O	1.99	0.79
27:BA:2693:A:OP1	67:BA:3117:HOH:O	2.00	0.79
27:BA:235:A:OP2	67:BA:3116:HOH:O	2.00	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:1520:G:O6	67:BA:3119:HOH:O	2.01	0.79
27:BA:1518:G:OP2	67:BA:3119:HOH:O	2.00	0.79
27:BA:856:C:OP1	67:BA:3122:HOH:O	2.01	0.78
27:BA:912:OMG:H5'	27:BA:913:G:OP1	1.82	0.78
27:BA:2576:G:N7	67:BA:3208:HOH:O	2.17	0.78
27:BA:833:OMG:N2	67:BA:3211:HOH:O	2.17	0.78
27:BA:1768:C:O2'	27:BA:1769:C:OP2	2.01	0.78
27:BA:1830:G:OP2	67:BA:3125:HOH:O	2.02	0.78
27:BA:1896:G:N7	67:BA:3203:HOH:O	2.16	0.78
27:BA:341:C:H5'	27:BA:341:C:C6	2.18	0.78
27:BA:1558:G:N7	38:BM:16:ARG:NH1	2.32	0.78
38:BM:46:ARG:NH2	67:BM:101:HOH:O	2.17	0.78
46:BV:71:GLN:OE1	46:BV:83:ARG:NH2	2.16	0.78
27:BA:231:U:O4	67:BA:3130:HOH:O	2.03	0.77
27:BA:1911:A:OP1	67:BA:3132:HOH:O	2.03	0.77
27:BA:2172:A:N7	67:BA:3213:HOH:O	2.17	0.77
28:BB:36:C:O2	41:BQ:148:HIS:NE2	2.17	0.77
27:BA:191:U:OP2	67:BA:3121:HOH:O	2.01	0.77
27:BA:236:G:N7	67:BA:3116:HOH:O	2.17	0.77
27:BA:1481:C:OP2	67:BA:3127:HOH:O	2.02	0.77
27:BA:1788:G:OP2	67:BA:3123:HOH:O	2.01	0.77
27:BA:959:G:OP2	67:BA:3126:HOH:O	2.02	0.77
27:BA:2053:U:O2'	27:BA:2054:C:OP2	2.00	0.77
27:BA:434:G:O2'	40:BP:91:SER:OG	2.02	0.76
31:BE:109:GLU:OE1	67:BE:301:HOH:O	2.03	0.76
27:BA:1397:G:N7	67:BA:3202:HOH:O	2.16	0.76
27:BA:629:G:N7	67:BA:3216:HOH:O	2.18	0.76
27:BA:341:C:H6	27:BA:341:C:C5'	1.97	0.76
27:BA:888:C:OP2	67:BA:3129:HOH:O	2.03	0.76
27:BA:636:U:OP2	34:BI:41:LYS:NZ	2.17	0.76
27:BA:1409:A:OP2	67:BA:3133:HOH:O	2.03	0.76
27:BA:2371:A:OP1	67:BA:3146:HOH:O	2.04	0.76
27:BA:2678:G:OP2	67:BA:3128:HOH:O	2.02	0.76
27:BA:1691:U:O2'	27:BA:1692:U:OP2	2.03	0.76
27:BA:2743:A:OP2	67:BA:3131:HOH:O	2.03	0.76
38:BM:8:ARG:NH2	38:BM:56:LEU:O	2.19	0.76
27:BA:823:G:N7	67:BA:3221:HOH:O	2.19	0.75
27:BA:1323:G:OP2	67:BA:3135:HOH:O	2.04	0.75
27:BA:1819:U:OP2	67:BA:3137:HOH:O	2.04	0.75
27:BA:2012:A:OP2	67:BA:3134:HOH:O	2.03	0.75
27:BA:2524:C:OP1	39:BO:61:ARG:NH2	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:2555:A:OP1	67:BA:3144:HOH:O	2.04	0.75
27:BA:1807:A:OP2	67:BA:3136:HOH:O	2.04	0.75
27:BA:1141:C:OP2	67:BA:3143:HOH:O	2.04	0.75
27:BA:1322:G:OP1	67:BA:3135:HOH:O	2.04	0.75
27:BA:1758:G:OP1	67:BA:3139:HOH:O	2.04	0.75
27:BA:2681:A:OP1	67:BA:3147:HOH:O	2.04	0.75
27:BA:3002:A:OP1	67:BA:3142:HOH:O	2.04	0.75
27:BA:195:A:OP1	67:BA:3141:HOH:O	2.04	0.75
27:BA:946:G:OP2	67:BA:3138:HOH:O	2.04	0.75
27:BA:1476:U:O2'	67:BA:3149:HOH:O	2.05	0.74
27:BA:1929:U:OP2	67:BA:3148:HOH:O	2.05	0.74
27:BA:2083:A:OP2	67:BA:3140:HOH:O	2.04	0.74
27:BA:507:OMG:HM22	27:BA:508:G:H5'	1.68	0.74
27:BA:1107:G:OP2	67:BA:3151:HOH:O	2.06	0.74
27:BA:3023:C:H5"	27:BA:3023:C:C6	2.20	0.74
48:BX:68:GLU:OE1	67:BX:201:HOH:O	2.05	0.74
27:BA:1824:A:OP2	67:BA:3150:HOH:O	2.06	0.74
27:BA:2865:G:OP2	67:BA:3154:HOH:O	2.07	0.73
27:BA:1945:G:OP1	29:BC:54:ARG:NH1	2.20	0.73
27:BA:1605:C:N3	67:BA:3227:HOH:O	2.20	0.73
27:BA:2850:A:OP2	67:BA:3153:HOH:O	2.06	0.73
27:BA:921:A:OP1	67:BA:3155:HOH:O	2.07	0.72
27:BA:1901:A:OP1	27:BA:1956:OMG:HM22	1.88	0.72
43:BS:81:LYS:HG2	43:BS:88:ARG:NH1	2.04	0.72
27:BA:120:U:OP1	50:BZ:63:ARG:NH1	2.23	0.72
27:BA:2603:C:OP2	67:BA:3157:HOH:O	2.07	0.72
36:BK:94:PHE:O	67:BK:201:HOH:O	2.08	0.72
27:BA:371:A:OP1	31:BE:191:TYR:OH	2.06	0.72
27:BA:2216:G:O2'	27:BA:2217:G:O4'	2.08	0.72
30:BD:273:GLU:HA	30:BD:301:ASP:OD1	1.90	0.72
40:BP:117:TYR:OH	40:BP:129:GLU:OE1	2.06	0.72
27:BA:905:G:OP2	67:BA:3160:HOH:O	2.07	0.71
27:BA:1812:A:OP2	67:BA:3152:HOH:O	2.06	0.71
28:BB:102:G:N7	67:BB:201:HOH:O	2.22	0.71
27:BA:585:G:OP2	67:BA:3156:HOH:O	2.07	0.71
27:BA:51:G:N2	27:BA:52:G:O6	2.24	0.71
39:BO:24:LYS:O	67:BO:201:HOH:O	2.08	0.71
27:BA:1564:G:OP1	67:BA:3168:HOH:O	2.09	0.71
27:BA:871:G:OP1	67:BA:3170:HOH:O	2.09	0.71
27:BA:2505:G:O6	67:BA:3159:HOH:O	2.07	0.71
27:BA:1498:G:OP2	67:BA:3158:HOH:O	2.07	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:2750:G:OP2	30:BD:324:ARG:NH2	2.24	0.71
27:BA:1153:U:O2'	27:BA:1158:C:N4	2.24	0.71
27:BA:2679:U:OP2	67:BA:3101:HOH:O	2.09	0.71
27:BA:492:A:OP2	67:BA:3163:HOH:O	2.08	0.70
27:BA:2642:OMG:HM22	27:BA:2642:OMG:H4'	1.71	0.70
27:BA:1956:OMG:OP2	67:BA:3169:HOH:O	2.09	0.70
27:BA:451:C:OP1	67:BA:3164:HOH:O	2.08	0.70
31:BE:233:GLY:O	31:BE:234:THR:OG1	2.09	0.70
27:BA:2345:U:OP1	67:BA:3165:HOH:O	2.09	0.70
27:BA:2674:G:N7	67:BA:3253:HOH:O	2.24	0.70
31:BE:156:GLN:OE1	67:BE:302:HOH:O	2.10	0.70
27:BA:814:U:O2	67:BA:3172:HOH:O	2.10	0.70
27:BA:2393:G:N7	67:BA:3262:HOH:O	2.25	0.70
27:BA:2696:G:OP1	67:BA:3167:HOH:O	2.09	0.70
27:BA:757:G:OP2	67:BA:3171:HOH:O	2.09	0.69
27:BA:2094:A:OP2	67:BA:3175:HOH:O	2.10	0.69
27:BA:492:A:OP1	67:BA:3177:HOH:O	2.10	0.69
27:BA:153:A:N1	67:BA:3120:HOH:O	2.26	0.69
27:BA:1945:G:O6	67:BA:3162:HOH:O	2.08	0.69
27:BA:630:G:N7	67:BA:3256:HOH:O	2.24	0.69
27:BA:2959:U:O2	30:BD:106:LYS:NZ	2.25	0.69
27:BA:1081:G:N7	67:BA:3257:HOH:O	2.24	0.69
27:BA:770:A:N7	67:BA:3254:HOH:O	2.24	0.69
27:BA:2216:G:O2'	27:BA:2217:G:O5'	2.10	0.68
27:BA:2516:G:O6	67:BA:3176:HOH:O	2.10	0.68
27:BA:1392:C:OP2	67:BA:3173:HOH:O	2.10	0.68
27:BA:2490:G:OP1	67:BA:3174:HOH:O	2.10	0.68
31:BE:190:ARG:O	67:BE:303:HOH:O	2.11	0.68
27:BA:36:G:OP2	67:BA:3179:HOH:O	2.11	0.68
27:BA:1482:G:OP2	67:BA:3127:HOH:O	2.11	0.68
27:BA:2021:G:N2	27:BA:2037:C:O2	2.27	0.68
27:BA:2427:5MU:H3'	27:BA:2428:G:H5"	1.74	0.68
28:BB:99:G:N7	67:BB:202:HOH:O	2.25	0.68
27:BA:1470:C:OP2	67:BA:3181:HOH:O	2.12	0.67
27:BA:548:U:OP2	67:BA:3183:HOH:O	2.12	0.67
27:BA:37:A:N1	67:BA:3274:HOH:O	2.28	0.67
27:BA:2986:G:OP2	67:BA:3180:HOH:O	2.11	0.67
45:BU:96:GLN:OE1	67:BU:101:HOH:O	2.11	0.67
27:BA:2462:C:OP2	67:BA:3188:HOH:O	2.13	0.67
27:BA:188:A:OP1	67:BA:3110:HOH:O	2.12	0.67
27:BA:1950:G:N7	67:BA:3277:HOH:O	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:670:OMG:H4'	27:BA:670:OMG:HM22	1.75	0.66
41:BQ:116:SER:O	41:BQ:120:VAL:HG23	1.95	0.66
27:BA:2482:A:O2'	27:BA:2483:A:OP1	2.12	0.66
27:BA:2685:G:N7	67:BA:3268:HOH:O	2.27	0.66
27:BA:2571:C:H2'	27:BA:2572:G:O4'	1.96	0.66
32:BF:22:ILE:HD12	32:BF:85:TYR:CE1	2.31	0.66
27:BA:1136:A:OP2	67:BA:3104:HOH:O	2.12	0.66
38:BM:8:ARG:NH2	38:BM:58:GLU:O	2.27	0.66
27:BA:2596:U:OP1	67:BA:3192:HOH:O	2.14	0.66
41:BQ:66:GLU:OE1	41:BQ:69:ARG:NH1	2.29	0.66
27:BA:693:G:N7	42:BR:85:LYS:NZ	2.43	0.65
27:BA:659:U:OP1	67:BA:3195:HOH:O	2.15	0.65
27:BA:2665:A:N7	67:BA:3276:HOH:O	2.28	0.65
27:BA:2160:G:OP1	67:BA:3196:HOH:O	2.15	0.65
27:BA:55:5MC:HM52	27:BA:205:G:C8	2.32	0.65
27:BA:2048:G:O6	67:BA:3182:HOH:O	2.12	0.65
27:BA:2817:G:OP2	67:BA:3193:HOH:O	2.14	0.65
31:BE:71:GLU:OE2	67:BE:304:HOH:O	2.14	0.65
38:BN:45:ARG:NH2	38:BN:66:ALA:O	2.30	0.65
49:BY:33:CYS:SG	67:BY:212:HOH:O	2.28	0.65
38:BM:4:ILE:O	38:BM:4:ILE:HG22	1.97	0.65
27:BA:1398:G:O6	67:BA:3189:HOH:O	2.13	0.64
27:BA:1180:A:H2	27:BA:2853:G:H22	1.45	0.64
27:BA:1818:C:OP1	67:BA:3137:HOH:O	2.15	0.64
27:BA:1408:C:OP2	67:BA:3133:HOH:O	2.15	0.64
27:BA:2799:G:N7	67:BA:3284:HOH:O	2.29	0.64
31:BE:33:ARG:NH1	67:BE:301:HOH:O	2.29	0.64
27:BA:2369:A:OP2	67:BA:3194:HOH:O	2.14	0.64
27:BA:1747:U:O4	67:BA:3102:HOH:O	2.13	0.64
31:BE:103:GLU:OE1	67:BE:305:HOH:O	2.15	0.64
27:BA:1362:G:N7	67:BA:3290:HOH:O	2.30	0.64
27:BA:160:G:O2'	27:BA:161:U:O4'	2.16	0.64
33:BG:143:ASP:O	33:BG:147:VAL:HG23	1.98	0.64
41:BQ:118:PHE:CD1	41:BQ:137:ILE:HD12	2.34	0.63
27:BA:55:5MC:HM52	27:BA:205:G:H8	1.62	0.63
27:BA:787:U:O4	67:BA:3166:HOH:O	2.09	0.63
48:BX:87:ASP:OD1	48:BX:88:GLY:N	2.31	0.63
35:BJ:19:ARG:NH1	35:BJ:21:GLU:OE2	2.32	0.63
27:BA:1776:OMU:H2'	27:BA:1777:G:O4'	1.99	0.63
45:BU:46:GLU:OE2	45:BU:48:SER:OG	2.16	0.63
27:BA:1412:G:OP1	67:BA:3197:HOH:O	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:2031:A:N3	27:BA:2032:A:N6	2.46	0.62
27:BA:1468:G:OP1	67:BA:3199:HOH:O	2.16	0.62
35:BJ:82:TYR:O	35:BJ:82:TYR:CD1	2.52	0.62
41:BQ:112:THR:OG1	41:BQ:115:SER:OG	2.16	0.62
27:BA:1002:G:O2'	27:BA:1003:G:O5'	2.16	0.62
36:BK:9:LEU:HD22	36:BK:118:ALA:O	2.00	0.62
27:BA:36:G:O2'	27:BA:37:A:OP2	2.13	0.62
27:BA:719:C:O2'	27:BA:783:U:OP1	2.15	0.62
27:BA:1624:A:HO2'	27:BA:1625:U:C5'	2.10	0.62
27:BA:2412:G:O2'	27:BA:2413:A:O4'	2.14	0.61
29:BC:31:VAL:HG12	29:BC:69:LYS:HE3	1.81	0.61
27:BA:1665:G:O6	67:BA:3187:HOH:O	2.13	0.61
34:BI:63:VAL:HG13	34:BI:66:LEU:HD12	1.81	0.61
27:BA:1671:A:H1'	27:BA:1672:U:OP2	2.00	0.61
27:BA:1945:G:OP2	29:BC:29:ARG:NH2	2.32	0.61
27:BA:670:OMG:O3'	27:BA:670:OMG:HM23	1.99	0.60
28:BB:51:G:N3	67:BB:203:HOH:O	2.31	0.60
27:BA:1849:A:O3'	27:BA:1893:OMG:HM21	2.02	0.60
27:BA:611:G:N7	38:BN:16:ARG:NH1	2.49	0.60
27:BA:1532:U:OP1	67:BA:3205:HOH:O	2.17	0.60
32:BF:42:GLU:OE1	67:BF:201:HOH:O	2.16	0.60
27:BA:968:G:HO2'	42:BR:2:VAL:N	2.00	0.59
43:BS:81:LYS:HG2	43:BS:88:ARG:HH12	1.67	0.59
27:BA:317:G:H5"	27:BA:317:G:C8	2.34	0.59
27:BA:1150:OMU:OP2	67:BA:3209:HOH:O	2.17	0.59
27:BA:1670:A:H1'	27:BA:1671:A:OP2	2.03	0.59
27:BA:2078:C:N3	67:BA:3298:HOH:O	2.31	0.59
31:BE:180:ARG:NE	31:BE:189:ARG:O	2.36	0.59
27:BA:248:A:OP2	67:BA:3200:HOH:O	2.16	0.59
27:BA:2534:A:O2'	27:BA:2535:G:OP2	2.20	0.59
32:BF:45:LEU:O	32:BF:49:VAL:HG22	2.01	0.59
27:BA:196:G:OP2	67:BA:3210:HOH:O	2.17	0.59
30:BD:269:ILE:HD11	30:BD:306:GLU:CG	2.33	0.59
27:BA:2642:OMG:O3'	27:BA:2642:OMG:HM23	2.03	0.59
39:BO:79:ASN:OD1	39:BO:80:ASP:N	2.35	0.59
27:BA:1949:U:OP2	67:BA:3204:HOH:O	2.17	0.58
27:BA:3023:C:C6	27:BA:3023:C:C5'	2.85	0.58
45:BU:89:HIS:ND1	45:BU:91:VAL:HG23	2.18	0.58
30:BD:269:ILE:HD11	30:BD:306:GLU:HG2	1.84	0.58
32:BF:57:ARG:NE	32:BF:70:GLY:O	2.34	0.58
45:BU:9:ARG:NH1	67:BU:102:HOH:O	2.30	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:1916:C:OP2	67:BA:3207:HOH:O	2.17	0.58
27:BA:2464:G:OP2	67:BA:3188:HOH:O	2.17	0.58
27:BA:2580:A:H2'	27:BA:2581:4SU:O4'	2.02	0.58
28:BB:40:U:O2'	28:BB:45:A:N6	2.36	0.58
27:BA:285:U:O4	67:BA:3206:HOH:O	2.17	0.57
27:BA:1560:C:OP1	38:BM:47:ARG:NH1	2.37	0.57
27:BA:147:U:H5"	27:BA:148:G:OP2	2.04	0.57
27:BA:1672:U:OP2	27:BA:1672:U:H4'	2.02	0.57
27:BA:1030:U:HO2'	27:BA:1031:C:P	2.26	0.57
27:BA:1381:U:OP1	39:BO:3:ARG:NH1	2.37	0.57
67:BA:3196:HOH:O	46:BV:70:SER:OG	2.15	0.57
32:BF:28:ASN:OD1	32:BF:29:ILE:N	2.37	0.57
27:BA:569:G:N7	67:BA:3303:HOH:O	2.32	0.57
31:BE:142:LEU:HD22	31:BE:241:ILE:HG23	1.85	0.57
45:BU:89:HIS:CE1	45:BU:91:VAL:HG23	2.39	0.57
27:BA:2069:G:H3'	27:BA:2070:5MC:HM51	1.87	0.57
27:BA:2042:G:OP2	27:BA:2042:G:N2	2.32	0.56
34:BI:39:THR:HG23	34:BI:100:ALA:HB2	1.87	0.56
27:BA:564:U:OP1	67:BA:3214:HOH:O	2.17	0.56
37:BL:84:ARG:NH2	37:BL:121:ALA:O	2.39	0.56
27:BA:2436:A:H5'	27:BA:2438:A:H1'	1.87	0.56
31:BE:123:ASN:OD1	31:BE:124:TYR:N	2.39	0.56
27:BA:2227:G:O2'	27:BA:2229:G:N7	2.24	0.56
35:BJ:163:ARG:NH2	35:BJ:173:THR:HG21	2.20	0.56
27:BA:1943:U:OP1	67:BA:3212:HOH:O	2.17	0.56
46:BV:153:GLU:OE1	46:BV:155:ARG:NH2	2.39	0.55
29:BC:36:VAL:HG12	29:BC:36:VAL:O	2.07	0.55
30:BD:111:ARG:HD2	30:BD:159:LYS:HE3	1.89	0.55
41:BQ:113:ARG:NH1	41:BQ:138:TYR:O	2.31	0.55
27:BA:2252:G:N1	27:BA:2264:G:O6	2.40	0.55
27:BA:507:OMG:HM23	31:BE:75:THR:OG1	2.07	0.55
27:BA:2482:A:HO2'	27:BA:2483:A:P	2.28	0.55
38:BM:2:PRO:O	67:BM:102:HOH:O	2.18	0.54
38:BN:70:GLU:N	38:BN:70:GLU:OE1	2.41	0.54
27:BA:2427:5MU:H3'	27:BA:2428:G:C5'	2.35	0.54
27:BA:1671:A:H4'	27:BA:1672:U:O5'	2.07	0.54
37:BL:74:ARG:NH1	67:BL:201:HOH:O	2.30	0.54
27:BA:55:5MC:HM51	27:BA:205:G:H3'	1.90	0.54
27:BA:932:A2M:HM'2	27:BA:934:C:C6	2.43	0.54
27:BA:2687:G:OP2	67:BA:3215:HOH:O	2.18	0.54
27:BA:303:U:H1'	27:BA:304:A:OP2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:2573:A:N6	27:BA:2585:G:O2'	2.39	0.54
27:BA:452:A:OP2	67:BA:3164:HOH:O	2.18	0.54
27:BA:1134:C:OP1	67:BA:3217:HOH:O	2.18	0.54
46:BV:70:SER:OG	46:BV:70:SER:O	2.25	0.54
27:BA:434:G:HO2'	40:BP:91:SER:HG	1.51	0.54
27:BA:2527:OMG:HM22	27:BA:2528:OMG:H5'	1.90	0.54
41:BQ:43:HIS:ND1	41:BQ:64:THR:OG1	2.33	0.53
27:BA:315:A:H2'	27:BA:316:G:C8	2.43	0.53
27:BA:2239:G:O2'	27:BA:2240:G:P	2.66	0.53
27:BA:257:G:O2'	67:BA:3107:HOH:O	1.92	0.53
27:BA:1469:C:OP2	67:BA:3219:HOH:O	2.18	0.53
27:BA:1907:U:OP2	27:BA:1912:A:N6	2.38	0.53
27:BA:1624:A:O2'	27:BA:1625:U:O4'	2.27	0.53
45:BU:61:ARG:NH2	67:BU:103:HOH:O	2.40	0.53
33:BG:90:LEU:HD23	33:BG:174:ILE:HA	1.91	0.53
27:BA:2215:G:N1	27:BA:2216:G:O6	2.41	0.53
27:BA:872:OMG:HN1	27:BA:881:U:H3	1.57	0.53
27:BA:2297:C:H2'	27:BA:2298:U:N1	2.23	0.53
27:BA:2829:C:OP1	67:BA:3223:HOH:O	2.19	0.53
27:BA:2836:G:HO2'	27:BA:2837:C:C5'	2.16	0.52
34:BI:6:TYR:OH	34:BI:55:GLU:O	2.22	0.52
28:BB:52:A:O2'	28:BB:53:A:O5'	2.22	0.52
27:BA:2571:C:O2'	27:BA:2572:G:O5'	2.19	0.52
38:BN:4:ILE:HG22	38:BN:4:ILE:O	2.09	0.52
41:BQ:8:ARG:NE	45:BU:22:ARG:O	2.42	0.52
27:BA:437:G:OP2	40:BP:68:ARG:NH2	2.42	0.52
38:BN:22:VAL:HA	38:BN:37:GLY:HA2	1.90	0.52
27:BA:1685:G:O6	43:BS:46:HIS:NE2	2.40	0.52
27:BA:2533:C:OP1	67:BA:3218:HOH:O	2.18	0.52
27:BA:2891:A:O2'	27:BA:3026:G:N2	2.39	0.52
31:BE:123:ASN:O	31:BE:127:VAL:HG23	2.09	0.52
34:BH:61:GLU:OE1	34:BH:61:GLU:N	2.38	0.52
27:BA:2025:A:H62	27:BA:2030:U:H3	1.57	0.52
27:BA:2496:C:O2'	67:BA:3145:HOH:O	2.04	0.51
27:BA:2882:C:H2'	27:BA:2882:C:O2	2.10	0.51
32:BF:25:VAL:CG2	32:BF:84:ALA:HB1	2.40	0.51
27:BA:314:G:H2'	27:BA:315:A:O4'	2.10	0.51
27:BA:404:G:O2'	27:BA:405:U:P	2.69	0.51
34:BH:10:GLU:O	34:BH:121:LEU:HD21	2.10	0.51
27:BA:341:C:C6	27:BA:341:C:C5'	2.85	0.51
27:BA:1178:A:HO2'	27:BA:1179:G:P	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:2562:C:OP2	67:BA:3220:HOH:O	2.19	0.51
28:BB:52:A:HO2'	28:BB:53:A:P	2.33	0.51
29:BC:85:ILE:HG23	29:BC:96:THR:HB	1.93	0.51
37:BL:108:THR:HG22	37:BL:109:PRO:HD2	1.92	0.51
38:BM:22:VAL:HG11	38:BM:35:VAL:CG1	2.40	0.51
27:BA:482:A:O2'	27:BA:1336:C:O2'	2.12	0.51
34:BI:32:ILE:HG22	34:BI:33:ARG:N	2.26	0.51
47:BW:11:LEU:HD12	47:BW:27:THR:HG22	1.92	0.51
27:BA:661:G:O6	67:BA:3201:HOH:O	2.16	0.51
27:BA:879:A2M:OP1	67:BA:3108:HOH:O	2.19	0.51
27:BA:1660:U:H2'	27:BA:1661:G:O4'	2.11	0.51
33:BG:155:GLU:OE2	33:BG:174:ILE:N	2.34	0.51
47:BW:12:VAL:HG13	47:BW:12:VAL:O	2.11	0.51
27:BA:2835:A:C2'	27:BA:2836:G:O4'	2.58	0.51
27:BA:2469:OMG:H8	27:BA:2469:OMG:H5"	1.76	0.51
29:BC:108:VAL:CG1	29:BC:157:ALA:HB1	2.41	0.51
27:BA:2268:G:H4'	27:BA:2269:G:OP1	2.11	0.50
30:BD:278:VAL:O	30:BD:334:ARG:NH2	2.44	0.50
40:BP:157:ARG:HA	40:BP:162:LEU:HD12	1.92	0.50
27:BA:317:G:C8	27:BA:317:G:C5'	2.94	0.50
27:BA:920:G:OP2	67:BA:3224:HOH:O	2.19	0.50
27:BA:2745:OMG:HM22	27:BA:2746:G:H5'	1.93	0.50
27:BA:2892:C:O2'	27:BA:3027:U:OP1	2.28	0.50
27:BA:997:U:H2'	27:BA:998:G:O4'	2.11	0.50
41:BQ:106:ILE:HD12	41:BQ:117:ILE:HG21	1.92	0.50
40:BP:144:PRO:O	67:BP:201:HOH:O	2.18	0.50
27:BA:1691:U:HO2'	27:BA:1692:U:P	2.28	0.50
27:BA:2936:A2M:H5'	67:BA:5614:HOH:O	2.11	0.50
27:BA:365:OMG:HM22	27:BA:366:G:H5'	1.93	0.50
27:BA:621:G:N7	67:BA:3308:HOH:O	2.33	0.50
48:BX:96:HIS:CE1	48:BX:98:SER:HG	2.27	0.50
32:BF:49:VAL:HG23	32:BF:50:GLY:N	2.26	0.50
27:BA:1759:A:N6	46:BV:136:ARG:O	2.45	0.50
30:BD:61:THR:HG22	30:BD:61:THR:O	2.12	0.50
30:BD:45:LYS:O	30:BD:313:PHE:O	2.30	0.49
27:BA:45:G:OP2	67:BA:3225:HOH:O	2.20	0.49
27:BA:1670:A:O2'	27:BA:1671:A:OP2	2.29	0.49
27:BA:687:A:H2'	27:BA:688:G:C8	2.47	0.49
27:BA:2176:C:H2'	27:BA:2177:C:C6	2.47	0.49
39:BO:32:GLY:O	39:BO:45:GLN:NE2	2.46	0.49
27:BA:1358:G:N2	27:BA:1360:G:H3'	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:2000:U:H2'	27:BA:2001:G:O4'	2.12	0.49
27:BA:2550:OMG:HM22	27:BA:2605:5MC:CM5	2.42	0.49
30:BD:292:PHE:O	30:BD:295:TYR:O	2.31	0.49
32:BF:104:PHE:CD1	32:BF:110:PHE:HB3	2.48	0.49
34:BI:18:LYS:HD2	34:BI:110:LEU:HD12	1.94	0.49
27:BA:2758:C:OP2	37:BL:2:ALA:N	2.46	0.49
38:BN:46:ARG:NH2	67:BN:101:HOH:O	2.29	0.49
27:BA:636:U:H2'	27:BA:637:G:O4'	2.12	0.49
27:BA:2252:G:N2	27:BA:2253:C:H41	2.10	0.49
27:BA:1910:U:OP1	67:BA:3226:HOH:O	2.20	0.48
47:BW:38:ASP:OD1	47:BW:41:ARG:NH1	2.46	0.48
27:BA:968:G:O2'	42:BR:2:VAL:N	2.46	0.48
27:BA:2529:A:O2'	27:BA:2530:U:OP2	2.22	0.48
41:BQ:67:LEU:HD23	41:BQ:89:LEU:HD11	1.95	0.48
27:BA:1565:C:O2	67:BA:3198:HOH:O	2.16	0.48
31:BE:29:ASP:OD1	31:BE:30:LEU:N	2.46	0.48
27:BA:2312:C:H6	27:BA:2312:C:O5'	1.95	0.48
27:BA:2571:C:O2'	27:BA:2572:G:P	2.72	0.48
27:BA:2252:G:O2'	27:BA:2253:C:O5'	2.30	0.48
27:BA:2260:G:O2'	27:BA:2261:G:O4'	2.26	0.48
29:BC:104:GLU:OE1	29:BC:104:GLU:N	2.44	0.48
34:BI:63:VAL:HG12	34:BI:63:VAL:O	2.13	0.48
42:BR:65:VAL:HG12	42:BR:67:GLY:H	1.78	0.48
27:BA:687:A:O2'	27:BA:688:G:P	2.72	0.48
32:BF:25:VAL:HG21	32:BF:84:ALA:HB1	1.96	0.48
27:BA:690:G:O2'	67:BE:301:HOH:O	2.04	0.48
27:BA:1773:G:N2	43:BS:58:GLN:OE1	2.46	0.48
27:BA:2038:U:H2'	27:BA:2038:U:O2	2.13	0.47
28:BB:56:U:H4'	28:BB:57:A:O5'	2.14	0.47
29:BC:185:ARG:O	29:BC:187:ARG:N	2.45	0.47
30:BD:84:ARG:NE	30:BD:98:GLU:OE2	2.47	0.47
41:BQ:104:LEU:HD21	41:BQ:106:ILE:HD11	1.95	0.47
42:BR:33:ASP:HA	42:BR:36:TRP:CD1	2.49	0.47
27:BA:527:G:N2	27:BA:530:A:OP2	2.45	0.47
27:BA:2482:A:O2'	27:BA:2483:A:P	2.72	0.47
46:BV:47:ASP:OD1	46:BV:50:ARG:NH2	2.42	0.47
27:BA:588:U:H3'	27:BA:589:G:H5'	1.97	0.47
34:BI:25:ILE:O	34:BI:29:THR:HG22	2.15	0.47
27:BA:598:C:H2'	27:BA:599:G:O4'	2.15	0.47
27:BA:1463:C:H2'	27:BA:1464:G:O4'	2.14	0.47
27:BA:1681:G:N2	27:BA:1684:A:H61	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:2252:G:HO2'	27:BA:2253:C:C5'	2.28	0.47
67:BA:4123:HOH:O	39:BO:9:ARG:HD3	2.15	0.47
38:BN:26:ASP:OD1	38:BN:27:ILE:N	2.48	0.47
27:BA:670:OMG:H5'	27:BA:2131:U:H5"	1.97	0.47
27:BA:657:OMU:H2'	27:BA:658:C:C6	2.50	0.47
27:BA:1353:G:OP1	67:BA:3229:HOH:O	2.20	0.47
27:BA:1411:A:OP2	67:BA:3230:HOH:O	2.20	0.47
27:BA:2267:U:O2	27:BA:2267:U:H2'	2.14	0.47
27:BA:1928:C:H1'	27:BA:1929:U:OP2	2.14	0.47
27:BA:1691:U:O2'	27:BA:1692:U:P	2.73	0.47
27:BA:2176:C:H2'	27:BA:2177:C:H6	1.79	0.47
38:BM:70:GLU:OE1	38:BM:70:GLU:N	2.44	0.47
27:BA:996:C:OP2	67:BA:3231:HOH:O	2.21	0.46
27:BA:2297:C:H2'	27:BA:2298:U:C6	2.50	0.46
27:BA:2250:C:H2'	27:BA:2251:C:C6	2.50	0.46
28:BB:45:A:OP1	32:BF:80:ARG:NH1	2.48	0.46
38:BM:22:VAL:HG11	38:BM:35:VAL:HG13	1.96	0.46
27:BA:1462:U:H5'	27:BA:2124:OMC:HM23	1.96	0.46
27:BA:1671:A:C1'	27:BA:1672:U:OP2	2.64	0.46
32:BF:23:ALA:HB3	32:BF:139:THR:HG23	1.96	0.46
39:BO:41:LYS:O	39:BO:42:ARG:HG2	2.15	0.46
33:BG:143:ASP:OD1	33:BG:146:ALA:HB3	2.15	0.46
34:BH:86:LEU:HD21	34:BH:99:VAL:HG23	1.98	0.46
47:BW:3:PRO:O	47:BW:4:TYR:HB2	2.14	0.46
27:BA:670:OMG:O3'	27:BA:670:OMG:CM2	2.62	0.46
27:BA:1672:U:O2'	27:BA:1673:G:OP2	2.30	0.46
27:BA:2642:OMG:H4'	27:BA:2642:OMG:CM2	2.41	0.46
32:BF:95:VAL:HG11	32:BF:114:ILE:HG22	1.97	0.46
38:BM:27:ILE:HG12	38:BM:33:VAL:HG12	1.98	0.46
43:BS:4:LEU:HA	43:BS:7:GLN:OE1	2.16	0.46
45:BU:31:PHE:HA	45:BU:91:VAL:HG22	1.97	0.46
27:BA:2124:OMC:HM23	27:BA:2124:OMC:H1'	1.52	0.46
27:BA:730:C:H2'	27:BA:731:G:O4'	2.16	0.46
27:BA:2394:U:OP1	27:BA:2486:C:O2'	2.34	0.46
42:BR:12:LEU:HG	42:BR:84:TRP:CZ2	2.50	0.46
27:BA:544:A:N3	67:BA:3340:HOH:O	2.36	0.46
27:BA:149:C:H2'	27:BA:150:C:C6	2.51	0.46
27:BA:1329:OMG:HM22	27:BA:1330:G:O4'	2.16	0.46
27:BA:14:G:H2'	27:BA:15:U:O4'	2.15	0.45
27:BA:2640:OMG:H1'	27:BA:2640:OMG:HM23	1.67	0.45
31:BE:33:ARG:NH1	31:BE:109:GLU:OE1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BF:104:PHE:HE2	32:BF:169:ILE:HA	1.80	0.45
34:BI:29:THR:HG23	34:BI:30:GLY:N	2.31	0.45
48:BX:48:VAL:O	48:BX:66:VAL:HB	2.15	0.45
27:BA:657:OMU:H1'	27:BA:657:OMU:HM23	1.55	0.45
27:BA:1979:U:H2'	27:BA:1980:G:O4'	2.16	0.45
27:BA:2107:OMC:OP2	67:BA:3234:HOH:O	2.21	0.45
27:BA:2958:U:C3'	27:BA:2959:U:H5'	2.45	0.45
27:BA:2035:C:H2'	27:BA:2036:U:O4'	2.16	0.45
27:BA:2338:U:H2'	27:BA:2339:G:O4'	2.17	0.45
37:BL:98:LYS:NZ	49:BY:38:GLU:OE2	2.43	0.45
38:BM:4:ILE:O	38:BM:4:ILE:CG2	2.64	0.45
27:BA:231:U:OP1	67:BA:3233:HOH:O	2.21	0.45
27:BA:1002:G:O2'	27:BA:1003:G:P	2.74	0.45
27:BA:1864:U:H2'	27:BA:1865:G:O4'	2.17	0.45
27:BA:2876:C:H2'	27:BA:2877:G:O4'	2.17	0.45
27:BA:712:C:OP2	31:BE:110:ARG:NH1	2.49	0.45
27:BA:1145:C:OP1	33:BG:61:ARG:NH2	2.49	0.45
27:BA:3034:G:H2'	27:BA:3035:G:O4'	2.16	0.45
27:BA:1242:G:N3	27:BA:1242:G:H2'	2.31	0.45
27:BA:1969:OMU:H2'	27:BA:1970:G:O4'	2.17	0.45
35:BJ:33:ILE:HG22	35:BJ:36:MET:SD	2.57	0.45
46:BV:22:SER:OG	46:BV:24:ARG:NE	2.49	0.45
27:BA:1750:C:H2'	27:BA:1751:G:O4'	2.16	0.45
27:BA:2220:G:H2'	27:BA:2221:U:O4'	2.17	0.45
27:BA:2642:OMG:CM2	27:BA:2642:OMG:C4'	2.95	0.45
28:BB:4:A:H2	28:BB:22:G:H21	1.63	0.45
38:BN:22:VAL:HB	38:BN:35:VAL:HG22	1.98	0.45
27:BA:1524:C:OP1	67:BA:3235:HOH:O	2.21	0.45
27:BA:2650:U:OP1	67:BA:3232:HOH:O	2.21	0.45
32:BF:176:LEU:O	32:BF:177:LYS:CG	2.64	0.45
34:BH:93:GLU:OE1	34:BH:93:GLU:N	2.50	0.45
27:BA:42:U:OP2	31:BE:186:MET:HG2	2.18	0.45
27:BA:699:A:H2'	27:BA:700:A:C8	2.52	0.45
27:BA:2171:A:H2'	27:BA:2172:A:O4'	2.17	0.45
27:BA:2219:G:N1	27:BA:2295:C:O2	2.50	0.45
27:BA:2231:A:H3'	27:BA:2232:G:H5"	1.98	0.45
30:BD:244:ALA:O	30:BD:245:ARG:HG3	2.17	0.45
27:BA:974:A:H1'	27:BA:975:G:OP2	2.17	0.44
27:BA:2642:OMG:HM22	27:BA:2642:OMG:C4'	2.44	0.44
42:BR:23:SER:OG	42:BR:28:VAL:O	2.31	0.44
27:BA:739:C:H2'	27:BA:740:G:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:1337:C:H5”	31:BE:189:ARG:HD3	1.98	0.44
27:BA:1360:G:H2’	27:BA:1361:A:C8	2.52	0.44
27:BA:1882:C:N3	27:BA:2819:C:O2’	2.51	0.44
27:BA:1993:A:H2’	27:BA:1994:A:O4’	2.17	0.44
27:BA:2039:U:H3	27:BA:2042:G:H22	1.65	0.44
27:BA:2412:G:H2’	27:BA:2413:A:C8	2.51	0.44
33:BG:5:ALA:O	33:BG:58:GLU:O	2.34	0.44
27:BA:1014:G:H22	27:BA:1024:U:H3	1.66	0.44
27:BA:1482:G:O2’	27:BA:1516:A:N3	2.45	0.44
27:BA:2420:C:H2’	27:BA:2421:G:O4’	2.18	0.44
32:BF:176:LEU:O	32:BF:177:LYS:HG2	2.17	0.44
35:BJ:18:THR:O	35:BJ:19:ARG:CG	2.65	0.44
42:BR:7:PRO:O	42:BR:13:ARG:NE	2.50	0.44
27:BA:2053:U:C2’	27:BA:2054:C:OP2	2.65	0.44
32:BF:68:ARG:HD2	32:BF:71:GLU:HB3	1.99	0.44
32:BF:142:ARG:HB3	32:BF:143:PRO:HD2	1.99	0.44
39:BO:122:ALA:HB1	39:BO:142:GLY:O	2.18	0.44
43:BS:9:ARG:HG3	43:BS:10:ILE:N	2.31	0.44
30:BD:151:PRO:O	30:BD:154:ILE:O	2.35	0.44
31:BE:82:PHE:O	31:BE:82:PHE:CD1	2.71	0.44
32:BF:166:GLU:HA	32:BF:169:ILE:HD12	1.99	0.44
27:BA:808:U:H3	27:BA:923:G:H1	1.66	0.44
27:BA:2159:C:O2’	27:BA:2949:A:N1	2.45	0.44
27:BA:2263:C:H2’	27:BA:2264:G:C8	2.53	0.44
30:BD:5:HIS:NE2	67:BD:402:HOH:O	2.31	0.44
27:BA:1151:G:OP2	67:BA:3209:HOH:O	2.21	0.44
31:BE:188:GLY:O	31:BE:190:ARG:N	2.50	0.44
32:BF:166:GLU:O	32:BF:170:VAL:HG13	2.18	0.44
35:BJ:82:TYR:O	35:BJ:82:TYR:CG	2.71	0.44
47:BW:85:LEU:HD23	47:BW:85:LEU:H	1.83	0.44
27:BA:2853:G:OP1	27:BA:2853:G:N2	2.49	0.44
29:BC:182:ALA:O	29:BC:185:ARG:O	2.35	0.44
34:BI:41:LYS:O	34:BI:45:ARG:HG2	2.18	0.44
27:BA:879:A2M:O5’	27:BA:879:A2M:H8	2.18	0.44
27:BA:2216:G:C2’	27:BA:2217:G:O4’	2.65	0.44
27:BA:2835:A:HO2’	27:BA:2836:G:C4’	2.18	0.44
27:BA:692:C:H2’	27:BA:693:G:O4’	2.18	0.43
27:BA:2688:5MC:H2’	27:BA:2689:U:H2’	1.99	0.43
27:BA:2053:U:H1’	27:BA:2054:C:OP2	2.18	0.43
27:BA:2162:U:H2’	27:BA:2163:G:O4’	2.17	0.43
27:BA:2379:OMG:OP2	67:BA:3236:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BG:58:GLU:O	33:BG:59:PHE:CD2	2.71	0.43
34:BI:31:ARG:HB2	34:BI:102:ILE:O	2.18	0.43
36:BK:84:PRO:O	36:BK:90:GLY:HA3	2.18	0.43
42:BR:96:GLU:O	42:BR:97:ALA:HB3	2.18	0.43
27:BA:2728:OMG:HM23	27:BA:2728:OMG:H1'	1.73	0.43
30:BD:324:ARG:O	30:BD:324:ARG:HG2	2.18	0.43
31:BE:37:ALA:O	31:BE:40:THR:OG1	2.30	0.43
32:BF:95:VAL:HG11	32:BF:114:ILE:CG2	2.48	0.43
27:BA:1676:C:H2'	27:BA:1677:U:O4'	2.18	0.43
34:BH:31:ARG:HB3	34:BH:102:ILE:O	2.19	0.43
27:BA:2431:A:H2'	27:BA:2432:G:C8	2.53	0.43
30:BD:49:THR:HG22	30:BD:72:ILE:HD11	2.00	0.43
41:BQ:133:HIS:NE2	41:BQ:135:GLU:OE2	2.51	0.43
27:BA:410:C:O2'	27:BA:411:U:P	2.77	0.43
39:BO:91:ALA:O	39:BO:93:ILE:N	2.44	0.43
27:BA:715:A:H2'	27:BA:715:A:N3	2.33	0.43
27:BA:2578:C:O2	27:BA:2578:C:H2'	2.18	0.43
28:BB:52:A:O2'	28:BB:53:A:H8	2.02	0.43
31:BE:140:ILE:HG22	31:BE:140:ILE:O	2.19	0.43
34:BI:18:LYS:HG3	34:BI:114:ILE:HD11	2.01	0.43
35:BJ:171:ASP:OD1	35:BJ:173:THR:HG22	2.19	0.43
38:BN:22:VAL:HG21	38:BN:35:VAL:HG21	1.99	0.43
27:BA:1995:OMC:HM23	27:BA:1995:OMC:H1'	1.71	0.43
27:BA:2032:A:H2'	27:BA:2032:A:N3	2.34	0.43
27:BA:2805:C:OP2	43:BS:62:ARG:NH2	2.41	0.43
41:BQ:104:LEU:CD2	41:BQ:106:ILE:HD11	2.49	0.43
27:BA:91:OMC:H1'	27:BA:91:OMC:HM23	1.44	0.43
27:BA:288:OMG:H1'	27:BA:288:OMG:HM23	1.53	0.43
27:BA:1014:G:N1	27:BA:1024:U:O4	2.51	0.43
27:BA:1160:A:H2'	27:BA:1161:A:C8	2.54	0.43
27:BA:1937:A:H2'	27:BA:1938:A:C8	2.54	0.43
30:BD:61:THR:HG21	30:BD:66:ILE:HG21	2.00	0.43
30:BD:269:ILE:HD11	30:BD:306:GLU:HG3	2.01	0.43
33:BG:50:ASP:OD1	33:BG:51:GLY:N	2.47	0.43
27:BA:770:A:H2'	27:BA:771:A:O4'	2.18	0.43
27:BA:873:C:H2'	27:BA:874:G:O4'	2.18	0.43
27:BA:1293:C:H2'	27:BA:1294:G:O4'	2.18	0.43
27:BA:2426:G:O2'	27:BA:2427:5MU:H5"	2.18	0.43
27:BA:2430:A:H2'	27:BA:2431:A:C8	2.53	0.43
48:BX:52:VAL:CG1	48:BX:100:VAL:HG21	2.49	0.43
49:BY:26:ASP:OD2	49:BY:28:ARG:NE	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BB:39:G:O2'	28:BB:40:U:O4'	2.34	0.42
27:BA:1946:U:HO2'	29:BC:121:TYR:HA	1.84	0.42
27:BA:2080:U:O2	27:BA:2080:U:O4'	2.36	0.42
33:BG:6:TRP:O	33:BG:6:TRP:CD1	2.71	0.42
40:BP:119:VAL:HG22	40:BP:119:VAL:O	2.18	0.42
27:BA:986:G:O2'	27:BA:987:G:H5'	2.19	0.42
27:BA:2565:C:H2'	27:BA:2566:U:C6	2.54	0.42
27:BA:2958:U:C4'	27:BA:2959:U:H5'	2.49	0.42
32:BF:22:ILE:HD12	32:BF:85:TYR:CD1	2.53	0.42
32:BF:131:ILE:H	32:BF:131:ILE:HD12	1.85	0.42
38:BN:38:ALA:HB3	38:BN:40:LEU:HD13	2.00	0.42
39:BO:14:SER:O	39:BO:15:HIS:HB3	2.19	0.42
41:BQ:87:GLY:HA2	41:BQ:90:ILE:HG22	2.01	0.42
41:BQ:99:ILE:O	41:BQ:99:ILE:HG13	2.19	0.42
27:BA:956:C:N4	67:BA:3507:HOH:O	2.50	0.42
27:BA:1109:A:OP1	67:BA:3151:HOH:O	2.21	0.42
27:BA:1684:A:OP1	43:BS:43:ARG:NE	2.52	0.42
27:BA:2410:A:H2'	27:BA:2411:G:C4	2.54	0.42
28:BB:56:U:H5"	32:BF:15:HIS:NE2	2.34	0.42
29:BC:238:ARG:NH2	67:BC:307:HOH:O	2.50	0.42
35:BJ:18:THR:HG22	35:BJ:92:GLN:HA	2.00	0.42
27:BA:849:A2M:HM'2	27:BA:850:U:O4'	2.19	0.42
27:BA:2186:U:H2'	27:BA:2187:U:C6	2.54	0.42
27:BA:2256:U:HO2'	27:BA:2259:G:H1	1.66	0.42
27:BA:2373:G:OP2	67:BA:3228:HOH:O	2.20	0.42
34:BH:53:ILE:HG22	34:BH:54:ALA:N	2.34	0.42
27:BA:230:U:H2'	27:BA:231:U:O4'	2.20	0.42
27:BA:1238:C:H2'	27:BA:1239:G:C8	2.54	0.42
27:BA:2239:G:O2'	27:BA:2240:G:O5'	2.36	0.42
27:BA:2521:OMG:H1'	27:BA:2521:OMG:HM23	1.68	0.42
27:BA:2595:OMC:O2'	27:BA:2596:U:P	2.78	0.42
27:BA:65:OMG:H1'	27:BA:65:OMG:HM23	1.78	0.42
27:BA:1088:A:H2'	27:BA:1089:A:C8	2.54	0.42
27:BA:2222:G:H4'	27:BA:2223:C:OP2	2.19	0.42
27:BA:2423:A:H2'	27:BA:2423:A:N3	2.35	0.42
34:BH:26:ALA:HB3	34:BH:32:ILE:HD11	2.02	0.42
42:BR:34:ILE:HD13	42:BR:64:ILE:HD13	2.00	0.42
27:BA:541:A:H4'	27:BA:542:A:OP1	2.20	0.42
27:BA:1488:A:H2'	27:BA:1489:A:C8	2.55	0.42
33:BG:6:TRP:O	33:BG:7:ILE:C	2.57	0.42
33:BG:61:ARG:O	33:BG:65:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:1860:C:H2'	27:BA:1861:G:O4'	2.20	0.42
45:BU:31:PHE:CD2	45:BU:91:VAL:HG21	2.54	0.42
27:BA:153:A:N6	67:BA:3120:HOH:O	2.45	0.42
27:BA:670:OMG:HM22	27:BA:670:OMG:C4'	2.48	0.42
27:BA:1776:OMU:HM23	27:BA:1776:OMU:H1'	1.52	0.42
27:BA:2124:OMC:H2'	27:BA:2125:G:O4'	2.20	0.42
27:BA:2140:C:H2'	27:BA:2141:G:O4'	2.20	0.42
27:BA:2250:C:N3	27:BA:2266:G:N2	2.68	0.42
27:BA:2483:A:H2'	27:BA:2484:A:C8	2.55	0.42
35:BJ:4:ARG:NH1	35:BJ:9:ASP:OD1	2.53	0.42
48:BX:27:MET:SD	48:BX:71:LEU:HD23	2.59	0.42
27:BA:93:A:OP2	48:BX:47:ARG:NH2	2.53	0.41
27:BA:471:U:O2'	27:BA:472:A:P	2.77	0.41
27:BA:1270:G:OP2	36:BK:52:ARG:NH2	2.42	0.41
27:BA:1386:C:O2	27:BA:1386:C:O5'	2.38	0.41
27:BA:2053:U:O2'	27:BA:2054:C:P	2.78	0.41
27:BA:2543:A:H4'	27:BA:2545:OMC:OP2	2.20	0.41
32:BF:141:GLU:HG3	32:BF:142:ARG:N	2.35	0.41
27:BA:993:G:H2'	27:BA:994:C:C6	2.55	0.41
27:BA:2545:OMC:H1'	27:BA:2545:OMC:HM23	1.56	0.41
30:BD:78:LEU:HD13	30:BD:147:VAL:HG11	2.02	0.41
32:BF:45:LEU:O	32:BF:49:VAL:HG13	2.21	0.41
27:BA:345:U:H2'	27:BA:346:G:O4'	2.21	0.41
27:BA:912:OMG:C5'	27:BA:913:G:OP1	2.63	0.41
27:BA:1285:C:H2'	27:BA:1286:G:O4'	2.20	0.41
27:BA:2239:G:O2'	27:BA:2240:G:OP1	2.38	0.41
47:BW:30:VAL:HG12	47:BW:31:ASP:N	2.35	0.41
27:BA:392:C:H2'	27:BA:393:G:O4'	2.19	0.41
27:BA:1828:U:H2'	27:BA:1829:G:O4'	2.20	0.41
27:BA:2413:A:N7	27:BA:2414:A:C8	2.89	0.41
27:BA:2414:A:H2'	27:BA:2415:U:O4'	2.20	0.41
27:BA:2673:G:N7	30:BD:3:LYS:HE3	2.35	0.41
30:BD:84:ARG:HD2	30:BD:146:LEU:HD21	2.02	0.41
30:BD:154:ILE:O	30:BD:156:LEU:N	2.52	0.41
41:BQ:60:VAL:HG12	41:BQ:61:SER:N	2.35	0.41
27:BA:1030:U:O2'	27:BA:1031:C:P	2.74	0.41
27:BA:1944:U:O2	27:BA:1944:U:O4'	2.39	0.41
27:BA:2640:OMG:H5"	27:BA:2640:OMG:H8	1.86	0.41
28:BB:83:U:H2'	28:BB:84:G:C8	2.56	0.41
31:BE:73:ILE:HG22	31:BE:75:THR:H	1.85	0.41
27:BA:1272:U:H4'	27:BA:1274:A:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BF:145:PHE:CD1	32:BF:157:ILE:HG13	2.55	0.41
27:BA:314:G:H2'	27:BA:315:A:C1'	2.50	0.41
27:BA:561:C:H2'	27:BA:562:G:O4'	2.21	0.41
28:BB:10:G:O6	41:BQ:12:ARG:NH1	2.54	0.41
28:BB:18:G:H2'	28:BB:19:G:O4'	2.21	0.41
32:BF:40:LYS:O	32:BF:43:THR:N	2.53	0.41
32:BF:88:LEU:HD21	32:BF:138:VAL:HG21	2.03	0.41
33:BG:6:TRP:O	33:BG:6:TRP:HD1	2.04	0.41
38:BM:22:VAL:CG1	38:BM:35:VAL:HG13	2.51	0.41
27:BA:2238:A:O3'	27:BA:2239:G:O4'	2.38	0.41
27:BA:2550:OMG:HM22	27:BA:2605:5MC:HM53	2.03	0.41
36:BK:22:LEU:O	36:BK:96:ARG:NH1	2.43	0.41
27:BA:493:A:H4'	27:BA:494:C:OP2	2.21	0.41
27:BA:1147:A:N1	27:BA:1272:U:O2'	2.40	0.41
27:BA:1241:C:OP2	27:BA:1242:G:N2	2.54	0.41
27:BA:1820:OMC:H2'	27:BA:1821:G:O4'	2.21	0.41
27:BA:2021:G:H3'	27:BA:2022:G:C8	2.56	0.41
27:BA:2127:A:H2'	27:BA:2128:A:C8	2.56	0.41
27:BA:2172:A:O2'	27:BA:2173:G:H3'	2.21	0.41
27:BA:2173:G:H5'	27:BA:2174:A:C2	2.56	0.41
27:BA:2264:G:H2'	27:BA:2265:G:C8	2.56	0.41
29:BC:54:ARG:O	29:BC:55:THR:CG2	2.69	0.41
30:BD:25:PRO:HB2	30:BD:202:ILE:HG22	2.02	0.41
38:BM:33:VAL:HG23	38:BM:35:VAL:HG23	2.03	0.41
38:BM:67:SER:HB3	38:BM:69:GLU:OE1	2.21	0.41
43:BS:132:PHE:O	43:BS:133:LYS:HB2	2.20	0.41
27:BA:2720:C:H2'	27:BA:2721:U:O4'	2.21	0.41
27:BA:2858:U:H4'	27:BA:2859:A:OP1	2.20	0.41
49:BY:3:ARG:HA	49:BY:3:ARG:NE	2.36	0.41
27:BA:185:G:H2'	27:BA:186:A:O4'	2.21	0.40
27:BA:312:C:H2'	27:BA:313:G:O4'	2.21	0.40
27:BA:982:A:H2'	27:BA:983:G:O4'	2.21	0.40
27:BA:1534:U:O2	27:BA:1534:U:H2'	2.20	0.40
27:BA:1946:U:O2'	29:BC:121:TYR:HA	2.20	0.40
27:BA:2824:A:OP1	67:BA:3237:HOH:O	2.22	0.40
27:BA:3032:C:H2'	27:BA:3033:C:C6	2.56	0.40
31:BE:137:VAL:HG12	31:BE:138:VAL:N	2.36	0.40
37:BL:119:ARG:HB3	37:BL:119:ARG:HH11	1.87	0.40
40:BP:180:GLU:OE1	40:BP:180:GLU:N	2.46	0.40
41:BQ:140:GLU:OE1	41:BQ:140:GLU:N	2.53	0.40
27:BA:143:C:H2'	27:BA:144:U:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:754:C:H2'	27:BA:755:G:O4'	2.21	0.40
27:BA:2075:5MC:OP2	27:BA:2075:5MC:H6	2.04	0.40
27:BA:2998:G:OP1	49:BY:63:ARG:NH1	2.50	0.40
30:BD:111:ARG:HG3	30:BD:160:PRO:O	2.21	0.40
27:BA:1907:U:H5	27:BA:1912:A:N7	2.20	0.40
31:BE:61:ILE:HG23	31:BE:62:GLY:N	2.36	0.40
43:BS:30:GLU:HG2	43:BS:31:ASP:N	2.36	0.40
47:BW:30:VAL:CG1	47:BW:31:ASP:N	2.84	0.40
27:BA:1033:C:C6	27:BA:1033:C:H5"	2.56	0.40
27:BA:2224:G:N3	27:BA:2224:G:H2'	2.35	0.40
27:BA:2595:OMC:HM23	27:BA:2595:OMC:H1'	1.50	0.40
30:BD:84:ARG:NH1	30:BD:98:GLU:OE2	2.55	0.40
32:BF:66:GLY:HA2	32:BF:73:ILE:HG13	2.02	0.40
32:BF:145:PHE:CG	32:BF:145:PHE:O	2.74	0.40
35:BJ:69:VAL:HG13	35:BJ:148:ALA:HB1	2.04	0.40
38:BM:36:THR:O	38:BM:36:THR:HG23	2.22	0.40
38:BN:37:GLY:O	38:BN:38:ALA:HB2	2.20	0.40
41:BQ:37:VAL:O	41:BQ:38:ARG:NH1	2.54	0.40
27:BA:934:C:OP2	39:BO:26:ARG:NH1	2.54	0.40
27:BA:1520:G:OP2	67:BA:3240:HOH:O	2.22	0.40
28:BB:24:G:N7	28:BB:56:U:O2'	2.29	0.40
30:BD:111:ARG:HD2	30:BD:111:ARG:HA	1.82	0.40
47:BW:44:GLU:O	47:BW:48:ASN:N	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Ab	194/201 (96%)	181 (93%)	13 (7%)	0	100	100
3	Ac	193/209 (92%)	185 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Ad	188/200 (94%)	175 (93%)	13 (7%)	0	100	100
5	Ae	172/180 (96%)	165 (96%)	7 (4%)	0	100	100
6	Af	240/243 (99%)	234 (98%)	6 (2%)	0	100	100
7	Ag	221/235 (94%)	209 (95%)	12 (5%)	0	100	100
8	Ah	121/125 (97%)	118 (98%)	3 (2%)	0	100	100
9	Ai	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
10	Aj	127/130 (98%)	119 (94%)	8 (6%)	0	100	100
11	Ak	123/130 (95%)	116 (94%)	7 (6%)	0	100	100
12	Al	131/135 (97%)	123 (94%)	8 (6%)	0	100	100
13	Am	98/102 (96%)	94 (96%)	4 (4%)	0	100	100
14	An	125/140 (89%)	118 (94%)	6 (5%)	1 (1%)	19	29
15	Ao	141/147 (96%)	135 (96%)	6 (4%)	0	100	100
16	Ap	133/149 (89%)	118 (89%)	15 (11%)	0	100	100
17	Aq	147/151 (97%)	141 (96%)	6 (4%)	0	100	100
18	Ar	52/56 (93%)	46 (88%)	6 (12%)	0	100	100
19	As	106/114 (93%)	102 (96%)	4 (4%)	0	100	100
20	At	62/67 (92%)	60 (97%)	2 (3%)	0	100	100
20	Bm	61/67 (91%)	58 (95%)	3 (5%)	0	100	100
21	Au	114/133 (86%)	111 (97%)	3 (3%)	0	100	100
22	Av	147/150 (98%)	139 (95%)	8 (5%)	0	100	100
23	Aw	93/98 (95%)	87 (94%)	6 (6%)	0	100	100
23	Bn	90/98 (92%)	85 (94%)	5 (6%)	0	100	100
24	Ax	59/65 (91%)	56 (95%)	3 (5%)	0	100	100
25	Ay	62/70 (89%)	60 (97%)	2 (3%)	0	100	100
26	Az	53/62 (86%)	51 (96%)	2 (4%)	0	100	100
29	BC	235/239 (98%)	221 (94%)	14 (6%)	0	100	100
30	BD	342/346 (99%)	322 (94%)	20 (6%)	0	100	100
31	BE	253/255 (99%)	241 (95%)	12 (5%)	0	100	100
32	BF	162/183 (88%)	132 (82%)	30 (18%)	0	100	100
33	BG	181/184 (98%)	169 (93%)	12 (7%)	0	100	100
34	BH	119/123 (97%)	113 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	BI	119/123 (97%)	108 (91%)	11 (9%)	0	100	100
35	BJ	167/182 (92%)	157 (94%)	10 (6%)	0	100	100
36	BK	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
37	BL	138/141 (98%)	128 (93%)	10 (7%)	0	100	100
38	BM	79/83 (95%)	70 (89%)	9 (11%)	0	100	100
38	BN	79/83 (95%)	72 (91%)	7 (9%)	0	100	100
39	BO	146/148 (99%)	134 (92%)	12 (8%)	0	100	100
40	BP	191/194 (98%)	182 (95%)	9 (5%)	0	100	100
41	BQ	158/201 (79%)	149 (94%)	9 (6%)	0	100	100
42	BR	118/121 (98%)	112 (95%)	6 (5%)	0	100	100
43	BS	144/150 (96%)	139 (96%)	5 (4%)	0	100	100
44	BT	72/77 (94%)	70 (97%)	2 (3%)	0	100	100
45	BU	94/98 (96%)	91 (97%)	3 (3%)	0	100	100
46	BV	152/156 (97%)	149 (98%)	3 (2%)	0	100	100
47	BW	83/86 (96%)	78 (94%)	5 (6%)	0	100	100
48	BX	118/121 (98%)	113 (96%)	5 (4%)	0	100	100
49	BY	60/67 (90%)	60 (100%)	0	0	100	100
50	BZ	56/66 (85%)	54 (96%)	2 (4%)	0	100	100
51	Ba	152/155 (98%)	147 (97%)	5 (3%)	0	100	100
52	Bb	94/102 (92%)	87 (93%)	7 (7%)	0	100	100
53	Bc	87/90 (97%)	80 (92%)	7 (8%)	0	100	100
54	Bd	122/125 (98%)	117 (96%)	5 (4%)	0	100	100
55	Be	87/90 (97%)	82 (94%)	5 (6%)	0	100	100
56	Bf	84/101 (83%)	80 (95%)	4 (5%)	0	100	100
57	Bg	82/86 (95%)	77 (94%)	5 (6%)	0	100	100
58	Bh	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
59	Bi	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
60	Bj	45/51 (88%)	43 (96%)	2 (4%)	0	100	100
61	Bk	34/37 (92%)	34 (100%)	0	0	100	100
62	Bl	91/94 (97%)	90 (99%)	1 (1%)	0	100	100
63	Bo	41/47 (87%)	38 (93%)	3 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
64	Bp	230/236 (98%)	213 (93%)	17 (7%)	0	100	100
65	Bq	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
All	All	8160/8603 (95%)	7713 (94%)	446 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	An	133	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Ab	170/175 (97%)	170 (100%)	0	100	100
3	Ac	156/168 (93%)	156 (100%)	0	100	100
4	Ad	162/169 (96%)	162 (100%)	0	100	100
5	Ae	153/156 (98%)	153 (100%)	0	100	100
6	Af	211/212 (100%)	211 (100%)	0	100	100
7	Ag	185/197 (94%)	185 (100%)	0	100	100
8	Ah	104/105 (99%)	104 (100%)	0	100	100
9	Ai	183/184 (100%)	183 (100%)	0	100	100
10	Aj	106/107 (99%)	106 (100%)	0	100	100
11	Ak	101/105 (96%)	101 (100%)	0	100	100
12	Al	110/112 (98%)	110 (100%)	0	100	100
13	Am	89/91 (98%)	89 (100%)	0	100	100
14	An	95/108 (88%)	94 (99%)	1 (1%)	73	85
15	Ao	117/120 (98%)	117 (100%)	0	100	100
16	Ap	111/123 (90%)	111 (100%)	0	100	100
17	Aq	129/131 (98%)	129 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	Ar	45/46 (98%)	45 (100%)	0	100	100
19	As	96/101 (95%)	96 (100%)	0	100	100
20	At	58/61 (95%)	58 (100%)	0	100	100
20	Bm	58/61 (95%)	58 (100%)	0	100	100
21	Au	104/117 (89%)	104 (100%)	0	100	100
22	Av	125/126 (99%)	125 (100%)	0	100	100
23	Aw	85/88 (97%)	85 (100%)	0	100	100
23	Bn	82/88 (93%)	82 (100%)	0	100	100
24	Ax	53/56 (95%)	53 (100%)	0	100	100
25	Ay	53/59 (90%)	53 (100%)	0	100	100
26	Az	49/55 (89%)	49 (100%)	0	100	100
29	BC	185/187 (99%)	185 (100%)	0	100	100
30	BD	288/289 (100%)	288 (100%)	0	100	100
31	BE	212/212 (100%)	212 (100%)	0	100	100
32	BF	140/155 (90%)	138 (99%)	2 (1%)	67	81
33	BG	158/159 (99%)	158 (100%)	0	100	100
34	BH	99/100 (99%)	99 (100%)	0	100	100
34	BI	99/100 (99%)	98 (99%)	1 (1%)	76	86
35	BJ	145/153 (95%)	145 (100%)	0	100	100
36	BK	120/120 (100%)	120 (100%)	0	100	100
37	BL	104/105 (99%)	104 (100%)	0	100	100
38	BM	63/65 (97%)	63 (100%)	0	100	100
38	BN	63/65 (97%)	63 (100%)	0	100	100
39	BO	116/116 (100%)	116 (100%)	0	100	100
40	BP	161/162 (99%)	161 (100%)	0	100	100
41	BQ	138/167 (83%)	137 (99%)	1 (1%)	84	91
42	BR	101/102 (99%)	101 (100%)	0	100	100
43	BS	120/124 (97%)	120 (100%)	0	100	100
44	BT	69/72 (96%)	69 (100%)	0	100	100
45	BU	84/85 (99%)	84 (100%)	0	100	100
46	BV	129/131 (98%)	129 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
47	BW	75/76 (99%)	75 (100%)	0	100 100
48	BX	109/109 (100%)	109 (100%)	0	100 100
49	BY	54/58 (93%)	54 (100%)	0	100 100
50	BZ	57/61 (93%)	57 (100%)	0	100 100
51	Ba	132/133 (99%)	132 (100%)	0	100 100
52	Bb	76/80 (95%)	76 (100%)	0	100 100
53	Bc	75/76 (99%)	75 (100%)	0	100 100
54	Bd	106/107 (99%)	106 (100%)	0	100 100
55	Be	80/80 (100%)	79 (99%)	1 (1%)	69 82
56	Bf	71/83 (86%)	71 (100%)	0	100 100
57	Bg	62/63 (98%)	62 (100%)	0	100 100
58	Bh	50/51 (98%)	50 (100%)	0	100 100
59	Bi	45/46 (98%)	44 (98%)	1 (2%)	52 70
60	Bj	36/38 (95%)	36 (100%)	0	100 100
61	Bk	34/35 (97%)	34 (100%)	0	100 100
62	Bl	83/84 (99%)	83 (100%)	0	100 100
63	Bo	36/39 (92%)	36 (100%)	0	100 100
64	Bp	196/200 (98%)	196 (100%)	0	100 100
All	All	6961/7209 (97%)	6954 (100%)	7 (0%)	93 97

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	An	130	ARG
32	BF	5	ARG
32	BF	179	LYS
34	BI	67	PRO
41	BQ	113	ARG
55	Be	63	ARG
59	Bi	3	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
12	Al	91	ASN

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Mol	Chain	Res	Type
17	Aq	104	GLN
18	Ar	7	ASN
23	Aw	54	GLN
31	BE	139	GLN
32	BF	60	GLN
35	BJ	83	HIS
35	BJ	141	HIS
41	BQ	42	ASN
41	BQ	145	ASN
45	BU	96	GLN
46	BV	12	ASN
48	BX	17	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Aa	1453/1498 (96%)	240 (16%)	0
27	BA	2929/3037 (96%)	488 (16%)	36 (1%)
28	BB	124/126 (98%)	15 (12%)	3 (2%)
All	All	4506/4661 (96%)	743 (16%)	39 (0%)

All (743) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	Aa	4	C
1	Aa	17	5MC
1	Aa	33	U
1	Aa	42	G
1	Aa	45	U
1	Aa	47	A
1	Aa	54	C
1	Aa	60	A
1	Aa	65	G
1	Aa	70	C
1	Aa	77	C
1	Aa	95	A
1	Aa	99	A
1	Aa	100	C
1	Aa	109	A
1	Aa	111	C
1	Aa	121	OMG

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Mol	Chain	Res	Type
1	Aa	137	G
1	Aa	143	C
1	Aa	179	G
1	Aa	188	G
1	Aa	192	A
1	Aa	194	A
1	Aa	195	G
1	Aa	214	G
1	Aa	219	OMG
1	Aa	228	C
1	Aa	231	A
1	Aa	232	U
1	Aa	233	U
1	Aa	235	G
1	Aa	239	G
1	Aa	254	G
1	Aa	255	C
1	Aa	268	A
1	Aa	270	A
1	Aa	277	C
1	Aa	289	G
1	Aa	291	G
1	Aa	294	A
1	Aa	316	C
1	Aa	317	A
1	Aa	318	C
1	Aa	320	OMG
1	Aa	335	G
1	Aa	337	G
1	Aa	340	5MC
1	Aa	341	A
1	Aa	342	G
1	Aa	350	G
1	Aa	352	A2M
1	Aa	355	C
1	Aa	360	C
1	Aa	372	C
1	Aa	381	OMG
1	Aa	385	A
1	Aa	386	C
1	Aa	391	A
1	Aa	394	G

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Mol	Chain	Res	Type
1	Aa	428	A
1	Aa	440	A
1	Aa	441	U
1	Aa	442	A
1	Aa	443	A
1	Aa	453	A
1	Aa	454	A
1	Aa	456	G
1	Aa	457	5MC
1	Aa	463	G
1	Aa	466	G
1	Aa	469	G
1	Aa	472	G
1	Aa	477	A
1	Aa	478	A
1	Aa	492	A
1	Aa	498	OMG
1	Aa	506	U
1	Aa	509	U
1	Aa	517	A
1	Aa	518	A
1	Aa	521	C
1	Aa	522	G
1	Aa	526	G
1	Aa	541	A
1	Aa	564	U
1	Aa	578	U
1	Aa	579	G
1	Aa	599	U
1	Aa	611	A
1	Aa	620	G
1	Aa	621	U
1	Aa	634	G
1	Aa	647	A
1	Aa	649	A
1	Aa	662	C
1	Aa	663	C
1	Aa	664	G
1	Aa	669	U
1	Aa	670	OMG
1	Aa	677	G
1	Aa	679	G

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Mol	Chain	Res	Type
1	Aa	694	G
1	Aa	695	U
1	Aa	701	G
1	Aa	707	G
1	Aa	719	G
1	Aa	723	A
1	Aa	727	A
1	Aa	738	A
1	Aa	739	U
1	Aa	761	A
1	Aa	763	G
1	Aa	774	A
1	Aa	787	G
1	Aa	793	A
1	Aa	822	A
1	Aa	840	G
1	Aa	864	A
1	Aa	869	A
1	Aa	876	G
1	Aa	877	G
1	Aa	884	C
1	Aa	886	A
1	Aa	889	A
1	Aa	890	G
1	Aa	911	U
1	Aa	917	5MU
1	Aa	920	A
1	Aa	922	G
1	Aa	925	G
1	Aa	926	G
1	Aa	927	G
1	Aa	928	A
1	Aa	929	A
1	Aa	941	G
1	Aa	943	G
1	Aa	944	A
1	Aa	947	G
1	Aa	959	C
1	Aa	961	A
1	Aa	963	OMG
1	Aa	968	A
1	Aa	969	G

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Mol	Chain	Res	Type
1	Aa	970	G
1	Aa	975	G
1	Aa	979	G
1	Aa	987	G
1	Aa	988	A
1	Aa	997	G
1	Aa	1004	5MC
1	Aa	1007	5MC
1	Aa	1009	U
1	Aa	1010	C
1	Aa	1038	G
1	Aa	1039	U
1	Aa	1044	U
1	Aa	1045	A
1	Aa	1069	U
1	Aa	1070	U
1	Aa	1076	U
1	Aa	1077	C
1	Aa	1084	G
1	Aa	1085	C
1	Aa	1086	U
1	Aa	1088	G
1	Aa	1092	G
1	Aa	1093	G
1	Aa	1094	A
1	Aa	1096	G
1	Aa	1098	A
1	Aa	1107	OMG
1	Aa	1111	C
1	Aa	1119	A
1	Aa	1120	U
1	Aa	1127	G
1	Aa	1136	G
1	Aa	1147	U
1	Aa	1148	A
1	Aa	1149	G
1	Aa	1154	G
1	Aa	1157	U
1	Aa	1158	G
1	Aa	1164	A
1	Aa	1165	A
1	Aa	1168	C

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Mol	Chain	Res	Type
1	Aa	1169	C
1	Aa	1171	C
1	Aa	1176	U
1	Aa	1179	A
1	Aa	1190	A
1	Aa	1193	G
1	Aa	1208	A
1	Aa	1209	U
1	Aa	1212	G
1	Aa	1217	C
1	Aa	1221	A
1	Aa	1222	G
1	Aa	1231	A
1	Aa	1232	A
1	Aa	1252	G
1	Aa	1253	U
1	Aa	1254	U
1	Aa	1255	C
1	Aa	1272	C
1	Aa	1288	U
1	Aa	1299	G
1	Aa	1305	G
1	Aa	1306	5MC
1	Aa	1311	C
1	Aa	1312	A
1	Aa	1316	U
1	Aa	1322	G
1	Aa	1328	U
1	Aa	1331	G
1	Aa	1334	C
1	Aa	1349	C
1	Aa	1350	A
1	Aa	1352	5MC
1	Aa	1355	C
1	Aa	1371	G
1	Aa	1376	G
1	Aa	1400	U
1	Aa	1401	C
1	Aa	1402	G
1	Aa	1403	G
1	Aa	1407	G
1	Aa	1423	G

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Mol	Chain	Res	Type
1	Aa	1431	G
1	Aa	1434	G
1	Aa	1436	G
1	Aa	1442	A
1	Aa	1446	G
1	Aa	1448	A
1	Aa	1451	A
1	Aa	1452	A
1	Aa	1453	G
1	Aa	1455	U
1	Aa	1466	G
1	Aa	1478	5MC
1	Aa	1479	G
27	BA	12	C
27	BA	15	U
27	BA	18	C
27	BA	19	A
27	BA	21	C
27	BA	32	G
27	BA	33	G
27	BA	37	A
27	BA	43	C
27	BA	51	G
27	BA	55	5MC
27	BA	64	G
27	BA	73	A
27	BA	80	A
27	BA	83	A
27	BA	84	G
27	BA	94	G
27	BA	100	G
27	BA	108	U
27	BA	109	C
27	BA	126	A
27	BA	127	A
27	BA	128	U
27	BA	129	G
27	BA	132	A
27	BA	133	C
27	BA	134	C
27	BA	135	U
27	BA	136	C

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Mol	Chain	Res	Type
27	BA	148	G
27	BA	153	A
27	BA	159	A
27	BA	160	G
27	BA	161	U
27	BA	162	C
27	BA	172	A
27	BA	187	A
27	BA	190	A
27	BA	206	G
27	BA	207	A
27	BA	208	A
27	BA	212	A
27	BA	213	A
27	BA	217	A
27	BA	219	A
27	BA	220	A
27	BA	221	G
27	BA	224	A
27	BA	239	G
27	BA	257	G
27	BA	277	C
27	BA	278	G
27	BA	287	G
27	BA	301	U
27	BA	302	G
27	BA	303	U
27	BA	304	A
27	BA	314	G
27	BA	316	G
27	BA	317	G
27	BA	323	U
27	BA	331	A
27	BA	332	A
27	BA	340	U
27	BA	341	C
27	BA	342	OMC
27	BA	343	G
27	BA	350	C
27	BA	360	G
27	BA	365	OMG
27	BA	368	G

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Mol	Chain	Res	Type
27	BA	369	A
27	BA	372	G
27	BA	377	G
27	BA	398	C
27	BA	401	G
27	BA	405	U
27	BA	408	C
27	BA	411	U
27	BA	414	G
27	BA	429	U
27	BA	430	A
27	BA	440	A
27	BA	445	G
27	BA	453	OMU
27	BA	456	G
27	BA	460	C
27	BA	472	A
27	BA	476	C
27	BA	495	U
27	BA	496	A
27	BA	506	G
27	BA	518	A
27	BA	519	A
27	BA	520	G
27	BA	531	G
27	BA	540	A
27	BA	542	A
27	BA	543	G
27	BA	546	C
27	BA	567	G
27	BA	568	A
27	BA	569	G
27	BA	570	G
27	BA	574	C
27	BA	581	A
27	BA	584	OMG
27	BA	589	G
27	BA	616	C
27	BA	622	A
27	BA	623	G
27	BA	654	C
27	BA	666	A

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Mol	Chain	Res	Type
27	BA	674	OMG
27	BA	677	A
27	BA	688	G
27	BA	694	A
27	BA	707	C
27	BA	708	A
27	BA	729	C
27	BA	733	C
27	BA	734	A
27	BA	736	G
27	BA	801	A
27	BA	802	A
27	BA	803	G
27	BA	812	U
27	BA	835	C
27	BA	840	A
27	BA	841	A
27	BA	842	C
27	BA	844	G
27	BA	846	G
27	BA	849	A2M
27	BA	852	G
27	BA	853	A
27	BA	856	C
27	BA	870	U
27	BA	875	5MU
27	BA	891	G
27	BA	892	A
27	BA	893	C
27	BA	903	G
27	BA	904	G
27	BA	910	A
27	BA	912	OMG
27	BA	913	G
27	BA	920	G
27	BA	933	G
27	BA	940	C
27	BA	950	U
27	BA	951	A
27	BA	955	C
27	BA	956	C
27	BA	974	A

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Mol	Chain	Res	Type
27	BA	975	G
27	BA	983	G
27	BA	988	G
27	BA	995	A
27	BA	998	G
27	BA	1001	U
27	BA	1003	G
27	BA	1006	G
27	BA	1008	U
27	BA	1012	G
27	BA	1014	G
27	BA	1016	C
27	BA	1017	G
27	BA	1018	A
27	BA	1019	A
27	BA	1021	G
27	BA	1022	C
27	BA	1023	C
27	BA	1026	C
27	BA	1031	C
27	BA	1036	U
27	BA	1039	A
27	BA	1041	C
27	BA	1048	C
27	BA	1066	G
27	BA	1076	G
27	BA	1077	G
27	BA	1102	G
27	BA	1103	A
27	BA	1117	G
27	BA	1119	C
27	BA	1129	G
27	BA	1130	G
27	BA	1136	A
27	BA	1139	U
27	BA	1140	G
27	BA	1144	G
27	BA	1149	G
27	BA	1158	C
27	BA	1159	A
27	BA	1165	U
27	BA	1175	C

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Mol	Chain	Res	Type
27	BA	1177	U
27	BA	1179	G
27	BA	1180	A
27	BA	1183	G
27	BA	1184	C
27	BA	1238	C
27	BA	1239	G
27	BA	1243	A
27	BA	1244	G
27	BA	1249	G
27	BA	1250	G
27	BA	1266	C
27	BA	1270	G
27	BA	1275	A
27	BA	1307	A
27	BA	1309	U
27	BA	1310	G
27	BA	1318	A
27	BA	1320	C
27	BA	1322	G
27	BA	1331	G
27	BA	1336	C
27	BA	1361	A
27	BA	1362	G
27	BA	1372	A
27	BA	1373	C
27	BA	1388	G
27	BA	1391	C
27	BA	1409	A
27	BA	1410	U
27	BA	1436	U
27	BA	1437	A
27	BA	1438	G
27	BA	1474	G
27	BA	1490	C
27	BA	1503	U
27	BA	1515	A
27	BA	1517	A
27	BA	1521	A
27	BA	1533	A
27	BA	1556	G
27	BA	1563	C

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Mol	Chain	Res	Type
27	BA	1568	G
27	BA	1581	C
27	BA	1606	A
27	BA	1608	A
27	BA	1623	U
27	BA	1638	U
27	BA	1639	G
27	BA	1640	C
27	BA	1664	A
27	BA	1671	A
27	BA	1672	U
27	BA	1673	G
27	BA	1680	C
27	BA	1681	G
27	BA	1683	A
27	BA	1685	G
27	BA	1692	U
27	BA	1693	C
27	BA	1696	C
27	BA	1699	A
27	BA	1706	G
27	BA	1715	A
27	BA	1734	U
27	BA	1742	G
27	BA	1743	A
27	BA	1752	A
27	BA	1754	A
27	BA	1755	A
27	BA	1762	C
27	BA	1764	G
27	BA	1767	G
27	BA	1768	C
27	BA	1769	C
27	BA	1785	U
27	BA	1792	U
27	BA	1793	G
27	BA	1795	C
27	BA	1801	A
27	BA	1811	G
27	BA	1822	G
27	BA	1848	A
27	BA	1859	G

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Mol	Chain	Res	Type
27	BA	1861	G
27	BA	1884	G
27	BA	1891	G
27	BA	1892	G
27	BA	1901	A
27	BA	1904	G
27	BA	1908	A
27	BA	1914	A
27	BA	1928	C
27	BA	1929	U
27	BA	1945	G
27	BA	1957	A
27	BA	1967	A
27	BA	1991	A
27	BA	2002	A
27	BA	2014	A
27	BA	2016	OMG
27	BA	2020	G
27	BA	2021	G
27	BA	2023	G
27	BA	2024	U
27	BA	2025	A
27	BA	2026	A
27	BA	2027	C
27	BA	2028	U
27	BA	2029	A
27	BA	2031	A
27	BA	2033	C
27	BA	2034	C
27	BA	2036	U
27	BA	2037	C
27	BA	2039	U
27	BA	2043	G
27	BA	2050	A
27	BA	2053	U
27	BA	2054	C
27	BA	2067	A
27	BA	2068	U
27	BA	2076	U
27	BA	2080	U
27	BA	2083	A
27	BA	2084	U

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Mol	Chain	Res	Type
27	BA	2085	G
27	BA	2104	U
27	BA	2133	U
27	BA	2139	G
27	BA	2142	C
27	BA	2143	A
27	BA	2144	U
27	BA	2145	A
27	BA	2167	A
27	BA	2174	A
27	BA	2175	C
27	BA	2181	G
27	BA	2205	G
27	BA	2207	C
27	BA	2219	G
27	BA	2220	G
27	BA	2222	G
27	BA	2223	C
27	BA	2224	G
27	BA	2225	C
27	BA	2226	A
27	BA	2227	G
27	BA	2228	C
27	BA	2229	G
27	BA	2230	U
27	BA	2234	C
27	BA	2237	G
27	BA	2238	A
27	BA	2240	G
27	BA	2242	G
27	BA	2243	U
27	BA	2244	C
27	BA	2245	G
27	BA	2248	G
27	BA	2249	C
27	BA	2257	C
27	BA	2260	G
27	BA	2261	G
27	BA	2269	G
27	BA	2270	A
27	BA	2271	G
27	BA	2275	C

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Mol	Chain	Res	Type
27	BA	2278	A
27	BA	2281	A
27	BA	2282	G
27	BA	2283	A
27	BA	2286	C
27	BA	2288	G
27	BA	2292	A
27	BA	2299	G
27	BA	2310	A
27	BA	2311	A
27	BA	2317	G
27	BA	2318	G
27	BA	2321	G
27	BA	2327	A
27	BA	2328	C
27	BA	2336	G
27	BA	2337	G
27	BA	2340	G
27	BA	2353	OMG
27	BA	2360	A
27	BA	2369	A
27	BA	2382	G
27	BA	2385	G
27	BA	2386	C
27	BA	2390	A
27	BA	2391	A
27	BA	2409	C
27	BA	2412	G
27	BA	2414	A
27	BA	2415	U
27	BA	2423	A
27	BA	2425	A
27	BA	2428	G
27	BA	2438	A
27	BA	2448	G
27	BA	2450	C
27	BA	2453	G
27	BA	2460	A
27	BA	2469	OMG
27	BA	2483	A
27	BA	2489	G
27	BA	2491	C

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Mol	Chain	Res	Type
27	BA	2498	A
27	BA	2527	OMG
27	BA	2531	G
27	BA	2534	A
27	BA	2535	G
27	BA	2536	A
27	BA	2542	OMU
27	BA	2545	OMC
27	BA	2551	G
27	BA	2552	A
27	BA	2557	A
27	BA	2572	G
27	BA	2573	A
27	BA	2574	G
27	BA	2579	C
27	BA	2580	A
27	BA	2595	OMC
27	BA	2596	U
27	BA	2602	C
27	BA	2606	G
27	BA	2609	G
27	BA	2622	A
27	BA	2633	G
27	BA	2638	A
27	BA	2640	OMG
27	BA	2642	OMG
27	BA	2670	A
27	BA	2671	G
27	BA	2677	C
27	BA	2682	G
27	BA	2686	G
27	BA	2703	G
27	BA	2706	A
27	BA	2707	G
27	BA	2713	A
27	BA	2717	U
27	BA	2718	A
27	BA	2719	U
27	BA	2733	U
27	BA	2744	G
27	BA	2749	A
27	BA	2750	G

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Mol	Chain	Res	Type
27	BA	2766	G
27	BA	2768	G
27	BA	2776	G
27	BA	2787	U
27	BA	2794	U
27	BA	2808	C
27	BA	2809	A
27	BA	2815	U
27	BA	2817	G
27	BA	2829	C
27	BA	2836	G
27	BA	2837	C
27	BA	2850	A
27	BA	2853	G
27	BA	2860	A
27	BA	2862	G
27	BA	2864	C
27	BA	2867	A
27	BA	2878	A
27	BA	2879	A
27	BA	2882	C
27	BA	2884	G
27	BA	2937	G
27	BA	2944	G
27	BA	2959	U
27	BA	2960	G
27	BA	2961	A
27	BA	2982	G
27	BA	2988	A
27	BA	2995	C
27	BA	3001	C
27	BA	3007	G
27	BA	3008	C
27	BA	3017	A
27	BA	3021	C
27	BA	3023	C
27	BA	3026	G
27	BA	3032	C
27	BA	3034	G
28	BB	4	A
28	BB	11	C
28	BB	13	A

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Mol	Chain	Res	Type
28	BB	27	A
28	BB	35	U
28	BB	41	U
28	BB	44	G
28	BB	47	C
28	BB	50	G
28	BB	53	A
28	BB	57	A
28	BB	79	G
28	BB	89	C
28	BB	95	G
28	BB	115	G

All (39) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	BA	108	U
27	BA	128	U
27	BA	134	C
27	BA	303	U
27	BA	317	G
27	BA	404	G
27	BA	410	C
27	BA	471	U
27	BA	687	A
27	BA	912	OMG
27	BA	974	A
27	BA	1002	G
27	BA	1030	U
27	BA	1178	A
27	BA	1360	G
27	BA	1670	A
27	BA	1671	A
27	BA	1691	U
27	BA	1741	C
27	BA	1742	G
27	BA	1754	A
27	BA	1767	G
27	BA	1928	C
27	BA	2053	U
27	BA	2173	G
27	BA	2174	A

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Mol	Chain	Res	Type
27	BA	2239	G
27	BA	2268	G
27	BA	2482	A
27	BA	2534	A
27	BA	2551	G
27	BA	2571	C
27	BA	2595	OMC
27	BA	2605	5MC
27	BA	2836	G
27	BA	3023	C
28	BB	34	G
28	BB	52	A
28	BB	56	U

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

145 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	Aa	825	1	19,22,23	2.97	8 (42%)	26,31,34	0.73	0
1	OMG	Aa	963	1	18,26,27	2.53	8 (44%)	19,38,41	1.47	4 (21%)
27	OMG	BA	215	27	18,26,27	2.47	8 (44%)	19,38,41	1.55	4 (21%)
27	5MU	BA	1854	27	19,22,23	4.88	7 (36%)	28,32,35	3.73	9 (32%)
27	5MC	BA	2070	27	18,22,23	3.50	7 (38%)	26,32,35	1.01	2 (7%)
1	MA6	Aa	1467	1	18,26,27	1.03	2 (11%)	19,38,41	3.52	2 (10%)
27	OMG	BA	1953	27	18,26,27	2.45	8 (44%)	19,38,41	1.48	4 (21%)
27	OMC	BA	2047	27	19,22,23	2.96	8 (42%)	26,31,34	0.74	0
1	OMG	Aa	574	1	18,26,27	2.52	8 (44%)	19,38,41	1.50	4 (21%)
1	OMU	Aa	8	1	19,22,23	3.02	8 (42%)	26,31,34	1.71	5 (19%)
27	OMG	BA	365	27	18,26,27	2.46	8 (44%)	19,38,41	1.50	4 (21%)
27	4SU	BA	2581	27	18,21,22	4.24	8 (44%)	26,30,33	2.23	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	OMG	Aa	446	1	18,26,27	2.48	8 (44%)	19,38,41	1.56	4 (21%)
1	5MC	Aa	464	1	18,22,23	3.59	7 (38%)	26,32,35	1.03	2 (7%)
1	5MC	Aa	349	1	18,22,23	3.54	7 (38%)	26,32,35	1.04	2 (7%)
27	OMG	BA	800	27	18,26,27	2.47	8 (44%)	19,38,41	1.52	4 (21%)
27	OMU	BA	2389	27	19,22,23	1.33	4 (21%)	26,31,34	2.01	7 (26%)
1	5MC	Aa	672	1	18,22,23	3.54	7 (38%)	26,32,35	1.02	2 (7%)
27	OMC	BA	2169	27	19,22,23	2.98	8 (42%)	26,31,34	0.75	0
1	OMG	Aa	994	1	18,26,27	2.51	8 (44%)	19,38,41	1.51	4 (21%)
1	5MC	Aa	1004	1	18,22,23	3.59	7 (38%)	26,32,35	1.01	2 (7%)
27	OMU	BA	2542	27	19,22,23	3.01	8 (42%)	26,31,34	1.66	4 (15%)
27	OMG	BA	2521	27	18,26,27	2.49	8 (44%)	19,38,41	1.56	4 (21%)
27	A2M	BA	932	27	18,25,26	4.28	7 (38%)	18,36,39	2.98	3 (16%)
27	A2M	BA	2329	27	18,25,26	0.99	1 (5%)	18,36,39	1.18	2 (11%)
27	OMG	BA	2168	27	18,26,27	2.46	8 (44%)	19,38,41	1.50	4 (21%)
1	5MC	Aa	923	1	18,22,23	3.54	7 (38%)	26,32,35	1.08	2 (7%)
1	5MC	Aa	1003	1	18,22,23	3.57	7 (38%)	26,32,35	1.01	2 (7%)
27	OMC	BA	2595	27	19,22,23	3.03	8 (42%)	26,31,34	0.92	1 (3%)
1	OMG	Aa	1107	1	18,26,27	2.51	8 (44%)	19,38,41	1.50	4 (21%)
1	OMG	Aa	836	1	18,26,27	2.51	8 (44%)	19,38,41	1.55	4 (21%)
1	5MC	Aa	17	1	18,22,23	3.51	7 (38%)	26,32,35	1.01	2 (7%)
1	5MC	Aa	1184	1	18,22,23	3.56	7 (38%)	26,32,35	1.01	2 (7%)
1	5MC	Aa	1321	1	18,22,23	3.51	7 (38%)	26,32,35	1.15	2 (7%)
27	OMG	BA	833	27	18,26,27	2.49	8 (44%)	19,38,41	1.50	4 (21%)
1	5MC	Aa	473	1	18,22,23	3.54	7 (38%)	26,32,35	1.07	2 (7%)
27	OMU	BA	453	27	19,22,23	3.03	8 (42%)	26,31,34	1.72	4 (15%)
27	OMG	BA	1525	27	18,26,27	2.46	8 (44%)	19,38,41	1.50	4 (21%)
27	OMG	BA	584	27	18,26,27	2.50	8 (44%)	19,38,41	1.52	4 (21%)
27	OMG	BA	2870	27	18,26,27	2.45	8 (44%)	19,38,41	1.48	4 (21%)
27	OMU	BA	1402	27	19,22,23	3.06	8 (42%)	26,31,34	1.67	4 (15%)
1	OMG	Aa	629	1	18,26,27	2.51	8 (44%)	19,38,41	1.54	4 (21%)
1	OMG	Aa	659	1	18,26,27	2.48	8 (44%)	19,38,41	1.47	4 (21%)
27	OMG	BA	2672	27	18,26,27	2.47	8 (44%)	19,38,41	1.52	4 (21%)
27	5MC	BA	1345	27	18,22,23	3.55	7 (38%)	26,32,35	1.02	1 (3%)
27	OMG	BA	2353	27	18,26,27	1.05	1 (5%)	19,38,41	1.03	2 (10%)
27	OMG	BA	2469	27	18,26,27	2.46	8 (44%)	19,38,41	1.47	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	OMG	BA	1508	27	18,26,27	2.50	8 (44%)	19,38,41	1.51	4 (21%)
27	OMG	BA	2527	27	18,26,27	2.48	8 (44%)	19,38,41	1.48	4 (21%)
27	OMU	BA	1150	27	19,22,23	3.03	8 (42%)	26,31,34	1.70	4 (15%)
27	OMC	BA	66	27	19,22,23	2.97	8 (42%)	26,31,34	0.76	0
1	OMC	Aa	112	1	19,22,23	2.99	8 (42%)	26,31,34	0.74	0
1	OMG	Aa	852	1	18,26,27	0.99	1 (5%)	19,38,41	1.06	2 (10%)
1	OMU	Aa	1358	1	19,22,23	3.00	8 (42%)	26,31,34	1.71	5 (19%)
1	OMG	Aa	219	1	18,26,27	2.48	8 (44%)	19,38,41	1.48	4 (21%)
1	OMU	Aa	753	1	19,22,23	3.05	8 (42%)	26,31,34	1.70	4 (15%)
1	OMC	Aa	752	1	19,22,23	3.01	8 (42%)	26,31,34	0.71	0
27	OMG	BA	1329	27	18,26,27	2.47	8 (44%)	19,38,41	1.59	4 (21%)
1	LV2	Aa	918	1	20,23,24	0.89	0	26,33,36	0.81	0
1	OMG	Aa	1223	1	18,26,27	2.52	8 (44%)	19,38,41	1.51	4 (21%)
27	5MC	BA	2075	27	18,22,23	3.51	7 (38%)	26,32,35	1.04	2 (7%)
27	5MC	BA	2605	27	18,22,23	3.55	7 (38%)	26,32,35	1.12	2 (7%)
1	5MC	Aa	1476	1	18,22,23	3.52	7 (38%)	26,32,35	0.99	2 (7%)
1	OMG	Aa	891	1	18,26,27	2.48	8 (44%)	19,38,41	1.51	4 (21%)
27	OMG	BA	872	27	18,26,27	2.44	8 (44%)	19,38,41	1.47	3 (15%)
1	OMG	Aa	532	1	18,26,27	2.49	8 (44%)	19,38,41	1.51	4 (21%)
27	OMC	BA	2124	27	19,22,23	2.97	8 (42%)	26,31,34	0.66	0
27	A2M	BA	849	27	18,25,26	4.19	7 (38%)	18,36,39	3.00	3 (16%)
27	OMG	BA	1956	27	18,26,27	2.49	8 (44%)	19,38,41	1.52	4 (21%)
1	5MC	Aa	457	1	18,22,23	3.58	7 (38%)	26,32,35	1.01	2 (7%)
27	5MU	BA	2427	27	19,22,23	4.92	7 (36%)	28,32,35	3.62	9 (32%)
27	OMG	BA	2528	27	18,26,27	2.46	8 (44%)	19,38,41	1.48	4 (21%)
27	OMC	BA	2967	27	19,22,23	3.00	8 (42%)	26,31,34	0.73	0
27	OMG	BA	2379	27	18,26,27	2.48	8 (44%)	19,38,41	1.53	4 (21%)
27	5MC	BA	1965	27	18,22,23	3.55	7 (38%)	26,32,35	1.04	2 (7%)
1	5MC	Aa	340	1	18,22,23	3.56	7 (38%)	26,32,35	1.11	2 (7%)
27	OMC	BA	91	27	19,22,23	2.99	8 (42%)	26,31,34	0.69	0
27	OMG	BA	2550	27	18,26,27	1.08	1 (5%)	19,38,41	0.99	2 (10%)
1	OMG	Aa	913	1	18,26,27	2.51	8 (44%)	19,38,41	1.49	4 (21%)
1	5MC	Aa	1478	1	18,22,23	3.58	7 (38%)	26,32,35	1.11	2 (7%)
27	A2M	BA	2936	27	18,25,26	4.23	7 (38%)	18,36,39	2.92	3 (16%)
27	5MU	BA	875	27	19,22,23	4.92	7 (36%)	28,32,35	3.63	10 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	5MC	Aa	1352	1	18,22,23	3.59	7 (38%)	26,32,35	0.98	1 (3%)
27	OMU	BA	657	27	19,22,23	3.01	8 (42%)	26,31,34	1.70	4 (15%)
1	OMG	Aa	636	1	18,26,27	2.50	8 (44%)	19,38,41	1.48	4 (21%)
1	5MC	Aa	1306	1	18,22,23	3.55	7 (38%)	26,32,35	1.01	2 (7%)
27	OMG	BA	65	27	18,26,27	2.46	8 (44%)	19,38,41	1.51	4 (21%)
1	OMG	Aa	147	1	18,26,27	2.50	8 (44%)	19,38,41	1.51	4 (21%)
1	5MC	Aa	685	1	18,22,23	3.53	7 (38%)	26,32,35	1.04	2 (7%)
1	5MC	Aa	854	1	18,22,23	3.55	7 (38%)	26,32,35	1.05	2 (7%)
27	OMG	BA	507	27	18,26,27	2.47	8 (44%)	19,38,41	1.53	3 (15%)
27	OMG	BA	2745	27	18,26,27	2.45	8 (44%)	19,38,41	1.56	3 (15%)
1	OMG	Aa	498	1	18,26,27	2.50	8 (44%)	19,38,41	1.55	4 (21%)
27	OMC	BA	2107	27	19,22,23	2.99	8 (42%)	26,31,34	0.77	0
27	OMG	BA	1893	27	18,26,27	2.49	8 (44%)	19,38,41	1.56	4 (21%)
1	OMG	Aa	381	1	18,26,27	2.52	8 (44%)	19,38,41	1.53	4 (21%)
1	OMG	Aa	320	1	18,26,27	2.49	8 (44%)	19,38,41	1.54	4 (21%)
27	OMG	BA	2640	27	18,26,27	2.50	8 (44%)	19,38,41	1.52	4 (21%)
1	OMC	Aa	229	1	19,22,23	3.00	8 (42%)	26,31,34	0.78	0
27	OMU	BA	1480	27	19,22,23	3.04	8 (42%)	26,31,34	1.70	4 (15%)
27	OMG	BA	912	27	18,26,27	2.47	8 (44%)	19,38,41	1.50	4 (21%)
27	OMC	BA	2545	27	19,22,23	3.02	8 (42%)	26,31,34	0.76	0
27	5MC	BA	55	27	18,22,23	3.48	7 (38%)	26,32,35	1.17	3 (11%)
1	A2M	Aa	352	1	18,25,26	4.20	7 (38%)	18,36,39	3.03	3 (16%)
27	A2M	BA	505	27	18,25,26	4.22	7 (38%)	18,36,39	2.93	3 (16%)
1	OMC	Aa	1354	1	19,22,23	2.97	8 (42%)	26,31,34	0.77	0
27	OMU	BA	1776	27	19,22,23	3.02	8 (42%)	26,31,34	1.65	4 (15%)
1	6MZ	Aa	1449	1	18,25,26	0.88	1 (5%)	16,36,39	1.93	3 (18%)
27	OMG	BA	674	27	18,26,27	2.47	8 (44%)	19,38,41	1.54	4 (21%)
1	OMG	Aa	670	1	18,26,27	2.51	8 (44%)	19,38,41	1.56	4 (21%)
27	OMC	BA	342	27	19,22,23	0.84	0	26,31,34	0.98	1 (3%)
27	5MC	BA	2688	27	18,22,23	3.55	7 (38%)	26,32,35	1.04	1 (3%)
27	5MU	BA	829	27	19,22,23	4.86	7 (36%)	28,32,35	3.68	10 (35%)
27	OMG	BA	63	27	18,26,27	2.48	8 (44%)	19,38,41	1.57	4 (21%)
27	OMG	BA	2728	27	18,26,27	2.48	8 (44%)	19,38,41	1.50	4 (21%)
1	5MC	Aa	1006	1	18,22,23	3.57	7 (38%)	26,32,35	1.04	2 (7%)
1	OMU	Aa	479	1	19,22,23	3.07	8 (42%)	26,31,34	1.70	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	OMG	Aa	450	1	18,26,27	1.05	1 (5%)	19,38,41	1.11	2 (10%)
27	OMG	BA	2466	27	18,26,27	2.46	8 (44%)	19,38,41	1.47	3 (15%)
27	A2M	BA	879	27	18,25,26	4.24	7 (38%)	18,36,39	2.99	3 (16%)
1	5MC	Aa	1266	1	18,22,23	3.56	7 (38%)	26,32,35	1.02	2 (7%)
1	OMC	Aa	924	1	19,22,23	3.01	8 (42%)	26,31,34	0.73	0
27	5MU	BA	1766	27	19,22,23	4.88	7 (36%)	28,32,35	3.67	9 (32%)
1	OMU	Aa	1020	1	19,22,23	3.04	8 (42%)	26,31,34	1.67	5 (19%)
27	OMC	BA	1995	27	19,22,23	3.00	8 (42%)	26,31,34	0.74	0
27	OMU	BA	1969	27	19,22,23	3.05	8 (42%)	26,31,34	1.73	5 (19%)
1	OMC	Aa	1361	1	19,22,23	3.02	8 (42%)	26,31,34	0.74	0
27	A2M	BA	2091	27	18,25,26	0.92	1 (5%)	18,36,39	1.19	2 (11%)
27	OMG	BA	288	27	18,26,27	2.51	8 (44%)	19,38,41	1.53	4 (21%)
27	OMG	BA	2016	27	18,26,27	2.47	8 (44%)	19,38,41	1.48	4 (21%)
1	5MC	Aa	1007	1	18,22,23	3.57	7 (38%)	26,32,35	1.05	1 (3%)
1	OMG	Aa	770	1	18,26,27	2.49	8 (44%)	19,38,41	1.55	4 (21%)
27	4SU	BA	2553	27	18,21,22	1.75	4 (22%)	26,30,33	2.19	5 (19%)
1	5MU	Aa	917	1	19,22,23	1.36	4 (21%)	28,32,35	2.15	6 (21%)
27	OMU	BA	2656	27	19,22,23	3.03	8 (42%)	26,31,34	1.70	4 (15%)
1	OMG	Aa	121	1	18,26,27	2.48	8 (44%)	19,38,41	1.50	4 (21%)
1	2MG	Aa	995	1	18,26,27	0.89	1 (5%)	16,38,41	1.14	2 (12%)
27	OMG	BA	670	27	18,26,27	2.47	8 (44%)	19,38,41	1.65	5 (26%)
1	OMG	Aa	495	1	18,26,27	2.50	8 (44%)	19,38,41	1.52	4 (21%)
27	OMC	BA	869	27	19,22,23	2.97	8 (42%)	26,31,34	0.70	0
27	OMG	BA	2642	27	18,26,27	2.48	8 (44%)	19,38,41	1.64	4 (21%)
27	OMC	BA	1820	27	19,22,23	3.00	8 (42%)	26,31,34	0.71	0
27	OMG	BA	2010	27	18,26,27	2.46	8 (44%)	19,38,41	1.53	4 (21%)
27	5MC	BA	2055	27	18,22,23	3.57	7 (38%)	26,32,35	1.00	1 (3%)
1	MA6	Aa	1468	1	18,26,27	1.04	2 (11%)	19,38,41	3.63	2 (10%)

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	Aa	825	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	Aa	963	1	-	2/5/27/28	0/3/3/3
27	OMG	BA	215	27	-	0/5/27/28	0/3/3/3
27	5MU	BA	1854	27	-	0/7/25/26	0/2/2/2
27	5MC	BA	2070	27	-	0/7/25/26	0/2/2/2
1	MA6	Aa	1467	1	-	0/7/29/30	0/3/3/3
27	OMG	BA	1953	27	-	1/5/27/28	0/3/3/3
27	OMC	BA	2047	27	-	3/9/27/28	0/2/2/2
1	OMG	Aa	574	1	-	1/5/27/28	0/3/3/3
1	OMU	Aa	8	1	-	6/9/27/28	0/2/2/2
27	OMG	BA	365	27	-	3/5/27/28	0/3/3/3
27	4SU	BA	2581	27	-	1/7/25/26	0/2/2/2
1	OMG	Aa	446	1	-	0/5/27/28	0/3/3/3
1	5MC	Aa	464	1	-	0/7/25/26	0/2/2/2
1	5MC	Aa	349	1	-	0/7/25/26	0/2/2/2
27	OMG	BA	800	27	-	1/5/27/28	0/3/3/3
27	OMU	BA	2389	27	-	2/9/27/28	0/2/2/2
1	5MC	Aa	672	1	-	0/7/25/26	0/2/2/2
27	OMC	BA	2169	27	-	0/9/27/28	0/2/2/2
1	OMG	Aa	994	1	-	0/5/27/28	0/3/3/3
1	5MC	Aa	1004	1	-	3/7/25/26	0/2/2/2
27	OMU	BA	2542	27	-	2/9/27/28	0/2/2/2
27	OMG	BA	2521	27	-	1/5/27/28	0/3/3/3
27	A2M	BA	932	27	-	0/5/27/28	0/3/3/3
27	A2M	BA	2329	27	-	2/5/27/28	0/3/3/3
27	OMG	BA	2168	27	-	0/5/27/28	0/3/3/3
1	5MC	Aa	923	1	-	0/7/25/26	0/2/2/2
1	5MC	Aa	1003	1	-	0/7/25/26	0/2/2/2
27	OMC	BA	2595	27	-	1/9/27/28	0/2/2/2
1	OMG	Aa	1107	1	-	2/5/27/28	0/3/3/3
1	OMG	Aa	836	1	-	0/5/27/28	0/3/3/3
1	5MC	Aa	17	1	-	2/7/25/26	0/2/2/2
1	5MC	Aa	1184	1	-	0/7/25/26	0/2/2/2
1	5MC	Aa	1321	1	-	0/7/25/26	0/2/2/2
27	OMG	BA	833	27	-	0/5/27/28	0/3/3/3
1	5MC	Aa	473	1	-	0/7/25/26	0/2/2/2
27	OMU	BA	453	27	-	2/9/27/28	0/2/2/2
27	OMG	BA	1525	27	-	2/5/27/28	0/3/3/3
27	OMG	BA	584	27	-	0/5/27/28	0/3/3/3
27	OMG	BA	2870	27	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	OMU	BA	1402	27	-	2/9/27/28	0/2/2/2
1	OMG	Aa	629	1	-	0/5/27/28	0/3/3/3
1	OMG	Aa	659	1	-	1/5/27/28	0/3/3/3
27	OMG	BA	2672	27	-	0/5/27/28	0/3/3/3
27	5MC	BA	1345	27	-	1/7/25/26	0/2/2/2
27	OMG	BA	2353	27	-	2/5/27/28	0/3/3/3
27	OMG	BA	2469	27	-	4/5/27/28	0/3/3/3
27	OMG	BA	1508	27	-	0/5/27/28	0/3/3/3
27	OMG	BA	2527	27	-	2/5/27/28	0/3/3/3
27	OMU	BA	1150	27	-	2/9/27/28	0/2/2/2
27	OMC	BA	66	27	-	1/9/27/28	0/2/2/2
1	OMC	Aa	112	1	-	0/9/27/28	0/2/2/2
1	OMG	Aa	852	1	-	0/5/27/28	0/3/3/3
1	OMU	Aa	1358	1	-	0/9/27/28	0/2/2/2
1	OMG	Aa	219	1	-	2/5/27/28	0/3/3/3
1	OMU	Aa	753	1	-	1/9/27/28	0/2/2/2
1	OMC	Aa	752	1	-	0/9/27/28	0/2/2/2
27	OMG	BA	1329	27	-	0/5/27/28	0/3/3/3
1	LV2	Aa	918	1	-	0/9/29/30	0/2/2/2
1	OMG	Aa	1223	1	-	0/5/27/28	0/3/3/3
27	5MC	BA	2075	27	-	0/7/25/26	0/2/2/2
27	5MC	BA	2605	27	-	4/7/25/26	0/2/2/2
1	5MC	Aa	1476	1	-	0/7/25/26	0/2/2/2
1	OMG	Aa	891	1	-	1/5/27/28	0/3/3/3
27	OMG	BA	872	27	-	0/5/27/28	0/3/3/3
1	OMG	Aa	532	1	-	0/5/27/28	0/3/3/3
27	OMC	BA	2124	27	-	1/9/27/28	0/2/2/2
27	A2M	BA	849	27	-	2/5/27/28	0/3/3/3
27	OMG	BA	1956	27	-	2/5/27/28	0/3/3/3
1	5MC	Aa	457	1	-	2/7/25/26	0/2/2/2
27	5MU	BA	2427	27	-	0/7/25/26	0/2/2/2
27	OMG	BA	2528	27	-	0/5/27/28	0/3/3/3
27	OMC	BA	2967	27	-	0/9/27/28	0/2/2/2
27	OMG	BA	2379	27	-	2/5/27/28	0/3/3/3
27	5MC	BA	1965	27	-	0/7/25/26	0/2/2/2
1	5MC	Aa	340	1	-	3/7/25/26	0/2/2/2
27	OMC	BA	91	27	-	1/9/27/28	0/2/2/2
27	OMG	BA	2550	27	-	0/5/27/28	0/3/3/3
1	OMG	Aa	913	1	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	Aa	1478	1	-	5/7/25/26	0/2/2/2
27	A2M	BA	2936	27	-	1/5/27/28	0/3/3/3
27	5MU	BA	875	27	-	0/7/25/26	0/2/2/2
1	5MC	Aa	1352	1	-	2/7/25/26	0/2/2/2
27	OMU	BA	657	27	-	1/9/27/28	0/2/2/2
1	OMG	Aa	636	1	-	1/5/27/28	0/3/3/3
1	5MC	Aa	1306	1	-	3/7/25/26	0/2/2/2
27	OMG	BA	65	27	-	1/5/27/28	0/3/3/3
1	OMG	Aa	147	1	-	1/5/27/28	0/3/3/3
1	5MC	Aa	685	1	-	0/7/25/26	0/2/2/2
1	5MC	Aa	854	1	-	0/7/25/26	0/2/2/2
27	OMG	BA	507	27	-	0/5/27/28	0/3/3/3
27	OMG	BA	2745	27	-	0/5/27/28	0/3/3/3
1	OMG	Aa	498	1	-	2/5/27/28	0/3/3/3
27	OMC	BA	2107	27	-	0/9/27/28	0/2/2/2
27	OMG	BA	1893	27	-	2/5/27/28	0/3/3/3
1	OMG	Aa	381	1	-	2/5/27/28	0/3/3/3
1	OMG	Aa	320	1	-	3/5/27/28	0/3/3/3
27	OMG	BA	2640	27	-	3/5/27/28	0/3/3/3
1	OMC	Aa	229	1	-	1/9/27/28	0/2/2/2
27	OMU	BA	1480	27	-	0/9/27/28	0/2/2/2
27	OMG	BA	912	27	-	1/5/27/28	0/3/3/3
27	OMC	BA	2545	27	-	3/9/27/28	0/2/2/2
27	5MC	BA	55	27	-	3/7/25/26	0/2/2/2
1	A2M	Aa	352	1	-	2/5/27/28	0/3/3/3
27	A2M	BA	505	27	-	0/5/27/28	0/3/3/3
1	OMC	Aa	1354	1	-	0/9/27/28	0/2/2/2
27	OMU	BA	1776	27	-	1/9/27/28	0/2/2/2
1	6MZ	Aa	1449	1	-	2/5/27/28	0/3/3/3
27	OMG	BA	674	27	-	2/5/27/28	0/3/3/3
1	OMG	Aa	670	1	-	2/5/27/28	0/3/3/3
27	OMC	BA	342	27	-	2/9/27/28	0/2/2/2
27	5MC	BA	2688	27	-	0/7/25/26	0/2/2/2
27	5MU	BA	829	27	-	0/7/25/26	0/2/2/2
27	OMG	BA	63	27	-	0/5/27/28	0/3/3/3
27	OMG	BA	2728	27	-	1/5/27/28	0/3/3/3
1	5MC	Aa	1006	1	-	0/7/25/26	0/2/2/2
1	OMU	Aa	479	1	-	0/9/27/28	0/2/2/2
1	OMG	Aa	450	1	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	OMG	BA	2466	27	-	0/5/27/28	0/3/3/3
27	A2M	BA	879	27	-	1/5/27/28	0/3/3/3
1	5MC	Aa	1266	1	-	0/7/25/26	0/2/2/2
1	OMC	Aa	924	1	-	1/9/27/28	0/2/2/2
27	5MU	BA	1766	27	-	0/7/25/26	0/2/2/2
1	OMU	Aa	1020	1	-	1/9/27/28	0/2/2/2
27	OMC	BA	1995	27	-	1/9/27/28	0/2/2/2
27	OMU	BA	1969	27	-	0/9/27/28	0/2/2/2
1	OMC	Aa	1361	1	-	1/9/27/28	0/2/2/2
27	A2M	BA	2091	27	-	0/5/27/28	0/3/3/3
27	OMG	BA	288	27	-	1/5/27/28	0/3/3/3
27	OMG	BA	2016	27	-	2/5/27/28	0/3/3/3
1	5MC	Aa	1007	1	-	2/7/25/26	0/2/2/2
1	OMG	Aa	770	1	-	0/5/27/28	0/3/3/3
27	4SU	BA	2553	27	-	0/7/25/26	0/2/2/2
1	5MU	Aa	917	1	-	2/7/25/26	0/2/2/2
27	OMU	BA	2656	27	-	0/9/27/28	0/2/2/2
1	OMG	Aa	121	1	-	2/5/27/28	0/3/3/3
1	2MG	Aa	995	1	-	0/5/27/28	0/3/3/3
27	OMG	BA	670	27	-	1/5/27/28	0/3/3/3
1	OMG	Aa	495	1	-	2/5/27/28	0/3/3/3
27	OMC	BA	869	27	-	0/9/27/28	0/2/2/2
27	OMG	BA	2642	27	-	3/5/27/28	0/3/3/3
27	OMC	BA	1820	27	-	1/9/27/28	0/2/2/2
27	OMG	BA	2010	27	-	0/5/27/28	0/3/3/3
27	5MC	BA	2055	27	-	0/7/25/26	0/2/2/2
1	MA6	Aa	1468	1	-	1/7/29/30	0/3/3/3

All (1024) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	932	A2M	O4'-C1'	15.41	1.62	1.41
27	BA	879	A2M	O4'-C1'	15.29	1.62	1.41
27	BA	2936	A2M	O4'-C1'	15.28	1.62	1.41
27	BA	505	A2M	O4'-C1'	15.18	1.62	1.41
1	Aa	352	A2M	O4'-C1'	15.09	1.62	1.41
27	BA	849	A2M	O4'-C1'	15.07	1.62	1.41
27	BA	875	5MU	C2-N1	11.41	1.56	1.38
27	BA	2427	5MU	C2-N1	11.33	1.56	1.38
27	BA	1854	5MU	C2-N1	11.29	1.56	1.38
27	BA	829	5MU	C2-N1	11.25	1.56	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	1766	5MU	C2-N1	11.22	1.56	1.38
27	BA	875	5MU	C6-N1	10.84	1.56	1.38
27	BA	2427	5MU	C6-N1	10.81	1.56	1.38
27	BA	1766	5MU	C6-N1	10.65	1.56	1.38
27	BA	829	5MU	C6-N1	10.63	1.56	1.38
27	BA	1854	5MU	C6-N1	10.60	1.56	1.38
27	BA	875	5MU	C4-C5	10.00	1.61	1.44
27	BA	829	5MU	C4-C5	9.93	1.61	1.44
27	BA	1766	5MU	C4-C5	9.90	1.61	1.44
27	BA	2427	5MU	C4-C5	9.89	1.61	1.44
27	BA	1854	5MU	C4-C5	9.88	1.61	1.44
27	BA	2581	4SU	C2-N1	9.25	1.53	1.38
27	BA	1965	5MC	C6-C5	9.24	1.49	1.34
1	Aa	1004	5MC	C6-C5	9.23	1.49	1.34
27	BA	2055	5MC	C6-C5	9.22	1.49	1.34
27	BA	2605	5MC	C6-C5	9.21	1.49	1.34
1	Aa	1352	5MC	C6-C5	9.20	1.49	1.34
1	Aa	854	5MC	C6-C5	9.17	1.49	1.34
1	Aa	1007	5MC	C6-C5	9.17	1.49	1.34
1	Aa	1003	5MC	C6-C5	9.15	1.49	1.34
1	Aa	1478	5MC	C6-C5	9.15	1.49	1.34
27	BA	2688	5MC	C6-C5	9.15	1.49	1.34
27	BA	1345	5MC	C6-C5	9.14	1.49	1.34
1	Aa	457	5MC	C6-C5	9.11	1.49	1.34
1	Aa	1006	5MC	C6-C5	9.09	1.49	1.34
1	Aa	1184	5MC	C6-C5	9.08	1.49	1.34
1	Aa	464	5MC	C6-C5	9.07	1.49	1.34
1	Aa	672	5MC	C6-C5	9.07	1.49	1.34
1	Aa	685	5MC	C6-C5	9.05	1.49	1.34
1	Aa	340	5MC	C6-C5	9.05	1.49	1.34
1	Aa	923	5MC	C6-C5	9.04	1.49	1.34
1	Aa	473	5MC	C6-C5	9.04	1.49	1.34
1	Aa	1306	5MC	C6-C5	9.03	1.49	1.34
1	Aa	1266	5MC	C6-C5	9.01	1.49	1.34
1	Aa	1476	5MC	C6-C5	9.00	1.49	1.34
27	BA	2075	5MC	C6-C5	8.97	1.49	1.34
1	Aa	349	5MC	C6-C5	8.96	1.49	1.34
27	BA	2070	5MC	C6-C5	8.96	1.49	1.34
27	BA	55	5MC	C6-C5	8.94	1.49	1.34
1	Aa	17	5MC	C6-C5	8.93	1.49	1.34
1	Aa	1321	5MC	C6-C5	8.92	1.49	1.34
27	BA	2581	4SU	C4-N3	8.37	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	1854	5MU	C4-N3	-7.50	1.24	1.38
27	BA	2427	5MU	C4-N3	-7.44	1.25	1.38
27	BA	1766	5MU	C4-N3	-7.42	1.25	1.38
27	BA	829	5MU	C4-N3	-7.31	1.25	1.38
1	Aa	479	OMU	C2-N1	7.22	1.50	1.38
27	BA	875	5MU	C4-N3	-7.21	1.25	1.38
1	Aa	753	OMU	C2-N1	7.16	1.49	1.38
27	BA	1480	OMU	C2-N1	7.16	1.49	1.38
27	BA	2656	OMU	C2-N1	7.16	1.49	1.38
27	BA	1150	OMU	C2-N1	7.15	1.49	1.38
27	BA	1402	OMU	C2-N1	7.14	1.49	1.38
27	BA	453	OMU	C2-N1	7.14	1.49	1.38
27	BA	2542	OMU	C2-N1	7.11	1.49	1.38
1	Aa	1020	OMU	C2-N1	7.10	1.49	1.38
27	BA	1776	OMU	C2-N1	7.09	1.49	1.38
1	Aa	8	OMU	C2-N1	7.05	1.49	1.38
27	BA	657	OMU	C2-N1	7.04	1.49	1.38
27	BA	1969	OMU	C2-N1	7.03	1.49	1.38
1	Aa	1358	OMU	C2-N1	6.99	1.49	1.38
27	BA	2581	4SU	C2-N3	6.89	1.50	1.38
27	BA	2581	4SU	C5-C4	6.82	1.51	1.42
1	Aa	1020	OMU	C2-N3	6.76	1.50	1.38
27	BA	1969	OMU	C2-N3	6.75	1.50	1.38
27	BA	1402	OMU	C2-N3	6.75	1.50	1.38
1	Aa	753	OMU	C2-N3	6.74	1.50	1.38
1	Aa	479	OMU	C2-N3	6.74	1.50	1.38
27	BA	453	OMU	C2-N3	6.68	1.49	1.38
27	BA	1776	OMU	C2-N3	6.67	1.49	1.38
27	BA	2656	OMU	C2-N3	6.64	1.49	1.38
1	Aa	1358	OMU	C2-N3	6.62	1.49	1.38
1	Aa	8	OMU	C2-N3	6.62	1.49	1.38
1	Aa	464	5MC	C4-N3	6.60	1.45	1.34
27	BA	1480	OMU	C2-N3	6.59	1.49	1.38
1	Aa	1352	5MC	C4-N3	6.59	1.45	1.34
27	BA	657	OMU	C2-N3	6.59	1.49	1.38
27	BA	2542	OMU	C2-N3	6.57	1.49	1.38
1	Aa	457	5MC	C4-N3	6.55	1.45	1.34
27	BA	2427	5MU	C6-C5	6.53	1.45	1.34
27	BA	875	5MU	C6-C5	6.51	1.45	1.34
27	BA	1150	OMU	C2-N3	6.51	1.49	1.38
1	Aa	1266	5MC	C4-N3	6.49	1.45	1.34
1	Aa	1006	5MC	C4-N3	6.47	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	1184	5MC	C4-N3	6.46	1.45	1.34
1	Aa	340	5MC	C4-N3	6.46	1.45	1.34
1	Aa	1306	5MC	C4-N3	6.46	1.45	1.34
1	Aa	1003	5MC	C4-N3	6.46	1.45	1.34
1	Aa	1004	5MC	C4-N3	6.46	1.45	1.34
1	Aa	923	5MC	C4-N3	6.44	1.45	1.34
1	Aa	1321	5MC	C4-N3	6.44	1.45	1.34
27	BA	1345	5MC	C4-N3	6.43	1.45	1.34
1	Aa	1478	5MC	C4-N3	6.43	1.45	1.34
1	Aa	349	5MC	C4-N3	6.43	1.45	1.34
1	Aa	1361	OMC	C2-N3	6.41	1.49	1.36
27	BA	2967	OMC	C2-N3	6.40	1.49	1.36
27	BA	2581	4SU	C6-C5	6.38	1.49	1.35
27	BA	91	OMC	C2-N3	6.38	1.49	1.36
27	BA	932	A2M	O4'-C4'	-6.37	1.30	1.45
1	Aa	473	5MC	C4-N3	6.37	1.44	1.34
1	Aa	112	OMC	C2-N3	6.36	1.49	1.36
1	Aa	1007	5MC	C4-N3	6.36	1.44	1.34
27	BA	2055	5MC	C4-N3	6.36	1.44	1.34
1	Aa	352	A2M	O4'-C4'	-6.36	1.30	1.45
1	Aa	924	OMC	C2-N3	6.35	1.49	1.36
27	BA	2688	5MC	C4-N3	6.35	1.44	1.34
27	BA	2595	OMC	C2-N3	6.35	1.49	1.36
27	BA	2545	OMC	C2-N3	6.35	1.49	1.36
1	Aa	17	5MC	C4-N3	6.35	1.44	1.34
27	BA	1995	OMC	C2-N3	6.35	1.49	1.36
27	BA	2075	5MC	C4-N3	6.34	1.44	1.34
1	Aa	672	5MC	C4-N3	6.34	1.44	1.34
27	BA	1820	OMC	C2-N3	6.34	1.49	1.36
1	Aa	1476	5MC	C4-N3	6.33	1.44	1.34
27	BA	505	A2M	O4'-C4'	-6.33	1.30	1.45
1	Aa	229	OMC	C2-N3	6.33	1.49	1.36
1	Aa	685	5MC	C4-N3	6.32	1.44	1.34
1	Aa	752	OMC	C2-N3	6.31	1.49	1.36
1	Aa	854	5MC	C4-N3	6.31	1.44	1.34
27	BA	1766	5MU	C6-C5	6.31	1.45	1.34
27	BA	2070	5MC	C4-N3	6.30	1.44	1.34
27	BA	869	OMC	C2-N3	6.30	1.49	1.36
27	BA	2107	OMC	C2-N3	6.29	1.49	1.36
27	BA	2169	OMC	C2-N3	6.28	1.49	1.36
27	BA	1854	5MU	C6-C5	6.28	1.44	1.34
27	BA	2124	OMC	C2-N3	6.27	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	55	5MC	C4-N3	6.25	1.44	1.34
27	BA	2605	5MC	C4-N3	6.25	1.44	1.34
27	BA	2047	OMC	C2-N3	6.23	1.49	1.36
27	BA	879	A2M	O4'-C4'	-6.21	1.31	1.45
1	Aa	1354	OMC	C2-N3	6.20	1.48	1.36
27	BA	66	OMC	C2-N3	6.20	1.48	1.36
1	Aa	825	OMC	C2-N3	6.20	1.48	1.36
27	BA	2936	A2M	O4'-C4'	-6.20	1.31	1.45
27	BA	1965	5MC	C4-N3	6.19	1.44	1.34
27	BA	849	A2M	O4'-C4'	-6.19	1.31	1.45
1	Aa	457	5MC	C2-N3	6.17	1.48	1.36
27	BA	829	5MU	C6-C5	6.17	1.44	1.34
1	Aa	464	5MC	C2-N3	6.17	1.48	1.36
1	Aa	1266	5MC	C2-N3	6.13	1.48	1.36
27	BA	2595	OMC	C6-C5	6.12	1.49	1.35
1	Aa	1006	5MC	C2-N3	6.12	1.48	1.36
27	BA	2545	OMC	C6-C5	6.10	1.49	1.35
1	Aa	1352	5MC	C2-N3	6.09	1.48	1.36
1	Aa	1184	5MC	C2-N3	6.09	1.48	1.36
1	Aa	340	5MC	C2-N3	6.08	1.48	1.36
1	Aa	924	OMC	C6-C5	6.05	1.49	1.35
1	Aa	349	5MC	C2-N3	6.05	1.48	1.36
1	Aa	1004	5MC	C2-N3	6.05	1.48	1.36
1	Aa	923	5MC	C2-N3	6.04	1.48	1.36
27	BA	2055	5MC	C2-N3	6.03	1.48	1.36
1	Aa	1478	5MC	C2-N3	6.02	1.48	1.36
1	Aa	1306	5MC	C2-N3	6.02	1.48	1.36
1	Aa	229	OMC	C6-C5	6.02	1.49	1.35
1	Aa	17	5MC	C2-N3	6.01	1.48	1.36
1	Aa	1007	5MC	C2-N3	6.01	1.48	1.36
1	Aa	854	5MC	C2-N3	6.01	1.48	1.36
1	Aa	752	OMC	C6-C5	6.01	1.49	1.35
1	Aa	1354	OMC	C6-C5	6.01	1.49	1.35
27	BA	2075	5MC	C2-N3	6.00	1.48	1.36
1	Aa	1003	5MC	C2-N3	6.00	1.48	1.36
1	Aa	473	5MC	C2-N3	6.00	1.48	1.36
1	Aa	1361	OMC	C6-C5	6.00	1.49	1.35
1	Aa	672	5MC	C2-N3	5.99	1.48	1.36
27	BA	1995	OMC	C6-C5	5.98	1.49	1.35
27	BA	1820	OMC	C6-C5	5.98	1.49	1.35
1	Aa	825	OMC	C6-C5	5.98	1.48	1.35
1	Aa	1476	5MC	C2-N3	5.97	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	112	OMC	C6-C5	5.97	1.48	1.35
27	BA	2047	OMC	C6-C5	5.96	1.48	1.35
27	BA	2688	5MC	C2-N3	5.96	1.48	1.36
27	BA	869	OMC	C6-C5	5.95	1.48	1.35
27	BA	1345	5MC	C2-N3	5.95	1.48	1.36
27	BA	1965	5MC	C2-N3	5.95	1.48	1.36
27	BA	2107	OMC	C6-C5	5.94	1.48	1.35
1	Aa	1321	5MC	C2-N3	5.94	1.48	1.36
27	BA	2169	OMC	C6-C5	5.94	1.48	1.35
27	BA	2124	OMC	C6-C5	5.94	1.48	1.35
27	BA	91	OMC	C6-C5	5.93	1.48	1.35
27	BA	2605	5MC	C2-N3	5.92	1.48	1.36
27	BA	2967	OMC	C6-C5	5.92	1.48	1.35
27	BA	66	OMC	C6-C5	5.91	1.48	1.35
1	Aa	685	5MC	C2-N3	5.91	1.48	1.36
27	BA	2070	5MC	C2-N3	5.90	1.48	1.36
27	BA	55	5MC	C2-N3	5.85	1.48	1.36
1	Aa	479	OMU	C6-C5	5.78	1.48	1.35
27	BA	1150	OMU	C6-C5	5.72	1.48	1.35
1	Aa	1020	OMU	C6-C5	5.72	1.48	1.35
1	Aa	8	OMU	C6-C5	5.71	1.48	1.35
27	BA	1969	OMU	C6-C5	5.69	1.48	1.35
1	Aa	1358	OMU	C6-C5	5.69	1.48	1.35
27	BA	1402	OMU	C6-C5	5.68	1.48	1.35
27	BA	1480	OMU	C6-C5	5.65	1.48	1.35
1	Aa	753	OMU	C6-C5	5.64	1.48	1.35
27	BA	2656	OMU	C6-C5	5.63	1.48	1.35
27	BA	2542	OMU	C6-C5	5.60	1.48	1.35
1	Aa	636	OMG	C2-N3	5.60	1.46	1.33
1	Aa	963	OMG	C2-N3	5.59	1.46	1.33
27	BA	1776	OMU	C6-C5	5.59	1.48	1.35
1	Aa	1223	OMG	C2-N3	5.59	1.46	1.33
1	Aa	670	OMG	C2-N3	5.58	1.46	1.33
1	Aa	1107	OMG	C2-N3	5.58	1.46	1.33
27	BA	2640	OMG	C2-N3	5.56	1.46	1.33
27	BA	657	OMU	C6-C5	5.56	1.48	1.35
1	Aa	994	OMG	C2-N3	5.55	1.46	1.33
27	BA	1508	OMG	C2-N3	5.55	1.46	1.33
27	BA	453	OMU	C6-C5	5.54	1.47	1.35
1	Aa	147	OMG	C2-N3	5.54	1.46	1.33
27	BA	288	OMG	C2-N3	5.54	1.46	1.33
1	Aa	659	OMG	C2-N3	5.54	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	629	OMG	C2-N3	5.53	1.46	1.33
1	Aa	381	OMG	C2-N3	5.52	1.46	1.33
27	BA	584	OMG	C2-N3	5.52	1.46	1.33
27	BA	1893	OMG	C2-N3	5.52	1.46	1.33
1	Aa	574	OMG	C2-N3	5.51	1.46	1.33
1	Aa	913	OMG	C2-N3	5.50	1.46	1.33
27	BA	670	OMG	C2-N3	5.50	1.46	1.33
27	BA	1956	OMG	C2-N3	5.49	1.46	1.33
27	BA	365	OMG	C2-N3	5.49	1.46	1.33
1	Aa	498	OMG	C2-N3	5.48	1.46	1.33
1	Aa	121	OMG	C2-N3	5.48	1.46	1.33
1	Aa	836	OMG	C2-N3	5.47	1.46	1.33
27	BA	833	OMG	C2-N3	5.47	1.46	1.33
1	Aa	770	OMG	C2-N3	5.47	1.46	1.33
1	Aa	891	OMG	C2-N3	5.47	1.46	1.33
27	BA	215	OMG	C2-N3	5.46	1.46	1.33
27	BA	2527	OMG	C2-N3	5.46	1.46	1.33
27	BA	2469	OMG	C2-N3	5.46	1.46	1.33
1	Aa	219	OMG	C2-N3	5.45	1.46	1.33
27	BA	2016	OMG	C2-N3	5.45	1.46	1.33
1	Aa	446	OMG	C2-N3	5.44	1.46	1.33
1	Aa	495	OMG	C2-N3	5.44	1.46	1.33
27	BA	2672	OMG	C2-N3	5.44	1.46	1.33
27	BA	872	OMG	C2-N3	5.44	1.46	1.33
27	BA	912	OMG	C2-N3	5.44	1.46	1.33
27	BA	2642	OMG	C2-N3	5.43	1.46	1.33
27	BA	65	OMG	C2-N3	5.43	1.46	1.33
27	BA	1329	OMG	C2-N3	5.43	1.46	1.33
1	Aa	532	OMG	C2-N3	5.43	1.46	1.33
1	Aa	320	OMG	C2-N3	5.42	1.46	1.33
27	BA	1525	OMG	C2-N3	5.42	1.46	1.33
27	BA	2466	OMG	C2-N3	5.41	1.46	1.33
27	BA	63	OMG	C2-N3	5.41	1.46	1.33
27	BA	2168	OMG	C2-N3	5.39	1.46	1.33
27	BA	2010	OMG	C2-N3	5.39	1.46	1.33
27	BA	2728	OMG	C2-N3	5.39	1.46	1.33
27	BA	2379	OMG	C2-N3	5.38	1.46	1.33
27	BA	800	OMG	C2-N3	5.38	1.46	1.33
27	BA	1953	OMG	C2-N3	5.38	1.46	1.33
27	BA	2528	OMG	C2-N3	5.37	1.46	1.33
27	BA	2870	OMG	C2-N3	5.37	1.46	1.33
27	BA	2521	OMG	C2-N3	5.35	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	674	OMG	C2-N3	5.35	1.46	1.33
27	BA	507	OMG	C2-N3	5.35	1.46	1.33
27	BA	2745	OMG	C2-N3	5.34	1.46	1.33
1	Aa	752	OMC	C4-N3	5.19	1.44	1.34
1	Aa	1361	OMC	C4-N3	5.18	1.44	1.34
27	BA	2967	OMC	C4-N3	5.17	1.44	1.34
1	Aa	924	OMC	C4-N3	5.16	1.44	1.34
27	BA	1820	OMC	C4-N3	5.15	1.44	1.34
27	BA	2595	OMC	C4-N3	5.14	1.44	1.34
27	BA	1995	OMC	C4-N3	5.10	1.44	1.34
1	Aa	229	OMC	C4-N3	5.09	1.44	1.34
1	Aa	112	OMC	C4-N3	5.08	1.44	1.34
27	BA	91	OMC	C4-N3	5.07	1.44	1.34
27	BA	2107	OMC	C4-N3	5.07	1.44	1.34
27	BA	2169	OMC	C4-N3	5.06	1.44	1.34
27	BA	2545	OMC	C4-N3	5.05	1.44	1.34
27	BA	2124	OMC	C4-N3	5.05	1.44	1.34
27	BA	66	OMC	C4-N3	5.04	1.44	1.34
1	Aa	825	OMC	C4-N3	5.02	1.44	1.34
1	Aa	1354	OMC	C4-N3	5.00	1.44	1.34
27	BA	869	OMC	C4-N3	4.97	1.44	1.34
27	BA	2047	OMC	C4-N3	4.96	1.44	1.34
1	Aa	1361	OMC	C4-N4	4.92	1.45	1.33
27	BA	1995	OMC	C4-N4	4.89	1.45	1.33
1	Aa	825	OMC	C4-N4	4.88	1.45	1.33
27	BA	2107	OMC	C4-N4	4.88	1.45	1.33
27	BA	2595	OMC	C4-N4	4.88	1.45	1.33
1	Aa	924	OMC	C4-N4	4.87	1.45	1.33
27	BA	2967	OMC	C4-N4	4.87	1.45	1.33
27	BA	91	OMC	C4-N4	4.85	1.45	1.33
1	Aa	752	OMC	C4-N4	4.84	1.45	1.33
1	Aa	229	OMC	C4-N4	4.84	1.45	1.33
1	Aa	963	OMG	C4-N3	4.84	1.49	1.37
27	BA	2545	OMC	C4-N4	4.84	1.45	1.33
1	Aa	994	OMG	C4-N3	4.83	1.49	1.37
1	Aa	1354	OMC	C4-N4	4.83	1.45	1.33
1	Aa	495	OMG	C4-N3	4.83	1.49	1.37
1	Aa	1107	OMG	C4-N3	4.83	1.49	1.37
1	Aa	112	OMC	C4-N4	4.83	1.45	1.33
1	Aa	1223	OMG	C4-N3	4.82	1.49	1.37
1	Aa	629	OMG	C4-N3	4.82	1.49	1.37
27	BA	2047	OMC	C4-N4	4.82	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	288	OMG	C4-N3	4.82	1.49	1.37
27	BA	833	OMG	C4-N3	4.82	1.49	1.37
27	BA	2169	OMC	C4-N4	4.82	1.45	1.33
1	Aa	574	OMG	C4-N3	4.81	1.49	1.37
27	BA	66	OMC	C4-N4	4.81	1.45	1.33
1	Aa	636	OMG	C4-N3	4.81	1.49	1.37
1	Aa	147	OMG	C4-N3	4.80	1.49	1.37
1	Aa	381	OMG	C4-N3	4.80	1.49	1.37
27	BA	2016	OMG	C4-N3	4.80	1.49	1.37
27	BA	584	OMG	C4-N3	4.79	1.49	1.37
1	Aa	498	OMG	C4-N3	4.79	1.49	1.37
27	BA	1508	OMG	C4-N3	4.79	1.49	1.37
1	Aa	836	OMG	C4-N3	4.78	1.49	1.37
27	BA	1820	OMC	C4-N4	4.78	1.45	1.33
1	Aa	670	OMG	C4-N3	4.78	1.49	1.37
1	Aa	659	OMG	C4-N3	4.78	1.49	1.37
27	BA	63	OMG	C4-N3	4.78	1.49	1.37
27	BA	1525	OMG	C4-N3	4.78	1.49	1.37
27	BA	365	OMG	C4-N3	4.78	1.49	1.37
1	Aa	913	OMG	C4-N3	4.78	1.49	1.37
27	BA	869	OMC	C4-N4	4.77	1.45	1.33
1	Aa	320	OMG	C4-N3	4.77	1.48	1.37
27	BA	2642	OMG	C4-N3	4.77	1.48	1.37
27	BA	2640	OMG	C4-N3	4.76	1.48	1.37
27	BA	2466	OMG	C4-N3	4.76	1.48	1.37
27	BA	2469	OMG	C4-N3	4.76	1.48	1.37
27	BA	912	OMG	C4-N3	4.76	1.48	1.37
1	Aa	121	OMG	C4-N3	4.76	1.48	1.37
27	BA	2672	OMG	C4-N3	4.76	1.48	1.37
27	BA	1956	OMG	C4-N3	4.75	1.48	1.37
1	Aa	891	OMG	C4-N3	4.75	1.48	1.37
27	BA	215	OMG	C4-N3	4.75	1.48	1.37
27	BA	2124	OMC	C4-N4	4.75	1.45	1.33
27	BA	800	OMG	C4-N3	4.75	1.48	1.37
1	Aa	219	OMG	C4-N3	4.75	1.48	1.37
27	BA	65	OMG	C4-N3	4.75	1.48	1.37
27	BA	2527	OMG	C4-N3	4.74	1.48	1.37
27	BA	1893	OMG	C4-N3	4.74	1.48	1.37
1	Aa	770	OMG	C4-N3	4.73	1.48	1.37
27	BA	2010	OMG	C4-N3	4.73	1.48	1.37
27	BA	2168	OMG	C4-N3	4.73	1.48	1.37
1	Aa	532	OMG	C4-N3	4.73	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2528	OMG	C4-N3	4.73	1.48	1.37
27	BA	1329	OMG	C4-N3	4.73	1.48	1.37
1	Aa	446	OMG	C4-N3	4.72	1.48	1.37
27	BA	674	OMG	C4-N3	4.71	1.48	1.37
27	BA	670	OMG	C4-N3	4.71	1.48	1.37
27	BA	2745	OMG	C4-N3	4.71	1.48	1.37
27	BA	2870	OMG	C4-N3	4.70	1.48	1.37
27	BA	2379	OMG	C4-N3	4.70	1.48	1.37
27	BA	507	OMG	C4-N3	4.70	1.48	1.37
27	BA	2521	OMG	C4-N3	4.69	1.48	1.37
27	BA	2728	OMG	C4-N3	4.68	1.48	1.37
27	BA	872	OMG	C4-N3	4.64	1.48	1.37
1	Aa	1478	5MC	C6-N1	4.60	1.45	1.38
1	Aa	464	5MC	C6-N1	4.58	1.45	1.38
27	BA	2055	5MC	C6-N1	4.57	1.45	1.38
27	BA	1953	OMG	C4-N3	4.57	1.48	1.37
27	BA	2595	OMC	C2-N1	4.56	1.49	1.40
27	BA	1965	5MC	C6-N1	4.55	1.45	1.38
1	Aa	1004	5MC	C6-N1	4.55	1.45	1.38
1	Aa	672	5MC	C6-N1	4.53	1.45	1.38
1	Aa	1306	5MC	C6-N1	4.53	1.45	1.38
27	BA	66	OMC	C2-N1	4.53	1.49	1.40
1	Aa	1007	5MC	C6-N1	4.52	1.45	1.38
1	Aa	1476	5MC	C6-N1	4.51	1.45	1.38
1	Aa	1006	5MC	C6-N1	4.51	1.45	1.38
27	BA	2605	5MC	C6-N1	4.51	1.45	1.38
1	Aa	685	5MC	C6-N1	4.51	1.45	1.38
27	BA	1820	OMC	C2-N1	4.50	1.49	1.40
1	Aa	1184	5MC	C6-N1	4.49	1.45	1.38
27	BA	2688	5MC	C6-N1	4.49	1.45	1.38
1	Aa	1352	5MC	C6-N1	4.49	1.45	1.38
1	Aa	1361	OMC	C2-N1	4.49	1.49	1.40
1	Aa	457	5MC	C6-N1	4.49	1.45	1.38
27	BA	2545	OMC	C2-N1	4.48	1.49	1.40
1	Aa	229	OMC	C2-N1	4.48	1.49	1.40
1	Aa	473	5MC	C6-N1	4.47	1.45	1.38
1	Aa	112	OMC	C2-N1	4.47	1.49	1.40
1	Aa	854	5MC	C6-N1	4.47	1.45	1.38
1	Aa	340	5MC	C6-N1	4.46	1.45	1.38
27	BA	1345	5MC	C6-N1	4.46	1.45	1.38
1	Aa	752	OMC	C2-N1	4.45	1.49	1.40
27	BA	2967	OMC	C2-N1	4.45	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	1266	5MC	C6-N1	4.45	1.45	1.38
1	Aa	349	5MC	C6-N1	4.45	1.45	1.38
1	Aa	1003	5MC	C6-N1	4.43	1.45	1.38
27	BA	2070	5MC	C6-N1	4.42	1.45	1.38
1	Aa	923	5MC	C6-N1	4.42	1.45	1.38
27	BA	2047	OMC	C2-N1	4.41	1.49	1.40
1	Aa	825	OMC	C2-N1	4.41	1.49	1.40
1	Aa	924	OMC	C2-N1	4.41	1.49	1.40
27	BA	1995	OMC	C2-N1	4.41	1.49	1.40
27	BA	2107	OMC	C2-N1	4.40	1.49	1.40
27	BA	869	OMC	C2-N1	4.40	1.49	1.40
1	Aa	1352	5MC	C4-N4	4.39	1.45	1.34
27	BA	2169	OMC	C2-N1	4.39	1.49	1.40
1	Aa	17	5MC	C6-N1	4.39	1.45	1.38
27	BA	2581	4SU	C4-S4	-4.37	1.60	1.68
27	BA	91	OMC	C2-N1	4.37	1.49	1.40
27	BA	2124	OMC	C2-N1	4.37	1.49	1.40
1	Aa	1478	5MC	C2-N1	4.36	1.49	1.40
1	Aa	1266	5MC	C4-N4	4.36	1.45	1.34
1	Aa	1003	5MC	C4-N4	4.36	1.45	1.34
1	Aa	464	5MC	C4-N4	4.35	1.45	1.34
1	Aa	457	5MC	C4-N4	4.35	1.45	1.34
27	BA	2688	5MC	C4-N4	4.35	1.45	1.34
1	Aa	1004	5MC	C4-N4	4.35	1.45	1.34
27	BA	2605	5MC	C4-N4	4.35	1.45	1.34
27	BA	2075	5MC	C6-N1	4.34	1.45	1.38
1	Aa	923	5MC	C4-N4	4.34	1.45	1.34
1	Aa	1006	5MC	C4-N4	4.34	1.45	1.34
1	Aa	464	5MC	C2-N1	4.33	1.49	1.40
1	Aa	1306	5MC	C4-N4	4.33	1.45	1.34
1	Aa	349	5MC	C4-N4	4.33	1.45	1.34
1	Aa	473	5MC	C4-N4	4.33	1.45	1.34
27	BA	2553	4SU	C4-S4	-4.33	1.60	1.68
27	BA	1345	5MC	C4-N4	4.33	1.45	1.34
1	Aa	1007	5MC	C4-N4	4.32	1.45	1.34
27	BA	2055	5MC	C4-N4	4.32	1.45	1.34
1	Aa	1321	5MC	C4-N4	4.32	1.45	1.34
1	Aa	854	5MC	C4-N4	4.31	1.45	1.34
1	Aa	340	5MC	C2-N1	4.31	1.49	1.40
27	BA	1965	5MC	C4-N4	4.30	1.45	1.34
1	Aa	1321	5MC	C6-N1	4.30	1.45	1.38
1	Aa	1184	5MC	C4-N4	4.30	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2070	5MC	C4-N4	4.30	1.45	1.34
27	BA	2075	5MC	C4-N4	4.30	1.45	1.34
1	Aa	685	5MC	C4-N4	4.30	1.45	1.34
1	Aa	1354	OMC	C2-N1	4.29	1.49	1.40
1	Aa	17	5MC	C4-N4	4.29	1.45	1.34
1	Aa	340	5MC	C4-N4	4.28	1.45	1.34
27	BA	55	5MC	C6-N1	4.28	1.45	1.38
1	Aa	1476	5MC	C4-N4	4.28	1.45	1.34
1	Aa	1478	5MC	C4-N4	4.27	1.45	1.34
1	Aa	479	OMU	C4-N3	4.27	1.46	1.38
1	Aa	457	5MC	C2-N1	4.26	1.49	1.40
1	Aa	1003	5MC	C2-N1	4.26	1.49	1.40
1	Aa	1007	5MC	C2-N1	4.26	1.49	1.40
27	BA	55	5MC	C4-N4	4.25	1.45	1.34
1	Aa	1004	5MC	C2-N1	4.25	1.49	1.40
1	Aa	1321	5MC	C2-N1	4.24	1.49	1.40
1	Aa	672	5MC	C4-N4	4.24	1.45	1.34
27	BA	55	5MC	C2-N1	4.24	1.49	1.40
1	Aa	349	5MC	C2-N1	4.24	1.49	1.40
1	Aa	473	5MC	C2-N1	4.23	1.49	1.40
1	Aa	923	5MC	C2-N1	4.23	1.49	1.40
1	Aa	1006	5MC	C2-N1	4.23	1.49	1.40
1	Aa	1306	5MC	C2-N1	4.22	1.49	1.40
1	Aa	1266	5MC	C2-N1	4.22	1.49	1.40
27	BA	2055	5MC	C2-N1	4.21	1.49	1.40
1	Aa	672	5MC	C2-N1	4.20	1.49	1.40
1	Aa	685	5MC	C2-N1	4.20	1.49	1.40
1	Aa	1352	5MC	C2-N1	4.20	1.49	1.40
27	BA	2075	5MC	C2-N1	4.19	1.49	1.40
27	BA	1965	5MC	C2-N1	4.19	1.49	1.40
27	BA	1480	OMU	C4-N3	4.18	1.46	1.38
1	Aa	753	OMU	C4-N3	4.18	1.46	1.38
27	BA	2688	5MC	C2-N1	4.17	1.49	1.40
1	Aa	1184	5MC	C2-N1	4.17	1.49	1.40
27	BA	1345	5MC	C2-N1	4.17	1.49	1.40
1	Aa	854	5MC	C2-N1	4.17	1.49	1.40
1	Aa	17	5MC	C2-N1	4.17	1.49	1.40
27	BA	1969	OMU	C4-N3	4.13	1.46	1.38
1	Aa	1476	5MC	C2-N1	4.12	1.48	1.40
27	BA	2605	5MC	C2-N1	4.12	1.48	1.40
27	BA	453	OMU	C4-N3	4.12	1.45	1.38
1	Aa	1020	OMU	C4-N3	4.11	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2070	5MC	C2-N1	4.10	1.48	1.40
27	BA	2656	OMU	C4-N3	4.09	1.45	1.38
1	Aa	963	OMG	C2-N2	4.07	1.43	1.34
27	BA	1402	OMU	C4-N3	4.06	1.45	1.38
1	Aa	994	OMG	C2-N2	4.05	1.43	1.34
1	Aa	1107	OMG	C2-N2	4.05	1.43	1.34
1	Aa	574	OMG	C2-N2	4.04	1.43	1.34
1	Aa	1223	OMG	C2-N2	4.04	1.43	1.34
1	Aa	1358	OMU	C4-N3	4.04	1.45	1.38
1	Aa	636	OMG	C2-N2	4.03	1.43	1.34
27	BA	1508	OMG	C2-N2	4.02	1.43	1.34
27	BA	1150	OMU	C4-N3	4.02	1.45	1.38
1	Aa	836	OMG	C2-N2	4.02	1.43	1.34
1	Aa	913	OMG	C2-N2	4.02	1.43	1.34
1	Aa	498	OMG	C2-N2	4.02	1.43	1.34
1	Aa	147	OMG	C2-N2	4.02	1.43	1.34
1	Aa	629	OMG	C2-N2	4.01	1.43	1.34
1	Aa	532	OMG	C2-N2	4.01	1.43	1.34
27	BA	288	OMG	C2-N2	4.01	1.43	1.34
1	Aa	8	OMU	C4-N3	4.00	1.45	1.38
27	BA	2542	OMU	C4-N3	4.00	1.45	1.38
27	BA	833	OMG	C2-N2	3.99	1.43	1.34
27	BA	2728	OMG	C2-N2	3.99	1.43	1.34
27	BA	2521	OMG	C2-N2	3.99	1.43	1.34
1	Aa	891	OMG	C2-N2	3.98	1.43	1.34
1	Aa	495	OMG	C2-N2	3.98	1.43	1.34
1	Aa	670	OMG	C2-N2	3.98	1.43	1.34
27	BA	2379	OMG	C2-N2	3.98	1.43	1.34
1	Aa	121	OMG	C2-N2	3.98	1.43	1.34
1	Aa	770	OMG	C2-N2	3.98	1.43	1.34
27	BA	912	OMG	C2-N2	3.97	1.43	1.34
27	BA	1776	OMU	C4-N3	3.97	1.45	1.38
27	BA	1953	OMG	C2-N2	3.97	1.43	1.34
27	BA	2640	OMG	C2-N2	3.97	1.43	1.34
1	Aa	446	OMG	C2-N2	3.96	1.43	1.34
1	Aa	219	OMG	C2-N2	3.96	1.43	1.34
1	Aa	381	OMG	C2-N2	3.96	1.43	1.34
27	BA	2672	OMG	C2-N2	3.96	1.43	1.34
1	Aa	659	OMG	C2-N2	3.96	1.43	1.34
27	BA	1956	OMG	C2-N2	3.95	1.43	1.34
27	BA	584	OMG	C2-N2	3.95	1.43	1.34
27	BA	2010	OMG	C2-N2	3.95	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2016	OMG	C2-N2	3.95	1.43	1.34
27	BA	215	OMG	C2-N2	3.94	1.43	1.34
27	BA	657	OMU	C4-N3	3.94	1.45	1.38
27	BA	674	OMG	C2-N2	3.94	1.43	1.34
27	BA	800	OMG	C2-N2	3.93	1.43	1.34
27	BA	1525	OMG	C2-N2	3.93	1.43	1.34
27	BA	2466	OMG	C2-N2	3.93	1.43	1.34
27	BA	2870	OMG	C2-N2	3.93	1.43	1.34
1	Aa	320	OMG	C2-N2	3.93	1.43	1.34
27	BA	1893	OMG	C2-N2	3.93	1.43	1.34
27	BA	1329	OMG	C2-N2	3.92	1.43	1.34
27	BA	872	OMG	C2-N2	3.92	1.43	1.34
27	BA	2168	OMG	C2-N2	3.91	1.43	1.34
27	BA	365	OMG	C2-N2	3.91	1.43	1.34
27	BA	2528	OMG	C2-N2	3.91	1.43	1.34
27	BA	2745	OMG	C2-N2	3.90	1.43	1.34
27	BA	507	OMG	C2-N2	3.90	1.43	1.34
27	BA	2527	OMG	C2-N2	3.90	1.43	1.34
27	BA	63	OMG	C2-N2	3.89	1.43	1.34
27	BA	65	OMG	C2-N2	3.88	1.43	1.34
27	BA	2642	OMG	C2-N2	3.88	1.43	1.34
27	BA	2469	OMG	C2-N2	3.88	1.43	1.34
1	Aa	963	OMG	C6-N1	3.88	1.43	1.37
1	Aa	913	OMG	C6-N1	3.85	1.43	1.37
27	BA	670	OMG	C2-N2	3.84	1.43	1.34
1	Aa	381	OMG	C6-N1	3.82	1.43	1.37
27	BA	2521	OMG	C6-N1	3.81	1.43	1.37
1	Aa	495	OMG	C6-N1	3.81	1.43	1.37
1	Aa	574	OMG	C6-N1	3.80	1.43	1.37
1	Aa	836	OMG	C6-N1	3.80	1.43	1.37
27	BA	1508	OMG	C6-N1	3.79	1.43	1.37
1	Aa	320	OMG	C6-N1	3.78	1.43	1.37
1	Aa	636	OMG	C6-N1	3.78	1.43	1.37
1	Aa	532	OMG	C6-N1	3.77	1.43	1.37
1	Aa	994	OMG	C6-N1	3.77	1.43	1.37
1	Aa	1107	OMG	C6-N1	3.77	1.43	1.37
1	Aa	1223	OMG	C6-N1	3.75	1.43	1.37
27	BA	584	OMG	C6-N1	3.75	1.43	1.37
27	BA	2379	OMG	C6-N1	3.74	1.43	1.37
1	Aa	147	OMG	C6-N1	3.73	1.43	1.37
1	Aa	629	OMG	C6-N1	3.73	1.43	1.37
27	BA	288	OMG	C6-N1	3.72	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2728	OMG	C6-N1	3.71	1.43	1.37
1	Aa	498	OMG	C6-N1	3.70	1.43	1.37
1	Aa	121	OMG	C6-N1	3.70	1.43	1.37
1	Aa	446	OMG	C6-N1	3.69	1.43	1.37
27	BA	63	OMG	C6-N1	3.67	1.43	1.37
27	BA	2168	OMG	C6-N1	3.66	1.43	1.37
1	Aa	891	OMG	C6-N1	3.66	1.43	1.37
1	Aa	219	OMG	C6-N1	3.66	1.43	1.37
1	Aa	670	OMG	C6-N1	3.65	1.43	1.37
27	BA	2469	OMG	C6-N1	3.65	1.43	1.37
27	BA	800	OMG	C6-N1	3.64	1.43	1.37
27	BA	2640	OMG	C6-N1	3.64	1.43	1.37
1	Aa	659	OMG	C6-N1	3.63	1.43	1.37
27	BA	507	OMG	C6-N1	3.63	1.43	1.37
27	BA	1956	OMG	C6-N1	3.63	1.43	1.37
1	Aa	770	OMG	C6-N1	3.62	1.43	1.37
27	BA	833	OMG	C6-N1	3.62	1.43	1.37
27	BA	2527	OMG	C6-N1	3.62	1.43	1.37
27	BA	674	OMG	C6-N1	3.62	1.43	1.37
27	BA	2528	OMG	C6-N1	3.62	1.43	1.37
27	BA	1953	OMG	C6-N1	3.61	1.43	1.37
27	BA	2553	4SU	C4-N3	-3.61	1.33	1.37
27	BA	215	OMG	C6-N1	3.59	1.43	1.37
27	BA	2870	OMG	C6-N1	3.58	1.43	1.37
27	BA	2745	OMG	C6-N1	3.57	1.43	1.37
27	BA	1329	OMG	C6-N1	3.57	1.43	1.37
27	BA	2010	OMG	C6-N1	3.57	1.43	1.37
27	BA	670	OMG	C6-N1	3.57	1.43	1.37
27	BA	65	OMG	C6-N1	3.54	1.43	1.37
27	BA	1525	OMG	C6-N1	3.54	1.43	1.37
27	BA	2642	OMG	C6-N1	3.54	1.43	1.37
27	BA	1893	OMG	C6-N1	3.54	1.43	1.37
27	BA	2466	OMG	C6-N1	3.53	1.43	1.37
27	BA	2016	OMG	C6-N1	3.53	1.43	1.37
27	BA	912	OMG	C6-N1	3.51	1.43	1.37
27	BA	872	OMG	C6-N1	3.46	1.43	1.37
27	BA	2672	OMG	C6-N1	3.44	1.43	1.37
27	BA	365	OMG	C6-N1	3.43	1.43	1.37
27	BA	2595	OMC	C6-N1	3.27	1.45	1.38
27	BA	2545	OMC	C6-N1	3.25	1.45	1.38
27	BA	1820	OMC	C6-N1	3.23	1.45	1.38
1	Aa	924	OMC	C6-N1	3.23	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	825	OMC	C6-N1	3.22	1.45	1.38
27	BA	2124	OMC	C6-N1	3.22	1.45	1.38
27	BA	1995	OMC	C6-N1	3.21	1.45	1.38
27	BA	869	OMC	C6-N1	3.20	1.45	1.38
27	BA	66	OMC	C6-N1	3.20	1.45	1.38
1	Aa	752	OMC	C6-N1	3.19	1.45	1.38
27	BA	91	OMC	C6-N1	3.19	1.45	1.38
27	BA	2107	OMC	C6-N1	3.19	1.45	1.38
1	Aa	1361	OMC	C6-N1	3.19	1.45	1.38
27	BA	2047	OMC	C6-N1	3.18	1.45	1.38
1	Aa	229	OMC	C6-N1	3.18	1.45	1.38
27	BA	2169	OMC	C6-N1	3.18	1.45	1.38
1	Aa	112	OMC	C6-N1	3.17	1.45	1.38
27	BA	657	OMU	O4-C4	-3.15	1.18	1.24
27	BA	2967	OMC	C6-N1	3.15	1.45	1.38
27	BA	2642	OMG	C5-C6	3.14	1.53	1.47
27	BA	2550	OMG	C6-N1	-3.14	1.33	1.37
27	BA	1854	5MU	O4-C4	-3.13	1.17	1.23
1	Aa	1354	OMC	C6-N1	3.13	1.45	1.38
27	BA	1402	OMU	O4-C4	-3.13	1.18	1.24
27	BA	932	A2M	C6-N6	3.12	1.45	1.34
27	BA	2656	OMU	O4-C4	-3.12	1.18	1.24
27	BA	932	A2M	O3'-C3'	-3.12	1.35	1.43
27	BA	1480	OMU	O4-C4	-3.11	1.18	1.24
27	BA	2936	A2M	C6-N6	3.10	1.45	1.34
27	BA	1776	OMU	O4-C4	-3.10	1.18	1.24
27	BA	849	A2M	C6-N6	3.09	1.45	1.34
1	Aa	8	OMU	O4-C4	-3.09	1.18	1.24
27	BA	829	5MU	O4-C4	-3.08	1.17	1.23
27	BA	1969	OMU	O4-C4	-3.08	1.18	1.24
27	BA	879	A2M	C6-N6	3.08	1.45	1.34
1	Aa	352	A2M	C6-N6	3.06	1.45	1.34
27	BA	2542	OMU	O4-C4	-3.06	1.18	1.24
27	BA	872	OMG	C5-C6	3.06	1.53	1.47
27	BA	1766	5MU	O4-C4	-3.05	1.17	1.23
1	Aa	574	OMG	C5-C6	3.05	1.53	1.47
27	BA	2466	OMG	C5-C6	3.04	1.53	1.47
27	BA	453	OMU	O4-C4	-3.04	1.18	1.24
27	BA	2527	OMG	C5-C6	3.04	1.53	1.47
27	BA	1150	OMU	O4-C4	-3.04	1.18	1.24
1	Aa	1020	OMU	O4-C4	-3.03	1.18	1.24
1	Aa	381	OMG	C5-C6	3.03	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	836	OMG	C5-C6	3.03	1.53	1.47
27	BA	2427	5MU	O4-C4	-3.02	1.17	1.23
27	BA	2521	OMG	C5-C6	3.01	1.53	1.47
27	BA	505	A2M	C6-N6	3.01	1.45	1.34
27	BA	800	OMG	C5-C6	3.01	1.53	1.47
1	Aa	1223	OMG	C5-C6	3.00	1.53	1.47
27	BA	670	OMG	C5-C6	3.00	1.53	1.47
1	Aa	994	OMG	C5-C6	3.00	1.53	1.47
1	Aa	219	OMG	C5-C6	3.00	1.53	1.47
1	Aa	495	OMG	C5-C6	3.00	1.53	1.47
1	Aa	753	OMU	O4-C4	-3.00	1.18	1.24
1	Aa	498	OMG	C5-C6	3.00	1.53	1.47
27	BA	288	OMG	C5-C6	3.00	1.53	1.47
1	Aa	670	OMG	C5-C6	2.99	1.53	1.47
27	BA	2528	OMG	C5-C6	2.99	1.53	1.47
27	BA	2728	OMG	C5-C6	2.99	1.53	1.47
27	BA	507	OMG	C5-C6	2.99	1.53	1.47
27	BA	2379	OMG	C5-C6	2.99	1.53	1.47
1	Aa	147	OMG	C5-C6	2.98	1.53	1.47
27	BA	584	OMG	C5-C6	2.97	1.53	1.47
27	BA	2745	OMG	C5-C6	2.97	1.53	1.47
1	Aa	17	5MC	O2-C2	-2.97	1.18	1.23
1	Aa	963	OMG	C5-C6	2.97	1.53	1.47
27	BA	912	OMG	C5-C6	2.97	1.53	1.47
27	BA	1965	5MC	O2-C2	-2.97	1.18	1.23
27	BA	1402	OMU	C6-N1	2.97	1.45	1.38
1	Aa	1107	OMG	C5-C6	2.96	1.53	1.47
1	Aa	852	OMG	C6-N1	-2.96	1.33	1.37
27	BA	2640	OMG	C5-C6	2.96	1.53	1.47
27	BA	2672	OMG	C5-C6	2.96	1.53	1.47
1	Aa	891	OMG	C5-C6	2.95	1.53	1.47
27	BA	2936	A2M	O3'-C3'	-2.95	1.36	1.43
1	Aa	1476	5MC	O2-C2	-2.95	1.18	1.23
27	BA	2070	5MC	O2-C2	-2.95	1.18	1.23
27	BA	2353	OMG	C6-N1	-2.95	1.33	1.37
27	BA	2016	OMG	C5-C6	2.95	1.53	1.47
1	Aa	672	5MC	O2-C2	-2.95	1.18	1.23
1	Aa	636	OMG	C5-C6	2.94	1.53	1.47
1	Aa	770	OMG	C5-C6	2.94	1.53	1.47
27	BA	1953	OMG	C5-C6	2.94	1.53	1.47
1	Aa	659	OMG	C5-C6	2.94	1.53	1.47
27	BA	1893	OMG	C5-C6	2.94	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	629	OMG	C5-C6	2.94	1.53	1.47
27	BA	1480	OMU	C6-N1	2.94	1.45	1.38
1	Aa	1321	5MC	O2-C2	-2.93	1.18	1.23
1	Aa	913	OMG	C5-C6	2.93	1.53	1.47
1	Aa	1358	OMU	O4-C4	-2.93	1.18	1.24
27	BA	2075	5MC	O2-C2	-2.93	1.18	1.23
1	Aa	121	OMG	C5-C6	2.93	1.53	1.47
1	Aa	917	5MU	C4-N3	-2.93	1.33	1.38
1	Aa	446	OMG	C5-C6	2.93	1.53	1.47
27	BA	833	OMG	C5-C6	2.92	1.53	1.47
27	BA	365	OMG	C5-C6	2.92	1.53	1.47
27	BA	2870	OMG	C5-C6	2.92	1.53	1.47
27	BA	63	OMG	C5-C6	2.91	1.53	1.47
27	BA	55	5MC	O2-C2	-2.91	1.18	1.23
1	Aa	532	OMG	C5-C6	2.91	1.53	1.47
27	BA	1508	OMG	C5-C6	2.91	1.53	1.47
27	BA	2055	5MC	O2-C2	-2.91	1.18	1.23
1	Aa	1007	5MC	O2-C2	-2.91	1.18	1.23
27	BA	2605	5MC	O2-C2	-2.91	1.18	1.23
27	BA	1345	5MC	O2-C2	-2.90	1.18	1.23
27	BA	1150	OMU	C6-N1	2.90	1.45	1.38
1	Aa	1306	5MC	O2-C2	-2.90	1.18	1.23
1	Aa	320	OMG	C5-C6	2.90	1.53	1.47
27	BA	674	OMG	C5-C6	2.90	1.53	1.47
27	BA	849	A2M	O3'-C3'	-2.90	1.36	1.43
27	BA	657	OMU	C6-N1	2.90	1.45	1.38
27	BA	65	OMG	C5-C6	2.90	1.53	1.47
27	BA	1776	OMU	C6-N1	2.90	1.45	1.38
1	Aa	685	5MC	O2-C2	-2.90	1.18	1.23
27	BA	2656	OMU	C6-N1	2.89	1.45	1.38
1	Aa	854	5MC	O2-C2	-2.89	1.18	1.23
1	Aa	479	OMU	O4-C4	-2.89	1.18	1.24
27	BA	875	5MU	O4-C4	-2.89	1.18	1.23
27	BA	2688	5MC	O2-C2	-2.89	1.18	1.23
27	BA	1969	OMU	C6-N1	2.88	1.45	1.38
1	Aa	479	OMU	C6-N1	2.88	1.44	1.38
1	Aa	8	OMU	C6-N1	2.88	1.44	1.38
1	Aa	473	5MC	O2-C2	-2.88	1.18	1.23
1	Aa	1184	5MC	O2-C2	-2.88	1.18	1.23
1	Aa	1478	5MC	O2-C2	-2.87	1.18	1.23
27	BA	2542	OMU	C6-N1	2.87	1.44	1.38
27	BA	2010	OMG	C5-C6	2.87	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	349	5MC	O2-C2	-2.87	1.18	1.23
27	BA	2168	OMG	C5-C6	2.87	1.53	1.47
1	Aa	1003	5MC	O2-C2	-2.86	1.18	1.23
27	BA	1956	OMG	C5-C6	2.86	1.53	1.47
27	BA	2107	OMC	O2-C2	-2.86	1.18	1.23
1	Aa	753	OMU	C6-N1	2.86	1.44	1.38
27	BA	1329	OMG	C5-C6	2.85	1.53	1.47
1	Aa	1006	5MC	O2-C2	-2.85	1.18	1.23
1	Aa	1004	5MC	O2-C2	-2.85	1.18	1.23
1	Aa	1266	5MC	O2-C2	-2.85	1.18	1.23
1	Aa	450	OMG	C6-N1	-2.85	1.33	1.37
1	Aa	340	5MC	O2-C2	-2.85	1.18	1.23
27	BA	453	OMU	C6-N1	2.85	1.44	1.38
27	BA	879	A2M	O2'-C2'	2.84	1.49	1.42
27	BA	505	A2M	O3'-C3'	-2.84	1.36	1.43
1	Aa	1352	5MC	O2-C2	-2.84	1.18	1.23
27	BA	869	OMC	O2-C2	-2.83	1.18	1.23
27	BA	2124	OMC	O2-C2	-2.83	1.18	1.23
27	BA	2469	OMG	C5-C6	2.83	1.53	1.47
1	Aa	1020	OMU	C6-N1	2.83	1.44	1.38
27	BA	2389	OMU	C4-N3	-2.83	1.33	1.38
1	Aa	352	A2M	O2'-C2'	2.83	1.49	1.42
27	BA	879	A2M	O3'-C3'	-2.82	1.36	1.43
27	BA	2169	OMC	O2-C2	-2.82	1.18	1.23
1	Aa	1354	OMC	O2-C2	-2.81	1.18	1.23
27	BA	849	A2M	O2'-C2'	2.80	1.49	1.42
27	BA	215	OMG	C5-C6	2.79	1.53	1.47
27	BA	2545	OMC	O2-C2	-2.79	1.18	1.23
27	BA	1820	OMC	O2-C2	-2.79	1.18	1.23
27	BA	932	A2M	O2'-C2'	2.79	1.49	1.42
27	BA	2936	A2M	O2'-C2'	2.79	1.49	1.42
1	Aa	923	5MC	O2-C2	-2.79	1.18	1.23
1	Aa	457	5MC	O2-C2	-2.78	1.18	1.23
1	Aa	752	OMC	O2-C2	-2.78	1.18	1.23
27	BA	1525	OMG	C5-C6	2.77	1.53	1.47
1	Aa	1358	OMU	C6-N1	2.76	1.44	1.38
27	BA	879	A2M	C5-C4	-2.76	1.33	1.40
1	Aa	464	5MC	O2-C2	-2.76	1.18	1.23
27	BA	66	OMC	O2-C2	-2.76	1.18	1.23
1	Aa	352	A2M	O3'-C3'	-2.74	1.36	1.43
1	Aa	352	A2M	C5-C4	-2.73	1.33	1.40
27	BA	849	A2M	C5-C4	-2.73	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	505	A2M	O2'-C2'	2.73	1.49	1.42
27	BA	2047	OMC	O2-C2	-2.73	1.18	1.23
27	BA	1766	5MU	O2-C2	-2.72	1.18	1.23
1	Aa	112	OMC	O2-C2	-2.72	1.18	1.23
27	BA	2936	A2M	C5-C4	-2.72	1.33	1.40
27	BA	91	OMC	O2-C2	-2.71	1.18	1.23
1	Aa	1467	MA6	C5-C4	-2.71	1.33	1.40
1	Aa	1468	MA6	C5-C4	-2.71	1.33	1.40
1	Aa	229	OMC	O2-C2	-2.71	1.18	1.23
27	BA	2521	OMG	C5-C4	-2.70	1.36	1.43
1	Aa	825	OMC	O2-C2	-2.70	1.18	1.23
27	BA	932	A2M	C5-C4	-2.70	1.33	1.40
27	BA	1329	OMG	O6-C6	-2.69	1.17	1.23
1	Aa	924	OMC	O2-C2	-2.69	1.18	1.23
27	BA	1956	OMG	O6-C6	-2.69	1.17	1.23
1	Aa	446	OMG	C5-C4	-2.69	1.36	1.43
27	BA	1995	OMC	O2-C2	-2.68	1.18	1.23
27	BA	2168	OMG	C5-C4	-2.68	1.36	1.43
27	BA	2595	OMC	O2-C2	-2.67	1.18	1.23
27	BA	1953	OMG	C5-C4	-2.67	1.36	1.43
1	Aa	532	OMG	C5-C4	-2.67	1.36	1.43
27	BA	63	OMG	C5-C4	-2.67	1.36	1.43
27	BA	507	OMG	C5-C4	-2.66	1.36	1.43
27	BA	505	A2M	C5-C4	-2.66	1.33	1.40
27	BA	2010	OMG	C5-C4	-2.66	1.36	1.43
27	BA	63	OMG	O6-C6	-2.66	1.17	1.23
27	BA	584	OMG	O6-C6	-2.66	1.17	1.23
27	BA	2967	OMC	O2-C2	-2.65	1.18	1.23
27	BA	215	OMG	O6-C6	-2.65	1.17	1.23
1	Aa	770	OMG	C5-C4	-2.65	1.36	1.43
27	BA	1329	OMG	C5-C4	-2.65	1.36	1.43
27	BA	670	OMG	C5-C4	-2.65	1.36	1.43
27	BA	2581	4SU	O2-C2	-2.65	1.18	1.23
27	BA	1893	OMG	C5-C4	-2.64	1.36	1.43
27	BA	2745	OMG	C5-C4	-2.64	1.36	1.43
27	BA	215	OMG	C5-C4	-2.64	1.36	1.43
27	BA	833	OMG	C5-C4	-2.64	1.36	1.43
27	BA	65	OMG	O6-C6	-2.64	1.17	1.23
1	Aa	1361	OMC	O2-C2	-2.63	1.18	1.23
27	BA	65	OMG	C5-C4	-2.63	1.36	1.43
27	BA	2672	OMG	O6-C6	-2.63	1.17	1.23
27	BA	2379	OMG	C5-C4	-2.63	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	912	OMG	C5-C4	-2.62	1.36	1.43
27	BA	507	OMG	O6-C6	-2.62	1.18	1.23
1	Aa	320	OMG	C5-C4	-2.62	1.36	1.43
1	Aa	381	OMG	C5-C4	-2.62	1.36	1.43
27	BA	2672	OMG	C5-C4	-2.62	1.36	1.43
27	BA	2528	OMG	C5-C4	-2.62	1.36	1.43
27	BA	674	OMG	O6-C6	-2.62	1.18	1.23
27	BA	674	OMG	C5-C4	-2.62	1.36	1.43
27	BA	1956	OMG	C5-C4	-2.61	1.36	1.43
27	BA	288	OMG	C5-C4	-2.61	1.36	1.43
27	BA	365	OMG	O6-C6	-2.61	1.18	1.23
27	BA	1953	OMG	O6-C6	-2.61	1.18	1.23
1	Aa	495	OMG	C5-C4	-2.61	1.36	1.43
27	BA	2870	OMG	O6-C6	-2.60	1.18	1.23
27	BA	2427	5MU	O2-C2	-2.60	1.18	1.23
27	BA	800	OMG	C5-C4	-2.60	1.36	1.43
27	BA	2642	OMG	C5-C4	-2.60	1.36	1.43
27	BA	2728	OMG	C5-C4	-2.60	1.36	1.43
1	Aa	836	OMG	C5-C4	-2.59	1.36	1.43
27	BA	2527	OMG	C5-C4	-2.59	1.36	1.43
27	BA	2521	OMG	O6-C6	-2.59	1.18	1.23
27	BA	1525	OMG	C5-C4	-2.59	1.36	1.43
1	Aa	498	OMG	C5-C4	-2.59	1.36	1.43
27	BA	2168	OMG	O6-C6	-2.59	1.18	1.23
1	Aa	219	OMG	C5-C4	-2.59	1.36	1.43
27	BA	1525	OMG	O6-C6	-2.59	1.18	1.23
1	Aa	147	OMG	C5-C4	-2.58	1.36	1.43
1	Aa	891	OMG	C5-C4	-2.58	1.36	1.43
27	BA	584	OMG	C5-C4	-2.58	1.36	1.43
27	BA	1893	OMG	O6-C6	-2.58	1.18	1.23
27	BA	2379	OMG	O6-C6	-2.58	1.18	1.23
1	Aa	629	OMG	C5-C4	-2.58	1.36	1.43
27	BA	2595	OMC	C5-C4	2.58	1.48	1.42
27	BA	912	OMG	O6-C6	-2.58	1.18	1.23
27	BA	2469	OMG	O6-C6	-2.58	1.18	1.23
27	BA	670	OMG	O6-C6	-2.57	1.18	1.23
1	Aa	670	OMG	C5-C4	-2.57	1.36	1.43
27	BA	365	OMG	C5-C4	-2.57	1.36	1.43
27	BA	833	OMG	O6-C6	-2.57	1.18	1.23
27	BA	1854	5MU	O2-C2	-2.57	1.18	1.23
1	Aa	770	OMG	O6-C6	-2.57	1.18	1.23
27	BA	829	5MU	O2-C2	-2.57	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2010	OMG	O6-C6	-2.57	1.18	1.23
27	BA	2016	OMG	C5-C4	-2.57	1.36	1.43
27	BA	2870	OMG	C5-C4	-2.57	1.36	1.43
1	Aa	574	OMG	C5-C4	-2.56	1.36	1.43
27	BA	2016	OMG	O6-C6	-2.56	1.18	1.23
27	BA	1508	OMG	C5-C4	-2.56	1.36	1.43
27	BA	1150	OMU	O2-C2	-2.56	1.18	1.23
27	BA	657	OMU	O2-C2	-2.56	1.18	1.23
1	Aa	670	OMG	O6-C6	-2.56	1.18	1.23
27	BA	2466	OMG	O6-C6	-2.56	1.18	1.23
27	BA	872	OMG	O6-C6	-2.56	1.18	1.23
27	BA	2728	OMG	O6-C6	-2.56	1.18	1.23
27	BA	2466	OMG	C5-C4	-2.55	1.36	1.43
27	BA	800	OMG	O6-C6	-2.55	1.18	1.23
27	BA	1776	OMU	O2-C2	-2.55	1.18	1.23
27	BA	2642	OMG	O6-C6	-2.55	1.18	1.23
27	BA	1402	OMU	O2-C2	-2.55	1.18	1.23
27	BA	2640	OMG	O6-C6	-2.55	1.18	1.23
1	Aa	574	OMG	O6-C6	-2.54	1.18	1.23
1	Aa	836	OMG	O6-C6	-2.54	1.18	1.23
27	BA	2745	OMG	O6-C6	-2.54	1.18	1.23
1	Aa	1223	OMG	C5-C4	-2.54	1.36	1.43
1	Aa	446	OMG	O6-C6	-2.54	1.18	1.23
27	BA	2169	OMC	C5-C4	2.54	1.48	1.42
1	Aa	121	OMG	C5-C4	-2.53	1.36	1.43
1	Aa	320	OMG	O6-C6	-2.53	1.18	1.23
1	Aa	532	OMG	O6-C6	-2.53	1.18	1.23
1	Aa	1354	OMC	C5-C4	2.53	1.48	1.42
1	Aa	963	OMG	C5-C4	-2.53	1.36	1.43
1	Aa	913	OMG	C5-C4	-2.52	1.36	1.43
27	BA	2527	OMG	O6-C6	-2.52	1.18	1.23
27	BA	2581	4SU	C6-N1	2.52	1.44	1.38
27	BA	2528	OMG	O6-C6	-2.52	1.18	1.23
1	Aa	995	2MG	C6-N1	-2.52	1.34	1.37
1	Aa	891	OMG	O6-C6	-2.52	1.18	1.23
1	Aa	659	OMG	C5-C4	-2.52	1.36	1.43
1	Aa	381	OMG	O6-C6	-2.52	1.18	1.23
27	BA	2469	OMG	C5-C4	-2.52	1.36	1.43
1	Aa	659	OMG	O6-C6	-2.52	1.18	1.23
1	Aa	994	OMG	C2-N1	2.51	1.43	1.37
27	BA	1995	OMC	C5-C4	2.51	1.48	1.42
27	BA	1480	OMU	O2-C2	-2.51	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	219	OMG	O6-C6	-2.51	1.18	1.23
27	BA	2640	OMG	C5-C4	-2.51	1.36	1.43
1	Aa	629	OMG	O6-C6	-2.51	1.18	1.23
27	BA	2545	OMC	C5-C4	2.51	1.48	1.42
1	Aa	994	OMG	C5-C4	-2.51	1.36	1.43
27	BA	1969	OMU	O2-C2	-2.51	1.18	1.23
1	Aa	963	OMG	C2-N1	2.51	1.43	1.37
1	Aa	913	OMG	O6-C6	-2.51	1.18	1.23
1	Aa	498	OMG	O6-C6	-2.50	1.18	1.23
27	BA	872	OMG	C5-C4	-2.50	1.36	1.43
1	Aa	913	OMG	C2-N1	2.50	1.43	1.37
1	Aa	381	OMG	C2-N1	2.50	1.43	1.37
1	Aa	1107	OMG	C2-N1	2.49	1.43	1.37
27	BA	875	5MU	O2-C2	-2.49	1.18	1.23
1	Aa	479	OMU	C5-C4	2.49	1.49	1.43
1	Aa	836	OMG	C2-N1	2.49	1.43	1.37
1	Aa	1223	OMG	O6-C6	-2.49	1.18	1.23
1	Aa	1468	MA6	C2-N3	2.49	1.36	1.32
27	BA	1508	OMG	O6-C6	-2.49	1.18	1.23
27	BA	288	OMG	O6-C6	-2.49	1.18	1.23
1	Aa	924	OMC	C5-C4	2.49	1.48	1.42
1	Aa	1449	6MZ	C5-C4	2.48	1.47	1.40
1	Aa	495	OMG	O6-C6	-2.48	1.18	1.23
1	Aa	1358	OMU	O2-C2	-2.48	1.18	1.23
1	Aa	1107	OMG	C5-C4	-2.48	1.36	1.43
1	Aa	1223	OMG	C2-N1	2.48	1.43	1.37
1	Aa	994	OMG	O6-C6	-2.48	1.18	1.23
1	Aa	1361	OMC	C5-C4	2.48	1.48	1.42
27	BA	2640	OMG	C2-N1	2.47	1.43	1.37
27	BA	2107	OMC	C5-C4	2.47	1.48	1.42
1	Aa	121	OMG	O6-C6	-2.47	1.18	1.23
1	Aa	121	OMG	C2-N1	2.47	1.43	1.37
1	Aa	636	OMG	O6-C6	-2.47	1.18	1.23
1	Aa	498	OMG	C2-N1	2.47	1.43	1.37
1	Aa	825	OMC	C5-C4	2.47	1.48	1.42
1	Aa	636	OMG	C5-C4	-2.46	1.36	1.43
27	BA	1969	OMU	C5-C4	2.46	1.49	1.43
27	BA	63	OMG	C2-N1	2.46	1.43	1.37
1	Aa	1467	MA6	C2-N3	2.46	1.36	1.32
1	Aa	636	OMG	C2-N1	2.45	1.43	1.37
27	BA	453	OMU	O2-C2	-2.45	1.18	1.23
1	Aa	219	OMG	C2-N1	2.45	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	770	OMG	C2-N1	2.45	1.43	1.37
1	Aa	147	OMG	C2-N1	2.45	1.43	1.37
27	BA	1820	OMC	C5-C4	2.45	1.48	1.42
1	Aa	574	OMG	C2-N1	2.45	1.43	1.37
1	Aa	229	OMC	C5-C4	2.44	1.48	1.42
1	Aa	320	OMG	C2-N1	2.44	1.43	1.37
1	Aa	963	OMG	O6-C6	-2.44	1.18	1.23
1	Aa	659	OMG	C2-N1	2.44	1.43	1.37
1	Aa	752	OMC	C5-C4	2.44	1.48	1.42
27	BA	2521	OMG	C2-N1	2.44	1.43	1.37
1	Aa	670	OMG	C2-N1	2.44	1.43	1.37
1	Aa	112	OMC	C5-C4	2.44	1.48	1.42
1	Aa	147	OMG	O6-C6	-2.44	1.18	1.23
27	BA	833	OMG	C2-N1	2.43	1.43	1.37
27	BA	91	OMC	C5-C4	2.43	1.48	1.42
1	Aa	891	OMG	C2-N1	2.43	1.43	1.37
27	BA	2010	OMG	C2-N1	2.43	1.43	1.37
1	Aa	753	OMU	C5-C4	2.43	1.49	1.43
27	BA	1508	OMG	C2-N1	2.43	1.43	1.37
27	BA	2016	OMG	C2-N1	2.42	1.43	1.37
27	BA	2047	OMC	C5-C4	2.42	1.48	1.42
1	Aa	495	OMG	C2-N1	2.42	1.43	1.37
27	BA	2728	OMG	C2-N1	2.42	1.43	1.37
27	BA	1953	OMG	C2-N1	2.42	1.43	1.37
1	Aa	8	OMU	O2-C2	-2.42	1.18	1.23
27	BA	2528	OMG	C2-N1	2.42	1.43	1.37
27	BA	2967	OMC	C5-C4	2.42	1.48	1.42
27	BA	869	OMC	C5-C4	2.42	1.48	1.42
27	BA	1525	OMG	C2-N1	2.42	1.43	1.37
1	Aa	446	OMG	C2-N1	2.42	1.43	1.37
27	BA	288	OMG	C2-N1	2.42	1.43	1.37
27	BA	674	OMG	C2-N1	2.41	1.43	1.37
27	BA	2656	OMU	O2-C2	-2.41	1.18	1.23
1	Aa	1107	OMG	O6-C6	-2.41	1.18	1.23
1	Aa	532	OMG	C2-N1	2.41	1.43	1.37
27	BA	2870	OMG	C2-N1	2.41	1.43	1.37
1	Aa	629	OMG	C2-N1	2.41	1.43	1.37
27	BA	800	OMG	C2-N1	2.41	1.43	1.37
1	Aa	1020	OMU	O2-C2	-2.40	1.18	1.23
27	BA	2466	OMG	C2-N1	2.40	1.43	1.37
27	BA	1150	OMU	C5-C4	2.40	1.48	1.43
27	BA	2642	OMG	C2-N1	2.40	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	507	OMG	C2-N1	2.39	1.43	1.37
27	BA	2168	OMG	C2-N1	2.39	1.43	1.37
27	BA	2124	OMC	C5-C4	2.39	1.48	1.42
1	Aa	917	5MU	C6-C5	2.39	1.38	1.34
27	BA	912	OMG	C2-N1	2.39	1.43	1.37
1	Aa	753	OMU	O2-C2	-2.39	1.18	1.23
27	BA	1956	OMG	C2-N1	2.39	1.43	1.37
27	BA	2553	4SU	C2-N3	-2.38	1.33	1.38
27	BA	2672	OMG	C2-N1	2.38	1.43	1.37
27	BA	2389	OMU	C2-N3	-2.38	1.33	1.38
27	BA	66	OMC	C5-C4	2.38	1.48	1.42
27	BA	2379	OMG	C2-N1	2.38	1.43	1.37
27	BA	657	OMU	C5-C4	2.37	1.48	1.43
1	Aa	8	OMU	C5-C4	2.37	1.48	1.43
27	BA	2542	OMU	O2-C2	-2.36	1.18	1.23
27	BA	2553	4SU	C5-C4	-2.36	1.39	1.42
1	Aa	1358	OMU	C5-C4	2.36	1.48	1.43
27	BA	2542	OMU	C5-C4	2.36	1.48	1.43
27	BA	2469	OMG	C2-N1	2.36	1.43	1.37
1	Aa	917	5MU	C6-N1	-2.35	1.34	1.38
27	BA	65	OMG	C2-N1	2.35	1.43	1.37
1	Aa	1020	OMU	C5-C4	2.34	1.48	1.43
27	BA	2527	OMG	C2-N1	2.34	1.43	1.37
27	BA	215	OMG	C2-N1	2.34	1.43	1.37
27	BA	365	OMG	C2-N1	2.34	1.43	1.37
27	BA	584	OMG	C2-N1	2.34	1.43	1.37
27	BA	1893	OMG	C2-N1	2.33	1.43	1.37
27	BA	1480	OMU	C5-C4	2.33	1.48	1.43
27	BA	1402	OMU	C5-C4	2.33	1.48	1.43
27	BA	872	OMG	C2-N1	2.33	1.43	1.37
27	BA	2745	OMG	C2-N1	2.31	1.43	1.37
27	BA	1329	OMG	C2-N1	2.31	1.43	1.37
27	BA	453	OMU	C5-C4	2.30	1.48	1.43
1	Aa	479	OMU	O2-C2	-2.29	1.18	1.23
27	BA	2656	OMU	C5-C4	2.28	1.48	1.43
27	BA	670	OMG	C2-N1	2.27	1.43	1.37
27	BA	1776	OMU	C5-C4	2.26	1.48	1.43
27	BA	2329	A2M	C5-C4	2.24	1.46	1.40
1	Aa	917	5MU	C2-N3	-2.22	1.34	1.38
27	BA	2389	OMU	C5-C4	-2.22	1.38	1.43
27	BA	2936	A2M	C2-N3	2.17	1.35	1.32
27	BA	932	A2M	C2-N3	2.14	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	505	A2M	C2-N3	2.13	1.35	1.32
1	Aa	352	A2M	C2-N3	2.08	1.35	1.32
27	BA	2091	A2M	C5-C4	2.07	1.46	1.40
27	BA	879	A2M	C2-N3	2.06	1.35	1.32
27	BA	849	A2M	C2-N3	2.05	1.35	1.32
27	BA	2389	OMU	C2-N1	2.01	1.41	1.38

All (446) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Aa	1468	MA6	N1-C6-N6	-14.53	101.77	117.06
1	Aa	1467	MA6	N1-C6-N6	-14.09	102.23	117.06
27	BA	1854	5MU	C5-C4-N3	12.41	125.90	115.31
27	BA	1766	5MU	C5-C4-N3	12.21	125.73	115.31
27	BA	829	5MU	C5-C4-N3	12.09	125.63	115.31
27	BA	2427	5MU	C5-C4-N3	12.06	125.61	115.31
27	BA	875	5MU	C5-C4-N3	11.95	125.51	115.31
27	BA	1854	5MU	C5-C6-N1	-10.39	112.65	123.34
27	BA	1766	5MU	C5-C6-N1	-10.17	112.87	123.34
27	BA	2427	5MU	C5-C6-N1	-9.98	113.07	123.34
27	BA	829	5MU	C5-C6-N1	-9.87	113.18	123.34
27	BA	875	5MU	C5-C6-N1	-9.86	113.20	123.34
27	BA	849	A2M	C5-C6-N6	9.24	134.40	120.35
1	Aa	352	A2M	C5-C6-N6	9.21	134.35	120.35
27	BA	932	A2M	C5-C6-N6	9.15	134.25	120.35
27	BA	879	A2M	C5-C6-N6	9.04	134.09	120.35
27	BA	505	A2M	C5-C6-N6	8.98	134.00	120.35
27	BA	2936	A2M	C5-C6-N6	8.93	133.93	120.35
27	BA	2581	4SU	C4-N3-C2	-7.90	119.66	127.34
27	BA	2553	4SU	C4-N3-C2	-6.63	120.90	127.34
1	Aa	352	A2M	N6-C6-N1	-6.32	105.45	118.57
27	BA	849	A2M	N6-C6-N1	-6.26	105.58	118.57
27	BA	879	A2M	N6-C6-N1	-6.21	105.68	118.57
27	BA	932	A2M	N6-C6-N1	-6.18	105.75	118.57
27	BA	505	A2M	N6-C6-N1	-6.14	105.84	118.57
1	Aa	1449	6MZ	C2-N1-C6	6.09	121.81	116.59
27	BA	2936	A2M	N6-C6-N1	-6.08	105.95	118.57
1	Aa	1467	MA6	N3-C2-N1	-5.61	119.90	128.68
27	BA	879	A2M	N3-C2-N1	-5.61	119.92	128.68
1	Aa	1468	MA6	N3-C2-N1	-5.60	119.92	128.68
27	BA	849	A2M	N3-C2-N1	-5.58	119.96	128.68
1	Aa	352	A2M	N3-C2-N1	-5.56	119.98	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BA	932	A2M	N3-C2-N1	-5.55	120.01	128.68
27	BA	2936	A2M	N3-C2-N1	-5.47	120.13	128.68
27	BA	2581	4SU	C5-C4-N3	5.38	119.68	114.69
27	BA	505	A2M	N3-C2-N1	-5.35	120.31	128.68
27	BA	657	OMU	C4-N3-C2	-5.34	119.53	126.58
1	Aa	8	OMU	C4-N3-C2	-5.30	119.59	126.58
27	BA	829	5MU	O4-C4-C5	-5.29	118.77	124.90
27	BA	1969	OMU	C4-N3-C2	-5.28	119.61	126.58
27	BA	1150	OMU	C4-N3-C2	-5.26	119.64	126.58
27	BA	2656	OMU	C4-N3-C2	-5.24	119.66	126.58
27	BA	453	OMU	C4-N3-C2	-5.24	119.67	126.58
1	Aa	479	OMU	C4-N3-C2	-5.22	119.69	126.58
1	Aa	753	OMU	C4-N3-C2	-5.21	119.71	126.58
27	BA	1480	OMU	C4-N3-C2	-5.20	119.72	126.58
1	Aa	917	5MU	C4-N3-C2	-5.19	120.63	127.35
27	BA	2542	OMU	C4-N3-C2	-5.17	119.76	126.58
27	BA	875	5MU	O4-C4-C5	-5.12	118.96	124.90
1	Aa	1020	OMU	C4-N3-C2	-5.12	119.83	126.58
1	Aa	1358	OMU	C4-N3-C2	-5.11	119.84	126.58
27	BA	1402	OMU	C4-N3-C2	-5.06	119.90	126.58
27	BA	1854	5MU	O4-C4-C5	-4.99	119.12	124.90
27	BA	1776	OMU	C4-N3-C2	-4.99	120.00	126.58
27	BA	2553	4SU	N3-C2-N1	4.97	121.48	114.89
27	BA	829	5MU	C4-N3-C2	-4.96	120.93	127.35
27	BA	1854	5MU	C4-N3-C2	-4.96	120.93	127.35
27	BA	1766	5MU	C4-N3-C2	-4.96	120.93	127.35
27	BA	1766	5MU	O4-C4-C5	-4.94	119.18	124.90
27	BA	2553	4SU	C5-C4-N3	4.93	119.26	114.69
1	Aa	917	5MU	N3-C2-N1	4.87	121.35	114.89
27	BA	2389	OMU	C4-N3-C2	-4.82	120.22	126.58
27	BA	875	5MU	C4-N3-C2	-4.76	121.19	127.35
1	Aa	917	5MU	C5-C4-N3	4.70	119.32	115.31
27	BA	2427	5MU	O4-C4-C5	-4.67	119.49	124.90
27	BA	2427	5MU	C4-N3-C2	-4.66	121.32	127.35
1	Aa	917	5MU	O4-C4-C5	-4.52	119.67	124.90
27	BA	2389	OMU	N3-C2-N1	4.40	120.73	114.89
27	BA	1766	5MU	N3-C2-N1	4.38	120.71	114.89
27	BA	829	5MU	N3-C2-N1	4.34	120.66	114.89
27	BA	875	5MU	N3-C2-N1	4.34	120.66	114.89
27	BA	829	5MU	C5M-C5-C6	-4.34	117.05	122.85
27	BA	1854	5MU	C5M-C5-C6	-4.32	117.08	122.85
27	BA	2427	5MU	N3-C2-N1	4.21	120.48	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BA	829	5MU	C5M-C5-C4	4.19	123.38	118.77
27	BA	1766	5MU	C5M-C5-C6	-4.16	117.29	122.85
27	BA	1854	5MU	C5M-C5-C4	4.14	123.32	118.77
27	BA	1854	5MU	N3-C2-N1	4.13	120.37	114.89
27	BA	2427	5MU	C5M-C5-C6	-4.11	117.36	122.85
27	BA	875	5MU	C5M-C5-C6	-4.11	117.36	122.85
27	BA	1150	OMU	N3-C2-N1	4.08	120.30	114.89
1	Aa	1358	OMU	N3-C2-N1	4.03	120.25	114.89
27	BA	55	5MC	C5-C6-N1	-4.01	119.21	123.34
27	BA	2427	5MU	C5M-C5-C4	4.01	123.18	118.77
27	BA	1766	5MU	C5M-C5-C4	3.96	123.13	118.77
27	BA	875	5MU	C5M-C5-C4	3.95	123.12	118.77
27	BA	2581	4SU	N3-C2-N1	3.89	120.06	114.89
1	Aa	8	OMU	N3-C2-N1	3.87	120.03	114.89
27	BA	2389	OMU	C5-C4-N3	3.85	120.60	114.84
27	BA	657	OMU	N3-C2-N1	3.85	120.00	114.89
27	BA	1969	OMU	N3-C2-N1	3.84	119.99	114.89
27	BA	453	OMU	N3-C2-N1	3.81	119.95	114.89
1	Aa	479	OMU	N3-C2-N1	3.80	119.94	114.89
27	BA	1402	OMU	N3-C2-N1	3.80	119.93	114.89
27	BA	1480	OMU	N3-C2-N1	3.78	119.91	114.89
1	Aa	1020	OMU	N3-C2-N1	3.78	119.91	114.89
27	BA	2656	OMU	N3-C2-N1	3.75	119.87	114.89
27	BA	1776	OMU	N3-C2-N1	3.74	119.86	114.89
1	Aa	753	OMU	N3-C2-N1	3.72	119.83	114.89
1	Aa	917	5MU	C5-C6-N1	-3.66	119.57	123.34
27	BA	1329	OMG	C5-C6-N1	3.65	120.40	113.95
27	BA	2542	OMU	N3-C2-N1	3.65	119.74	114.89
27	BA	2605	5MC	C5-C6-N1	-3.62	119.61	123.34
27	BA	215	OMG	C5-C6-N1	3.60	120.30	113.95
1	Aa	923	5MC	C5-C6-N1	-3.59	119.64	123.34
1	Aa	1321	5MC	C5-C6-N1	-3.59	119.64	123.34
27	BA	1893	OMG	C5-C6-N1	3.58	120.28	113.95
27	BA	63	OMG	C5-C6-N1	3.58	120.28	113.95
1	Aa	670	OMG	C5-C6-N1	3.58	120.28	113.95
1	Aa	446	OMG	C5-C6-N1	3.58	120.27	113.95
27	BA	2688	5MC	C5-C6-N1	-3.57	119.66	123.34
27	BA	2010	OMG	C5-C6-N1	3.56	120.24	113.95
1	Aa	770	OMG	C5-C6-N1	3.56	120.24	113.95
1	Aa	836	OMG	C5-C6-N1	3.55	120.23	113.95
27	BA	65	OMG	C5-C6-N1	3.54	120.20	113.95
27	BA	2379	OMG	C5-C6-N1	3.53	120.19	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Aa	495	OMG	C5-C6-N1	3.53	120.19	113.95
1	Aa	498	OMG	C5-C6-N1	3.53	120.19	113.95
1	Aa	629	OMG	C5-C6-N1	3.52	120.18	113.95
27	BA	670	OMG	C5-C6-N1	3.52	120.17	113.95
27	BA	1508	OMG	C5-C6-N1	3.52	120.17	113.95
1	Aa	994	OMG	C5-C6-N1	3.52	120.17	113.95
27	BA	674	OMG	C5-C6-N1	3.52	120.16	113.95
27	BA	1525	OMG	C5-C6-N1	3.51	120.16	113.95
1	Aa	1007	5MC	C5-C6-N1	-3.51	119.73	123.34
1	Aa	320	OMG	C5-C6-N1	3.51	120.14	113.95
27	BA	288	OMG	C5-C6-N1	3.50	120.13	113.95
1	Aa	147	OMG	C5-C6-N1	3.50	120.13	113.95
27	BA	2745	OMG	C5-C6-N1	3.49	120.12	113.95
27	BA	657	OMU	C5-C4-N3	3.49	120.07	114.84
27	BA	2642	OMG	C5-C6-N1	3.49	120.11	113.95
27	BA	584	OMG	C5-C6-N1	3.48	120.10	113.95
1	Aa	1107	OMG	C5-C6-N1	3.48	120.10	113.95
1	Aa	381	OMG	C5-C6-N1	3.48	120.09	113.95
27	BA	365	OMG	C5-C6-N1	3.47	120.08	113.95
27	BA	2672	OMG	C5-C6-N1	3.47	120.08	113.95
27	BA	800	OMG	C5-C6-N1	3.47	120.08	113.95
1	Aa	532	OMG	C5-C6-N1	3.47	120.08	113.95
27	BA	2640	OMG	C5-C6-N1	3.47	120.08	113.95
27	BA	2168	OMG	C5-C6-N1	3.47	120.07	113.95
1	Aa	636	OMG	C5-C6-N1	3.46	120.07	113.95
1	Aa	121	OMG	C5-C6-N1	3.46	120.06	113.95
27	BA	2542	OMU	C5-C4-N3	3.46	120.01	114.84
27	BA	2527	OMG	C5-C6-N1	3.46	120.06	113.95
27	BA	2521	OMG	C5-C6-N1	3.46	120.06	113.95
27	BA	833	OMG	C5-C6-N1	3.46	120.05	113.95
1	Aa	574	OMG	C5-C6-N1	3.45	120.05	113.95
27	BA	2656	OMU	C5-C4-N3	3.45	120.00	114.84
1	Aa	659	OMG	C5-C6-N1	3.45	120.04	113.95
1	Aa	891	OMG	C5-C6-N1	3.44	120.03	113.95
1	Aa	854	5MC	C5-C6-N1	-3.44	119.80	123.34
1	Aa	1223	OMG	C5-C6-N1	3.44	120.02	113.95
27	BA	2466	OMG	C5-C6-N1	3.44	120.02	113.95
27	BA	2016	OMG	C5-C6-N1	3.44	120.02	113.95
27	BA	1953	OMG	C5-C6-N1	3.43	120.02	113.95
27	BA	1345	5MC	C5-C6-N1	-3.43	119.81	123.34
1	Aa	913	OMG	C5-C6-N1	3.43	120.01	113.95
1	Aa	8	OMU	C5-C4-N3	3.43	119.97	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BA	1956	OMG	C5-C6-N1	3.42	120.00	113.95
27	BA	1480	OMU	C5-C4-N3	3.42	119.96	114.84
1	Aa	219	OMG	C5-C6-N1	3.42	119.98	113.95
27	BA	2728	OMG	C5-C6-N1	3.41	119.98	113.95
27	BA	912	OMG	C5-C6-N1	3.41	119.97	113.95
27	BA	872	OMG	C5-C6-N1	3.41	119.97	113.95
27	BA	2870	OMG	C5-C6-N1	3.40	119.96	113.95
27	BA	2528	OMG	C5-C6-N1	3.39	119.94	113.95
27	BA	507	OMG	C5-C6-N1	3.39	119.94	113.95
1	Aa	685	5MC	C5-C6-N1	-3.39	119.85	123.34
27	BA	2469	OMG	C5-C6-N1	3.39	119.93	113.95
27	BA	1969	OMU	C5-C4-N3	3.38	119.90	114.84
27	BA	1965	5MC	C5-C6-N1	-3.37	119.87	123.34
27	BA	2055	5MC	C5-C6-N1	-3.36	119.88	123.34
1	Aa	963	OMG	C5-C6-N1	3.36	119.88	113.95
1	Aa	1004	5MC	C5-C6-N1	-3.35	119.89	123.34
1	Aa	753	OMU	C5-C4-N3	3.34	119.84	114.84
27	BA	453	OMU	C5-C4-N3	3.34	119.84	114.84
27	BA	2581	4SU	C5-C4-S4	-3.33	120.18	124.47
27	BA	1150	OMU	C5-C4-N3	3.32	119.81	114.84
1	Aa	479	OMU	C5-C4-N3	3.30	119.77	114.84
27	BA	1402	OMU	C5-C4-N3	3.28	119.75	114.84
27	BA	2075	5MC	C5-C6-N1	-3.28	119.96	123.34
1	Aa	672	5MC	C5-C6-N1	-3.28	119.97	123.34
1	Aa	473	5MC	C5-C6-N1	-3.27	119.97	123.34
27	BA	1776	OMU	C5-C4-N3	3.27	119.73	114.84
27	BA	2389	OMU	O4-C4-C5	-3.24	119.46	125.16
1	Aa	340	5MC	C5-C6-N1	-3.24	120.01	123.34
1	Aa	1003	5MC	C5-C6-N1	-3.23	120.01	123.34
1	Aa	349	5MC	C5-C6-N1	-3.23	120.02	123.34
27	BA	2091	A2M	N3-C2-N1	-3.22	123.64	128.68
1	Aa	1020	OMU	C5-C4-N3	3.21	119.64	114.84
1	Aa	1006	5MC	C5-C6-N1	-3.19	120.06	123.34
1	Aa	1306	5MC	C5-C6-N1	-3.18	120.07	123.34
1	Aa	457	5MC	C5-C6-N1	-3.18	120.07	123.34
1	Aa	464	5MC	C5-C6-N1	-3.17	120.07	123.34
1	Aa	1476	5MC	C5-C6-N1	-3.15	120.10	123.34
1	Aa	1184	5MC	C5-C6-N1	-3.15	120.10	123.34
1	Aa	636	OMG	C2-N1-C6	-3.11	119.36	125.10
1	Aa	1358	OMU	C5-C4-N3	3.11	119.50	114.84
1	Aa	1352	5MC	C5-C6-N1	-3.09	120.16	123.34
27	BA	2070	5MC	C5-C6-N1	-3.09	120.16	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BA	1508	OMG	C2-N1-C6	-3.09	119.41	125.10
1	Aa	1449	6MZ	N3-C2-N1	-3.09	123.85	128.68
27	BA	1893	OMG	C2-N1-C6	-3.09	119.42	125.10
1	Aa	670	OMG	C2-N1-C6	-3.08	119.42	125.10
27	BA	2640	OMG	C2-N1-C6	-3.08	119.42	125.10
1	Aa	836	OMG	C2-N1-C6	-3.08	119.43	125.10
27	BA	2329	A2M	N3-C2-N1	-3.04	123.93	128.68
1	Aa	1266	5MC	C5-C6-N1	-3.03	120.22	123.34
1	Aa	1478	5MC	C5-C6-N1	-3.02	120.23	123.34
27	BA	63	OMG	C2-N1-C6	-3.02	119.54	125.10
1	Aa	1107	OMG	C2-N1-C6	-3.01	119.55	125.10
27	BA	872	OMG	C2-N1-C6	-3.01	119.55	125.10
27	BA	365	OMG	C2-N1-C6	-3.01	119.56	125.10
27	BA	1329	OMG	C2-N1-C6	-3.01	119.56	125.10
1	Aa	994	OMG	C2-N1-C6	-3.00	119.58	125.10
27	BA	2010	OMG	C2-N1-C6	-3.00	119.58	125.10
27	BA	2521	OMG	C2-N1-C6	-2.99	119.58	125.10
27	BA	215	OMG	C2-N1-C6	-2.99	119.59	125.10
27	BA	453	OMU	O4-C4-C5	-2.99	119.90	125.16
1	Aa	1223	OMG	C2-N1-C6	-2.99	119.59	125.10
27	BA	1525	OMG	C2-N1-C6	-2.99	119.59	125.10
1	Aa	629	OMG	C2-N1-C6	-2.99	119.60	125.10
1	Aa	320	OMG	C2-N1-C6	-2.99	119.60	125.10
1	Aa	446	OMG	C2-N1-C6	-2.98	119.61	125.10
27	BA	2469	OMG	C2-N1-C6	-2.97	119.64	125.10
27	BA	2379	OMG	C2-N1-C6	-2.97	119.64	125.10
1	Aa	147	OMG	C2-N1-C6	-2.97	119.64	125.10
27	BA	65	OMG	C2-N1-C6	-2.96	119.64	125.10
1	Aa	659	OMG	C2-N1-C6	-2.96	119.65	125.10
1	Aa	495	OMG	C2-N1-C6	-2.96	119.65	125.10
27	BA	584	OMG	C2-N1-C6	-2.96	119.65	125.10
1	Aa	219	OMG	C2-N1-C6	-2.95	119.67	125.10
1	Aa	574	OMG	C2-N1-C6	-2.94	119.68	125.10
1	Aa	498	OMG	C2-N1-C6	-2.94	119.68	125.10
27	BA	670	OMG	C2-N1-C6	-2.94	119.68	125.10
27	BA	2527	OMG	C2-N1-C6	-2.94	119.68	125.10
27	BA	288	OMG	C2-N1-C6	-2.94	119.69	125.10
27	BA	912	OMG	C2-N1-C6	-2.94	119.69	125.10
27	BA	2642	OMG	C2-N1-C6	-2.93	119.70	125.10
27	BA	1953	OMG	C2-N1-C6	-2.93	119.70	125.10
1	Aa	121	OMG	C2-N1-C6	-2.93	119.70	125.10
1	Aa	381	OMG	C2-N1-C6	-2.93	119.70	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BA	2870	OMG	C2-N1-C6	-2.93	119.71	125.10
27	BA	2016	OMG	C2-N1-C6	-2.93	119.71	125.10
27	BA	2168	OMG	C2-N1-C6	-2.92	119.72	125.10
27	BA	800	OMG	C2-N1-C6	-2.92	119.73	125.10
1	Aa	770	OMG	C2-N1-C6	-2.91	119.73	125.10
27	BA	674	OMG	C2-N1-C6	-2.91	119.74	125.10
1	Aa	532	OMG	C2-N1-C6	-2.91	119.75	125.10
27	BA	2728	OMG	C2-N1-C6	-2.90	119.75	125.10
27	BA	2466	OMG	C2-N1-C6	-2.90	119.76	125.10
1	Aa	913	OMG	C2-N1-C6	-2.90	119.76	125.10
27	BA	833	OMG	C2-N1-C6	-2.89	119.77	125.10
27	BA	2672	OMG	C2-N1-C6	-2.88	119.79	125.10
1	Aa	891	OMG	C2-N1-C6	-2.88	119.79	125.10
27	BA	1480	OMU	O4-C4-C5	-2.88	120.10	125.16
27	BA	1956	OMG	C2-N1-C6	-2.88	119.80	125.10
27	BA	2528	OMG	C2-N1-C6	-2.88	119.80	125.10
27	BA	507	OMG	C2-N1-C6	-2.87	119.80	125.10
27	BA	2656	OMU	O4-C4-C5	-2.87	120.11	125.16
1	Aa	479	OMU	O4-C4-C5	-2.87	120.11	125.16
1	Aa	753	OMU	O4-C4-C5	-2.85	120.15	125.16
27	BA	2745	OMG	C2-N1-C6	-2.85	119.85	125.10
1	Aa	1020	OMU	O4-C4-C5	-2.84	120.16	125.16
27	BA	2542	OMU	O4-C4-C5	-2.83	120.18	125.16
1	Aa	963	OMG	C2-N1-C6	-2.83	119.89	125.10
27	BA	2521	OMG	C8-N7-C5	2.82	108.37	102.99
27	BA	2642	OMG	C8-N7-C5	2.81	108.35	102.99
27	BA	63	OMG	C8-N7-C5	2.80	108.33	102.99
1	Aa	17	5MC	C5-C6-N1	-2.80	120.46	123.34
27	BA	800	OMG	C8-N7-C5	2.80	108.33	102.99
27	BA	1969	OMU	O4-C4-C5	-2.79	120.25	125.16
27	BA	2672	OMG	C8-N7-C5	2.78	108.29	102.99
1	Aa	836	OMG	C8-N7-C5	2.78	108.28	102.99
27	BA	2010	OMG	C8-N7-C5	2.78	108.28	102.99
27	BA	584	OMG	C8-N7-C5	2.77	108.27	102.99
1	Aa	8	OMU	O4-C4-C5	-2.77	120.29	125.16
27	BA	507	OMG	C8-N7-C5	2.77	108.26	102.99
27	BA	670	OMG	C8-N7-C5	2.76	108.24	102.99
1	Aa	320	OMG	C8-N7-C5	2.76	108.24	102.99
1	Aa	381	OMG	C8-N7-C5	2.75	108.24	102.99
27	BA	342	OMC	C2'-C1'-N1	-2.75	108.88	114.22
1	Aa	770	OMG	C8-N7-C5	2.75	108.23	102.99
1	Aa	1223	OMG	C8-N7-C5	2.75	108.23	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Aa	994	OMG	C8-N7-C5	2.75	108.23	102.99
27	BA	288	OMG	C8-N7-C5	2.75	108.23	102.99
27	BA	2329	A2M	C4-C5-N7	-2.75	106.54	109.40
27	BA	833	OMG	C8-N7-C5	2.75	108.22	102.99
27	BA	1776	OMU	O4-C4-C5	-2.74	120.34	125.16
1	Aa	498	OMG	C8-N7-C5	2.74	108.21	102.99
27	BA	872	OMG	C8-N7-C5	2.74	108.21	102.99
27	BA	2379	OMG	C8-N7-C5	2.74	108.20	102.99
1	Aa	532	OMG	C8-N7-C5	2.74	108.20	102.99
1	Aa	670	OMG	C8-N7-C5	2.73	108.20	102.99
27	BA	65	OMG	C8-N7-C5	2.73	108.19	102.99
27	BA	1508	OMG	C8-N7-C5	2.73	108.19	102.99
27	BA	1329	OMG	C8-N7-C5	2.73	108.19	102.99
27	BA	657	OMU	O4-C4-C5	-2.73	120.37	125.16
27	BA	2745	OMG	C8-N7-C5	2.72	108.18	102.99
27	BA	2427	5MU	O4-C4-N3	-2.72	114.90	120.12
1	Aa	891	OMG	C8-N7-C5	2.72	108.17	102.99
27	BA	1402	OMU	O4-C4-C5	-2.72	120.38	125.16
1	Aa	1321	5MC	CM5-C5-C6	-2.72	119.22	122.85
1	Aa	446	OMG	C8-N7-C5	2.72	108.17	102.99
1	Aa	495	OMG	C8-N7-C5	2.71	108.16	102.99
1	Aa	629	OMG	C8-N7-C5	2.71	108.15	102.99
27	BA	2527	OMG	C8-N7-C5	2.71	108.15	102.99
27	BA	2728	OMG	C8-N7-C5	2.71	108.15	102.99
1	Aa	574	OMG	C8-N7-C5	2.71	108.14	102.99
27	BA	1956	OMG	C8-N7-C5	2.70	108.14	102.99
1	Aa	913	OMG	C8-N7-C5	2.70	108.14	102.99
27	BA	912	OMG	C8-N7-C5	2.70	108.14	102.99
1	Aa	121	OMG	C8-N7-C5	2.70	108.14	102.99
27	BA	1893	OMG	C8-N7-C5	2.70	108.13	102.99
1	Aa	147	OMG	C8-N7-C5	2.69	108.12	102.99
27	BA	365	OMG	C8-N7-C5	2.69	108.12	102.99
27	BA	2469	OMG	C8-N7-C5	2.69	108.11	102.99
1	Aa	219	OMG	C8-N7-C5	2.69	108.11	102.99
1	Aa	659	OMG	C8-N7-C5	2.69	108.11	102.99
27	BA	1854	5MU	O4-C4-N3	-2.68	114.98	120.12
27	BA	2528	OMG	C8-N7-C5	2.68	108.09	102.99
27	BA	2016	OMG	C8-N7-C5	2.67	108.08	102.99
27	BA	2640	OMG	C8-N7-C5	2.67	108.08	102.99
27	BA	674	OMG	C8-N7-C5	2.65	108.05	102.99
27	BA	2466	OMG	C8-N7-C5	2.65	108.04	102.99
1	Aa	1449	6MZ	C4-C5-N7	-2.65	106.64	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BA	1953	OMG	C8-N7-C5	2.65	108.03	102.99
1	Aa	450	OMG	C5-C6-N1	2.64	118.62	113.95
1	Aa	1107	OMG	C8-N7-C5	2.64	108.02	102.99
1	Aa	1358	OMU	O4-C4-C5	-2.64	120.53	125.16
27	BA	2168	OMG	C8-N7-C5	2.63	108.01	102.99
27	BA	1766	5MU	O4-C4-N3	-2.62	115.09	120.12
1	Aa	963	OMG	C8-N7-C5	2.62	107.98	102.99
27	BA	215	OMG	C8-N7-C5	2.61	107.97	102.99
27	BA	2870	OMG	C8-N7-C5	2.61	107.97	102.99
27	BA	2553	4SU	C5-C4-S4	-2.59	121.13	124.47
27	BA	2389	OMU	O4'-C1'-C2'	-2.59	102.03	106.57
27	BA	1525	OMG	C8-N7-C5	2.57	107.89	102.99
1	Aa	636	OMG	C8-N7-C5	2.56	107.87	102.99
1	Aa	917	5MU	O2-C2-N1	-2.53	119.42	122.79
1	Aa	852	OMG	C5-C6-N1	2.52	118.40	113.95
27	BA	2550	OMG	C5-C6-N1	2.50	118.37	113.95
27	BA	1150	OMU	O4-C4-C5	-2.50	120.77	125.16
27	BA	829	5MU	O2-C2-N1	-2.46	119.51	122.79
27	BA	2553	4SU	O2-C2-N1	-2.43	119.56	122.79
27	BA	2091	A2M	C4-C5-N7	-2.42	106.87	109.40
1	Aa	340	5MC	CM5-C5-C6	-2.41	119.63	122.85
27	BA	2075	5MC	CM5-C5-C6	-2.40	119.64	122.85
27	BA	875	5MU	O4-C4-N3	-2.40	115.53	120.12
27	BA	829	5MU	O4-C4-N3	-2.36	115.60	120.12
27	BA	2353	OMG	C5-C6-N1	2.35	118.10	113.95
27	BA	1508	OMG	O6-C6-C5	-2.35	119.79	124.37
27	BA	2168	OMG	O6-C6-C5	-2.35	119.79	124.37
27	BA	670	OMG	CM2-O2'-C2'	2.35	120.68	114.52
1	Aa	381	OMG	O6-C6-C5	-2.33	119.81	124.37
1	Aa	995	2MG	C5-C6-N1	2.33	118.07	113.95
1	Aa	1107	OMG	O6-C6-C5	-2.32	119.83	124.37
27	BA	2389	OMU	O3'-C3'-C4'	-2.32	104.34	111.05
27	BA	1329	OMG	O6-C6-C5	-2.32	119.84	124.37
27	BA	2642	OMG	CM2-O2'-C2'	2.32	120.60	114.52
27	BA	2640	OMG	O6-C6-C5	-2.31	119.86	124.37
27	BA	215	OMG	O6-C6-C5	-2.30	119.88	124.37
1	Aa	852	OMG	C8-N7-C5	2.29	107.36	102.99
27	BA	2353	OMG	C8-N7-C5	2.29	107.34	102.99
27	BA	2010	OMG	O6-C6-C5	-2.28	119.92	124.37
1	Aa	450	OMG	C8-N7-C5	2.28	107.33	102.99
1	Aa	995	2MG	C8-N7-C5	2.28	107.33	102.99
1	Aa	636	OMG	O6-C6-C5	-2.27	119.94	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BA	1766	5MU	O2-C2-N1	-2.27	119.77	122.79
1	Aa	498	OMG	O6-C6-C5	-2.26	119.95	124.37
1	Aa	670	OMG	O6-C6-C5	-2.26	119.96	124.37
27	BA	1525	OMG	O6-C6-C5	-2.26	119.96	124.37
27	BA	2550	OMG	C8-N7-C5	2.26	107.29	102.99
1	Aa	923	5MC	CM5-C5-C6	-2.25	119.84	122.85
27	BA	63	OMG	O6-C6-C5	-2.25	119.97	124.37
1	Aa	532	OMG	O6-C6-C5	-2.25	119.98	124.37
1	Aa	17	5MC	CM5-C5-C6	-2.25	119.84	122.85
1	Aa	629	OMG	O6-C6-C5	-2.24	119.99	124.37
1	Aa	963	OMG	O6-C6-C5	-2.24	119.99	124.37
1	Aa	994	OMG	O6-C6-C5	-2.24	120.00	124.37
1	Aa	320	OMG	O6-C6-C5	-2.23	120.01	124.37
1	Aa	349	5MC	CM5-C5-C6	-2.23	119.87	122.85
1	Aa	1266	5MC	CM5-C5-C6	-2.23	119.87	122.85
1	Aa	770	OMG	O6-C6-C5	-2.23	120.01	124.37
1	Aa	1223	OMG	O6-C6-C5	-2.23	120.02	124.37
27	BA	2605	5MC	CM5-C5-C6	-2.22	119.88	122.85
1	Aa	473	5MC	CM5-C5-C6	-2.22	119.88	122.85
1	Aa	446	OMG	O6-C6-C5	-2.22	120.05	124.37
1	Aa	495	OMG	O6-C6-C5	-2.21	120.05	124.37
27	BA	2070	5MC	CM5-C5-C6	-2.21	119.90	122.85
27	BA	875	5MU	C1'-N1-C2	2.20	121.56	117.57
1	Aa	836	OMG	O6-C6-C5	-2.20	120.08	124.37
27	BA	1956	OMG	O6-C6-C5	-2.19	120.09	124.37
1	Aa	1006	5MC	CM5-C5-C6	-2.19	119.92	122.85
27	BA	1893	OMG	O6-C6-C5	-2.19	120.09	124.37
27	BA	288	OMG	O6-C6-C5	-2.19	120.10	124.37
1	Aa	121	OMG	O6-C6-C5	-2.18	120.12	124.37
27	BA	2389	OMU	C1'-N1-C2	2.17	121.51	117.57
27	BA	584	OMG	O6-C6-C5	-2.17	120.13	124.37
27	BA	1969	OMU	O2-C2-N1	-2.17	119.90	122.79
1	Aa	854	5MC	CM5-C5-C6	-2.17	119.95	122.85
27	BA	674	OMG	O6-C6-C5	-2.17	120.14	124.37
27	BA	2469	OMG	O6-C6-C5	-2.17	120.14	124.37
1	Aa	913	OMG	O6-C6-C5	-2.16	120.14	124.37
27	BA	55	5MC	CM5-C5-C6	-2.16	119.96	122.85
1	Aa	1306	5MC	CM5-C5-C6	-2.16	119.96	122.85
1	Aa	574	OMG	O6-C6-C5	-2.16	120.16	124.37
27	BA	2427	5MU	C1'-N1-C2	2.16	121.48	117.57
1	Aa	1358	OMU	O2-C2-N1	-2.16	119.92	122.79
27	BA	65	OMG	O6-C6-C5	-2.16	120.16	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Aa	1003	5MC	CM5-C5-C6	-2.15	119.98	122.85
27	BA	2521	OMG	O6-C6-C5	-2.14	120.18	124.37
1	Aa	659	OMG	O6-C6-C5	-2.14	120.20	124.37
27	BA	2595	OMC	O3'-C3'-C2'	2.13	117.22	111.17
1	Aa	219	OMG	O6-C6-C5	-2.13	120.21	124.37
27	BA	2379	OMG	O6-C6-C5	-2.12	120.23	124.37
27	BA	875	5MU	O2-C2-N1	-2.12	119.97	122.79
1	Aa	8	OMU	O2-C2-N1	-2.12	119.97	122.79
1	Aa	457	5MC	CM5-C5-C6	-2.11	120.03	122.85
27	BA	2728	OMG	O6-C6-C5	-2.11	120.25	124.37
1	Aa	891	OMG	O6-C6-C5	-2.11	120.26	124.37
1	Aa	1184	5MC	CM5-C5-C6	-2.11	120.04	122.85
27	BA	800	OMG	O6-C6-C5	-2.11	120.26	124.37
27	BA	833	OMG	O6-C6-C5	-2.11	120.26	124.37
1	Aa	685	5MC	CM5-C5-C6	-2.10	120.04	122.85
27	BA	829	5MU	C1'-N1-C2	2.09	121.36	117.57
1	Aa	464	5MC	CM5-C5-C6	-2.09	120.06	122.85
27	BA	365	OMG	O6-C6-C5	-2.08	120.30	124.37
1	Aa	147	OMG	O6-C6-C5	-2.08	120.31	124.37
27	BA	2672	OMG	O6-C6-C5	-2.08	120.31	124.37
1	Aa	1004	5MC	CM5-C5-C6	-2.07	120.08	122.85
27	BA	670	OMG	O6-C6-C5	-2.07	120.33	124.37
27	BA	2016	OMG	O6-C6-C5	-2.06	120.34	124.37
27	BA	912	OMG	O6-C6-C5	-2.06	120.35	124.37
1	Aa	672	5MC	CM5-C5-C6	-2.06	120.10	122.85
1	Aa	1476	5MC	CM5-C5-C6	-2.05	120.11	122.85
27	BA	1953	OMG	O6-C6-C5	-2.04	120.38	124.37
27	BA	2870	OMG	O6-C6-C5	-2.04	120.38	124.37
27	BA	2527	OMG	O6-C6-C5	-2.04	120.39	124.37
27	BA	2528	OMG	O6-C6-C5	-2.04	120.39	124.37
1	Aa	1020	OMU	O2-C2-N1	-2.04	120.08	122.79
1	Aa	1478	5MC	CM5-C5-C6	-2.01	120.16	122.85
27	BA	2581	4SU	O2-C2-N1	-2.01	120.11	122.79
27	BA	55	5MC	C5-C4-N3	-2.01	119.50	121.67
27	BA	1854	5MU	O2-C2-N1	-2.01	120.12	122.79
27	BA	1965	5MC	CM5-C5-C6	-2.00	120.17	122.85

There are no chirality outliers.

All (144) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	Aa	147	OMG	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
1	Aa	320	OMG	C3'-C4'-C5'-O5'
1	Aa	352	A2M	C1'-C2'-O2'-CM'
1	Aa	381	OMG	O4'-C4'-C5'-O5'
1	Aa	381	OMG	C3'-C4'-C5'-O5'
1	Aa	498	OMG	O4'-C4'-C5'-O5'
1	Aa	498	OMG	C3'-C4'-C5'-O5'
1	Aa	636	OMG	C1'-C2'-O2'-CM2
1	Aa	659	OMG	C1'-C2'-O2'-CM2
1	Aa	753	OMU	C1'-C2'-O2'-CM2
1	Aa	891	OMG	C1'-C2'-O2'-CM2
1	Aa	917	5MU	C3'-C4'-C5'-O5'
1	Aa	917	5MU	O4'-C4'-C5'-O5'
1	Aa	924	OMC	C3'-C2'-O2'-CM2
1	Aa	963	OMG	C3'-C4'-C5'-O5'
1	Aa	1004	5MC	O4'-C4'-C5'-O5'
1	Aa	1004	5MC	C3'-C4'-C5'-O5'
1	Aa	1020	OMU	C1'-C2'-O2'-CM2
1	Aa	1107	OMG	C3'-C4'-C5'-O5'
1	Aa	1306	5MC	O4'-C4'-C5'-O5'
1	Aa	1306	5MC	C3'-C4'-C5'-O5'
1	Aa	1361	OMC	C1'-C2'-O2'-CM2
1	Aa	1449	6MZ	C5-C6-N6-C9
1	Aa	1449	6MZ	N1-C6-N6-C9
27	BA	66	OMC	C1'-C2'-O2'-CM2
27	BA	91	OMC	C1'-C2'-O2'-CM2
27	BA	288	OMG	C1'-C2'-O2'-CM2
27	BA	342	OMC	C3'-C4'-C5'-O5'
27	BA	342	OMC	O4'-C4'-C5'-O5'
27	BA	453	OMU	C3'-C4'-C5'-O5'
27	BA	453	OMU	O4'-C4'-C5'-O5'
27	BA	657	OMU	C1'-C2'-O2'-CM2
27	BA	670	OMG	C3'-C2'-O2'-CM2
27	BA	674	OMG	O4'-C4'-C5'-O5'
27	BA	674	OMG	C3'-C4'-C5'-O5'
27	BA	849	A2M	C3'-C4'-C5'-O5'
27	BA	879	A2M	C1'-C2'-O2'-CM'
27	BA	1525	OMG	C1'-C2'-O2'-CM2
27	BA	1776	OMU	C1'-C2'-O2'-CM2
27	BA	1820	OMC	C1'-C2'-O2'-CM2
27	BA	1995	OMC	C1'-C2'-O2'-CM2
27	BA	2016	OMG	O4'-C4'-C5'-O5'
27	BA	2016	OMG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
27	BA	2124	OMC	C1'-C2'-O2'-CM2
27	BA	2353	OMG	O4'-C4'-C5'-O5'
27	BA	2353	OMG	C3'-C4'-C5'-O5'
27	BA	2469	OMG	C3'-C4'-C5'-O5'
27	BA	2521	OMG	C1'-C2'-O2'-CM2
27	BA	2527	OMG	C3'-C4'-C5'-O5'
27	BA	2542	OMU	C3'-C4'-C5'-O5'
27	BA	2542	OMU	O4'-C4'-C5'-O5'
27	BA	2545	OMC	C1'-C2'-O2'-CM2
27	BA	2545	OMC	C3'-C4'-C5'-O5'
27	BA	2545	OMC	O4'-C4'-C5'-O5'
27	BA	2595	OMC	C1'-C2'-O2'-CM2
27	BA	2640	OMG	C1'-C2'-O2'-CM2
27	BA	2642	OMG	C3'-C2'-O2'-CM2
27	BA	2728	OMG	C1'-C2'-O2'-CM2
1	Aa	17	5MC	O4'-C4'-C5'-O5'
1	Aa	121	OMG	O4'-C4'-C5'-O5'
1	Aa	121	OMG	C3'-C4'-C5'-O5'
1	Aa	495	OMG	C3'-C4'-C5'-O5'
1	Aa	670	OMG	O4'-C4'-C5'-O5'
1	Aa	913	OMG	C3'-C4'-C5'-O5'
1	Aa	963	OMG	O4'-C4'-C5'-O5'
1	Aa	1007	5MC	O4'-C4'-C5'-O5'
1	Aa	1107	OMG	O4'-C4'-C5'-O5'
1	Aa	1352	5MC	O4'-C4'-C5'-O5'
27	BA	55	5MC	O4'-C4'-C5'-O5'
27	BA	55	5MC	C3'-C4'-C5'-O5'
27	BA	2527	OMG	O4'-C4'-C5'-O5'
27	BA	2640	OMG	O4'-C4'-C5'-O5'
27	BA	2640	OMG	C3'-C4'-C5'-O5'
27	BA	2642	OMG	O4'-C4'-C5'-O5'
1	Aa	17	5MC	C3'-C4'-C5'-O5'
1	Aa	219	OMG	C3'-C4'-C5'-O5'
1	Aa	340	5MC	O4'-C4'-C5'-O5'
1	Aa	340	5MC	C3'-C4'-C5'-O5'
1	Aa	495	OMG	O4'-C4'-C5'-O5'
1	Aa	670	OMG	C3'-C4'-C5'-O5'
1	Aa	913	OMG	O4'-C4'-C5'-O5'
27	BA	849	A2M	O4'-C4'-C5'-O5'
27	BA	1150	OMU	O4'-C4'-C5'-O5'
27	BA	2642	OMG	C3'-C4'-C5'-O5'
1	Aa	320	OMG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	Aa	1352	5MC	C3'-C4'-C5'-O5'
1	Aa	8	OMU	C2'-C1'-N1-C6
27	BA	365	OMG	C3'-C4'-C5'-O5'
27	BA	1893	OMG	C3'-C4'-C5'-O5'
1	Aa	1007	5MC	C3'-C4'-C5'-O5'
27	BA	1150	OMU	C3'-C4'-C5'-O5'
27	BA	2047	OMC	O4'-C4'-C5'-O5'
27	BA	2389	OMU	C3'-C4'-C5'-O5'
27	BA	2389	OMU	O4'-C4'-C5'-O5'
27	BA	2469	OMG	O4'-C4'-C5'-O5'
27	BA	1893	OMG	O4'-C4'-C5'-O5'
27	BA	2379	OMG	C4'-C5'-O5'-P
1	Aa	219	OMG	O4'-C4'-C5'-O5'
27	BA	2329	A2M	O4'-C4'-C5'-O5'
1	Aa	8	OMU	O4'-C4'-C5'-O5'
1	Aa	229	OMC	C1'-C2'-O2'-CM2
27	BA	65	OMG	C1'-C2'-O2'-CM2
27	BA	2469	OMG	C1'-C2'-O2'-CM2
1	Aa	8	OMU	O4'-C1'-N1-C6
27	BA	365	OMG	O4'-C4'-C5'-O5'
27	BA	1956	OMG	O4'-C4'-C5'-O5'
27	BA	800	OMG	C3'-C2'-O2'-CM2
27	BA	2936	A2M	C3'-C2'-O2'-CM'
1	Aa	1478	5MC	C4'-C5'-O5'-P
1	Aa	8	OMU	C2'-C1'-N1-C2
27	BA	2605	5MC	C2'-C1'-N1-C6
27	BA	55	5MC	C4'-C5'-O5'-P
1	Aa	1478	5MC	O4'-C1'-N1-C6
1	Aa	320	OMG	C4'-C5'-O5'-P
1	Aa	574	OMG	C3'-C4'-C5'-O5'
27	BA	1345	5MC	O4'-C4'-C5'-O5'
27	BA	2329	A2M	C3'-C4'-C5'-O5'
1	Aa	1478	5MC	C2'-C1'-N1-C2
1	Aa	1478	5MC	C2'-C1'-N1-C6
1	Aa	8	OMU	O4'-C1'-N1-C2
1	Aa	352	A2M	O4'-C4'-C5'-O5'
27	BA	2047	OMC	C3'-C4'-C5'-O5'
27	BA	1402	OMU	C2'-C1'-N1-C6
1	Aa	8	OMU	C3'-C2'-O2'-CM2
27	BA	365	OMG	C3'-C2'-O2'-CM2
27	BA	2469	OMG	C3'-C2'-O2'-CM2
27	BA	2605	5MC	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
1	Aa	340	5MC	C4'-C5'-O5'-P
1	Aa	1468	MA6	O4'-C4'-C5'-O5'
27	BA	912	OMG	C3'-C4'-C5'-O5'
27	BA	1525	OMG	O4'-C4'-C5'-O5'
27	BA	2379	OMG	C3'-C4'-C5'-O5'
27	BA	2581	4SU	O4'-C4'-C5'-O5'
27	BA	1953	OMG	C3'-C4'-C5'-O5'
27	BA	1956	OMG	C3'-C4'-C5'-O5'
27	BA	1402	OMU	C2'-C1'-N1-C2
1	Aa	1478	5MC	O4'-C1'-N1-C2
27	BA	2605	5MC	O4'-C1'-N1-C2
1	Aa	457	5MC	C2'-C1'-N1-C2
1	Aa	1004	5MC	C2'-C1'-N1-C2
27	BA	2047	OMC	C2'-C1'-N1-C2
1	Aa	1306	5MC	C2'-C1'-N1-C2
27	BA	2605	5MC	C2'-C1'-N1-C2
1	Aa	457	5MC	C3'-C4'-C5'-O5'

There are no ring outliers.

43 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	BA	2070	5MC	1	0
27	BA	365	OMG	1	0
27	BA	2581	4SU	1	0
27	BA	2521	OMG	1	0
27	BA	932	A2M	1	0
27	BA	2595	OMC	2	0
27	BA	833	OMG	1	0
27	BA	2469	OMG	1	0
27	BA	2527	OMG	1	0
27	BA	1150	OMU	1	0
27	BA	1329	OMG	1	0
27	BA	2075	5MC	1	0
27	BA	2605	5MC	2	0
27	BA	872	OMG	1	0
27	BA	2124	OMC	3	0
27	BA	849	A2M	1	0
27	BA	1956	OMG	2	0
27	BA	2427	5MU	3	0
27	BA	2528	OMG	1	0
27	BA	2379	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	BA	91	OMC	1	0
27	BA	2550	OMG	2	0
27	BA	2936	A2M	1	0
27	BA	657	OMU	2	0
27	BA	65	OMG	1	0
27	BA	507	OMG	2	0
27	BA	2745	OMG	1	0
27	BA	2107	OMC	1	0
27	BA	1893	OMG	1	0
27	BA	2640	OMG	2	0
27	BA	912	OMG	2	0
27	BA	2545	OMC	2	0
27	BA	55	5MC	3	0
27	BA	1776	OMU	2	0
27	BA	2688	5MC	1	0
27	BA	2728	OMG	1	0
27	BA	879	A2M	2	0
27	BA	1995	OMC	1	0
27	BA	1969	OMU	1	0
27	BA	288	OMG	1	0
27	BA	670	OMG	5	0
27	BA	2642	OMG	5	0
27	BA	1820	OMC	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 14 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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.

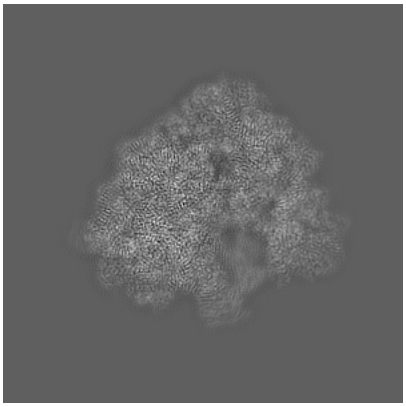
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10224. These allow visual inspection of the internal detail of the map and identification of artifacts.

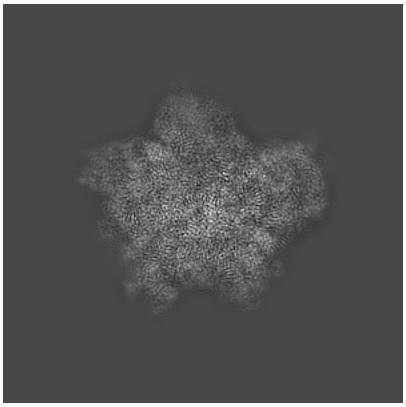
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

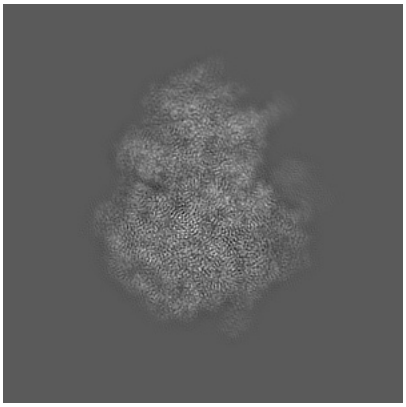
6.1.1 Primary map



X



Y

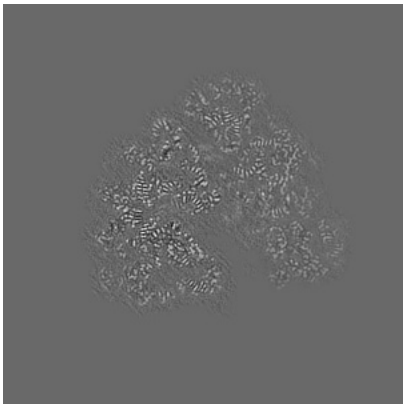


Z

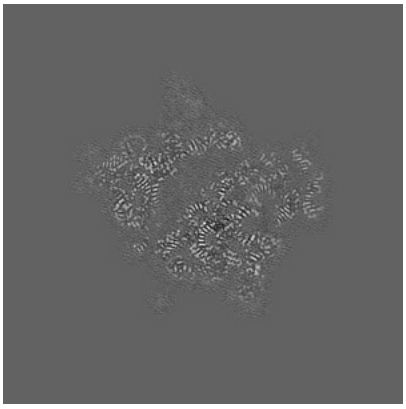
The images above show the map projected in three orthogonal directions.

6.2 Central slices

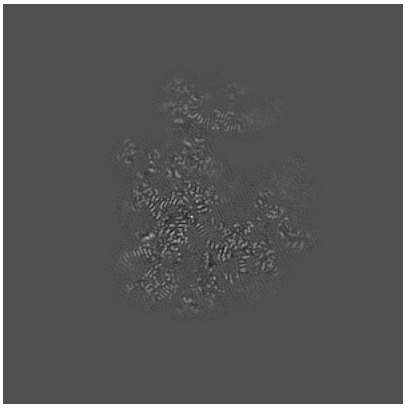
6.2.1 Primary map



X Index: 240



Y Index: 240

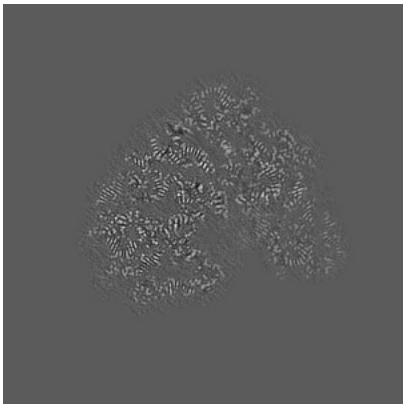


Z Index: 240

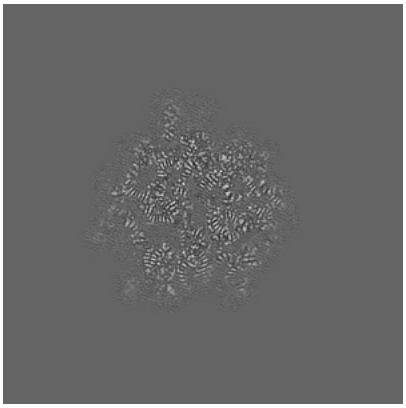
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

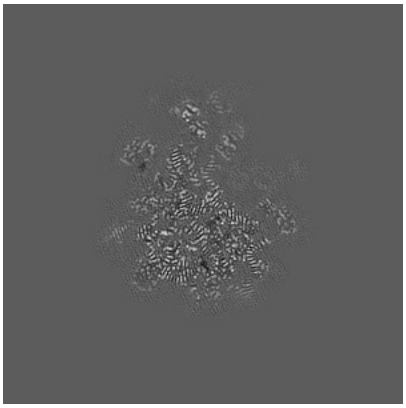
6.3.1 Primary map



X Index: 231



Y Index: 182

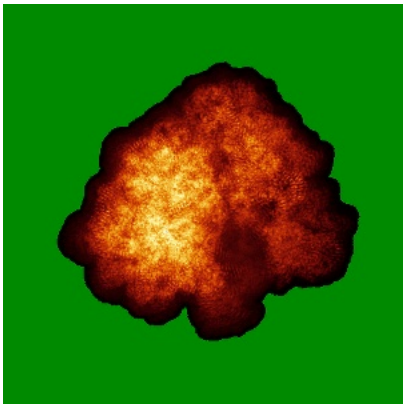


Z Index: 264

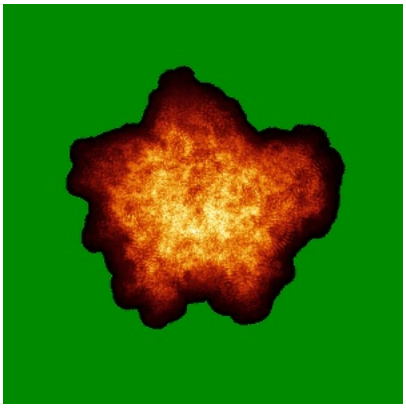
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

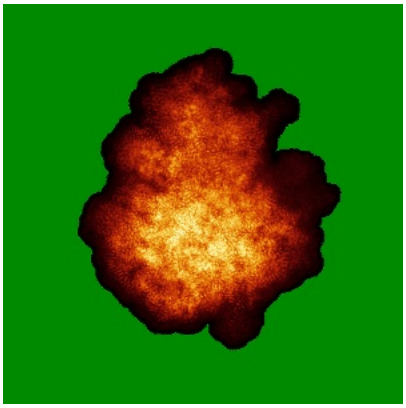
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

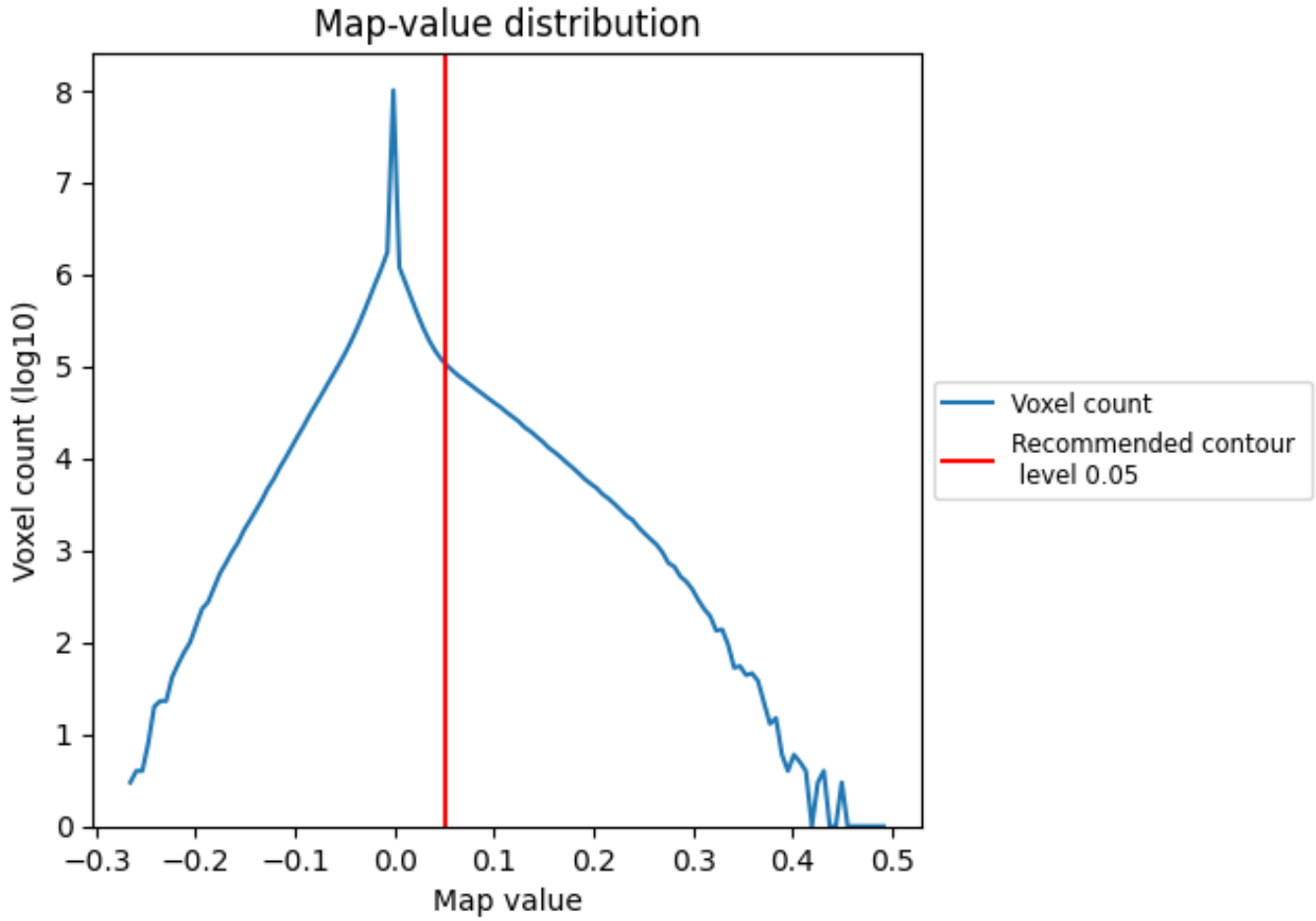
6.6 Mask visualisation (i)

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

7 Map analysis

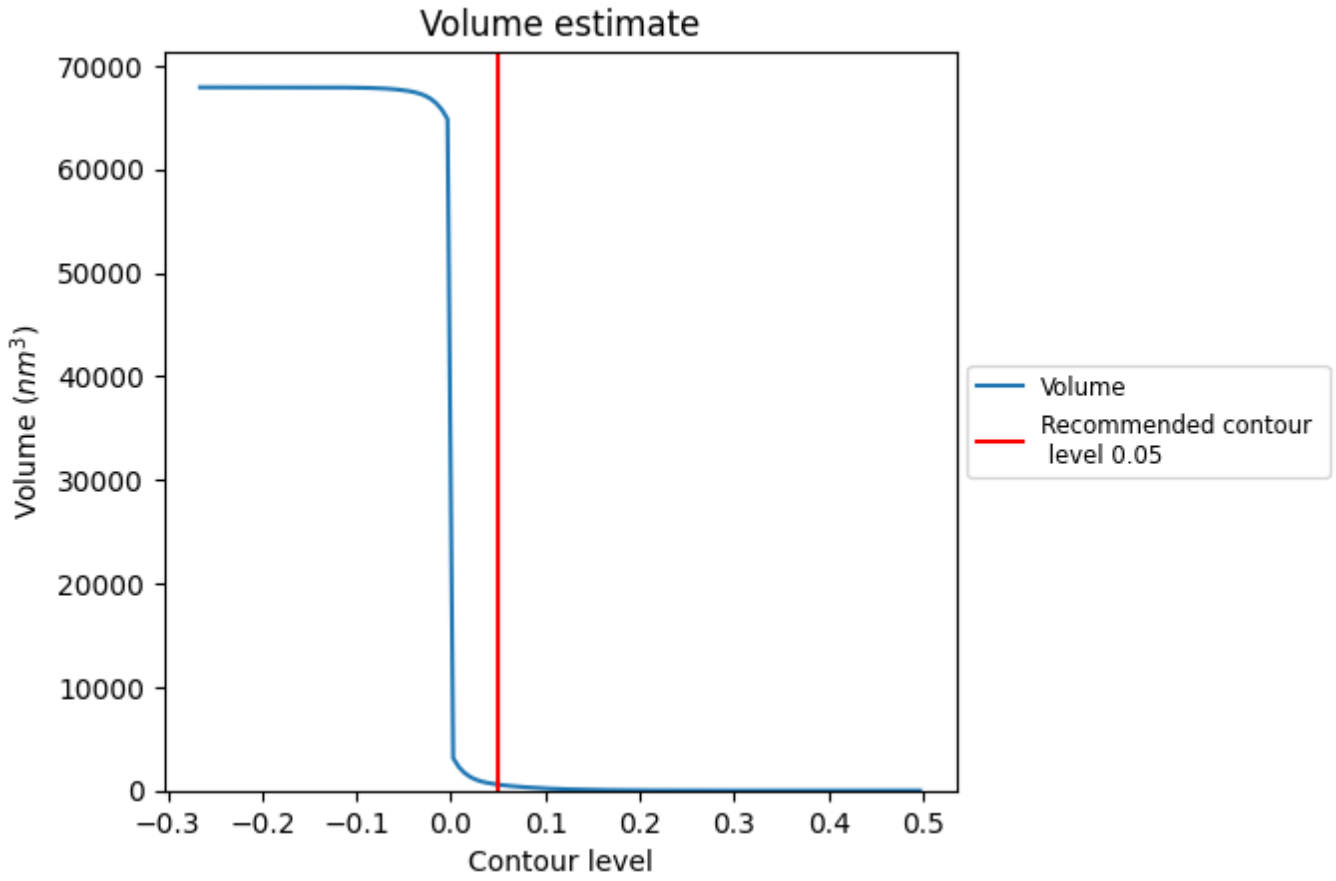
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

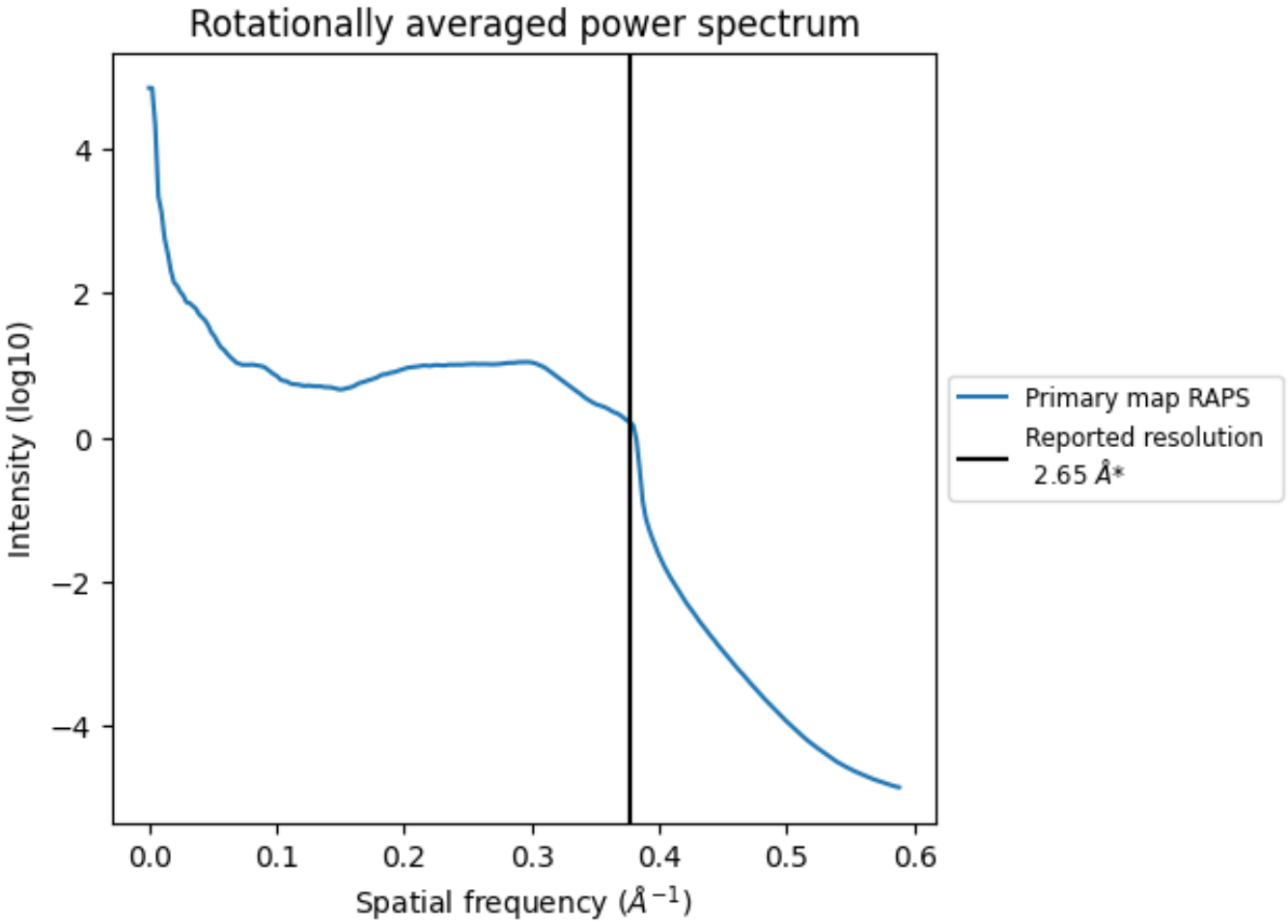
7.2 Volume estimate



The volume at the recommended contour level is 576 nm^3; this corresponds to an approximate mass of 520 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 (i)



*Reported resolution corresponds to spatial frequency of 0.377 Å^{-1}

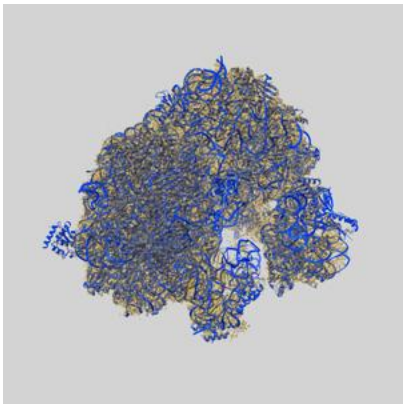
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

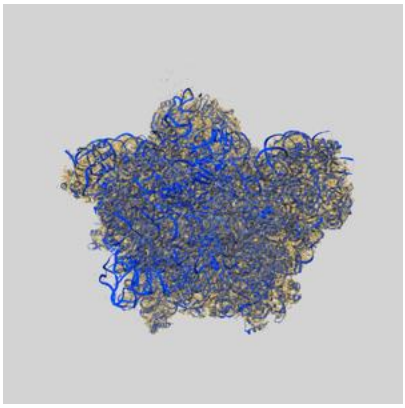
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10224 and PDB model 6SKG. Per-residue inclusion information can be found in section 3 on page 19.

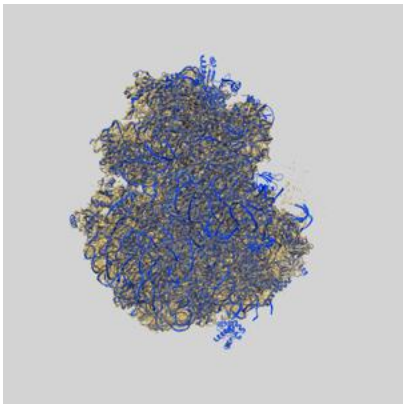
9.1 Map-model overlay



X



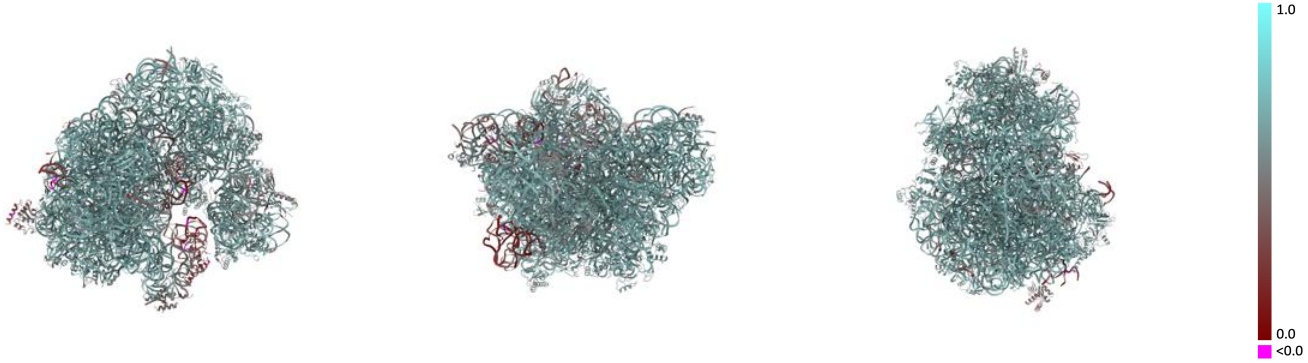
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

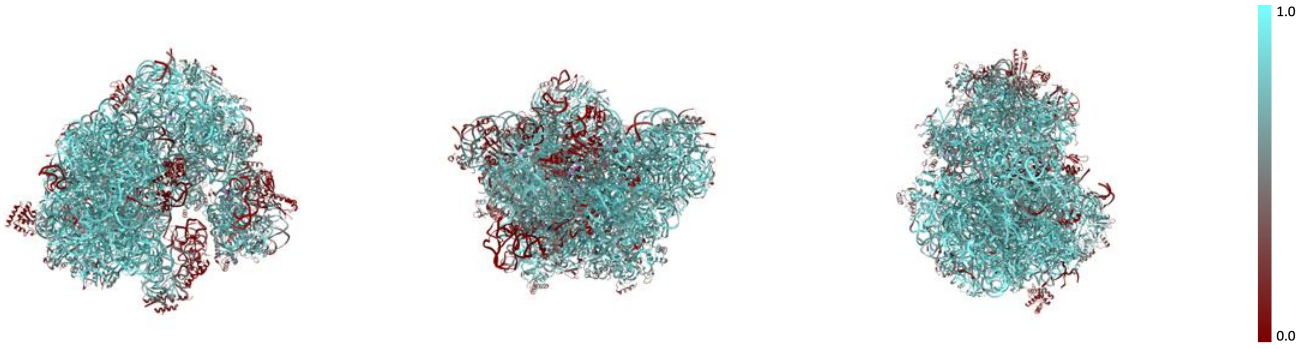
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

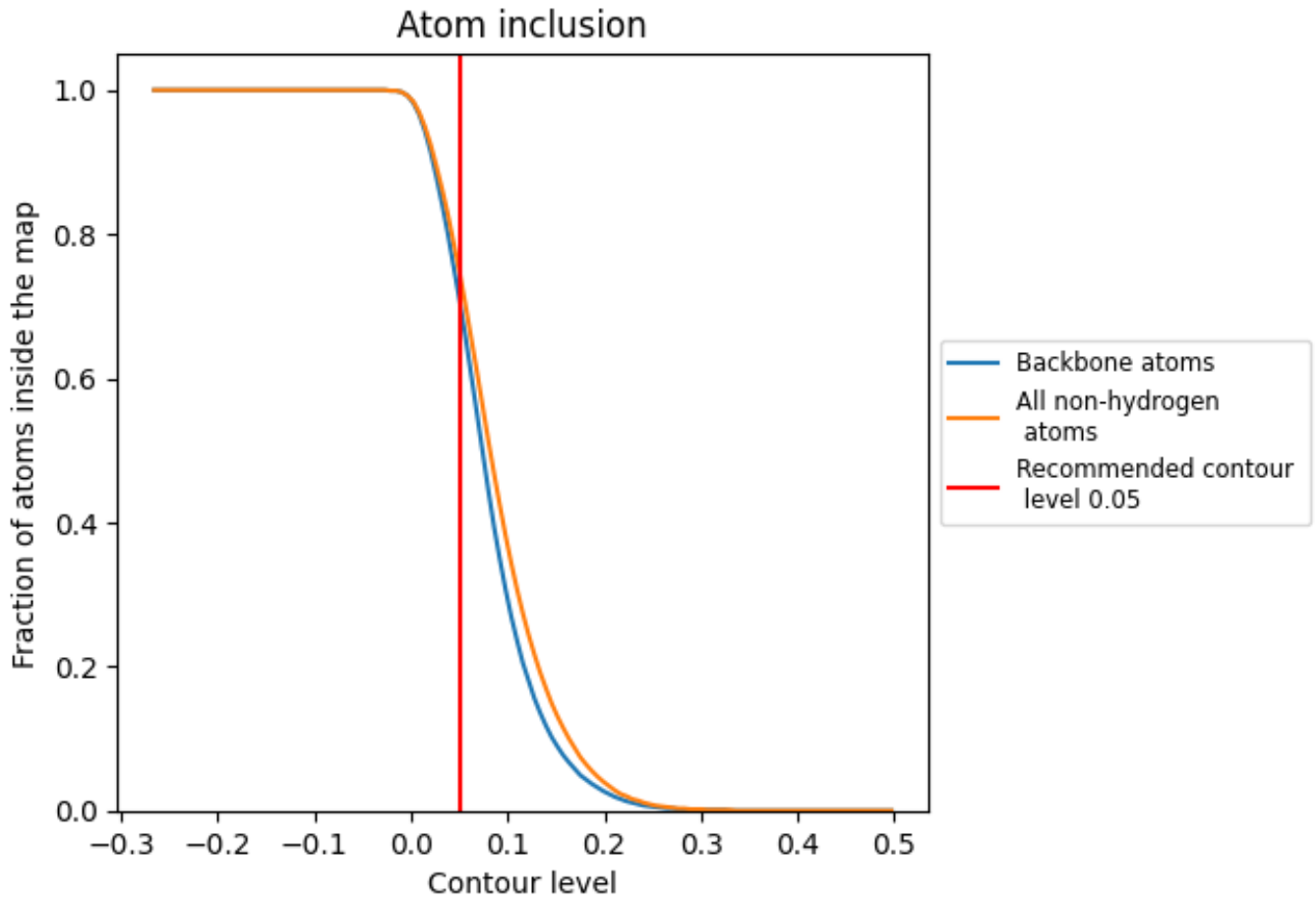
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 75% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7490	0.6140
Aa	0.7930	0.6280
Ab	0.5920	0.6100
Ac	0.2460	0.5360
Ad	0.5660	0.5980
Ae	0.6810	0.6190
Af	0.7270	0.6350
Ag	0.7100	0.6200
Ah	0.4000	0.5690
Ai	0.4940	0.5990
Aj	0.7550	0.6300
Ak	0.7110	0.6310
Al	0.5270	0.5990
Am	0.2700	0.5380
An	0.6040	0.6020
Ao	0.6920	0.6310
Ap	0.5220	0.5790
Aq	0.6910	0.6190
Ar	0.4750	0.5880
As	0.7240	0.6360
At	0.3020	0.5440
Au	0.5400	0.6000
Av	0.5910	0.6110
Aw	0.6090	0.5970
Ax	0.5550	0.5970
Ay	0.3010	0.5600
Az	0.7260	0.6200
BA	0.8480	0.6220
BB	0.6380	0.5600
BC	0.8460	0.6450
BD	0.8390	0.6530
BE	0.8160	0.6360
BF	0.1500	0.3600
BG	0.6960	0.6090
BH	0.5730	0.5750

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Chain	Atom inclusion	Q-score
BI	0.0570	0.3850
BJ	0.7460	0.6240
BK	0.8160	0.6490
BL	0.7820	0.6350
BM	0.5860	0.5680
BN	0.6080	0.5780
BO	0.6680	0.6110
BP	0.8950	0.6670
BQ	0.5270	0.5510
BR	0.8240	0.6440
BS	0.8030	0.6340
BT	0.6930	0.6170
BU	0.8370	0.6540
BV	0.8380	0.6560
BW	0.7220	0.6220
BX	0.7980	0.6320
BY	0.7940	0.6420
BZ	0.6170	0.5890
Ba	0.8070	0.6440
Bb	0.6500	0.5960
Bc	0.7730	0.6340
Bd	0.8350	0.6530
Be	0.8230	0.6360
Bf	0.7600	0.6300
Bg	0.7890	0.6300
Bh	0.9500	0.6770
Bi	0.8500	0.6450
Bj	0.7640	0.6420
Bk	0.8020	0.6360
Bl	0.7510	0.6440
Bm	0.5270	0.5600
Bn	0.5290	0.6000
Bo	0.8140	0.6430
Bp	0.0130	0.3690
Bq	0.0240	0.4650