Full wwPDB EM Validation Report (i)

Apr 17, 2024 – 04:08 am BST

PDB ID	:	6TH6
EMDB ID	:	EMD-10503
Title	:	Cryo-EM Structure of T. kodakarensis 70S ribosome
Authors	:	Matzov, D.; Sas-Chen, A.; Thomas, J.M.; Santangelo, T.; Meier, J.L.; Schwartz, S.; Shalev-Benami, M.
Deposited on	:	2019-11-18
Resolution	:	2.55 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 (i) 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 (i)) were used in the production of this report:

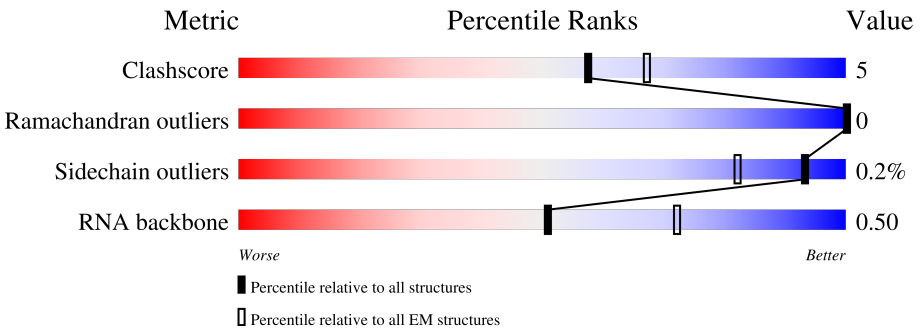
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.55 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	11% 80% 17% •
2	Ab	201	25% 98% •
3	Ac	209	81% 91% 9%
4	Ad	200	30% 95% 5%
5	Ae	180	16% 97% •
6	Af	243	8% 99% •
7	Ag	235	13% 94% 5%

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Mol	Chain	Length	Quality of chain
8	Ah	125	58% 98%
9	Ai	215	39% 99%
10	Aj	130	5% 99%
11	Ak	130	11% 96%
12	Al	135	30% 99%
13	Am	102	74% 98%
14	An	140	32% 87% 9%
15	Ao	147	11% 97%
16	Ap	149	40% 91% 9%
17	Aq	151	11% 99%
18	Ar	56	39% 96%
19	As	114	32% 93% 6%
20	At	67	94% 96%
21	Au	133	37% 87% 13%
22	Av	150	27% 99%
23	Aw	98	24% 97%
24	Ax	65	22% 94% 6%
25	Ay	70	66% 91% 9%
26	Az	62	11% 89% 11%
27	BA	3037	13% 62% 27% 7%
28	BB	126	40% 67% 23% 10%
29	BC	239	6% 89% 10%
30	BD	346	6% 89% 10%
31	BE	255	5% 88% 12%
32	BF	183	85% 57% 33% 9%

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Mol	Chain	Length	Quality of chain
33	BG	184	20% 93% 7%
34	BH	123	34% 88% 11%
34	BI	123	98% 74% 24%
35	BJ	182	22% 79% 14% 8%
36	BK	142	6% 94% 6%
37	BL	141	9% 94% 6%
38	BM	83	33% 77% 19%
38	BN	83	49% 80% 18%
39	BO	148	34% 88% 12%
40	BP	194	95%
41	BQ	201	36% 69% 12% 18%
42	BR	121	86% 13%
43	BS	150	87% 10%
44	BT	77	34% 88% 8%
45	BU	98	89% 9%
46	BV	156	5% 85% 13%
47	BW	86	14% 92% 7%
48	BX	121	6% 90% 9%
49	BY	67	16% 85% 7% 7%
50	BZ	66	27% 82% 9% 9%
51	Ba	155	8% 99%
52	Bb	102	26% 94% 6%
53	Bc	90	10% 99%
54	Bd	125	5% 98%
55	Be	90	97%

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Mol	Chain	Length	Quality of chain
56	Bg	86	6% 97%
57	Bh	63	98%
58	Bi	51	12% 96%
59	Bj	51	12% 92% 8%
60	Bk	37	97%
61	Bl	94	7% 99%

2 Entry composition (i)

There are 63 unique types of molecules in this entry. The entry contains 161508 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	31499	14027	5837	10172	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	191	1513	967	276	267	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	241	1945	1256	348	336	5	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	Ai	213	1706	1082	316	300	8	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	As	107	868	554	160	151	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	At	64	538	338	103	95	2	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	Aw	95	777	497	131	146	3	0	0

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ax	64	GLU	LEU	conflict	UNP Q5JE50
Ax	65	LEU	GLU	conflict	UNP Q5JE50

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

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

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
27	BA	2934	63188	28147	11754	20352	2934	1	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	BF	166	1338	839	258	234	7	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	BJ	168	1378	877	258	236	7	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	BO	148	1162	740	221	198	3	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 56 is a protein called 50S ribosomal protein L37Ae.

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

- Molecule 57 is a protein called 50S ribosomal protein L37e.

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

- Molecule 58 is a protein called 50S ribosomal protein L39e.

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

- Molecule 59 is a protein called 50S ribosomal protein L40e.

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

- Molecule 60 is a protein called LSU ribosomal protein L41E.

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

- Molecule 61 is a protein called 50S ribosomal protein L44e.

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

- Molecule 62 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 63 is water.

Mol	Chain	Residues	Atoms	AltConf
63	Aa	153	Total O 153 153	0
63	Ae	1	Total O 1 1	0
63	Af	5	Total O 5 5	0
63	Ag	1	Total O 1 1	0
63	Ai	1	Total O 1 1	0
63	Aj	1	Total O 1 1	0
63	Ak	2	Total O 2 2	0
63	Al	2	Total O 2 2	0
63	An	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
63	Ao	2	Total O 2 2	0
63	Ap	1	Total O 1 1	0
63	Aq	5	Total O 5 5	0
63	Av	1	Total O 1 1	0
63	Az	1	Total O 1 1	0
63	BA	1674	Total O 1674 1674	0
63	BB	7	Total O 7 7	0
63	BC	29	Total O 29 29	0
63	BD	30	Total O 30 30	0
63	BE	24	Total O 24 24	0
63	BF	1	Total O 1 1	0
63	BH	1	Total O 1 1	0
63	BJ	4	Total O 4 4	0
63	BK	7	Total O 7 7	0
63	BL	8	Total O 8 8	0
63	BN	1	Total O 1 1	0
63	BO	19	Total O 19 19	0
63	BP	23	Total O 23 23	0
63	BQ	5	Total O 5 5	0
63	BR	1	Total O 1 1	0
63	BS	12	Total O 12 12	0

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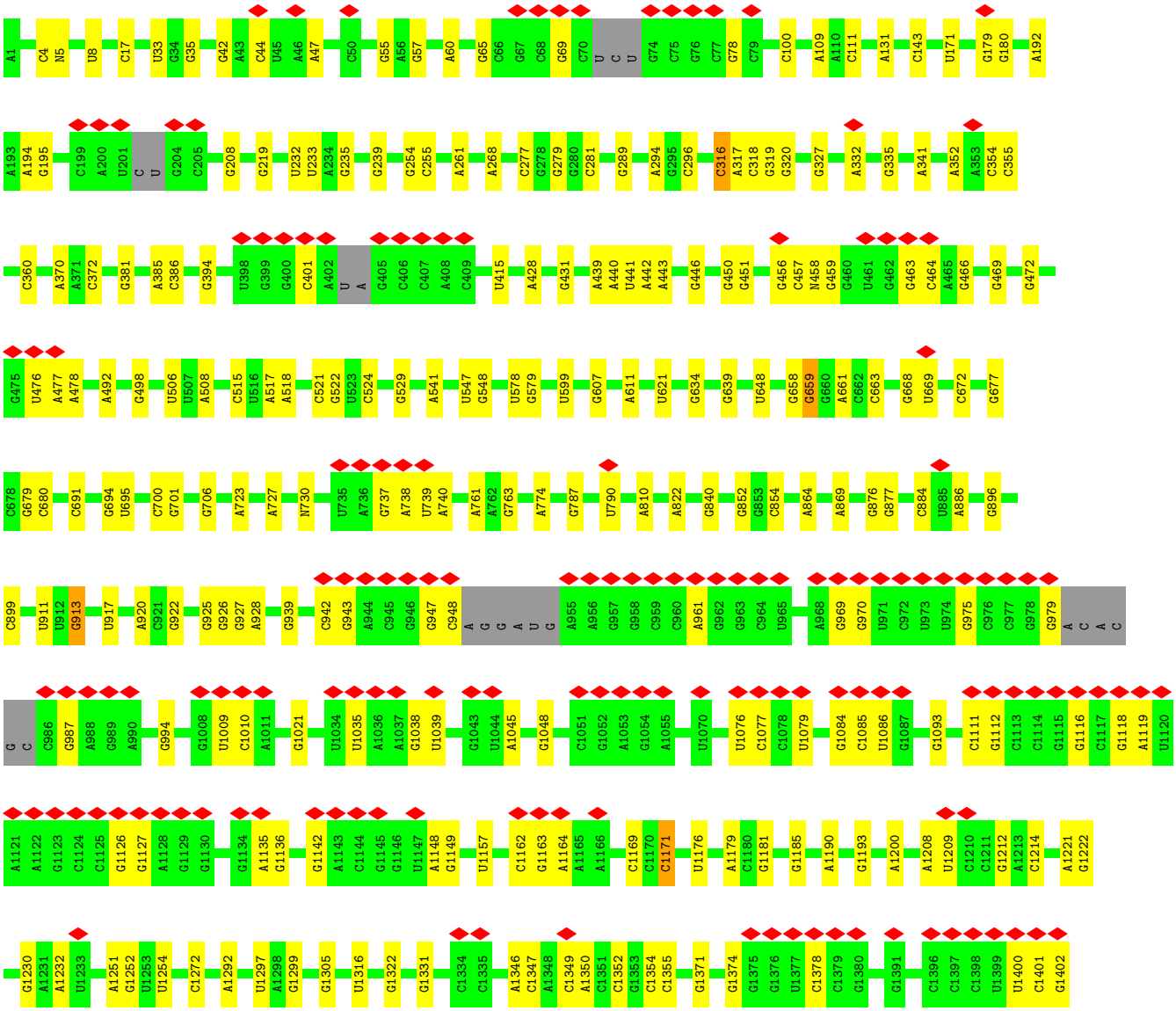
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
63	BV	17	17	17	0
			Total	O	
63	BW	3	3	3	0
			Total	O	
63	BX	7	7	7	0
			Total	O	
63	BY	5	5	5	0
			Total	O	
63	BZ	3	3	3	0
			Total	O	
63	Ba	6	6	6	0
			Total	O	
63	Bb	1	1	1	0
			Total	O	
63	Bc	7	7	7	0
			Total	O	
63	Bd	12	12	12	0
			Total	O	
63	Be	7	7	7	0
			Total	O	
63	Bg	6	6	6	0
			Total	O	
63	Bh	18	18	18	0
			Total	O	
63	Bi	5	5	5	0
			Total	O	
63	Bk	6	6	6	0
			Total	O	
63	Bl	3	3	3	0

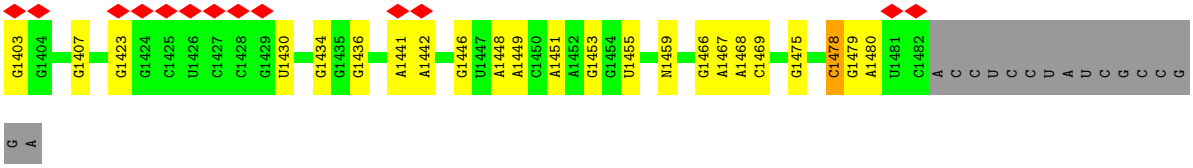
3 Residue-property plots (i)

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

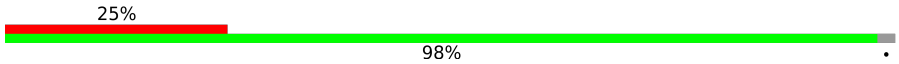
Chain Aa:

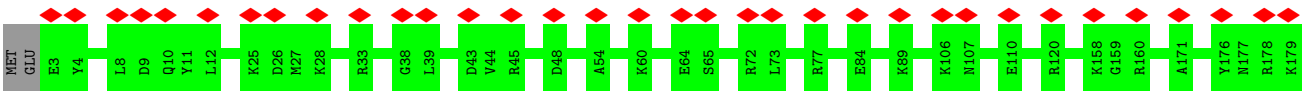


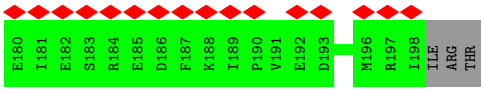


• Molecule 2: 30S ribosomal protein S2

Chain Ab:

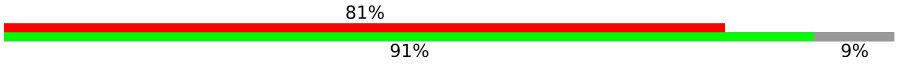


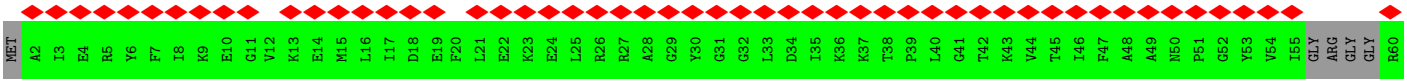


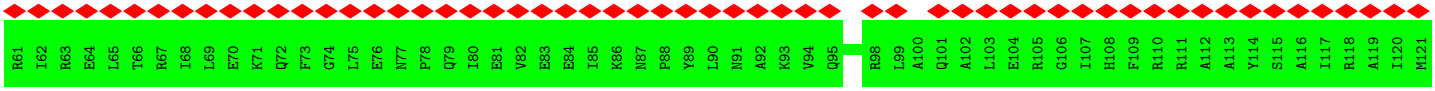


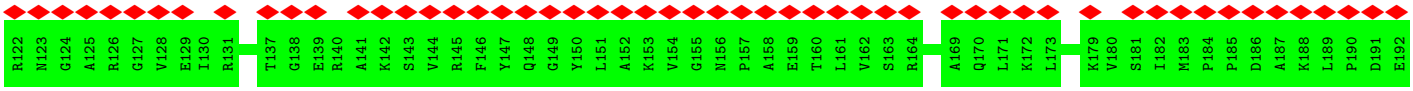
• Molecule 3: 30S ribosomal protein S3

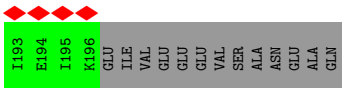
Chain Ac:





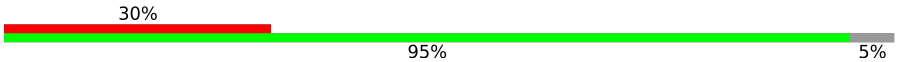


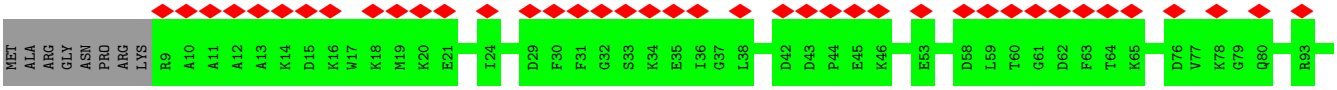


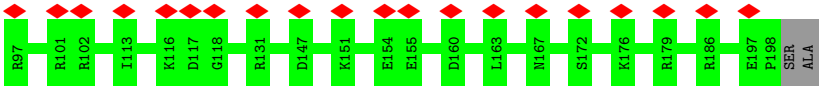


• Molecule 4: 30S ribosomal protein S3Ae

Chain Ad:

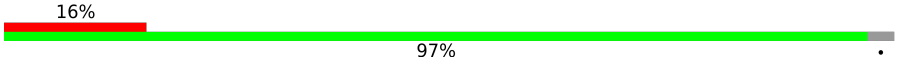


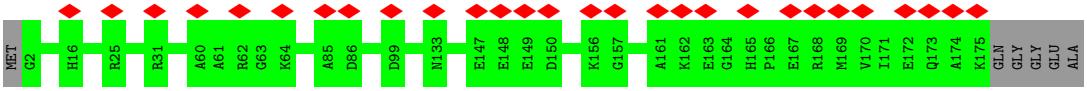




• Molecule 5: 30S ribosomal protein S4

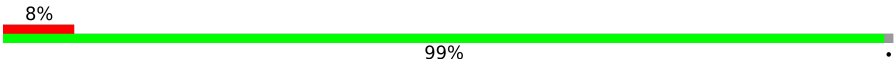
Chain Ae:

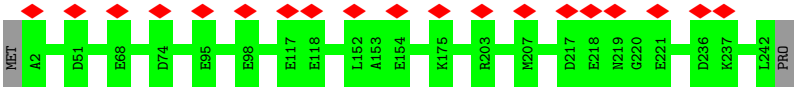




• Molecule 6: 30S ribosomal protein S4e

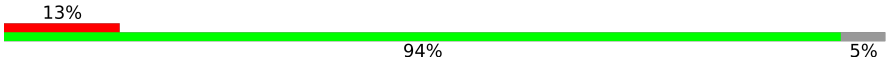
Chain Af:

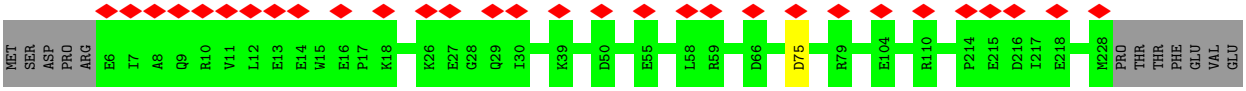




• Molecule 7: 30S ribosomal protein S5

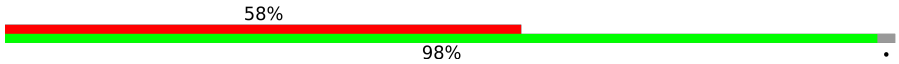
Chain Ag:





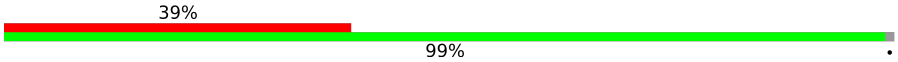
• Molecule 8: 30S ribosomal protein S6e

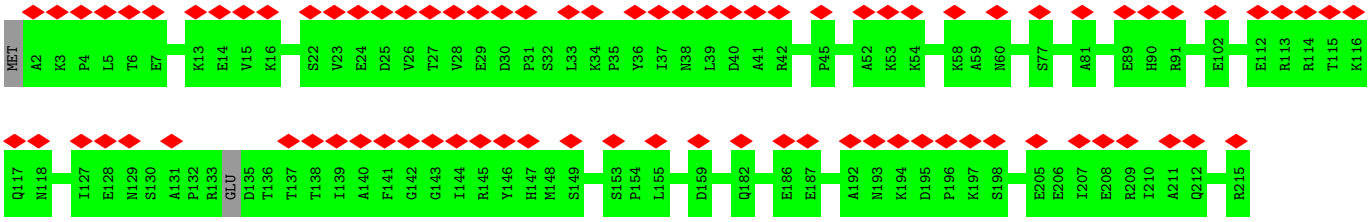
Chain Ah:



• Molecule 9: 30S ribosomal protein S7

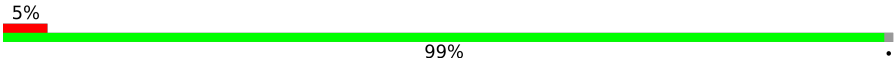
Chain Ai:

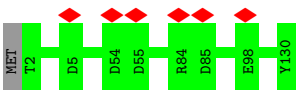




• Molecule 10: 30S ribosomal protein S8

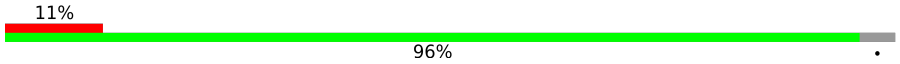
Chain Aj:

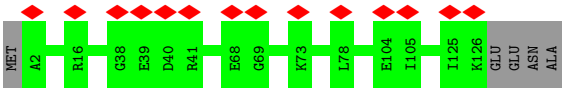




• Molecule 11: 30S ribosomal protein S8e

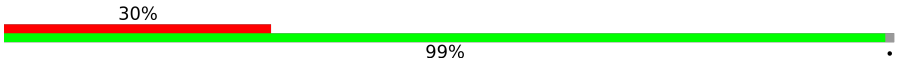
Chain Ak:

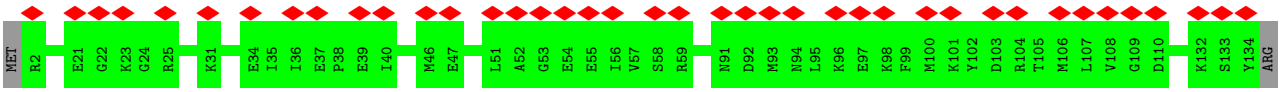




• Molecule 12: 30S ribosomal protein S9

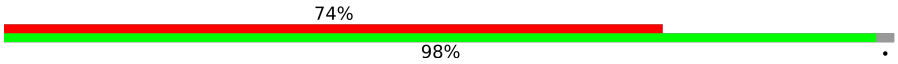
Chain Al:

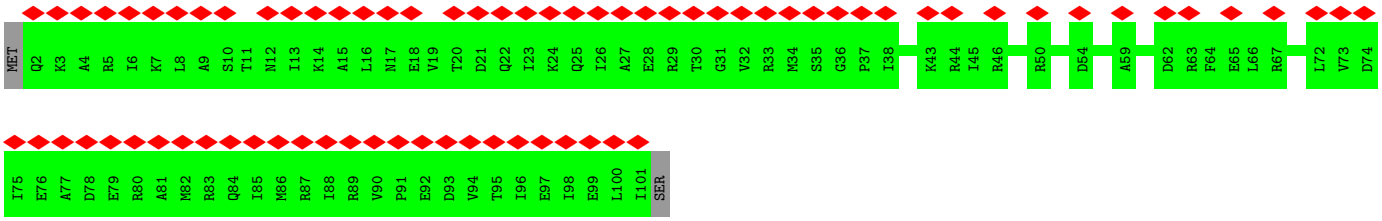




• Molecule 13: 30S ribosomal protein S10

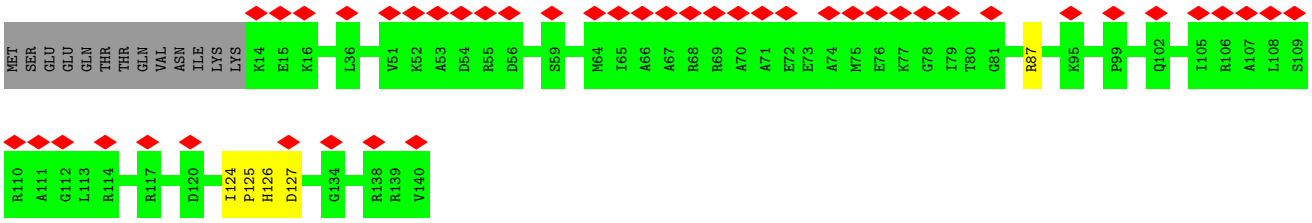
Chain Am:





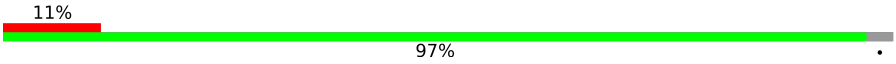
• Molecule 14: 30S ribosomal protein S11

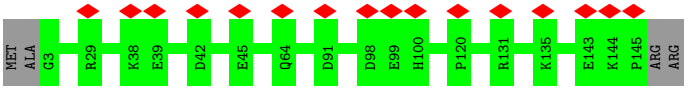
Chain An:



• Molecule 15: 30S ribosomal protein S12

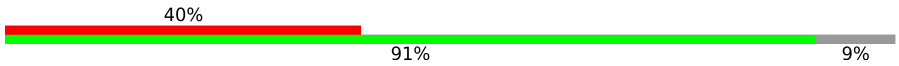
Chain Ao:

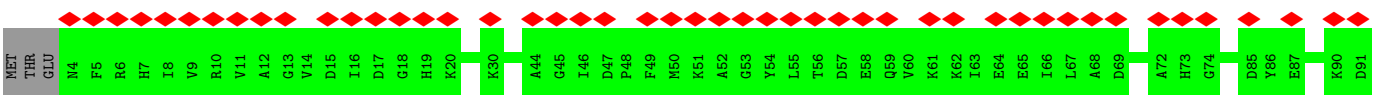


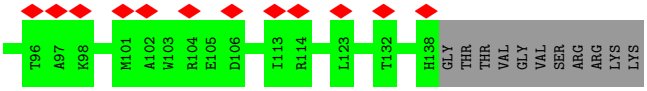


• Molecule 16: 30S ribosomal protein S13

Chain Ap:

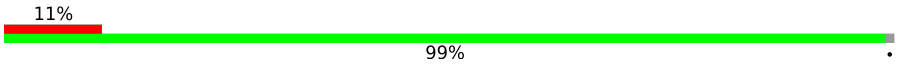


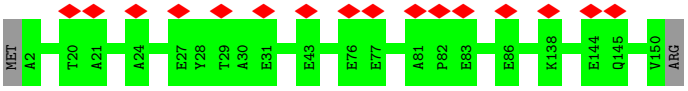




• Molecule 17: 30S ribosomal protein S15

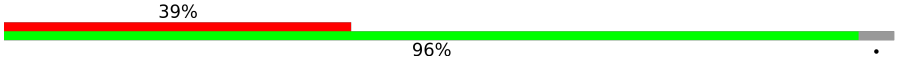
Chain Aq:

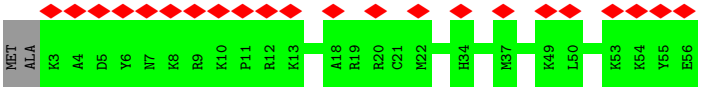




• Molecule 18: 30S ribosomal protein S14 type Z

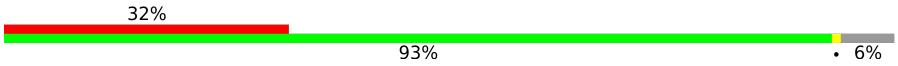
Chain Ar:

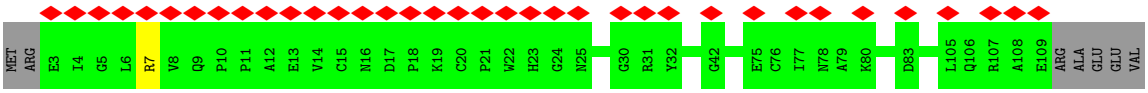




• Molecule 19: 30S ribosomal protein S17

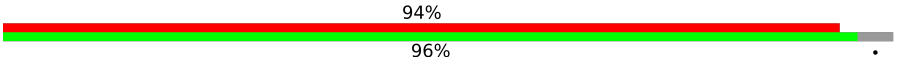
Chain As:





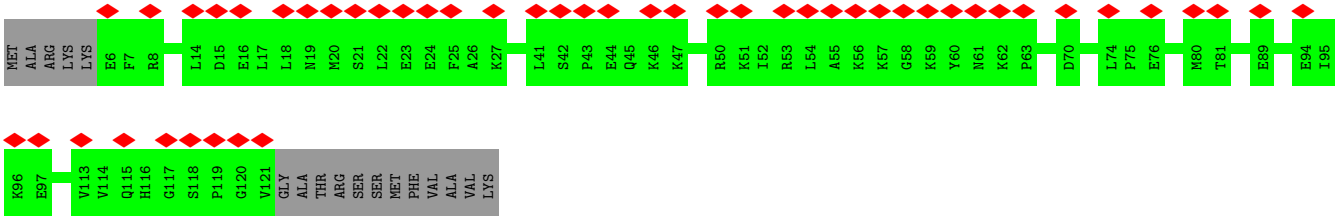
• Molecule 20: 30S ribosomal protein S17e

Chain At:



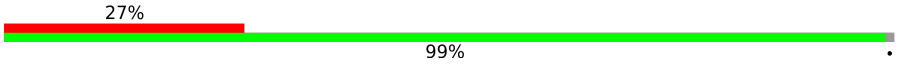
• Molecule 21: 30S ribosomal protein S19

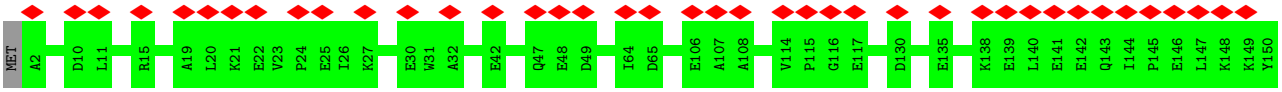
Chain Au:



• Molecule 22: 30S ribosomal protein S19e

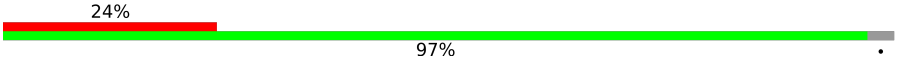
Chain Av:

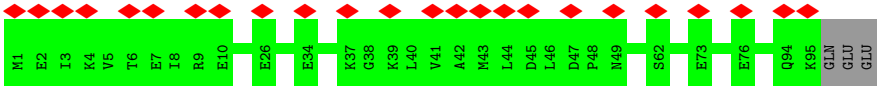




• Molecule 23: 30S ribosomal protein S24e

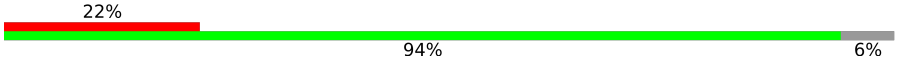
Chain Aw:

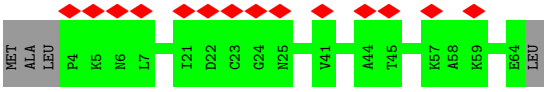




• Molecule 24: 30S ribosomal protein S27e

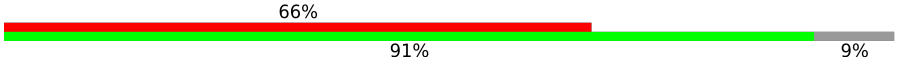
Chain Ax:

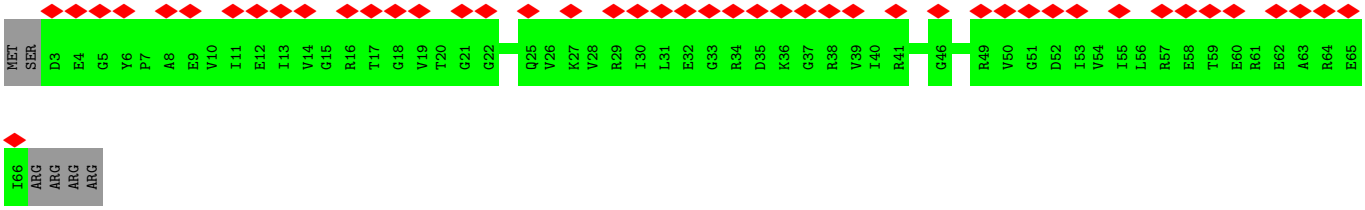




• Molecule 25: 30S ribosomal protein S28e

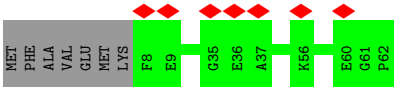
Chain Ay:





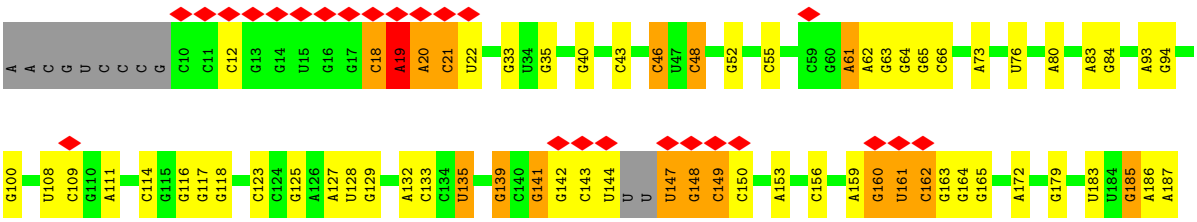
• Molecule 26: Predicted zinc-ribbon RNA-binding protein involved in translation

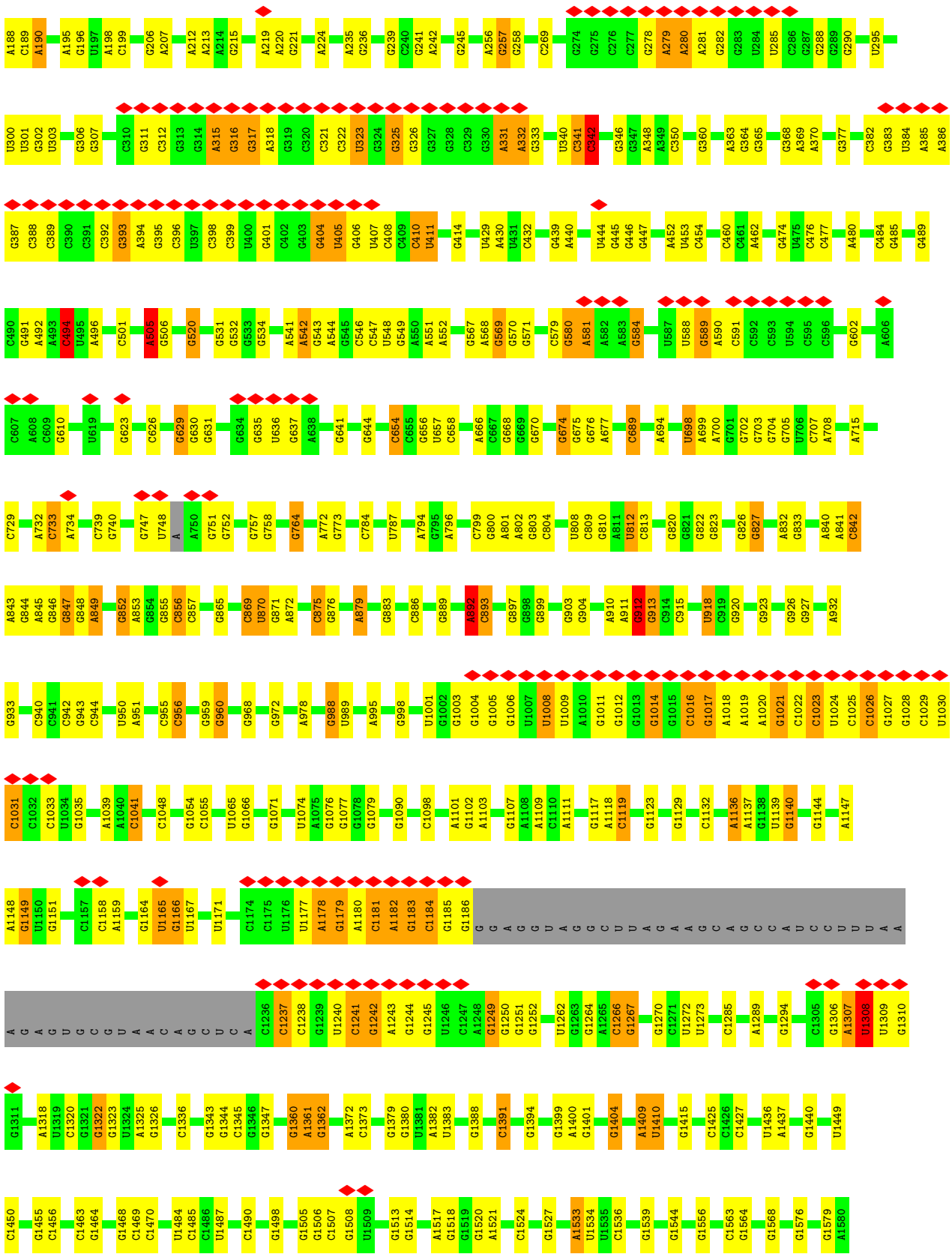
Chain Az:



• Molecule 27: 23S ribosomal RNA

Chain BA:

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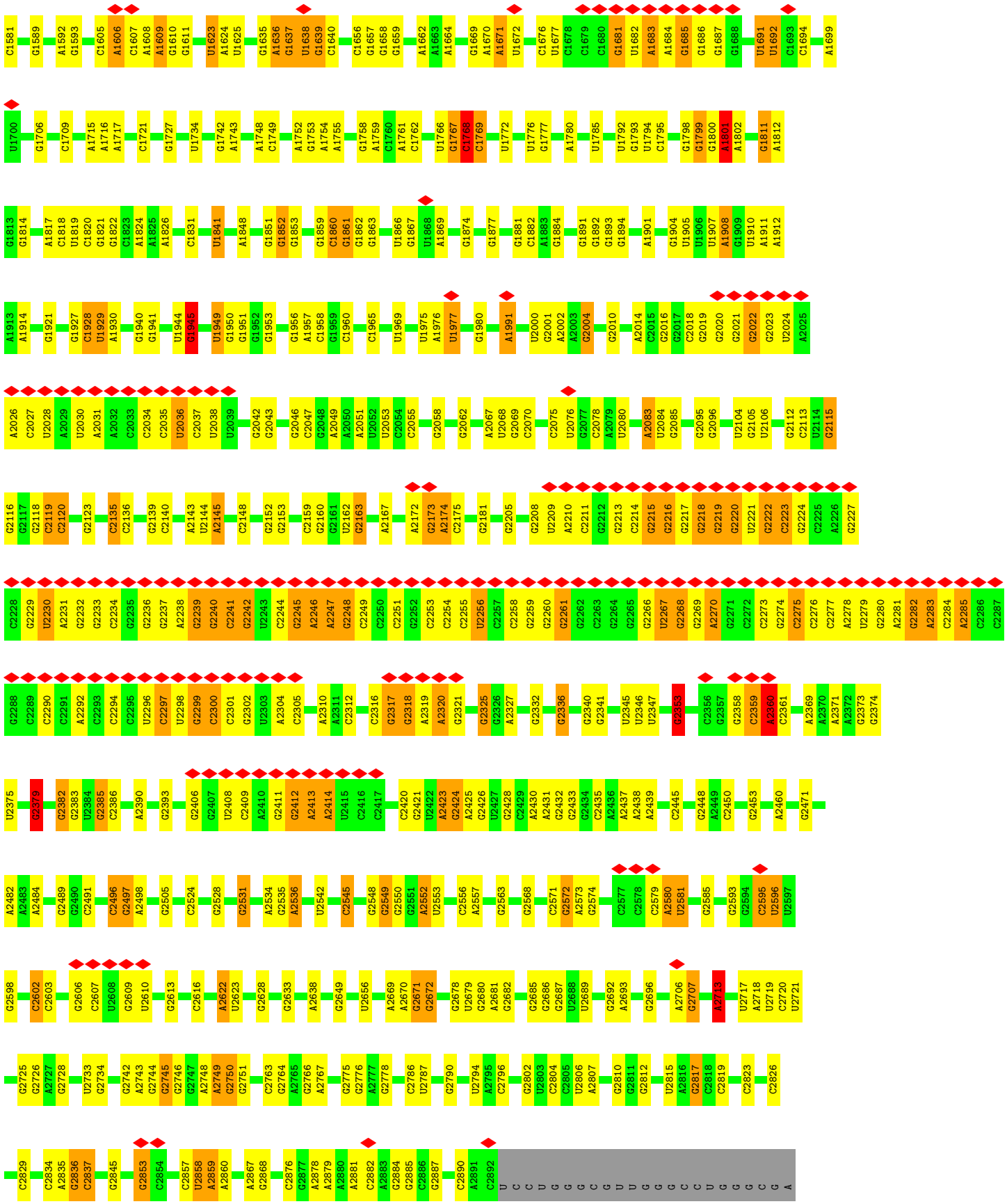
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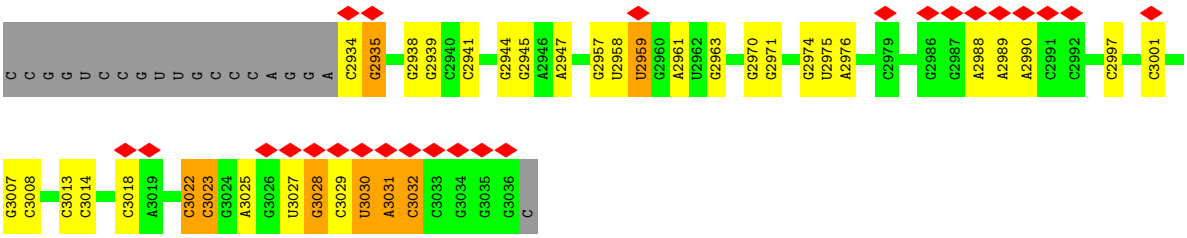
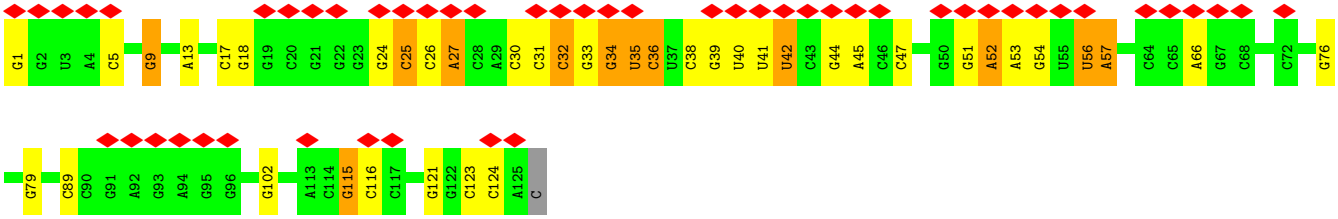


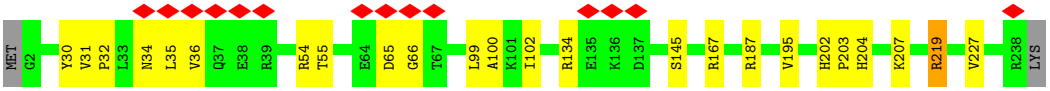
• Molecule 28: 5S ribosomal RNA

Chain BB:



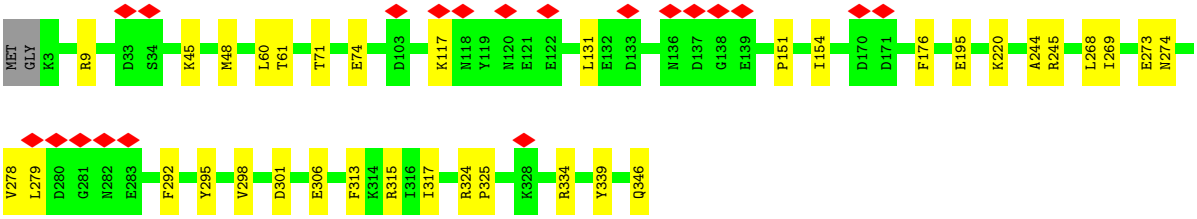
• Molecule 29: 50S ribosomal protein L2

Chain BC:



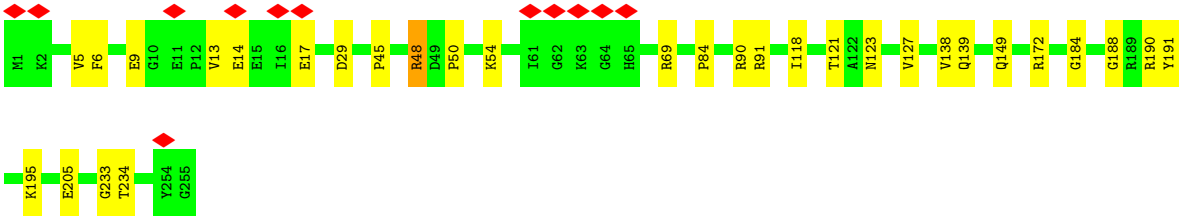
• Molecule 30: 50S ribosomal protein L3

Chain BD:



• Molecule 31: 50S ribosomal protein L4

Chain BE:

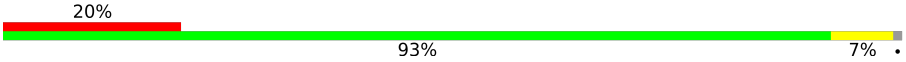


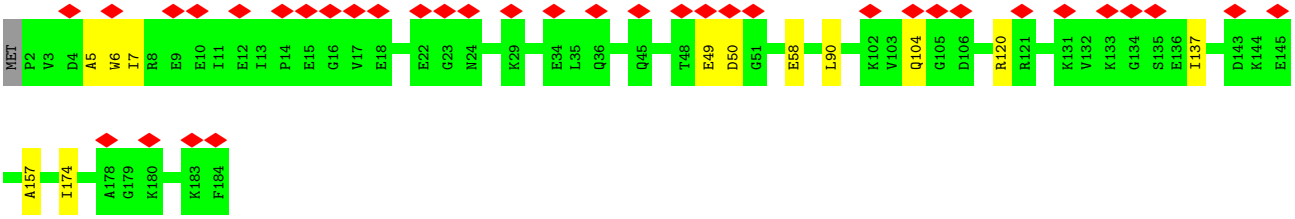
• Molecule 32: 50S ribosomal protein L5

Chain BF:

- Molecule 33: 50S ribosomal protein L6

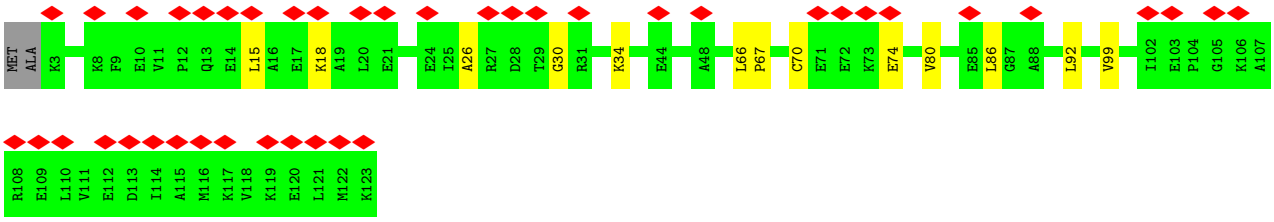
Chain BG:





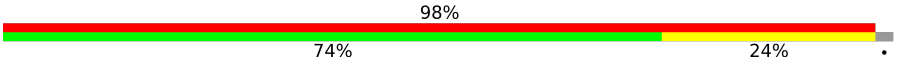
- Molecule 34: 50S ribosomal protein L7Ae

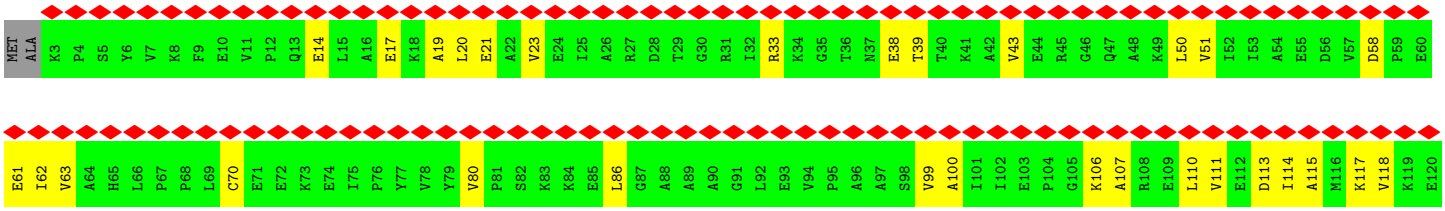
Chain BH:



- Molecule 34: 50S ribosomal protein L7Ae

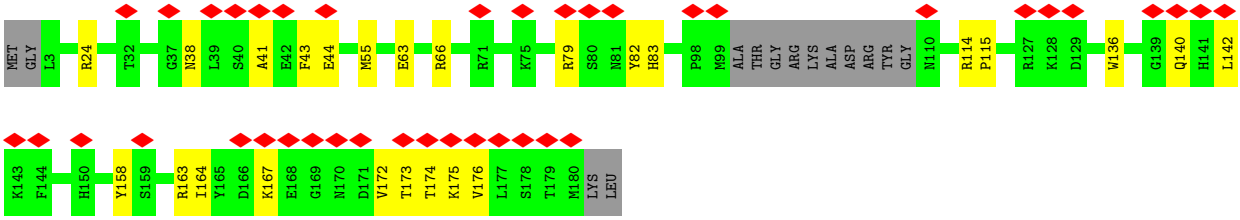
Chain BI:





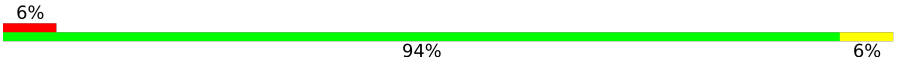
• Molecule 35: 50S ribosomal protein L10e

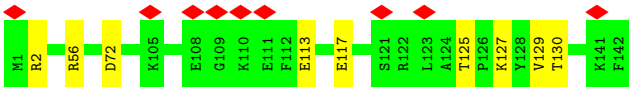
Chain BJ:



• Molecule 36: 50S ribosomal protein L13

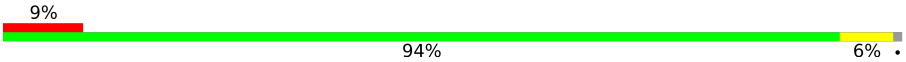
Chain BK:





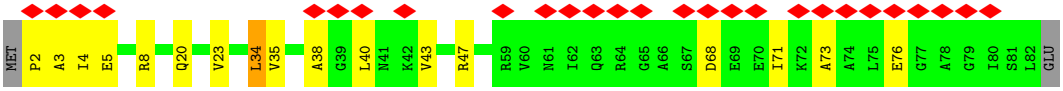
• Molecule 37: 50S ribosomal protein L14

Chain BL:



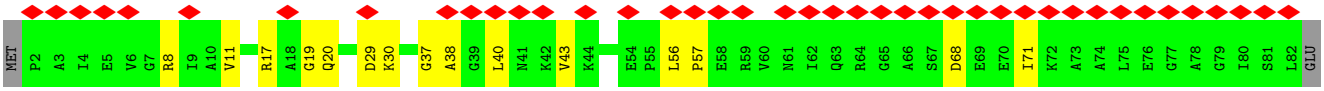
• Molecule 38: 50S ribosomal protein L14e

Chain BM:



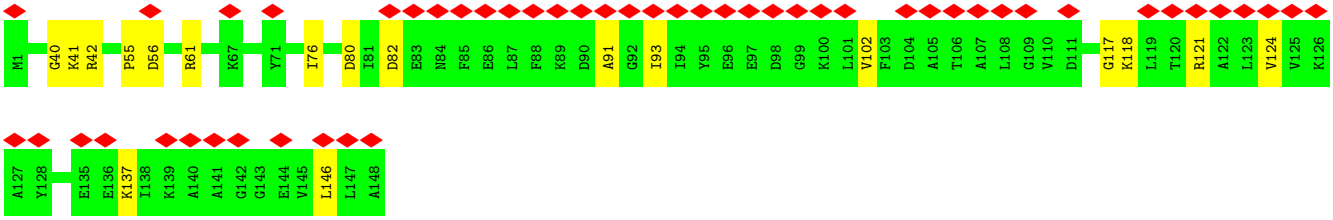
• Molecule 38: 50S ribosomal protein L14e

Chain BN:



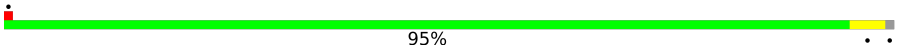
• Molecule 39: 50S ribosomal protein L15

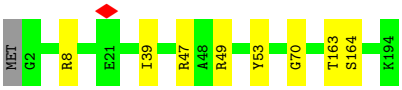
Chain BO:



- Molecule 40: 50S ribosomal protein L15e

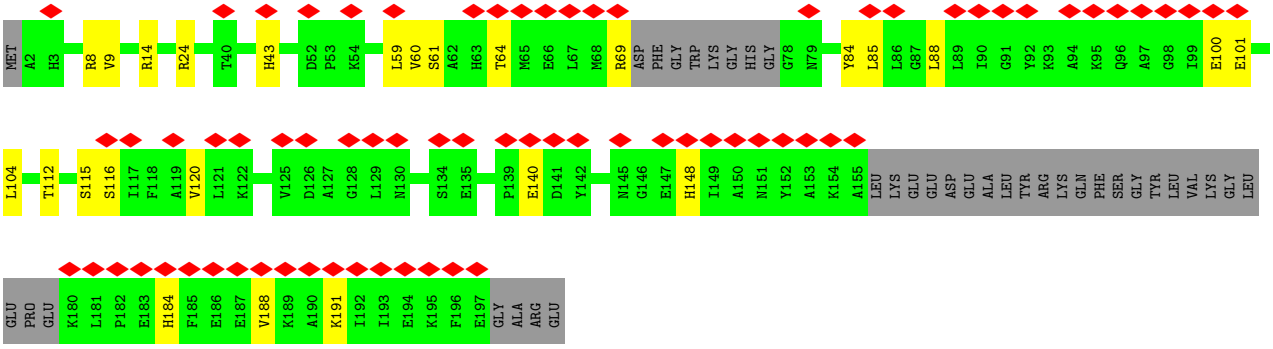
Chain BP:





- Molecule 41: 50S ribosomal protein L18

Chain BQ:

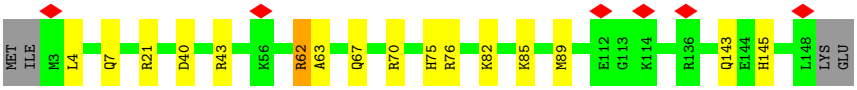


- Molecule 42: 50S ribosomal protein L18e

Chain BR:

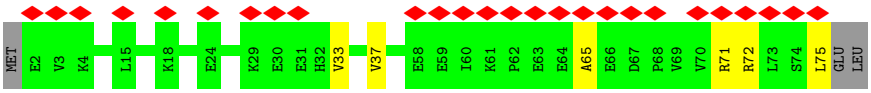
- Molecule 43: 50S ribosomal protein L19e

Chain BS:



- Molecule 44: 50S ribosomal protein L18Ae

Chain BT:



• Molecule 45: 50S ribosomal protein L21e

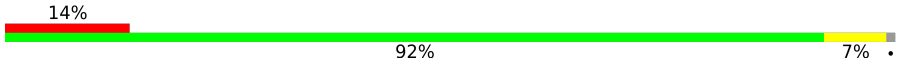
Chain BU:

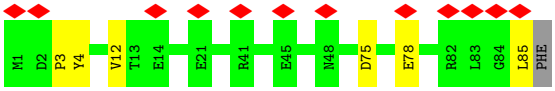
• Molecule 46: 50S ribosomal protein L22

Chain BV:

• Molecule 47: 50S ribosomal protein L23

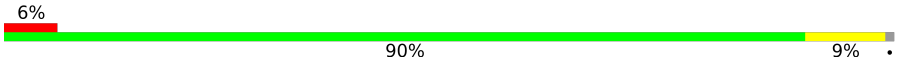
Chain BW:

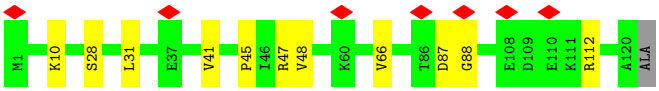




• Molecule 48: 50S ribosomal protein L24

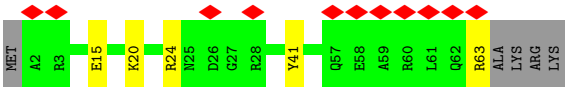
Chain BX:





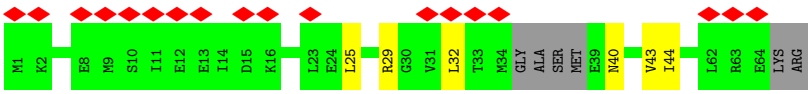
• Molecule 49: 50S ribosomal protein L24e

Chain BY:

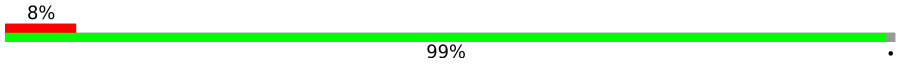


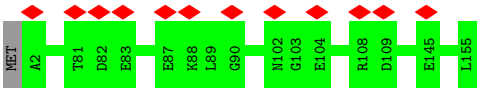
• Molecule 50: 50S ribosomal protein L29

Chain BZ:

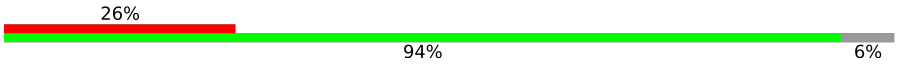


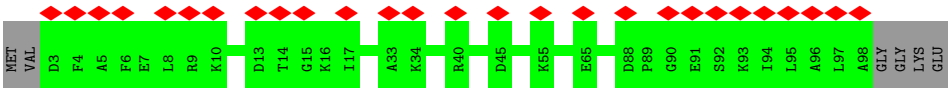
• Molecule 51: 50S ribosomal protein L30

Chain Ba: 

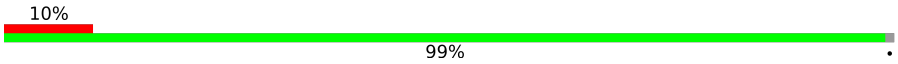


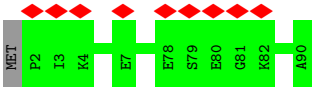
- Molecule 52: 50S ribosomal protein L30e

Chain Bb: 

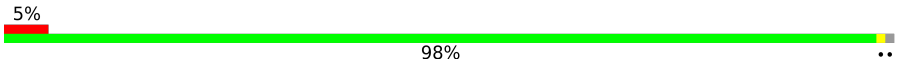


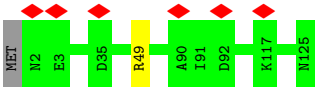
- Molecule 53: 50S ribosomal protein L31e

Chain Bc: 

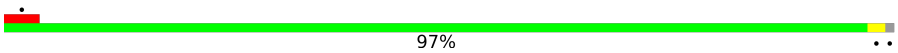


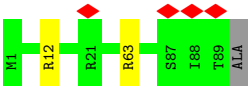
- Molecule 54: 50S ribosomal protein L32e

Chain Bd: 

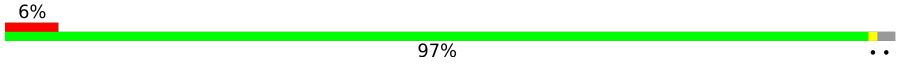


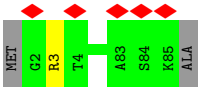
- Molecule 55: 50S ribosomal protein L34e

Chain Be: 

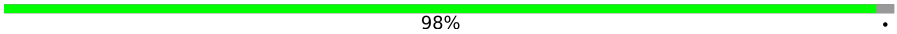


- Molecule 56: 50S ribosomal protein L37Ae

Chain Bg: 

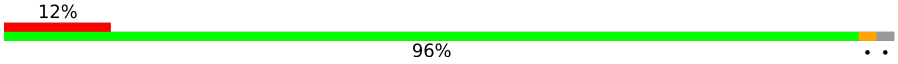


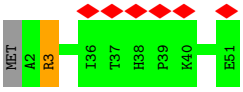
- Molecule 57: 50S ribosomal protein L37e

Chain Bh: 

• Molecule 58: 50S ribosomal protein L39e

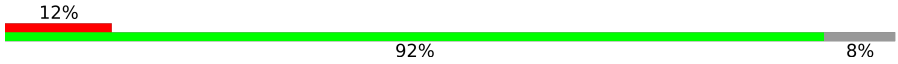
Chain Bi:

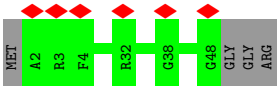




• Molecule 59: 50S ribosomal protein L40e

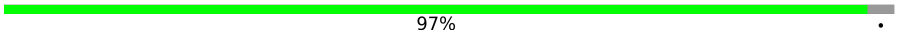
Chain Bj:





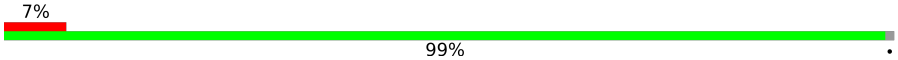
• Molecule 60: LSU ribosomal protein L41E

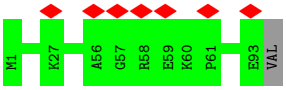
Chain Bk:



• Molecule 61: 50S ribosomal protein L44e

Chain Bl:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	283424	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	0.506	Depositor
Minimum map value	-0.277	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: 5MU, OMC, LHH, ZN, OMU, 6MZ, A2M, 4AC, OMG, 5MC, LV2, 4SU, MA6

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	0.81	0/34630	0.97	20/54028 (0.0%)
2	Ab	0.42	0/1611	0.51	0/2179
3	Ac	0.31	0/1534	0.48	0/2057
4	Ad	0.41	0/1578	0.53	0/2119
5	Ae	0.45	0/1477	0.55	0/1980
6	Af	0.51	0/1991	0.57	0/2688
7	Ag	0.48	0/1778	0.58	1/2393 (0.0%)
8	Ah	0.37	0/968	0.54	0/1300
9	Ai	0.39	0/1738	0.50	0/2332
10	Aj	0.50	0/1039	0.58	0/1397
11	Ak	0.51	0/991	0.59	0/1322
12	Al	0.38	0/1068	0.54	0/1430
13	Am	0.32	0/810	0.49	0/1087
14	An	0.62	2/971 (0.2%)	0.60	1/1308 (0.1%)
15	Ao	0.49	0/1139	0.56	0/1518
16	Ap	0.38	0/1113	0.52	0/1500
17	Aq	0.51	0/1241	0.57	0/1667
18	Ar	0.37	0/457	0.50	0/602
19	As	0.54	0/888	0.54	0/1200
20	At	0.30	0/545	0.47	0/725
21	Au	0.40	0/970	0.48	0/1295
22	Av	0.45	0/1249	0.49	0/1687
23	Aw	0.45	0/790	0.52	0/1063
24	Ax	0.44	0/469	0.54	0/633
25	Ay	0.36	0/501	0.54	0/672
26	Az	0.47	0/440	0.48	0/599
27	BA	1.03	1/69303 (0.0%)	1.13	90/108170 (0.1%)
28	BB	0.60	0/2993	0.93	2/4668 (0.0%)
29	BC	0.58	0/1860	0.74	4/2511 (0.2%)
30	BD	0.56	0/2815	0.65	0/3795
31	BE	0.53	0/2066	0.64	0/2785
32	BF	0.34	0/1355	0.57	0/1806

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	BG	0.43	0/1490	0.55	0/2006
34	BH	0.43	0/941	0.53	0/1272
34	BI	0.32	0/941	0.55	0/1272
35	BJ	0.46	0/1407	0.57	0/1891
36	BK	0.54	0/1165	0.66	0/1558
37	BL	0.53	0/1067	0.63	0/1435
38	BM	0.49	0/614	0.65	0/824
38	BN	0.42	0/614	0.60	0/824
39	BO	0.49	0/1184	0.65	0/1581
40	BP	0.63	0/1621	0.68	0/2163
41	BQ	0.40	0/1342	0.56	0/1804
42	BR	0.50	0/971	0.62	0/1301
43	BS	0.51	0/1216	0.65	0/1607
44	BT	0.41	0/636	0.57	0/852
45	BU	0.56	0/806	0.61	0/1080
46	BV	0.51	0/1259	0.60	0/1688
47	BW	0.47	0/690	0.60	0/925
48	BX	0.51	0/1007	0.64	0/1344
49	BY	0.61	0/538	0.59	0/716
50	BZ	0.44	0/506	0.63	0/668
51	Ba	0.51	0/1259	0.64	0/1680
52	Bb	0.42	0/742	0.53	0/1001
53	Bc	0.52	0/736	0.59	0/990
54	Bd	0.53	0/1044	0.63	1/1394 (0.1%)
55	Be	0.54	0/746	0.62	0/997
56	Bg	0.57	0/640	0.69	0/855
57	Bh	0.75	0/524	0.75	0/692
58	Bi	0.58	0/441	0.69	1/588 (0.2%)
59	Bj	0.42	0/381	0.56	0/505
60	Bk	0.78	0/351	0.70	0/454
61	Bl	0.55	0/796	0.59	0/1056
All	All	0.81	3/170053 (0.0%)	0.94	120/251539 (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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	An	125	PRO	N-CA	13.69	1.70	1.47
14	An	124	ILE	C-N	5.96	1.45	1.34
27	BA	190	A	C6-N6	-5.19	1.29	1.33

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BA	549	G	O4'-C1'-N9	9.49	115.80	108.20
27	BA	2297	C	N1-C2-O2	8.28	123.87	118.90
14	An	125	PRO	CA-N-CD	-7.97	100.34	111.50
1	Aa	700	C	C2-N1-C1'	7.58	127.14	118.80
1	Aa	1469	C	C2-N1-C1'	7.21	126.74	118.80
27	BA	2742	G	O4'-C1'-N9	7.19	113.95	108.20
27	BA	1237	C	N3-C2-O2	-6.99	117.00	121.90
29	BC	195	VAL	CG1-CB-CG2	6.96	122.04	110.90
27	BA	2135	C	C2-N1-C1'	6.96	126.45	118.80
27	BA	76	U	N3-C4-O4	6.90	124.23	119.40
27	BA	19	A	O4'-C1'-N9	6.86	113.69	108.20
27	BA	2297	C	N3-C2-O2	-6.64	117.25	121.90
27	BA	1450	C	C2-N1-C1'	6.60	126.06	118.80
27	BA	654	C	C2-N1-C1'	6.57	126.03	118.80
27	BA	76	U	C5-C4-O4	-6.56	121.97	125.90
27	BA	2312	C	C2-N1-C1'	6.54	125.99	118.80
27	BA	1449	U	C2-N1-C1'	6.53	125.53	117.70
1	Aa	316	C	C2-N1-C1'	6.46	125.91	118.80
1	Aa	700	C	C6-N1-C1'	-6.43	113.08	120.80
29	BC	219	ARG	NE-CZ-NH1	-6.41	117.10	120.30
27	BA	2360	A	C8-N9-C4	-6.37	103.25	105.80
27	BA	1536	C	C2-N1-C1'	6.32	125.75	118.80
27	BA	1799	G	O4'-C1'-N9	6.30	113.24	108.20
1	Aa	515	C	C2-N1-C1'	6.27	125.70	118.80
27	BA	892	A	C8-N9-C4	-6.25	103.30	105.80
58	Bi	3	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	Aa	1478	C	C2-N1-C1'	6.15	125.57	118.80
27	BA	1958	C	C2-N1-C1'	6.13	125.55	118.80
27	BA	2136	C	C2-N1-C1'	6.13	125.54	118.80
27	BA	942	C	C2-N1-C1'	6.12	125.53	118.80
27	BA	1391	C	C2-N1-C1'	6.11	125.52	118.80
28	BB	31	C	N1-C2-O2	6.04	122.52	118.90
27	BA	1132	C	C2-N1-C1'	6.02	125.42	118.80
27	BA	1469	C	C2-N1-C1'	6.02	125.42	118.80
27	BA	2159	C	C2-N1-C1'	6.00	125.41	118.80
27	BA	1484	U	O4'-C1'-N1	6.00	113.00	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BA	2136	C	N1-C2-O2	5.99	122.49	118.90
27	BA	892	A	P-O3'-C3'	5.91	126.79	119.70
27	BA	48	C	C2-N1-C1'	5.90	125.29	118.80
27	BA	1767	G	C8-N9-C4	-5.89	104.05	106.40
27	BA	1119	C	C2-N1-C1'	5.88	125.27	118.80
27	BA	1801	A	O4'-C1'-N9	5.88	112.90	108.20
1	Aa	1469	C	C6-N1-C1'	-5.87	113.76	120.80
27	BA	300	U	O4'-C1'-N1	5.84	112.87	108.20
27	BA	2113	C	C2-N1-C1'	5.78	125.15	118.80
27	BA	809	C	N1-C2-O2	5.77	122.36	118.90
27	BA	2796	C	C2-N1-C1'	5.75	125.12	118.80
27	BA	1237	C	N1-C2-O2	5.74	122.34	118.90
27	BA	1041	C	C2-N1-C1'	5.71	125.09	118.80
27	BA	855	G	C8-N9-C4	-5.70	104.12	106.40
27	BA	2119	C	C5-C4-N4	-5.70	116.21	120.20
27	BA	855	G	N7-C8-N9	5.68	115.94	113.10
27	BA	2037	C	N3-C2-O2	-5.66	117.94	121.90
27	BA	2796	C	N1-C2-O2	5.66	122.30	118.90
27	BA	2826	C	C2-N1-C1'	5.64	125.00	118.80
1	Aa	1171	C	C2-N1-C1'	5.63	124.99	118.80
29	BC	195	VAL	CA-CB-CG1	5.60	119.30	110.90
27	BA	1768	C	O4'-C1'-N1	5.59	112.67	108.20
27	BA	784	C	N1-C2-O2	5.55	122.23	118.90
27	BA	1811	G	N1-C6-O6	-5.55	116.57	119.90
27	BA	913	G	C5-C6-O6	5.54	131.92	128.60
1	Aa	296	C	N1-C2-O2	5.50	122.20	118.90
1	Aa	1347	C	N1-C2-O2	5.48	122.19	118.90
27	BA	876	G	O4'-C1'-N9	5.47	112.58	108.20
27	BA	1450	C	C6-N1-C1'	-5.46	114.25	120.80
54	Bd	49	ARG	NE-CZ-NH2	-5.46	117.57	120.30
27	BA	1308	U	C2-N1-C1'	5.45	124.24	117.70
27	BA	918	U	C2-N1-C1'	5.41	124.19	117.70
27	BA	944	C	C2-N1-C1'	5.38	124.72	118.80
1	Aa	680	C	C2-N1-C1'	5.37	124.70	118.80
27	BA	784	C	C2-N1-C1'	5.36	124.69	118.80
29	BC	219	ARG	NE-CZ-NH2	5.34	122.97	120.30
27	BA	494	C	N1-C2-O2	5.33	122.10	118.90
27	BA	2251	C	C2-N1-C1'	5.32	124.65	118.80
27	BA	2140	C	N3-C4-C5	5.29	124.02	121.90
1	Aa	281	C	C2-N1-C1'	5.28	124.61	118.80
27	BA	804	C	C2-N1-C1'	5.28	124.61	118.80
1	Aa	316	C	N3-C2-O2	-5.25	118.22	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Aa	1347	C	N3-C2-O2	-5.24	118.23	121.90
27	BA	2713	A	N1-C6-N6	5.24	121.74	118.60
27	BA	1811	G	N9-C4-C5	5.22	107.49	105.40
1	Aa	316	C	N1-C2-O2	5.22	122.03	118.90
27	BA	494	C	C2-N1-C1'	5.21	124.53	118.80
27	BA	2148	C	C2-N1-C1'	5.21	124.53	118.80
7	Ag	75	ASP	CB-CG-OD2	5.20	122.98	118.30
27	BA	1767	G	P-O3'-C3'	5.20	125.93	119.70
27	BA	2136	C	C6-N1-C1'	-5.19	114.57	120.80
27	BA	698	U	C2-N1-C1'	-5.19	111.47	117.70
27	BA	1831	C	C2-N1-C1'	5.19	124.51	118.80
27	BA	1427	C	C2-N1-C1'	5.19	124.51	118.80
27	BA	2360	A	C5-C6-N6	5.19	127.85	123.70
27	BA	2360	A	N1-C6-N6	-5.18	115.49	118.60
27	BA	2804	C	N3-C4-C5	5.16	123.96	121.90
27	BA	1533	A	N1-C6-N6	-5.13	115.52	118.60
1	Aa	691	C	C2-N1-C1'	5.12	124.43	118.80
28	BB	31	C	N3-C2-O2	-5.12	118.32	121.90
27	BA	1811	G	C4-C5-N7	-5.11	108.76	110.80
27	BA	2300	C	C2-N1-C1'	5.10	124.41	118.80
27	BA	1404	G	C8-N9-C4	-5.08	104.37	106.40
27	BA	1958	C	N1-C2-O2	5.07	121.94	118.90
27	BA	2445	C	C2-N1-C1'	5.07	124.38	118.80
27	BA	196	G	O4'-C1'-N9	5.06	112.25	108.20
1	Aa	1478	C	N1-C2-O2	5.06	121.94	118.90
27	BA	1289	A	C6-C5-N7	-5.06	128.76	132.30
1	Aa	691	C	N1-C2-O2	5.05	121.93	118.90
1	Aa	1469	C	N1-C2-O2	5.05	121.93	118.90
27	BA	1860	C	C2-N1-C1'	5.05	124.35	118.80
27	BA	547	C	C2-N1-C1'	5.04	124.35	118.80
27	BA	185	G	C8-N9-C4	-5.04	104.38	106.40
27	BA	1098	C	C2-N1-C1'	5.04	124.34	118.80
1	Aa	508	A	C4-N9-C1'	5.04	135.37	126.30
27	BA	1960	C	C2-N1-C1'	5.04	124.34	118.80
27	BA	66	C	N1-C2-O2	5.03	121.92	118.90
27	BA	654	C	C6-N1-C1'	-5.03	114.76	120.80
27	BA	1536	C	N1-C2-O2	5.03	121.92	118.90
27	BA	46	C	C2-N1-C1'	5.03	124.33	118.80
27	BA	2159	C	N1-C2-O2	5.02	121.91	118.90
27	BA	892	A	N7-C8-N9	5.01	116.31	113.80
27	BA	2058	G	C4-N9-C1'	5.01	133.01	126.50
27	BA	733	C	C6-N1-C2	-5.01	118.30	120.30

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	31499	0	15927	0	0
2	Ab	1580	0	1634	0	0
3	Ac	1513	0	1598	0	0
4	Ad	1550	0	1618	0	0
5	Ae	1454	0	1521	0	0
6	Af	1945	0	2028	0	0
7	Ag	1753	0	1820	0	0
8	Ah	952	0	997	0	0
9	Ai	1706	0	1772	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	868	0	895	0	0
20	At	538	0	560	0	0
21	Au	952	0	1000	0	0
22	Av	1216	0	1236	0	0
23	Aw	777	0	797	0	0
24	Ax	461	0	494	0	0
25	Ay	499	0	528	0	0
26	Az	426	0	403	0	0
27	BA	63188	0	31965	584	0
28	BB	2678	0	1361	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	BC	1820	0	1902	16	0
30	BD	2746	0	2840	26	0
31	BE	2026	0	2128	19	0
32	BF	1338	0	1403	48	0
33	BG	1463	0	1520	9	0
34	BH	928	0	970	7	0
34	BI	928	0	970	21	0
35	BJ	1378	0	1409	18	0
36	BK	1146	0	1213	6	0
37	BL	1055	0	1134	5	0
38	BM	610	0	660	18	0
38	BN	610	0	660	10	0
39	BO	1162	0	1218	11	0
40	BP	1582	0	1677	8	0
41	BQ	1314	0	1359	20	0
42	BR	959	0	1018	9	0
43	BS	1200	0	1298	11	0
44	BT	624	0	647	3	0
45	BU	784	0	821	7	0
46	BV	1234	0	1274	15	0
47	BW	683	0	743	4	0
48	BX	991	0	1053	8	0
49	BY	524	0	512	4	0
50	BZ	506	0	559	3	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	785	0	0
56	Bg	630	0	675	0	0
57	Bh	512	0	527	0	0
58	Bi	432	0	488	0	0
59	Bj	373	0	391	0	0
60	Bk	345	0	407	0	0
61	Bl	778	0	833	0	0
62	Ag	1	0	0	0	0
62	Ar	1	0	0	0	0
62	As	1	0	0	0	0
62	Ax	1	0	0	0	0
62	Az	2	0	0	0	0
62	BY	1	0	0	0	0
62	Be	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	Bg	1	0	0	0	0
62	Bh	1	0	0	0	0
62	Bj	1	0	0	0	0
62	Bl	1	0	0	0	0
63	Aa	153	0	0	0	0
63	Ae	1	0	0	0	0
63	Af	5	0	0	0	0
63	Ag	1	0	0	0	0
63	Ai	1	0	0	0	0
63	Aj	1	0	0	0	0
63	Ak	2	0	0	0	0
63	Al	2	0	0	0	0
63	An	1	0	0	0	0
63	Ao	2	0	0	0	0
63	Ap	1	0	0	0	0
63	Aq	5	0	0	0	0
63	Av	1	0	0	0	0
63	Az	1	0	0	0	0
63	BA	1674	0	0	277	0
63	BB	7	0	0	1	0
63	BC	29	0	0	3	0
63	BD	30	0	0	0	0
63	BE	24	0	0	1	0
63	BF	1	0	0	0	0
63	BH	1	0	0	0	0
63	BJ	4	0	0	0	0
63	BK	7	0	0	1	0
63	BL	8	0	0	1	0
63	BN	1	0	0	1	0
63	BO	19	0	0	0	0
63	BP	23	0	0	3	0
63	BQ	5	0	0	0	0
63	BR	1	0	0	0	0
63	BS	12	0	0	1	0
63	BV	17	0	0	5	0
63	BW	3	0	0	0	0
63	BX	7	0	0	1	0
63	BY	5	0	0	0	0
63	BZ	3	0	0	0	0
63	Ba	6	0	0	0	0
63	Bb	1	0	0	0	0
63	Bc	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	Bd	12	0	0	0	0
63	Be	7	0	0	0	0
63	Bg	6	0	0	0	0
63	Bh	18	0	0	0	0
63	Bi	5	0	0	0	0
63	Bk	6	0	0	0	0
63	Bl	3	0	0	0	0
All	All	161508	0	114403	875	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 5.

All (875) 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:1904:G:OP2	63:BA:3101:HOH:O	1.79	0.99
27:BA:1181:C:O2'	27:BA:1182:A:O5'	1.81	0.99
27:BA:1181:C:O2	27:BA:2853:G:N2	1.96	0.98
27:BA:2616:C:OP1	30:BD:9:ARG:NH1	1.99	0.95
27:BA:2744:G:N7	63:BA:3108:HOH:O	2.01	0.94
27:BA:480:A:N7	63:BA:3138:HOH:O	2.03	0.92
27:BA:189:C:OP2	63:BA:3103:HOH:O	1.88	0.92
27:BA:845:A:N7	63:BA:3131:HOH:O	2.02	0.92
27:BA:857:C:OP2	63:BA:3102:HOH:O	1.87	0.91
27:BA:321:C:N4	27:BA:394:A:N7	2.18	0.91
48:BX:112:ARG:NH1	63:BX:201:HOH:O	2.02	0.91
27:BA:847:G:N7	63:BA:3136:HOH:O	2.03	0.91
27:BA:2941:C:N3	63:BA:3139:HOH:O	2.04	0.91
27:BA:2728:G:N7	63:BA:3142:HOH:O	2.04	0.90
28:BB:102:G:N7	63:BB:201:HOH:O	2.03	0.90
38:BM:38:ALA:HA	38:BM:68:ASP:OD1	1.70	0.90
27:BA:245:G:N7	63:BA:3144:HOH:O	2.05	0.90
28:BB:47:C:OP2	32:BF:146:ARG:NH2	2.04	0.90
27:BA:2353:OMG:OP2	63:BA:3106:HOH:O	1.89	0.90
27:BA:2970:G:N7	63:BA:3153:HOH:O	2.05	0.90
27:BA:2743:A:OP2	63:BA:3108:HOH:O	1.90	0.89
27:BA:2693:A:OP1	63:BA:3104:HOH:O	1.89	0.89
27:BA:871:G:OP2	63:BA:3107:HOH:O	1.90	0.89
27:BA:1165:U:O4	63:BA:3105:HOH:O	1.89	0.89
27:BA:1249:G:N7	63:BA:3164:HOH:O	2.07	0.88
27:BA:1252:G:N7	63:BA:3165:HOH:O	2.07	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:1250:G:N7	63:BA:3105:HOH:O	2.04	0.88
27:BA:1742:G:N7	63:BA:3159:HOH:O	2.06	0.88
46:BV:70:SER:OG	63:BV:201:HOH:O	1.91	0.88
27:BA:799:C:N3	63:BA:3147:HOH:O	2.05	0.88
46:BV:112:ARG:NH2	46:BV:154:ILE:O	2.06	0.88
27:BA:1181:C:C2	27:BA:2853:G:N2	2.41	0.88
27:BA:280:A:O2'	27:BA:281:A:O4'	1.90	0.88
27:BA:164:G:N7	63:BA:3157:HOH:O	2.06	0.88
27:BA:1669:G:N7	63:BA:3168:HOH:O	2.07	0.88
27:BA:1861:G:N7	63:BA:3171:HOH:O	2.08	0.87
27:BA:474:G:N7	63:BA:3170:HOH:O	2.07	0.87
27:BA:125:G:N7	63:BA:3174:HOH:O	2.08	0.87
27:BA:2549:G:N7	63:BA:3169:HOH:O	2.07	0.87
27:BA:1107:G:N7	63:BA:3156:HOH:O	2.06	0.87
27:BA:2945:G:N7	63:BA:3163:HOH:O	2.06	0.87
27:BA:1079:G:N7	63:BA:3172:HOH:O	2.08	0.87
27:BA:1380:G:N7	63:BA:3166:HOH:O	2.07	0.86
27:BA:2776:G:N7	63:BA:3175:HOH:O	2.08	0.86
46:BV:2:SER:OG	63:BV:202:HOH:O	1.93	0.86
27:BA:290:G:N7	63:BA:3183:HOH:O	2.09	0.86
27:BA:810:G:N7	63:BA:3173:HOH:O	2.08	0.86
27:BA:848:G:N7	63:BA:3180:HOH:O	2.08	0.86
27:BA:703:G:N7	63:BA:3178:HOH:O	2.08	0.86
27:BA:548:U:OP2	63:BA:3109:HOH:O	1.92	0.85
27:BA:2371:A:OP1	63:BA:3110:HOH:O	1.94	0.85
27:BA:20:A:O2'	27:BA:21:C:O4'	1.93	0.85
27:BA:331:A:O2'	27:BA:332:A:O5'	1.93	0.85
27:BA:2939:G:N7	63:BA:3179:HOH:O	2.08	0.85
27:BA:1470:C:OP2	63:BA:3111:HOH:O	1.94	0.85
44:BT:65:ALA:O	44:BT:71:ARG:NH2	2.09	0.85
27:BA:2116:G:N7	63:BA:3192:HOH:O	2.10	0.85
27:BA:1071:G:N7	63:BA:3193:HOH:O	2.10	0.84
27:BA:1819:U:OP2	63:BA:3116:HOH:O	1.95	0.84
27:BA:841:A:N7	63:BA:3191:HOH:O	2.10	0.84
27:BA:1853:G:N7	63:BA:3186:HOH:O	2.10	0.84
27:BA:956:C:OP1	63:BA:3115:HOH:O	1.95	0.84
27:BA:2685:G:N7	63:BA:3182:HOH:O	2.09	0.84
27:BA:2787:U:OP2	63:BA:3114:HOH:O	1.94	0.84
27:BA:2775:G:N7	63:BA:3207:HOH:O	2.11	0.84
27:BA:1344:G:N7	63:BA:3189:HOH:O	2.10	0.83
27:BA:2696:G:OP1	63:BA:3112:HOH:O	1.94	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:446:G:N7	63:BA:3194:HOH:O	2.10	0.83
27:BA:1862:G:N7	63:BA:3190:HOH:O	2.10	0.83
27:BA:2845:G:N7	63:BA:3206:HOH:O	2.11	0.83
27:BA:1345:C:N3	63:BA:3187:HOH:O	2.10	0.83
27:BA:2046:G:N7	63:BA:3204:HOH:O	2.11	0.83
31:BE:69:ARG:NH1	63:BE:302:HOH:O	2.10	0.83
27:BA:147:U:O2'	27:BA:148:G:OP1	1.97	0.83
27:BA:1404:G:OP2	63:BA:3113:HOH:O	1.94	0.83
27:BA:705:G:N7	63:BA:3200:HOH:O	2.11	0.83
27:BA:2505:G:N7	63:BA:3211:HOH:O	2.12	0.83
27:BA:1399:G:N7	63:BA:3197:HOH:O	2.11	0.82
27:BA:764:G:N7	63:BA:3199:HOH:O	2.11	0.82
27:BA:923:G:O6	63:BA:3117:HOH:O	1.95	0.82
27:BA:1941:G:N7	63:BA:3208:HOH:O	2.11	0.82
27:BA:2373:G:OP2	63:BA:3119:HOH:O	1.97	0.82
27:BA:1182:A:O2'	27:BA:1183:G:O5'	1.97	0.82
27:BA:2944:G:N7	63:BA:3212:HOH:O	2.13	0.82
27:BA:704:G:N7	63:BA:3203:HOH:O	2.11	0.82
27:BA:912:OMG:OP1	63:BA:3120:HOH:O	1.97	0.81
29:BC:187:ARG:O	63:BC:301:HOH:O	1.99	0.81
27:BA:629:G:N7	63:BA:3223:HOH:O	2.14	0.81
27:BA:236:G:N7	63:BA:3151:HOH:O	2.14	0.81
32:BF:14:ALA:O	32:BF:15:HIS:ND1	2.14	0.81
27:BA:2078:C:N3	63:BA:3213:HOH:O	2.13	0.81
27:BA:1852:G:N7	63:BA:3218:HOH:O	2.14	0.81
27:BA:2885:G:N7	63:BA:3216:HOH:O	2.14	0.81
27:BA:630:G:N7	63:BA:3221:HOH:O	2.14	0.81
28:BB:9:G:OP1	41:BQ:24:ARG:NH2	2.14	0.81
46:BV:2:SER:O	63:BV:203:HOH:O	1.97	0.81
27:BA:160:G:O2'	27:BA:161:U:O4'	1.99	0.80
27:BA:1841:U:OP1	63:BA:3125:HOH:O	2.00	0.80
27:BA:2713:A:N3	63:BA:3220:HOH:O	2.14	0.80
27:BA:188:A:OP1	63:BA:3103:HOH:O	1.98	0.80
27:BA:1410:U:OP2	63:BA:3121:HOH:O	1.98	0.80
27:BA:1911:A:OP1	63:BA:3122:HOH:O	1.98	0.80
27:BA:2385:G:N7	63:BA:3224:HOH:O	2.14	0.80
32:BF:142:ARG:HH21	32:BF:163:LEU:HD23	1.46	0.80
27:BA:1066:G:N7	63:BA:3214:HOH:O	2.13	0.79
27:BA:2887:G:N7	63:BA:3226:HOH:O	2.15	0.79
27:BA:1400:A:OP2	63:BA:3129:HOH:O	2.01	0.79
27:BA:1921:G:N7	63:BA:3232:HOH:O	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:1166:G:N7	63:BA:3230:HOH:O	2.15	0.79
27:BA:1881:G:N7	63:BA:3219:HOH:O	2.14	0.79
27:BA:602:G:OP1	63:BA:3126:HOH:O	2.00	0.79
27:BA:1811:G:N7	63:BA:3217:HOH:O	2.14	0.79
27:BA:2062:G:N7	63:BA:3225:HOH:O	2.14	0.79
27:BA:2375:U:OP1	63:BA:3128:HOH:O	2.01	0.79
27:BA:2836:G:O2'	27:BA:2837:C:O5'	2.00	0.79
27:BA:139:G:N7	63:BA:3241:HOH:O	2.16	0.79
27:BA:1137:A:OP2	63:BA:3124:HOH:O	1.99	0.79
27:BA:1576:G:N7	63:BA:3235:HOH:O	2.15	0.79
27:BA:165:G:N7	63:BA:3239:HOH:O	2.16	0.79
27:BA:1518:G:OP2	63:BA:3123:HOH:O	1.99	0.78
27:BA:1605:C:N3	63:BA:3246:HOH:O	2.16	0.78
31:BE:172:ARG:NH1	31:BE:195:LYS:O	2.15	0.78
27:BA:1691:U:O2'	27:BA:1692:U:OP2	2.01	0.78
27:BA:1818:C:OP1	63:BA:3116:HOH:O	2.02	0.78
27:BA:2393:G:N7	63:BA:3248:HOH:O	2.17	0.78
27:BA:865:G:N7	63:BA:3238:HOH:O	2.16	0.78
27:BA:2963:G:N7	63:BA:3242:HOH:O	2.16	0.78
27:BA:1151:G:OP2	63:BA:3127:HOH:O	2.00	0.78
30:BD:339:TYR:OH	49:BY:15:GLU:OE1	2.00	0.78
27:BA:1749:C:OP2	63:BA:3132:HOH:O	2.02	0.78
27:BA:1267:G:N7	63:BA:3231:HOH:O	2.15	0.78
27:BA:532:G:N7	63:BA:3247:HOH:O	2.16	0.78
27:BA:856:C:OP1	63:BA:3135:HOH:O	2.02	0.78
27:BA:2810:G:N7	63:BA:3240:HOH:O	2.16	0.78
27:BA:1863:G:N7	63:BA:3228:HOH:O	2.15	0.77
30:BD:48:MET:SD	30:BD:71:THR:OG1	2.42	0.77
27:BA:118:G:N7	63:BA:3229:HOH:O	2.15	0.77
27:BA:631:G:N7	63:BA:3245:HOH:O	2.16	0.77
27:BA:827:G:N7	63:BA:3251:HOH:O	2.17	0.77
27:BA:1251:G:N7	63:BA:3243:HOH:O	2.16	0.77
27:BA:2971:G:N7	63:BA:3252:HOH:O	2.17	0.77
44:BT:33:VAL:O	44:BT:37:VAL:HG23	1.84	0.77
27:BA:306:G:N7	63:BA:3254:HOH:O	2.18	0.77
27:BA:2678:G:OP1	63:BA:3133:HOH:O	2.02	0.77
27:BA:492:A:OP1	63:BA:3130:HOH:O	2.01	0.77
27:BA:1409:A:OP2	63:BA:3121:HOH:O	2.02	0.77
27:BA:1659:G:N7	63:BA:3237:HOH:O	2.15	0.77
39:BO:82:ASP:OD1	39:BO:121:ARG:NH1	2.17	0.77
27:BA:1777:G:O2'	63:BA:3118:HOH:O	1.96	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:489:G:O6	63:BA:3130:HOH:O	2.01	0.76
42:BR:20:ARG:NH2	42:BR:39:GLU:OE2	2.17	0.76
27:BA:1766:U:OP2	63:BA:3134:HOH:O	2.02	0.76
27:BA:2548:G:N7	63:BA:3255:HOH:O	2.18	0.76
27:BA:1322:G:OP1	63:BA:3141:HOH:O	2.04	0.76
27:BA:2947:A:N1	63:BA:3249:HOH:O	2.17	0.76
28:BB:36:C:O2	41:BQ:148:HIS:NE2	2.18	0.75
27:BA:1513:G:N7	63:BA:3262:HOH:O	2.19	0.75
27:BA:2004:G:N7	63:BA:3267:HOH:O	2.20	0.75
27:BA:2374:G:OP1	45:BU:57:ARG:NH2	2.19	0.75
27:BA:2679:U:OP2	63:BA:3133:HOH:O	2.03	0.75
27:BA:2681:A:OP1	63:BA:3140:HOH:O	2.04	0.75
27:BA:959:G:OP2	63:BA:3143:HOH:O	2.04	0.75
27:BA:1123:G:N7	63:BA:3258:HOH:O	2.18	0.75
27:BA:1182:A:O2'	27:BA:1183:G:O4'	2.05	0.75
27:BA:1893:G:N7	63:BA:3272:HOH:O	2.20	0.75
29:BC:30:TYR:O	29:BC:31:VAL:HG13	1.86	0.75
27:BA:452:A:OP2	63:BA:3137:HOH:O	2.03	0.75
27:BA:1611:G:N7	63:BA:3256:HOH:O	2.18	0.75
27:BA:1768:C:O2'	27:BA:1769:C:OP2	2.04	0.75
27:BA:1798:G:N7	63:BA:3259:HOH:O	2.18	0.75
27:BA:644:G:N7	63:BA:3264:HOH:O	2.19	0.74
27:BA:1748:A:OP1	63:BA:3132:HOH:O	2.05	0.74
27:BA:235:A:OP2	63:BA:3151:HOH:O	2.05	0.74
27:BA:2678:G:OP2	63:BA:3150:HOH:O	2.05	0.74
27:BA:2593:G:N7	63:BA:3270:HOH:O	2.20	0.74
27:BA:968:G:N7	63:BA:3263:HOH:O	2.19	0.74
27:BA:812:U:OP2	63:BA:3146:HOH:O	2.05	0.74
27:BA:1818:C:OP2	63:BA:3149:HOH:O	2.05	0.74
27:BA:2083:A:OP2	63:BA:3152:HOH:O	2.05	0.74
27:BA:2246:A:O2'	27:BA:2247:A:O4'	2.05	0.74
27:BA:588:U:N3	34:BI:58:ASP:O	2.19	0.74
27:BA:1323:G:OP2	63:BA:3141:HOH:O	2.05	0.74
27:BA:852:G:O6	63:BA:3160:HOH:O	2.06	0.74
27:BA:1362:G:N7	63:BA:3273:HOH:O	2.20	0.74
27:BA:111:A:OP1	63:BA:3155:HOH:O	2.06	0.74
27:BA:1824:A:OP2	63:BA:3145:HOH:O	2.05	0.74
46:BV:17:ARG:NH1	46:BV:152:GLU:OE2	2.20	0.74
27:BA:2246:A:O2'	27:BA:2247:A:O5'	2.06	0.73
27:BA:2536:A:OP2	63:BA:3158:HOH:O	2.06	0.73
27:BA:1759:A:OP1	63:BA:3161:HOH:O	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:1308:U:OP1	63:BA:3167:HOH:O	2.07	0.73
27:BA:148:G:O2'	27:BA:149:C:OP1	2.06	0.73
27:BA:2957:G:N7	63:BA:3277:HOH:O	2.22	0.73
27:BA:2649:G:N7	63:BA:3268:HOH:O	2.20	0.73
27:BA:1821:G:OP1	63:BA:3162:HOH:O	2.06	0.73
27:BA:365:G:N7	63:BA:3274:HOH:O	2.21	0.73
30:BD:195:GLU:OE1	30:BD:334:ARG:HD3	1.89	0.73
27:BA:2680:G:N7	63:BA:3182:HOH:O	2.22	0.73
27:BA:892:A:O2'	27:BA:893:C:OP1	2.04	0.73
35:BJ:38:ASN:OD1	35:BJ:41:ALA:HB2	1.88	0.73
27:BA:1514:G:OP2	63:BA:3148:HOH:O	2.05	0.72
27:BA:1468:G:OP1	63:BA:3154:HOH:O	2.05	0.72
27:BA:2823:C:O2'	30:BD:346:GLN:O	2.06	0.72
41:BQ:8:ARG:NH2	41:BQ:9:VAL:O	2.23	0.72
27:BA:2471:G:N7	63:BA:3282:HOH:O	2.22	0.72
27:BA:447:G:N7	63:BA:3280:HOH:O	2.22	0.72
27:BA:1498:G:N7	63:BA:3287:HOH:O	2.23	0.71
27:BA:1101:A:N3	63:BA:3285:HOH:O	2.23	0.71
27:BA:520:G:O2'	27:BA:544:A:N6	2.22	0.71
27:BA:2750:G:N7	63:BA:3283:HOH:O	2.22	0.71
27:BA:1912:A:OP2	63:BA:3122:HOH:O	2.08	0.71
27:BA:2556:C:OP2	63:BA:3177:HOH:O	2.08	0.71
27:BA:1544:G:N7	63:BA:3279:HOH:O	2.22	0.71
27:BA:1727:G:N7	63:BA:3284:HOH:O	2.23	0.71
38:BM:40:LEU:HD22	38:BM:40:LEU:H	1.55	0.71
27:BA:1681:G:O6	27:BA:1685:G:N2	2.22	0.71
31:BE:118:ILE:O	31:BE:121:THR:OG1	2.08	0.71
27:BA:2345:U:OP1	63:BA:3181:HOH:O	2.09	0.70
30:BD:273:GLU:OE2	30:BD:274:ASN:ND2	2.24	0.70
27:BA:1379:G:N7	63:BA:3288:HOH:O	2.23	0.70
27:BA:364:G:N7	63:BA:3286:HOH:O	2.23	0.70
27:BA:1004:G:N7	63:BA:3296:HOH:O	2.25	0.70
27:BA:2160:G:OP1	63:BV:201:HOH:O	2.10	0.70
31:BE:50:PRO:O	31:BE:54:LYS:NZ	2.22	0.70
27:BA:348:A:N1	63:BA:3187:HOH:O	2.23	0.70
31:BE:233:GLY:O	31:BE:234:THR:OG1	2.07	0.70
41:BQ:43:HIS:HD1	41:BQ:64:THR:HG1	1.36	0.70
27:BA:822:G:N7	63:BA:3289:HOH:O	2.23	0.70
27:BA:2160:G:N7	63:BA:3291:HOH:O	2.24	0.70
27:BA:1149:G:O6	63:BA:3184:HOH:O	2.09	0.70
27:BA:1812:A:OP2	63:BA:3185:HOH:O	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BB:34:G:N7	28:BB:44:G:O2'	2.25	0.70
27:BA:918:U:OP2	63:BA:3176:HOH:O	2.08	0.69
38:BM:40:LEU:HD22	38:BM:40:LEU:N	2.06	0.69
27:BA:899:G:N7	63:BA:3300:HOH:O	2.25	0.69
27:BA:1181:C:HO2'	27:BA:1182:A:P	2.15	0.69
27:BA:813:C:OP2	63:BA:3146:HOH:O	2.08	0.69
27:BA:1894:G:N7	63:BA:3298:HOH:O	2.25	0.69
27:BA:2602:C:OP2	63:BA:3188:HOH:O	2.10	0.69
27:BA:2707:G:N7	63:BA:3295:HOH:O	2.25	0.69
27:BA:658:C:OP1	63:BA:3198:HOH:O	2.11	0.69
27:BA:3022:C:O2'	27:BA:3023:C:OP1	2.11	0.69
27:BA:1008:U:O4	27:BA:1027:G:O6	2.10	0.69
27:BA:1325:A:OP2	63:BA:3201:HOH:O	2.11	0.69
27:BA:2096:G:N7	63:BA:3293:HOH:O	2.24	0.69
27:BA:2336:G:N7	63:BA:3290:HOH:O	2.24	0.69
46:BV:112:ARG:NH1	46:BV:153:GLU:OE2	2.26	0.69
27:BA:489:G:OP2	63:BA:3202:HOH:O	2.11	0.69
27:BA:258:G:N7	63:BA:3306:HOH:O	2.26	0.68
27:BA:288:G:N7	63:BA:3310:HOH:O	2.26	0.68
27:BA:307:G:N7	63:BA:3308:HOH:O	2.26	0.68
27:BA:1910:U:OP1	63:BA:3205:HOH:O	2.11	0.68
27:BA:278:G:N2	27:BA:281:A:OP2	2.26	0.68
27:BA:676:G:N7	63:BA:3312:HOH:O	2.27	0.68
28:BB:123:C:OP1	41:BQ:69:ARG:NE	2.24	0.68
27:BA:2120:5MC:OP1	63:BV:201:HOH:O	2.10	0.68
43:BS:70:ARG:NH1	43:BS:75:HIS:O	2.26	0.68
27:BA:195:A:OP1	63:BA:3209:HOH:O	2.12	0.68
27:BA:1589:G:N7	63:BA:3299:HOH:O	2.25	0.68
34:BH:86:LEU:HD21	34:BH:99:VAL:HG23	1.76	0.68
34:BI:61:GLU:OE1	34:BI:61:GLU:N	2.26	0.68
40:BP:70:GLY:O	63:BP:201:HOH:O	2.12	0.68
27:BA:1785:U:OP1	63:BA:3195:HOH:O	2.10	0.67
32:BF:62:ASN:ND2	32:BF:65:PHE:O	2.25	0.67
27:BA:787:U:OP1	63:BA:3196:HOH:O	2.10	0.67
27:BA:1956:G:OP1	63:BA:3210:HOH:O	2.12	0.67
27:BA:64:G:N7	63:BA:3305:HOH:O	2.26	0.67
27:BA:2139:G:N7	63:BA:3319:HOH:O	2.28	0.67
32:BF:28:ASN:OD1	32:BF:29:ILE:N	2.27	0.67
38:BM:4:ILE:O	38:BM:4:ILE:HG22	1.95	0.67
27:BA:2628:G:N7	63:BA:3309:HOH:O	2.26	0.67
27:BA:1326:G:N7	63:BA:3201:HOH:O	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:1237:C:O2'	27:BA:1238:C:O4'	2.13	0.66
27:BA:1164:G:N7	63:BA:3314:HOH:O	2.27	0.66
27:BA:2746:G:N7	63:BA:3313:HOH:O	2.27	0.66
39:BO:76:ILE:HD11	39:BO:80:ASP:OD2	1.95	0.66
27:BA:2812:G:N7	63:BA:3318:HOH:O	2.28	0.66
28:BB:42:U:O2'	32:BF:52:LYS:O	2.08	0.66
37:BL:69:GLY:O	37:BL:74:ARG:NH1	2.28	0.66
27:BA:926:G:N7	63:BA:3317:HOH:O	2.27	0.66
27:BA:2248:G:O6	27:BA:2268:G:N2	2.28	0.66
38:BM:3:ALA:O	38:BM:8:ARG:NH1	2.28	0.66
27:BA:3030:U:N3	27:BA:3031:A:N7	2.43	0.66
27:BA:1054:G:N7	63:BA:3323:HOH:O	2.29	0.66
27:BA:2325:G:N7	63:BA:3326:HOH:O	2.29	0.66
27:BA:1539:G:N7	63:BA:3327:HOH:O	2.29	0.66
27:BA:2020:G:O6	27:BA:2036:U:O2	2.14	0.66
27:BA:2267:U:O2'	27:BA:2268:G:OP1	2.13	0.66
42:BR:16:ILE:HD13	42:BR:39:GLU:HG3	1.78	0.66
31:BE:123:ASN:O	31:BE:127:VAL:HG23	1.96	0.66
27:BA:462:A:OP2	63:BA:3222:HOH:O	2.14	0.65
27:BA:1388:G:N7	63:BA:3324:HOH:O	2.29	0.65
27:BA:656:G:N7	63:BA:3325:HOH:O	2.29	0.65
27:BA:1455:G:N7	63:BA:3320:HOH:O	2.28	0.65
27:BA:675:G:N7	63:BA:3336:HOH:O	2.30	0.65
27:BA:1008:U:O2'	27:BA:1009:U:O4'	2.13	0.65
27:BA:2552:A:OP2	63:BA:3188:HOH:O	2.15	0.65
27:BA:1440:G:N7	63:BA:3335:HOH:O	2.30	0.64
27:BA:2751:G:N7	63:BA:3331:HOH:O	2.30	0.64
27:BA:1911:A:OP2	63:BA:3205:HOH:O	2.15	0.64
27:BA:2603:C:OP2	63:BA:3188:HOH:O	2.15	0.64
28:BB:39:G:O2'	28:BB:40:U:O4'	2.12	0.64
27:BA:1507:C:H2'	27:BA:1508:G:N7	2.12	0.64
27:BA:1980:G:N7	63:BA:3332:HOH:O	2.30	0.64
27:BA:2332:G:OP2	63:BA:3236:HOH:O	2.15	0.64
27:BA:1111:A:OP2	63:BA:3233:HOH:O	2.15	0.64
27:BA:1147:A:N1	27:BA:1272:U:O2'	2.29	0.64
43:BS:82:LYS:NZ	63:BS:201:HOH:O	2.14	0.64
37:BL:52:ARG:O	63:BL:201:HOH:O	2.15	0.63
27:BA:494:C:O2	63:BA:3215:HOH:O	2.13	0.63
27:BA:1749:C:OP1	63:BA:3227:HOH:O	2.15	0.63
27:BA:2119:C:C5	27:BA:2120:5MC:HM52	2.34	0.63
27:BA:2229:G:O2'	27:BA:2230:U:OP2	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BE:17:GLU:N	31:BE:17:GLU:OE1	2.28	0.63
27:BA:2242:G:O2'	27:BA:2245:G:O2'	2.15	0.63
27:BA:2255:C:H2'	27:BA:2256:U:O4'	1.98	0.63
27:BA:183:U:OP1	63:BA:3181:HOH:O	2.16	0.62
27:BA:1505:G:N7	63:BA:3343:HOH:O	2.31	0.62
27:BA:2750:G:OP2	27:BA:2834:C:O2'	2.17	0.62
28:BB:24:G:N7	28:BB:56:U:O2'	2.30	0.62
32:BF:68:ARG:N	32:BF:71:GLU:OE2	2.31	0.62
35:BJ:63:GLU:OE2	35:BJ:66:ARG:NH1	2.28	0.62
38:BM:38:ALA:CA	38:BM:68:ASP:OD1	2.46	0.62
38:BN:29:ASP:OD1	38:BN:30:LYS:N	2.32	0.62
27:BA:702:G:N7	63:BA:3345:HOH:O	2.31	0.62
41:BQ:43:HIS:ND1	41:BQ:64:THR:OG1	2.27	0.62
27:BA:826:G:N7	63:BA:3338:HOH:O	2.31	0.61
27:BA:1758:G:OP1	63:BA:3244:HOH:O	2.16	0.61
48:BX:87:ASP:OD1	48:BX:88:GLY:N	2.33	0.61
27:BA:897:G:N7	63:BA:3339:HOH:O	2.31	0.61
27:BA:1008:U:O4	27:BA:1027:G:C6	2.54	0.61
46:BV:35:GLU:OE1	46:BV:38:ARG:NH1	2.34	0.61
46:BV:41:ARG:NH2	46:BV:118:ALA:O	2.32	0.61
27:BA:2552:A:OP1	63:BA:3234:HOH:O	2.15	0.61
49:BY:24:ARG:NH2	49:BY:41:TYR:OH	2.34	0.61
27:BA:1382:A:N7	63:BA:3340:HOH:O	2.31	0.60
38:BM:40:LEU:H	38:BM:40:LEU:CD2	2.14	0.60
30:BD:45:LYS:O	30:BD:313:PHE:O	2.18	0.60
27:BA:889:G:OP1	63:BA:3102:HOH:O	2.16	0.60
27:BA:1814:G:OP1	37:BL:102:ASN:ND2	2.31	0.60
27:BA:2220:G:H2'	27:BA:2221:U:O4'	2.01	0.60
35:BJ:41:ALA:HB3	35:BJ:43:PHE:CE1	2.36	0.60
27:BA:2266:G:N2	27:BA:2268:G:H22	1.99	0.60
27:BA:2112:G:N7	63:BA:3347:HOH:O	2.32	0.59
27:BA:2301:C:H2'	27:BA:2302:G:O4'	2.01	0.59
34:BI:86:LEU:HD21	34:BI:99:VAL:HG23	1.84	0.59
38:BM:47:ARG:O	38:BM:47:ARG:HG3	2.01	0.59
40:BP:39:ILE:O	63:BP:202:HOH:O	2.16	0.59
27:BA:1023:C:O2'	27:BA:1024:U:O5'	2.18	0.59
27:BA:2424:G:N3	27:BA:2424:G:H2'	2.15	0.59
27:BA:1181:C:O2	27:BA:2853:G:C2	2.55	0.59
29:BC:219:ARG:NE	63:BC:303:HOH:O	2.30	0.59
27:BA:2239:G:O2'	27:BA:2240:G:OP1	2.17	0.59
35:BJ:82:TYR:O	35:BJ:82:TYR:CD1	2.56	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:2038:U:H3	27:BA:2042:G:H22	1.51	0.58
27:BA:1623:OMU:HM22	27:BA:1624:A:H5'	1.84	0.58
27:BA:2413:A:O2'	32:BF:61:THR:O	2.08	0.58
32:BF:45:LEU:O	32:BF:49:VAL:HG22	2.03	0.58
34:BI:86:LEU:HD21	34:BI:99:VAL:CG2	2.34	0.58
29:BC:34:ASN:OD1	29:BC:35:LEU:HD12	2.04	0.57
32:BF:68:ARG:NH1	32:BF:70:GLY:O	2.37	0.57
38:BN:68:ASP:HA	38:BN:71:ILE:HG12	1.85	0.57
27:BA:2692:G:OP1	63:BA:3120:HOH:O	2.16	0.57
27:BA:796:A:OP1	63:BA:3257:HOH:O	2.18	0.57
27:BA:2358:G:H2'	27:BA:2359:C:O4'	2.04	0.57
32:BF:105:ASP:OD1	32:BF:109:ASN:N	2.35	0.57
27:BA:1065:U:OP2	63:BA:3214:HOH:O	2.17	0.57
27:BA:1817:A:OP2	63:BA:3149:HOH:O	2.17	0.57
37:BL:58:VAL:HG23	37:BL:85:GLN:OE1	2.04	0.57
34:BI:39:THR:HG21	34:BI:51:VAL:HG13	1.86	0.57
36:BK:117:GLU:OE1	63:BK:201:HOH:O	2.18	0.57
27:BA:2817:G:OP2	63:BA:3253:HOH:O	2.18	0.56
27:BA:569:G:N7	63:BA:3353:HOH:O	2.32	0.56
27:BA:2836:G:O2'	27:BA:2837:C:O4'	2.23	0.56
27:BA:2383:G:N7	63:BA:3352:HOH:O	2.32	0.56
46:BV:40:ILE:HA	46:BV:43:MET:SD	2.46	0.56
27:BA:2790:G:OP1	49:BY:20:LYS:NZ	2.30	0.56
28:BB:40:U:O2'	28:BB:45:A:N6	2.39	0.56
29:BC:65:ASP:OD1	29:BC:66:GLY:N	2.38	0.56
27:BA:2216:G:O2'	27:BA:2217:G:O4'	2.21	0.56
47:BW:85:LEU:HD23	47:BW:85:LEU:H	1.70	0.56
27:BA:35:G:N7	63:BA:3351:HOH:O	2.32	0.55
27:BA:2024:U:O4	27:BA:2031:A:O2'	2.15	0.55
27:BA:2835:A:H2'	27:BA:2836:G:O4'	2.05	0.55
27:BA:3029:C:H2'	27:BA:3030:U:O4'	2.06	0.55
27:BA:1008:U:C4	27:BA:1027:G:O6	2.59	0.55
27:BA:2210:A:H2'	27:BA:2211:C:O4'	2.07	0.55
42:BR:23:SER:OG	42:BR:28:VAL:O	2.24	0.55
27:BA:2229:G:O6	27:BA:2282:G:N1	2.39	0.55
34:BH:34:LYS:HE3	34:BH:92:LEU:HD21	1.89	0.55
39:BO:40:GLY:O	39:BO:41:LYS:HB3	2.06	0.55
27:BA:1181:C:N3	27:BA:2853:G:N1	2.54	0.55
34:BI:43:VAL:HG11	34:BI:70:CYS:SG	2.46	0.55
45:BU:31:PHE:HA	45:BU:91:VAL:HG22	1.88	0.55
31:BE:9:GLU:N	31:BE:9:GLU:OE1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:BD:60:LEU:O	30:BD:61:THR:HB	2.06	0.54
27:BA:758:G:N7	63:BA:3278:HOH:O	2.34	0.54
27:BA:808:U:H3	27:BA:923:G:H1	1.54	0.54
32:BF:42:GLU:HG2	32:BF:53:PRO:HG2	1.89	0.54
27:BA:325:G:H2'	27:BA:326:G:C8	2.42	0.54
32:BF:95:VAL:HG11	32:BF:114:ILE:HG21	1.89	0.54
38:BN:11:VAL:HG23	38:BN:56:LEU:HD11	1.90	0.54
27:BA:2231:A:N6	27:BA:2281:A:N7	2.55	0.54
32:BF:115:GLN:OE1	32:BF:115:GLN:N	2.41	0.54
27:BA:40:G:OP1	63:BA:3260:HOH:O	2.18	0.54
27:BA:3022:C:O2'	27:BA:3023:C:P	2.65	0.54
34:BI:39:THR:HG23	34:BI:100:ALA:HB2	1.88	0.54
27:BA:1579:G:N7	63:BA:3354:HOH:O	2.33	0.54
27:BA:1360:G:O2'	27:BA:1361:A:OP1	2.17	0.54
32:BF:42:GLU:HG2	32:BF:53:PRO:CG	2.38	0.54
27:BA:2119:C:C4	27:BA:2120:5MC:HM52	2.42	0.54
36:BK:129:VAL:HG22	36:BK:130:THR:H	1.73	0.54
27:BA:1401:G:N7	46:BV:29:SER:OG	2.33	0.54
27:BA:1683:A:H2'	27:BA:1684:A:C8	2.42	0.54
27:BA:1908:A:OP1	63:BA:3261:HOH:O	2.19	0.54
27:BA:2482:A:C2	41:BQ:104:LEU:HD23	2.43	0.53
27:BA:2359:C:H4'	27:BA:2360:A:OP1	2.08	0.53
27:BA:2253:C:H2'	27:BA:2254:C:C6	2.44	0.53
27:BA:2726:G:N7	63:BA:3359:HOH:O	2.34	0.53
27:BA:404:G:C2	27:BA:405:U:C5	2.97	0.53
27:BA:2240:G:H2'	27:BA:2241:C:O4'	2.09	0.53
27:BA:1180:A:N6	27:BA:2853:G:N1	2.57	0.53
27:BA:1671:A:H2'	27:BA:1671:A:N3	2.24	0.53
30:BD:292:PHE:O	30:BD:295:TYR:O	2.27	0.53
27:BA:1023:C:H2'	27:BA:1024:U:H6	1.74	0.53
32:BF:25:VAL:HG13	32:BF:138:VAL:HG22	1.91	0.53
32:BF:176:LEU:O	32:BF:177:LYS:HB2	2.09	0.53
36:BK:72:ASP:OD1	36:BK:72:ASP:N	2.42	0.53
27:BA:1240:U:O3'	27:BA:1241:C:O4'	2.27	0.53
27:BA:2267:U:HO2'	27:BA:2268:G:P	2.30	0.53
27:BA:1826:A:N1	63:BA:3361:HOH:O	2.34	0.53
28:BB:32:C:N3	28:BB:51:G:N2	2.56	0.53
38:BN:19:GLY:O	38:BN:20:GLN:HG3	2.09	0.53
27:BA:2595:C:HO2'	27:BA:2596:U:P	2.33	0.52
27:BA:2379:OMG:OP2	35:BJ:115:PRO:HD2	2.10	0.52
39:BO:102:VAL:HG23	39:BO:124:VAL:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:BR:11:ASN:OD1	42:BR:14:ARG:NH1	2.43	0.52
27:BA:580:G:N2	27:BA:641:G:O6	2.40	0.52
27:BA:405:U:H2'	27:BA:406:G:O4'	2.09	0.52
27:BA:911:A:OP2	63:BA:3104:HOH:O	2.18	0.52
27:BA:1179:G:N2	27:BA:1245:G:O4'	2.43	0.52
43:BS:62:ARG:HH11	43:BS:62:ARG:HG2	1.75	0.52
36:BK:2:ARG:NH1	36:BK:113:GLU:OE1	2.41	0.52
43:BS:40:ASP:OD1	43:BS:43:ARG:NH2	2.43	0.51
27:BA:590:A:H2'	27:BA:591:C:O4'	2.10	0.51
27:BA:2115:OMG:HM22	27:BA:2116:G:H5'	1.90	0.51
29:BC:54:ARG:O	29:BC:55:THR:HB	2.09	0.51
27:BA:48:C:H4'	31:BE:45:PRO:HG2	1.93	0.51
46:BV:114:LYS:HD2	46:BV:154:ILE:HD11	1.93	0.51
27:BA:1685:G:C2	27:BA:1686:G:C8	2.99	0.51
34:BI:110:LEU:O	34:BI:114:ILE:HG12	2.10	0.51
41:BQ:84:TYR:CE2	41:BQ:88:LEU:HD11	2.46	0.51
27:BA:820:G:N7	63:BA:3363:HOH:O	2.34	0.51
27:BA:915:C:OP1	63:BA:3176:HOH:O	2.19	0.51
27:BA:2299:G:H2'	27:BA:2300:C:C6	2.46	0.51
27:BA:1011:G:H22	27:BA:1026:C:N4	2.09	0.51
27:BA:2748:A:O2'	27:BA:2749:A:O4'	2.28	0.51
33:BG:5:ALA:O	33:BG:58:GLU:O	2.29	0.51
27:BA:2802:G:N7	63:BA:3365:HOH:O	2.34	0.51
28:BB:1:G:H1	28:BB:124:C:H42	1.58	0.51
34:BI:107:ALA:O	34:BI:111:VAL:HG23	2.11	0.51
27:BA:1307:A:H4'	27:BA:1308:U:OP1	2.11	0.51
30:BD:151:PRO:O	30:BD:154:ILE:O	2.29	0.51
34:BH:80:VAL:HG21	34:BH:86:LEU:HD12	1.92	0.51
34:BI:17:GLU:O	34:BI:21:GLU:OE1	2.28	0.51
27:BA:316:G:H4'	27:BA:317:G:OP1	2.10	0.50
30:BD:61:THR:HG22	30:BD:61:THR:O	2.10	0.50
27:BA:46:C:O2'	31:BE:48:ARG:NH1	2.44	0.50
27:BA:2023:G:N2	27:BA:2034:C:C2	2.79	0.50
27:BA:579:C:H2'	27:BA:580:G:C1'	2.41	0.50
32:BF:23:ALA:HB3	32:BF:139:THR:O	2.11	0.50
27:BA:2172:A:N3	27:BA:2173:G:O2'	2.37	0.50
27:BA:2385:G:O2'	27:BA:2531:G:O6	2.28	0.50
27:BA:2687:G:OP2	63:BA:3265:HOH:O	2.20	0.50
27:BA:2997:C:O3'	49:BY:63:ARG:NH1	2.44	0.50
27:BA:739:C:H2'	27:BA:740:G:O4'	2.10	0.50
27:BA:1023:C:O2'	27:BA:1024:U:O4'	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:2409:C:O2'	27:BA:2412:G:N7	2.45	0.50
30:BD:195:GLU:HA	30:BD:268:LEU:HD22	1.92	0.50
32:BF:99:LEU:O	32:BF:180:VAL:N	2.45	0.50
27:BA:147:U:HO2'	27:BA:148:G:P	2.30	0.50
27:BA:2215:G:H22	27:BA:2298:U:H3	1.58	0.50
27:BA:2411:G:N7	27:BA:2412:G:N2	2.60	0.50
27:BA:579:C:H2'	27:BA:580:G:O4'	2.11	0.50
27:BA:883:G:N7	63:BA:3360:HOH:O	2.34	0.50
27:BA:1237:C:HO2'	27:BA:1238:C:C1'	2.23	0.50
41:BQ:184:HIS:O	41:BQ:188:VAL:HG12	2.12	0.50
29:BC:219:ARG:NH1	63:BC:303:HOH:O	2.40	0.50
47:BW:12:VAL:HG13	47:BW:12:VAL:O	2.12	0.50
27:BA:148:G:C2'	27:BA:149:C:OP1	2.59	0.50
27:BA:346:G:N7	63:BA:3368:HOH:O	2.35	0.50
27:BA:1636:A:H4'	27:BA:1637:G:OP1	2.12	0.50
27:BA:1874:G:O6	43:BS:76:ARG:NH2	2.45	0.50
27:BA:2317:G:H2'	27:BA:2318:G:C5'	2.42	0.49
32:BF:14:ALA:O	32:BF:15:HIS:CG	2.65	0.49
32:BF:40:LYS:HB2	32:BF:129:ILE:CD1	2.42	0.49
27:BA:1415:G:N7	63:BA:3367:HOH:O	2.35	0.49
34:BI:50:LEU:HD12	34:BI:51:VAL:H	1.77	0.49
38:BM:34:LEU:HD12	38:BM:35:VAL:N	2.27	0.49
27:BA:61:A2M:H2'	27:BA:62:A:C8	2.48	0.49
32:BF:29:ILE:HG22	32:BF:29:ILE:O	2.12	0.49
34:BI:115:ALA:O	34:BI:118:VAL:HG12	2.13	0.49
27:BA:162:C:H2'	27:BA:163:G:O4'	2.12	0.49
27:BA:2173:G:O2'	27:BA:2174:A:OP2	2.31	0.49
40:BP:47:ARG:HE	40:BP:47:ARG:HA	1.77	0.49
27:BA:2237:G:C2	27:BA:2285:A:N6	2.81	0.49
38:BN:38:ALA:HB3	38:BN:40:LEU:HB2	1.94	0.49
45:BU:89:HIS:ND1	45:BU:91:VAL:HG23	2.27	0.49
27:BA:123:C:O2'	27:BA:135:U:O2'	2.28	0.49
27:BA:1945:OMG:HM23	27:BA:1949:OMU:HM21	1.95	0.49
34:BH:15:LEU:O	34:BH:18:LYS:N	2.45	0.49
27:BA:179:G:OP2	63:BA:3269:HOH:O	2.20	0.49
27:BA:2245:G:N3	27:BA:2245:G:H2'	2.28	0.49
27:BA:2382:G:OP1	35:BJ:24:ARG:NE	2.41	0.49
27:BA:879:A2M:OP1	63:BA:3161:HOH:O	2.19	0.48
27:BA:1975:U:H2'	27:BA:1976:A:O4'	2.13	0.48
27:BA:2070:C:H5	63:BA:4106:HOH:O	1.96	0.48
27:BA:2420:C:H2'	27:BA:2421:G:O4'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:541:A:H4'	27:BA:542:A:OP1	2.13	0.48
27:BA:2282:G:H1'	27:BA:2283:A:C8	2.48	0.48
30:BD:315:ARG:O	30:BD:317:ILE:HD12	2.13	0.48
32:BF:67:ILE:N	32:BF:71:GLU:OE2	2.46	0.48
46:BV:20:ARG:HG2	46:BV:150:VAL:HG22	1.95	0.48
34:BI:19:ALA:O	34:BI:23:VAL:HG23	2.14	0.48
38:BM:20:GLN:OE1	38:BM:43:VAL:HG23	2.13	0.48
39:BO:117:GLY:O	39:BO:137:LYS:NZ	2.38	0.48
27:BA:2241:C:C4	27:BA:2242:G:N7	2.81	0.48
48:BX:48:VAL:O	48:BX:66:VAL:O	2.31	0.48
32:BF:91:LEU:O	32:BF:95:VAL:HG22	2.13	0.48
34:BH:26:ALA:O	34:BH:30:GLY:N	2.47	0.48
38:BM:40:LEU:N	38:BM:40:LEU:CD2	2.74	0.48
38:BN:37:GLY:O	38:BN:38:ALA:HB2	2.13	0.48
40:BP:49:ARG:NE	40:BP:53:TYR:O	2.46	0.48
45:BU:96:GLN:O	45:BU:97:LYS:HB2	2.14	0.48
27:BA:392:C:H2'	27:BA:393:G:O4'	2.14	0.48
27:BA:1181:C:O2'	27:BA:1182:A:C8	2.66	0.48
27:BA:2000:U:H2'	27:BA:2001:G:O4'	2.14	0.48
29:BC:32:PRO:HB2	29:BC:34:ASN:OD1	2.14	0.48
27:BA:1609:A:C2	27:BA:1610:G:H1'	2.48	0.48
27:BA:2218:G:H4'	27:BA:2219:G:OP1	2.14	0.48
29:BC:100:ALA:O	29:BC:134:ARG:NH2	2.47	0.48
38:BM:73:ALA:O	38:BM:76:GLU:N	2.45	0.48
27:BA:988:G:O2'	27:BA:989:U:OP2	2.29	0.48
28:BB:56:U:H1'	28:BB:57:A:OP2	2.14	0.48
27:BA:1180:A:N1	27:BA:2853:G:N2	2.62	0.48
27:BA:1867:G:HO2'	27:BA:1869:A:H8	1.60	0.48
34:BI:17:GLU:O	34:BI:20:LEU:HB3	2.14	0.48
27:BA:1608:A:H3'	27:BA:1609:A:C8	2.49	0.47
27:BA:2430:A:H2'	27:BA:2431:A:C8	2.49	0.47
33:BG:6:TRP:O	33:BG:6:TRP:CD1	2.67	0.47
41:BQ:60:VAL:HG12	41:BQ:61:SER:N	2.29	0.47
45:BU:61:ARG:NH1	45:BU:78:THR:O	2.45	0.47
27:BA:147:U:O2'	27:BA:148:G:P	2.72	0.47
27:BA:404:G:O2'	27:BA:405:U:P	2.72	0.47
27:BA:2152:G:N7	63:BA:3372:HOH:O	2.35	0.47
27:BA:2496:C:H4'	27:BA:2497:G:OP1	2.13	0.47
27:BA:871:G:OP1	63:BA:3271:HOH:O	2.20	0.47
27:BA:317:G:O2'	27:BA:318:A:OP2	2.32	0.47
38:BM:2:PRO:N	38:BM:8:ARG:NH2	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:1635:G:O2'	27:BA:1636:A:OP2	2.24	0.47
27:BA:341:C:C5	27:BA:342:5MC:HM52	2.50	0.47
27:BA:2853:G:N3	27:BA:2853:G:H2'	2.29	0.47
27:BA:1691:U:O2'	27:BA:1692:U:P	2.72	0.47
27:BA:2021:G:H3'	27:BA:2022:G:H5"	1.96	0.47
27:BA:2316:C:H2'	27:BA:2317:G:O4'	2.14	0.47
29:BC:202:HIS:O	29:BC:204:HIS:O	2.32	0.47
32:BF:88:LEU:HD23	32:BF:175:GLU:OE2	2.14	0.47
27:BA:2020:G:O6	27:BA:2036:U:C2	2.68	0.47
42:BR:91:ARG:O	42:BR:95:ILE:HG12	2.14	0.47
27:BA:1180:A:N6	27:BA:2853:G:C6	2.83	0.47
27:BA:2435:C:O2	27:BA:2435:C:O5'	2.32	0.47
27:BA:2671:G:H2'	27:BA:2672:OMG:O4'	2.15	0.47
32:BF:8:ILE:O	32:BF:11:ASP:OD1	2.33	0.47
27:BA:1030:U:O2'	27:BA:1031:C:OP1	2.28	0.46
27:BA:1907:U:H5	27:BA:1912:A:N7	2.13	0.46
27:BA:2095:G:N7	63:BA:3376:HOH:O	2.36	0.46
27:BA:2304:A:H2'	27:BA:2305:C:O4'	2.15	0.46
27:BA:2988:A:H2'	27:BA:2989:A:O4'	2.15	0.46
27:BA:454:C:O2'	27:BA:1991:A:N6	2.48	0.46
27:BA:1520:G:O6	63:BA:3123:HOH:O	2.16	0.46
27:BA:2413:A:N7	27:BA:2414:A:C8	2.83	0.46
28:BB:32:C:C2	28:BB:51:G:N2	2.83	0.46
27:BA:842:C:H2'	27:BA:843:A:O4'	2.15	0.46
27:BA:1394:G:N7	63:BA:3370:HOH:O	2.35	0.46
27:BA:3031:A:H2'	27:BA:3032:C:C4'	2.46	0.46
32:BF:64:ASP:O	32:BF:65:PHE:CD2	2.68	0.46
34:BH:66:LEU:HB2	34:BH:67:PRO:HD3	1.97	0.46
39:BO:55:PRO:O	39:BO:56:ASP:HB2	2.16	0.46
39:BO:91:ALA:O	39:BO:93:ILE:N	2.44	0.46
50:BZ:25:LEU:HD21	50:BZ:29:ARG:NH2	2.30	0.46
27:BA:1777:G:N1	27:BA:1780:A:OP2	2.43	0.46
35:BJ:82:TYR:O	35:BJ:82:TYR:CG	2.69	0.46
27:BA:1607:C:H2'	27:BA:1608:A:O4'	2.14	0.46
27:BA:2260:G:C2'	27:BA:2261:G:O5'	2.64	0.46
30:BD:45:LYS:HB3	30:BD:313:PHE:O	2.15	0.46
27:BA:1882:C:N3	27:BA:2819:C:O2'	2.43	0.46
27:BA:2278:A:H2'	27:BA:2279:U:H5'	1.98	0.46
32:BF:99:LEU:HB2	32:BF:177:LYS:HG2	1.98	0.46
27:BA:18:C:O3'	27:BA:19:A:H4'	2.16	0.46
27:BA:331:A:O2'	27:BA:332:A:P	2.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:1685:G:O2'	27:BA:1686:G:H5'	2.15	0.46
29:BC:219:ARG:HG2	29:BC:219:ARG:HH21	1.80	0.46
41:BQ:100:GLU:O	41:BQ:101:GLU:HG2	2.16	0.46
32:BF:8:ILE:HG21	32:BF:170:VAL:HG21	1.97	0.46
38:BN:8:ARG:NH2	38:BN:57:PRO:HA	2.30	0.46
41:BQ:140:GLU:OE1	41:BQ:140:GLU:N	2.43	0.46
27:BA:321:C:H2'	27:BA:322:C:O4'	2.16	0.45
27:BA:2173:G:H1'	27:BA:2174:A:OP2	2.16	0.45
32:BF:71:GLU:HG3	32:BF:73:ILE:HG12	1.98	0.45
27:BA:2300:C:H2'	27:BA:2301:C:C6	2.52	0.45
27:BA:2958:U:H4'	27:BA:2959:U:H5"	1.96	0.45
30:BD:74:GLU:OE1	30:BD:298:VAL:HG13	2.17	0.45
27:BA:581:A:N1	27:BA:584:G:O6	2.49	0.45
27:BA:1181:C:C2	27:BA:2853:G:C2	3.02	0.45
27:BA:1976:A:O2'	27:BA:1977:U:O5'	2.26	0.45
27:BA:2426:G:H1	27:BA:2435:C:H5	1.65	0.45
34:BH:70:CYS:O	34:BH:74:GLU:N	2.49	0.45
35:BJ:163:ARG:HE	35:BJ:163:ARG:HA	1.81	0.45
35:BJ:164:ILE:HD12	35:BJ:173:THR:HA	1.99	0.45
41:BQ:100:GLU:N	41:BQ:100:GLU:OE1	2.50	0.45
43:BS:63:ALA:O	43:BS:67:GLN:HG2	2.17	0.45
27:BA:19:A:N6	27:BA:3028:G:C5	2.84	0.45
27:BA:185:G:H2'	27:BA:186:A:O4'	2.17	0.45
27:BA:1927:G:N7	29:BC:145:SER:OG	2.39	0.45
32:BF:31:VAL:HG13	32:BF:32:GLY:H	1.82	0.45
47:BW:3:PRO:O	47:BW:4:TYR:HB2	2.16	0.45
47:BW:75:ASP:O	47:BW:78:GLU:HG2	2.17	0.45
27:BA:1178:A:H4'	27:BA:1179:G:OP1	2.16	0.45
32:BF:22:ILE:HD12	32:BF:85:TYR:CE1	2.51	0.45
39:BO:41:LYS:O	39:BO:42:ARG:HG2	2.16	0.45
27:BA:636:U:H2'	27:BA:637:G:C8	2.51	0.45
27:BA:840:A:H3'	63:BA:3369:HOH:O	2.17	0.45
27:BA:1360:G:H4'	27:BA:1361:A:OP1	2.16	0.45
27:BA:2413:A:N6	32:BF:64:ASP:HB3	2.32	0.45
27:BA:1684:A:P	43:BS:43:ARG:HE	2.39	0.45
27:BA:2260:G:H2'	27:BA:2261:G:O5'	2.16	0.45
27:BA:1949:OMU:HM22	27:BA:1950:G:O4'	2.17	0.45
30:BD:269:ILE:HD12	30:BD:306:GLU:HB3	1.98	0.45
33:BG:120:ARG:HD3	33:BG:157:ALA:O	2.17	0.45
34:BI:14:GLU:O	34:BI:17:GLU:HG3	2.17	0.45
27:BA:143:C:H2'	27:BA:144:U:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:2034:C:C2	27:BA:2035:C:C5	3.05	0.45
27:BA:2431:A:H2'	27:BA:2432:G:C8	2.51	0.45
33:BG:6:TRP:O	33:BG:7:ILE:C	2.54	0.45
50:BZ:40:ASN:O	50:BZ:43:VAL:HG23	2.17	0.44
27:BA:1463:C:H2'	27:BA:1464:G:O4'	2.16	0.44
27:BA:2208:G:H2'	27:BA:2209:U:C6	2.51	0.44
27:BA:2975:U:H4'	27:BA:2976:A:H5'	1.99	0.44
38:BM:23:VAL:HG11	38:BM:71:ILE:HG21	1.99	0.44
27:BA:674:OMG:HM22	27:BA:675:G:H5'	1.99	0.44
27:BA:972:G:N7	63:BA:3377:HOH:O	2.36	0.44
27:BA:1140:G:OP2	63:BA:3276:HOH:O	2.21	0.44
27:BA:2379:OMG:OP2	35:BJ:114:ARG:HA	2.17	0.44
28:BB:26:C:C5	28:BB:27:A:C8	3.06	0.44
50:BZ:32:LEU:HD22	50:BZ:44:ILE:CD1	2.47	0.44
27:BA:114:C:HO2'	27:BA:332:A:HO2'	1.62	0.44
27:BA:734:A:N1	39:BO:118:LYS:HG2	2.32	0.44
27:BA:2934:C:C2'	27:BA:2935:G:O5'	2.66	0.44
33:BG:90:LEU:HD23	33:BG:174:ILE:HA	2.00	0.44
27:BA:1148:A:N1	27:BA:1272:U:H5	2.16	0.44
27:BA:1241:C:H5"	27:BA:1242:G:OP2	2.18	0.44
28:BB:35:U:C2'	28:BB:36:C:O5'	2.65	0.44
31:BE:29:ASP:OD1	31:BE:29:ASP:N	2.51	0.44
48:BX:48:VAL:O	48:BX:66:VAL:HB	2.18	0.44
31:BE:84:PRO:HA	31:BE:90:ARG:O	2.18	0.44
45:BU:31:PHE:CD1	45:BU:91:VAL:HG21	2.52	0.44
27:BA:1343:G:N7	63:BA:3386:HOH:O	2.37	0.44
27:BA:2935:G:H1'	27:BA:3025:A:H61	1.83	0.44
30:BD:278:VAL:HG12	30:BD:279:LEU:O	2.18	0.44
44:BT:72:ARG:O	44:BT:75:LEU:HG	2.18	0.44
27:BA:505:A2M:H8	27:BA:505:A2M:C5'	2.47	0.44
27:BA:588:U:H4'	27:BA:589:G:OP2	2.17	0.44
27:BA:1294:G:N7	63:BA:3383:HOH:O	2.36	0.44
29:BC:36:VAL:HG22	29:BC:36:VAL:O	2.18	0.44
42:BR:105:GLU:HA	42:BR:108:MET:HG2	2.00	0.44
27:BA:494:C:O2	27:BA:494:C:H2'	2.16	0.43
27:BA:803:G:O6	63:BA:3266:HOH:O	2.20	0.43
27:BA:1136:A:N3	27:BA:1285:C:O2'	2.49	0.43
27:BA:2274:G:C2	27:BA:2275:C:C4	3.06	0.43
32:BF:97:ARG:HG2	32:BF:98:LYS:N	2.33	0.43
41:BQ:85:LEU:HA	41:BQ:88:LEU:HD12	2.00	0.43
27:BA:315:A:H4'	27:BA:315:A:OP1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:534:G:N7	46:BV:2:SER:HB3	2.33	0.43
27:BA:751:G:O2'	27:BA:752:G:H5'	2.18	0.43
30:BD:61:THR:O	30:BD:61:THR:CG2	2.66	0.43
34:BI:99:VAL:HG12	34:BI:100:ALA:N	2.33	0.43
27:BA:1009:U:N3	27:BA:1027:G:N7	2.63	0.43
27:BA:1014:G:H22	27:BA:1024:U:H3	1.65	0.43
27:BA:2162:U:H2'	27:BA:2163:G:O4'	2.18	0.43
30:BD:244:ALA:O	30:BD:245:ARG:HG3	2.18	0.43
27:BA:279:A:C2	27:BA:323:U:H5'	2.53	0.43
27:BA:772:A:H2'	27:BA:773:G:O4'	2.18	0.43
27:BA:2437:A:OP2	41:BQ:14:ARG:NH2	2.41	0.43
29:BC:203:PRO:HG2	29:BC:227:VAL:HG21	2.01	0.43
30:BD:273:GLU:HA	30:BD:301:ASP:OD1	2.18	0.43
35:BJ:44:GLU:OE1	35:BJ:167:LYS:NZ	2.38	0.43
39:BO:146:LEU:HG	39:BO:146:LEU:O	2.18	0.43
40:BP:163:THR:HG22	40:BP:164:SER:H	1.83	0.43
27:BA:960:G:N7	63:BA:3381:HOH:O	2.36	0.43
27:BA:1185:G:H2'	27:BA:1186:G:C8	2.54	0.43
27:BA:2216:G:O2'	27:BA:2217:G:O5'	2.37	0.43
27:BA:2230:U:H3'	27:BA:2231:A:H5'	2.00	0.43
27:BA:2297:C:H2'	27:BA:2298:U:N1	2.34	0.43
27:BA:2433:G:N7	63:BA:3378:HOH:O	2.36	0.43
27:BA:2580:A:C2'	27:BA:2581:U:O5'	2.67	0.43
27:BA:2766:G:H2'	27:BA:2767:A:O4'	2.18	0.43
31:BE:149:GLN:O	31:BE:205:GLU:O	2.37	0.43
46:BV:124:PRO:O	46:BV:144:THR:OG1	2.35	0.43
27:BA:2255:C:H2'	27:BA:2256:U:C6	2.54	0.43
35:BJ:140:GLN:OE1	35:BJ:140:GLN:N	2.50	0.43
35:BJ:142:LEU:HD13	35:BJ:176:VAL:CG1	2.48	0.43
27:BA:2119:C:C6	27:BA:2120:5MC:HM52	2.54	0.43
31:BE:190:ARG:O	31:BE:191:TYR:HB2	2.19	0.43
27:BA:699:A:H2'	27:BA:700:A:C8	2.53	0.43
27:BA:927:G:N7	63:BA:3388:HOH:O	2.37	0.43
27:BA:2246:A:C2	27:BA:2270:A:O4'	2.71	0.43
27:BA:2595:C:O2'	27:BA:2596:U:OP1	2.28	0.43
30:BD:131:LEU:HD23	30:BD:176:PHE:HE1	1.83	0.43
31:BE:13:VAL:HG23	31:BE:14:GLU:N	2.34	0.43
32:BF:176:LEU:C	32:BF:176:LEU:HD23	2.39	0.43
35:BJ:55:MET:SD	35:BJ:158:TYR:HB2	2.59	0.43
27:BA:1687:G:H2'	27:BA:1687:G:N3	2.34	0.43
27:BA:1716:A:H2'	27:BA:1717:A:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:2890:C:OP1	30:BD:117:LYS:NZ	2.50	0.43
63:BA:3138:HOH:O	48:BX:10:LYS:NZ	2.19	0.43
31:BE:138:VAL:HG23	31:BE:139:GLN:N	2.32	0.43
27:BA:2236:G:C6	27:BA:2237:G:C4	3.07	0.43
32:BF:177:LYS:HD3	32:BF:178:ALA:H	1.83	0.43
33:BG:104:GLN:O	33:BG:104:GLN:HG3	2.19	0.43
27:BA:241:G:H2'	27:BA:242:A:C8	2.54	0.42
27:BA:1023:C:HO2'	27:BA:1024:U:C5'	2.28	0.42
27:BA:1606:A:H2'	27:BA:1607:C:O4'	2.18	0.42
27:BA:2035:C:C4	27:BA:2036:U:C6	3.07	0.42
27:BA:2423:A:H2'	27:BA:2423:A:N3	2.34	0.42
27:BA:386:A:C4	27:BA:387:G:C8	3.07	0.42
27:BA:410:C:HO2'	27:BA:411:U:P	2.42	0.42
27:BA:571:G:N7	63:BA:3384:HOH:O	2.36	0.42
27:BA:1928:C:H1'	27:BA:1929:U:OP2	2.19	0.42
27:BA:2222:G:H4'	27:BA:2223:C:OP2	2.19	0.42
27:BA:2233:G:H2'	27:BA:2234:C:O4'	2.19	0.42
27:BA:2720:C:H2'	27:BA:2721:U:O4'	2.19	0.42
27:BA:395:G:H2'	27:BA:396:C:O4'	2.18	0.42
27:BA:2173:G:H4'	27:BA:2174:A:O4'	2.18	0.42
27:BA:2524:C:OP1	39:BO:61:ARG:NH2	2.50	0.42
35:BJ:83:HIS:HB3	35:BJ:136:TRP:HB2	2.00	0.42
27:BA:331:A:H4'	27:BA:332:A:OP1	2.19	0.42
27:BA:2248:G:N3	27:BA:2248:G:H2'	2.35	0.42
30:BD:278:VAL:O	30:BD:334:ARG:NH1	2.51	0.42
31:BE:184:GLY:O	31:BE:188:GLY:O	2.36	0.42
32:BF:68:ARG:O	32:BF:68:ARG:HD3	2.20	0.42
34:BI:113:ASP:O	34:BI:117:LYS:HD2	2.18	0.42
38:BM:38:ALA:HA	38:BM:68:ASP:CG	2.36	0.42
27:BA:18:C:N3	27:BA:19:A:C8	2.87	0.42
43:BS:143:GLN:O	43:BS:145:HIS:O	2.37	0.42
46:BV:45:LEU:HD23	46:BV:115:ILE:HD11	2.01	0.42
27:BA:1022:C:H3'	27:BA:1023:C:H5'	2.02	0.42
27:BA:1798:G:H2'	27:BA:1799:G:O4'	2.20	0.42
33:BG:90:LEU:HB2	33:BG:137:ILE:HB	2.02	0.42
41:BQ:116:SER:O	41:BQ:120:VAL:HG23	2.20	0.42
42:BR:65:VAL:HG12	42:BR:67:GLY:H	1.83	0.42
27:BA:869:OMC:H5'	27:BA:870:U:O5'	2.19	0.42
27:BA:1564:G:OP1	63:BA:3275:HOH:O	2.21	0.42
33:BG:6:TRP:O	33:BG:6:TRP:HD1	2.03	0.42
34:BI:33:ARG:HG2	34:BI:38:GLU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:2304:A:H2'	27:BA:2305:C:C6	2.55	0.42
38:BM:4:ILE:O	38:BM:4:ILE:CG2	2.65	0.42
41:BQ:112:THR:OG1	41:BQ:115:SER:OG	2.38	0.42
27:BA:1944:U:O2	27:BA:1944:U:O4'	2.38	0.42
27:BA:2216:G:C2'	27:BA:2217:G:O4'	2.68	0.42
28:BB:53:A:C8	28:BB:54:G:C8	3.07	0.42
30:BD:324:ARG:N	30:BD:325:PRO:HD3	2.35	0.42
36:BK:125:THR:HG22	36:BK:127:LYS:H	1.84	0.42
40:BP:8:ARG:HG2	40:BP:8:ARG:HH11	1.85	0.42
27:BA:19:A:C6	27:BA:20:A:C2	3.08	0.41
27:BA:116:G:H2'	27:BA:117:G:O4'	2.20	0.41
27:BA:845:A:H2'	27:BA:846:G:O4'	2.20	0.41
27:BA:2413:A:C4	32:BF:62:ASN:HB2	2.55	0.41
38:BN:17:ARG:NH1	63:BN:101:HOH:O	2.25	0.41
27:BA:160:G:O2'	27:BA:161:U:O5'	2.34	0.41
27:BA:1308:U:OP2	27:BA:1308:U:H3'	2.20	0.41
27:BA:1592:A:H2'	27:BA:1593:G:O4'	2.20	0.41
27:BA:1684:A:OP1	43:BS:43:ARG:NH1	2.48	0.41
28:BB:17:C:H2'	28:BB:18:G:O4'	2.19	0.41
35:BJ:79:ARG:HA	35:BJ:82:TYR:CE2	2.56	0.41
43:BS:85:LYS:O	43:BS:89:MET:HG3	2.20	0.41
27:BA:331:A:H2'	27:BA:332:A:C8	2.55	0.41
27:BA:439:G:N7	63:BA:3390:HOH:O	2.37	0.41
27:BA:1980:G:N1	27:BA:2002:A:OP2	2.53	0.41
34:BI:106:LYS:HG2	34:BI:106:LYS:O	2.21	0.41
38:BM:3:ALA:HB3	38:BM:5:GLU:HG2	2.03	0.41
27:BA:1016:C:H3'	27:BA:1017:G:H4'	2.02	0.41
27:BA:1638:U:H3'	27:BA:1639:G:C5'	2.49	0.41
27:BA:2239:G:H4'	27:BA:2240:G:OP1	2.21	0.41
27:BA:2571:C:H2'	27:BA:2572:G:O4'	2.21	0.41
63:BA:4449:HOH:O	29:BC:167:ARG:HD2	2.20	0.41
38:BN:17:ARG:HG2	38:BN:43:VAL:HG22	2.03	0.41
27:BA:388:C:H2'	27:BA:389:C:C6	2.56	0.41
27:BA:689:C:OP1	42:BR:5:THR:O	2.39	0.41
27:BA:1183:G:C3'	27:BA:1184:C:H5"	2.51	0.41
27:BA:2260:G:H2'	27:BA:2261:G:O4'	2.20	0.41
28:BB:115:G:H2'	28:BB:116:C:C6	2.56	0.41
32:BF:150:ARG:CG	32:BF:151:LYS:N	2.84	0.41
48:BX:31:LEU:HD12	48:BX:41:VAL:O	2.20	0.41
27:BA:484:C:H2'	27:BA:485:G:O4'	2.21	0.41
27:BA:757:G:OP2	63:BA:3278:HOH:O	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:1183:G:C2'	27:BA:1184:C:H5"	2.50	0.41
27:BA:1949:OMU:O5'	27:BA:1949:OMU:H6	2.21	0.41
27:BA:2023:G:H2'	27:BA:2024:U:C6	2.55	0.41
27:BA:2806:U:H2'	27:BA:2807:A:H8	1.86	0.41
27:BA:2858:U:H4'	27:BA:2859:A:OP1	2.20	0.41
27:BA:2935:G:C2'	27:BA:3025:A:H61	2.34	0.41
35:BJ:174:THR:OG1	35:BJ:175:LYS:N	2.53	0.41
38:BN:68:ASP:HA	38:BN:71:ILE:CG1	2.50	0.41
27:BA:1074:U:O2	27:BA:1074:U:O5'	2.39	0.41
27:BA:2556:C:H2'	27:BA:2557:A:H8	1.86	0.41
32:BF:142:ARG:HB2	32:BF:143:PRO:HD2	2.03	0.41
40:BP:47:ARG:NH1	63:BP:205:HOH:O	2.52	0.41
45:BU:55:ASP:OD2	45:BU:57:ARG:HB2	2.20	0.41
27:BA:698:U:C6	27:BA:715:A:N7	2.89	0.41
27:BA:2255:C:C2'	27:BA:2256:U:O4'	2.67	0.41
28:BB:51:G:C2'	28:BB:52:A:O5'	2.69	0.41
33:BG:49:GLU:O	33:BG:50:ASP:C	2.59	0.41
27:BA:198:A:H2'	27:BA:199:C:O4'	2.21	0.41
27:BA:551:A:H2'	27:BA:552:A:O4'	2.21	0.41
27:BA:1266:C:H5'	27:BA:1267:G:OP2	2.21	0.41
27:BA:1383:U:O2	31:BE:91:ARG:HD2	2.21	0.41
27:BA:1684:A:C8	27:BA:1685:G:C1'	3.03	0.41
27:BA:1799:G:O2'	27:BA:1801:A:H1'	2.21	0.41
27:BA:2233:G:O6	27:BA:2290:C:C4	2.74	0.41
27:BA:2299:G:H2'	27:BA:2300:C:C5	2.56	0.41
27:BA:2745:OMG:H5"	36:BK:56:ARG:NH1	2.36	0.41
30:BD:268:LEU:C	30:BD:268:LEU:HD23	2.41	0.41
32:BF:57:ARG:HG3	32:BF:71:GLU:N	2.36	0.41
32:BF:59:LYS:O	32:BF:60:GLN:C	2.59	0.41
34:BI:80:VAL:CG2	34:BI:86:LEU:HD12	2.51	0.41
35:BJ:172:VAL:O	35:BJ:172:VAL:HG12	2.21	0.41
38:BM:73:ALA:O	38:BM:76:GLU:HB3	2.21	0.41
43:BS:4:LEU:HA	43:BS:7:GLN:OE1	2.21	0.41
48:BX:28:SER:HA	48:BX:45:PRO:HA	2.03	0.41
27:BA:20:A:H2'	27:BA:21:C:C6	2.55	0.41
27:BA:93:A:OP2	48:BX:47:ARG:NH2	2.54	0.41
27:BA:1184:C:H5	27:BA:1185:G:C5	2.39	0.41
27:BA:2320:A:OP2	27:BA:2320:A:C8	2.74	0.41
27:BA:2346:U:H2'	27:BA:2347:U:O4'	2.20	0.41
27:BA:2622:A:OP2	63:BA:3281:HOH:O	2.22	0.41
32:BF:23:ALA:HB2	32:BF:141:GLU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:BP:163:THR:HG22	40:BP:164:SER:N	2.36	0.41
27:BA:636:U:O2'	27:BA:637:G:O4'	2.31	0.40
28:BB:57:A:O2'	32:BF:18:ARG:NH2	2.51	0.40
30:BD:269:ILE:O	30:BD:334:ARG:HG3	2.20	0.40
41:BQ:84:TYR:HE2	41:BQ:88:LEU:HD11	1.86	0.40
42:BR:96:GLU:O	42:BR:97:ALA:HB3	2.20	0.40
27:BA:147:U:C2	27:BA:148:G:C8	3.09	0.40
27:BA:2248:G:C6	27:BA:2249:C:C6	3.10	0.40
27:BA:2763:C:H2'	27:BA:2764:G:O4'	2.21	0.40
27:BA:1524:C:OP2	27:BA:1534:U:H5	2.04	0.40
27:BA:1866:U:C2'	27:BA:1867:G:O5'	2.70	0.40
27:BA:2172:A:O2'	27:BA:2173:G:H3'	2.21	0.40
28:BB:36:C:O2	41:BQ:148:HIS:CD2	2.74	0.40
32:BF:8:ILE:HG23	32:BF:9:LEU:HD22	2.03	0.40
32:BF:18:ARG:HD3	32:BF:142:ARG:NH1	2.36	0.40
27:BA:141:G:H2'	27:BA:142:G:C8	2.57	0.40
27:BA:383:G:H2'	27:BA:384:U:O4'	2.22	0.40
27:BA:1017:G:O2'	27:BA:1021:G:O6	2.10	0.40
27:BA:1676:C:H2'	27:BA:1677:U:O4'	2.22	0.40
28:BB:25:C:H2'	28:BB:26:C:O4'	2.22	0.40
31:BE:5:VAL:HG12	31:BE:6:PHE:N	2.37	0.40
27:BA:256:A:H4'	27:BA:257:G:OP1	2.22	0.40
27:BA:2239:G:O6	27:BA:2274:G:C2	2.74	0.40
28:BB:56:U:P	32:BF:15:HIS:HE2	2.45	0.40
29:BC:99:LEU:HA	29:BC:102:ILE:HD12	2.03	0.40
32:BF:12:TRP:CE3	32:BF:13:GLU:N	2.90	0.40
34:BI:62:ILE:HG22	34:BI:63:VAL:HG13	2.02	0.40
37:BL:84:ARG:NE	37:BL:121:ALA:O	2.53	0.40
41:BQ:59:LEU:C	41:BQ:60:VAL:HG23	2.41	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%)	175 (90%)	19 (10%)	0	100	100
3	Ac	187/209 (90%)	173 (92%)	14 (8%)	0	100	100
4	Ad	188/200 (94%)	176 (94%)	12 (6%)	0	100	100
5	Ae	172/180 (96%)	166 (96%)	6 (4%)	0	100	100
6	Af	239/243 (98%)	229 (96%)	10 (4%)	0	100	100
7	Ag	219/235 (93%)	197 (90%)	22 (10%)	0	100	100
8	Ah	121/125 (97%)	113 (93%)	8 (7%)	0	100	100
9	Ai	209/215 (97%)	197 (94%)	12 (6%)	0	100	100
10	Aj	127/130 (98%)	117 (92%)	10 (8%)	0	100	100
11	Ak	123/130 (95%)	111 (90%)	12 (10%)	0	100	100
12	Al	131/135 (97%)	124 (95%)	7 (5%)	0	100	100
13	Am	98/102 (96%)	90 (92%)	8 (8%)	0	100	100
14	An	125/140 (89%)	114 (91%)	11 (9%)	0	100	100
15	Ao	141/147 (96%)	134 (95%)	7 (5%)	0	100	100
16	Ap	133/149 (89%)	114 (86%)	19 (14%)	0	100	100
17	Aq	147/151 (97%)	135 (92%)	12 (8%)	0	100	100
18	Ar	52/56 (93%)	45 (86%)	7 (14%)	0	100	100
19	As	105/114 (92%)	98 (93%)	7 (7%)	0	100	100
20	At	62/67 (92%)	56 (90%)	6 (10%)	0	100	100
21	Au	114/133 (86%)	107 (94%)	7 (6%)	0	100	100
22	Av	147/150 (98%)	143 (97%)	4 (3%)	0	100	100
23	Aw	93/98 (95%)	87 (94%)	6 (6%)	0	100	100
24	Ax	59/65 (91%)	51 (86%)	8 (14%)	0	100	100
25	Ay	62/70 (89%)	56 (90%)	6 (10%)	0	100	100
26	Az	53/62 (86%)	47 (89%)	6 (11%)	0	100	100
29	BC	235/239 (98%)	216 (92%)	19 (8%)	0	100	100
30	BD	342/346 (99%)	325 (95%)	17 (5%)	0	100	100
31	BE	253/255 (99%)	242 (96%)	11 (4%)	0	100	100
32	BF	162/183 (88%)	122 (75%)	40 (25%)	0	100	100
33	BG	181/184 (98%)	163 (90%)	18 (10%)	0	100	100
34	BH	119/123 (97%)	110 (92%)	9 (8%)	0	100	100
34	BI	119/123 (97%)	105 (88%)	14 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	BJ	164/182 (90%)	147 (90%)	17 (10%)	0	100	100
36	BK	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
37	BL	138/141 (98%)	132 (96%)	6 (4%)	0	100	100
38	BM	79/83 (95%)	65 (82%)	14 (18%)	0	100	100
38	BN	79/83 (95%)	61 (77%)	18 (23%)	0	100	100
39	BO	146/148 (99%)	130 (89%)	16 (11%)	0	100	100
40	BP	191/194 (98%)	184 (96%)	7 (4%)	0	100	100
41	BQ	158/201 (79%)	142 (90%)	16 (10%)	0	100	100
42	BR	118/121 (98%)	113 (96%)	5 (4%)	0	100	100
43	BS	144/150 (96%)	140 (97%)	4 (3%)	0	100	100
44	BT	72/77 (94%)	67 (93%)	5 (7%)	0	100	100
45	BU	94/98 (96%)	91 (97%)	3 (3%)	0	100	100
46	BV	152/156 (97%)	145 (95%)	7 (5%)	0	100	100
47	BW	83/86 (96%)	80 (96%)	3 (4%)	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%)	52 (93%)	4 (7%)	0	100	100
51	Ba	152/155 (98%)	140 (92%)	12 (8%)	0	100	100
52	Bb	94/102 (92%)	84 (89%)	10 (11%)	0	100	100
53	Bc	87/90 (97%)	80 (92%)	7 (8%)	0	100	100
54	Bd	122/125 (98%)	119 (98%)	3 (2%)	0	100	100
55	Be	87/90 (97%)	77 (88%)	10 (12%)	0	100	100
56	Bg	82/86 (95%)	76 (93%)	6 (7%)	0	100	100
57	Bh	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
58	Bi	48/51 (94%)	42 (88%)	6 (12%)	0	100	100
59	Bj	45/51 (88%)	41 (91%)	4 (9%)	0	100	100
60	Bk	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
61	Bl	91/94 (97%)	91 (100%)	0	0	100	100
All	All	7606/8020 (95%)	7033 (92%)	573 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	155/168 (92%)	155 (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	210/212 (99%)	210 (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	182/184 (99%)	182 (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	83
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
18	Ar	45/46 (98%)	45 (100%)	0	100	100
19	As	95/101 (94%)	94 (99%)	1 (1%)	73	83
20	At	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
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%)	184 (100%)	1 (0%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	BD	288/289 (100%)	287 (100%)	1 (0%)	92	96
31	BE	212/212 (100%)	211 (100%)	1 (0%)	88	93
32	BF	140/155 (90%)	137 (98%)	3 (2%)	53	68
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%)	99 (100%)	0	100	100
35	BJ	144/153 (94%)	144 (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%)	62 (98%)	1 (2%)	62	77
38	BN	63/65 (97%)	63 (100%)	0	100	100
39	BO	115/116 (99%)	115 (100%)	0	100	100
40	BP	161/162 (99%)	161 (100%)	0	100	100
41	BQ	138/167 (83%)	137 (99%)	1 (1%)	84	90
42	BR	101/102 (99%)	101 (100%)	0	100	100
43	BS	120/124 (97%)	118 (98%)	2 (2%)	60	75
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
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%)	78 (98%)	2 (2%)	47	62
56	Bg	62/63 (98%)	61 (98%)	1 (2%)	62	77
57	Bh	50/51 (98%)	50 (100%)	0	100	100
58	Bi	45/46 (98%)	44 (98%)	1 (2%)	52	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	Bj	36/38 (95%)	36 (100%)	0	100	100
60	Bk	34/35 (97%)	34 (100%)	0	100	100
61	Bl	83/84 (99%)	83 (100%)	0	100	100
All	All	6512/6738 (97%)	6496 (100%)	16 (0%)	93	97

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	An	87	ARG
19	As	7	ARG
29	BC	207	LYS
30	BD	220	LYS
31	BE	48	ARG
32	BF	57	ARG
32	BF	90	ARG
32	BF	179	LYS
38	BM	34	LEU
41	BQ	191	LYS
43	BS	21	ARG
43	BS	62	ARG
55	Be	12	ARG
55	Be	63	ARG
56	Bg	3	ARG
58	Bi	3	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
3	Ac	79	GLN
6	Af	37	HIS
9	Ai	84	HIS
9	Ai	117	GLN
12	Al	94	ASN
29	BC	186	ASN
30	BD	136	ASN
30	BD	274	ASN
32	BF	47	GLN
35	BJ	150	HIS
39	BO	84	ASN
54	Bd	83	HIS

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Mol	Chain	Res	Type
56	Bg	57	GLN
61	Bl	78	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Aa	1449/1498 (96%)	235 (16%)	0
27	BA	2928/3037 (96%)	525 (17%)	36 (1%)
28	BB	124/126 (98%)	22 (17%)	1 (0%)
All	All	4501/4661 (96%)	782 (17%)	37 (0%)

All (782) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	Aa	4	C
1	Aa	17	C
1	Aa	33	U
1	Aa	35	G
1	Aa	42	G
1	Aa	44	C
1	Aa	47	A
1	Aa	55	G
1	Aa	57	G
1	Aa	60	A
1	Aa	65	G
1	Aa	69	G
1	Aa	78	G
1	Aa	100	C
1	Aa	109	A
1	Aa	111	C
1	Aa	131	A
1	Aa	143	C
1	Aa	171	U
1	Aa	179	G
1	Aa	180	G
1	Aa	192	A
1	Aa	194	A
1	Aa	195	G
1	Aa	208	G
1	Aa	219	G
1	Aa	232	U

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Mol	Chain	Res	Type
1	Aa	233	U
1	Aa	235	G
1	Aa	239	G
1	Aa	254	G
1	Aa	255	C
1	Aa	261	A
1	Aa	268	A
1	Aa	277	C
1	Aa	279	G
1	Aa	289	G
1	Aa	294	A
1	Aa	316	C
1	Aa	317	A
1	Aa	318	C
1	Aa	319	G
1	Aa	320	G
1	Aa	327	G
1	Aa	332	A
1	Aa	335	G
1	Aa	341	A
1	Aa	354	C
1	Aa	355	C
1	Aa	360	C
1	Aa	370	A
1	Aa	372	C
1	Aa	381	G
1	Aa	385	A
1	Aa	386	C
1	Aa	394	G
1	Aa	401	C
1	Aa	415	U
1	Aa	428	A
1	Aa	431	G
1	Aa	439	A
1	Aa	440	A
1	Aa	441	U
1	Aa	442	A
1	Aa	443	A
1	Aa	451	G
1	Aa	456	G
1	Aa	457	C
1	Aa	459	G

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Mol	Chain	Res	Type
1	Aa	463	G
1	Aa	464	C
1	Aa	466	G
1	Aa	469	G
1	Aa	472	G
1	Aa	476	U
1	Aa	477	A
1	Aa	478	A
1	Aa	492	A
1	Aa	506	U
1	Aa	517	A
1	Aa	518	A
1	Aa	521	C
1	Aa	522	G
1	Aa	524	C
1	Aa	541	A
1	Aa	547	U
1	Aa	578	U
1	Aa	579	G
1	Aa	599	U
1	Aa	607	G
1	Aa	611	A
1	Aa	621	U
1	Aa	634	G
1	Aa	639	G
1	Aa	648	U
1	Aa	659	OMG
1	Aa	661	A
1	Aa	663	C
1	Aa	668	G
1	Aa	669	U
1	Aa	677	G
1	Aa	679	G
1	Aa	694	G
1	Aa	695	U
1	Aa	701	G
1	Aa	706	G
1	Aa	723	A
1	Aa	727	A
1	Aa	737	G
1	Aa	738	A
1	Aa	739	U

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Mol	Chain	Res	Type
1	Aa	740	A
1	Aa	761	A
1	Aa	763	G
1	Aa	774	A
1	Aa	787	G
1	Aa	790	U
1	Aa	810	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	896	G
1	Aa	899	C
1	Aa	911	U
1	Aa	913	OMG
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	939	G
1	Aa	942	C
1	Aa	943	G
1	Aa	947	G
1	Aa	948	C
1	Aa	961	A
1	Aa	969	G
1	Aa	970	G
1	Aa	975	G
1	Aa	979	G
1	Aa	987	G
1	Aa	994	G
1	Aa	1009	U
1	Aa	1010	C
1	Aa	1021	G
1	Aa	1035	U
1	Aa	1038	G

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Mol	Chain	Res	Type
1	Aa	1039	U
1	Aa	1045	A
1	Aa	1048	G
1	Aa	1076	U
1	Aa	1077	C
1	Aa	1079	U
1	Aa	1084	G
1	Aa	1085	C
1	Aa	1086	U
1	Aa	1093	G
1	Aa	1111	C
1	Aa	1112	G
1	Aa	1116	G
1	Aa	1118	G
1	Aa	1119	A
1	Aa	1126	G
1	Aa	1127	G
1	Aa	1135	A
1	Aa	1136	G
1	Aa	1142	G
1	Aa	1148	A
1	Aa	1149	G
1	Aa	1157	U
1	Aa	1162	C
1	Aa	1163	G
1	Aa	1164	A
1	Aa	1169	C
1	Aa	1171	C
1	Aa	1176	U
1	Aa	1179	A
1	Aa	1181	G
1	Aa	1185	G
1	Aa	1190	A
1	Aa	1193	G
1	Aa	1200	A
1	Aa	1208	A
1	Aa	1209	U
1	Aa	1212	G
1	Aa	1214	C
1	Aa	1221	A
1	Aa	1222	G
1	Aa	1230	G

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Mol	Chain	Res	Type
1	Aa	1232	A
1	Aa	1251	A
1	Aa	1252	G
1	Aa	1254	U
1	Aa	1272	C
1	Aa	1292	A
1	Aa	1297	U
1	Aa	1299	G
1	Aa	1305	G
1	Aa	1316	U
1	Aa	1322	G
1	Aa	1331	G
1	Aa	1346	A
1	Aa	1349	C
1	Aa	1350	A
1	Aa	1355	C
1	Aa	1371	G
1	Aa	1374	G
1	Aa	1378	C
1	Aa	1400	U
1	Aa	1401	C
1	Aa	1402	G
1	Aa	1403	G
1	Aa	1407	G
1	Aa	1423	G
1	Aa	1430	U
1	Aa	1434	G
1	Aa	1436	G
1	Aa	1441	A
1	Aa	1442	A
1	Aa	1446	G
1	Aa	1448	A
1	Aa	1451	A
1	Aa	1453	G
1	Aa	1455	U
1	Aa	1466	G
1	Aa	1475	G
1	Aa	1478	C
1	Aa	1479	G
1	Aa	1480	A
27	BA	12	C
27	BA	18	C

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Mol	Chain	Res	Type
27	BA	19	A
27	BA	20	A
27	BA	21	C
27	BA	22	U
27	BA	33	G
27	BA	43	C
27	BA	52	G
27	BA	55	C
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	127	A
27	BA	128	U
27	BA	129	G
27	BA	132	A
27	BA	133	C
27	BA	135	U
27	BA	139	G
27	BA	141	G
27	BA	148	G
27	BA	149	C
27	BA	150	C
27	BA	153	A
27	BA	156	C
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	206	G
27	BA	207	A
27	BA	212	A
27	BA	213	A
27	BA	219	A
27	BA	220	A
27	BA	221	G

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Mol	Chain	Res	Type
27	BA	224	A
27	BA	239	G
27	BA	257	G
27	BA	269	C
27	BA	279	A
27	BA	280	A
27	BA	282	G
27	BA	285	U
27	BA	295	U
27	BA	301	U
27	BA	302	G
27	BA	303	U
27	BA	311	G
27	BA	312	C
27	BA	315	A
27	BA	316	G
27	BA	317	G
27	BA	323	U
27	BA	325	G
27	BA	332	A
27	BA	333	G
27	BA	340	U
27	BA	341	C
27	BA	342	5MC
27	BA	350	C
27	BA	360	G
27	BA	363	A
27	BA	368	G
27	BA	369	A
27	BA	370	A
27	BA	377	G
27	BA	382	C
27	BA	385	A
27	BA	393	G
27	BA	398	C
27	BA	399	C
27	BA	401	G
27	BA	405	U
27	BA	407	U
27	BA	408	C
27	BA	411	U
27	BA	414	G

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Mol	Chain	Res	Type
27	BA	429	U
27	BA	430	A
27	BA	432	C
27	BA	440	A
27	BA	444	U
27	BA	445	G
27	BA	460	C
27	BA	476	C
27	BA	494	C
27	BA	496	A
27	BA	505	A2M
27	BA	506	G
27	BA	520	G
27	BA	531	G
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	580	G
27	BA	581	A
27	BA	584	G
27	BA	589	G
27	BA	610	G
27	BA	623	G
27	BA	626	C
27	BA	629	G
27	BA	635	G
27	BA	654	C
27	BA	666	A
27	BA	670	G
27	BA	677	A
27	BA	689	C
27	BA	694	A
27	BA	707	C
27	BA	708	A
27	BA	729	C
27	BA	732	A
27	BA	733	C
27	BA	747	G

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Mol	Chain	Res	Type
27	BA	748	U
27	BA	764	G
27	BA	794	A
27	BA	801	A
27	BA	802	A
27	BA	812	U
27	BA	823	G
27	BA	827	G
27	BA	832	A
27	BA	842	C
27	BA	844	G
27	BA	847	G
27	BA	849	A2M
27	BA	852	G
27	BA	853	A
27	BA	856	C
27	BA	870	U
27	BA	875	5MC
27	BA	886	C
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	960	G
27	BA	978	A
27	BA	988	G
27	BA	995	A
27	BA	998	G
27	BA	1001	U
27	BA	1003	G
27	BA	1005	G
27	BA	1006	G

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Mol	Chain	Res	Type
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	1020	A
27	BA	1021	G
27	BA	1023	C
27	BA	1025	C
27	BA	1026	C
27	BA	1028	G
27	BA	1029	C
27	BA	1031	C
27	BA	1033	C
27	BA	1035	G
27	BA	1039	A
27	BA	1041	C
27	BA	1048	C
27	BA	1055	C
27	BA	1076	G
27	BA	1077	G
27	BA	1090	G
27	BA	1102	G
27	BA	1103	A
27	BA	1117	G
27	BA	1118	A
27	BA	1119	C
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	1166	G
27	BA	1167	U
27	BA	1171	U
27	BA	1177	U
27	BA	1179	G

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Mol	Chain	Res	Type
27	BA	1182	A
27	BA	1183	G
27	BA	1184	C
27	BA	1241	C
27	BA	1242	G
27	BA	1243	A
27	BA	1244	G
27	BA	1249	G
27	BA	1262	U
27	BA	1264	G
27	BA	1266	C
27	BA	1267	G
27	BA	1270	G
27	BA	1273	U
27	BA	1306	G
27	BA	1307	A
27	BA	1308	U
27	BA	1309	U
27	BA	1310	G
27	BA	1318	A
27	BA	1320	C
27	BA	1322	G
27	BA	1336	C
27	BA	1347	G
27	BA	1361	A
27	BA	1362	G
27	BA	1372	A
27	BA	1373	C
27	BA	1391	C
27	BA	1409	A
27	BA	1410	U
27	BA	1425	C
27	BA	1436	U
27	BA	1437	A
27	BA	1456	C
27	BA	1485	C
27	BA	1487	U
27	BA	1490	C
27	BA	1506	G
27	BA	1517	A
27	BA	1521	A
27	BA	1527	G

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Mol	Chain	Res	Type
27	BA	1533	A
27	BA	1556	G
27	BA	1563	C
27	BA	1568	G
27	BA	1581	C
27	BA	1606	A
27	BA	1609	A
27	BA	1625	U
27	BA	1637	G
27	BA	1638	U
27	BA	1639	G
27	BA	1640	C
27	BA	1656	C
27	BA	1657	G
27	BA	1658	G
27	BA	1662	A
27	BA	1664	A
27	BA	1670	A
27	BA	1671	A
27	BA	1672	U
27	BA	1681	G
27	BA	1682	U
27	BA	1683	A
27	BA	1685	G
27	BA	1692	U
27	BA	1694	C
27	BA	1699	A
27	BA	1706	G
27	BA	1715	A
27	BA	1734	U
27	BA	1743	A
27	BA	1752	A
27	BA	1754	A
27	BA	1755	A
27	BA	1761	A
27	BA	1762	C
27	BA	1767	G
27	BA	1768	C
27	BA	1769	C
27	BA	1772	U
27	BA	1792	U
27	BA	1793	G

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Mol	Chain	Res	Type
27	BA	1794	U
27	BA	1795	C
27	BA	1800	G
27	BA	1801	A
27	BA	1802	A
27	BA	1822	G
27	BA	1841	U
27	BA	1848	A
27	BA	1851	G
27	BA	1852	G
27	BA	1859	G
27	BA	1860	C
27	BA	1861	G
27	BA	1877	G
27	BA	1884	G
27	BA	1891	G
27	BA	1892	G
27	BA	1901	A
27	BA	1908	A
27	BA	1914	A
27	BA	1928	C
27	BA	1929	U
27	BA	1930	A
27	BA	1940	G
27	BA	1945	OMG
27	BA	1951	G
27	BA	1957	A
27	BA	1977	U
27	BA	1991	A
27	BA	2004	G
27	BA	2014	A
27	BA	2018	C
27	BA	2019	G
27	BA	2022	G
27	BA	2026	A
27	BA	2027	C
27	BA	2028	U
27	BA	2030	U
27	BA	2036	U
27	BA	2043	G
27	BA	2049	A
27	BA	2051	A

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Mol	Chain	Res	Type
27	BA	2053	U
27	BA	2067	A
27	BA	2068	U
27	BA	2069	G
27	BA	2076	U
27	BA	2080	U
27	BA	2083	A
27	BA	2084	U
27	BA	2085	G
27	BA	2104	U
27	BA	2105	G
27	BA	2106	U
27	BA	2118	G
27	BA	2123	G
27	BA	2135	C
27	BA	2143	A
27	BA	2144	U
27	BA	2145	A2M
27	BA	2153	G
27	BA	2163	G
27	BA	2167	A
27	BA	2173	G
27	BA	2174	A
27	BA	2175	C
27	BA	2181	G
27	BA	2205	G
27	BA	2213	G
27	BA	2214	C
27	BA	2215	G
27	BA	2216	G
27	BA	2219	G
27	BA	2220	G
27	BA	2222	G
27	BA	2223	C
27	BA	2224	G
27	BA	2227	G
27	BA	2230	U
27	BA	2232	G
27	BA	2238	A
27	BA	2240	G
27	BA	2241	C
27	BA	2242	G

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Mol	Chain	Res	Type
27	BA	2244	C
27	BA	2245	G
27	BA	2246	A
27	BA	2247	A
27	BA	2248	G
27	BA	2256	U
27	BA	2258	C
27	BA	2259	G
27	BA	2261	G
27	BA	2267	U
27	BA	2268	G
27	BA	2269	G
27	BA	2270	A
27	BA	2273	C
27	BA	2275	C
27	BA	2276	C
27	BA	2277	C
27	BA	2280	G
27	BA	2282	G
27	BA	2283	A
27	BA	2284	C
27	BA	2285	A
27	BA	2292	A
27	BA	2294	C
27	BA	2296	U
27	BA	2299	G
27	BA	2310	A
27	BA	2317	G
27	BA	2318	G
27	BA	2319	A
27	BA	2320	A
27	BA	2321	G
27	BA	2325	G
27	BA	2327	A
27	BA	2336	G
27	BA	2340	G
27	BA	2341	G
27	BA	2353	OMG
27	BA	2359	C
27	BA	2360	A
27	BA	2361	C
27	BA	2369	A

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Mol	Chain	Res	Type
27	BA	2379	OMG
27	BA	2382	G
27	BA	2385	G
27	BA	2386	C
27	BA	2390	A
27	BA	2406	G
27	BA	2408	U
27	BA	2412	G
27	BA	2413	A
27	BA	2414	A
27	BA	2423	A
27	BA	2424	G
27	BA	2425	A
27	BA	2428	G
27	BA	2438	A
27	BA	2439	A
27	BA	2448	G
27	BA	2450	C
27	BA	2453	G
27	BA	2460	A
27	BA	2484	A
27	BA	2489	G
27	BA	2491	C
27	BA	2497	G
27	BA	2498	A
27	BA	2531	G
27	BA	2535	G
27	BA	2536	A
27	BA	2545	OMC
27	BA	2549	G
27	BA	2552	A
27	BA	2563	G
27	BA	2568	G
27	BA	2572	G
27	BA	2573	A
27	BA	2574	G
27	BA	2579	C
27	BA	2580	A
27	BA	2581	U
27	BA	2585	G
27	BA	2596	U
27	BA	2598	G

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Mol	Chain	Res	Type
27	BA	2602	C
27	BA	2606	G
27	BA	2607	C
27	BA	2609	G
27	BA	2610	U
27	BA	2622	A
27	BA	2623	U
27	BA	2633	G
27	BA	2638	A
27	BA	2669	A
27	BA	2670	A
27	BA	2671	G
27	BA	2682	G
27	BA	2686	G
27	BA	2689	U
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	2725	G
27	BA	2733	U
27	BA	2734	G
27	BA	2749	A
27	BA	2750	G
27	BA	2778	G
27	BA	2794	U
27	BA	2815	U
27	BA	2817	G
27	BA	2829	C
27	BA	2836	G
27	BA	2837	C
27	BA	2853	G
27	BA	2857	C
27	BA	2859	A
27	BA	2860	A
27	BA	2867	A
27	BA	2868	G
27	BA	2878	A
27	BA	2879	A
27	BA	2882	C

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Mol	Chain	Res	Type
27	BA	2884	G
27	BA	2935	G
27	BA	2938	G
27	BA	2959	U
27	BA	2961	A
27	BA	2974	G
27	BA	2990	A
27	BA	3001	C
27	BA	3007	G
27	BA	3008	C
27	BA	3013	C
27	BA	3014	C
27	BA	3018	C
27	BA	3023	C
27	BA	3027	U
27	BA	3028	G
27	BA	3030	U
27	BA	3031	A
27	BA	3032	C
28	BB	5	C
28	BB	9	G
28	BB	13	A
28	BB	25	C
28	BB	27	A
28	BB	30	C
28	BB	32	C
28	BB	33	G
28	BB	34	G
28	BB	35	U
28	BB	36	C
28	BB	38	C
28	BB	41	U
28	BB	42	U
28	BB	52	A
28	BB	57	A
28	BB	66	A
28	BB	76	G
28	BB	79	G
28	BB	89	C
28	BB	115	G
28	BB	121	G

All (37) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	BA	108	U
27	BA	147	U
27	BA	148	G
27	BA	187	A
27	BA	190	A
27	BA	331	A
27	BA	404	G
27	BA	410	C
27	BA	892	A
27	BA	912	OMG
27	BA	1178	A
27	BA	1181	C
27	BA	1182	A
27	BA	1360	G
27	BA	1636	A
27	BA	1670	A
27	BA	1671	A
27	BA	1681	G
27	BA	1691	U
27	BA	1753	G
27	BA	1754	A
27	BA	1767	G
27	BA	1928	C
27	BA	2173	G
27	BA	2218	G
27	BA	2239	G
27	BA	2246	A
27	BA	2267	U
27	BA	2496	C
27	BA	2534	A
27	BA	2536	A
27	BA	2595	C
27	BA	2836	G
27	BA	2858	U
27	BA	2881	A
27	BA	3022	C
28	BB	56	U

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

81 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	$\#\|Z\| > 2$
27	A2M	BA	2145	27	18,25,26	4.12	8 (44%)	18,36,39	2.86	3 (16%)
27	OMG	BA	2672	27	18,26,27	2.25	7 (38%)	19,38,41	1.37	3 (15%)
1	MA6	Aa	1467	1	18,26,27	1.10	1 (5%)	19,38,41	3.13	2 (10%)
1	OMG	Aa	913	1	18,26,27	2.37	8 (44%)	19,38,41	1.46	3 (15%)
1	OMC	Aa	1354	1	19,22,23	2.82	8 (42%)	26,31,34	0.81	0
27	OMG	BA	2745	27	18,26,27	2.22	7 (38%)	19,38,41	1.35	3 (15%)
27	OMU	BA	1969	27	19,22,23	2.91	7 (36%)	26,31,34	1.78	6 (23%)
27	OMU	BA	2542	27	19,22,23	2.86	7 (36%)	26,31,34	1.60	5 (19%)
1	OMG	Aa	446	1	18,26,27	2.27	7 (38%)	19,38,41	1.34	3 (15%)
27	5MC	BA	2075	27	18,22,23	3.27	7 (38%)	26,32,35	0.94	0
27	OMC	BA	1820	27	19,22,23	2.70	7 (36%)	26,31,34	0.99	2 (7%)
27	OMG	BA	2550	27	18,26,27	2.21	7 (38%)	19,38,41	1.25	2 (10%)
1	4AC	Aa	1459	1	21,24,25	3.00	11 (52%)	29,34,37	1.08	3 (10%)
27	OMG	BA	2016	27	18,26,27	2.22	7 (38%)	19,38,41	1.24	3 (15%)
27	A2M	BA	872	27	18,25,26	4.07	8 (44%)	18,36,39	2.80	3 (16%)
1	5MC	Aa	1352	1	18,22,23	3.43	7 (38%)	26,32,35	1.00	2 (7%)
27	OMG	BA	1953	27	18,26,27	2.18	7 (38%)	19,38,41	1.35	3 (15%)
27	OMG	BA	491	27	18,26,27	2.11	7 (38%)	19,38,41	1.50	4 (21%)
27	5MC	BA	342	27	18,22,23	3.37	7 (38%)	26,32,35	0.98	2 (7%)
1	6MZ	Aa	1449	1	18,25,26	0.84	1 (5%)	16,36,39	2.14	4 (25%)
1	4AC	Aa	458	1	21,24,25	1.07	1 (4%)	29,34,37	1.13	3 (10%)
27	A2M	BA	1109	27	18,25,26	4.13	7 (38%)	18,36,39	3.09	4 (22%)
27	OMU	BA	1905	27	19,22,23	2.76	8 (42%)	26,31,34	1.55	5 (19%)
27	OMG	BA	2115	27	18,26,27	2.15	6 (33%)	19,38,41	1.23	3 (15%)
27	5MC	BA	2120	27	18,22,23	3.07	7 (38%)	26,32,35	1.28	3 (11%)
27	OMG	BA	215	27	18,26,27	2.29	8 (44%)	19,38,41	1.36	3 (15%)
1	5MC	Aa	854	1	18,22,23	0.96	2 (11%)	26,32,35	1.27	3 (11%)
1	OMG	Aa	498	1	18,26,27	2.23	8 (44%)	19,38,41	1.37	3 (15%)
27	5MC	BA	2055	27	18,22,23	3.41	7 (38%)	26,32,35	1.23	4 (15%)
27	OMG	BA	1129	27	18,26,27	2.22	8 (44%)	19,38,41	1.31	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
27	OMG	BA	912	27	18,26,27	2.19	7 (38%)	19,38,41	1.86	5 (26%)
27	OMG	BA	2010	27	18,26,27	2.23	7 (38%)	19,38,41	1.28	3 (15%)
27	OMU	BA	2656	27	19,22,23	2.91	7 (36%)	26,31,34	1.71	5 (19%)
27	OMC	BA	1709	27	19,22,23	2.82	7 (36%)	26,31,34	0.83	0
1	4AC	Aa	730	1	21,24,25	3.21	10 (47%)	29,34,37	0.96	2 (6%)
27	OMC	BA	2786	27	19,22,23	2.63	7 (36%)	26,31,34	0.93	1 (3%)
27	A2M	BA	879	27	18,25,26	4.03	7 (38%)	18,36,39	3.06	3 (16%)
27	OMG	BA	674	27	18,26,27	2.12	6 (33%)	19,38,41	1.24	3 (15%)
27	A2M	BA	61	27	18,25,26	4.10	7 (38%)	18,36,39	3.10	5 (27%)
27	OMG	BA	2613	27	18,26,27	2.16	8 (44%)	19,38,41	1.30	3 (15%)
1	OMG	Aa	658	1	18,26,27	2.28	7 (38%)	19,38,41	1.60	5 (26%)
27	OMC	BA	869	27	19,22,23	2.62	7 (36%)	26,31,34	1.06	2 (7%)
27	5MC	BA	1965	27	18,22,23	3.31	7 (38%)	26,32,35	0.95	3 (11%)
27	OMG	BA	2353	27	18,26,27	2.47	8 (44%)	19,38,41	1.48	4 (21%)
27	OMC	BA	2545	27	19,22,23	2.70	7 (36%)	26,31,34	0.81	1 (3%)
1	OMG	Aa	852	1	18,26,27	2.16	7 (38%)	19,38,41	1.38	3 (15%)
1	4AC	Aa	5	1	21,24,25	3.15	10 (47%)	29,34,37	0.93	2 (6%)
27	OMG	BA	668	27	18,26,27	2.21	7 (38%)	19,38,41	1.31	3 (15%)
27	OMC	BA	2047	27	19,22,23	2.69	7 (36%)	26,31,34	0.88	0
1	OMG	Aa	529	1	18,26,27	2.18	7 (38%)	19,38,41	1.26	3 (15%)
27	OMU	BA	1949	27	19,22,23	2.85	7 (36%)	26,31,34	1.66	5 (19%)
27	OMU	BA	1776	27	19,22,23	2.86	7 (36%)	26,31,34	1.62	6 (23%)
27	OMC	BA	2876	27	19,22,23	2.72	7 (36%)	26,31,34	1.00	0
27	OMC	BA	1721	27	19,22,23	2.71	7 (36%)	26,31,34	0.97	0
27	OMG	BA	800	27	18,26,27	2.16	7 (38%)	19,38,41	1.37	4 (21%)
27	OMG	BA	943	27	18,26,27	2.23	7 (38%)	19,38,41	1.75	6 (31%)
27	4SU	BA	2553	27	18,21,22	4.08	8 (44%)	26,30,33	1.94	5 (19%)
27	OMG	BA	63	27	18,26,27	2.26	8 (44%)	19,38,41	1.40	4 (21%)
27	OMU	BA	657	27	19,22,23	2.80	7 (36%)	26,31,34	1.67	4 (15%)
27	OMU	BA	453	27	19,22,23	2.90	7 (36%)	26,31,34	1.71	5 (19%)
27	OMC	BA	477	27	19,22,23	2.88	7 (36%)	26,31,34	0.97	1 (3%)
27	5MC	BA	875	27	18,22,23	3.33	7 (38%)	26,32,35	1.22	6 (23%)
1	5MC	Aa	672	1	18,22,23	3.25	7 (38%)	26,32,35	1.00	2 (7%)
27	OMG	BA	1945	27	18,26,27	2.15	7 (38%)	19,38,41	1.48	3 (15%)
27	OMU	BA	1623	27	19,22,23	2.85	8 (42%)	26,31,34	1.65	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	OMU	Aa	8	1	19,22,23	2.82	7 (36%)	26,31,34	1.80	5 (19%)
1	MA6	Aa	1468	1	18,26,27	1.14	2 (11%)	19,38,41	3.36	2 (10%)
27	OMG	BA	65	27	18,26,27	2.19	7 (38%)	19,38,41	1.43	4 (21%)
27	OMG	BA	2528	27	18,26,27	2.33	8 (44%)	19,38,41	1.31	3 (15%)
27	A2M	BA	849	27	18,25,26	4.13	6 (33%)	18,36,39	2.96	3 (16%)
1	LV2	Aa	918	1	20,23,24	0.91	0	26,33,36	0.77	0
1	A2M	Aa	352	1	18,25,26	4.17	6 (33%)	18,36,39	3.14	3 (16%)
1	OMG	Aa	450	1	18,26,27	1.06	1 (5%)	19,38,41	1.07	2 (10%)
27	OMG	BA	833	27	18,26,27	2.23	7 (38%)	19,38,41	1.34	3 (15%)
27	LHH	BA	501	27	22,25,26	2.41	4 (18%)	29,35,38	1.23	4 (13%)
1	5MU	Aa	917	1	19,22,23	1.40	5 (26%)	28,32,35	2.18	6 (21%)
1	OMG	Aa	548	1	18,26,27	2.31	8 (44%)	19,38,41	1.40	3 (15%)
27	A2M	BA	505	27	18,25,26	4.24	8 (44%)	18,36,39	3.12	3 (16%)
1	OMG	Aa	659	1	18,26,27	2.29	8 (44%)	19,38,41	1.33	3 (15%)
27	OMG	BA	2379	27	18,26,27	2.17	7 (38%)	19,38,41	1.36	4 (21%)
27	A2M	BA	932	27	18,25,26	4.14	7 (38%)	18,36,39	3.02	3 (16%)

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
27	A2M	BA	2145	27	-	0/5/27/28	0/3/3/3
27	OMG	BA	2672	27	-	2/5/27/28	0/3/3/3
1	MA6	Aa	1467	1	-	0/7/29/30	0/3/3/3
1	OMG	Aa	913	1	-	2/5/27/28	0/3/3/3
1	OMC	Aa	1354	1	-	0/9/27/28	0/2/2/2
27	OMG	BA	2745	27	-	0/5/27/28	0/3/3/3
27	OMU	BA	1969	27	-	0/9/27/28	0/2/2/2
27	OMU	BA	2542	27	-	0/9/27/28	0/2/2/2
1	OMG	Aa	446	1	-	1/5/27/28	0/3/3/3
27	5MC	BA	2075	27	-	2/7/25/26	0/2/2/2
27	OMC	BA	1820	27	-	0/9/27/28	0/2/2/2
27	OMG	BA	2550	27	-	0/5/27/28	0/3/3/3
1	4AC	Aa	1459	1	-	0/11/29/30	0/2/2/2
27	OMG	BA	2016	27	-	0/5/27/28	0/3/3/3
27	A2M	BA	872	27	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	Aa	1352	1	-	0/7/25/26	0/2/2/2
27	OMG	BA	1953	27	-	1/5/27/28	0/3/3/3
27	OMG	BA	491	27	-	1/5/27/28	0/3/3/3
27	5MC	BA	342	27	-	2/7/25/26	0/2/2/2
1	6MZ	Aa	1449	1	-	0/5/27/28	0/3/3/3
1	4AC	Aa	458	1	-	3/11/29/30	0/2/2/2
27	A2M	BA	1109	27	-	0/5/27/28	0/3/3/3
27	OMU	BA	1905	27	-	0/9/27/28	0/2/2/2
27	OMG	BA	2115	27	-	1/5/27/28	0/3/3/3
27	5MC	BA	2120	27	-	0/7/25/26	0/2/2/2
27	OMG	BA	215	27	-	0/5/27/28	0/3/3/3
1	5MC	Aa	854	1	-	0/7/25/26	0/2/2/2
1	OMG	Aa	498	1	-	0/5/27/28	0/3/3/3
27	5MC	BA	2055	27	-	0/7/25/26	0/2/2/2
27	OMG	BA	1129	27	-	0/5/27/28	0/3/3/3
27	OMG	BA	912	27	-	0/5/27/28	0/3/3/3
27	OMG	BA	2010	27	-	0/5/27/28	0/3/3/3
27	OMU	BA	2656	27	-	0/9/27/28	0/2/2/2
27	OMC	BA	1709	27	-	0/9/27/28	0/2/2/2
1	4AC	Aa	730	1	-	0/11/29/30	0/2/2/2
27	OMC	BA	2786	27	-	2/9/27/28	0/2/2/2
27	A2M	BA	879	27	-	0/5/27/28	0/3/3/3
27	OMG	BA	674	27	-	2/5/27/28	0/3/3/3
27	A2M	BA	61	27	-	2/5/27/28	0/3/3/3
27	OMG	BA	2613	27	-	0/5/27/28	0/3/3/3
1	OMG	Aa	658	1	-	0/5/27/28	0/3/3/3
27	OMC	BA	869	27	-	2/9/27/28	0/2/2/2
27	5MC	BA	1965	27	-	0/7/25/26	0/2/2/2
27	OMG	BA	2353	27	-	2/5/27/28	0/3/3/3
27	OMC	BA	2545	27	-	1/9/27/28	0/2/2/2
1	OMG	Aa	852	1	-	1/5/27/28	0/3/3/3
1	4AC	Aa	5	1	-	2/11/29/30	0/2/2/2
27	OMG	BA	668	27	-	1/5/27/28	0/3/3/3
27	OMC	BA	2047	27	-	0/9/27/28	0/2/2/2
1	OMG	Aa	529	1	-	0/5/27/28	0/3/3/3
27	OMU	BA	1949	27	-	0/9/27/28	0/2/2/2
27	OMU	BA	1776	27	-	0/9/27/28	0/2/2/2
27	OMC	BA	2876	27	-	0/9/27/28	0/2/2/2
27	OMC	BA	1721	27	-	0/9/27/28	0/2/2/2
27	OMG	BA	800	27	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	OMG	BA	943	27	-	0/5/27/28	0/3/3/3
27	4SU	BA	2553	27	-	0/7/25/26	0/2/2/2
27	OMG	BA	63	27	-	0/5/27/28	0/3/3/3
27	OMU	BA	657	27	-	0/9/27/28	0/2/2/2
27	OMU	BA	453	27	-	0/9/27/28	0/2/2/2
27	OMC	BA	477	27	-	0/9/27/28	0/2/2/2
27	5MC	BA	875	27	-	2/7/25/26	0/2/2/2
1	5MC	Aa	672	1	-	0/7/25/26	0/2/2/2
27	OMG	BA	1945	27	-	2/5/27/28	0/3/3/3
27	OMU	BA	1623	27	-	2/9/27/28	0/2/2/2
1	OMU	Aa	8	1	-	3/9/27/28	0/2/2/2
1	MA6	Aa	1468	1	-	1/7/29/30	0/3/3/3
27	OMG	BA	65	27	-	2/5/27/28	0/3/3/3
27	OMG	BA	2528	27	-	0/5/27/28	0/3/3/3
27	A2M	BA	849	27	-	2/5/27/28	0/3/3/3
1	LV2	Aa	918	1	-	2/9/29/30	0/2/2/2
1	A2M	Aa	352	1	-	0/5/27/28	0/3/3/3
1	OMG	Aa	450	1	-	0/5/27/28	0/3/3/3
27	OMG	BA	833	27	-	0/5/27/28	0/3/3/3
27	LHH	BA	501	27	-	0/13/31/32	0/2/2/2
1	5MU	Aa	917	1	-	0/7/25/26	0/2/2/2
1	OMG	Aa	548	1	-	0/5/27/28	0/3/3/3
27	A2M	BA	505	27	-	2/5/27/28	0/3/3/3
1	OMG	Aa	659	1	-	2/5/27/28	0/3/3/3
27	OMG	BA	2379	27	-	3/5/27/28	0/3/3/3
27	A2M	BA	932	27	-	0/5/27/28	0/3/3/3

All (544) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	505	A2M	O4'-C1'	14.94	1.61	1.41
1	Aa	352	A2M	O4'-C1'	14.90	1.61	1.41
27	BA	1109	A2M	O4'-C1'	14.81	1.61	1.41
27	BA	849	A2M	O4'-C1'	14.79	1.61	1.41
27	BA	932	A2M	O4'-C1'	14.68	1.61	1.41
27	BA	2145	A2M	O4'-C1'	14.42	1.61	1.41
27	BA	61	A2M	O4'-C1'	14.36	1.61	1.41
27	BA	872	A2M	O4'-C1'	14.35	1.61	1.41
27	BA	879	A2M	O4'-C1'	14.22	1.60	1.41
27	BA	2553	4SU	C2-N1	8.76	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	1965	5MC	C6-C5	8.50	1.48	1.34
1	Aa	1352	5MC	C6-C5	8.48	1.48	1.34
27	BA	501	LHH	O2-C2	8.45	1.39	1.23
27	BA	342	5MC	C6-C5	8.44	1.48	1.34
27	BA	2075	5MC	C6-C5	8.29	1.48	1.34
27	BA	2055	5MC	C6-C5	8.28	1.48	1.34
1	Aa	672	5MC	C6-C5	8.16	1.48	1.34
27	BA	875	5MC	C6-C5	8.12	1.47	1.34
27	BA	2553	4SU	C4-N3	7.65	1.45	1.37
27	BA	1969	OMU	C2-N1	7.11	1.49	1.38
27	BA	2120	5MC	C6-C5	7.09	1.46	1.34
27	BA	2542	OMU	C2-N1	7.04	1.49	1.38
27	BA	2553	4SU	C2-N3	6.92	1.50	1.38
27	BA	1776	OMU	C2-N1	6.89	1.49	1.38
1	Aa	730	4AC	C4-N3	6.88	1.44	1.32
27	BA	657	OMU	C2-N1	6.78	1.49	1.38
27	BA	1949	OMU	C2-N1	6.76	1.49	1.38
1	Aa	5	4AC	C4-N3	6.74	1.44	1.32
27	BA	2656	OMU	C2-N1	6.71	1.49	1.38
27	BA	453	OMU	C2-N1	6.71	1.49	1.38
27	BA	505	A2M	O4'-C4'	-6.65	1.30	1.45
27	BA	61	A2M	O4'-C4'	-6.65	1.30	1.45
27	BA	932	A2M	O4'-C4'	-6.60	1.30	1.45
27	BA	1623	OMU	C2-N1	6.52	1.48	1.38
1	Aa	352	A2M	O4'-C4'	-6.52	1.30	1.45
1	Aa	1459	4AC	C4-N3	6.51	1.44	1.32
27	BA	879	A2M	O4'-C4'	-6.51	1.30	1.45
27	BA	2145	A2M	O4'-C4'	-6.48	1.30	1.45
1	Aa	1352	5MC	C4-N3	6.45	1.45	1.34
27	BA	2656	OMU	C2-N3	6.45	1.49	1.38
27	BA	2553	4SU	C5-C4	6.44	1.50	1.42
1	Aa	8	OMU	C2-N1	6.40	1.48	1.38
27	BA	1905	OMU	C2-N1	6.38	1.48	1.38
27	BA	872	A2M	O4'-C4'	-6.37	1.30	1.45
27	BA	477	OMC	C2-N3	6.33	1.49	1.36
27	BA	1109	A2M	O4'-C4'	-6.31	1.30	1.45
27	BA	453	OMU	C2-N3	6.29	1.49	1.38
27	BA	1623	OMU	C2-N3	6.26	1.49	1.38
27	BA	2553	4SU	C6-C5	6.24	1.49	1.35
27	BA	875	5MC	C4-N3	6.23	1.44	1.34
27	BA	2055	5MC	C4-N3	6.22	1.44	1.34
27	BA	1969	OMU	C2-N3	6.21	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	849	A2M	O4'-C4'	-6.20	1.31	1.45
27	BA	1949	OMU	C2-N3	6.19	1.49	1.38
1	Aa	730	4AC	C6-C5	6.18	1.49	1.35
27	BA	342	5MC	C4-N3	6.17	1.44	1.34
1	Aa	8	OMU	C2-N3	6.10	1.48	1.38
27	BA	1709	OMC	C2-N3	6.08	1.48	1.36
1	Aa	5	4AC	C6-C5	6.07	1.49	1.35
27	BA	1776	OMU	C2-N3	6.05	1.48	1.38
1	Aa	1352	5MC	C2-N3	6.00	1.48	1.36
27	BA	2542	OMU	C2-N3	5.97	1.48	1.38
27	BA	2120	5MC	C4-N3	5.94	1.44	1.34
1	Aa	1354	OMC	C2-N3	5.90	1.48	1.36
1	Aa	672	5MC	C4-N3	5.90	1.44	1.34
27	BA	2075	5MC	C4-N3	5.89	1.44	1.34
27	BA	2055	5MC	C2-N3	5.85	1.48	1.36
27	BA	1820	OMC	C2-N3	5.82	1.48	1.36
27	BA	1965	5MC	C4-N3	5.82	1.44	1.34
27	BA	1721	OMC	C2-N3	5.81	1.48	1.36
27	BA	342	5MC	C2-N3	5.77	1.48	1.36
27	BA	657	OMU	C2-N3	5.77	1.48	1.38
27	BA	1905	OMU	C2-N3	5.77	1.48	1.38
27	BA	2047	OMC	C2-N3	5.76	1.48	1.36
27	BA	875	5MC	C2-N3	5.71	1.47	1.36
27	BA	2876	OMC	C2-N3	5.67	1.47	1.36
27	BA	869	OMC	C2-N3	5.65	1.47	1.36
27	BA	2786	OMC	C2-N3	5.61	1.47	1.36
1	Aa	1459	4AC	C6-C5	5.60	1.48	1.35
27	BA	2075	5MC	C2-N3	5.56	1.47	1.36
27	BA	2545	OMC	C6-C5	5.54	1.47	1.35
27	BA	2120	5MC	C2-N3	5.53	1.47	1.36
27	BA	2545	OMC	C2-N3	5.50	1.47	1.36
27	BA	2353	OMG	C2-N3	5.50	1.46	1.33
1	Aa	672	5MC	C2-N3	5.48	1.47	1.36
27	BA	477	OMC	C6-C5	5.45	1.47	1.35
1	Aa	1354	OMC	C6-C5	5.42	1.47	1.35
27	BA	1709	OMC	C6-C5	5.42	1.47	1.35
27	BA	1965	5MC	C2-N3	5.40	1.47	1.36
1	Aa	913	OMG	C2-N3	5.39	1.46	1.33
1	Aa	8	OMU	C6-C5	5.38	1.47	1.35
27	BA	2656	OMU	C6-C5	5.31	1.47	1.35
27	BA	453	OMU	C6-C5	5.31	1.47	1.35
27	BA	2786	OMC	C6-C5	5.23	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	658	OMG	C2-N3	5.22	1.45	1.33
27	BA	2528	OMG	C2-N3	5.21	1.45	1.33
27	BA	1969	OMU	C6-C5	5.20	1.47	1.35
27	BA	1623	OMU	C6-C5	5.20	1.47	1.35
27	BA	2047	OMC	C6-C5	5.19	1.47	1.35
1	Aa	548	OMG	C2-N3	5.12	1.45	1.33
1	Aa	659	OMG	C2-N3	5.12	1.45	1.33
27	BA	943	OMG	C2-N3	5.11	1.45	1.33
27	BA	215	OMG	C2-N3	5.08	1.45	1.33
27	BA	2055	5MC	C6-N1	5.07	1.46	1.38
27	BA	1776	OMU	C6-C5	5.03	1.46	1.35
27	BA	2876	OMC	C6-C5	5.02	1.46	1.35
27	BA	668	OMG	C2-N3	5.02	1.45	1.33
1	Aa	446	OMG	C2-N3	5.02	1.45	1.33
27	BA	2016	OMG	C2-N3	5.01	1.45	1.33
27	BA	1820	OMC	C6-C5	4.99	1.46	1.35
27	BA	2672	OMG	C2-N3	4.98	1.45	1.33
27	BA	2550	OMG	C2-N3	4.98	1.45	1.33
27	BA	1721	OMC	C6-C5	4.98	1.46	1.35
1	Aa	498	OMG	C2-N3	4.97	1.45	1.33
27	BA	657	OMU	C6-C5	4.95	1.46	1.35
1	Aa	5	4AC	C2-N1	4.95	1.50	1.40
27	BA	833	OMG	C2-N3	4.95	1.45	1.33
27	BA	63	OMG	C2-N3	4.95	1.45	1.33
27	BA	2115	OMG	C2-N3	4.94	1.45	1.33
27	BA	2010	OMG	C2-N3	4.92	1.45	1.33
27	BA	2745	OMG	C2-N3	4.92	1.45	1.33
27	BA	912	OMG	C2-N3	4.92	1.45	1.33
1	Aa	852	OMG	C2-N3	4.92	1.45	1.33
27	BA	2542	OMU	C6-C5	4.92	1.46	1.35
27	BA	477	OMC	C4-N3	4.91	1.44	1.34
27	BA	65	OMG	C2-N3	4.90	1.45	1.33
1	Aa	529	OMG	C2-N3	4.90	1.45	1.33
27	BA	2876	OMC	C4-N3	4.89	1.44	1.34
1	Aa	730	4AC	C2-N1	4.89	1.50	1.40
27	BA	1949	OMU	C6-C5	4.88	1.46	1.35
27	BA	1129	OMG	C2-N3	4.87	1.45	1.33
1	Aa	1354	OMC	C4-N3	4.87	1.44	1.34
27	BA	1709	OMC	C4-N3	4.86	1.44	1.34
27	BA	1905	OMU	C6-C5	4.84	1.46	1.35
27	BA	1953	OMG	C2-N3	4.83	1.44	1.33
27	BA	1945	OMG	C2-N3	4.79	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2613	OMG	C2-N3	4.78	1.44	1.33
27	BA	674	OMG	C2-N3	4.78	1.44	1.33
1	Aa	730	4AC	C7-N4	4.77	1.46	1.37
27	BA	800	OMG	C2-N3	4.77	1.44	1.33
27	BA	869	OMC	C4-N3	4.77	1.44	1.34
27	BA	2379	OMG	C2-N3	4.75	1.44	1.33
27	BA	477	OMC	C4-N4	4.72	1.45	1.33
27	BA	2353	OMG	C4-N3	4.70	1.48	1.37
27	BA	1721	OMC	C4-N3	4.69	1.44	1.34
1	Aa	1459	4AC	C7-N4	4.66	1.45	1.37
1	Aa	730	4AC	C2-N3	4.66	1.45	1.36
27	BA	1820	OMC	C4-N3	4.65	1.43	1.34
27	BA	2528	OMG	C4-N3	4.64	1.48	1.37
27	BA	491	OMG	C2-N3	4.63	1.44	1.33
1	Aa	5	4AC	C2-N3	4.61	1.45	1.36
1	Aa	1459	4AC	C2-N1	4.61	1.50	1.40
27	BA	2047	OMC	C4-N3	4.58	1.43	1.34
27	BA	869	OMC	C6-C5	4.57	1.45	1.35
1	Aa	5	4AC	C7-N4	4.57	1.45	1.37
1	Aa	913	OMG	C4-N3	4.56	1.48	1.37
27	BA	2016	OMG	C4-N3	4.54	1.48	1.37
27	BA	501	LHH	C7-N4	4.53	1.45	1.37
1	Aa	659	OMG	C4-N3	4.51	1.48	1.37
1	Aa	658	OMG	C4-N3	4.49	1.48	1.37
27	BA	1709	OMC	C4-N4	4.49	1.44	1.33
1	Aa	548	OMG	C4-N3	4.47	1.48	1.37
27	BA	215	OMG	C4-N3	4.47	1.48	1.37
27	BA	2786	OMC	C4-N3	4.44	1.43	1.34
27	BA	477	OMC	C2-N1	4.43	1.49	1.40
27	BA	943	OMG	C4-N3	4.42	1.48	1.37
27	BA	1820	OMC	C2-N1	4.41	1.49	1.40
27	BA	833	OMG	C4-N3	4.40	1.48	1.37
27	BA	2553	4SU	C4-S4	-4.39	1.60	1.68
27	BA	63	OMG	C4-N3	4.38	1.48	1.37
1	Aa	1354	OMC	C2-N1	4.38	1.49	1.40
27	BA	875	5MC	C2-N1	4.38	1.49	1.40
1	Aa	1354	OMC	C4-N4	4.38	1.44	1.33
27	BA	869	OMC	C2-N1	4.38	1.49	1.40
27	BA	668	OMG	C4-N3	4.37	1.48	1.37
27	BA	2745	OMG	C4-N3	4.37	1.48	1.37
27	BA	2545	OMC	C4-N3	4.37	1.43	1.34
1	Aa	446	OMG	C4-N3	4.35	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2010	OMG	C4-N3	4.32	1.47	1.37
27	BA	1721	OMC	C2-N1	4.32	1.49	1.40
27	BA	2672	OMG	C4-N3	4.31	1.47	1.37
27	BA	2545	OMC	C2-N1	4.31	1.49	1.40
1	Aa	1459	4AC	C2-N3	4.28	1.45	1.36
1	Aa	498	OMG	C4-N3	4.27	1.47	1.37
27	BA	1721	OMC	C4-N4	4.27	1.44	1.33
27	BA	2876	OMC	C2-N1	4.27	1.49	1.40
27	BA	1129	OMG	C4-N3	4.26	1.47	1.37
27	BA	1965	5MC	C6-N1	4.25	1.45	1.38
27	BA	1709	OMC	C2-N1	4.25	1.49	1.40
27	BA	912	OMG	C4-N3	4.24	1.47	1.37
27	BA	65	OMG	C4-N3	4.22	1.47	1.37
27	BA	2550	OMG	C4-N3	4.21	1.47	1.37
1	Aa	1352	5MC	C2-N1	4.20	1.49	1.40
27	BA	2115	OMG	C4-N3	4.19	1.47	1.37
1	Aa	1352	5MC	C4-N4	4.18	1.45	1.34
27	BA	674	OMG	C4-N3	4.18	1.47	1.37
1	Aa	852	OMG	C4-N3	4.17	1.47	1.37
27	BA	342	5MC	C2-N1	4.16	1.49	1.40
27	BA	2075	5MC	C6-N1	4.15	1.45	1.38
27	BA	342	5MC	C6-N1	4.13	1.45	1.38
1	Aa	1352	5MC	C6-N1	4.12	1.45	1.38
27	BA	2120	5MC	C2-N1	4.11	1.48	1.40
27	BA	1945	OMG	C4-N3	4.10	1.47	1.37
1	Aa	672	5MC	C2-N1	4.10	1.48	1.40
27	BA	2379	OMG	C4-N3	4.09	1.47	1.37
27	BA	2047	OMC	C4-N4	4.09	1.43	1.33
27	BA	875	5MC	C6-N1	4.08	1.45	1.38
27	BA	2613	OMG	C4-N3	4.08	1.47	1.37
27	BA	1820	OMC	C4-N4	4.08	1.43	1.33
27	BA	2047	OMC	C2-N1	4.07	1.48	1.40
27	BA	2055	5MC	C2-N1	4.06	1.48	1.40
27	BA	2876	OMC	C4-N4	4.06	1.43	1.33
27	BA	2786	OMC	C2-N1	4.06	1.48	1.40
27	BA	1949	OMU	C4-N3	4.06	1.45	1.38
1	Aa	730	4AC	C4-N4	4.05	1.45	1.39
27	BA	2545	OMC	C4-N4	4.04	1.43	1.33
27	BA	491	OMG	C4-N3	4.04	1.47	1.37
27	BA	1953	OMG	C4-N3	4.01	1.47	1.37
27	BA	800	OMG	C4-N3	4.00	1.47	1.37
1	Aa	529	OMG	C4-N3	3.99	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	342	5MC	C4-N4	3.96	1.44	1.34
27	BA	1965	5MC	C2-N1	3.94	1.48	1.40
27	BA	2353	OMG	C2-N2	3.94	1.43	1.34
1	Aa	672	5MC	C6-N1	3.93	1.44	1.38
27	BA	453	OMU	C4-N3	3.93	1.45	1.38
1	Aa	730	4AC	CM7-C7	3.86	1.58	1.50
27	BA	2075	5MC	C2-N1	3.84	1.48	1.40
27	BA	1905	OMU	C4-N3	3.84	1.45	1.38
1	Aa	5	4AC	C4-N4	3.81	1.45	1.39
27	BA	1969	OMU	C4-N3	3.74	1.45	1.38
27	BA	1623	OMU	C4-N3	3.74	1.45	1.38
27	BA	2656	OMU	C4-N3	3.72	1.45	1.38
27	BA	1965	5MC	C4-N4	3.71	1.43	1.34
1	Aa	5	4AC	CM7-C7	3.68	1.58	1.50
27	BA	875	5MC	C4-N4	3.67	1.43	1.34
27	BA	2055	5MC	C4-N4	3.67	1.43	1.34
27	BA	2528	OMG	C2-N2	3.66	1.42	1.34
1	Aa	672	5MC	C4-N4	3.66	1.43	1.34
1	Aa	1459	4AC	CM7-C7	3.64	1.58	1.50
27	BA	215	OMG	C2-N2	3.60	1.42	1.34
1	Aa	913	OMG	C2-N2	3.60	1.42	1.34
27	BA	2075	5MC	C4-N4	3.60	1.43	1.34
27	BA	869	OMC	C4-N4	3.59	1.42	1.33
27	BA	2542	OMU	C4-N3	3.58	1.45	1.38
1	Aa	730	4AC	C5-C4	3.58	1.48	1.40
27	BA	1776	OMU	C4-N3	3.57	1.44	1.38
27	BA	657	OMU	O4-C4	-3.56	1.17	1.24
1	Aa	5	4AC	C5-C4	3.56	1.48	1.40
27	BA	2786	OMC	C4-N4	3.55	1.42	1.33
1	Aa	8	OMU	C4-N3	3.54	1.44	1.38
27	BA	2120	5MC	C6-N1	3.54	1.44	1.38
27	BA	1776	OMU	O4-C4	-3.54	1.17	1.24
27	BA	2542	OMU	O4-C4	-3.51	1.17	1.24
27	BA	2353	OMG	C6-N1	3.48	1.43	1.37
27	BA	2656	OMU	O4-C4	-3.48	1.17	1.24
1	Aa	659	OMG	C2-N2	3.45	1.42	1.34
1	Aa	446	OMG	C2-N2	3.42	1.42	1.34
27	BA	501	LHH	C4-N4	3.41	1.44	1.39
27	BA	1905	OMU	O4-C4	-3.40	1.17	1.24
27	BA	1969	OMU	O4-C4	-3.39	1.17	1.24
1	Aa	658	OMG	C2-N2	3.38	1.42	1.34
27	BA	657	OMU	C4-N3	3.37	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	1949	OMU	O4-C4	-3.35	1.18	1.24
27	BA	63	OMG	C2-N2	3.35	1.42	1.34
27	BA	505	A2M	O5'-C5'	-3.35	1.36	1.44
27	BA	1965	5MC	O2-C2	-3.34	1.17	1.23
1	Aa	548	OMG	C2-N2	3.33	1.42	1.34
27	BA	2010	OMG	C2-N2	3.33	1.42	1.34
27	BA	1129	OMG	C2-N2	3.32	1.42	1.34
27	BA	2550	OMG	C2-N2	3.32	1.42	1.34
27	BA	2545	OMC	O2-C2	-3.31	1.17	1.23
27	BA	2120	5MC	O2-C2	-3.30	1.17	1.23
27	BA	2672	OMG	C2-N2	3.30	1.42	1.34
27	BA	501	LHH	C2-N3	3.29	1.43	1.36
27	BA	2786	OMC	O2-C2	-3.25	1.17	1.23
1	Aa	8	OMU	O4-C4	-3.25	1.18	1.24
27	BA	2120	5MC	C4-N4	3.25	1.42	1.34
27	BA	833	OMG	C2-N2	3.25	1.41	1.34
27	BA	2379	OMG	C2-N2	3.24	1.41	1.34
27	BA	1623	OMU	O4-C4	-3.24	1.18	1.24
1	Aa	672	5MC	O2-C2	-3.24	1.17	1.23
1	Aa	1459	4AC	C4-N4	3.22	1.44	1.39
27	BA	2745	OMG	C2-N2	3.22	1.41	1.34
27	BA	875	5MC	O2-C2	-3.21	1.17	1.23
1	Aa	498	OMG	C2-N2	3.21	1.41	1.34
27	BA	2075	5MC	O2-C2	-3.20	1.17	1.23
27	BA	2876	OMC	O2-C2	-3.18	1.17	1.23
1	Aa	913	OMG	C6-N1	3.18	1.42	1.37
27	BA	2016	OMG	C2-N2	3.18	1.41	1.34
27	BA	872	A2M	C5-C4	-3.18	1.32	1.40
27	BA	65	OMG	C2-N2	3.16	1.41	1.34
1	Aa	529	OMG	C2-N2	3.16	1.41	1.34
27	BA	453	OMU	O4-C4	-3.15	1.18	1.24
27	BA	1953	OMG	C2-N2	3.15	1.41	1.34
27	BA	2047	OMC	O2-C2	-3.12	1.17	1.23
27	BA	2145	A2M	C5-C4	-3.12	1.32	1.40
27	BA	869	OMC	O2-C2	-3.09	1.18	1.23
27	BA	943	OMG	C2-N2	3.09	1.41	1.34
27	BA	61	A2M	C5-C4	-3.09	1.32	1.40
27	BA	912	OMG	O6-C6	-3.07	1.17	1.23
27	BA	1820	OMC	O2-C2	-3.07	1.18	1.23
27	BA	491	OMG	O6-C6	-3.06	1.17	1.23
27	BA	1945	OMG	O6-C6	-3.05	1.17	1.23
1	Aa	548	OMG	C6-N1	3.03	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2055	5MC	O2-C2	-3.03	1.18	1.23
27	BA	491	OMG	C5-C4	-3.02	1.35	1.43
1	Aa	1459	4AC	C5-C4	3.01	1.47	1.40
27	BA	657	OMU	O2-C2	-3.01	1.17	1.23
27	BA	2553	4SU	O2-C2	-3.00	1.17	1.23
1	Aa	450	OMG	C6-N1	-3.00	1.33	1.37
27	BA	912	OMG	C2-N2	2.99	1.41	1.34
1	Aa	852	OMG	C2-N2	2.99	1.41	1.34
1	Aa	446	OMG	C6-N1	2.99	1.42	1.37
27	BA	1953	OMG	O6-C6	-2.99	1.17	1.23
27	BA	1721	OMC	O2-C2	-2.98	1.18	1.23
27	BA	849	A2M	C5-C4	-2.98	1.33	1.40
27	BA	505	A2M	C5-C4	-2.98	1.33	1.40
27	BA	668	OMG	C2-N2	2.97	1.41	1.34
27	BA	342	5MC	O2-C2	-2.96	1.18	1.23
27	BA	932	A2M	C5-C4	-2.96	1.33	1.40
1	Aa	352	A2M	C5-C4	-2.95	1.33	1.40
27	BA	800	OMG	C2-N2	2.95	1.41	1.34
27	BA	65	OMG	O6-C6	-2.95	1.17	1.23
27	BA	61	A2M	O2'-C2'	2.95	1.50	1.42
27	BA	65	OMG	C5-C4	-2.94	1.35	1.43
1	Aa	1468	MA6	C5-C4	-2.94	1.33	1.40
27	BA	2550	OMG	O6-C6	-2.94	1.17	1.23
27	BA	1709	OMC	O2-C2	-2.94	1.18	1.23
1	Aa	352	A2M	C6-N6	2.94	1.44	1.34
1	Aa	529	OMG	O6-C6	-2.93	1.17	1.23
27	BA	2672	OMG	O6-C6	-2.93	1.17	1.23
27	BA	477	OMC	C6-N1	2.93	1.45	1.38
27	BA	2613	OMG	C2-N2	2.93	1.41	1.34
27	BA	668	OMG	C5-C4	-2.92	1.35	1.43
27	BA	1776	OMU	O2-C2	-2.92	1.17	1.23
27	BA	2745	OMG	O6-C6	-2.92	1.17	1.23
1	Aa	1354	OMC	O2-C2	-2.92	1.18	1.23
27	BA	1109	A2M	C5-C4	-2.92	1.33	1.40
1	Aa	498	OMG	C6-N1	2.91	1.42	1.37
27	BA	1905	OMU	O2-C2	-2.91	1.17	1.23
27	BA	674	OMG	O6-C6	-2.90	1.17	1.23
27	BA	668	OMG	O6-C6	-2.90	1.17	1.23
27	BA	215	OMG	O6-C6	-2.90	1.17	1.23
1	Aa	852	OMG	O6-C6	-2.89	1.17	1.23
1	Aa	852	OMG	C5-C4	-2.89	1.35	1.43
27	BA	833	OMG	O6-C6	-2.89	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	1945	OMG	C2-N2	2.88	1.41	1.34
27	BA	453	OMU	C6-N1	2.88	1.44	1.38
27	BA	800	OMG	O6-C6	-2.88	1.17	1.23
1	Aa	1354	OMC	C6-N1	2.88	1.44	1.38
27	BA	2115	OMG	O6-C6	-2.88	1.17	1.23
27	BA	2542	OMU	O2-C2	-2.87	1.17	1.23
27	BA	2613	OMG	C5-C4	-2.87	1.35	1.43
1	Aa	1467	MA6	C5-C4	-2.86	1.33	1.40
27	BA	1709	OMC	C6-N1	2.86	1.44	1.38
1	Aa	917	5MU	C4-N3	-2.85	1.33	1.38
1	Aa	446	OMG	C5-C4	-2.84	1.35	1.43
27	BA	1129	OMG	C6-N1	2.84	1.42	1.37
1	Aa	1459	4AC	O7-C7	-2.84	1.16	1.23
27	BA	879	A2M	C5-C4	-2.84	1.33	1.40
27	BA	2745	OMG	C5-C4	-2.84	1.35	1.43
27	BA	2672	OMG	C5-C4	-2.84	1.35	1.43
27	BA	63	OMG	O6-C6	-2.83	1.17	1.23
27	BA	2115	OMG	C2-N2	2.83	1.40	1.34
27	BA	2379	OMG	C5-C4	-2.83	1.35	1.43
27	BA	1820	OMC	C6-N1	2.83	1.44	1.38
1	Aa	658	OMG	C6-N1	2.83	1.42	1.37
27	BA	2613	OMG	O6-C6	-2.83	1.17	1.23
27	BA	1969	OMU	O2-C2	-2.83	1.17	1.23
27	BA	1949	OMU	O2-C2	-2.83	1.17	1.23
27	BA	63	OMG	C5-C4	-2.82	1.35	1.43
27	BA	1953	OMG	C5-C6	2.82	1.53	1.47
1	Aa	8	OMU	O2-C2	-2.82	1.17	1.23
27	BA	800	OMG	C5-C4	-2.82	1.35	1.43
1	Aa	659	OMG	C6-N1	2.82	1.42	1.37
27	BA	1953	OMG	C5-C4	-2.82	1.35	1.43
27	BA	2047	OMC	C6-N1	2.82	1.44	1.38
27	BA	2016	OMG	O6-C6	-2.82	1.17	1.23
27	BA	215	OMG	C5-C4	-2.81	1.35	1.43
27	BA	2010	OMG	C6-N1	2.81	1.42	1.37
27	BA	674	OMG	C5-C4	-2.81	1.35	1.43
1	Aa	458	4AC	C4-N4	-2.80	1.35	1.39
27	BA	674	OMG	C2-N2	2.80	1.40	1.34
27	BA	2528	OMG	C6-N1	2.79	1.42	1.37
1	Aa	548	OMG	O6-C6	-2.79	1.17	1.23
27	BA	2528	OMG	O6-C6	-2.78	1.17	1.23
27	BA	2010	OMG	O6-C6	-2.78	1.17	1.23
27	BA	2115	OMG	C5-C4	-2.78	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	659	OMG	O6-C6	-2.78	1.17	1.23
27	BA	491	OMG	C2-N2	2.78	1.40	1.34
27	BA	2876	OMC	C6-N1	2.78	1.44	1.38
27	BA	477	OMC	O2-C2	-2.78	1.18	1.23
27	BA	1623	OMU	O2-C2	-2.77	1.18	1.23
1	Aa	548	OMG	C5-C6	2.77	1.53	1.47
27	BA	1721	OMC	C6-N1	2.77	1.44	1.38
27	BA	833	OMG	C5-C6	2.76	1.53	1.47
27	BA	1129	OMG	O6-C6	-2.76	1.17	1.23
27	BA	879	A2M	C6-N6	2.76	1.44	1.34
1	Aa	529	OMG	C5-C4	-2.76	1.36	1.43
27	BA	912	OMG	C5-C4	-2.75	1.36	1.43
27	BA	63	OMG	C6-N1	2.75	1.42	1.37
27	BA	833	OMG	C5-C4	-2.75	1.36	1.43
27	BA	2379	OMG	O6-C6	-2.75	1.17	1.23
27	BA	1129	OMG	C5-C4	-2.74	1.36	1.43
27	BA	2672	OMG	C5-C6	2.74	1.53	1.47
1	Aa	1352	5MC	O2-C2	-2.74	1.18	1.23
27	BA	2016	OMG	C5-C4	-2.74	1.36	1.43
27	BA	2010	OMG	C5-C4	-2.73	1.36	1.43
27	BA	943	OMG	O6-C6	-2.73	1.17	1.23
27	BA	2545	OMC	C6-N1	2.73	1.44	1.38
27	BA	2379	OMG	C5-C6	2.73	1.53	1.47
1	Aa	498	OMG	O6-C6	-2.73	1.17	1.23
27	BA	2528	OMG	C5-C4	-2.73	1.36	1.43
27	BA	453	OMU	O2-C2	-2.73	1.18	1.23
27	BA	2550	OMG	C5-C4	-2.73	1.36	1.43
1	Aa	352	A2M	O2'-C2'	2.72	1.49	1.42
27	BA	932	A2M	O3'-C3'	-2.72	1.36	1.43
27	BA	2656	OMU	O2-C2	-2.72	1.18	1.23
27	BA	1945	OMG	C5-C4	-2.72	1.36	1.43
27	BA	849	A2M	C6-N6	2.71	1.43	1.34
1	Aa	854	5MC	C6-N1	-2.71	1.33	1.38
1	Aa	446	OMG	C5-C6	2.71	1.52	1.47
27	BA	869	OMC	C6-N1	2.71	1.44	1.38
27	BA	2115	OMG	C5-C6	2.71	1.52	1.47
27	BA	2786	OMC	C6-N1	2.70	1.44	1.38
1	Aa	548	OMG	C5-C4	-2.70	1.36	1.43
27	BA	61	A2M	O3'-C3'	-2.70	1.36	1.43
1	Aa	498	OMG	C5-C4	-2.69	1.36	1.43
27	BA	1109	A2M	O3'-C3'	-2.69	1.36	1.43
27	BA	2145	A2M	O3'-C3'	-2.69	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2353	OMG	C5-C6	2.68	1.52	1.47
27	BA	849	A2M	O2'-C2'	2.68	1.49	1.42
1	Aa	659	OMG	C5-C4	-2.67	1.36	1.43
1	Aa	913	OMG	C5-C4	-2.67	1.36	1.43
1	Aa	658	OMG	C5-C6	2.67	1.52	1.47
27	BA	800	OMG	C6-N1	2.66	1.41	1.37
27	BA	2353	OMG	O6-C6	-2.66	1.17	1.23
1	Aa	529	OMG	C6-N1	2.66	1.41	1.37
1	Aa	913	OMG	C5-C6	2.66	1.52	1.47
27	BA	2656	OMU	C6-N1	2.65	1.44	1.38
27	BA	2745	OMG	C6-N1	2.65	1.41	1.37
1	Aa	529	OMG	C5-C6	2.65	1.52	1.47
27	BA	943	OMG	C5-C4	-2.64	1.36	1.43
1	Aa	446	OMG	O6-C6	-2.64	1.17	1.23
27	BA	943	OMG	C5-C6	2.63	1.52	1.47
1	Aa	352	A2M	O3'-C3'	-2.62	1.36	1.43
1	Aa	658	OMG	C5-C4	-2.62	1.36	1.43
27	BA	2010	OMG	C5-C6	2.61	1.52	1.47
27	BA	2016	OMG	C5-C6	2.61	1.52	1.47
1	Aa	913	OMG	O6-C6	-2.61	1.18	1.23
27	BA	2145	A2M	C6-N6	2.60	1.43	1.34
27	BA	63	OMG	C5-C6	2.60	1.52	1.47
27	BA	1776	OMU	C6-N1	2.60	1.44	1.38
27	BA	932	A2M	C6-N6	2.59	1.43	1.34
27	BA	2353	OMG	C2-N1	2.59	1.44	1.37
27	BA	1129	OMG	C5-C6	2.59	1.52	1.47
27	BA	657	OMU	C6-N1	2.59	1.44	1.38
27	BA	61	A2M	C6-N6	2.58	1.43	1.34
27	BA	800	OMG	C5-C6	2.58	1.52	1.47
1	Aa	658	OMG	O6-C6	-2.58	1.18	1.23
27	BA	491	OMG	C6-N1	2.57	1.41	1.37
1	Aa	659	OMG	C5-C6	2.57	1.52	1.47
27	BA	912	OMG	C5-C6	2.57	1.52	1.47
27	BA	505	A2M	O3'-C3'	-2.56	1.36	1.43
27	BA	2353	OMG	C5-C4	-2.56	1.36	1.43
27	BA	879	A2M	O3'-C3'	-2.56	1.36	1.43
27	BA	879	A2M	O2'-C2'	2.56	1.49	1.42
27	BA	2542	OMU	C6-N1	2.55	1.44	1.38
27	BA	2613	OMG	C6-N1	2.55	1.41	1.37
27	BA	1623	OMU	C6-N1	2.55	1.44	1.38
1	Aa	8	OMU	C6-N1	2.55	1.44	1.38
1	Aa	730	4AC	O7-C7	-2.55	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	668	OMG	C5-C6	2.54	1.52	1.47
27	BA	872	A2M	C6-N6	2.54	1.43	1.34
1	Aa	5	4AC	O7-C7	-2.53	1.17	1.23
1	Aa	498	OMG	C5-C6	2.53	1.52	1.47
27	BA	872	A2M	O2'-C2'	2.53	1.49	1.42
27	BA	833	OMG	C6-N1	2.53	1.41	1.37
27	BA	2550	OMG	C5-C6	2.52	1.52	1.47
27	BA	1945	OMG	C5-C6	2.52	1.52	1.47
27	BA	2145	A2M	O2'-C2'	2.51	1.49	1.42
1	Aa	917	5MU	C6-N1	-2.50	1.33	1.38
27	BA	505	A2M	C6-N6	2.50	1.43	1.34
27	BA	2528	OMG	C5-C6	2.49	1.52	1.47
27	BA	2613	OMG	C5-C6	2.49	1.52	1.47
27	BA	215	OMG	C6-N1	2.49	1.41	1.37
27	BA	1945	OMG	C6-N1	2.49	1.41	1.37
27	BA	943	OMG	C6-N1	2.47	1.41	1.37
27	BA	65	OMG	C6-N1	2.46	1.41	1.37
27	BA	849	A2M	O3'-C3'	-2.46	1.37	1.43
27	BA	2550	OMG	C6-N1	2.45	1.41	1.37
27	BA	2016	OMG	C6-N1	2.45	1.41	1.37
27	BA	932	A2M	O2'-C2'	2.44	1.48	1.42
27	BA	2745	OMG	C5-C6	2.43	1.52	1.47
27	BA	1109	A2M	C6-N6	2.43	1.42	1.34
27	BA	505	A2M	O2'-C2'	2.43	1.48	1.42
27	BA	2145	A2M	O5'-C5'	-2.42	1.38	1.44
27	BA	2553	4SU	C6-N1	2.42	1.43	1.38
27	BA	215	OMG	C5-C6	2.41	1.52	1.47
27	BA	1969	OMU	C6-N1	2.41	1.43	1.38
27	BA	674	OMG	C5-C6	2.41	1.52	1.47
27	BA	1109	A2M	O2'-C2'	2.40	1.48	1.42
1	Aa	917	5MU	C6-C5	2.39	1.38	1.34
27	BA	1905	OMU	C6-N1	2.37	1.43	1.38
1	Aa	852	OMG	C5-C6	2.35	1.52	1.47
27	BA	912	OMG	C6-N1	2.34	1.41	1.37
27	BA	2379	OMG	C6-N1	2.33	1.41	1.37
1	Aa	917	5MU	C2-N3	-2.31	1.33	1.38
27	BA	1953	OMG	C6-N1	2.30	1.41	1.37
27	BA	872	A2M	O3'-C3'	-2.29	1.37	1.43
27	BA	1949	OMU	C6-N1	2.29	1.43	1.38
27	BA	2672	OMG	C6-N1	2.28	1.41	1.37
1	Aa	913	OMG	C2-N1	2.27	1.43	1.37
27	BA	668	OMG	C6-N1	2.25	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	1459	4AC	O2-C2	-2.24	1.19	1.23
27	BA	491	OMG	C5-C6	2.24	1.52	1.47
27	BA	872	A2M	O5'-C5'	-2.23	1.39	1.44
27	BA	65	OMG	C5-C6	2.23	1.51	1.47
1	Aa	1459	4AC	C6-N1	2.23	1.43	1.38
1	Aa	852	OMG	C6-N1	2.22	1.41	1.37
1	Aa	854	5MC	C6-C5	2.21	1.38	1.34
27	BA	215	OMG	C2-N1	2.20	1.43	1.37
27	BA	1109	A2M	O5'-C5'	-2.19	1.39	1.44
1	Aa	1468	MA6	C2-N3	2.18	1.35	1.32
27	BA	2145	A2M	C5-N7	-2.18	1.31	1.39
27	BA	879	A2M	O5'-C5'	-2.17	1.39	1.44
1	Aa	548	OMG	C2-N1	2.14	1.43	1.37
1	Aa	5	4AC	C6-N1	2.13	1.43	1.38
1	Aa	730	4AC	C6-N1	2.12	1.43	1.38
1	Aa	1449	6MZ	C5-C4	2.12	1.46	1.40
27	BA	932	A2M	O5'-C5'	-2.10	1.39	1.44
27	BA	2528	OMG	C2-N1	2.09	1.42	1.37
1	Aa	498	OMG	C2-N1	2.08	1.42	1.37
1	Aa	1354	OMC	C5-C4	2.07	1.47	1.42
27	BA	1623	OMU	C5-C4	2.07	1.48	1.43
27	BA	63	OMG	C2-N1	2.05	1.42	1.37
27	BA	61	A2M	O5'-C5'	-2.04	1.39	1.44
1	Aa	659	OMG	C2-N1	2.04	1.42	1.37
27	BA	505	A2M	C5-N7	-2.04	1.32	1.39
27	BA	872	A2M	C5-N7	-2.04	1.32	1.39
27	BA	2613	OMG	C2-N1	2.01	1.42	1.37
1	Aa	917	5MU	C4-C5	2.01	1.48	1.44
27	BA	1129	OMG	C2-N1	2.01	1.42	1.37
27	BA	1905	OMU	C5-C4	2.00	1.48	1.43

All (253) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Aa	1468	MA6	N1-C6-N6	-13.55	102.80	117.06
1	Aa	1467	MA6	N1-C6-N6	-12.53	103.87	117.06
1	Aa	352	A2M	C5-C6-N6	9.73	135.14	120.35
27	BA	1109	A2M	C5-C6-N6	9.49	134.77	120.35
27	BA	505	A2M	C5-C6-N6	9.37	134.59	120.35
27	BA	932	A2M	C5-C6-N6	9.35	134.56	120.35
27	BA	879	A2M	C5-C6-N6	9.29	134.47	120.35
27	BA	849	A2M	C5-C6-N6	9.21	134.35	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BA	2145	A2M	C5-C6-N6	8.98	134.00	120.35
27	BA	61	A2M	C5-C6-N6	8.98	134.00	120.35
27	BA	872	A2M	C5-C6-N6	8.48	133.24	120.35
27	BA	1109	A2M	N6-C6-N1	-7.10	103.83	118.57
1	Aa	1449	6MZ	C2-N1-C6	6.96	122.56	116.59
27	BA	505	A2M	N6-C6-N1	-6.81	104.44	118.57
27	BA	932	A2M	N6-C6-N1	-6.72	104.62	118.57
1	Aa	352	A2M	N6-C6-N1	-6.68	104.71	118.57
27	BA	2553	4SU	C4-N3-C2	-6.62	120.91	127.34
27	BA	879	A2M	N6-C6-N1	-6.58	104.92	118.57
27	BA	61	A2M	N6-C6-N1	-6.52	105.05	118.57
27	BA	849	A2M	N6-C6-N1	-6.50	105.08	118.57
27	BA	872	A2M	N6-C6-N1	-6.13	105.85	118.57
27	BA	2145	A2M	N6-C6-N1	-6.08	105.96	118.57
1	Aa	917	5MU	C4-N3-C2	-5.35	120.42	127.35
1	Aa	352	A2M	N3-C2-N1	-5.26	120.46	128.68
27	BA	61	A2M	N3-C2-N1	-5.24	120.48	128.68
27	BA	879	A2M	N3-C2-N1	-5.12	120.67	128.68
1	Aa	8	OMU	C4-N3-C2	-5.09	119.86	126.58
27	BA	932	A2M	N3-C2-N1	-5.08	120.74	128.68
1	Aa	1468	MA6	N3-C2-N1	-5.03	120.82	128.68
27	BA	849	A2M	N3-C2-N1	-4.99	120.88	128.68
27	BA	1623	OMU	C4-N3-C2	-4.94	120.06	126.58
1	Aa	917	5MU	N3-C2-N1	4.93	121.44	114.89
1	Aa	1467	MA6	N3-C2-N1	-4.93	120.97	128.68
27	BA	2656	OMU	C4-N3-C2	-4.91	120.10	126.58
27	BA	1969	OMU	C4-N3-C2	-4.89	120.13	126.58
27	BA	453	OMU	C4-N3-C2	-4.87	120.16	126.58
1	Aa	917	5MU	C5-C4-N3	4.81	119.41	115.31
27	BA	505	A2M	N3-C2-N1	-4.78	121.21	128.68
27	BA	872	A2M	N3-C2-N1	-4.73	121.28	128.68
27	BA	1109	A2M	N3-C2-N1	-4.71	121.31	128.68
27	BA	657	OMU	C4-N3-C2	-4.64	120.45	126.58
27	BA	1905	OMU	C4-N3-C2	-4.57	120.55	126.58
27	BA	1949	OMU	C4-N3-C2	-4.54	120.59	126.58
27	BA	2145	A2M	N3-C2-N1	-4.42	121.77	128.68
27	BA	2542	OMU	C4-N3-C2	-4.29	120.92	126.58
1	Aa	8	OMU	N3-C2-N1	4.23	120.50	114.89
27	BA	1969	OMU	N3-C2-N1	4.19	120.46	114.89
27	BA	1776	OMU	C4-N3-C2	-4.11	121.16	126.58
27	BA	912	OMG	O3'-C3'-C4'	4.11	122.93	111.05
1	Aa	917	5MU	O4-C4-C5	-4.09	120.16	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BA	453	OMU	N3-C2-N1	4.01	120.22	114.89
27	BA	2553	4SU	C5-C4-N3	3.97	118.37	114.69
27	BA	2553	4SU	N3-C2-N1	3.87	120.03	114.89
27	BA	2656	OMU	N3-C2-N1	3.81	119.95	114.89
27	BA	943	OMG	O3'-C3'-C2'	3.79	121.92	111.17
27	BA	657	OMU	N3-C2-N1	3.78	119.91	114.89
27	BA	1776	OMU	N3-C2-N1	3.76	119.88	114.89
1	Aa	917	5MU	C5-C6-N1	-3.72	119.51	123.34
27	BA	1949	OMU	O4-C4-C5	-3.57	118.88	125.16
1	Aa	854	5MC	C5-C6-N1	-3.52	119.72	123.34
27	BA	1623	OMU	N3-C2-N1	3.50	119.53	114.89
27	BA	912	OMG	O3'-C3'-C2'	3.49	121.08	111.17
27	BA	1905	OMU	N3-C2-N1	3.47	119.50	114.89
27	BA	2353	OMG	C5-C6-N1	3.40	119.96	113.95
27	BA	2055	5MC	O4'-C1'-N1	3.37	116.08	108.36
27	BA	2542	OMU	O4-C4-C5	-3.32	119.32	125.16
27	BA	2542	OMU	N3-C2-N1	3.30	119.27	114.89
1	Aa	913	OMG	C5-C6-N1	3.30	119.78	113.95
1	Aa	1449	6MZ	N3-C2-N1	-3.27	123.56	128.68
27	BA	2656	OMU	O4-C4-C5	-3.24	119.46	125.16
1	Aa	658	OMG	C5-C6-N1	3.21	119.62	113.95
27	BA	1623	OMU	C5-C4-N3	3.21	119.64	114.84
1	Aa	548	OMG	C5-C6-N1	3.20	119.60	113.95
27	BA	1945	OMG	C5-C6-N1	3.20	119.59	113.95
27	BA	2656	OMU	C5-C4-N3	3.18	119.59	114.84
27	BA	657	OMU	O4-C4-C5	-3.17	119.59	125.16
27	BA	943	OMG	O3'-C3'-C4'	3.13	120.10	111.05
27	BA	453	OMU	O4-C4-C5	-3.10	119.72	125.16
27	BA	2120	5MC	CM5-C5-C6	-3.09	118.72	122.85
27	BA	1945	OMG	C2-N1-C6	-3.09	119.40	125.10
27	BA	2353	OMG	C2-N1-C6	-3.08	119.44	125.10
1	Aa	659	OMG	C5-C6-N1	3.06	119.35	113.95
27	BA	215	OMG	C5-C6-N1	3.05	119.35	113.95
27	BA	2528	OMG	C5-C6-N1	3.05	119.33	113.95
27	BA	1949	OMU	C5-C4-N3	3.03	119.38	114.84
27	BA	1969	OMU	O4-C4-C5	-3.03	119.84	125.16
1	Aa	498	OMG	C5-C6-N1	3.02	119.28	113.95
27	BA	2550	OMG	C5-C6-N1	2.99	119.24	113.95
27	BA	833	OMG	C5-C6-N1	2.99	119.24	113.95
27	BA	2745	OMG	C5-C6-N1	2.99	119.23	113.95
27	BA	491	OMG	C5-C6-N1	2.99	119.23	113.95
27	BA	65	OMG	C5-C6-N1	2.99	119.23	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Aa	913	OMG	C2-N1-C6	-2.98	119.61	125.10
1	Aa	852	OMG	C5-C6-N1	2.98	119.22	113.95
27	BA	2379	OMG	C5-C6-N1	2.97	119.20	113.95
1	Aa	658	OMG	C2-N1-C6	-2.97	119.62	125.10
27	BA	1949	OMU	N3-C2-N1	2.97	118.83	114.89
1	Aa	548	OMG	C2-N1-C6	-2.97	119.64	125.10
27	BA	63	OMG	C5-C6-N1	2.96	119.18	113.95
27	BA	1953	OMG	C5-C6-N1	2.93	119.12	113.95
1	Aa	446	OMG	C5-C6-N1	2.92	119.11	113.95
27	BA	800	OMG	C5-C6-N1	2.92	119.11	113.95
27	BA	2613	OMG	C2-N1-C6	-2.90	119.76	125.10
1	Aa	529	OMG	C2-N1-C6	-2.90	119.76	125.10
27	BA	1129	OMG	C5-C6-N1	2.89	119.06	113.95
27	BA	453	OMU	C5-C4-N3	2.89	119.17	114.84
27	BA	1623	OMU	O4-C4-C5	-2.88	120.09	125.16
27	BA	912	OMG	C5-C6-N1	2.88	119.04	113.95
1	Aa	8	OMU	C5-C4-N3	2.88	119.15	114.84
27	BA	501	LHH	C6-C5-C4	2.87	120.48	116.96
27	BA	912	OMG	C2-N1-C6	-2.87	119.81	125.10
1	Aa	852	OMG	C2-N1-C6	-2.87	119.81	125.10
27	BA	657	OMU	C5-C4-N3	2.87	119.13	114.84
27	BA	1776	OMU	C1'-N1-C2	2.85	122.74	117.57
27	BA	2542	OMU	C5-C4-N3	2.85	119.11	114.84
1	Aa	529	OMG	C5-C6-N1	2.85	118.99	113.95
1	Aa	658	OMG	O4'-C4'-C5'	2.82	118.64	109.37
27	BA	2672	OMG	C5-C6-N1	2.82	118.92	113.95
27	BA	2016	OMG	C5-C6-N1	2.81	118.92	113.95
27	BA	1905	OMU	C5-C4-N3	2.81	119.04	114.84
27	BA	2672	OMG	C8-N7-C5	2.81	108.34	102.99
27	BA	1953	OMG	C2-N1-C6	-2.80	119.93	125.10
27	BA	491	OMG	C2-N1-C6	-2.80	119.95	125.10
1	Aa	458	4AC	C6-C5-C4	2.79	120.37	116.96
1	Aa	659	OMG	C2-N1-C6	-2.78	119.98	125.10
27	BA	668	OMG	C5-C6-N1	2.77	118.85	113.95
27	BA	2010	OMG	C5-C6-N1	2.77	118.85	113.95
27	BA	943	OMG	C5-C6-N1	2.76	118.83	113.95
27	BA	2613	OMG	C5-C6-N1	2.74	118.79	113.95
27	BA	1969	OMU	C5-C4-N3	2.73	118.93	114.84
1	Aa	498	OMG	C2-N1-C6	-2.73	120.07	125.10
27	BA	2115	OMG	C5-C6-N1	2.72	118.75	113.95
27	BA	800	OMG	C2-N1-C6	-2.71	120.11	125.10
27	BA	833	OMG	C2-N1-C6	-2.70	120.14	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BA	1776	OMU	O4-C4-C5	-2.68	120.45	125.16
27	BA	2120	5MC	C5-C4-N4	-2.68	117.48	121.48
27	BA	2010	OMG	C2-N1-C6	-2.67	120.17	125.10
27	BA	1953	OMG	C8-N7-C5	2.67	108.08	102.99
27	BA	2550	OMG	C2-N1-C6	-2.66	120.20	125.10
1	Aa	458	4AC	N4-C4-N3	2.66	118.31	113.85
27	BA	2553	4SU	C5-C4-S4	-2.66	121.04	124.47
27	BA	1129	OMG	C2-N1-C6	-2.65	120.22	125.10
27	BA	2672	OMG	C2-N1-C6	-2.64	120.23	125.10
27	BA	674	OMG	C5-C6-N1	2.63	118.60	113.95
27	BA	2055	5MC	C5-C6-N1	-2.63	120.64	123.34
27	BA	668	OMG	C8-N7-C5	2.62	107.98	102.99
27	BA	869	OMC	C5-C4-N4	-2.61	116.47	120.57
27	BA	833	OMG	C8-N7-C5	2.60	107.94	102.99
27	BA	1949	OMU	C1'-N1-C2	2.60	122.28	117.57
27	BA	943	OMG	C2-N1-C6	-2.60	120.32	125.10
27	BA	674	OMG	C2-N1-C6	-2.59	120.33	125.10
1	Aa	1449	6MZ	C4-C5-N7	-2.57	106.72	109.40
1	Aa	8	OMU	O4-C4-C5	-2.57	120.64	125.16
27	BA	215	OMG	C2-N1-C6	-2.57	120.36	125.10
27	BA	491	OMG	CM2-O2'-C2'	2.57	121.26	114.52
27	BA	65	OMG	C2-N1-C6	-2.56	120.38	125.10
27	BA	1776	OMU	C6-N1-C2	-2.56	117.71	120.99
27	BA	2379	OMG	C2-N1-C6	-2.55	120.41	125.10
1	Aa	913	OMG	C8-N7-C5	2.54	107.84	102.99
27	BA	1905	OMU	O4-C4-C5	-2.54	120.70	125.16
1	Aa	450	OMG	C5-C6-N1	2.52	118.41	113.95
1	Aa	917	5MU	O2-C2-N1	-2.51	119.44	122.79
27	BA	2528	OMG	C2-N1-C6	-2.50	120.50	125.10
27	BA	501	LHH	N4-C4-N3	2.50	118.04	113.85
27	BA	943	OMG	C8-N7-C5	2.49	107.74	102.99
27	BA	2016	OMG	C8-N7-C5	2.49	107.73	102.99
1	Aa	548	OMG	C8-N7-C5	2.48	107.72	102.99
27	BA	668	OMG	C2-N1-C6	-2.48	120.53	125.10
27	BA	2353	OMG	C8-N7-C5	2.48	107.72	102.99
1	Aa	446	OMG	C2-N1-C6	-2.48	120.53	125.10
27	BA	1776	OMU	C5-C4-N3	2.48	118.55	114.84
1	Aa	672	5MC	C5-C6-N1	-2.47	120.80	123.34
27	BA	2010	OMG	C8-N7-C5	2.46	107.69	102.99
27	BA	1969	OMU	C1'-N1-C2	2.45	122.00	117.57
27	BA	342	5MC	C5-C6-N1	-2.44	120.82	123.34
27	BA	2613	OMG	C8-N7-C5	2.44	107.64	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Aa	8	OMU	O2-C2-N1	-2.44	119.55	122.79
27	BA	912	OMG	C8-N7-C5	2.43	107.62	102.99
27	BA	63	OMG	C2-N1-C6	-2.42	120.63	125.10
27	BA	342	5MC	CM5-C5-C6	-2.42	119.61	122.85
1	Aa	659	OMG	C8-N7-C5	2.40	107.57	102.99
27	BA	65	OMG	CM2-O2'-C2'	2.39	120.79	114.52
1	Aa	1352	5MC	C5-C6-N1	-2.39	120.88	123.34
27	BA	2016	OMG	C2-N1-C6	-2.38	120.71	125.10
1	Aa	730	4AC	C6-C5-C4	2.37	119.86	116.96
1	Aa	658	OMG	C8-N7-C5	2.36	107.49	102.99
27	BA	2542	OMU	C1'-N1-C2	2.36	121.84	117.57
27	BA	875	5MC	CM5-C5-C6	-2.36	119.70	122.85
27	BA	2745	OMG	C2-N1-C6	-2.35	120.77	125.10
27	BA	63	OMG	C8-N7-C5	2.34	107.45	102.99
1	Aa	529	OMG	C8-N7-C5	2.33	107.43	102.99
27	BA	2120	5MC	C5-C6-N1	-2.33	120.94	123.34
1	Aa	854	5MC	O2-C2-N3	-2.33	118.55	122.33
27	BA	2528	OMG	C8-N7-C5	2.32	107.41	102.99
1	Aa	498	OMG	C8-N7-C5	2.32	107.41	102.99
27	BA	61	A2M	C3'-C2'-C1'	2.31	107.23	102.89
1	Aa	446	OMG	C8-N7-C5	2.31	107.39	102.99
27	BA	2553	4SU	O2-C2-N1	-2.31	119.72	122.79
1	Aa	1459	4AC	N4-C4-N3	2.30	117.72	113.85
27	BA	2115	OMG	C2-N1-C6	-2.30	120.86	125.10
27	BA	1969	OMU	C6-N1-C2	-2.29	118.06	120.99
1	Aa	1459	4AC	C6-C5-C4	2.29	119.76	116.96
27	BA	501	LHH	CM7-C7-N4	2.28	119.23	115.29
27	BA	2055	5MC	C2'-C1'-N1	2.27	119.64	113.22
27	BA	2353	OMG	O6-C6-C5	-2.27	119.95	124.37
27	BA	2745	OMG	C8-N7-C5	2.26	107.30	102.99
27	BA	1820	OMC	O2-C2-N3	-2.26	118.65	122.33
27	BA	215	OMG	C8-N7-C5	2.26	107.30	102.99
27	BA	875	5MC	C1'-N1-C2	2.26	123.47	118.42
27	BA	61	A2M	O2'-C2'-C1'	2.26	113.57	109.09
27	BA	2379	OMG	C8-N7-C5	2.25	107.28	102.99
1	Aa	658	OMG	C5'-C4'-C3'	2.25	123.61	115.18
27	BA	1129	OMG	C8-N7-C5	2.25	107.27	102.99
1	Aa	854	5MC	C5-C4-N3	-2.24	119.26	121.67
1	Aa	730	4AC	N4-C4-N3	2.24	117.61	113.85
1	Aa	672	5MC	CM5-C5-C6	-2.23	119.87	122.85
27	BA	800	OMG	C8-N7-C5	2.23	107.23	102.99
27	BA	674	OMG	C8-N7-C5	2.22	107.22	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BA	875	5MC	C5-C4-N4	-2.19	118.19	121.48
1	Aa	852	OMG	C8-N7-C5	2.19	107.16	102.99
27	BA	875	5MC	C1'-N1-C6	-2.18	117.50	121.12
27	BA	477	OMC	N4-C4-N3	2.17	121.77	117.97
27	BA	65	OMG	C8-N7-C5	2.16	107.11	102.99
27	BA	1109	A2M	C3'-C2'-C1'	2.16	106.96	102.89
27	BA	1965	5MC	C5-C6-N1	-2.16	121.12	123.34
1	Aa	5	4AC	N4-C4-N3	2.14	117.45	113.85
27	BA	943	OMG	C2'-C3'-C4'	2.14	106.64	101.99
27	BA	1945	OMG	C8-N7-C5	2.14	107.06	102.99
27	BA	491	OMG	C8-N7-C5	2.13	107.06	102.99
1	Aa	458	4AC	C2'-C1'-N1	-2.13	107.17	113.22
27	BA	2055	5MC	CM5-C5-C6	-2.13	120.00	122.85
1	Aa	1449	6MZ	C9-N6-C6	2.13	124.71	122.87
27	BA	2115	OMG	C8-N7-C5	2.12	107.03	102.99
27	BA	869	OMC	N4-C4-N3	2.12	121.69	117.97
1	Aa	450	OMG	C8-N7-C5	2.12	107.03	102.99
1	Aa	1459	4AC	O2-C2-N3	-2.11	118.89	122.33
27	BA	2379	OMG	N2-C2-N1	2.11	121.21	116.71
27	BA	1623	OMU	O2-C2-N1	-2.11	119.98	122.79
27	BA	63	OMG	N2-C2-N1	2.10	121.19	116.71
27	BA	1905	OMU	C1'-N1-C2	2.08	121.34	117.57
27	BA	2786	OMC	O2'-C2'-C1'	2.07	113.13	109.08
27	BA	2545	OMC	O2-C2-N3	-2.07	118.96	122.33
27	BA	1965	5MC	CM5-C5-C6	-2.07	120.09	122.85
27	BA	1965	5MC	O2-C2-N3	-2.06	118.98	122.33
27	BA	501	LHH	O2-C2-N3	-2.05	119.00	122.33
27	BA	2656	OMU	O2-C2-N1	-2.04	120.07	122.79
27	BA	875	5MC	C5-C6-N1	-2.02	121.25	123.34
27	BA	875	5MC	O2-C2-N3	-2.02	119.05	122.33
27	BA	800	OMG	N2-C2-N1	2.02	121.01	116.71
27	BA	1820	OMC	C1'-N1-C2	2.01	122.91	118.42
1	Aa	5	4AC	C6-C5-C4	2.01	119.42	116.96
27	BA	453	OMU	O2-C2-N1	-2.00	120.12	122.79
1	Aa	1352	5MC	CM5-C5-C6	-2.00	120.17	122.85

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	Aa	5	4AC	O4'-C4'-C5'-O5'
1	Aa	5	4AC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	Aa	659	OMG	C3'-C4'-C5'-O5'
1	Aa	913	OMG	O4'-C4'-C5'-O5'
27	BA	61	A2M	C1'-C2'-O2'-CM'
27	BA	65	OMG	C1'-C2'-O2'-CM2
27	BA	342	5MC	O4'-C4'-C5'-O5'
27	BA	342	5MC	C3'-C4'-C5'-O5'
27	BA	491	OMG	C1'-C2'-O2'-CM2
27	BA	505	A2M	C3'-C4'-C5'-O5'
27	BA	849	A2M	C3'-C4'-C5'-O5'
27	BA	875	5MC	O4'-C4'-C5'-O5'
27	BA	875	5MC	C3'-C4'-C5'-O5'
27	BA	1945	OMG	O4'-C4'-C5'-O5'
27	BA	2353	OMG	O4'-C4'-C5'-O5'
27	BA	2353	OMG	C3'-C4'-C5'-O5'
27	BA	2379	OMG	O4'-C4'-C5'-O5'
1	Aa	458	4AC	C3'-C4'-C5'-O5'
1	Aa	659	OMG	O4'-C4'-C5'-O5'
1	Aa	913	OMG	C3'-C4'-C5'-O5'
27	BA	505	A2M	O4'-C4'-C5'-O5'
27	BA	2379	OMG	C3'-C4'-C5'-O5'
1	Aa	458	4AC	O4'-C4'-C5'-O5'
27	BA	869	OMC	O4'-C4'-C5'-O5'
27	BA	1945	OMG	C3'-C4'-C5'-O5'
27	BA	674	OMG	C3'-C4'-C5'-O5'
27	BA	849	A2M	O4'-C4'-C5'-O5'
27	BA	869	OMC	C3'-C4'-C5'-O5'
27	BA	2672	OMG	O4'-C4'-C5'-O5'
1	Aa	1468	MA6	C5-C6-N6-C9
27	BA	1623	OMU	O4'-C4'-C5'-O5'
27	BA	65	OMG	C3'-C2'-O2'-CM2
27	BA	674	OMG	O4'-C4'-C5'-O5'
1	Aa	918	LV2	O4'-C4'-C5'-O5'
27	BA	2545	OMC	C4'-C5'-O5'-P
27	BA	1953	OMG	C3'-C4'-C5'-O5'
27	BA	2379	OMG	C4'-C5'-O5'-P
27	BA	2786	OMC	O4'-C4'-C5'-O5'
1	Aa	446	OMG	O4'-C4'-C5'-O5'
27	BA	800	OMG	C3'-C2'-O2'-CM2
27	BA	2115	OMG	C3'-C2'-O2'-CM2
27	BA	668	OMG	C3'-C2'-O2'-CM2
1	Aa	8	OMU	C2'-C1'-N1-C6
1	Aa	8	OMU	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
27	BA	2075	5MC	O4'-C4'-C5'-O5'
27	BA	2672	OMG	C3'-C4'-C5'-O5'
27	BA	1623	OMU	C3'-C4'-C5'-O5'
27	BA	2786	OMC	C3'-C4'-C5'-O5'
1	Aa	458	4AC	C2'-C1'-N1-C2
1	Aa	8	OMU	O4'-C4'-C5'-O5'
1	Aa	918	LV2	C3'-C4'-C5'-O5'
27	BA	2075	5MC	C3'-C4'-C5'-O5'
27	BA	61	A2M	C3'-C2'-O2'-CM'
1	Aa	852	OMG	C4'-C5'-O5'-P

There are no ring outliers.

16 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	BA	2672	OMG	1	0
27	BA	2745	OMG	1	0
27	BA	342	5MC	1	0
27	BA	2115	OMG	1	0
27	BA	2120	5MC	4	0
27	BA	912	OMG	1	0
27	BA	879	A2M	1	0
27	BA	674	OMG	1	0
27	BA	61	A2M	1	0
27	BA	869	OMC	1	0
27	BA	2353	OMG	1	0
27	BA	1949	OMU	3	0
27	BA	1945	OMG	1	0
27	BA	1623	OMU	1	0
27	BA	505	A2M	1	0
27	BA	2379	OMG	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 12 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
27	BA	1
7	Ag	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	582:A	O3'	583:A	P	4.39
1	Ag	75:ASP	C	76:SER	N	3.06

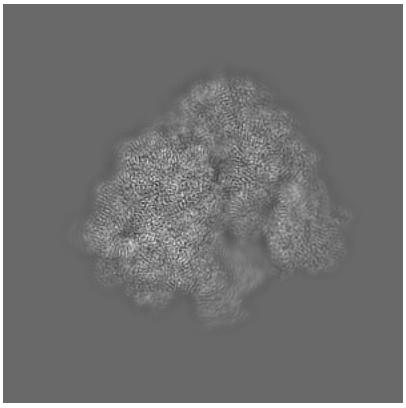
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10503. These allow visual inspection of the internal detail of the map and identification of artifacts.

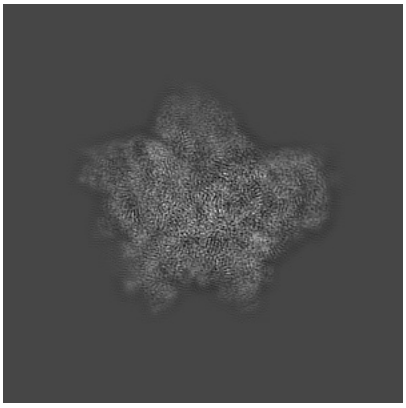
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

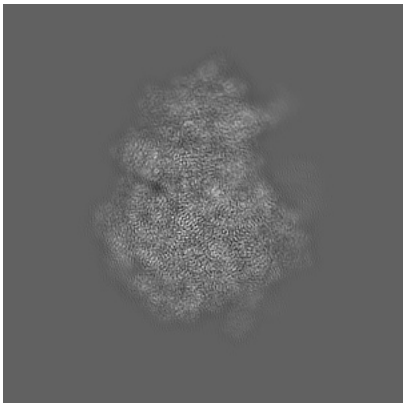
6.1.1 Primary map



X



Y

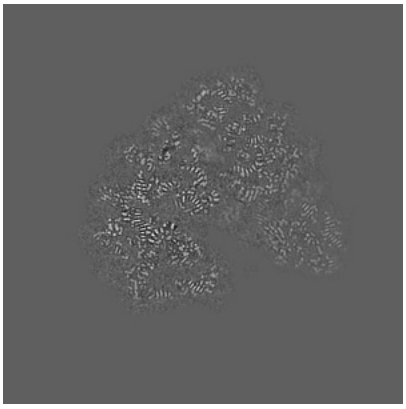


Z

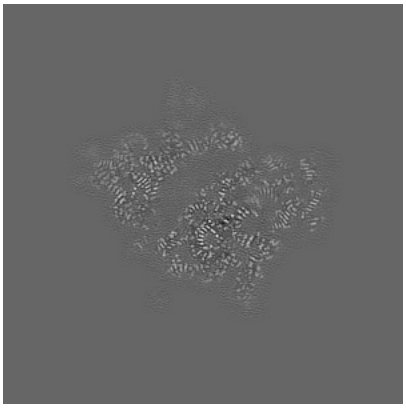
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

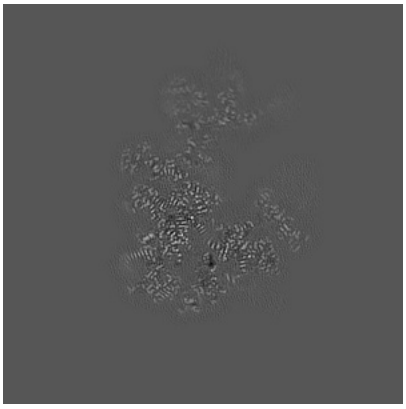
6.2.1 Primary map



X Index: 240



Y Index: 240

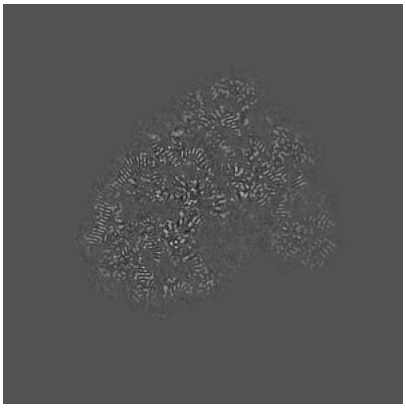


Z Index: 240

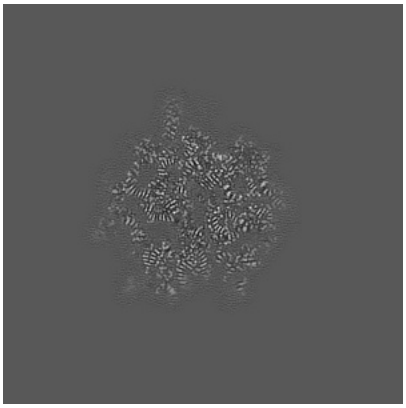
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

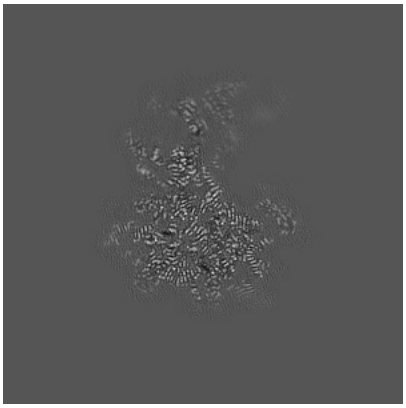
6.3.1 Primary map



X Index: 227



Y Index: 181

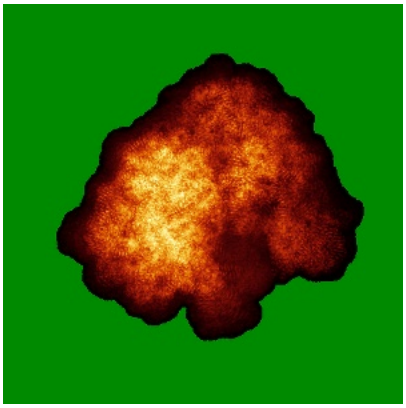


Z Index: 265

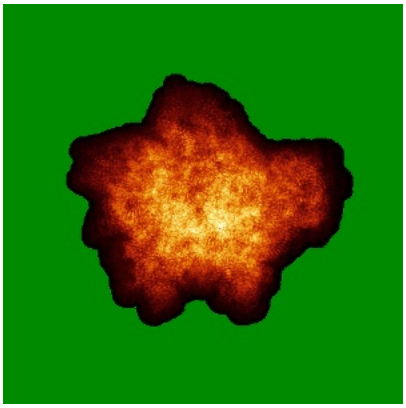
The images above show the largest variance slices of the map in three orthogonal directions.

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

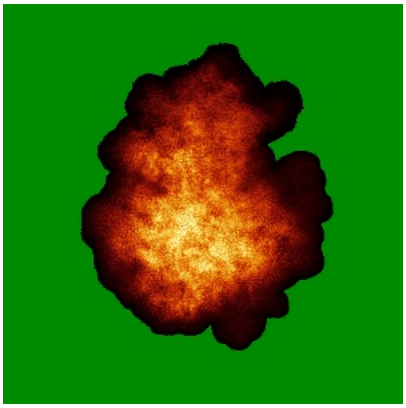
6.4.1 Primary map



X



Y

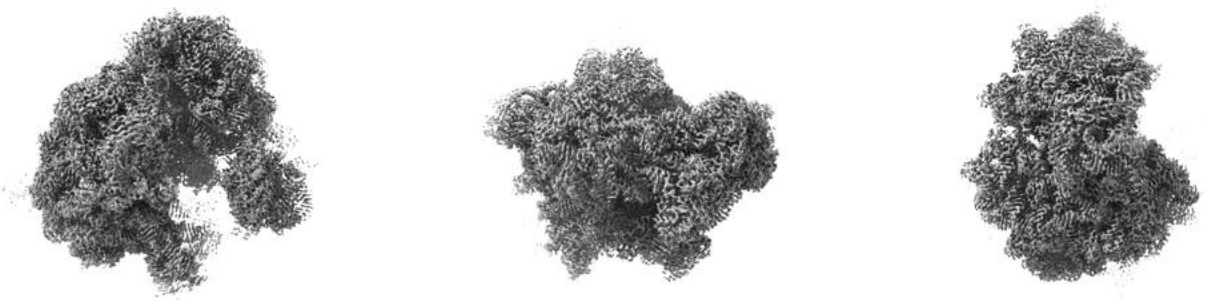


Z

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.

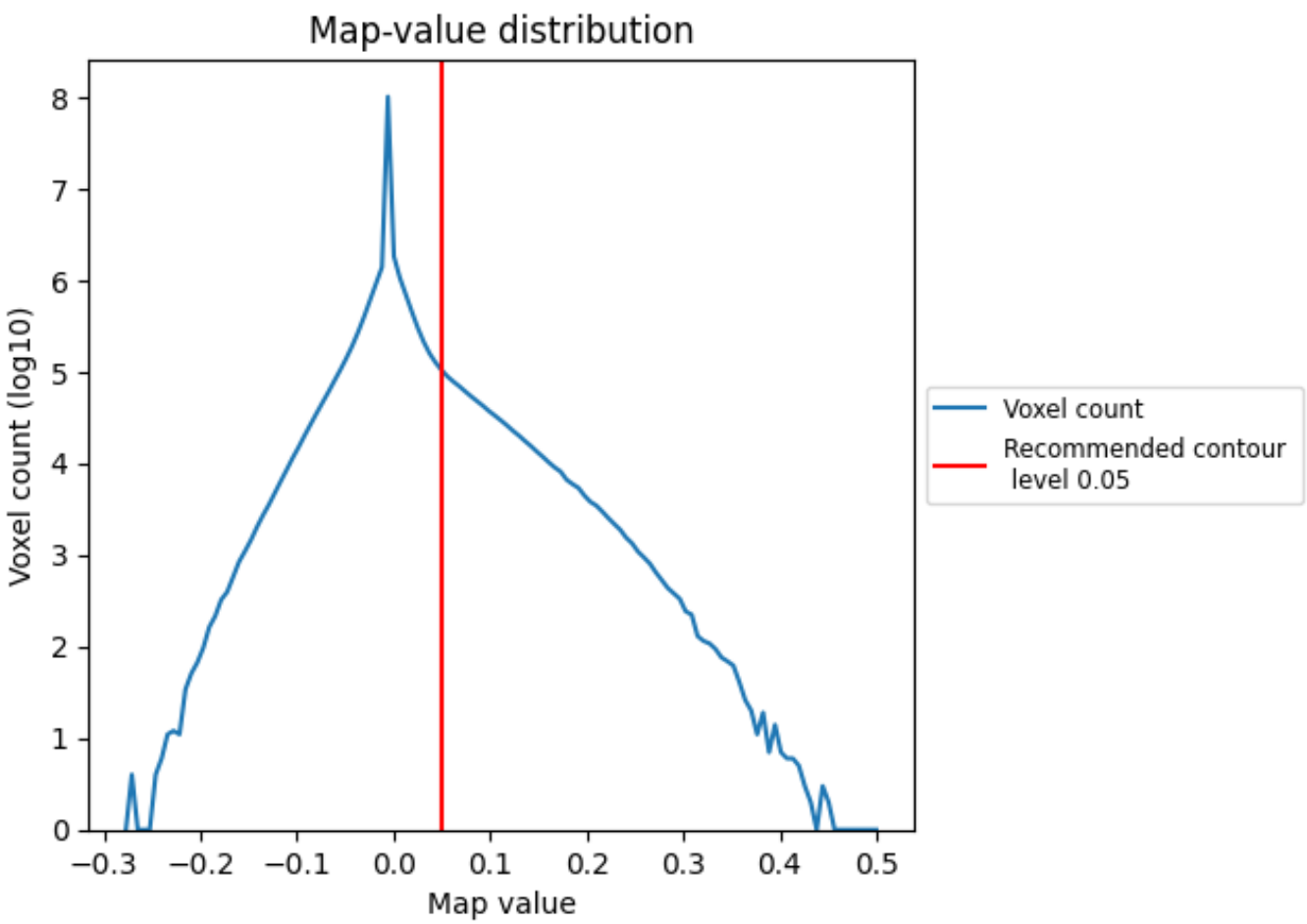
6.6 Mask visualisation (i)

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

7 Map analysis (i)

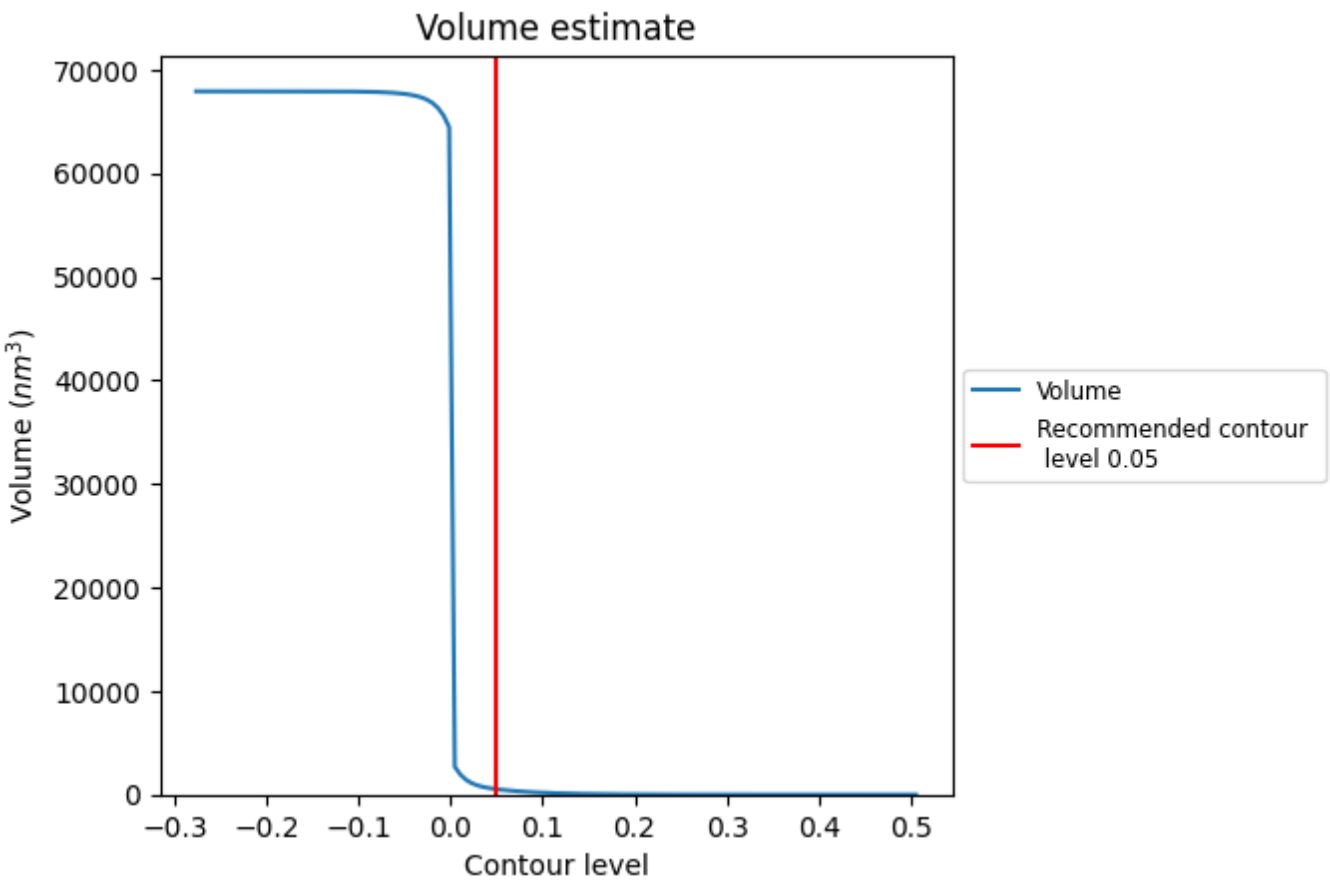
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

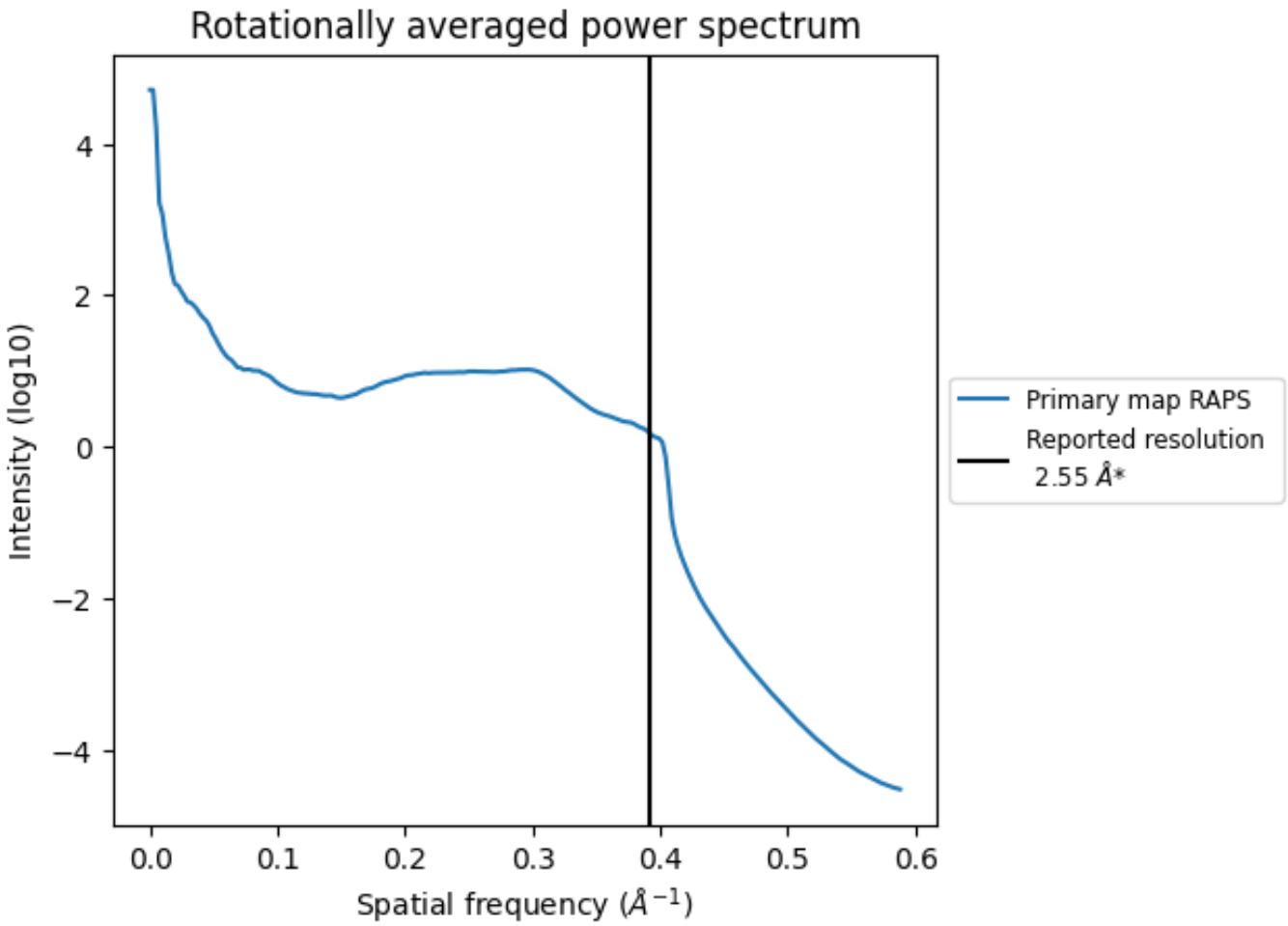
7.2 Volume estimate (i)



The volume at the recommended contour level is 518 nm^3; this corresponds to an approximate mass of 468 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 0.392 Å^{-1}

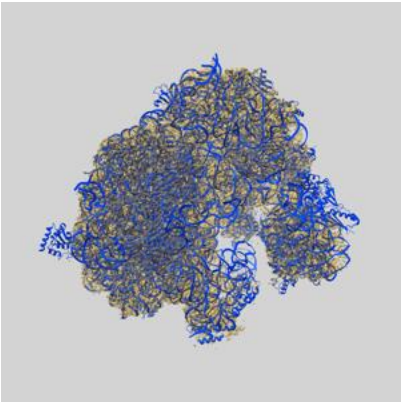
8 Fourier-Shell correlation (i)

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

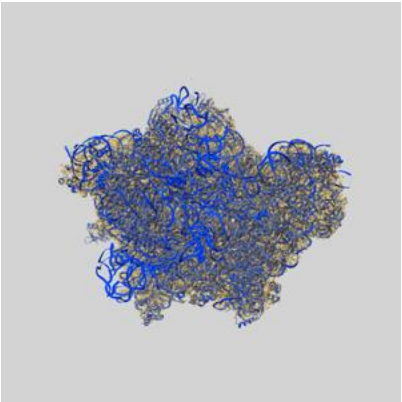
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-10503 and PDB model 6TH6. Per-residue inclusion information can be found in section 3 on page 18.

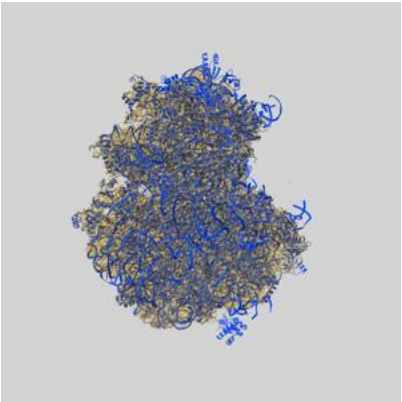
9.1 Map-model overlay (i)



X



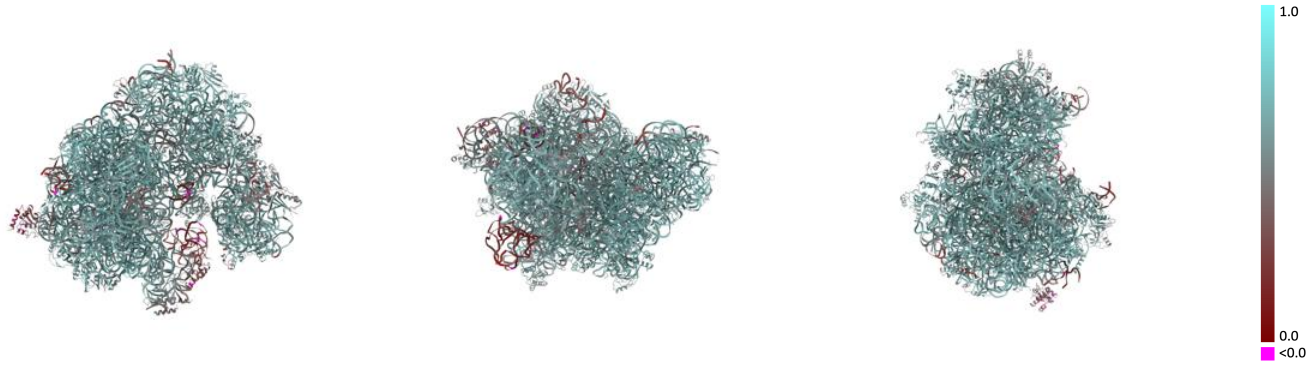
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

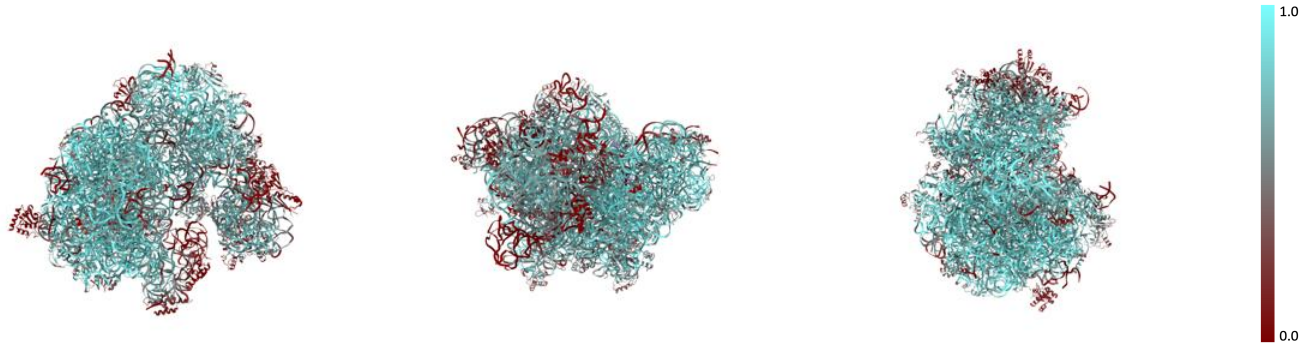
9.2 Q-score mapped to coordinate model (i)



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.

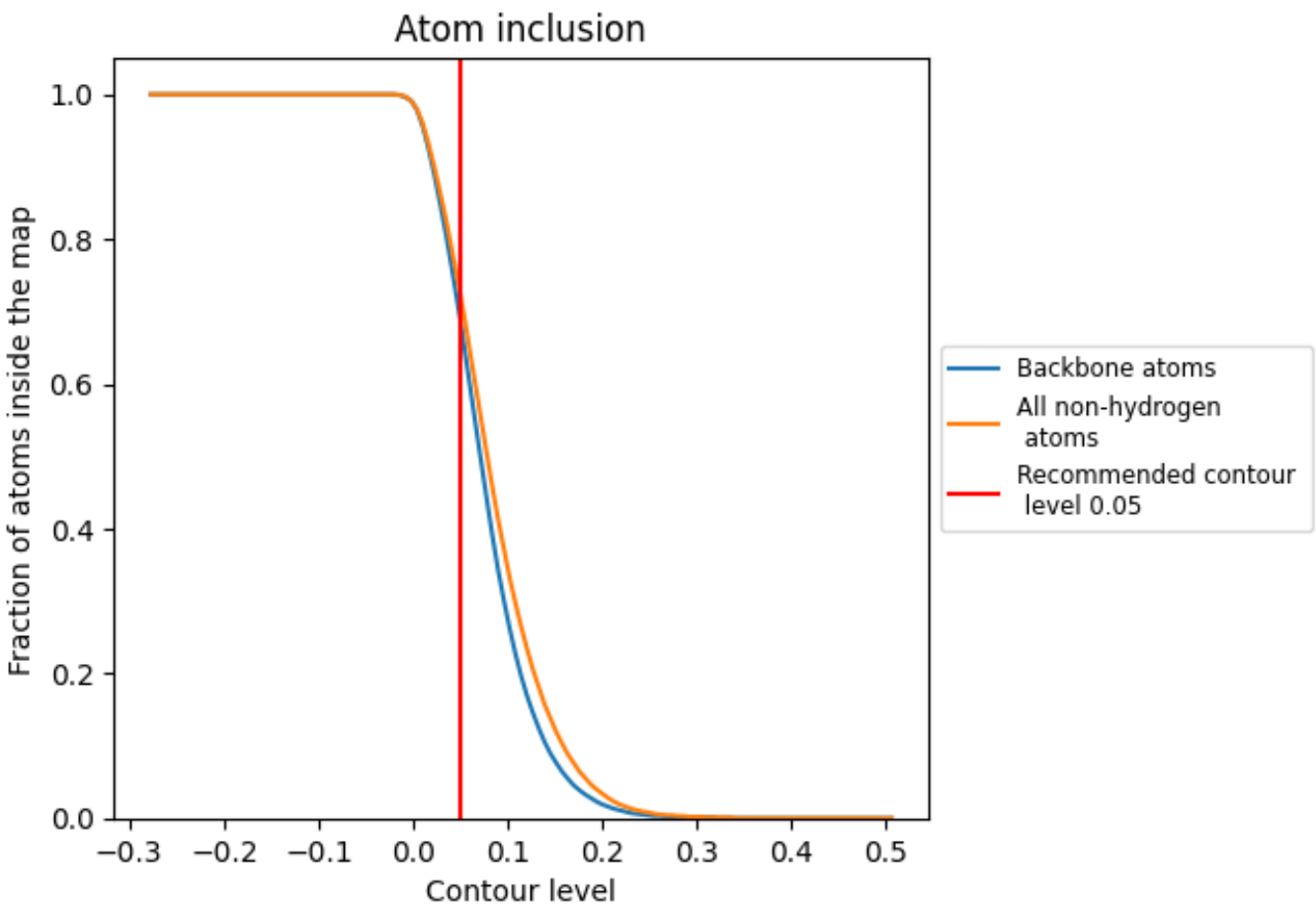
9.3 Atom inclusion mapped to coordinate model (i)



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, 69% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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	0.7250	0.6220
Aa	0.7550	0.6320
Ab	0.5560	0.6270
Ac	0.1560	0.5370
Ad	0.5400	0.6070
Ae	0.6830	0.6450
Af	0.7640	0.6520
Ag	0.7200	0.6340
Ah	0.3250	0.5650
Ai	0.4630	0.5940
Aj	0.7980	0.6580
Ak	0.7300	0.6350
Al	0.5050	0.6260
Am	0.2270	0.5540
An	0.5050	0.6120
Ao	0.7050	0.6510
Ap	0.4540	0.5650
Aq	0.7170	0.6350
Ar	0.4240	0.5780
As	0.5790	0.5960
At	0.0350	0.5090
Au	0.4660	0.6130
Av	0.5750	0.6340
Aw	0.5660	0.6110
Ax	0.6150	0.6110
Ay	0.2680	0.5710
Az	0.7060	0.6440
BA	0.8080	0.6240
BB	0.5070	0.5460
BC	0.8580	0.6730
BD	0.8420	0.6770
BE	0.8270	0.6680
BF	0.1190	0.3620
BG	0.5790	0.6030
BH	0.5470	0.5880

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Chain	Atom inclusion	Q-score
BI	0.0010	0.3030
BJ	0.6400	0.6170
BK	0.8160	0.6720
BL	0.7960	0.6530
BM	0.5930	0.5990
BN	0.4260	0.5440
BO	0.6060	0.6120
BP	0.8920	0.6800
BQ	0.4630	0.5670
BR	0.7930	0.6570
BS	0.8370	0.6620
BT	0.5550	0.6250
BU	0.8450	0.6780
BV	0.8610	0.6740
BW	0.7250	0.6410
BX	0.7810	0.6450
BY	0.7700	0.6460
BZ	0.5780	0.5810
Ba	0.7890	0.6560
Bb	0.6060	0.5970
Bc	0.7770	0.6660
Bd	0.8160	0.6700
Be	0.8170	0.6530
Bg	0.7970	0.6600
Bh	0.9420	0.6990
Bi	0.7720	0.6250
Bj	0.6970	0.6420
Bk	0.8770	0.6490
Bl	0.7700	0.6600