



Full wwPDB EM Validation Report ⓘ

Oct 28, 2025 – 07:49 pm GMT

PDB ID : 9QF6 / pdb_00009qf6
EMDB ID : EMD-53100
Title : Structure of P. furiosus 70S ribosome in RsmB deleted strain
Authors : Matzov, D.; Georgeson, J.; Westhof, E.; Schwartz, S.; Shalev-Benami, M.
Deposited on : 2025-03-11
Resolution : 2.67 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev129
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

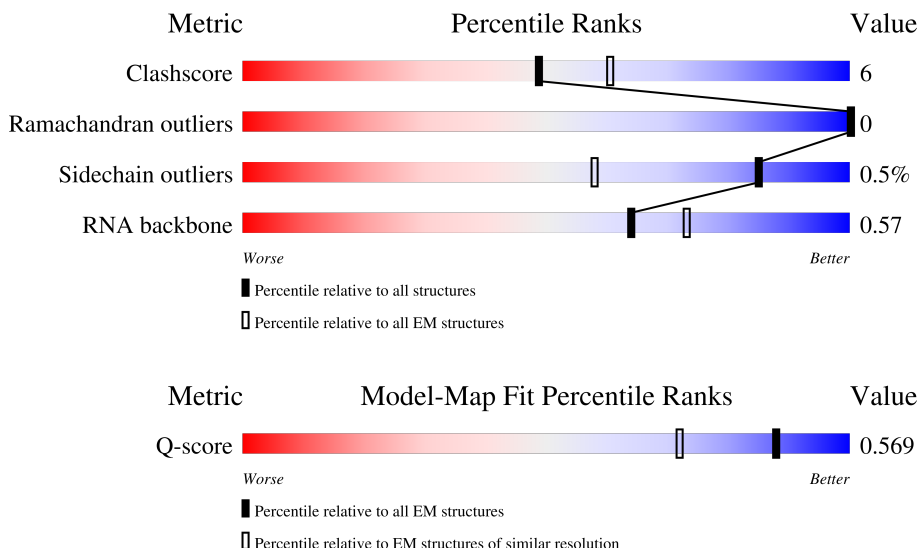
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.67 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.










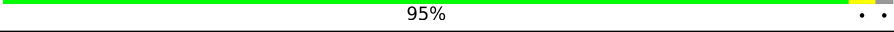



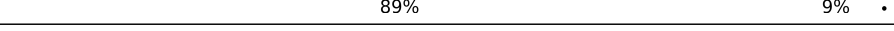







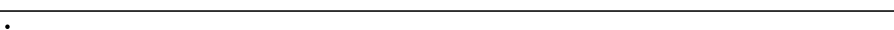

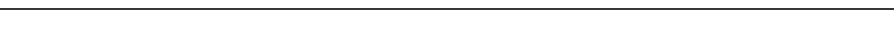
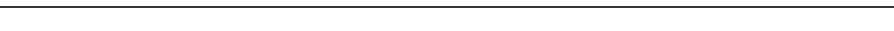


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	9182 (2.17 - 3.17)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A1	1497	
2	Aa	202	
3	Ab	210	

























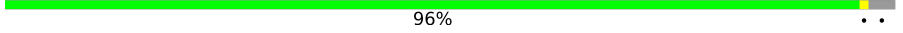
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	Ac	198	
5	Ad	180	
6	Ae	243	
7	Af	236	
8	Ag	125	
9	Ah	215	
10	Ai	130	
11	Aj	127	
12	Ak	135	
13	Al	102	
14	Am	137	
15	An	147	
16	Ao	148	
17	Ap	56	
18	Aq	158	
19	Ar	113	
20	As	67	
21	At	132	
22	Au	150	
23	Av	99	
23	Bl	99	
24	Aw	63	
25	Ax	71	
26	Az	60	
27	B1	3051	


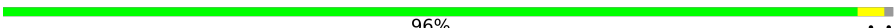





Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	B2	125	
29	BA	239	
30	BB	365	
31	BC	255	
32	BD	186	
33	BE	184	
34	BF	123	
34	BG	123	
35	BH	181	
36	BI	142	
37	BJ	141	
38	BK	83	
38	BL	83	
39	BM	147	
40	BN	194	
41	BO	203	
42	BP	120	
43	BQ	150	
44	BR	97	
45	BS	155	
46	BT	86	
47	BU	121	
48	BV	66	
49	BW	72	
50	BX	155	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
51	BY	99	 84% 14% .
52	BZ	95	 96% . .
53	Ba	130	 95% . .
54	Bb	89	 91% 8% .
55	Bc	87	 91% 8% .
56	Bd	62	 87% 10% .
57	Be	83	 84% 14% .
58	Bf	51	 92% 6% .
59	Bg	51	 84% 6% 10%
60	Bh	37	 84% 14% .
61	Bi	94	 99% .
62	Bj	77	 94% 6%
63	Bk	64	 81% 16% .

2 Entry composition [i](#)

There are 65 unique types of molecules in this entry. The entry contains 164601 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 rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A1	1490	Total	C	N	O	P	S	0	0
			32212	14384	5942	10395	1490	1		

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Aa	196	Total	C	N	O	S	0	0
			1572	1017	270	281	4		

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Ab	195	Total	C	N	O	S	0	0
			1513	968	276	266	3		

- Molecule 4 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Ac	185	Total	C	N	O	S	0	0
			1516	981	264	266	5		

- Molecule 5 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Ad	173	Total	C	N	O	S	0	0
			1452	913	280	255	4		

- Molecule 6 is a protein called Small ribosomal subunit protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Ae	242	Total	C	N	O	S	0	0
			1975	1277	353	340	5		

- Molecule 7 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Af	226	Total	C	N	O	S	0	0
			1784	1129	333	315	7		

- Molecule 8 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Ag	124	Total	C	N	O	S	0	0
			963	610	177	175	1		

- Molecule 9 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Ah	214	Total	C	N	O	S	0	0
			1722	1089	325	301	7		

- Molecule 10 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Ai	129	Total	C	N	O	S	0	0
			1028	668	178	180	2		

- Molecule 11 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Aj	125	Total	C	N	O	S	0	0
			972	603	200	169			

- Molecule 12 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Ak	134	Total	C	N	O	S	0	0
			1048	657	200	186	5		

- Molecule 13 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Al	99	Total	C	N	O	S	0	0
			770	479	146	142	3		

- Molecule 14 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Am	128	Total	C	N	O	S	0	0
			963	597	192	172	2		

- Molecule 15 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	An	144	Total	C	N	O	S	0	0
			1124	715	215	191	3		

- Molecule 16 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Ao	137	Total	C	N	O	S	0	0
			1102	693	219	185	5		

- Molecule 17 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Ap	55	Total	C	N	O	S	0	0
			450	285	94	66	5		

- Molecule 18 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Aq	156	Total	C	N	O	S	0	0
			1290	823	245	218	4		

- Molecule 19 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Ar	107	Total	C	N	O	S	0	0
			877	560	165	149	3		

- Molecule 20 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	As	63	Total	C	N	O	S	0	0
			522	330	100	90	2		

- Molecule 21 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	At	121	Total	C	N	O	S	0	0
			985	632	184	163	6		

- Molecule 22 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Au	149	Total	C	N	O		0	0
			1221	790	219	212			

- Molecule 23 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Av	95	Total	C	N	O	S	0	0
			791	514	129	145	3		
23	Bl	92	Total	C	N	O	S	0	0
			765	498	125	140	2		

- Molecule 24 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Aw	61	Total	C	N	O	S	0	0
			464	298	83	78	5		

- Molecule 25 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Ax	64	Total	C	N	O		0	0
			495	305	98	92			

- Molecule 26 is a protein called Zn-ribbon RNA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Az	56	Total	C	N	O	S	0	0
			434	272	78	76	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
27	B1	2931	Total	C	N	O	P	S	0	0
			63424	28311	11737	20444	2931	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	B2	125	Total	C	N	O	P	0	0
			2689	1198	494	872	125		

- Molecule 29 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BA	237	Total	C	N	O	S	0	0
			1814	1155	341	314	4		

- Molecule 30 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BB	363	Total	C	N	O	S	0	0
			2888	1854	522	498	14		

- Molecule 31 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BC	255	Total	C	N	O	S	0	0
			2026	1288	391	342	5		

- Molecule 32 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BD	182	Total	C	N	O	S	0	0
			1415	886	272	249	8		

- Molecule 33 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BE	183	Total	C	N	O	S	0	0
			1468	951	251	265	1		

- Molecule 34 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BF	122	Total	C	N	O	S	0	0
			927	591	153	180	3		
34	BG	121	Total	C	N	O	S	0	0
			921	588	152	178	3		

- Molecule 35 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BH	169	Total	C	N	O	S	0	0
			1383	879	263	235	6		

- Molecule 36 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BI	142	Total	C	N	O	S	0	0
			1150	737	215	195	3		

- Molecule 37 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BJ	140	Total	C	N	O	S	0	0
			1058	657	213	185	3		

- Molecule 38 is a protein called Large ribosomal subunit protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BK	81	Total	C	N	O	S	0	0
			614	386	119	108	1		
38	BL	82	Total	C	N	O	S	0	0
			621	391	120	109	1		

- Molecule 39 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BM	147	Total	C	N	O	S	0	0
			1154	727	227	195	5		

- Molecule 40 is a protein called Large ribosomal subunit protein eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BN	193	Total	C	N	O	S	0	0
			1587	1015	315	252	5		

- Molecule 41 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BO	196	Total	C	N	O	S	0	0
			1564	999	295	269	1		

- Molecule 42 is a protein called Large ribosomal subunit protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BP	120	Total	C	N	O	S	0	0
			966	606	186	171	3		

- Molecule 43 is a protein called Large ribosomal subunit protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BQ	148	Total	C	N	O	S	0	0
			1238	783	252	199	4		

- Molecule 44 is a protein called Large ribosomal subunit protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BR	96	Total	C	N	O	S	0	0
			790	503	160	126	1		

- Molecule 45 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BS	151	Total	C	N	O	S	0	0
			1198	767	225	202	4		

- Molecule 46 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	BT	84	Total	C	N	O	0	0
			674	434	118	122		

- Molecule 47 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BU	120	Total	C	N	O	S	0	0
			1003	635	194	170	4		

- Molecule 48 is a protein called Large ribosomal subunit protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BV	63	Total	C	N	O	S	0	0
			533	339	103	85	6		

- Molecule 49 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BW	70	Total	C	N	O	S	0	0
			565	351	111	99	4		

- Molecule 50 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BX	154	Total	C	N	O	S	0	0
			1235	783	234	212	6		

- Molecule 51 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BY	97	Total	C	N	O	S	0	0
			734	478	116	139	1		

- Molecule 52 is a protein called Large ribosomal subunit protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BZ	94	Total	C	N	O	S	0	0
			746	487	138	121			

- Molecule 53 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Ba	128	Total	C	N	O	S	0	0
			1082	693	218	170	1		

- Molecule 54 is a protein called Large ribosomal subunit protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Bb	88	Total	C	N	O	S	0	0
			733	460	157	105	11		

- Molecule 55 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Bc	86	Total	C	N	O	S	0	0
			677	429	131	116	1		

- Molecule 56 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Bd	60	Total	C	N	O	S	0	0
			483	298	106	75	4		

- Molecule 57 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Be	82	Total	C	N	O	S	0	0
			616	383	127	101	5		

- Molecule 58 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Bf	50	Total	C	N	O	S	0	0
			437	279	97	61			

- Molecule 59 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Bg	46	Total	C	N	O	S	0	0
			375	238	77	56	4		

- Molecule 60 is a protein called Small ribosomal subunit protein eS32.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Bh	36	Total	C	N	O	S	0	0
			336	212	83	39	2		

- Molecule 61 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Bi	94	Total	C	N	O	S	0	0
			787	499	161	122	5		

- Molecule 62 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Bj	77	Total	C	N	O	S	0	0
			652	420	118	113	1		

- Molecule 63 is a protein called C2H2-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Bk	62	Total	C	N	O	S	0	0
			514	330	103	78	3		

- Molecule 64 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
64	Af	1	Total	Zn	0
			1	1	
64	Ap	1	Total	Zn	0
			1	1	
64	Ar	1	Total	Zn	0
			1	1	
64	Aw	1	Total	Zn	0
			1	1	
64	Az	2	Total	Zn	0
			2	2	
64	BV	1	Total	Zn	0
			1	1	
64	Bb	1	Total	Zn	0
			1	1	
64	Bd	1	Total	Zn	0
			1	1	
64	Be	1	Total	Zn	0
			1	1	
64	Bg	1	Total	Zn	0
			1	1	
64	Bi	1	Total	Zn	0
			1	1	
64	Bk	1	Total	Zn	0
			1	1	

- Molecule 65 is water.

Mol	Chain	Residues	Atoms		AltConf
65	A1	151	Total	O	0
			151	151	
65	Ae	3	Total	O	0
			3	3	
65	Ag	1	Total	O	0
			1	1	
65	Ah	1	Total	O	0
			1	1	
65	Aj	1	Total	O	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
65	Ak	1	Total 1	O 1	0
65	Al	3	Total 3	O 3	0
65	Am	2	Total 2	O 2	0
65	Ao	2	Total 2	O 2	0
65	Ap	1	Total 1	O 1	0
65	Aq	2	Total 2	O 2	0
65	Au	1	Total 1	O 1	0
65	Av	1	Total 1	O 1	0
65	B1	1173	Total 1173	O 1173	0
65	B2	19	Total 19	O 19	0
65	BA	10	Total 10	O 10	0
65	BB	6	Total 6	O 6	0
65	BC	7	Total 7	O 7	0
65	BE	1	Total 1	O 1	0
65	BF	1	Total 1	O 1	0
65	BH	6	Total 6	O 6	0
65	BI	7	Total 7	O 7	0
65	BJ	2	Total 2	O 2	0
65	BM	11	Total 11	O 11	0
65	BN	14	Total 14	O 14	0
65	BO	2	Total 2	O 2	0

Continued on next page...

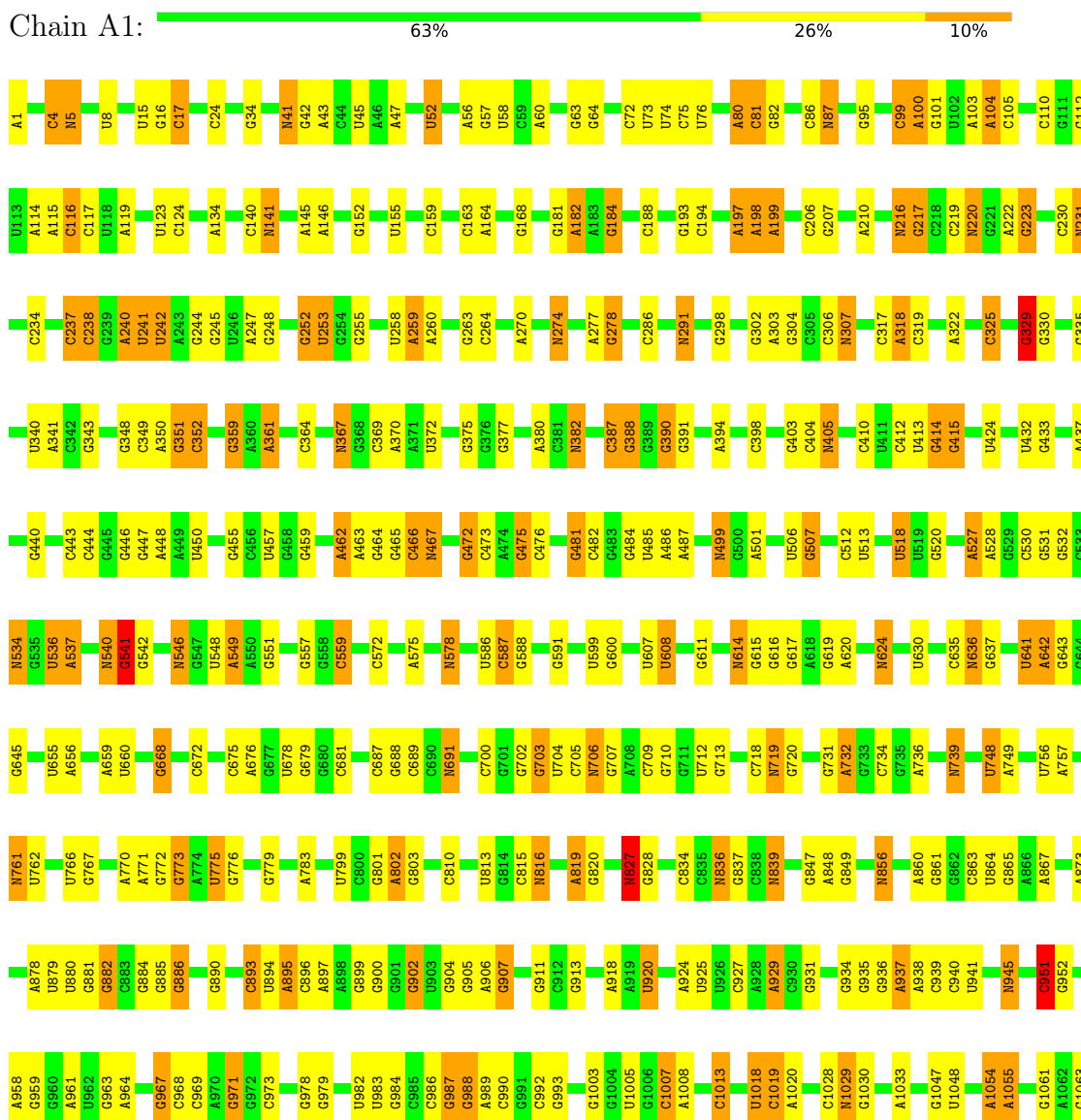
Continued from previous page...

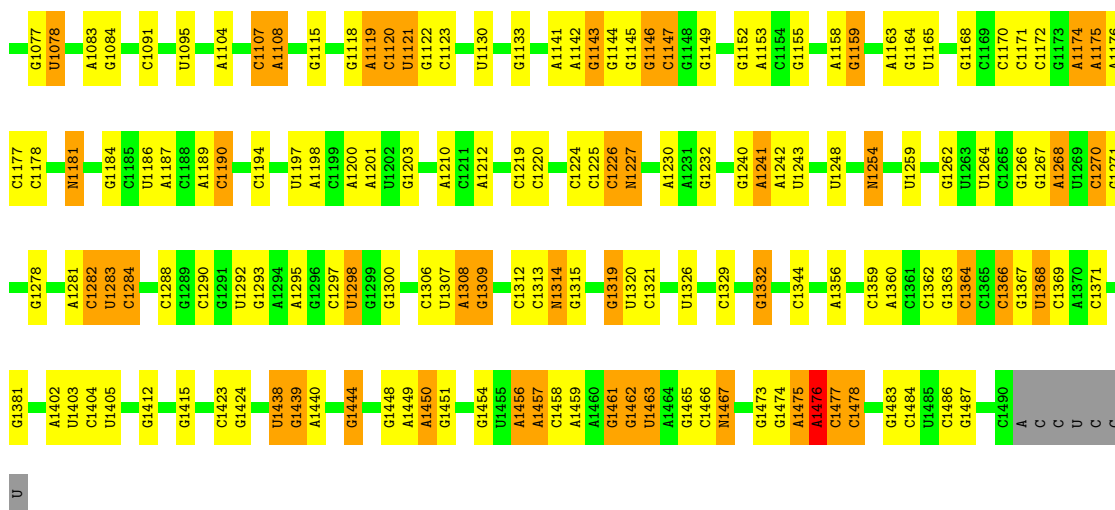
Mol	Chain	Residues	Atoms		AltConf
65	BP	8	Total 8	O 8	0
65	BQ	3	Total 3	O 3	0
65	BR	7	Total 7	O 7	0
65	BS	6	Total 6	O 6	0
65	BT	2	Total 2	O 2	0
65	BU	2	Total 2	O 2	0
65	BW	1	Total 1	O 1	0
65	BX	11	Total 11	O 11	0
65	BZ	2	Total 2	O 2	0
65	Ba	6	Total 6	O 6	0
65	Bb	3	Total 3	O 3	0
65	Bc	4	Total 4	O 4	0
65	Bd	5	Total 5	O 5	0
65	Bf	3	Total 3	O 3	0
65	Bi	3	Total 3	O 3	0
65	Bj	4	Total 4	O 4	0
65	Bk	2	Total 2	O 2	0

3 Residue-property plots

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

• Molecule 1: 16S rRNA





- Molecule 2: Small ribosomal subunit protein uS2

Chain Aa: 86% 11% .



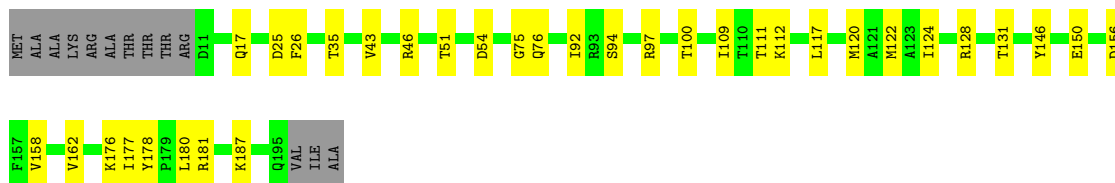
- Molecule 3: Small ribosomal subunit protein uS3

Chain Ab: 82% 10% 7%



- Molecule 4: Small ribosomal subunit protein eS1

Chain Ac: 76% 17% 7%



- Molecule 5: Small ribosomal subunit protein uS4

Chain Ad: 82% 14% .



- Molecule 6: Small ribosomal subunit protein eS4

Chain Ae: 87% 12%



- Molecule 7: Small ribosomal subunit protein uS5

Chain Af: 89% 7%



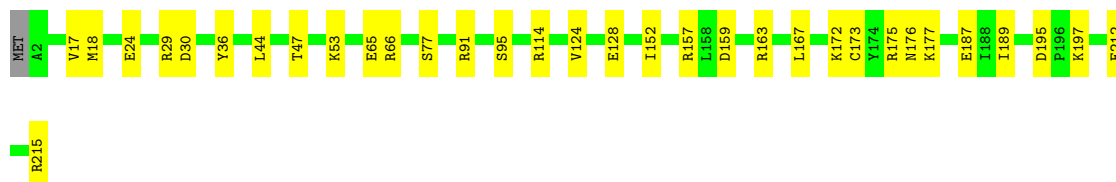
- Molecule 8: Small ribosomal subunit protein eS6

Chain Ag: 87% 12%



- Molecule 9: Small ribosomal subunit protein uS7

Chain Ah: 84% 15%



- Molecule 10: Small ribosomal subunit protein uS8

Chain Ai: 87% 12%



- Molecule 11: Small ribosomal subunit protein eS8

Chain Aj: 95%

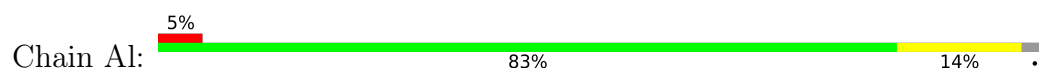


- Molecule 12: Small ribosomal subunit protein uS9

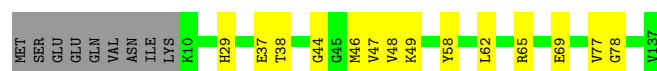
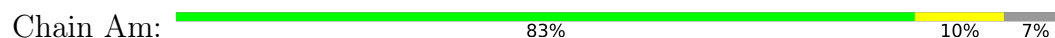
Chain Ak: 81% 19%



- Molecule 13: Small ribosomal subunit protein uS10



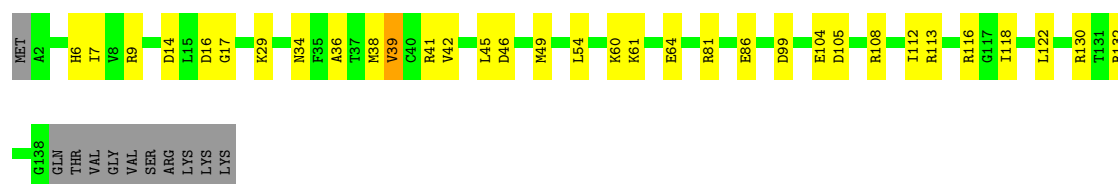
- Molecule 14: Small ribosomal subunit protein uS11



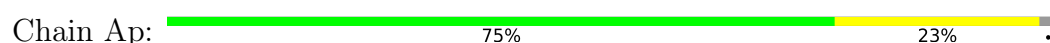
- Molecule 15: Small ribosomal subunit protein uS12



- Molecule 16: Small ribosomal subunit protein uS13



- Molecule 17: Small ribosomal subunit protein uS14



- Molecule 18: Small ribosomal subunit protein uS15



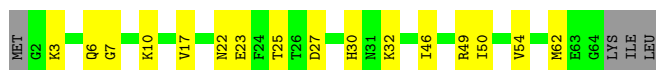
- Molecule 19: Small ribosomal subunit protein uS17





- Molecule 20: Small ribosomal subunit protein eS17

Chain As: 70% 24% 6%



- Molecule 21: Small ribosomal subunit protein uS19

Chain At: 80% 11% 8%



- Molecule 22: Small ribosomal subunit protein eS19

Chain Au: 87% 11% ..



- Molecule 23: Small ribosomal subunit protein eS24

Chain Av: 85% 11% .



- Molecule 23: Small ribosomal subunit protein eS24

Chain Bl: 82% 11% 7%



- Molecule 24: Small ribosomal subunit protein eS27

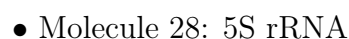
Chain Aw: 81% 16% .

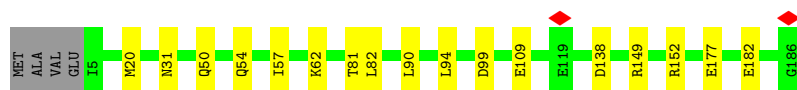


- Molecule 25: Small ribosomal subunit protein eS28

Chain Ax: 73% 17% 10%

C2619	C2603	U2401	G2276	G2185	C2090	A2005	A1881	U1778	A1678	G1574	G1455	C1359	G1247	A1186
C2634	C2503	A2402	G2277	A2186	A2091	N2008	N1885	G1779	A1679	A1574	C1458	N1360	G1250	G1157
C2637	C2504	A2403	C2187	C2187	U2092	G2093	G2093	C1780	U1680	A1575	C1459	G1363	A1251	A1188
G2645	A2506	G2405	G2194	G2194	A2094	A2094	G1889	C1782	G1681	C1577	A1466	U1367	G1252	G1191
G2648	A2510	U2406	G2281	G2193	U2096	C2017	C1894	G1789	G1696	C1578	A1465	A1368	U1254	C
C2649	A2511	C2407	A2282	U2198	G2097	N2020	G1898	A1790	G1697	N1579	A1466	A1369	C1255	G
A2650	C2519	U2419	G2287	G2207	G2108	G2021	G1899	G1791	G1698	C1589	C1471	G1370	N1264	G
A2680	C2520	A2420	C2288	G2207	G2108	G2022	A1899	A1792	G1699	G1590	G1476	C1373	N1269	G
A2681	N2526	G2423	U2291	N2213	C2112	U2023	C1900	G1793	U1700	N1478	A1477	G1375	A1269	G
A2682	G2540	U2427	G2294	G2217	U2116	A2026	G1904	G1796	N1706	G1594	G1476	C1373	A1269	G
G2684	G2541	C2428	A2295	G2117	U2118	A2027	N1911	U1804	A1708	G1600	G1482	G1377	G1272	G
G2691	U2542	N2429	C2298	U2118	U2118	G2028	A1913	G1805	U1709	C1603	N1478	G1376	A1273	A
G2692	G2543	G2430	C2298	C2119	C2119	G2031	C1914	U1806	G1710	G1595	G1488	U1377	G1273	G
A2693	A2544	C2431	C2302	C2120	C2121	G2032	U1919	C1807	G1712	N1608	A1496	C1382	G1276	C
C2694	C2546	N2432	A2304	G2229	G2122	G2033	A1920	G1810	G1715	G1613	A1497	N1383	G1278	A
C2695	G2547	A2435	G2309	G2230	G2123	G2034	C1937	G1811	A1724	G1616	C1500	G1388	U1280	G
U2696	A2548	G2436	C2309	G2232	G2124	G2035	A1938	G1812	A1725	G1617	N1501	G1392	C1281	A
G2697	A2549	A2437	C2309	U2233	C2126	A2036	G1939	A1813	G1735	A1617	C1500	C1398	U1282	G
G2698	A2550	G2437	G2314	G2234	G2127	A2037	C1940	A1814	G1738	G1618	N1505	G1399	G1287	C
G2699	G2440	U2440	A2322	C2235	G2128	A2038	U1941	N1818	U1722	G1623	A1408	G1412	U1296	C
U2700	C2441	G2441	A2322	G2236	G2128	C2039	A1942	G1819	G1723	C1394	C1301	G1413	C1308	A
G2704	A2442	A2442	G2329	C2237	N2133	U2040	G1947	C1830	G1738	G1624	G1308	G1414	G1309	G
A2705	A2450	A2450	G2339	A2238	A2138	U2041	C1937	U1831	A1739	U1625	A1529	A1415	A1315	A
G2711	G2455	G2455	C2340	U2243	G2146	A2044	G1965	C1832	C1742	G1643	C1532	G1416	U1316	A
G2714	N2469	N2469	A2347	G2246	C2152	U2050	C1966	G1833	G1747	U1644	U1537	U1418	U1317	A
G2715	G2470	G2470	G2352	G2247	C2154	U2051	G1967	G1834	C1747	U1646	U1540	C1434	G1318	G
A2718	A2471	A2471	G2353	G2248	C2155	A2052	N1846	C1845	N1761	G1647	U1540	N1435	A1326	G
C2722	G2473	G2473	G2365	A2250	C2156	A2053	G1968	C1846	A1755	C1648	U1541	N1436	U1327	C
U2729	C2474	C2474	G2365	G2252	C2160	G2055	N1967	C1846	A1755	N1649	U1542	A1437	G1328	G
A2730	A2475	A2475	A2372	G2254	G2163	C2059	G1968	U1853	G1758	G1658	N1546	C1439	G1329	U
G2736	A2476	A2476	U2377	U2255	A2166	A2061	A1969	C1854	A1758	A1659	U1551	N1442	U1331	A
G2737	G2477	G2477	C2378	G2256	C2167	A2063	C1977	G1855	U1759	G1660	G1557	G1443	U1332	C
U2745	G2478	G2478	G2379	G2257	C2170	U2064	C1978	G1856	A1760	A1661	G1557	A1444	G1337	G
N2749	A2487	A2487	G2380	A2258	C2171	U2065	U1981	G1857	G1761	G1665	G1561	G1446	C1344	U
G2757	C2491	C2491	A2381	G2260	G2172	C2067	G1982	A1858	N1762	G1666	G1567	G1447	N1345	A
A2760	N2492	N2492	A2384	C2261	U2171	C2068	G1986	A1860	G1765	G1666	C1568	G1448	U1333	C
A2761	G2493	G2493	G2385	C2262	U2174	U2090	U1987	A1861	A1766	G1666	A1569	G1449	G1365	C
G2762	A2496	A2496	G2386	G2264	G2175	A2085	A1988	G1870	G1768	G1666	G1570	C1450		
C2769	G2497	G2497	G2391	C2266	A2179	C2086	A1993	G1871	N1769	A1670				
	G2498	G2498	C2398	C2267	G2180	U2087	A2003	U1876	A1773	G1677				
	G2501	G2501		C2270	A2184	G2089	C2004	G1877	C1774					





- Molecule 33: Large ribosomal subunit protein uL6

Chain BE: 92% 7%



- Molecule 34: Large ribosomal subunit protein eL8

Chain BF: 85% 14%



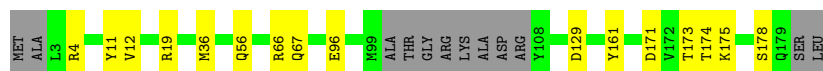
- Molecule 34: Large ribosomal subunit protein eL8

Chain BG: 77% 21%



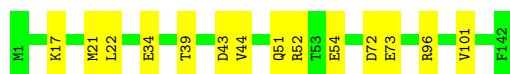
- Molecule 35: Large ribosomal subunit protein uL16

Chain BH: 85% 9% 7%



- Molecule 36: Large ribosomal subunit protein uL13

Chain BI: 90% 10%



- Molecule 37: Large ribosomal subunit protein uL14

Chain BJ: 93% 6%



- Molecule 38: Large ribosomal subunit protein eL14

Chain BK: 90% 7%



- Molecule 38: Large ribosomal subunit protein eL14

Chain BL: 72% 27%



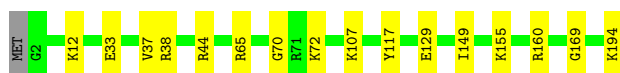
- Molecule 39: Large ribosomal subunit protein uL15

Chain BM: 82% 18%



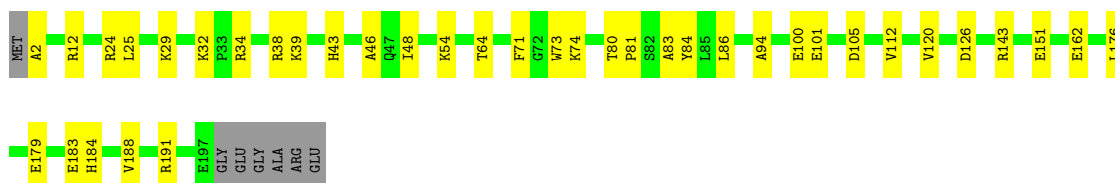
- Molecule 40: Large ribosomal subunit protein eL15

Chain BN: 91% 8%



- Molecule 41: Large ribosomal subunit protein uL18

Chain BO: 78% 19%



- Molecule 42: Large ribosomal subunit protein eL18

Chain BP: 88% 12%




- Molecule 43: Large ribosomal subunit protein eL19

Chain BQ: 89% 9%



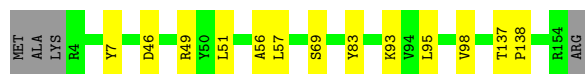
- Molecule 44: Large ribosomal subunit protein eL21

Chain BR:  87% 12% .




- Molecule 45: Large ribosomal subunit protein uL22

Chain BS:  89% 8% .




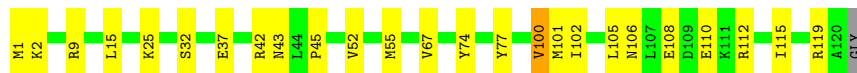
- Molecule 46: Large ribosomal subunit protein uL23

Chain BT:  85% 13% .



- Molecule 47: Large ribosomal subunit protein uL24

Chain BU:  79% 20% ..



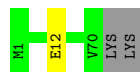
- Molecule 48: Large ribosomal subunit protein eL24

Chain BV:  91% 5% 5%




- Molecule 49: Large ribosomal subunit protein uL29

Chain BW:  96% ..




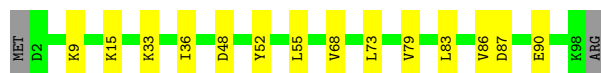
- Molecule 50: Large ribosomal subunit protein uL30

Chain BX:  86% 13% .



- Molecule 51: Large ribosomal subunit protein eL30

Chain BY:  84% 14% .



- Molecule 52: Large ribosomal subunit protein eL31

Chain BZ:  96% ..



- Molecule 53: Large ribosomal subunit protein eL32

Chain Ba:  95% ..



- Molecule 54: Large ribosomal subunit protein eL34

Chain Bb:  91% 8% .




- Molecule 55: Large ribosomal subunit protein eL33

Chain Bc:  91% 8% .




- Molecule 56: Large ribosomal subunit protein eL37

Chain Bd:  87% 10% .



- Molecule 57: Large ribosomal subunit protein eL43

Chain Be:  84% 14% .




- Molecule 58: Large ribosomal subunit protein eL39

Chain Bf:  92% 6% .




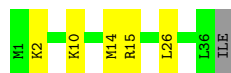
- Molecule 59: Large ribosomal subunit protein eL40

Chain Bg:  84% 6% 10%



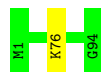
- Molecule 60: Small ribosomal subunit protein eS32

Chain Bh:  84% 14% .



- Molecule 61: Large ribosomal subunit protein eL42

Chain Bi:  99% .




- Molecule 62: Large ribosomal subunit protein eL20

Chain Bj:  94% 6%



- Molecule 63: C2H2-type domain-containing protein

Chain Bk:  81% 16% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91960	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.01	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.600	Depositor
Minimum map value	-1.451	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.074	Depositor
Recommended contour level	0.0083	Depositor
Map size (Å)	443.52002, 443.52002, 443.52002	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.99000007, 0.99000007, 0.99000007	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4SU, A1I59, 5MC, LHH, A2M, OMU, OMG, G7M, UR3, ZN, OMC, 5MU, MA6, 4AC

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	A1	0.12	1/33844 (0.0%)	0.24	0/52748
2	Aa	0.10	0/1603	0.26	0/2167
3	Ab	0.10	0/1535	0.26	0/2065
4	Ac	0.10	0/1542	0.29	0/2067
5	Ad	0.11	0/1476	0.26	0/1980
6	Ae	0.10	0/2024	0.27	0/2732
7	Af	0.09	0/1814	0.25	0/2444
8	Ag	0.13	0/978	0.34	0/1311
9	Ah	0.12	0/1758	0.30	0/2362
10	Ai	0.11	0/1049	0.28	0/1408
11	Aj	0.07	0/981	0.21	0/1312
12	Ak	0.11	0/1064	0.29	0/1426
13	Al	0.10	0/778	0.28	0/1049
14	Am	0.10	0/981	0.27	0/1320
15	An	0.11	0/1141	0.27	0/1518
16	Ao	0.13	0/1121	0.33	0/1507
17	Ap	0.10	0/459	0.32	0/605
18	Aq	0.34	1/1318 (0.1%)	0.54	4/1773 (0.2%)
19	Ar	0.08	0/899	0.22	0/1215
20	As	0.15	0/528	0.36	0/701
21	At	0.09	0/1005	0.23	0/1343
22	Au	0.10	0/1251	0.25	0/1686
23	Av	0.11	0/807	0.27	0/1082
23	Bl	0.10	0/781	0.31	0/1049
24	Aw	0.12	0/471	0.34	0/634
25	Ax	0.10	0/497	0.28	0/668
26	Az	0.17	0/448	0.40	1/610 (0.2%)
27	B1	0.11	2/67034 (0.0%)	0.25	2/104432 (0.0%)
28	B2	0.08	0/2927	0.23	0/4559
29	BA	0.11	0/1859	0.27	0/2512
30	BB	0.10	0/2954	0.26	0/3976
31	BC	0.11	0/2068	0.26	0/2787

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	BD	0.11	0/1437	0.29	0/1925
33	BE	0.09	0/1499	0.24	0/2022
34	BF	0.10	0/939	0.26	0/1267
34	BG	0.13	0/933	0.34	0/1260
35	BH	0.09	0/1413	0.25	0/1897
36	BI	0.10	0/1168	0.23	0/1561
37	BJ	0.08	0/1071	0.23	0/1444
38	BK	0.11	0/618	0.25	0/829
38	BL	0.10	0/626	0.28	0/840
39	BM	0.11	0/1175	0.29	0/1563
40	BN	0.10	0/1626	0.25	0/2169
41	BO	0.09	0/1602	0.24	0/2158
42	BP	0.12	0/980	0.27	0/1313
43	BQ	0.09	0/1254	0.25	0/1655
44	BR	0.10	0/811	0.25	0/1086
45	BS	0.10	0/1225	0.31	0/1651
46	BT	0.11	0/682	0.30	0/915
47	BU	0.13	0/1019	0.31	0/1360
48	BV	0.09	0/548	0.21	0/731
49	BW	0.12	0/566	0.23	0/749
50	BX	0.10	0/1254	0.27	0/1677
51	BY	0.11	0/744	0.26	0/1004
52	BZ	0.10	0/760	0.25	0/1024
53	Ba	0.10	0/1107	0.26	0/1477
54	Bb	0.11	0/751	0.26	0/999
55	Bc	0.10	0/686	0.30	0/916
56	Bd	0.09	0/493	0.24	0/652
57	Be	0.12	0/625	0.30	0/832
58	Bf	0.10	0/445	0.25	0/593
59	Bg	0.08	0/384	0.23	0/509
60	Bh	0.16	0/342	0.33	0/443
61	Bi	0.10	0/805	0.22	0/1064
62	Bj	0.11	0/662	0.24	0/875
63	Bk	0.19	0/524	0.45	1/691 (0.1%)
All	All	0.11	4/169769 (0.0%)	0.26	8/250199 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Aq	89	PRO	CG-CD	-9.98	1.16	1.50
1	A1	775	OMU	O3'-P	5.13	1.61	1.56
27	B1	857	A2M	O3'-P	5.06	1.61	1.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	506	A2M	O3'-P	5.01	1.61	1.56

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Aq	89	PRO	N-CD-CG	-14.76	81.06	103.20
18	Aq	89	PRO	CA-N-CD	-9.29	98.99	112.00
18	Aq	89	PRO	CA-CB-CG	-7.79	89.69	104.50
63	Bk	11	ASP	CA-CB-CG	6.72	119.32	112.60
26	Az	60	PRO	CA-N-CD	-6.42	103.01	112.00
18	Aq	89	PRO	N-CA-CB	-5.98	98.30	103.32
27	B1	2541	A	C1'-C2'-O2'	5.73	120.39	111.80
27	B1	2541	A	C3'-C2'-O2'	5.72	123.18	114.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	32212	0	16327	350	0
2	Aa	1572	0	1629	17	0
3	Ab	1513	0	1580	19	0
4	Ac	1516	0	1597	26	0
5	Ad	1452	0	1521	21	0
6	Ae	1975	0	2040	23	0
7	Af	1784	0	1836	12	0
8	Ag	963	0	1006	12	0
9	Ah	1722	0	1768	31	0
10	Ai	1028	0	1065	11	0
11	Aj	972	0	1037	4	0
12	Ak	1048	0	1085	19	0
13	Al	770	0	797	11	0
14	Am	963	0	994	9	0
15	An	1124	0	1217	12	0
16	Ao	1102	0	1143	24	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Ap	450	0	473	15	0
18	Aq	1290	0	1367	10	0
19	Ar	877	0	898	6	0
20	As	522	0	557	12	0
21	At	985	0	1046	12	0
22	Au	1221	0	1263	13	0
23	Av	791	0	819	8	0
23	Bl	765	0	788	8	0
24	Aw	464	0	503	8	0
25	Ax	495	0	516	9	0
26	Az	434	0	402	3	0
27	B1	63424	0	32104	644	0
28	B2	2689	0	1367	33	0
29	BA	1814	0	1878	19	0
30	BB	2888	0	3025	28	0
31	BC	2026	0	2137	20	0
32	BD	1415	0	1433	15	0
33	BE	1468	0	1507	8	0
34	BF	927	0	971	10	0
34	BG	921	0	969	17	0
35	BH	1383	0	1410	11	0
36	BI	1150	0	1240	8	0
37	BJ	1058	0	1116	6	0
38	BK	614	0	670	4	0
38	BL	621	0	678	16	0
39	BM	1154	0	1219	27	0
40	BN	1587	0	1683	13	0
41	BO	1564	0	1572	31	0
42	BP	966	0	1019	8	0
43	BQ	1238	0	1365	12	0
44	BR	790	0	825	11	0
45	BS	1198	0	1242	10	0
46	BT	674	0	732	8	0
47	BU	1003	0	1074	20	0
48	BV	533	0	523	3	0
49	BW	565	0	618	1	0
50	BX	1235	0	1314	16	0
51	BY	734	0	779	9	0
52	BZ	746	0	803	2	0
53	Ba	1082	0	1172	3	0
54	Bb	733	0	800	7	0
55	Bc	677	0	729	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	Bd	483	0	495	5	0
57	Be	616	0	655	11	0
58	Bf	437	0	498	3	0
59	Bg	375	0	394	2	0
60	Bh	336	0	387	7	0
61	Bi	787	0	833	1	0
62	Bj	652	0	686	4	0
63	Bk	514	0	555	6	0
64	Af	1	0	0	0	0
64	Ap	1	0	0	0	0
64	Ar	1	0	0	0	0
64	Aw	1	0	0	0	0
64	Az	2	0	0	0	0
64	BV	1	0	0	0	0
64	Bb	1	0	0	0	0
64	Bd	1	0	0	0	0
64	Be	1	0	0	0	0
64	Bg	1	0	0	0	0
64	Bi	1	0	0	0	0
64	Bk	1	0	0	0	0
65	A1	151	0	0	34	0
65	Ae	3	0	0	0	0
65	Ag	1	0	0	1	0
65	Ah	1	0	0	0	0
65	Aj	1	0	0	0	0
65	Ak	1	0	0	0	0
65	Al	3	0	0	1	0
65	Am	2	0	0	0	0
65	Ao	2	0	0	0	0
65	Ap	1	0	0	0	0
65	Aq	2	0	0	0	0
65	Au	1	0	0	1	0
65	Av	1	0	0	0	0
65	B1	1173	0	0	153	0
65	B2	19	0	0	0	0
65	BA	10	0	0	1	0
65	BB	6	0	0	0	0
65	BC	7	0	0	2	0
65	BE	1	0	0	0	0
65	BF	1	0	0	0	0
65	BH	6	0	0	1	0
65	BI	7	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
65	BJ	2	0	0	1	0
65	BM	11	0	0	1	0
65	BN	14	0	0	1	0
65	BO	2	0	0	0	0
65	BP	8	0	0	0	0
65	BQ	3	0	0	0	0
65	BR	7	0	0	2	0
65	BS	6	0	0	0	0
65	BT	2	0	0	0	0
65	BU	2	0	0	0	0
65	BW	1	0	0	0	0
65	BX	11	0	0	2	0
65	BZ	2	0	0	0	0
65	Ba	6	0	0	0	0
65	Bb	3	0	0	0	0
65	Bc	4	0	0	0	0
65	Bd	5	0	0	1	0
65	Bf	3	0	0	1	0
65	Bi	3	0	0	0	0
65	Bj	4	0	0	0	0
65	Bk	2	0	0	0	0
All	All	164601	0	117751	1551	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 6.

All (1551) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:945:4AC:HM73	1:A1:1181:4AC:HM71	1.47	0.96
1:A1:302:G:HO2'	5:Ad:2:GLY:N	1.63	0.95
27:B1:574:G:N2	55:Bc:76:PRO:O	2.03	0.91
1:A1:1145:G:O2'	1:A1:1146:G:OP1	1.91	0.89
1:A1:1462:G:O2'	1:A1:1463:U:OP2	1.89	0.89
5:Ad:52:ARG:NH2	7:Af:161:ARG:O	2.07	0.88
1:A1:1146:G:O2'	1:A1:1147:C:OP1	1.93	0.87
1:A1:74:U:O2'	1:A1:76:U:OP2	1.94	0.85
27:B1:2123:G:HO2'	27:B1:2839:U:HO2'	1.14	0.85
1:A1:899:G:O3'	9:Ah:163:ARG:NH2	2.09	0.85
25:Ax:59:GLU:OE1	25:Ax:59:GLU:N	2.09	0.85
27:B1:1919:U:OP2	27:B1:1924:A:N6	2.10	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B1:1987:U:O2'	27:B1:1988:A:N7	2.10	0.82
9:Ah:176:ASN:OD1	9:Ah:177:LYS:N	2.13	0.81
1:A1:624:4AC:HM73	1:A1:691:4AC:HM73	1.62	0.81
12:Ak:55:GLU:OE1	12:Ak:55:GLU:N	2.13	0.81
27:B1:333:A:N1	27:B1:386:U:O2'	2.14	0.81
51:BY:48:ASP:OD1	54:Bb:85:ARG:NH2	2.13	0.81
4:Ac:158:VAL:O	4:Ac:162:VAL:HG23	1.80	0.81
27:B1:1337:G:N7	39:BM:10:LYS:NZ	2.27	0.81
1:A1:801:G:O2'	4:Ac:176:LYS:O	1.97	0.81
1:A1:1307:U:OP1	12:Ak:127:ARG:NH1	2.14	0.81
33:BE:102:LYS:NZ	33:BE:111:GLU:OE2	2.14	0.80
27:B1:115:C:O2'	27:B1:127:U:O2'	1.97	0.80
27:B1:849:A:O2'	27:B1:851:C:OP2	1.99	0.80
1:A1:1084:G:OP1	12:Ak:20:ARG:NH2	2.15	0.80
27:B1:765:G:OP1	42:BP:51:LYS:NZ	2.16	0.79
27:B1:942:C:OP1	27:B1:966:A:O2'	2.01	0.79
27:B1:2475:A:OP2	44:BR:81:SER:OG	2.00	0.79
1:A1:624:4AC:HM73	1:A1:691:4AC:CM7	2.13	0.79
27:B1:1769:4AC:OP2	65:B1:3101:HOH:O	1.99	0.79
1:A1:702:G:O2'	18:Aq:55:ARG:NH1	2.16	0.78
27:B1:662:G:O6	65:B1:3105:HOH:O	2.02	0.78
1:A1:197:A:O2'	1:A1:198:A:O5'	2.01	0.78
27:B1:1459:C:OP2	65:B1:3102:HOH:O	1.99	0.78
27:B1:821:C:OP1	65:B1:3104:HOH:O	2.01	0.78
40:BN:117:TYR:OH	40:BN:129:GLU:OE1	2.00	0.78
1:A1:482:C:N4	15:An:66:ASN:OD1	2.16	0.78
1:A1:897:A:O2'	25:Ax:23:ASP:OD2	2.02	0.78
27:B1:2799:U:OP2	65:B1:3103:HOH:O	2.01	0.78
27:B1:1476:G:OP1	65:B1:3102:HOH:O	2.01	0.77
27:B1:2836:A:OP1	65:B1:3103:HOH:O	2.02	0.77
28:B2:35:U:O4'	41:BO:143:ARG:NH2	2.17	0.77
30:BB:284:LYS:NZ	30:BB:327:SER:O	2.17	0.77
1:A1:100:A:OP2	65:A1:1503:HOH:O	2.03	0.77
41:BO:84:TYR:OH	41:BO:126:ASP:OD2	2.03	0.77
27:B1:259:C:OP1	65:B1:3108:HOH:O	2.03	0.77
29:BA:122:VAL:HG12	29:BA:122:VAL:O	1.83	0.77
1:A1:398:C:O2'	1:A1:575:A:N3	2.17	0.77
1:A1:551:G:H21	10:Ai:124:ARG:HH21	1.33	0.77
1:A1:940:C:OP2	65:A1:1501:HOH:O	2.02	0.76
16:Ao:86:GLU:N	16:Ao:86:GLU:OE1	2.18	0.76
40:BN:70:GLY:O	65:BN:201:HOH:O	2.03	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B1:463:A:OP2	65:B1:3109:HOH:O	2.03	0.76
27:B1:2024:A:N1	65:B1:3216:HOH:O	2.19	0.76
1:A1:1230:A:N3	1:A1:1288:C:O2'	2.18	0.76
1:A1:1297:C:O2'	9:Ah:175:ARG:NH1	2.18	0.76
9:Ah:197:LYS:O	9:Ah:197:LYS:NZ	2.18	0.76
27:B1:1328:C:OP2	65:B1:3106:HOH:O	2.03	0.76
27:B1:182:U:OP1	65:B1:3110:HOH:O	2.03	0.76
27:B1:2691:U:O2'	30:BB:255:SER:OG	2.00	0.76
29:BA:117:ASP:OD1	29:BA:118:GLY:N	2.18	0.76
39:BM:72:GLU:N	39:BM:72:GLU:OE1	2.18	0.76
1:A1:463:A:OP2	65:A1:1502:HOH:O	2.02	0.76
28:B2:7:G:OP1	41:BO:24:ARG:NH1	2.19	0.76
27:B1:1330:G:OP1	65:B1:3107:HOH:O	2.03	0.76
27:B1:1084:G:OP1	65:B1:3112:HOH:O	2.04	0.76
27:B1:1937:C:OP1	29:BA:233:ARG:NH1	2.19	0.75
27:B1:2031:G:N1	27:B1:2051:U:O4	2.20	0.75
1:A1:1462:G:OP1	65:A1:1504:HOH:O	2.03	0.75
27:B1:1418:U:OP2	65:B1:3117:HOH:O	2.05	0.75
27:B1:178:G:OP2	65:B1:3120:HOH:O	2.05	0.75
27:B1:1478:4AC:OP2	65:B1:3111:HOH:O	2.04	0.75
58:Bf:39:PRO:O	65:Bf:101:HOH:O	2.03	0.75
1:A1:940:C:OP1	65:A1:1507:HOH:O	2.04	0.74
27:B1:261:A:OP1	65:B1:3123:HOH:O	2.05	0.74
27:B1:28:G:O2'	27:B1:29:A:OP2	2.06	0.74
27:B1:208:A:OP2	65:B1:3116:HOH:O	2.04	0.74
27:B1:678:A:OP2	65:B1:3113:HOH:O	2.04	0.74
27:B1:1885:4AC:OP2	43:BQ:76:ARG:NH1	2.19	0.74
1:A1:512:C:OP1	65:A1:1506:HOH:O	2.04	0.74
27:B1:2615:C:OP1	65:B1:3105:HOH:O	2.05	0.74
29:BA:169:GLU:O	57:Be:24:ARG:NH1	2.20	0.74
1:A1:828:G:N7	65:A1:1524:HOH:O	2.19	0.74
1:A1:911:G:OP2	16:Ao:130:ARG:NH1	2.20	0.74
1:A1:1241:A:O2'	1:A1:1243:U:OP2	2.05	0.74
1:A1:1366:A1I59:O2	1:A1:1476:MA6:O2'	2.05	0.74
27:B1:765:G:OP2	65:B1:3118:HOH:O	2.05	0.74
27:B1:885:C:OP2	65:B1:3129:HOH:O	2.06	0.74
27:B1:188:C:OP2	65:B1:3115:HOH:O	2.04	0.74
27:B1:1780:C:O2'	27:B1:1781:C:OP2	2.06	0.74
27:B1:1154:U:OP1	27:B1:1175:U:O2'	2.06	0.74
27:B1:1412:G:OP2	65:B1:3114:HOH:O	2.04	0.74
1:A1:1266:G:OP2	65:A1:1508:HOH:O	2.05	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ad:26:GLU:OE1	5:Ad:38:LYS:NZ	2.21	0.74
27:B1:1416:C:OP2	65:B1:3117:HOH:O	2.05	0.74
1:A1:348:G:OP2	1:A1:348:G:N2	2.15	0.73
1:A1:476:C:OP2	65:A1:1505:HOH:O	2.03	0.73
1:A1:904:G:OP1	65:A1:1509:HOH:O	2.06	0.73
27:B1:413:G:N7	65:B1:3109:HOH:O	2.21	0.73
27:B1:1102:U:OP1	65:B1:3124:HOH:O	2.06	0.73
27:B1:1489:OMC:OP2	65:B1:3131:HOH:O	2.06	0.73
27:B1:1127:C:O2'	53:Ba:62:SER:OG	2.05	0.73
27:B1:1359:C:C4	27:B1:1360:4AC:HM73	2.23	0.73
1:A1:1369:C:O2'	27:B1:2044:A:N3	2.20	0.73
27:B1:1333:A:OP1	65:B1:3122:HOH:O	2.05	0.73
23:Av:33:ARG:NH1	23:Av:90:ASP:OD1	2.20	0.73
27:B1:2163:G:OP1	65:B1:3125:HOH:O	2.06	0.73
1:A1:387:C:O2'	1:A1:388:G:OP1	2.07	0.73
1:A1:1466:C:OP1	60:Bh:10:LYS:NZ	2.20	0.73
27:B1:234:A:OP2	65:B1:3132:HOH:O	2.06	0.73
27:B1:1095:U:OP1	65:B1:3130:HOH:O	2.06	0.73
27:B1:1108:G:OP1	65:B1:3127:HOH:O	2.06	0.73
27:B1:163:G:OP2	65:B1:3135:HOH:O	2.07	0.73
27:B1:2401:5MU:O4	65:B1:3126:HOH:O	2.06	0.73
31:BC:71:GLU:OE1	65:BC:301:HOH:O	2.06	0.73
5:Ad:61:ALA:O	5:Ad:70:ARG:NH2	2.22	0.73
27:B1:429:A:N7	65:B1:3202:HOH:O	2.22	0.72
27:B1:1718:C:OP1	57:Be:33:ARG:NH1	2.22	0.72
1:A1:1159:G:OP1	65:A1:1510:HOH:O	2.07	0.72
23:Bl:5:ILE:HD13	23:Bl:43:MET:HE1	1.70	0.72
27:B1:1408:A:OP2	65:B1:3119:HOH:O	2.05	0.72
27:B1:1652:A:OP1	65:B1:3128:HOH:O	2.06	0.72
27:B1:1923:A:OP1	65:B1:3139:HOH:O	2.07	0.72
27:B1:2498:G:OP1	41:BO:29:LYS:NZ	2.22	0.72
31:BC:42:ARG:O	65:BC:302:HOH:O	2.08	0.72
27:B1:946:U:OP1	65:B1:3133:HOH:O	2.06	0.72
27:B1:2501:G:OP2	65:B1:3147:HOH:O	2.08	0.72
10:Ai:18:GLU:OE2	26:Az:16:ARG:NH1	2.21	0.72
27:B1:117:G:OP2	65:B1:3148:HOH:O	2.08	0.72
27:B1:934:G:N7	65:B1:3231:HOH:O	2.22	0.72
47:BU:43:ASN:O	47:BU:119:ARG:NH1	2.23	0.72
1:A1:1298:U:O4	9:Ah:91:ARG:NH2	2.23	0.71
27:B1:926:OMU:OP2	65:B1:3138:HOH:O	2.07	0.71
31:BC:138:PRO:O	23:Bl:13:LEU:HD21	1.90	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:24:C:OP1	5:Ad:9:LYS:NZ	2.22	0.71
27:B1:2862:A:OP2	65:B1:3151:HOH:O	2.09	0.71
29:BA:154:MET:HA	29:BA:154:MET:HE2	1.71	0.71
1:A1:837:G:OP2	15:An:4:LYS:NZ	2.22	0.71
27:B1:923:C:OP1	65:B1:3138:HOH:O	2.08	0.71
1:A1:1143:G:O2'	1:A1:1144:G:N7	2.23	0.71
29:BA:26:GLY:O	65:BA:301:HOH:O	2.07	0.71
51:BY:33:LYS:NZ	51:BY:86:VAL:O	2.16	0.71
1:A1:1282:C:OP2	65:A1:1512:HOH:O	2.09	0.71
27:B1:114:C:OP2	65:B1:3150:HOH:O	2.09	0.71
27:B1:920:OMG:OP1	65:B1:3154:HOH:O	2.09	0.71
1:A1:472:G:N2	15:An:65:PRO:O	2.23	0.71
27:B1:493:A:OP1	65:B1:3134:HOH:O	2.09	0.71
27:B1:32:G:OP1	65:B1:3141:HOH:O	2.08	0.71
27:B1:490:G:O6	65:B1:3134:HOH:O	2.07	0.71
27:B1:829:G:OP2	65:B1:3145:HOH:O	2.08	0.71
35:BH:11:TYR:O	65:BH:201:HOH:O	2.09	0.71
27:B1:1377:U:O4'	65:B1:3158:HOH:O	2.09	0.71
27:B1:1393:G:O6	65:B1:3157:HOH:O	2.09	0.71
27:B1:2749:4AC:O2'	30:BB:132:ILE:O	2.07	0.71
1:A1:462:A:OP2	65:A1:1502:HOH:O	2.08	0.70
27:B1:1333:A:OP2	65:B1:3140:HOH:O	2.08	0.70
1:A1:1077:G:N2	1:A1:1078:U:O4	2.24	0.70
1:A1:1212:A:N3	1:A1:1332:G:O2'	2.23	0.70
27:B1:867:G:N7	65:B1:3243:HOH:O	2.24	0.70
27:B1:877:C:OP1	65:B1:3143:HOH:O	2.08	0.70
27:B1:879:G:OP2	65:B1:3163:HOH:O	2.09	0.70
27:B1:1861:A:OP2	65:B1:3144:HOH:O	2.08	0.70
27:B1:2493:G:OP2	65:B1:3160:HOH:O	2.09	0.70
27:B1:2955:C:O2	27:B1:3031:A:O2'	2.09	0.70
27:B1:2503:C:OP2	65:B1:3137:HOH:O	2.07	0.70
28:B2:28:C:OP1	32:BD:149:ARG:NH1	2.23	0.70
27:B1:2847:A:O3'	30:BB:346:LYS:NZ	2.24	0.70
27:B1:179:G:OP2	65:B1:3149:HOH:O	2.08	0.70
27:B1:662:G:O4'	27:B1:1119:A:N6	2.24	0.70
27:B1:795:G:OP1	65:B1:3159:HOH:O	2.09	0.70
27:B1:1277:G:OP2	65:B1:3162:HOH:O	2.09	0.70
27:B1:1145:A:OP2	65:B1:3152:HOH:O	2.09	0.70
1:A1:1465:G:OP1	65:A1:1504:HOH:O	2.08	0.70
27:B1:209:A:N3	27:B1:224:U:O2'	2.24	0.70
48:BV:48:ARG:NH2	48:BV:62:GLN:OE1	2.25	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B1:1947:G:N7	65:B1:3242:HOH:O	2.24	0.70
34:BG:39:THR:HG23	34:BG:100:ALA:HB2	1.72	0.70
46:BT:73:GLU:N	46:BT:73:GLU:OE1	2.25	0.70
56:Bd:31:LYS:O	65:Bd:201:HOH:O	2.08	0.70
27:B1:220:G:O2'	65:B1:3167:HOH:O	2.10	0.69
27:B1:1073:U:OP2	65:B1:3142:HOH:O	2.08	0.69
27:B1:1388:G:OP2	65:B1:3156:HOH:O	2.09	0.69
27:B1:1542:U:OP1	65:B1:3165:HOH:O	2.09	0.69
1:A1:1007:C:OP2	65:A1:1513:HOH:O	2.09	0.69
9:Ah:29:ARG:O	9:Ah:29:ARG:NE	2.25	0.69
27:B1:809:A:OP1	65:B1:3168:HOH:O	2.10	0.69
1:A1:16:G:OP1	65:A1:1514:HOH:O	2.10	0.69
27:B1:586:G:OP2	65:B1:3166:HOH:O	2.10	0.69
16:Ao:9:ARG:NH2	16:Ao:14:ASP:OD2	2.24	0.69
27:B1:2501:G:N7	65:B1:3236:HOH:O	2.23	0.69
27:B1:2693:A:OP1	65:B1:3172:HOH:O	2.10	0.69
1:A1:864:U:OP2	60:Bh:2:LYS:NZ	2.21	0.69
27:B1:485:4AC:HM72	47:BU:9:ARG:NH1	2.08	0.69
27:B1:879:G:OP1	65:B1:3171:HOH:O	2.10	0.69
27:B1:1524:A:OP1	65:B1:3181:HOH:O	2.11	0.69
27:B1:1537:U:OP2	65:B1:3174:HOH:O	2.10	0.69
1:A1:528:A:OP2	65:A1:1515:HOH:O	2.10	0.69
1:A1:925:U:OP1	65:A1:1516:HOH:O	2.11	0.69
27:B1:933:4AC:O2'	56:Bd:51:TRP:O	2.09	0.69
27:B1:1830:C:OP1	65:B1:3173:HOH:O	2.10	0.69
27:B1:2194:G:OP2	65:B1:3153:HOH:O	2.09	0.69
47:BU:108:GLU:N	47:BU:108:GLU:OE1	2.25	0.69
9:Ah:215:ARG:OXT	25:Ax:62:ARG:NH2	2.26	0.69
12:Ak:80:MET:HE2	12:Ak:105:THR:HG22	1.73	0.69
27:B1:887:OMG:OP1	65:B1:3175:HOH:O	2.10	0.69
30:BB:224:VAL:O	30:BB:334:ARG:NH1	2.26	0.69
27:B1:183:U:OP1	65:B1:3146:HOH:O	2.08	0.69
27:B1:288:G:N7	65:B1:3250:HOH:O	2.25	0.69
27:B1:1471:C:OP2	65:B1:3170:HOH:O	2.10	0.69
27:B1:1778:U:OP2	65:B1:3164:HOH:O	2.09	0.69
22:Au:82:ASN:OD1	65:Au:201:HOH:O	2.10	0.69
27:B1:2493:G:N2	27:B1:2496:A:OP2	2.25	0.69
42:BP:102:THR:OG1	42:BP:105:GLU:OE1	2.04	0.69
27:B1:1107:4AC:OP2	65:B1:3169:HOH:O	2.10	0.68
1:A1:642:A:O2'	1:A1:656:A:N6	2.26	0.68
27:B1:489:A:OP2	65:B1:3161:HOH:O	2.09	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B1:557:G:N7	65:B1:3257:HOH:O	2.26	0.68
32:BD:90:LEU:O	32:BD:94:LEU:HD12	1.92	0.68
10:AI:51:GLU:OE2	10:AI:62:ARG:NH1	2.26	0.68
27:B1:367:G:OP1	65:B1:3185:HOH:O	2.11	0.68
27:B1:1331:G:OP2	65:B1:3107:HOH:O	2.11	0.68
44:BR:55:ASP:OD2	65:BR:101:HOH:O	2.11	0.68
16:Ao:64:GLU:N	16:Ao:64:GLU:OE2	2.26	0.68
27:B1:1360:4AC:O7	27:B1:1374:4AC:HM73	1.93	0.68
27:B1:1661:A:OP1	65:B1:3176:HOH:O	2.10	0.68
27:B1:2637:C:O2'	27:B1:2680:A:N3	2.25	0.68
3:Ab:88:PRO:O	3:Ab:95:GLN:NE2	2.27	0.68
27:B1:2380:G:OP1	65:B1:3178:HOH:O	2.11	0.68
27:B1:1938:A:O2'	27:B1:1942:A:N3	2.27	0.68
27:B1:2347:A:OP1	65:B1:3188:HOH:O	2.12	0.68
37:BJ:16:ARG:NH1	37:BJ:17:PRO:O	2.26	0.68
27:B1:2504:C:OP1	65:B1:3183:HOH:O	2.11	0.68
1:A1:1288:C:OP1	22:Au:81:LYS:NZ	2.26	0.68
27:B1:486:G:OP1	65:B1:3177:HOH:O	2.11	0.68
27:B1:1094:G:N2	27:B1:1097:A:OP2	2.18	0.68
27:B1:195:G:OP2	65:B1:3187:HOH:O	2.12	0.68
1:A1:513:U:O4	65:A1:1511:HOH:O	2.08	0.67
1:A1:1091:C:O2'	22:Au:130:ASP:OD2	2.12	0.67
27:B1:722:G:OP2	65:B1:3179:HOH:O	2.11	0.67
27:B1:2185:G:O2'	27:B1:2187:C:N4	2.20	0.67
1:A1:207:G:N2	1:A1:210:A:OP2	2.24	0.67
27:B1:137:U:O2'	27:B1:138:A:O4'	2.11	0.67
27:B1:999:G:OP2	65:B1:3186:HOH:O	2.11	0.67
27:B1:1149:C:OP2	65:B1:3190:HOH:O	2.13	0.67
27:B1:2404:G:OP1	65:B1:3137:HOH:O	2.11	0.67
21:At:81:ILE:HD12	21:At:94:ILE:HD11	1.77	0.67
27:B1:939:U:OP2	65:B1:3189:HOH:O	2.12	0.67
27:B1:1781:C:H1'	54:Bb:6:ARG:NH1	2.10	0.67
27:B1:2839:U:OP2	65:B1:3182:HOH:O	2.11	0.67
27:B1:2054:G:N2	27:B1:2054:G:OP2	2.28	0.67
27:B1:2829:G:OP2	65:B1:3184:HOH:O	2.11	0.67
6:Ae:89:ASP:OD1	6:Ae:90:VAL:N	2.28	0.66
27:B1:879:G:O2'	27:B1:1819:G:OP1	2.14	0.66
38:BK:26:ASP:OD1	38:BK:27:ILE:N	2.28	0.66
39:BM:42:ARG:O	65:BM:201:HOH:O	2.13	0.66
27:B1:1978:C:O2	65:B1:3155:HOH:O	2.09	0.66
1:A1:1159:G:OP2	65:A1:1513:HOH:O	2.13	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B1:2146:G:N7	65:B1:3268:HOH:O	2.28	0.66
27:B1:2730:A:N1	65:B1:3263:HOH:O	2.27	0.66
63:Bk:30:ARG:O	63:Bk:34:THR:HG23	1.96	0.66
6:Ae:15:ALA:O	6:Ae:23:ARG:NH2	2.28	0.66
27:B1:1280:U:OP2	36:Bi:39:THR:OG1	2.12	0.66
34:BF:3:LYS:NZ	34:BF:10:GLU:OE2	2.28	0.66
1:A1:924:A:N3	1:A1:929:A:O2'	2.25	0.66
13:Al:54:ASP:OD1	65:Al:201:HOH:O	2.12	0.66
27:B1:2166:A:O2'	27:B1:2167:C:OP1	2.14	0.66
2:Aa:102:THR:OG1	2:Aa:129:GLU:OE1	2.13	0.66
27:B1:1831:U:OP2	65:B1:3173:HOH:O	2.13	0.66
27:B1:1922:U:OP1	65:B1:3194:HOH:O	2.14	0.66
27:B1:2970:G:OP2	30:BB:130:ARG:NH2	2.28	0.66
1:A1:15:U:O2'	1:A1:527:A:N6	2.29	0.66
1:A1:188:C:OP2	6:Ae:134:LYS:NZ	2.26	0.66
25:Ax:36:ASP:OD2	25:Ax:60:THR:OG1	2.06	0.66
27:B1:2052:A:O2'	27:B1:2053:A:O5'	2.13	0.66
1:A1:578:4AC:OP1	6:Ae:24:LYS:NZ	2.20	0.66
27:B1:3007:G:N7	65:B1:3274:HOH:O	2.29	0.66
27:B1:127:U:OP1	58:Bf:12:ARG:NH2	2.29	0.65
27:B1:1824:A:OP2	65:B1:3193:HOH:O	2.14	0.65
1:A1:1271:G:OP1	16:Ao:116:ARG:NH1	2.29	0.65
27:B1:484:C:N4	27:B1:485:4AC:O7	2.29	0.65
27:B1:1004:C:O2'	27:B1:1005:U:OP1	2.14	0.65
50:BX:71:ARG:O	65:BX:201:HOH:O	2.13	0.65
27:B1:2868:U:O4	65:B1:3151:HOH:O	2.12	0.65
27:B1:2962:A:N7	65:B1:3277:HOH:O	2.29	0.65
1:A1:527:A:OP2	65:A1:1515:HOH:O	2.13	0.65
27:B1:1939:G:N7	29:BA:145:SER:OG	2.29	0.65
27:B1:2617:5MC:O2'	27:B1:2618:G:OP1	2.14	0.65
27:B1:167:G:OP2	27:B1:167:G:N2	2.23	0.65
27:B1:2229:G:O6	27:B1:2309:C:N4	2.30	0.65
1:A1:766:U:O2'	1:A1:860:A:N1	2.29	0.65
27:B1:1287:G:O2'	62:Bj:49:ARG:NE	2.30	0.65
27:B1:2377:U:OP2	44:BR:4:LYS:NZ	2.30	0.65
27:B1:2835:C:O2'	30:BB:365:GLN:OXT	2.13	0.65
28:B2:85:C:O2'	28:B2:87:C:OP1	2.13	0.65
51:BY:15:LYS:N	51:BY:87:ASP:OD1	2.30	0.65
33:BE:56:TYR:OH	33:BE:58:ASP:OD1	2.07	0.65
27:B1:1122:C:O3'	50:BX:131:LYS:NZ	2.28	0.64
27:B1:2989:A:OP2	65:B1:3196:HOH:O	2.14	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Ag:94:PHE:O	65:Ag:201:HOH:O	2.15	0.64
27:B1:897:G:OP1	65:B1:3191:HOH:O	2.13	0.64
27:B1:1920:A:OP1	65:B1:3194:HOH:O	2.15	0.64
51:BY:36:ILE:HD12	51:BY:83:LEU:HD11	1.78	0.64
1:A1:1020:A:N1	1:A1:1061:G:O2'	2.26	0.64
1:A1:1438:U:O2'	1:A1:1439:G:OP1	2.15	0.64
27:B1:1576:G:OP1	54:Bb:59:LYS:NZ	2.30	0.64
1:A1:712:U:OP1	18:Aq:7:ARG:NH2	2.31	0.64
13:Al:92:GLU:OE1	13:Al:92:GLU:N	2.31	0.64
19:Ar:57:LEU:HD11	19:Ar:64:GLU:OE2	1.98	0.64
27:B1:177:G:OP1	40:BN:194:LYS:NZ	2.30	0.64
1:A1:317:C:OP1	1:A1:1423:C:O2'	2.14	0.64
4:Ac:35:THR:OG1	4:Ac:46:ARG:NH1	2.31	0.64
6:Ae:207:MET:HE3	19:Ar:7:LEU:HD23	1.80	0.64
9:Ah:24:GLU:N	9:Ah:24:GLU:OE1	2.29	0.64
22:Au:18:GLN:OE1	22:Au:21:LYS:NZ	2.29	0.64
27:B1:2634:A:OP2	65:B1:3198:HOH:O	2.15	0.64
41:BO:71:PHE:O	41:BO:191:ARG:NH1	2.31	0.64
27:B1:238:G:OP2	65:B1:3197:HOH:O	2.15	0.64
27:B1:1315:A:OP1	23:Bl:57:ARG:NH2	2.31	0.64
10:Ai:36:GLU:OE1	10:Ai:39:ARG:NH1	2.30	0.64
27:B1:32:G:O2'	27:B1:1381:G:OP1	2.16	0.64
27:B1:1414:A:N3	27:B1:2128:G:O2'	2.24	0.64
8:Ag:68:ASP:OD2	8:Ag:108:ARG:NE	2.31	0.63
27:B1:1898:G:OP1	65:B1:3199:HOH:O	2.15	0.63
1:A1:252:G:O2'	1:A1:253:U:OP1	2.16	0.63
1:A1:779:G:OP1	18:Aq:2:ALA:N	2.31	0.63
1:A1:971:G:N1	1:A1:982:U:O4	2.31	0.63
27:B1:1831:U:O4	65:B1:3195:HOH:O	2.14	0.63
27:B1:430:U:OP1	27:B1:431:A:N6	2.26	0.63
31:BC:118:ILE:O	31:BC:121:THR:HG22	1.98	0.63
1:A1:197:A:OP2	65:A1:1518:HOH:O	2.15	0.63
27:B1:1458:C:OP1	65:B1:3102:HOH:O	2.15	0.63
27:B1:262:A:H62	27:B1:298:G:H21	1.46	0.63
44:BR:11:LYS:NZ	65:BR:102:HOH:O	2.23	0.63
1:A1:608:U:OP1	18:Aq:16:ARG:NH1	2.31	0.63
27:B1:298:G:O2'	27:B1:299:G:O5'	2.13	0.63
1:A1:518:U:O4	65:A1:1517:HOH:O	2.13	0.63
1:A1:1314:4AC:CM7	12:Ak:124:LYS:HA	2.29	0.63
20:As:25:THR:HG22	20:As:30:HIS:ND1	2.14	0.63
27:B1:1144:A:H61	55:Bc:14:LYS:HG2	1.63	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:532:G:OP1	65:A1:1519:HOH:O	2.16	0.62
27:B1:321:C:O2'	63:Bk:34:THR:HG22	1.98	0.62
39:BM:87:GLU:N	39:BM:87:GLU:OE1	2.32	0.62
27:B1:1739:A:O2'	27:B1:1742:C:O2	2.18	0.62
27:B1:2563:G:O4'	27:B1:2617:5MC:HM52	1.99	0.62
27:B1:985:U:N3	27:B1:1064:4AC:HM73	2.14	0.62
27:B1:341:G:OP2	47:BU:42:ARG:NH2	2.32	0.62
27:B1:2421:C:OP2	27:B1:2422:A:O2'	2.11	0.62
27:B1:2762:G:OP2	27:B1:2846:C:O2'	2.18	0.62
27:B1:2856:G:OP1	59:Bg:33:LYS:NZ	2.28	0.61
1:A1:1178:C:O2	17:Ap:7:ASN:ND2	2.33	0.61
27:B1:658:U:O2'	39:BM:22:LYS:NZ	2.33	0.61
27:B1:1589:C:O2'	27:B1:1724:A:OP1	2.11	0.61
27:B1:1977:5MC:O2'	27:B1:2052:A:N3	2.32	0.61
1:A1:849:G:O2'	1:A1:865:G:O6	2.15	0.61
27:B1:2251:G:O2'	27:B1:2252:G:O5'	2.16	0.61
1:A1:207:G:O2'	1:A1:210:A:N6	2.32	0.61
1:A1:968:C:OP2	17:Ap:3:LYS:NZ	2.32	0.61
26:Az:41:GLU:O	26:Az:45:VAL:HG23	2.00	0.61
27:B1:534:G:OP1	45:BS:7:TYR:OH	2.15	0.61
27:B1:2240:C:N4	27:B1:2241:G:O6	2.33	0.61
27:B1:2645:G:OP1	33:BE:166:ARG:NH2	2.32	0.61
4:Ac:17:GLN:OE1	4:Ac:76:GLN:NE2	2.33	0.61
27:B1:778:A:N1	27:B1:2487:A:O2'	2.34	0.61
27:B1:1696:G:O2'	27:B1:1697:G:OP1	2.17	0.61
41:BO:25:LEU:HD13	44:BR:28:LEU:HD12	1.83	0.61
41:BO:100:GLU:N	41:BO:100:GLU:OE1	2.32	0.61
19:Ar:38:VAL:HG13	19:Ar:47:VAL:HG13	1.82	0.61
40:BN:169:GLY:O	40:BN:194:LYS:NZ	2.33	0.61
27:B1:401:U:O4	65:B1:3200:HOH:O	2.16	0.61
27:B1:1396:G:N7	65:B1:3133:HOH:O	2.31	0.60
27:B1:2562:OMG:H2'	27:B1:2617:5MC:HM51	1.81	0.60
27:B1:2564:A:OP1	65:B1:3105:HOH:O	2.16	0.60
1:A1:81:C:HO2'	1:A1:82:G:H8	1.48	0.60
9:Ah:17:VAL:HG12	9:Ah:18:MET:HG3	1.83	0.60
27:B1:55:OMG:O2'	56:Bd:58:LYS:NZ	2.33	0.60
34:BG:67:PRO:HG2	34:BG:68:PRO:HD2	1.84	0.60
1:A1:1184:G:OP2	1:A1:1284:C:N4	2.31	0.60
2:Aa:36:ARG:NH1	2:Aa:38:ASP:OD1	2.34	0.60
27:B1:2473:A:O2'	44:BR:79:ASP:OD2	2.18	0.60
27:B1:1540:U:OP1	65:B1:3203:HOH:O	2.17	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BS:46:ASP:OD1	45:BS:49:ARG:NH2	2.34	0.60
3:Ab:15:MET:CE	17:Ap:46:VAL:HG21	2.32	0.60
41:BO:184:HIS:O	41:BO:188:VAL:HG23	2.02	0.60
1:A1:676:A:OP2	4:Ac:128:ARG:NH1	2.35	0.60
16:Ao:60:LYS:O	16:Ao:64:GLU:OE2	2.19	0.60
27:B1:2958:G:O2'	27:B1:2960:A:N7	2.25	0.60
8:Ag:57:GLU:OE1	8:Ag:57:GLU:N	2.33	0.60
1:A1:245:G:N2	11:Aj:13:SER:O	2.29	0.60
27:B1:198:C:OP2	56:Bd:50:ARG:NH1	2.35	0.60
27:B1:1482:G:O3'	46:BT:13:THR:HG21	2.02	0.60
27:B1:503:G:N2	27:B1:506:A2M:OP2	2.33	0.59
31:BC:123:ASN:OD1	31:BC:124:TYR:N	2.35	0.59
1:A1:900:G:OP1	9:Ah:163:ARG:NH1	2.34	0.59
2:Aa:101:MET:HE1	2:Aa:115:LEU:CD1	2.33	0.59
5:Ad:132:VAL:N	5:Ad:135:GLN:O	2.35	0.59
6:Ae:49:VAL:HG21	6:Ae:66:LEU:HD21	1.84	0.59
1:A1:1033:A:OP1	7:Af:102:HIS:NE2	2.33	0.59
3:Ab:67:ARG:HE	3:Ab:71:LYS:HE3	1.67	0.59
5:Ad:71:GLU:OE1	5:Ad:71:GLU:N	2.36	0.59
6:Ae:219:GLU:N	6:Ae:219:GLU:OE1	2.36	0.59
13:Al:8:ILE:HG22	13:Al:96:ILE:HG12	1.85	0.59
47:BU:67:VAL:N	47:BU:77:TYR:O	2.34	0.59
1:A1:1005:U:O2'	1:A1:1008:A:OP2	2.15	0.59
27:B1:594:C:OP1	55:Bc:54:LYS:NZ	2.35	0.59
28:B2:14:G:HO2'	41:BO:2:ALA:N	2.01	0.59
38:BL:54:GLU:OE1	51:BY:52:TYR:OH	2.21	0.59
1:A1:304:G:OP2	1:A1:304:G:N2	2.25	0.59
27:B1:1623:G:O2'	27:B1:1700:U:O2'	2.13	0.59
27:B1:2589:C:OP1	27:B1:2645:G:N2	2.34	0.59
1:A1:1197:U:OP1	65:A1:1520:HOH:O	2.16	0.59
12:Ak:86:LEU:O	12:Ak:90:THR:HG22	2.03	0.59
25:Ax:61:GLU:OE1	25:Ax:61:GLU:N	2.36	0.59
1:A1:1121:U:OP2	20:As:49:ARG:NH2	2.36	0.59
16:Ao:29:LYS:NZ	16:Ao:99:ASP:OD1	2.27	0.59
27:B1:148:C:OP1	40:BN:107:LYS:NZ	2.28	0.59
27:B1:2259:A:O2'	27:B1:2260:G:OP1	2.20	0.59
1:A1:259:A:OP2	11:Aj:54:LYS:NZ	2.34	0.59
1:A1:907:G:HO2'	1:A1:1268:A:HO2'	1.46	0.59
27:B1:726:G:N3	27:B1:774:U:O2'	2.36	0.59
30:BB:170:GLN:O	30:BB:173:VAL:HG12	2.03	0.59
1:A1:1007:C:OP1	65:A1:1510:HOH:O	2.16	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Ae:38:ASN:O	6:Ae:42:SER:OG	2.19	0.59
27:B1:1360:4AC:CM7	27:B1:1360:4AC:H5	2.33	0.58
30:BB:75:THR:O	30:BB:75:THR:HG22	2.02	0.58
51:BY:87:ASP:OD1	51:BY:87:ASP:O	2.19	0.58
6:Ae:55:TYR:OH	6:Ae:98:GLU:OE1	2.21	0.58
30:BB:346:LYS:HD2	30:BB:346:LYS:N	2.18	0.58
17:Ap:48:PRO:O	17:Ap:53:ARG:NH1	2.36	0.58
57:Be:21:ILE:O	57:Be:25:VAL:HG23	2.04	0.58
27:B1:2525:C:OP2	65:B1:3204:HOH:O	2.17	0.58
1:A1:1467:4AC:H5	1:A1:1467:4AC:CM7	2.34	0.58
7:Af:136:ARG:NH1	7:Af:219:GLU:OE1	2.36	0.58
50:BX:62:GLU:OE1	50:BX:62:GLU:N	2.25	0.58
50:BX:120:HIS:NE2	65:BX:202:HOH:O	2.21	0.58
1:A1:675:C:O2'	4:Ac:100:THR:O	2.19	0.58
27:B1:2563:G:OP1	65:B1:3201:HOH:O	2.16	0.58
6:Ae:185:VAL:HG11	6:Ae:199:ILE:HD11	1.85	0.58
15:An:143:GLU:OE1	15:An:143:GLU:N	2.37	0.57
27:B1:948:C:OP2	65:B1:3205:HOH:O	2.17	0.57
27:B1:2053:A:O2'	27:B1:2054:G:O4'	2.22	0.57
1:A1:1119:A:N7	1:A1:1142:A:N6	2.52	0.57
27:B1:888:5MU:O2'	27:B1:889:U:OP2	2.17	0.57
31:BC:233:GLY:O	31:BC:234:THR:OG1	2.17	0.57
38:BK:75:LEU:CD2	38:BK:80:ILE:HD11	2.34	0.57
27:B1:2987:G:O2'	27:B1:2988:U:OP2	2.19	0.57
50:BX:70:LYS:HE3	50:BX:155:LEU:HD23	1.87	0.57
1:A1:703:G:N2	24:Aw:11:SER:O	2.34	0.57
22:Au:20:LEU:HD12	22:Au:23:ILE:HD13	1.85	0.57
31:BC:175:GLU:OE1	31:BC:175:GLU:C	2.47	0.57
41:BO:151:GLU:OE2	41:BO:151:GLU:N	2.37	0.57
27:B1:380:U:O2'	27:B1:381:A:OP1	2.23	0.57
39:BM:124:ILE:HD12	39:BM:124:ILE:O	2.05	0.57
27:B1:2419:G:H22	27:B1:2427:U:H3	1.51	0.57
27:B1:2617:5MC:H4'	27:B1:2618:G:OP2	2.04	0.57
12:Ak:36:ILE:O	12:Ak:42:ARG:NH1	2.36	0.57
27:B1:1309:G:N7	65:B1:3290:HOH:O	2.32	0.57
27:B1:2243:A:O4'	27:B1:2294:G:N2	2.37	0.57
28:B2:47:C:OP2	41:BO:39:LYS:NZ	2.38	0.57
1:A1:1454:G:H1'	1:A1:1475:MA6:H2	1.87	0.57
27:B1:253:A:O2'	27:B1:470:A:N3	2.36	0.57
16:Ao:104:GLU:OE2	16:Ao:104:GLU:O	2.23	0.56
27:B1:2471:U:OP2	27:B1:2472:A:O2'	2.17	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Ao:112:ILE:HD13	21:At:97:GLU:HG2	1.86	0.56
27:B1:1368:A:O2'	27:B1:1369:A:O5'	2.23	0.56
51:BY:9:LYS:NZ	51:BY:90:GLU:O	2.31	0.56
1:A1:1308:A:O2'	9:Ah:53:LYS:HD3	2.05	0.56
10:Ai:104:VAL:HG22	10:Ai:125:LEU:HD23	1.88	0.56
27:B1:442:A:OP2	40:BN:12:LYS:NZ	2.37	0.56
27:B1:1331:G:O2'	27:B1:1332:U:O5'	2.23	0.56
27:B1:1359:C:C5	27:B1:1360:4AC:HM73	2.40	0.56
27:B1:3013:C:OP2	27:B1:3014:U:O2'	2.13	0.56
46:BT:13:THR:HG22	46:BT:14:GLU:OE1	2.05	0.56
57:Be:78:VAL:O	57:Be:82:THR:HG22	2.05	0.56
1:A1:940:C:O2	17:Ap:17:GLY:N	2.39	0.56
27:B1:1526:G:OP2	65:B1:3208:HOH:O	2.18	0.56
1:A1:679:G:OP1	1:A1:813:U:O2'	2.24	0.56
1:A1:1457:MA6:OP1	65:A1:1521:HOH:O	2.17	0.56
47:BU:52:VAL:HG13	47:BU:100:VAL:HG13	1.88	0.56
1:A1:635:C:H2'	1:A1:636:4AC:H6	1.88	0.56
1:A1:939:C:O2	17:Ap:12:ARG:NH1	2.39	0.56
27:B1:1050:U:C4	27:B1:1052:4AC:HM72	2.41	0.56
1:A1:1402:A:O2'	48:BV:62:GLN:O	2.24	0.56
13:Al:82:MET:HE3	13:Al:83:ARG:HB2	1.86	0.56
27:B1:2776:G:N2	27:B1:2779:A:OP2	2.37	0.56
27:B1:2961:G:N7	65:B1:3275:HOH:O	2.33	0.56
34:BF:60:GLU:OE2	34:BF:60:GLU:N	2.38	0.56
63:Bk:38:ASN:OD1	63:Bk:47:ARG:NH1	2.39	0.56
1:A1:112:G:O2'	19:Ar:30:HIS:ND1	2.38	0.56
27:B1:338:G:N1	27:B1:380:U:OP2	2.36	0.56
47:BU:1:MET:HE2	47:BU:1:MET:HA	1.87	0.56
27:B1:490:G:OP2	65:B1:3207:HOH:O	2.18	0.55
27:B1:2198:U:OP1	65:B1:3209:HOH:O	2.18	0.55
4:Ac:51:THR:OG1	4:Ac:54:ASP:OD2	2.24	0.55
27:B1:1003:A:N3	65:B1:3292:HOH:O	2.33	0.55
40:BN:33:GLU:O	40:BN:65:ARG:NH2	2.40	0.55
4:Ac:76:GLN:OE1	4:Ac:76:GLN:HA	2.05	0.55
23:Av:49:GLU:N	23:Av:49:GLU:OE1	2.38	0.55
27:B1:735:C:O2'	27:B1:736:A:OP1	2.23	0.55
27:B1:2185:G:H21	27:B1:2186:A:H61	1.53	0.55
12:Ak:4:ILE:HD12	12:Ak:89:TRP:HE3	1.72	0.55
27:B1:90:C:OP2	27:B1:91:A:O2'	2.22	0.55
1:A1:1367:G:H2'	1:A1:1368:OMU:H6	1.88	0.55
9:Ah:124:VAL:O	9:Ah:128:GLU:HG3	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Aq:137:LYS:NZ	18:Aq:146:TRP:O	2.36	0.55
27:B1:1758:G:OP2	65:B1:3206:HOH:O	2.18	0.55
27:B1:2711:G:N2	27:B1:2714:A:OP2	2.34	0.55
1:A1:945:4AC:CM7	1:A1:1181:4AC:HM71	2.29	0.55
32:BD:109:GLU:N	32:BD:109:GLU:OE1	2.39	0.55
41:BO:73:TRP:HE3	41:BO:188:VAL:HG21	1.71	0.55
47:BU:37:GLU:HA	47:BU:37:GLU:OE1	2.07	0.55
27:B1:996:G:O2'	27:B1:1053:G:O6	2.25	0.55
1:A1:1314:4AC:HM71	12:Ak:124:LYS:HA	1.88	0.55
6:Ae:189:GLN:NE2	6:Ae:229:TYR:CE1	2.75	0.55
27:B1:426:U:O2'	27:B1:428:G:N7	2.35	0.55
27:B1:937:G:N7	31:BC:54:LYS:NZ	2.51	0.54
33:BE:4:ASP:OD1	33:BE:5:ALA:N	2.40	0.54
24:Aw:43:THR:HG21	24:Aw:46:GLU:OE2	2.06	0.54
27:B1:793:A:N3	31:BC:33:ARG:NH2	2.52	0.54
50:BX:150:LEU:O	50:BX:154:MET:HG3	2.07	0.54
47:BU:55:MET:HE1	47:BU:101:MET:HB3	1.90	0.54
1:A1:168:G:N7	65:A1:1541:HOH:O	2.34	0.54
27:B1:1116:A:O2'	27:B1:1117:A:O5'	2.18	0.54
27:B1:2067:5MC:OP2	27:B1:2068:U:O2'	2.21	0.54
27:B1:298:G:C2'	27:B1:299:G:O5'	2.55	0.54
8:Ag:62:GLU:HA	8:Ag:62:GLU:OE1	2.08	0.54
27:B1:212:A:OP1	65:B1:3211:HOH:O	2.18	0.54
27:B1:1782:C:O2'	54:Bb:1:MET:SD	2.66	0.54
1:A1:110:C:OP1	1:A1:559:C:O2'	2.19	0.54
32:BD:182:GLU:N	32:BD:182:GLU:OE1	2.41	0.54
1:A1:116:C:O2'	1:A1:259:A:N3	2.36	0.54
2:Aa:198:LYS:HD3	2:Aa:198:LYS:C	2.33	0.54
46:BT:16:ALA:O	46:BT:20:ILE:HG13	2.08	0.54
1:A1:615:G:H2'	1:A1:616:G:C8	2.42	0.53
1:A1:897:A:OP2	65:A1:1522:HOH:O	2.18	0.53
12:Ak:31:LYS:NZ	12:Ak:35:ILE:O	2.38	0.53
27:B1:603:G:OP1	50:BX:123:ARG:NH2	2.41	0.53
50:BX:69:ARG:NH1	50:BX:82:ASP:OD2	2.40	0.53
5:Ad:48:LEU:O	5:Ad:52:ARG:HG3	2.07	0.53
39:BM:103:VAL:CG1	39:BM:124:ILE:HG22	2.38	0.53
1:A1:101:G:OP2	65:A1:1523:HOH:O	2.19	0.53
1:A1:1466:C:C4	1:A1:1467:4AC:HM73	2.44	0.53
33:BE:18:GLU:OE2	33:BE:20:THR:OG1	2.19	0.53
41:BO:54:LYS:HD3	41:BO:54:LYS:C	2.34	0.53
27:B1:1070:A:N3	27:B1:1308:C:O2'	2.34	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B1:1455:G:OP2	27:B1:1455:G:N2	2.30	0.53
29:BA:122:VAL:O	29:BA:122:VAL:CG1	2.55	0.53
50:BX:95:GLU:OE2	50:BX:95:GLU:HA	2.08	0.53
1:A1:771:A:OP1	1:A1:1483:G:O2'	2.24	0.53
1:A1:802:A:O2'	4:Ac:177:ILE:O	2.26	0.53
1:A1:902:G:OP2	9:Ah:77:SER:OG	2.25	0.53
27:B1:1857:G:OP2	27:B1:1858:A:O2'	2.18	0.53
1:A1:512:C:OP2	1:A1:513:U:O2'	2.20	0.53
10:Ai:18:GLU:C	10:Ai:18:GLU:OE1	2.51	0.53
27:B1:1296:G:O6	65:B1:3210:HOH:O	2.18	0.53
1:A1:1462:G:HO2'	1:A1:1463:U:P	2.26	0.53
1:A1:372:U:OP1	6:Ae:50:ARG:NH1	2.42	0.53
5:Ad:148:GLU:C	5:Ad:148:GLU:OE1	2.51	0.53
8:Ag:49:GLU:OE1	8:Ag:49:GLU:N	2.42	0.53
27:B1:583:A:OP2	65:B1:3212:HOH:O	2.19	0.53
27:B1:2207:G:OP1	40:BN:72:LYS:NZ	2.38	0.53
1:A1:372:U:O2'	6:Ae:28:TRP:O	2.27	0.53
14:Am:58:TYR:CZ	14:Am:62:LEU:HD11	2.44	0.53
27:B1:337:4AC:HM73	27:B1:380:U:OP2	2.08	0.53
27:B1:978:C:H2'	27:B1:979:4AC:H6	1.91	0.53
23:Bl:5:ILE:HD12	23:Bl:5:ILE:N	2.24	0.53
1:A1:252:G:O2'	1:A1:253:U:P	2.67	0.52
13:Al:52:SER:O	17:Ap:40:ARG:NH1	2.41	0.52
27:B1:2698:G:OP2	65:B1:3215:HOH:O	2.19	0.52
32:BD:177:GLU:OE1	32:BD:177:GLU:HA	2.09	0.52
57:Be:25:VAL:O	57:Be:29:GLU:HG3	2.08	0.52
7:Af:213:ILE:O	10:Ai:68:ARG:NH2	2.42	0.52
21:At:17:MET:HE1	21:At:74:PRO:C	2.34	0.52
27:B1:913:G:OP2	65:B1:3214:HOH:O	2.19	0.52
41:BO:183:GLU:OE1	41:BO:183:GLU:N	2.42	0.52
50:BX:70:LYS:CE	50:BX:155:LEU:HD23	2.39	0.52
2:Aa:6:LEU:O	2:Aa:173:ARG:NH2	2.41	0.52
16:Ao:6:HIS:C	16:Ao:7:ILE:HD12	2.35	0.52
27:B1:2234:G:O6	27:B1:2304:A:N6	2.42	0.52
31:BC:29:ASP:OD1	31:BC:29:ASP:N	2.41	0.52
46:BT:4:TYR:OH	46:BT:41:ARG:NH2	2.43	0.52
1:A1:820:G:O6	1:A1:828:G:N2	2.43	0.52
3:Ab:21:LEU:HD21	3:Ab:65:LEU:HD11	1.90	0.52
12:Ak:103:ASP:OD1	12:Ak:105:THR:N	2.40	0.52
27:B1:1760:A:OP1	65:B1:3213:HOH:O	2.19	0.52
1:A1:351:G:H3'	1:A1:352:5MC:HM53	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:1240:G:H4'	1:A1:1241:A:OP2	2.09	0.52
27:B1:1488:OMU:OP1	27:B1:1489:OMC:N4	2.41	0.52
27:B1:1696:G:O2'	27:B1:1697:G:P	2.68	0.52
27:B1:2094:A:O2'	27:B1:2097:G:N3	2.35	0.52
39:BM:73:VAL:O	39:BM:73:VAL:HG13	2.10	0.52
1:A1:387:C:O2'	1:A1:388:G:P	2.68	0.52
1:A1:432:U:O2'	23:Av:56:ILE:O	2.28	0.52
27:B1:298:G:HO2'	27:B1:299:G:C5'	2.21	0.52
41:BO:162:GLU:N	41:BO:162:GLU:OE1	2.42	0.52
1:A1:377:G:N2	1:A1:380:A:OP2	2.37	0.52
1:A1:1118:G:OP1	20:As:32:LYS:NZ	2.39	0.52
13:Al:30:THR:HG22	13:Al:32:VAL:HG23	1.91	0.52
38:BL:67:SER:OG	38:BL:70:GLU:OE1	2.27	0.52
41:BO:43:HIS:ND1	41:BO:64:THR:OG1	2.41	0.52
7:Af:51:ASP:OD1	7:Af:58:ASN:ND2	2.42	0.52
7:Af:219:GLU:OE1	7:Af:219:GLU:O	2.27	0.52
42:BP:87:GLU:OE1	42:BP:87:GLU:HA	2.09	0.52
1:A1:642:A:N1	1:A1:655:U:O2'	2.41	0.51
35:BH:129:ASP:OD2	35:BH:161:TYR:OH	2.26	0.51
23:Bl:2:GLU:O	23:Bl:23:ILE:HD12	2.10	0.51
1:A1:1438:U:HO2'	1:A1:1439:G:P	2.32	0.51
27:B1:2386:G:OP1	44:BR:57:ARG:NH1	2.43	0.51
27:B1:2696:U:OP1	65:B1:3171:HOH:O	2.19	0.51
27:B1:2897:G:H21	30:BB:95:THR:HG21	1.76	0.51
34:BG:85:GLU:OE1	34:BG:85:GLU:N	2.43	0.51
1:A1:641:U:O2'	1:A1:642:A:O5'	2.26	0.51
1:A1:252:G:HO2'	1:A1:253:U:P	2.33	0.51
30:BB:75:THR:HG21	30:BB:209:VAL:HB	1.92	0.51
1:A1:624:4AC:O7	1:A1:624:4AC:H5	2.11	0.51
1:A1:1030:G:N2	1:A1:1033:A:OP2	2.32	0.51
27:B1:313:G:N2	27:B1:403:G:C5	2.79	0.51
55:Bc:72:GLU:O	55:Bc:72:GLU:OE1	2.28	0.51
1:A1:182:A:O3'	19:Ar:3:ARG:NH2	2.44	0.51
27:B1:2406:U:O2'	27:B1:2492:4AC:O2	2.28	0.51
1:A1:691:4AC:O7	1:A1:691:4AC:H5	2.11	0.51
3:Ab:15:MET:HE3	17:Ap:46:VAL:HG11	1.92	0.51
4:Ac:43:VAL:HG22	4:Ac:43:VAL:O	2.09	0.51
15:An:69:MET:HE3	15:An:69:MET:HA	1.92	0.51
27:B1:415:G:OP2	40:BN:44:ARG:NH1	2.43	0.51
27:B1:472:U:O2'	27:B1:473:A:P	2.69	0.51
31:BC:33:ARG:NH1	31:BC:109:GLU:OE2	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:BX:89:LEU:HB3	50:BX:91:MET:HE3	1.93	0.51
16:Ao:113:ARG:NH1	27:B1:1026:A:O2'	2.42	0.51
27:B1:1931:A:C2	27:B1:1969:A:H4'	2.46	0.51
34:BG:3:LYS:O	34:BG:7:VAL:HG22	2.11	0.51
27:B1:460:C:OP2	65:B1:3218:HOH:O	2.19	0.51
27:B1:2173:G:O2'	27:B1:2174:U:P	2.68	0.51
1:A1:104:A:OP1	11:Aj:11:LYS:NZ	2.28	0.51
27:B1:2648:G:N2	27:B1:2780:G:O2'	2.44	0.51
1:A1:893:C:O2'	1:A1:1306:C:OP2	2.29	0.50
5:Ad:148:GLU:O	5:Ad:150:ASP:N	2.44	0.50
12:Ak:133:SER:OG	12:Ak:135:ARG:O	2.25	0.50
27:B1:1445:A:OP2	27:B1:1780:C:N4	2.45	0.50
27:B1:1570:A:N1	27:B1:1666:G:O2'	2.39	0.50
27:B1:2251:G:O2'	27:B1:2252:G:P	2.70	0.50
32:BD:99:ASP:OD1	32:BD:99:ASP:C	2.54	0.50
34:BG:58:ASP:OD1	34:BG:58:ASP:C	2.54	0.50
1:A1:306:C:H2'	1:A1:307:4AC:H6	1.93	0.50
1:A1:937:A:N6	1:A1:1186:U:O5'	2.44	0.50
1:A1:945:4AC:O7	1:A1:945:4AC:H5	2.12	0.50
1:A1:1146:G:O2'	1:A1:1147:C:P	2.70	0.50
2:Aa:48:THR:HG23	2:Aa:155:PRO:O	2.11	0.50
1:A1:1054:A:H4'	1:A1:1055:A:O5'	2.11	0.50
9:Ah:29:ARG:NE	9:Ah:29:ARG:C	2.69	0.50
27:B1:1445:A:P	27:B1:1780:C:H41	2.35	0.50
27:B1:2578:U:O2'	27:B1:2579:C:H5'	2.12	0.50
28:B2:30:4AC:H6	28:B2:30:4AC:O5'	2.11	0.50
28:B2:46:C:H4'	41:BO:112:VAL:HG21	1.93	0.50
34:BF:105:GLY:O	34:BF:108:ARG:NH2	2.45	0.50
43:BQ:39:GLU:CD	43:BQ:39:GLU:H	2.20	0.50
16:Ao:16:ASP:OD1	16:Ao:17:GLY:N	2.42	0.50
27:B1:311:C:O2'	27:B1:312:C:P	2.70	0.50
27:B1:348:G:N1	27:B1:351:A:OP2	2.37	0.50
27:B1:2237:C:N4	27:B1:2291:U:O2'	2.44	0.50
27:B1:1331:G:N2	27:B1:1332:U:O4	2.41	0.50
28:B2:8:G:O6	41:BO:12:ARG:NH1	2.44	0.50
41:BO:105:ASP:OD1	41:BO:105:ASP:C	2.55	0.50
50:BX:81:THR:HG23	50:BX:84:TYR:H	1.77	0.50
1:A1:1054:A:H1'	1:A1:1055:A:OP2	2.12	0.50
1:A1:1121:U:OP2	20:As:3:LYS:NZ	2.45	0.50
18:Aq:25:TRP:NE1	24:Aw:63:GLU:OE2	2.45	0.50
27:B1:834:G:O2'	27:B1:1790:A:N3	2.43	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B1:1603:C:O3'	43:BQ:60:ARG:NH1	2.45	0.50
27:B1:1824:A:H61	27:B1:2121:C:H42	1.58	0.50
27:B1:2048:U:O2'	27:B1:2049:C:O5'	2.15	0.50
27:B1:2996:A:N1	65:B1:3307:HOH:O	2.34	0.50
38:BL:5:ASP:N	38:BL:5:ASP:OD1	2.44	0.50
1:A1:1181:4AC:H5	1:A1:1181:4AC:O7	2.11	0.50
27:B1:933:4AC:O7	27:B1:933:4AC:H5	2.12	0.50
1:A1:87:4AC:H5	1:A1:87:4AC:O7	2.12	0.50
6:Ae:89:ASP:OD1	6:Ae:89:ASP:C	2.54	0.50
24:Aw:24:GLU:OE1	24:Aw:24:GLU:HA	2.12	0.50
27:B1:498:G:O2'	27:B1:509:G:O6	2.28	0.50
27:B1:1374:4AC:O7	27:B1:1374:4AC:H5	2.12	0.50
27:B1:1434:C:H2'	27:B1:1435:4AC:H6	1.94	0.50
27:B1:2962:A:OP1	30:BB:230:THR:OG1	2.26	0.50
1:A1:80:A:O2'	1:A1:81:C:P	2.69	0.49
6:Ae:201:GLU:HA	6:Ae:201:GLU:OE1	2.11	0.49
27:B1:1437:A:O2'	52:BZ:56:GLU:OE2	2.29	0.49
27:B1:1677:G:OP2	27:B1:1678:A:O2'	2.28	0.49
27:B1:2266:C:H2'	27:B1:2267:C:C6	2.47	0.49
27:B1:3005:C:H2'	27:B1:3006:4AC:H6	1.94	0.49
28:B2:29:C:H2'	28:B2:30:4AC:H6	1.94	0.49
28:B2:37:A:O2'	28:B2:38:U:O4'	2.30	0.49
2:Aa:80:VAL:HG12	2:Aa:91:ALA:HB1	1.93	0.49
5:Ad:148:GLU:OE1	5:Ad:148:GLU:O	2.30	0.49
27:B1:227:4AC:H5	27:B1:227:4AC:O7	2.12	0.49
27:B1:868:C:H5'	27:B1:896:4AC:HM71	1.94	0.49
27:B1:1608:4AC:O7	27:B1:1608:4AC:H5	2.12	0.49
27:B1:1743:4AC:H5	27:B1:1743:4AC:O7	2.12	0.49
38:BK:75:LEU:HD22	38:BK:80:ILE:HD11	1.94	0.49
30:BB:346:LYS:N	30:BB:346:LYS:CD	2.74	0.49
34:BG:15:LEU:HA	34:BG:18:LYS:HD3	1.94	0.49
58:Bf:12:ARG:NH1	58:Bf:51:GLU:OE2	2.45	0.49
63:Bk:4:LEU:HD13	63:Bk:37:VAL:HG13	1.94	0.49
1:A1:624:4AC:HM73	1:A1:691:4AC:HM71	1.91	0.49
27:B1:1177:C:H2'	27:B1:1178:4AC:H6	1.93	0.49
27:B1:2617:5MC:O2'	27:B1:2618:G:P	2.71	0.49
30:BB:73:ILE:HD11	30:BB:324:ILE:CD1	2.42	0.49
27:B1:732:4AC:O7	27:B1:732:4AC:H5	2.12	0.49
27:B1:1501:4AC:O7	27:B1:1501:4AC:H5	2.12	0.49
27:B1:1751:4AC:O7	27:B1:1751:4AC:H5	2.13	0.49
27:B1:1827:G:O2'	27:B1:2116:U:O4	2.24	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:475:G:N7	15:An:70:ARG:NH1	2.60	0.49
1:A1:951:5MC:O4'	1:A1:951:5MC:OP1	2.31	0.49
1:A1:1146:G:HO2'	1:A1:1147:C:P	2.33	0.49
1:A1:1283:U:OP2	1:A1:1284:C:O2'	2.31	0.49
13:Al:93:ASP:C	13:Al:93:ASP:OD1	2.55	0.49
24:Aw:17:LYS:HG2	24:Aw:59:LEU:HD11	1.93	0.49
27:B1:380:U:HO2'	27:B1:381:A:P	2.34	0.49
27:B1:643:G:O2'	27:B1:1363:G:OP1	2.25	0.49
27:B1:1142:C:OP2	27:B1:1143:A:O2'	2.18	0.49
27:B1:1292:C:H2'	27:B1:1293:4AC:H6	1.94	0.49
27:B1:2052:A:C2'	27:B1:2053:A:O5'	2.61	0.49
1:A1:761:4AC:H5	1:A1:761:4AC:O7	2.13	0.49
27:B1:344:4AC:H5	27:B1:344:4AC:O7	2.13	0.49
27:B1:666:C:O2	27:B1:2156:C:O2'	2.31	0.49
27:B1:950:4AC:O7	27:B1:950:4AC:H5	2.13	0.49
30:BB:73:ILE:HD11	30:BB:324:ILE:HD11	1.94	0.49
34:BG:6:TYR:O	34:BG:79:TYR:OH	2.30	0.49
41:BO:46:ALA:CB	41:BO:86:LEU:HD21	2.43	0.49
1:A1:951:5MC:O4'	1:A1:951:5MC:P	2.71	0.49
7:Af:95:TYR:OH	7:Af:123:GLU:OE2	2.26	0.49
10:Ai:23:ARG:NH2	10:Ai:65:LEU:O	2.46	0.49
27:B1:419:4AC:H5	27:B1:419:4AC:O7	2.13	0.49
27:B1:1567:G:N2	27:B1:1570:A:OP2	2.40	0.49
27:B1:2844:4AC:O7	27:B1:2844:4AC:H5	2.13	0.49
28:B2:30:4AC:O7	28:B2:30:4AC:H5	2.13	0.49
28:B2:88:4AC:H5	28:B2:88:4AC:O7	2.13	0.49
28:B2:115:4AC:H5	28:B2:115:4AC:O7	2.13	0.49
31:BC:121:THR:HG21	31:BC:242:TRP:HZ2	1.77	0.49
31:BC:242:TRP:CZ3	31:BC:250:LEU:HD11	2.48	0.49
18:Aq:122:LEU:O	18:Aq:126:GLU:HG2	2.13	0.49
27:B1:613:G:N2	27:B1:616:A:OP2	2.40	0.49
27:B1:1445:A:O2'	27:B1:1447:G:N7	2.33	0.49
51:BY:73:LEU:C	51:BY:73:LEU:HD23	2.37	0.49
1:A1:739:4AC:H5	1:A1:739:4AC:O7	2.13	0.48
27:B1:1150:4AC:H5	27:B1:1150:4AC:O7	2.13	0.48
27:B1:1639:4AC:H5	27:B1:1639:4AC:O7	2.13	0.48
27:B1:1762:4AC:H5	27:B1:1762:4AC:O7	2.13	0.48
27:B1:2035:G:H5'	27:B1:2036:U:OP2	2.13	0.48
30:BB:65:GLU:OE1	48:BV:2:ALA:N	2.46	0.48
34:BG:3:LYS:NZ	34:BG:55:GLU:O	2.34	0.48
1:A1:291:4AC:O7	1:A1:291:4AC:H5	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:827:4AC:O7	1:A1:827:4AC:H5	2.13	0.48
1:A1:1145:G:H3'	1:A1:1146:G:H5''	1.96	0.48
1:A1:1367:G:H4'	60:Bh:14:MET:HE2	1.94	0.48
9:Ah:47:THR:OG1	9:Ah:65:GLU:OE2	2.29	0.48
27:B1:434:4AC:H5	27:B1:434:4AC:O7	2.13	0.48
27:B1:953:4AC:H5	27:B1:953:4AC:O7	2.14	0.48
27:B1:1004:C:HO2'	27:B1:1005:U:P	2.35	0.48
27:B1:1293:4AC:H5	27:B1:1293:4AC:O7	2.12	0.48
27:B1:1940:C:H1'	27:B1:1941:U:OP2	2.12	0.48
27:B1:2792:4AC:H5	27:B1:2792:4AC:O7	2.13	0.48
27:B1:3006:4AC:H5	27:B1:3006:4AC:O7	2.13	0.48
34:BF:56:ASP:OD1	34:BF:56:ASP:N	2.43	0.48
35:BH:171:ASP:OD1	35:BH:173:THR:HG22	2.13	0.48
1:A1:216:4AC:O7	1:A1:216:4AC:H5	2.13	0.48
1:A1:1456:A:OP2	65:A1:1525:HOH:O	2.20	0.48
7:Af:20:THR:OG1	7:Af:46:GLU:OE2	2.31	0.48
27:B1:337:4AC:O7	27:B1:337:4AC:H5	2.14	0.48
27:B1:896:4AC:H5	27:B1:896:4AC:O7	2.14	0.48
28:B2:38:U:H3'	28:B2:39:U:H4'	1.93	0.48
29:BA:54:ARG:O	29:BA:55:THR:HB	2.13	0.48
1:A1:614:4AC:O7	1:A1:614:4AC:H5	2.13	0.48
27:B1:46:G:H3'	27:B1:205:G:H2'	1.95	0.48
27:B1:1846:4AC:H5	27:B1:1846:4AC:O7	2.13	0.48
27:B1:3020:4AC:H5	27:B1:3020:4AC:O7	2.13	0.48
33:BE:98:PRO:O	33:BE:112:ASN:ND2	2.43	0.48
1:A1:231:4AC:H5	1:A1:231:4AC:O7	2.14	0.48
1:A1:534:4AC:O7	1:A1:534:4AC:H5	2.13	0.48
27:B1:479:4AC:O7	27:B1:479:4AC:H5	2.13	0.48
27:B1:1066:C:H2'	27:B1:1067:4AC:H6	1.96	0.48
1:A1:199:A:N1	1:A1:217:G:O2'	2.40	0.48
1:A1:705:C:N4	1:A1:706:4AC:O7	2.47	0.48
27:B1:48:4AC:HM71	27:B1:204:G:OP2	2.14	0.48
27:B1:1505:4AC:H5	27:B1:1505:4AC:O7	2.14	0.48
27:B1:2454:4AC:O7	27:B1:2454:4AC:H5	2.13	0.48
27:B1:2809:4AC:H5	27:B1:2809:4AC:O7	2.14	0.48
27:B1:2821:4AC:H5	27:B1:2821:4AC:O7	2.14	0.48
27:B1:3011:4AC:O7	27:B1:3011:4AC:H5	2.13	0.48
42:BP:7:THR:O	42:BP:7:THR:HG22	2.14	0.48
1:A1:636:4AC:H5	1:A1:636:4AC:O7	2.14	0.48
1:A1:719:4AC:O7	1:A1:719:4AC:H5	2.13	0.48
1:A1:1254:4AC:H5	1:A1:1254:4AC:O7	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:1444:G:H4'	60:Bh:26:LEU:HD11	1.95	0.48
27:B1:378:4AC:O7	27:B1:378:4AC:H5	2.13	0.48
27:B1:1100:4AC:H5	27:B1:1100:4AC:O7	2.14	0.48
1:A1:499:4AC:O7	1:A1:499:4AC:H5	2.14	0.48
5:Ad:33:TYR:HA	5:Ad:118:MET:HE2	1.96	0.48
27:B1:162:4AC:O7	27:B1:162:4AC:H5	2.14	0.48
27:B1:200:4AC:O7	27:B1:200:4AC:H5	2.14	0.48
27:B1:1061:4AC:O7	27:B1:1061:4AC:H5	2.14	0.48
27:B1:1993:A:OP2	27:B1:2013:G:N2	2.43	0.48
27:B1:2026:A:O2'	29:BA:215:THR:OG1	2.04	0.48
27:B1:2171:4AC:O7	27:B1:2171:4AC:H5	2.14	0.48
27:B1:2469:4AC:O7	27:B1:2469:4AC:H5	2.13	0.48
27:B1:3037:4AC:H5	27:B1:3037:4AC:O7	2.13	0.48
32:BD:54:GLN:NE2	32:BD:81:THR:O	2.45	0.48
38:BL:29:ASP:C	38:BL:29:ASP:OD1	2.57	0.48
1:A1:274:4AC:O7	1:A1:274:4AC:H5	2.14	0.48
1:A1:330:G:O2'	8:Ag:102:ARG:O	2.32	0.48
1:A1:414:G:H2'	1:A1:415:G:C8	2.48	0.48
1:A1:1290:C:OP1	16:Ao:34:ASN:ND2	2.42	0.48
3:Ab:6:TYR:O	3:Ab:9:ARG:HG2	2.14	0.48
14:Am:49:LYS:H	14:Am:49:LYS:HD2	1.79	0.48
27:B1:1064:4AC:O7	27:B1:1064:4AC:H5	2.13	0.48
27:B1:1649:4AC:H5	27:B1:1649:4AC:O7	2.13	0.48
27:B1:2185:G:N2	27:B1:2186:A:H61	2.11	0.48
27:B1:2736:C:O2'	30:BB:236:ARG:NH2	2.47	0.48
28:B2:21:G:H2'	28:B2:22:G:C8	2.49	0.48
29:BA:207:LYS:NZ	29:BA:208:GLU:OE2	2.44	0.48
1:A1:1292:U:H2'	1:A1:1293:G:O4'	2.14	0.48
6:Ae:217:ASP:OD1	6:Ae:221:GLU:N	2.46	0.48
27:B1:98:4AC:O7	27:B1:98:4AC:H5	2.13	0.48
27:B1:979:4AC:O7	27:B1:979:4AC:H5	2.14	0.48
27:B1:1052:4AC:H5	27:B1:1052:4AC:O7	2.14	0.48
29:BA:55:THR:O	29:BA:55:THR:HG22	2.13	0.48
23:Bl:82:GLU:OE2	23:Bl:86:ILE:HG21	2.14	0.48
1:A1:141:4AC:H5	1:A1:141:4AC:O7	2.14	0.47
1:A1:405:4AC:H5	1:A1:405:4AC:O7	2.14	0.47
3:Ab:43:LYS:HZ3	3:Ab:43:LYS:HB2	1.79	0.47
4:Ac:111:THR:HG22	4:Ac:112:LYS:N	2.29	0.47
9:Ah:36:TYR:OH	25:Ax:53:ASP:OD2	2.26	0.47
27:B1:688:4AC:O7	27:B1:688:4AC:H5	2.13	0.47
27:B1:954:G:OP2	65:B1:3223:HOH:O	2.20	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B1:1579:4AC:O7	27:B1:1579:4AC:H5	2.14	0.47
27:B1:2008:4AC:O7	27:B1:2008:4AC:H5	2.14	0.47
27:B1:2173:G:HO2'	27:B1:2174:U:P	2.37	0.47
35:BH:173:THR:HG23	35:BH:174:THR:N	2.28	0.47
1:A1:540:4AC:O7	1:A1:540:4AC:H5	2.14	0.47
1:A1:1119:A:H4'	1:A1:1120:C:O4'	2.13	0.47
1:A1:1438:U:O2'	1:A1:1439:G:P	2.72	0.47
8:Ag:10:ASP:OD1	8:Ag:13:SER:N	2.46	0.47
27:B1:360:4AC:H5	27:B1:360:4AC:O7	2.13	0.47
27:B1:1706:4AC:H5	27:B1:1706:4AC:O7	2.13	0.47
27:B1:1818:4AC:O7	27:B1:1818:4AC:H5	2.13	0.47
27:B1:1911:4AC:H5	27:B1:1911:4AC:O7	2.14	0.47
27:B1:2112:C:H2'	27:B1:2113:4AC:H6	1.95	0.47
27:B1:2491:C:H2'	27:B1:2492:4AC:H6	1.96	0.47
29:BA:161:VAL:HG23	57:Be:78:VAL:HG21	1.96	0.47
47:BU:110:GLU:H	47:BU:110:GLU:CD	2.20	0.47
1:A1:119:A:H1'	1:A1:322:A:C5	2.49	0.47
1:A1:367:4AC:O7	1:A1:367:4AC:H5	2.13	0.47
1:A1:457:U:OP1	65:A1:1526:HOH:O	2.20	0.47
1:A1:467:4AC:O7	1:A1:467:4AC:H5	2.14	0.47
1:A1:1141:A:H2'	1:A1:1142:A:O4'	2.15	0.47
1:A1:1309:G:O6	12:Ak:10:ARG:NH2	2.44	0.47
6:Ae:81:TYR:CD1	6:Ae:81:TYR:C	2.93	0.47
27:B1:80:4AC:H5	27:B1:80:4AC:O7	2.13	0.47
27:B1:1383:4AC:H5	27:B1:1383:4AC:O7	2.14	0.47
27:B1:1551:4AC:H5	27:B1:1551:4AC:O7	2.15	0.47
27:B1:2526:4AC:O7	27:B1:2526:4AC:H5	2.13	0.47
27:B1:2876:4AC:H5	27:B1:2876:4AC:O7	2.14	0.47
30:BB:35:GLU:OE2	30:BB:214:LYS:NZ	2.42	0.47
32:BD:138:ASP:OD1	32:BD:138:ASP:N	2.43	0.47
39:BM:105:VAL:O	39:BM:105:VAL:HG22	2.14	0.47
23:Bl:50:THR:HA	23:Bl:78:MET:HE1	1.97	0.47
13:Al:6:ILE:HG22	13:Al:98:ILE:HD12	1.96	0.47
14:Am:44:GLY:O	14:Am:48:VAL:HG22	2.15	0.47
27:B1:262:A:N6	27:B1:298:G:H21	2.13	0.47
27:B1:1001:G:H2'	27:B1:1002:C:C6	2.49	0.47
27:B1:1004:C:O2'	27:B1:1005:U:P	2.72	0.47
27:B1:1276:G:O6	65:B1:3221:HOH:O	2.20	0.47
27:B1:1345:4AC:H5	27:B1:1345:4AC:O7	2.14	0.47
27:B1:1442:4AC:H5	27:B1:1442:4AC:O7	2.15	0.47
27:B1:1742:C:H2'	27:B1:1743:4AC:H6	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B1:2133:4AC:H5	27:B1:2133:4AC:O7	2.14	0.47
27:B1:2213:4AC:O7	27:B1:2213:4AC:H5	2.15	0.47
1:A1:546:4AC:H5	1:A1:546:4AC:O7	2.14	0.47
1:A1:713:G:N7	65:A1:1543:HOH:O	2.35	0.47
27:B1:2968:4AC:H5	27:B1:2968:4AC:O7	2.13	0.47
41:BO:74:LYS:HB3	41:BO:176:LEU:HD12	1.96	0.47
41:BO:179:GLU:N	41:BO:179:GLU:OE1	2.47	0.47
1:A1:220:4AC:O7	1:A1:220:4AC:H5	2.14	0.47
1:A1:241:U:H4'	1:A1:242:U:C5'	2.45	0.47
1:A1:816:4AC:H5	1:A1:816:4AC:O7	2.14	0.47
1:A1:884:G:O2'	1:A1:886:G:OP1	2.31	0.47
27:B1:19:4AC:O7	27:B1:19:4AC:H5	2.14	0.47
27:B1:1546:4AC:O7	27:B1:1546:4AC:H5	2.13	0.47
27:B1:2432:4AC:H5	27:B1:2432:4AC:O7	2.14	0.47
39:BM:124:ILE:HD13	39:BM:129:PHE:CE2	2.49	0.47
1:A1:41:4AC:H5	1:A1:41:4AC:O7	2.14	0.47
1:A1:382:4AC:H5	1:A1:382:4AC:O7	2.15	0.47
1:A1:499:4AC:OP1	5:Ad:38:LYS:NZ	2.45	0.47
1:A1:506:U:O4'	15:An:106:GLU:OE1	2.33	0.47
1:A1:536:U:OP2	1:A1:713:G:N1	2.42	0.47
1:A1:578:4AC:O7	1:A1:578:4AC:H5	2.13	0.47
1:A1:1013:5MC:OP1	17:Ap:44:ARG:NH2	2.41	0.47
1:A1:1029:4AC:O7	1:A1:1029:4AC:H5	2.15	0.47
3:Ab:21:LEU:CD2	3:Ab:65:LEU:HD11	2.45	0.47
4:Ac:109:ILE:HD11	4:Ac:117:LEU:HD12	1.97	0.47
4:Ac:178:TYR:O	4:Ac:180:LEU:HD12	2.15	0.47
10:Ai:102:LEU:O	10:Ai:104:VAL:HG23	2.15	0.47
17:Ap:42:CYS:O	17:Ap:46:VAL:HG23	2.14	0.47
27:B1:243:4AC:H5	27:B1:243:4AC:O7	2.14	0.47
27:B1:324:U:O2'	27:B1:326:G:N7	2.45	0.47
27:B1:580:4AC:H5	27:B1:580:4AC:O7	2.15	0.47
27:B1:663:A:O2'	65:B1:3121:HOH:O	2.05	0.47
27:B1:715:4AC:O7	27:B1:715:4AC:H5	2.14	0.47
27:B1:866:4AC:O7	27:B1:866:4AC:H5	2.14	0.47
27:B1:1047:A:O2'	27:B1:2379:4AC:O2'	2.31	0.47
27:B1:1435:4AC:O7	27:B1:1435:4AC:H5	2.15	0.47
27:B1:1967:4AC:H5	27:B1:1967:4AC:O7	2.15	0.47
1:A1:839:4AC:H5	1:A1:839:4AC:O7	2.14	0.47
1:A1:951:5MC:HN41	1:A1:1175:A:H62	1.63	0.47
1:A1:1314:4AC:O7	1:A1:1314:4AC:H5	2.14	0.47
3:Ab:136:LEU:O	3:Ab:137:THR:OG1	2.23	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Ah:29:ARG:O	9:Ah:29:ARG:CZ	2.62	0.47
9:Ah:29:ARG:O	9:Ah:30:ASP:C	2.58	0.47
9:Ah:152:ILE:HG22	9:Ah:157:ARG:HG3	1.97	0.47
27:B1:418:C:H2'	27:B1:419:4AC:H6	1.96	0.47
27:B1:1151:G:H21	62:Bj:43:SER:HB2	1.80	0.47
27:B1:2602:4AC:H5	27:B1:2602:4AC:O7	2.14	0.47
39:BM:105:VAL:CG1	39:BM:126:ALA:HB2	2.45	0.47
1:A1:5:4AC:H5	1:A1:5:4AC:O7	2.14	0.47
1:A1:1171:C:C2	1:A1:1172:C:C5	3.02	0.47
14:Am:65:ARG:O	14:Am:69:GLU:HG3	2.14	0.47
16:Ao:81:ARG:NH1	16:Ao:105:ASP:OD2	2.48	0.47
21:At:97:GLU:O	21:At:97:GLU:HG3	2.14	0.47
27:B1:652:4AC:O7	27:B1:652:4AC:H5	2.15	0.47
27:B1:721:4AC:O7	27:B1:721:4AC:H5	2.15	0.47
27:B1:1128:4AC:H5	27:B1:1128:4AC:O7	2.15	0.47
27:B1:1822:4AC:O7	27:B1:1822:4AC:H5	2.14	0.47
27:B1:2113:4AC:O7	27:B1:2113:4AC:H5	2.15	0.47
1:A1:836:4AC:O7	1:A1:836:4AC:H5	2.14	0.47
15:An:136:GLU:OE1	15:An:141:ARG:NE	2.47	0.47
27:B1:311:C:O2'	27:B1:312:C:O5'	2.31	0.47
27:B1:1107:4AC:H5	27:B1:1107:4AC:O7	2.15	0.47
27:B1:1107:4AC:H6	27:B1:1107:4AC:O5'	2.14	0.47
27:B1:1885:4AC:O7	27:B1:1885:4AC:H5	2.15	0.47
62:Bj:45:HIS:O	62:Bj:46:LYS:C	2.57	0.47
27:B1:130:4AC:H5	27:B1:130:4AC:O7	2.14	0.46
27:B1:663:A:O2'	27:B1:665:A:OP2	2.34	0.46
27:B1:786:4AC:H5	27:B1:786:4AC:O7	2.14	0.46
27:B1:1049:C:OP1	35:BH:19:ARG:NH2	2.48	0.46
27:B1:1264:4AC:H5	27:B1:1264:4AC:O7	2.14	0.46
27:B1:1290:4AC:O7	27:B1:1290:4AC:H5	2.15	0.46
27:B1:2262:C:H2'	27:B1:2263:C:C1'	2.44	0.46
27:B1:2850:4AC:O7	27:B1:2850:4AC:H5	2.15	0.46
38:BL:24:VAL:HG13	38:BL:33:VAL:CG1	2.45	0.46
45:BS:137:THR:HG23	45:BS:138:PRO:HD2	1.97	0.46
6:Ae:45:LEU:HD23	6:Ae:66:LEU:HD22	1.97	0.46
15:An:116:MET:SD	15:An:116:MET:C	2.98	0.46
27:B1:561:G:N3	27:B1:646:U:O2'	2.48	0.46
27:B1:982:A:H1'	27:B1:983:G:OP2	2.16	0.46
27:B1:2749:4AC:H5	27:B1:2749:4AC:O7	2.14	0.46
37:BJ:25:ALA:HB3	37:BJ:40:ILE:HD12	1.97	0.46
38:BL:67:SER:O	38:BL:71:VAL:HG23	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:BM:103:VAL:HG13	39:BM:124:ILE:HG22	1.98	0.46
1:A1:700:C:OP1	1:A1:810:C:O2'	2.25	0.46
1:A1:856:4AC:H5	1:A1:856:4AC:O7	2.15	0.46
6:Ae:216:GLU:C	6:Ae:216:GLU:OE1	2.58	0.46
7:Af:86:LEU:HD22	7:Af:195:VAL:HA	1.98	0.46
27:B1:527:4AC:O7	27:B1:527:4AC:H5	2.14	0.46
27:B1:584:A:H3'	27:B1:585:G:C5'	2.46	0.46
27:B1:1522:G:OP2	65:B1:3225:HOH:O	2.20	0.46
27:B1:1986:G:H2'	27:B1:1987:U:O4'	2.16	0.46
4:Ac:124:ILE:O	4:Ac:181:ARG:N	2.49	0.46
27:B1:1769:4AC:H5	27:B1:1769:4AC:O7	2.15	0.46
1:A1:952:G:H22	1:A1:1174:A:P	2.38	0.46
9:Ah:66:ARG:NH2	9:Ah:159:ASP:OD1	2.48	0.46
27:B1:2491:C:N4	27:B1:2492:4AC:C7	2.78	0.46
57:Be:45:ALA:O	57:Be:57:GLN:N	2.41	0.46
1:A1:706:4AC:O7	1:A1:706:4AC:H5	2.16	0.46
1:A1:1122:G:C2	1:A1:1123:C:C6	3.03	0.46
3:Ab:69:LEU:HD23	3:Ab:69:LEU:C	2.41	0.46
27:B1:23:4AC:H5	27:B1:23:4AC:O7	2.14	0.46
27:B1:1789:G:OP1	65:B1:3222:HOH:O	2.20	0.46
34:BG:67:PRO:HG2	34:BG:68:PRO:CD	2.45	0.46
2:Aa:115:LEU:CD2	2:Aa:117:VAL:HG13	2.45	0.46
9:Ah:195:ASP:C	9:Ah:195:ASP:OD1	2.59	0.46
17:Ap:39:CYS:SG	17:Ap:40:ARG:N	2.89	0.46
27:B1:1067:4AC:H5	27:B1:1067:4AC:O7	2.16	0.46
28:B2:115:4AC:OP2	28:B2:115:4AC:H6	2.15	0.46
39:BM:123:VAL:O	39:BM:123:VAL:HG13	2.16	0.46
59:Bg:17:CYS:HA	59:Bg:39:LEU:HD23	1.97	0.46
1:A1:1259:U:O3'	9:Ah:177:LYS:NZ	2.49	0.46
1:A1:1308:A:H1'	1:A1:1309:G:OP2	2.15	0.46
1:A1:1314:4AC:HM73	12:Ak:123:THR:O	2.16	0.46
8:Ag:47:LEU:O	8:Ag:47:LEU:HD23	2.15	0.46
14:Am:47:VAL:HG11	14:Am:62:LEU:HB2	1.97	0.46
23:Av:76:GLU:N	23:Av:76:GLU:OE1	2.49	0.46
27:B1:48:4AC:O7	27:B1:48:4AC:H5	2.15	0.46
27:B1:1178:4AC:H5	27:B1:1178:4AC:O7	2.15	0.46
27:B1:1478:4AC:H5	27:B1:1478:4AC:O7	2.16	0.46
27:B1:2050:U:N3	27:B1:2051:U:O4	2.49	0.46
27:B1:2492:4AC:O7	27:B1:2492:4AC:H5	2.15	0.46
1:A1:307:4AC:H5	1:A1:307:4AC:O7	2.15	0.46
4:Ac:94:SER:O	4:Ac:97:ARG:NH2	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:At:82:TYR:HB3	21:At:89:PHE:HB3	1.98	0.46
27:B1:1046:A:O2'	27:B1:1048:A:OP2	2.31	0.46
31:BC:224:ASN:OD1	31:BC:224:ASN:N	2.49	0.46
38:BL:49:ASN:OD1	38:BL:50:ILE:N	2.49	0.46
40:BN:149:ILE:O	63:Bk:12:ARG:NH2	2.48	0.46
1:A1:63:G:H2'	1:A1:64:G:C8	2.51	0.46
1:A1:1329:C:OP1	12:Ak:120:ASN:N	2.48	0.46
27:B1:945:G:OP2	39:BM:22:LYS:NZ	2.44	0.46
27:B1:1894:C:N3	27:B1:2831:C:O2'	2.49	0.46
27:B1:2429:4AC:O7	27:B1:2429:4AC:H5	2.15	0.46
34:BG:11:VAL:HG21	34:BG:79:TYR:HB2	1.98	0.46
38:BL:23:VAL:HG21	38:BL:71:VAL:HG11	1.98	0.46
1:A1:660:U:O2	1:A1:660:U:O4'	2.34	0.45
22:Au:7:VAL:HG13	22:Au:136:LEU:HD22	1.98	0.45
27:B1:583:A:N3	27:B1:1374:4AC:O2'	2.48	0.45
28:B2:6:C:OP1	41:BO:38:ARG:NE	2.35	0.45
28:B2:37:A:C2	28:B2:42:G:C2	3.04	0.45
28:B2:87:C:H2'	28:B2:88:4AC:H6	1.98	0.45
36:BI:43:ASP:OD1	36:BI:44:VAL:HG23	2.15	0.45
42:BP:16:ARG:HB2	42:BP:16:ARG:NH1	2.32	0.45
3:Ab:15:MET:HE3	17:Ap:46:VAL:HG21	1.98	0.45
27:B1:1124:A:OP2	65:B1:3227:HOH:O	2.21	0.45
27:B1:1368:A:H4'	27:B1:1369:A:OP1	2.16	0.45
27:B1:1713:U:OP1	54:Bb:48:ARG:NH2	2.47	0.45
27:B1:1957:G:OP1	29:BA:123:ARG:NH2	2.49	0.45
28:B2:56:A:N3	28:B2:57:G:C8	2.84	0.45
1:A1:748:U:O2	1:A1:748:U:C2'	2.64	0.45
2:Aa:65:GLN:OE1	2:Aa:65:GLN:N	2.34	0.45
27:B1:116:4AC:H5	27:B1:116:4AC:O7	2.15	0.45
27:B1:332:G:N1	27:B1:387:A:OP2	2.42	0.45
27:B1:383:G:O6	47:BU:2:LYS:NZ	2.50	0.45
27:B1:1368:A:O2'	27:B1:1369:A:P	2.75	0.45
27:B1:2020:4AC:O7	27:B1:2020:4AC:H5	2.15	0.45
31:BC:180:ARG:NE	31:BC:189:ARG:O	2.49	0.45
42:BP:21:LYS:HZ2	42:BP:107:ILE:HG21	1.81	0.45
27:B1:1359:C:C4	27:B1:1360:4AC:CM7	2.98	0.45
27:B1:2035:G:H3'	27:B1:2036:U:H5''	1.99	0.45
1:A1:404:C:H2'	1:A1:405:4AC:H6	1.97	0.45
14:Am:29:HIS:NE2	14:Am:38:THR:HG23	2.31	0.45
27:B1:85:A:C2	27:B1:103:A:C5	3.04	0.45
27:B1:362:G:O2'	27:B1:381:A:N3	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B1:453:A:H1'	27:B1:2005:A:C2	2.51	0.45
27:B1:1946:4AC:H5	27:B1:1946:4AC:O7	2.16	0.45
27:B1:2186:A:OP1	27:B1:2619:C:N4	2.49	0.45
27:B1:2511:A:N3	39:BM:41:LYS:NZ	2.62	0.45
52:BZ:93:THR:HG22	52:BZ:94:LEU:N	2.31	0.45
55:Bc:63:THR:HG22	55:Bc:63:THR:O	2.16	0.45
1:A1:541:OMG:N1	1:A1:709:C:OP2	2.44	0.45
1:A1:619:G:OP1	4:Ac:131:THR:N	2.50	0.45
1:A1:945:4AC:HM73	1:A1:1181:4AC:CM7	2.32	0.45
1:A1:1225:C:H2'	1:A1:1226:OMC:H6	1.82	0.45
7:Af:28:GLU:N	7:Af:28:GLU:OE1	2.49	0.45
27:B1:840:A:OP1	57:Be:4:THR:OG1	2.29	0.45
27:B1:949:C:H2'	27:B1:950:4AC:H6	1.99	0.45
31:BC:243:THR:HG22	31:BC:244:VAL:N	2.32	0.45
34:BF:53:ILE:HG22	34:BF:54:ALA:N	2.31	0.45
37:BJ:26:TYR:O	65:BJ:201:HOH:O	2.21	0.45
37:BJ:93:ASP:OD1	37:BJ:93:ASP:C	2.60	0.45
1:A1:1227:4AC:H5	1:A1:1227:4AC:O7	2.17	0.45
16:Ao:46:ASP:O	16:Ao:49:MET:HG2	2.16	0.45
22:Au:146:GLU:OE1	22:Au:146:GLU:N	2.50	0.45
27:B1:1613:G:O2'	27:B1:2818:U:O4	2.28	0.45
43:BQ:13:GLU:OE1	43:BQ:14:ILE:N	2.50	0.45
1:A1:1248:U:OP2	22:Au:72:ARG:NH1	2.46	0.45
23:Av:43:MET:HG2	23:Av:44:LEU:HD22	1.98	0.45
27:B1:1180:G:H21	35:BH:178:SER:HB3	1.82	0.45
27:B1:2061:A:H4'	27:B1:2062:A:O5'	2.17	0.45
30:BB:195:LYS:O	30:BB:199:ILE:HG13	2.17	0.45
27:B1:266:A:C2	27:B1:295:U:C2	3.04	0.45
9:Ah:44:LEU:HD11	12:Ak:40:ILE:HD12	1.97	0.45
27:B1:485:4AC:O7	27:B1:485:4AC:H5	2.17	0.45
27:B1:589:U:H4'	27:B1:590:G:OP2	2.17	0.45
1:A1:99:C:H4'	1:A1:100:A:O5'	2.17	0.44
1:A1:184:G:H2'	1:A1:184:G:N3	2.32	0.44
1:A1:304:G:N1	5:Ad:3:ASP:OD2	2.48	0.44
5:Ad:42:TRP:O	5:Ad:46:THR:OG1	2.33	0.44
16:Ao:118:ILE:O	16:Ao:122:LEU:HD12	2.15	0.44
27:B1:1546:4AC:O5'	27:B1:1546:4AC:H6	2.16	0.44
27:B1:1568:C:O2'	38:BL:52:HIS:ND1	2.38	0.44
27:B1:2379:4AC:O7	27:B1:2379:4AC:H5	2.16	0.44
45:BS:95:LEU:O	45:BS:98:VAL:HG12	2.16	0.44
1:A1:611:G:OP1	18:Aq:4:MET:N	2.45	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B1:2124:G:OP1	27:B1:2838:C:O2'	2.35	0.44
27:B1:2848:G:O2'	27:B1:2849:C:O5'	2.34	0.44
1:A1:99:C:H1'	1:A1:100:A:OP2	2.17	0.44
1:A1:849:G:C8	60:Bh:2:LYS:HB2	2.52	0.44
1:A1:1145:G:HO2'	1:A1:1146:G:P	2.31	0.44
20:As:62:MET:SD	20:As:62:MET:C	3.00	0.44
22:Au:141:GLU:OE1	22:Au:148:LYS:NZ	2.50	0.44
27:B1:28:G:H22	27:B1:550:G:H1'	1.82	0.44
27:B1:1670:A:N3	27:B1:1712:C:O2'	2.47	0.44
27:B1:2809:4AC:O2	27:B1:2986:U:O2'	2.32	0.44
51:BY:68:VAL:HG22	51:BY:79:VAL:HG12	1.99	0.44
1:A1:689:C:O2	1:A1:689:C:O4'	2.34	0.44
2:Aa:65:GLN:H	2:Aa:65:GLN:CD	2.23	0.44
4:Ac:156:ASP:OD1	4:Ac:156:ASP:N	2.49	0.44
27:B1:472:U:O2'	27:B1:473:A:OP1	2.32	0.44
27:B1:1515:C:C2	27:B1:1516:G:C8	3.04	0.44
27:B1:2947:C:H2'	27:B1:2948:G:O4'	2.17	0.44
39:BM:76:VAL:HG11	39:BM:105:VAL:HG21	1.99	0.44
43:BQ:95:TRP:O	43:BQ:99:ILE:HG22	2.18	0.44
45:BS:69:SER:O	45:BS:69:SER:OG	2.31	0.44
1:A1:986:C:H2'	1:A1:987:G:O5'	2.17	0.44
3:Ab:4:GLU:OE1	13:Al:68:VAL:HG21	2.17	0.44
27:B1:149:C:OP1	40:BN:38:ARG:NH1	2.48	0.44
27:B1:365:A:N6	27:B1:380:U:O4'	2.51	0.44
27:B1:837:U:H2'	27:B1:838:G:O4'	2.18	0.44
27:B1:1057:C:O2'	27:B1:2384:A:N7	2.49	0.44
27:B1:2066:C:N4	27:B1:2090:C:O4'	2.51	0.44
27:B1:2212:C:H2'	27:B1:2213:4AC:H6	1.99	0.44
27:B1:2262:C:H2'	27:B1:2263:C:O4'	2.18	0.44
27:B1:2901:C:O3'	30:BB:137:LYS:NZ	2.50	0.44
28:B2:95:G:H2'	28:B2:96:G:H8	1.82	0.44
30:BB:60:LEU:HD23	37:BJ:14:ALA:HA	1.98	0.44
34:BG:39:THR:O	34:BG:43:VAL:HG13	2.18	0.44
1:A1:340:U:O2'	1:A1:343:G:O6	2.29	0.44
8:Ag:23:GLY:O	8:Ag:25:GLU:N	2.50	0.44
20:As:23:GLU:N	20:As:23:GLU:CD	2.76	0.44
20:As:25:THR:HG23	20:As:27:ASP:H	1.82	0.44
27:B1:453:A:H2'	27:B1:454:OMU:H6	2.00	0.44
33:BE:18:GLU:C	33:BE:18:GLU:CD	2.85	0.44
34:BG:20:LEU:O	34:BG:23:VAL:HG12	2.17	0.44
36:BI:72:ASP:OD1	36:BI:73:GLU:N	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B1:530:OMG:O6	45:BS:93:LYS:NZ	2.39	0.44
27:B1:2173:G:O2'	27:B1:2174:U:O5'	2.36	0.44
34:BG:3:LYS:HZ1	34:BG:57:VAL:H	1.66	0.44
38:BL:21:LYS:O	38:BL:41:ASN:ND2	2.51	0.44
41:BO:46:ALA:HB2	41:BO:86:LEU:HD21	2.00	0.44
62:Bj:38:TYR:CD1	62:Bj:49:ARG:HG2	2.53	0.44
1:A1:163:C:C2	1:A1:164:A:C8	3.06	0.44
1:A1:607:U:O4	1:A1:707:G:O2'	2.34	0.44
1:A1:1008:A:C2	1:A1:1168:G:C4	3.05	0.44
8:Ag:25:GLU:H	8:Ag:25:GLU:CD	2.25	0.44
10:Ai:118:GLU:HA	10:Ai:118:GLU:OE1	2.17	0.44
27:B1:84:G:O5'	47:BU:115:ILE:HD11	2.18	0.44
27:B1:946:U:OP2	39:BM:15:HIS:NE2	2.46	0.44
27:B1:1367:U:OP1	53:Ba:66:SER:OG	2.29	0.44
27:B1:1578:C:H2'	27:B1:1579:4AC:H6	2.00	0.44
27:B1:2051:U:N3	27:B1:2054:G:O6	2.51	0.44
47:BU:15:LEU:O	47:BU:74:TYR:OH	2.33	0.44
1:A1:443:C:N3	1:A1:444:C:C5	2.86	0.44
1:A1:964:A:N6	1:A1:987:G:O2'	2.51	0.44
1:A1:1278:G:N1	1:A1:1281:A:OP2	2.50	0.44
1:A1:1320:U:OP2	1:A1:1321:C:N4	2.38	0.44
16:Ao:108:ARG:HG3	21:At:97:GLU:OE1	2.18	0.44
18:Aq:126:GLU:OE1	18:Aq:148:TYR:CE2	2.71	0.44
27:B1:1181:G:O3'	35:BH:175:LYS:NZ	2.51	0.44
27:B1:1767:A:OP1	27:B1:1769:4AC:HM71	2.18	0.44
27:B1:1889:G:HO2'	27:B1:2997:A:HO2'	1.64	0.44
27:B1:2519:G:OP1	61:Bi:76:LYS:NZ	2.39	0.44
6:Ae:40:ARG:NH1	6:Ae:40:ARG:HB3	2.33	0.43
12:Ak:40:ILE:HG23	12:Ak:41:ALA:N	2.33	0.43
27:B1:95:A:H2'	27:B1:96:G:O4'	2.17	0.43
27:B1:146:C:O2'	27:B1:147:U:P	2.75	0.43
27:B1:1301:C:OP1	65:B1:3226:HOH:O	2.20	0.43
27:B1:1617:A:C2	27:B1:1618:G:H1'	2.53	0.43
27:B1:2242:U:O2	27:B1:2242:U:O4'	2.34	0.43
32:BD:31:ASN:O	32:BD:138:ASP:OD1	2.35	0.43
39:BM:14:SER:O	39:BM:15:HIS:HB3	2.18	0.43
39:BM:77:ASN:OD1	39:BM:115:THR:HB	2.18	0.43
1:A1:643:G:O5'	14:Am:46:MET:HB3	2.18	0.43
1:A1:672:C:O2'	1:A1:689:C:O4'	2.32	0.43
1:A1:1367:G:H4'	60:Bh:14:MET:CE	2.48	0.43
1:A1:1475:MA6:H2'	1:A1:1476:MA6:O4'	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Aa:101:MET:HE1	2:Aa:115:LEU:HD11	1.99	0.43
9:Ah:212:GLU:OE1	9:Ah:215:ARG:NE	2.50	0.43
27:B1:614:C:O2	27:B1:614:C:O4'	2.34	0.43
27:B1:1532:C:O2'	27:B1:1626:A:N3	2.45	0.43
27:B1:1889:G:O2'	27:B1:2997:A:O2'	2.35	0.43
27:B1:2840:A:C4	27:B1:2842:G:C8	3.06	0.43
27:B1:2880:G:C2	27:B1:2881:C:C6	3.05	0.43
29:BA:100:ALA:O	29:BA:134:ARG:NH1	2.46	0.43
34:BG:5:SER:HB3	34:BG:60:GLU:OE2	2.17	0.43
36:BI:22:LEU:O	36:BI:96:ARG:NH1	2.51	0.43
43:BQ:13:GLU:OE1	43:BQ:13:GLU:C	2.61	0.43
1:A1:1018:U:H4'	1:A1:1019:C:O5'	2.17	0.43
9:Ah:172:LYS:NZ	9:Ah:187:GLU:OE1	2.49	0.43
23:Av:94:GLU:OE2	23:Av:94:GLU:HA	2.17	0.43
27:B1:240:G:OP1	27:B1:2511:A:O2'	2.33	0.43
27:B1:2052:A:HO2'	27:B1:2053:A:P	2.42	0.43
41:BO:32:LYS:NZ	41:BO:101:GLU:OE2	2.44	0.43
42:BP:8:ASP:OD1	42:BP:10:ASN:N	2.50	0.43
1:A1:720:G:H1	1:A1:767:G:HO2'	1.61	0.43
1:A1:906:A:H2'	1:A1:907:G:C8	2.54	0.43
1:A1:987:G:H2'	1:A1:988:G:C4	2.52	0.43
4:Ac:120:MET:HB2	4:Ac:187:LYS:HB3	2.00	0.43
25:Ax:18:THR:CG2	25:Ax:19:GLY:N	2.82	0.43
27:B1:380:U:O2'	27:B1:381:A:P	2.77	0.43
27:B1:1981:U:C2	27:B1:1982:G:C8	3.06	0.43
27:B1:2254:G:O2'	27:B1:2282:A:N1	2.52	0.43
27:B1:2791:C:O2'	37:BJ:47:HIS:O	2.36	0.43
27:B1:2870:U:H4'	27:B1:2871:A:OP1	2.18	0.43
28:B2:37:A:HO2'	28:B2:38:U:C5'	2.32	0.43
30:BB:143:MET:HA	30:BB:146:GLN:HG2	2.01	0.43
33:BE:22:GLU:N	33:BE:22:GLU:OE1	2.52	0.43
34:BF:43:VAL:HG13	34:BF:75:ILE:HD12	1.99	0.43
1:A1:537:A:N6	1:A1:713:G:O2'	2.42	0.43
1:A1:1450:A:H2'	1:A1:1450:A:N3	2.33	0.43
2:Aa:186:GLU:N	2:Aa:186:GLU:CD	2.76	0.43
8:Ag:69:LYS:C	8:Ag:69:LYS:CD	2.91	0.43
23:Av:11:ASN:O	23:Av:14:ILE:O	2.37	0.43
27:B1:146:C:HO2'	27:B1:147:U:P	2.41	0.43
27:B1:1360:4AC:HM73	27:B1:1360:4AC:H5	2.01	0.43
27:B1:2035:G:OP1	27:B1:2035:G:H4'	2.18	0.43
27:B1:2562:OMG:H2'	27:B1:2617:5MC:CM5	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B1:3006:4AC:H6	27:B1:3006:4AC:O5'	2.18	0.43
31:BC:63:LYS:HG2	31:BC:64:GLY:N	2.34	0.43
54:Bb:80:MET:O	54:Bb:84:ILE:HG22	2.19	0.43
5:Ad:48:LEU:HB2	5:Ad:100:ILE:HD12	2.01	0.43
27:B1:103:A:C4	27:B1:104:A:C8	3.06	0.43
27:B1:1796:C:O2	27:B1:2815:U:O2'	2.37	0.43
28:B2:11:A:OP2	44:BR:22:ARG:NH1	2.51	0.43
1:A1:718:C:H2'	1:A1:719:4AC:H6	1.99	0.43
1:A1:839:4AC:HM71	15:An:5:LYS:HA	2.01	0.43
8:Ag:32:LYS:O	8:Ag:112:ILE:HD12	2.19	0.43
27:B1:280:G:H21	27:B1:323:C:H1'	1.83	0.43
27:B1:667:A:OP2	27:B1:2615:C:O2'	2.37	0.43
29:BA:18:LYS:O	29:BA:186:ASN:ND2	2.45	0.43
39:BM:68:GLU:C	39:BM:68:GLU:OE2	2.62	0.43
39:BM:102:ILE:HA	39:BM:123:VAL:HG13	1.99	0.43
43:BQ:4:LEU:HD13	43:BQ:32:VAL:CG1	2.48	0.43
1:A1:240:A:H4'	1:A1:241:U:O5'	2.18	0.43
1:A1:1283:U:O2'	21:At:110:ARG:NH1	2.44	0.43
4:Ac:46:ARG:NH2	14:Am:37:GLU:OE2	2.51	0.43
4:Ac:75:GLY:O	4:Ac:76:GLN:HB2	2.18	0.43
27:B1:259:C:H2'	27:B1:259:C:O2	2.18	0.43
27:B1:337:4AC:HM71	47:BU:1:MET:O	2.19	0.43
27:B1:566:A:H2'	27:B1:566:A:N3	2.34	0.43
27:B1:1781:C:H2'	27:B1:1782:C:C6	2.53	0.43
47:BU:102:ILE:HG21	47:BU:105:LEU:HD23	2.00	0.43
1:A1:572:C:OP2	65:A1:1527:HOH:O	2.21	0.43
1:A1:731:G:N2	1:A1:757:A:OP2	2.47	0.43
1:A1:815:C:H2'	1:A1:816:4AC:H6	2.00	0.43
10:Ai:101:ILE:HD12	10:Ai:103:ILE:HD11	2.00	0.43
27:B1:83:C:O2'	47:BU:25:LYS:NZ	2.52	0.43
27:B1:146:C:O2'	27:B1:147:U:OP1	2.36	0.43
27:B1:662:G:H2'	27:B1:2154:C:C5	2.54	0.43
27:B1:2166:A:HO2'	27:B1:2167:C:P	2.39	0.43
27:B1:2276:G:C6	27:B1:2277:G:C5	3.07	0.43
39:BM:55:PRO:O	39:BM:56:ASP:OD1	2.37	0.43
39:BM:108:PHE:O	39:BM:109:ALA:HB3	2.18	0.43
1:A1:58:U:H4'	1:A1:375:G:H22	1.83	0.43
1:A1:847:G:OP2	1:A1:848:A:O2'	2.31	0.43
1:A1:913:G:N7	16:Ao:132:ARG:NH2	2.66	0.43
1:A1:939:C:C4	1:A1:940:C:C5	3.07	0.43
1:A1:967:G:C6	1:A1:986:C:N4	2.87	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:1120:C:O3'	20:As:49:ARG:NH1	2.52	0.43
5:Ad:164:GLN:O	5:Ad:169:MET:HE2	2.19	0.43
6:Ae:216:GLU:OE1	6:Ae:216:GLU:O	2.36	0.43
21:At:12:THR:HG22	21:At:13:LEU:N	2.34	0.43
27:B1:561:G:OP1	27:B1:578:C:O2'	2.37	0.43
43:BQ:6:MET:HE1	43:BQ:36:ILE:O	2.19	0.43
1:A1:472:G:O2'	1:A1:484:G:N2	2.52	0.42
1:A1:878:A:C2	1:A1:879:U:C5	3.07	0.42
1:A1:881:G:H2'	1:A1:882:G:C8	2.53	0.42
1:A1:920:U:H2'	1:A1:1187:A:H62	1.84	0.42
1:A1:986:C:H2'	1:A1:986:C:O2	2.18	0.42
1:A1:1119:A:H4'	1:A1:1120:C:O5'	2.18	0.42
14:Am:77:VAL:HG23	14:Am:78:GLY:N	2.34	0.42
16:Ao:61:LYS:O	16:Ao:64:GLU:OE2	2.37	0.42
27:B1:1375:G:C2	27:B1:1376:G:C8	3.07	0.42
27:B1:2152:C:H2'	27:B1:2153:G:O4'	2.19	0.42
50:BX:145:GLU:O	50:BX:148:ASN:ND2	2.45	0.42
1:A1:1240:G:O5'	1:A1:1241:A:H5'	2.19	0.42
27:B1:1162:A:N3	65:B1:3314:HOH:O	2.36	0.42
35:BH:4:ARG:HD3	35:BH:96:GLU:OE2	2.19	0.42
38:BK:3:ALA:O	38:BK:4:ILE:HG22	2.19	0.42
43:BQ:4:LEU:HD13	43:BQ:32:VAL:HG11	2.01	0.42
1:A1:75:C:O2	1:A1:75:C:O4'	2.37	0.42
1:A1:1363:G:H2'	1:A1:1364:OMC:O4'	2.19	0.42
1:A1:1423:C:H2'	1:A1:1424:G:O4'	2.19	0.42
18:Aq:41:ARG:NH2	18:Aq:89:PRO:HD3	2.34	0.42
27:B1:736:A:N6	39:BM:117:LYS:O	2.50	0.42
27:B1:1794:G:O2'	27:B1:1900:C:O2'	2.27	0.42
27:B1:2185:G:H21	27:B1:2186:A:N6	2.15	0.42
34:BG:103:GLU:HG3	34:BG:103:GLU:O	2.19	0.42
36:BI:51:GLN:HA	36:BI:54:GLU:HG3	2.00	0.42
41:BO:83:ALA:HB1	41:BO:120:VAL:HG23	2.00	0.42
1:A1:4:C:OP2	7:Af:187:THR:OG1	2.37	0.42
1:A1:712:U:H2'	1:A1:713:G:O4'	2.18	0.42
1:A1:1083:A:H4'	12:Ak:18:VAL:HG21	2.01	0.42
9:Ah:163:ARG:NH1	9:Ah:163:ARG:HG3	2.34	0.42
27:B1:260:A:OP2	27:B1:299:G:N1	2.50	0.42
27:B1:576:G:O4'	55:Bc:76:PRO:HB3	2.20	0.42
27:B1:603:G:OP1	50:BX:155:LEU:HD22	2.20	0.42
27:B1:918:A:N3	65:B1:3315:HOH:O	2.36	0.42
27:B1:2138:A:O2'	45:BS:137:THR:HG22	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B1:2170:C:H2'	27:B1:2171:4AC:H6	2.01	0.42
27:B1:2329:G:N2	27:B1:2332:A:OP2	2.45	0.42
27:B1:2585:A:N6	27:B1:2597:G:O2'	2.52	0.42
28:B2:69:U:H2'	28:B2:70:C:C6	2.55	0.42
1:A1:145:A:H2'	1:A1:146:A:O4'	2.18	0.42
1:A1:867:A:OP1	15:An:31:LYS:NZ	2.42	0.42
1:A1:880:U:H2'	1:A1:881:G:O4'	2.20	0.42
1:A1:1477:C:HO2'	1:A1:1478:C:H6	1.56	0.42
27:B1:168:G:OP1	56:Bd:44:ARG:NH2	2.52	0.42
27:B1:698:U:H2'	27:B1:699:U:O4'	2.20	0.42
27:B1:2435:A:N3	27:B1:2435:A:H2'	2.34	0.42
28:B2:40:U:H6	32:BD:57:ILE:HD11	1.85	0.42
30:BB:296:LYS:O	30:BB:353:ARG:NH1	2.52	0.42
46:BT:31:ASP:OD2	46:BT:33:ARG:HD2	2.19	0.42
1:A1:527:A:O2'	1:A1:528:A:O4'	2.32	0.42
1:A1:599:U:C2	1:A1:600:G:C8	3.08	0.42
1:A1:939:C:O2	1:A1:939:C:H2'	2.20	0.42
1:A1:1440:A:H2	27:B1:2085:A:O4'	2.03	0.42
3:Ab:42:THR:HG21	3:Ab:75:LEU:HD13	2.00	0.42
4:Ac:111:THR:HG22	4:Ac:112:LYS:H	1.85	0.42
4:Ac:146:TYR:O	4:Ac:150:GLU:HG2	2.19	0.42
13:Al:82:MET:HE3	13:Al:83:ARG:N	2.35	0.42
16:Ao:39:VAL:HA	16:Ao:42:VAL:HG12	2.02	0.42
27:B1:857:A2M:HM'2	27:B1:858:U:O4'	2.19	0.42
27:B1:920:OMG:H5'	27:B1:921:OMG:OP1	2.20	0.42
27:B1:1449:G:C2'	27:B1:1450:C:O5'	2.68	0.42
27:B1:1940:C:H4'	27:B1:1941:U:O5'	2.20	0.42
27:B1:2249:G:H21	27:B1:2298:C:H42	1.68	0.42
45:BS:57:LEU:HD23	45:BS:83:TYR:CG	2.55	0.42
1:A1:773:G:O2'	1:A1:775:OMU:H6	2.20	0.42
1:A1:918:A:C2	21:At:87:LYS:HG3	2.55	0.42
1:A1:1155:G:OP2	3:Ab:131:ARG:NH2	2.52	0.42
27:B1:970:U:O2'	27:B1:2476:G:N3	2.47	0.42
27:B1:2420:U:H2'	27:B1:2421:C:C6	2.55	0.42
27:B1:2431:C:H2'	27:B1:2432:4AC:H6	2.01	0.42
27:B1:3036:C:H2'	27:B1:3037:4AC:H6	2.01	0.42
34:BF:67:PRO:HB2	34:BF:68:PRO:HD3	2.02	0.42
1:A1:905:G:C2	1:A1:906:A:C8	3.08	0.42
1:A1:1170:C:C2	1:A1:1171:C:C6	3.08	0.42
1:A1:1473:G:N2	1:A1:1476:MA6:OP2	2.50	0.42
3:Ab:189:LEU:N	3:Ab:192:GLU:OE1	2.44	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ad:148:GLU:OE2	5:Ad:151:THR:OG1	2.38	0.42
9:Ah:163:ARG:O	9:Ah:167:LEU:HD23	2.20	0.42
27:B1:314:U:O2	27:B1:314:U:O5'	2.38	0.42
27:B1:1810:G:O2'	27:B1:1811:G:H5'	2.20	0.42
27:B1:2838:C:H2'	27:B1:2839:U:O4'	2.19	0.42
41:BO:101:GLU:N	41:BO:101:GLU:OE1	2.53	0.42
44:BR:28:LEU:N	44:BR:28:LEU:HD22	2.34	0.42
53:Ba:46:ILE:HG13	53:Ba:47:ASP:N	2.33	0.42
1:A1:390:G:C2	1:A1:391:G:C8	3.08	0.42
1:A1:446:G:H2'	1:A1:447:G:O4'	2.20	0.42
1:A1:557:G:C6	1:A1:591:G:C5	3.08	0.42
6:Ae:48:ILE:CD1	6:Ae:85:VAL:HG21	2.50	0.42
27:B1:1052:4AC:OP1	44:BR:19:HIS:NE2	2.41	0.42
27:B1:1500:C:H2'	27:B1:1501:4AC:H6	2.02	0.42
27:B1:2835:C:C2	27:B1:2836:A:C8	3.07	0.42
39:BM:105:VAL:HG13	39:BM:126:ALA:HB2	2.02	0.42
46:BT:73:GLU:N	46:BT:73:GLU:CD	2.78	0.42
63:Bk:9:VAL:HG12	63:Bk:10:LYS:N	2.35	0.42
1:A1:414:G:H2'	1:A1:415:G:H8	1.84	0.42
1:A1:884:G:C2	1:A1:886:G:C8	3.07	0.42
20:As:50:ILE:O	20:As:54:VAL:HG22	2.19	0.42
22:Au:88:GLU:OE1	22:Au:88:GLU:N	2.42	0.42
27:B1:138:A:H2'	27:B1:139:U:O4'	2.20	0.42
27:B1:165:A:N6	27:B1:166:G:O6	2.53	0.42
27:B1:971:G:C4	27:B1:972:G:C8	3.07	0.42
27:B1:1853:U:H4'	27:B1:1854:C:OP2	2.20	0.42
27:B1:2429:4AC:OP2	27:B1:2429:4AC:H6	2.20	0.42
28:B2:43:A:O3'	32:BD:152:ARG:NH1	2.53	0.42
28:B2:56:A:O2'	28:B2:57:G:P	2.78	0.42
31:BC:218:ASP:OD1	31:BC:218:ASP:N	2.53	0.42
38:BL:48:MET:HE2	38:BL:48:MET:HB3	1.99	0.42
38:BL:80:ILE:CG2	38:BL:81:SER:N	2.83	0.42
45:BS:56:ALA:O	45:BS:57:LEU:HB2	2.20	0.42
55:Bc:3:ILE:HG22	55:Bc:4:LYS:N	2.35	0.42
60:Bh:14:MET:CG	60:Bh:15:ARG:N	2.82	0.42
1:A1:140:C:N4	1:A1:152:G:O6	2.52	0.41
1:A1:318:A:N7	1:A1:325:C:O2'	2.52	0.41
1:A1:506:U:H2'	1:A1:507:OMG:H8	1.85	0.41
1:A1:1367:G:O2'	1:A1:1475:MA6:O2'	2.21	0.41
3:Ab:15:MET:HE1	17:Ap:46:VAL:HG21	2.02	0.41
27:B1:670:G:OP1	27:B1:1398:U:O2'	2.28	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B1:1876:U:H2'	27:B1:1877:G:O4'	2.20	0.41
27:B1:2174:U:H2'	27:B1:2175:G:O4'	2.20	0.41
34:BF:27:ARG:NH1	34:BF:89:ALA:O	2.53	0.41
34:BG:10:GLU:C	34:BG:10:GLU:CD	2.87	0.41
35:BH:12:VAL:HG12	35:BH:56:GLN:HG3	2.01	0.41
23:BI:72:TYR:HB2	23:BI:78:MET:HE2	2.02	0.41
1:A1:896:C:C2	1:A1:897:A:C8	3.09	0.41
13:AI:82:MET:O	13:AI:86:MET:HG2	2.20	0.41
27:B1:347:U:H2'	27:B1:348:G:O4'	2.19	0.41
27:B1:1026:A:H4'	27:B1:1027:A:OP1	2.20	0.41
27:B1:1590:G:O4'	27:B1:1723:G:H2'	2.20	0.41
27:B1:1854:C:OP1	57:Be:22:ARG:NH1	2.53	0.41
27:B1:2038:A:H3'	27:B1:2039:C:H5''	2.02	0.41
34:BF:15:LEU:HD13	34:BF:117:LYS:HD2	2.01	0.41
47:BU:110:GLU:OE2	47:BU:110:GLU:N	2.39	0.41
1:A1:258:U:OP1	11:Aj:30:ARG:NH1	2.44	0.41
1:A1:675:C:OP2	1:A1:676:A:O2'	2.14	0.41
1:A1:1063:G:O2'	20:As:6:GLN:NE2	2.50	0.41
2:Aa:96:PHE:CZ	2:Aa:101:MET:HE3	2.55	0.41
4:Ac:25:ASP:OD1	4:Ac:26:PHE:N	2.54	0.41
9:Ah:29:ARG:C	9:Ah:29:ARG:HE	2.27	0.41
27:B1:242:C:H2'	27:B1:243:4AC:H6	2.03	0.41
27:B1:548:C:C2	27:B1:549:U:C5	3.08	0.41
27:B1:858:U:O2'	27:B1:1653:A:H4'	2.21	0.41
27:B1:958:C:C2	27:B1:959:A:N7	2.88	0.41
27:B1:2265:G:H2'	27:B1:2266:C:O4'	2.21	0.41
27:B1:2407:C:H2'	27:B1:2408:G:H8	1.84	0.41
27:B1:2843:C:H2'	27:B1:2844:4AC:H6	2.03	0.41
30:BB:220:ASP:OD1	30:BB:341:ALA:HA	2.20	0.41
35:BH:66:ARG:NH2	35:BH:67:GLN:OE1	2.53	0.41
36:BI:17:LYS:O	36:BI:21:MET:HG3	2.20	0.41
57:Be:82:THR:O	57:Be:82:THR:OG1	2.37	0.41
1:A1:52:OMU:O5'	1:A1:52:OMU:H6	2.21	0.41
1:A1:277:A:H3'	1:A1:278:G:H5'	2.02	0.41
1:A1:881:G:C2'	1:A1:882:G:O5'	2.69	0.41
3:Ab:69:LEU:HD21	3:Ab:75:LEU:HD12	2.02	0.41
16:Ao:41:ARG:NE	22:Au:48:GLU:OE1	2.53	0.41
16:Ao:45:LEU:HD13	16:Ao:54:LEU:HD21	2.02	0.41
20:As:7:GLY:HA2	20:As:10:LYS:NZ	2.36	0.41
27:B1:538:U:H2'	27:B1:539:G:O4'	2.21	0.41
27:B1:855:G:H2'	27:B1:856:OMG:O4'	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B1:2331:A:H2'	27:B1:2332:A:O4'	2.20	0.41
27:B1:2541:A:O2'	27:B1:2542:U:OP2	2.29	0.41
29:BA:31:ILE:HG23	29:BA:32:PRO:HD2	2.02	0.41
31:BC:134:ILE:O	31:BC:137:VAL:HG22	2.20	0.41
36:BI:34:GLU:OE1	36:BI:101:VAL:HA	2.20	0.41
38:BL:75:LEU:HD23	38:BL:80:ILE:HB	2.02	0.41
39:BM:126:ALA:HB3	39:BM:129:PHE:CZ	2.55	0.41
47:BU:106:ASN:OD1	47:BU:106:ASN:C	2.62	0.41
1:A1:1:A:O5'	5:Ad:49:LYS:NZ	2.52	0.41
1:A1:86:C:H2'	1:A1:87:4AC:H6	2.02	0.41
1:A1:913:G:O2'	21:At:121:GLY:O	2.30	0.41
1:A1:1366:A1I59:N5	1:A1:1366:A1I59:OP2	2.53	0.41
6:Ae:155:LYS:NZ	6:Ae:156:ASP:OD1	2.53	0.41
25:Ax:20:THR:HG22	25:Ax:21:THR:HG23	2.02	0.41
27:B1:1449:G:H21	54:Bb:1:MET:H3	1.68	0.41
27:B1:1870:U:O4	43:BQ:74:ARG:NH2	2.54	0.41
34:BG:33:ARG:CG	34:BG:38:GLU:HB3	2.50	0.41
1:A1:222:A:H2'	1:A1:223:G:O4'	2.20	0.41
1:A1:252:G:H2'	1:A1:253:U:C6	2.56	0.41
1:A1:1319:G:H2'	1:A1:1320:U:O4'	2.20	0.41
1:A1:1404:C:H2'	1:A1:1405:U:C6	2.55	0.41
1:A1:1457:MA6:O5'	1:A1:1457:MA6:H8	2.20	0.41
3:Ab:64:GLU:OE1	3:Ab:64:GLU:HA	2.20	0.41
9:Ah:30:ASP:OD1	9:Ah:128:GLU:OE2	2.38	0.41
22:Au:10:ASP:OD1	22:Au:11:LEU:N	2.52	0.41
24:Aw:3:LYS:N	24:Aw:4:PRO:HD2	2.36	0.41
27:B1:37:G:N3	27:B1:490:G:O2'	2.54	0.41
27:B1:1912:G:N2	27:B1:1914:OMC:OP1	2.51	0.41
27:B1:1913:A:C5	27:B1:1914:OMC:C6	3.09	0.41
27:B1:1931:A:C2	27:B1:1969:A:C4'	3.04	0.41
43:BQ:30:ASP:OD1	43:BQ:30:ASP:N	2.54	0.41
45:BS:51:LEU:HD12	45:BS:95:LEU:HD12	2.02	0.41
1:A1:1107:C:H4'	1:A1:1108:A:O5'	2.21	0.41
1:A1:1108:A:N3	1:A1:1108:A:H2'	2.36	0.41
1:A1:1403:U:H2'	1:A1:1404:C:C6	2.55	0.41
5:Ad:148:GLU:O	5:Ad:149:GLU:C	2.62	0.41
26:Az:32:CYS:HB3	26:Az:55:CYS:SG	2.59	0.41
27:B1:576:G:C2	27:B1:577:G:C8	3.09	0.41
27:B1:1465:A:C4	27:B1:1466:A:C8	3.09	0.41
27:B1:2705:A:N1	27:B1:2722:C:N4	2.69	0.41
28:B2:37:A:H2'	28:B2:38:U:C6	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BA:78:LEU:HD12	57:Be:63:PHE:HB3	2.02	0.41
1:A1:967:G:C2'	1:A1:968:C:O5'	2.69	0.41
1:A1:1149:G:H21	17:Ap:56:GLU:CB	2.34	0.41
4:Ac:43:VAL:HG23	4:Ac:46:ARG:HD2	2.01	0.41
21:At:17:MET:HE1	21:At:75:GLU:HA	2.03	0.41
24:Aw:58:ILE:O	24:Aw:58:ILE:HG22	2.21	0.41
27:B1:377:C:H2'	27:B1:378:4AC:H6	2.02	0.41
27:B1:1360:4AC:H5	27:B1:1360:4AC:HM72	2.03	0.41
30:BB:106:LEU:HD22	30:BB:127:LEU:HD23	2.03	0.41
38:BL:4:ILE:C	38:BL:4:ILE:HD12	2.45	0.41
41:BO:34:ARG:NH1	41:BO:105:ASP:OD2	2.54	0.41
47:BU:32:SER:HA	47:BU:101:MET:SD	2.60	0.41
1:A1:668:OMG:N2	1:A1:732:A:O2'	2.54	0.41
1:A1:938:A:C2	1:A1:1281:A:C4	3.09	0.41
1:A1:1146:G:OP1	1:A1:1146:G:H3'	2.20	0.41
1:A1:1458:C:OP2	1:A1:1461:G:O2'	2.24	0.41
2:Aa:21:THR:HG22	2:Aa:143:THR:OG1	2.20	0.41
2:Aa:194:GLU:C	2:Aa:194:GLU:OE2	2.64	0.41
3:Ab:150:TYR:N	3:Ab:150:TYR:CD1	2.87	0.41
4:Ac:92:ILE:HD12	4:Ac:122:MET:HE1	2.02	0.41
5:Ad:163:PRO:HA	5:Ad:168:ARG:HD3	2.02	0.41
23:Av:14:ILE:O	23:Av:16:ARG:N	2.53	0.41
27:B1:424:G:N2	40:BN:194:LYS:OXT	2.51	0.41
27:B1:429:A:H2'	27:B1:429:A:N3	2.36	0.41
27:B1:662:G:C1'	27:B1:1119:A:N6	2.84	0.41
27:B1:994:G:O2'	27:B1:995:G:H5'	2.21	0.41
27:B1:1326:A:C4	50:BX:116:VAL:HG11	2.56	0.41
27:B1:2585:A:H2'	27:B1:2586:G:O4'	2.20	0.41
28:B2:49:G:O2'	28:B2:50:A:O4'	2.37	0.41
28:B2:52:G:H21	32:BD:20:MET:CE	2.34	0.41
32:BD:54:GLN:NE2	32:BD:82:LEU:HD13	2.36	0.41
34:BF:113:GLU:OE2	34:BF:117:LYS:NZ	2.54	0.41
35:BH:36:MET:HE1	35:BH:66:ARG:HG3	2.02	0.41
41:BO:25:LEU:HD11	44:BR:31:PHE:CD1	2.56	0.41
42:BP:47:VAL:HG12	42:BP:48:ASN:N	2.36	0.41
50:BX:82:ASP:HA	50:BX:85:VAL:HG12	2.03	0.41
1:A1:636:4AC:N3	1:A1:637:G:N7	2.69	0.41
1:A1:895:A:H2'	1:A1:896:C:C6	2.56	0.41
1:A1:973:C:OP1	21:At:61:LYS:NZ	2.53	0.41
1:A1:1224:C:H2'	1:A1:1225:C:H6	1.86	0.41
2:Aa:46:ARG:H	2:Aa:46:ARG:HD3	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Ao:38:MET:HG2	22:Au:34:PHE:HD1	1.85	0.41
27:B1:1144:A:N6	55:Bc:14:LYS:HG2	2.33	0.41
27:B1:1624:C:O2'	27:B1:1625:U:H5'	2.21	0.41
27:B1:2280:G:H5''	27:B1:2281:G:P	2.61	0.41
27:B1:2406:U:H2'	27:B1:2407:C:C6	2.56	0.41
27:B1:3023:C:H4'	30:BB:314:TYR:O	2.21	0.41
39:BM:61:ARG:HG3	39:BM:62:GLY:H	1.85	0.41
40:BN:155:LYS:O	40:BN:160:ARG:NH2	2.52	0.41
41:BO:80:THR:N	41:BO:81:PRO:HD2	2.36	0.41
43:BQ:13:GLU:C	43:BQ:13:GLU:CD	2.90	0.41
49:BW:12:GLU:OE1	49:BW:12:GLU:N	2.46	0.41
1:A1:234:C:OP1	19:Ar:68:SER:OG	2.30	0.40
1:A1:951:5MC:OP1	1:A1:951:5MC:H6	2.04	0.40
27:B1:2683:G:H2'	27:B1:2684:OMG:C8	2.55	0.40
28:B2:37:A:O2'	28:B2:38:U:C5'	2.69	0.40
32:BD:81:THR:O	32:BD:82:LEU:HD13	2.21	0.40
47:BU:45:PRO:O	47:BU:112:ARG:NH2	2.50	0.40
1:A1:548:U:C2'	1:A1:549:A:O5'	2.69	0.40
27:B1:2704:G:OP2	65:B1:3230:HOH:O	2.22	0.40
38:BL:33:VAL:HG12	38:BL:34:LEU:N	2.36	0.40
46:BT:31:ASP:OD1	46:BT:32:ARG:N	2.55	0.40
1:A1:586:U:O5'	1:A1:587:C:H5'	2.22	0.40
1:A1:904:G:N1	1:A1:1300:G:OP2	2.50	0.40
1:A1:1312:C:N3	9:Ah:95:SER:OG	2.55	0.40
12:Ak:97:GLU:OE1	12:Ak:101:LYS:HE2	2.22	0.40
16:Ao:36:ALA:O	16:Ao:39:VAL:HG12	2.22	0.40
20:As:46:ILE:O	20:As:50:ILE:HD12	2.21	0.40
24:Aw:24:GLU:OE1	24:Aw:24:GLU:CA	2.69	0.40
25:Ax:66:GLU:OE1	25:Ax:66:GLU:N	2.52	0.40
27:B1:29:A:C2	27:B1:551:A:C8	3.09	0.40
27:B1:1277:G:OP1	36:BI:52:ARG:NH2	2.53	0.40
27:B1:1496:A:H2'	27:B1:1497:A:C8	2.56	0.40
27:B1:1633:U:C2	27:B1:1634:A:C8	3.09	0.40
27:B1:1769:4AC:H6	27:B1:1769:4AC:O5'	2.20	0.40
27:B1:1818:4AC:HM73	27:B1:2126:C:N4	2.37	0.40
27:B1:2423:G:N3	27:B1:2423:G:H2'	2.37	0.40
27:B1:2577:C:C2	27:B1:2578:U:C5	3.09	0.40
27:B1:2888:C:H2'	27:B1:2889:G:O4'	2.21	0.40
28:B2:21:G:O2'	28:B2:22:G:O4'	2.33	0.40
30:BB:260:HIS:HA	30:BB:261:PRO:C	2.47	0.40
1:A1:103:A:C4	1:A1:237:C:N4	2.90	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:123:U:H2'	1:A1:124:C:C6	2.57	0.40
1:A1:219:C:H2'	1:A1:220:4AC:H6	2.03	0.40
1:A1:319:C:N3	1:A1:329:OMG:N2	2.69	0.40
1:A1:359:G:O3'	15:An:79:LYS:NZ	2.54	0.40
1:A1:958:A:H2'	1:A1:959:G:O4'	2.22	0.40
4:Ac:150:GLU:OE1	4:Ac:150:GLU:CA	2.69	0.40
7:Af:65:VAL:O	7:Af:65:VAL:HG13	2.20	0.40
9:Ah:114:ARG:HD2	9:Ah:189:ILE:HD13	2.03	0.40
17:Ap:49:LYS:C	17:Ap:49:LYS:HD2	2.47	0.40
27:B1:1594:C:H2'	27:B1:1595:G:H8	1.86	0.40
27:B1:2697:G:OP2	27:B1:2697:G:N2	2.54	0.40
29:BA:25:ARG:HG2	29:BA:25:ARG:HH11	1.87	0.40
2:Aa:21:THR:HG21	2:Aa:144:GLU:HB3	2.03	0.40
27:B1:146:C:C2'	27:B1:147:U:O5'	2.69	0.40
27:B1:548:C:O2	27:B1:548:C:H2'	2.22	0.40
27:B1:637:G:H2'	27:B1:638:G:O4'	2.22	0.40
27:B1:891:G:H2'	27:B1:892:C:C6	2.57	0.40
27:B1:1845:C:H2'	27:B1:1846:4AC:H6	2.04	0.40
31:BC:41:HIS:NE2	31:BC:103:GLU:O	2.43	0.40
32:BD:62:LYS:HD3	32:BD:62:LYS:N	2.37	0.40
38:BL:11:VAL:HG22	38:BL:54:GLU:HB3	2.04	0.40
41:BO:48:ILE:CD1	41:BO:94:ALA:HB2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Aa	194/202 (96%)	190 (98%)	4 (2%)	0	100	100
3	Ab	193/210 (92%)	189 (98%)	4 (2%)	0	100	100
4	Ac	183/198 (92%)	179 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Ad	171/180 (95%)	169 (99%)	2 (1%)	0	100	100
6	Ae	240/243 (99%)	232 (97%)	8 (3%)	0	100	100
7	Af	224/236 (95%)	215 (96%)	9 (4%)	0	100	100
8	Ag	122/125 (98%)	110 (90%)	12 (10%)	0	100	100
9	Ah	212/215 (99%)	202 (95%)	10 (5%)	0	100	100
10	Ai	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
11	Aj	123/127 (97%)	118 (96%)	5 (4%)	0	100	100
12	Ak	132/135 (98%)	126 (96%)	6 (4%)	0	100	100
13	Al	97/102 (95%)	93 (96%)	4 (4%)	0	100	100
14	Am	126/137 (92%)	118 (94%)	8 (6%)	0	100	100
15	An	142/147 (97%)	137 (96%)	5 (4%)	0	100	100
16	Ao	135/148 (91%)	134 (99%)	1 (1%)	0	100	100
17	Ap	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
18	Aq	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
19	Ar	105/113 (93%)	104 (99%)	1 (1%)	0	100	100
20	As	61/67 (91%)	60 (98%)	1 (2%)	0	100	100
21	At	119/132 (90%)	117 (98%)	2 (2%)	0	100	100
22	Au	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
23	Av	93/99 (94%)	92 (99%)	1 (1%)	0	100	100
23	Bl	90/99 (91%)	89 (99%)	1 (1%)	0	100	100
24	Aw	59/63 (94%)	58 (98%)	1 (2%)	0	100	100
25	Ax	62/71 (87%)	61 (98%)	1 (2%)	0	100	100
26	Az	54/60 (90%)	53 (98%)	1 (2%)	0	100	100
29	BA	235/239 (98%)	223 (95%)	12 (5%)	0	100	100
30	BB	361/365 (99%)	348 (96%)	13 (4%)	0	100	100
31	BC	253/255 (99%)	247 (98%)	6 (2%)	0	100	100
32	BD	180/186 (97%)	163 (91%)	17 (9%)	0	100	100
33	BE	181/184 (98%)	178 (98%)	3 (2%)	0	100	100
34	BF	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
34	BG	119/123 (97%)	116 (98%)	3 (2%)	0	100	100
35	BH	165/181 (91%)	161 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	BI	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
37	BJ	138/141 (98%)	138 (100%)	0	0	100	100
38	BK	79/83 (95%)	72 (91%)	7 (9%)	0	100	100
38	BL	80/83 (96%)	77 (96%)	3 (4%)	0	100	100
39	BM	145/147 (99%)	136 (94%)	9 (6%)	0	100	100
40	BN	191/194 (98%)	183 (96%)	8 (4%)	0	100	100
41	BO	194/203 (96%)	190 (98%)	4 (2%)	0	100	100
42	BP	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
43	BQ	146/150 (97%)	143 (98%)	3 (2%)	0	100	100
44	BR	94/97 (97%)	94 (100%)	0	0	100	100
45	BS	149/155 (96%)	144 (97%)	5 (3%)	0	100	100
46	BT	82/86 (95%)	80 (98%)	2 (2%)	0	100	100
47	BU	118/121 (98%)	116 (98%)	2 (2%)	0	100	100
48	BV	61/66 (92%)	61 (100%)	0	0	100	100
49	BW	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
50	BX	152/155 (98%)	149 (98%)	3 (2%)	0	100	100
51	BY	95/99 (96%)	94 (99%)	1 (1%)	0	100	100
52	BZ	92/95 (97%)	90 (98%)	2 (2%)	0	100	100
53	Ba	126/130 (97%)	125 (99%)	1 (1%)	0	100	100
54	Bb	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
55	Bc	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
56	Bd	58/62 (94%)	55 (95%)	3 (5%)	0	100	100
57	Be	80/83 (96%)	73 (91%)	7 (9%)	0	100	100
58	Bf	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
59	Bg	44/51 (86%)	44 (100%)	0	0	100	100
60	Bh	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
61	Bi	92/94 (98%)	92 (100%)	0	0	100	100
62	Bj	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
63	Bk	60/64 (94%)	59 (98%)	1 (2%)	0	100	100
All	All	7961/8293 (96%)	7729 (97%)	232 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Aa	168/173 (97%)	168 (100%)	0	100	100
3	Ab	149/167 (89%)	148 (99%)	1 (1%)	81	92
4	Ac	161/171 (94%)	161 (100%)	0	100	100
5	Ad	156/160 (98%)	156 (100%)	0	100	100
6	Ae	211/213 (99%)	210 (100%)	1 (0%)	86	95
7	Af	186/197 (94%)	185 (100%)	1 (0%)	86	95
8	Ag	103/108 (95%)	103 (100%)	0	100	100
9	Ah	182/184 (99%)	181 (100%)	1 (0%)	86	95
10	Ai	107/108 (99%)	106 (99%)	1 (1%)	75	89
11	Aj	98/103 (95%)	98 (100%)	0	100	100
12	Ak	106/111 (96%)	106 (100%)	0	100	100
13	Al	82/91 (90%)	82 (100%)	0	100	100
14	Am	95/104 (91%)	95 (100%)	0	100	100
15	An	117/121 (97%)	117 (100%)	0	100	100
16	Ao	112/122 (92%)	111 (99%)	1 (1%)	75	89
17	Ap	44/46 (96%)	44 (100%)	0	100	100
18	Aq	141/143 (99%)	141 (100%)	0	100	100
19	Ar	96/102 (94%)	96 (100%)	0	100	100
20	As	57/61 (93%)	55 (96%)	2 (4%)	31	57
21	At	104/114 (91%)	103 (99%)	1 (1%)	73	88
22	Au	126/127 (99%)	125 (99%)	1 (1%)	79	91
23	Av	86/89 (97%)	86 (100%)	0	100	100
23	Bl	83/89 (93%)	83 (100%)	0	100	100
24	Aw	53/54 (98%)	53 (100%)	0	100	100
25	Ax	51/60 (85%)	51 (100%)	0	100	100
26	Az	48/53 (91%)	48 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	BA	186/189 (98%)	185 (100%)	1 (0%)	86	95
30	BB	308/312 (99%)	306 (99%)	2 (1%)	84	93
31	BC	213/213 (100%)	209 (98%)	4 (2%)	52	77
32	BD	142/158 (90%)	141 (99%)	1 (1%)	81	92
33	BE	155/156 (99%)	154 (99%)	1 (1%)	84	93
34	BF	97/99 (98%)	97 (100%)	0	100	100
34	BG	97/99 (98%)	95 (98%)	2 (2%)	48	74
35	BH	143/152 (94%)	143 (100%)	0	100	100
36	BI	122/122 (100%)	122 (100%)	0	100	100
37	BJ	106/108 (98%)	105 (99%)	1 (1%)	75	89
38	BK	64/66 (97%)	64 (100%)	0	100	100
38	BL	65/66 (98%)	64 (98%)	1 (2%)	60	82
39	BM	117/117 (100%)	116 (99%)	1 (1%)	75	89
40	BN	161/162 (99%)	160 (99%)	1 (1%)	84	93
41	BO	158/169 (94%)	158 (100%)	0	100	100
42	BP	101/101 (100%)	99 (98%)	2 (2%)	50	76
43	BQ	128/130 (98%)	127 (99%)	1 (1%)	79	91
44	BR	85/87 (98%)	83 (98%)	2 (2%)	44	70
45	BS	125/130 (96%)	125 (100%)	0	100	100
46	BT	74/77 (96%)	73 (99%)	1 (1%)	62	82
47	BU	110/110 (100%)	109 (99%)	1 (1%)	75	89
48	BV	54/56 (96%)	54 (100%)	0	100	100
49	BW	60/66 (91%)	60 (100%)	0	100	100
50	BX	132/133 (99%)	132 (100%)	0	100	100
51	BY	78/80 (98%)	77 (99%)	1 (1%)	65	84
52	BZ	76/83 (92%)	76 (100%)	0	100	100
53	Ba	115/117 (98%)	115 (100%)	0	100	100
54	Bb	80/81 (99%)	80 (100%)	0	100	100
55	Bc	73/74 (99%)	73 (100%)	0	100	100
56	Bd	48/51 (94%)	47 (98%)	1 (2%)	48	74
57	Be	60/61 (98%)	60 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	Bf	46/47 (98%)	46 (100%)	0	100	100
59	Bg	37/39 (95%)	37 (100%)	0	100	100
60	Bh	32/35 (91%)	32 (100%)	0	100	100
61	Bi	82/83 (99%)	82 (100%)	0	100	100
62	Bj	70/72 (97%)	70 (100%)	0	100	100
63	Bk	53/55 (96%)	53 (100%)	0	100	100
All	All	6775/7027 (96%)	6741 (100%)	34 (0%)	85	95

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Ab	146	PHE
6	Ae	189	GLN
7	Af	143	PHE
9	Ah	173	CYS
10	Ai	112	SER
16	Ao	39	VAL
20	As	17	VAL
20	As	22	ASN
21	At	80	THR
22	Au	34	PHE
29	BA	31	ILE
30	BB	255	SER
30	BB	365	GLN
31	BC	154	THR
31	BC	164	LEU
31	BC	218	ASP
31	BC	224	ASN
32	BD	50	GLN
33	BE	82	VAL
34	BG	21	GLN
34	BG	70	CYS
37	BJ	76	GLN
38	BL	26	ASP
39	BM	124	ILE
40	BN	37	VAL
42	BP	58	ASP
42	BP	119	MET
43	BQ	69	GLN
44	BR	7	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	BR	94	ARG
46	BT	85	LEU
47	BU	100	VAL
51	BY	55	LEU
56	Bd	29	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
29	BA	7	GLN
29	BA	229	HIS
30	BB	365	GLN
34	BG	21	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A1	1487/1497 (99%)	247 (16%)	17 (1%)
27	B1	2928/3051 (95%)	437 (14%)	29 (0%)
28	B2	124/125 (99%)	16 (12%)	0
All	All	4539/4673 (97%)	700 (15%)	46 (1%)

All (700) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A1	4	C
1	A1	17	5MC
1	A1	34	G
1	A1	42	G
1	A1	43	A
1	A1	45	U
1	A1	47	A
1	A1	56	A
1	A1	57	G
1	A1	60	A
1	A1	72	C
1	A1	73	U
1	A1	80	A
1	A1	81	C
1	A1	95	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A1	100	A
1	A1	104	A
1	A1	105	C
1	A1	114	A
1	A1	115	A
1	A1	116	C
1	A1	134	A
1	A1	155	U
1	A1	159	C
1	A1	181	G
1	A1	182	A
1	A1	184	G
1	A1	193	G
1	A1	194	C
1	A1	197	A
1	A1	198	A
1	A1	199	A
1	A1	206	C
1	A1	217	G
1	A1	223	G
1	A1	237	C
1	A1	238	LHH
1	A1	241	U
1	A1	242	U
1	A1	244	G
1	A1	247	A
1	A1	248	G
1	A1	253	U
1	A1	255	G
1	A1	259	A
1	A1	260	A
1	A1	263	G
1	A1	264	C
1	A1	270	A
1	A1	278	G
1	A1	286	C
1	A1	298	G
1	A1	303	A
1	A1	318	A
1	A1	325	C
1	A1	329	OMG
1	A1	335	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A1	341	A
1	A1	349	C
1	A1	350	A
1	A1	351	G
1	A1	359	G
1	A1	361	A2M
1	A1	364	C
1	A1	369	C
1	A1	370	A
1	A1	387	C
1	A1	388	G
1	A1	390	G
1	A1	394	A
1	A1	403	G
1	A1	410	C
1	A1	412	C
1	A1	413	U
1	A1	414	G
1	A1	415	G
1	A1	424	U
1	A1	433	G
1	A1	437	A
1	A1	440	G
1	A1	448	A
1	A1	450	U
1	A1	462	A
1	A1	464	G
1	A1	465	G
1	A1	466	5MC
1	A1	472	G
1	A1	475	G
1	A1	481	G7M
1	A1	485	U
1	A1	486	A
1	A1	487	A
1	A1	501	A
1	A1	518	U
1	A1	520	G
1	A1	527	A
1	A1	530	C
1	A1	531	G
1	A1	536	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A1	537	A
1	A1	541	OMG
1	A1	542	G
1	A1	549	A
1	A1	559	C
1	A1	587	C
1	A1	588	G
1	A1	608	U
1	A1	617	G
1	A1	620	A
1	A1	630	U
1	A1	641	U
1	A1	642	A
1	A1	659	A
1	A1	678	U
1	A1	688	G
1	A1	703	G
1	A1	704	U
1	A1	710	G
1	A1	732	A
1	A1	734	C
1	A1	736	A
1	A1	748	U
1	A1	749	A
1	A1	770	A
1	A1	772	G
1	A1	773	G
1	A1	776	G
1	A1	783	A
1	A1	799	U
1	A1	802	A
1	A1	803	G
1	A1	819	A2M
1	A1	827	4AC
1	A1	873	A
1	A1	882	G
1	A1	885	G
1	A1	886	G
1	A1	890	G
1	A1	893	C
1	A1	894	U
1	A1	895	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A1	902	G
1	A1	907	G
1	A1	920	U
1	A1	929	A
1	A1	931	G
1	A1	934	G
1	A1	935	G
1	A1	936	G
1	A1	937	A
1	A1	941	U
1	A1	951	5MC
1	A1	961	A
1	A1	963	G
1	A1	967	G
1	A1	969	C
1	A1	971	G
1	A1	978	G
1	A1	979	G
1	A1	983	U
1	A1	984	G
1	A1	987	G
1	A1	988	G
1	A1	989	A
1	A1	990	C
1	A1	992	C
1	A1	993	G
1	A1	1007	C
1	A1	1018	U
1	A1	1019	C
1	A1	1047	G
1	A1	1048	U
1	A1	1054	A
1	A1	1055	A
1	A1	1078	U
1	A1	1095	U
1	A1	1104	A
1	A1	1108	A
1	A1	1120	C
1	A1	1121	U
1	A1	1130	U
1	A1	1133	G
1	A1	1143	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A1	1146	G
1	A1	1147	C
1	A1	1153	A
1	A1	1158	A
1	A1	1159	G
1	A1	1163	A
1	A1	1164	G
1	A1	1174	A
1	A1	1175	A
1	A1	1176	A
1	A1	1177	C
1	A1	1189	A
1	A1	1190	5MC
1	A1	1198	A
1	A1	1200	A
1	A1	1201	A
1	A1	1203	G
1	A1	1210	A
1	A1	1219	C
1	A1	1220	C
1	A1	1232	G
1	A1	1241	A
1	A1	1242	A
1	A1	1262	G
1	A1	1264	U
1	A1	1267	G
1	A1	1268	A
1	A1	1270	OMC
1	A1	1282	C
1	A1	1283	U
1	A1	1284	C
1	A1	1295	A
1	A1	1298	U
1	A1	1308	A
1	A1	1309	G
1	A1	1313	C
1	A1	1315	G
1	A1	1319	G
1	A1	1326	U
1	A1	1332	G
1	A1	1344	C
1	A1	1356	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A1	1359	C
1	A1	1360	A
1	A1	1381	G
1	A1	1412	G
1	A1	1415	G
1	A1	1439	G
1	A1	1444	G
1	A1	1448	G
1	A1	1449	A
1	A1	1450	A
1	A1	1451	G
1	A1	1456	A
1	A1	1459	A
1	A1	1461	G
1	A1	1462	G
1	A1	1463	U
1	A1	1474	G
1	A1	1476	MA6
1	A1	1477	C
1	A1	1478	C
1	A1	1486	C
1	A1	1487	G
27	B1	14	U
27	B1	15	A
27	B1	47	C
27	B1	55	OMG
27	B1	70	C
27	B1	72	A
27	B1	75	A
27	B1	76	G
27	B1	92	G
27	B1	100	U
27	B1	118	A
27	B1	120	U
27	B1	121	G
27	B1	124	A
27	B1	125	C
27	B1	127	U
27	B1	131	G
27	B1	134	G
27	B1	137	U
27	B1	138	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	B1	147	U
27	B1	155	U
27	B1	157	A
27	B1	158	U
27	B1	171	A
27	B1	186	A
27	B1	205	G
27	B1	206	A
27	B1	212	A
27	B1	217	A
27	B1	219	A
27	B1	220	G
27	B1	223	A
27	B1	238	G
27	B1	255	A
27	B1	256	G
27	B1	278	A
27	B1	279	C
27	B1	299	G
27	B1	302	G
27	B1	303	U
27	B1	307	G
27	B1	312	C
27	B1	316	U
27	B1	333	A
27	B1	335	G
27	B1	342	U
27	B1	343	C
27	B1	352	C
27	B1	362	G
27	B1	364	G
27	B1	370	G
27	B1	371	A
27	B1	372	U
27	B1	379	G
27	B1	381	A
27	B1	408	A
27	B1	415	G
27	B1	431	A
27	B1	441	A
27	B1	451	G
27	B1	452	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	B1	470	A
27	B1	473	A
27	B1	476	U
27	B1	477	C
27	B1	497	A
27	B1	501	OMC
27	B1	507	G
27	B1	521	G
27	B1	524	C
27	B1	543	A
27	B1	546	G
27	B1	547	C
27	B1	567	G
27	B1	569	A
27	B1	570	G
27	B1	571	G
27	B1	575	C
27	B1	585	G
27	B1	586	G
27	B1	590	G
27	B1	591	A
27	B1	617	C
27	B1	624	G
27	B1	655	C
27	B1	667	A
27	B1	671	G
27	B1	678	A
27	B1	679	G
27	B1	695	A
27	B1	731	C
27	B1	735	C
27	B1	736	A
27	B1	737	U
27	B1	741	C
27	B1	778	A
27	B1	782	C
27	B1	809	A
27	B1	810	A
27	B1	820	U
27	B1	843	C
27	B1	848	A
27	B1	850	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	B1	853	A
27	B1	856	OMG
27	B1	857	A2M
27	B1	860	G
27	B1	864	C
27	B1	875	U
27	B1	878	U
27	B1	883	U
27	B1	888	5MU
27	B1	889	U
27	B1	900	A
27	B1	911	G
27	B1	912	G
27	B1	918	A
27	B1	920	OMG
27	B1	921	OMG
27	B1	925	A
27	B1	938	A
27	B1	941	G
27	B1	948	C
27	B1	958	C
27	B1	959	A
27	B1	962	C
27	B1	964	G
27	B1	966	A
27	B1	979	4AC
27	B1	982	A
27	B1	983	G
27	B1	996	G
27	B1	1003	A
27	B1	1005	U
27	B1	1016	G
27	B1	1017	C
27	B1	1018	A
27	B1	1019	G
27	B1	1020	G
27	B1	1023	G
27	B1	1026	A
27	B1	1027	A
27	B1	1028	A
27	B1	1030	C
27	B1	1033	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	B1	1047	A
27	B1	1049	C
27	B1	1084	G
27	B1	1085	G
27	B1	1110	G
27	B1	1116	A
27	B1	1117	A
27	B1	1119	A
27	B1	1120	A
27	B1	1125	G
27	B1	1127	C
27	B1	1140	C
27	B1	1144	A
27	B1	1146	G
27	B1	1147	U
27	B1	1148	G
27	B1	1167	A
27	B1	1173	U
27	B1	1174	G
27	B1	1181	G
27	B1	1182	C
27	B1	1184	U
27	B1	1185	U
27	B1	1186	A
27	B1	1187	G
27	B1	1188	A
27	B1	1250	G
27	B1	1251	A
27	B1	1252	G
27	B1	1254	U
27	B1	1255	C
27	B1	1269	A
27	B1	1272	G
27	B1	1274	C
27	B1	1275	G
27	B1	1278	G
27	B1	1282	A
27	B1	1293	4AC
27	B1	1315	A
27	B1	1316	U
27	B1	1317	U
27	B1	1318	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	B1	1326	A
27	B1	1328	C
27	B1	1332	U
27	B1	1355	G
27	B1	1369	A
27	B1	1370	G
27	B1	1373	C
27	B1	1379	G
27	B1	1381	G
27	B1	1392	C
27	B1	1395	G
27	B1	1396	G
27	B1	1398	U
27	B1	1399	C
27	B1	1417	G
27	B1	1418	U
27	B1	1439	LHH
27	B1	1445	A
27	B1	1446	G
27	B1	1450	C
27	B1	1489	OMC
27	B1	1517	C
27	B1	1521	G
27	B1	1523	A
27	B1	1525	A
27	B1	1529	A
27	B1	1532	C
27	B1	1541	A
27	B1	1561	G
27	B1	1574	A
27	B1	1576	G
27	B1	1589	C
27	B1	1600	A
27	B1	1608	4AC
27	B1	1616	G
27	B1	1617	A
27	B1	1636	G
27	B1	1643	G
27	B1	1644	A
27	B1	1645	G
27	B1	1646	U
27	B1	1647	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	B1	1658	G
27	B1	1659	A
27	B1	1665	G
27	B1	1670	A
27	B1	1679	A
27	B1	1681	G
27	B1	1697	G
27	B1	1699	G
27	B1	1700	U
27	B1	1701	U
27	B1	1708	A
27	B1	1710	C
27	B1	1715	G
27	B1	1721	G
27	B1	1723	G
27	B1	1724	A
27	B1	1725	A
27	B1	1735	G
27	B1	1738	A
27	B1	1747	C
27	B1	1755	A
27	B1	1766	A
27	B1	1767	A
27	B1	1773	A
27	B1	1774	C
27	B1	1779	G
27	B1	1780	C
27	B1	1781	C
27	B1	1782	C
27	B1	1791	G
27	B1	1792	A
27	B1	1804	U
27	B1	1805	G
27	B1	1807	C
27	B1	1812	G
27	B1	1813	A
27	B1	1814	A
27	B1	1834	G
27	B1	1856	G
27	B1	1860	A
27	B1	1871	G
27	B1	1881	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	B1	1904	OMG
27	B1	1913	A
27	B1	1920	A
27	B1	1931	A
27	B1	1940	C
27	B1	1941	U
27	B1	1969	A
27	B1	2003	A
27	B1	2017	C
27	B1	2026	A
27	B1	2031	G
27	B1	2033	G
27	B1	2034	G
27	B1	2035	G
27	B1	2036	U
27	B1	2037	A
27	B1	2038	A
27	B1	2039	C
27	B1	2040	U
27	B1	2042	U
27	B1	2044	A
27	B1	2049	C
27	B1	2050	U
27	B1	2051	U
27	B1	2052	A
27	B1	2053	A
27	B1	2055	G
27	B1	2062	A
27	B1	2063	A
27	B1	2064	U
27	B1	2080	U
27	B1	2089	G
27	B1	2092	U
27	B1	2096	U
27	B1	2097	G
27	B1	2116	U
27	B1	2118	U
27	B1	2155	G
27	B1	2156	C
27	B1	2157	A
27	B1	2160	C
27	B1	2167	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	B1	2174	U
27	B1	2179	A
27	B1	2183	A
27	B1	2185	G
27	B1	2186	A
27	B1	2193	G
27	B1	2217	G
27	B1	2220	A
27	B1	2226	C
27	B1	2231	G
27	B1	2232	G
27	B1	2234	G
27	B1	2235	C
27	B1	2236	G
27	B1	2237	C
27	B1	2238	A
27	B1	2239	G
27	B1	2240	C
27	B1	2241	G
27	B1	2246	C
27	B1	2247	G
27	B1	2252	G
27	B1	2255	U
27	B1	2257	G
27	B1	2260	G
27	B1	2263	C
27	B1	2270	C
27	B1	2281	G
27	B1	2282	A
27	B1	2287	U
27	B1	2289	C
27	B1	2290	A
27	B1	2294	G
27	B1	2295	A
27	B1	2302	C
27	B1	2304	A
27	B1	2314	G
27	B1	2322	A
27	B1	2339	A
27	B1	2340	C
27	B1	2352	G
27	B1	2353	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	B1	2372	A
27	B1	2381	A
27	B1	2391	OMG
27	B1	2398	C
27	B1	2402	A
27	B1	2403	A
27	B1	2420	U
27	B1	2423	G
27	B1	2429	4AC
27	B1	2435	A
27	B1	2437	A
27	B1	2440	G
27	B1	2442	A
27	B1	2450	A
27	B1	2460	G
27	B1	2465	G
27	B1	2472	A
27	B1	2478	G
27	B1	2501	G
27	B1	2503	C
27	B1	2510	A
27	B1	2519	G
27	B1	2520	C
27	B1	2543	G
27	B1	2545	C
27	B1	2547	G
27	B1	2548	A
27	B1	2549	A
27	B1	2550	A
27	B1	2557	OMC
27	B1	2564	A
27	B1	2591	C
27	B1	2594	A
27	B1	2607	OMC
27	B1	2614	C
27	B1	2618	G
27	B1	2619	C
27	B1	2634	A
27	B1	2645	G
27	B1	2650	A
27	B1	2682	A
27	B1	2683	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	B1	2694	G
27	B1	2698	G
27	B1	2715	G
27	B1	2718	A
27	B1	2729	U
27	B1	2730	A
27	B1	2737	G
27	B1	2745	U
27	B1	2760	A
27	B1	2761	A
27	B1	2762	G
27	B1	2769	C
27	B1	2806	U
27	B1	2827	U
27	B1	2829	G
27	B1	2841	C
27	B1	2848	G
27	B1	2849	C
27	B1	2862	A
27	B1	2865	G
27	B1	2879	A
27	B1	2880	G
27	B1	2890	A
27	B1	2891	A
27	B1	2893	A
27	B1	2894	U
27	B1	2895	A
27	B1	2949	A
27	B1	2959	U
27	B1	2962	A
27	B1	2972	U
27	B1	2974	A
27	B1	2989	A
27	B1	2998	G
27	B1	3002	C
27	B1	3021	G
27	B1	3022	C
27	B1	3028	C
27	B1	3040	G
28	B2	2	A
28	B2	3	C
28	B2	23	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	B2	30	4AC
28	B2	39	U
28	B2	44	A
28	B2	51	A
28	B2	54	U
28	B2	56	A
28	B2	57	G
28	B2	87	C
28	B2	93	G
28	B2	94	G
28	B2	113	G
28	B2	114	C
28	B2	115	4AC

All (46) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A1	80	A
1	A1	99	C
1	A1	197	A
1	A1	240	A
1	A1	252	G
1	A1	387	C
1	A1	541	OMG
1	A1	1018	U
1	A1	1054	A
1	A1	1107	C
1	A1	1119	A
1	A1	1146	G
1	A1	1152	G
1	A1	1163	A
1	A1	1308	A
1	A1	1438	U
1	A1	1462	G
27	B1	120	U
27	B1	126	C
27	B1	146	C
27	B1	311	C
27	B1	315	A
27	B1	380	U
27	B1	472	U
27	B1	542	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	B1	677	G
27	B1	877	C
27	B1	888	5MU
27	B1	920	OMG
27	B1	982	A
27	B1	1004	C
27	B1	1331	G
27	B1	1368	A
27	B1	1394	C
27	B1	1444	G
27	B1	1696	G
27	B1	1765	G
27	B1	1940	C
27	B1	2166	A
27	B1	2173	G
27	B1	2251	G
27	B1	2259	A
27	B1	2280	G
27	B1	2617	5MC
27	B1	2893	A
27	B1	2958	G

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

243 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	OMG	B1	856	27	18,26,27	2.60	8 (44%)	19,38,41	1.53	4 (21%)
27	4AC	B1	2492	27	21,24,25	3.27	10 (47%)	29,34,37	1.05	4 (13%)
27	4AC	B1	786	27	21,24,25	3.26	9 (42%)	29,34,37	1.05	4 (13%)
1	4AC	A1	761	1	21,24,25	3.29	9 (42%)	29,34,37	1.08	4 (13%)
27	5MC	B1	1344	27	18,22,23	3.17	7 (38%)	26,32,35	1.00	2 (7%)
27	OMC	B1	1489	27	19,22,23	3.10	8 (42%)	26,31,34	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	A1	863	1	18,22,23	3.19	7 (38%)	26,32,35	1.01	2 (7%)
27	4AC	B1	721	27	21,24,25	3.24	9 (42%)	29,34,37	1.03	4 (13%)
27	4AC	B1	3006	27	21,24,25	3.27	9 (42%)	29,34,37	1.07	4 (13%)
27	4AC	B1	1579	27	21,24,25	3.29	9 (42%)	29,34,37	1.08	4 (13%)
27	OMG	B1	808	27	18,26,27	2.59	8 (44%)	19,38,41	1.53	4 (21%)
27	4AC	B1	2020	27	21,24,25	3.25	10 (47%)	29,34,37	1.03	4 (13%)
27	4AC	B1	527	27	21,24,25	3.26	9 (42%)	29,34,37	1.07	4 (13%)
1	4AC	A1	856	1	21,24,25	3.24	10 (47%)	29,34,37	1.05	4 (13%)
27	OMG	B1	2365	27	18,26,27	2.59	8 (44%)	19,38,41	1.49	4 (21%)
1	4AC	A1	1254	1	21,24,25	3.26	9 (42%)	29,34,37	1.26	6 (20%)
1	LHH	A1	238	1	22,25,26	2.93	6 (27%)	29,35,38	1.51	4 (13%)
1	5MC	A1	473	1	18,22,23	3.19	7 (38%)	26,32,35	0.99	2 (7%)
27	OMG	B1	921	27	18,26,27	2.59	8 (44%)	19,38,41	1.49	4 (21%)
27	4AC	B1	1067	27	21,24,25	3.25	10 (47%)	29,34,37	1.05	4 (13%)
27	4AC	B1	1064	27	21,24,25	3.25	10 (47%)	29,34,37	1.07	4 (13%)
27	OMC	B1	1914	27	19,22,23	3.09	8 (42%)	26,31,34	0.78	0
27	4AC	B1	1967	27	21,24,25	3.23	9 (42%)	29,34,37	1.01	4 (13%)
27	4AC	B1	2432	27	21,24,25	3.27	10 (47%)	29,34,37	1.05	4 (13%)
27	4AC	B1	2749	27	21,24,25	3.24	10 (47%)	29,34,37	1.04	4 (13%)
1	4AC	A1	839	1	21,24,25	3.25	9 (42%)	29,34,37	1.06	4 (13%)
1	G7M	A1	481	1	20,26,27	4.09	10 (50%)	17,39,42	0.98	1 (5%)
27	OMG	B1	2108	27	18,26,27	2.58	8 (44%)	19,38,41	1.53	4 (21%)
1	4AC	A1	1467	1	21,24,25	3.29	9 (42%)	29,34,37	1.45	5 (17%)
1	5MC	A1	1013	1	18,22,23	3.19	7 (38%)	26,32,35	0.99	2 (7%)
1	5MC	A1	17	1	18,22,23	3.16	7 (38%)	26,32,35	0.98	2 (7%)
1	4AC	A1	827	1	21,24,25	3.28	10 (47%)	29,34,37	1.07	4 (13%)
27	4SU	B1	2565	27	18,21,22	3.87	8 (44%)	26,30,33	2.23	5 (19%)
1	OMC	A1	1270	1	19,22,23	3.13	8 (42%)	26,31,34	0.72	0
27	4AC	B1	1762	27	21,24,25	3.25	10 (47%)	29,34,37	1.04	4 (13%)
27	UR3	B1	2700	27	19,22,23	3.17	7 (36%)	26,32,35	1.41	3 (11%)
27	OMG	B1	530	27	18,26,27	2.61	8 (44%)	19,38,41	1.48	4 (21%)
27	OMC	B1	2557	27	19,22,23	3.13	8 (42%)	26,31,34	1.02	2 (7%)
27	4AC	B1	1608	27	21,24,25	3.30	9 (42%)	29,34,37	1.29	6 (20%)
27	4AC	B1	896	27	21,24,25	3.25	9 (42%)	29,34,37	1.03	3 (10%)
27	4AC	B1	688	27	21,24,25	3.27	10 (47%)	29,34,37	1.04	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4AC	A1	467	1	21,24,25	3.15	10 (47%)	29,34,37	0.94	2 (6%)
27	4AC	B1	1818	27	21,24,25	3.24	10 (47%)	29,34,37	1.03	4 (13%)
1	4AC	A1	274	1	21,24,25	3.27	9 (42%)	29,34,37	1.05	4 (13%)
27	4AC	B1	1639	27	21,24,25	3.27	10 (47%)	29,34,37	1.05	4 (13%)
27	4AC	B1	1345	27	21,24,25	3.24	10 (47%)	29,34,37	1.02	4 (13%)
27	LHH	B1	1439	27	22,25,26	2.92	6 (27%)	29,35,38	1.33	2 (6%)
1	OMU	A1	52	1	19,22,23	3.31	7 (36%)	26,31,34	1.68	5 (19%)
27	4AC	B1	337	27	21,24,25	3.25	10 (47%)	29,34,37	1.03	4 (13%)
27	4AC	B1	419	27	21,24,25	3.26	9 (42%)	29,34,37	1.05	4 (13%)
27	OMG	B1	1904	27	18,26,27	2.58	8 (44%)	19,38,41	1.52	4 (21%)
27	4AC	B1	2008	27	21,24,25	3.27	10 (47%)	29,34,37	1.02	4 (13%)
27	4AC	B1	48	27	21,24,25	3.21	10 (47%)	29,34,37	0.98	3 (10%)
1	4AC	A1	546	1	21,24,25	3.28	9 (42%)	29,34,37	1.06	4 (13%)
1	5MC	A1	1190	1	18,22,23	3.18	7 (38%)	26,32,35	0.96	2 (7%)
1	OMU	A1	1165	1	19,22,23	3.30	7 (36%)	26,31,34	1.68	5 (19%)
27	4AC	B1	1478	27	21,24,25	3.24	10 (47%)	29,34,37	1.02	4 (13%)
27	OMG	B1	887	27	18,26,27	2.61	8 (44%)	19,38,41	1.51	4 (21%)
1	4AC	A1	499	1	21,24,25	3.27	9 (42%)	29,34,37	1.05	4 (13%)
1	4AC	A1	1227	1	21,24,25	3.13	10 (47%)	29,34,37	0.96	1 (3%)
1	4AC	A1	739	1	21,24,25	3.30	9 (42%)	29,34,37	1.06	4 (13%)
27	4AC	B1	243	27	21,24,25	3.25	10 (47%)	29,34,37	1.03	4 (13%)
27	4AC	B1	2850	27	21,24,25	3.25	10 (47%)	29,34,37	1.03	4 (13%)
27	A2M	B1	880	27	18,25,26	4.24	7 (38%)	18,36,39	2.20	4 (22%)
27	4AC	B1	2876	27	21,24,25	3.27	10 (47%)	29,34,37	1.06	4 (13%)
1	5MC	A1	1484	1	18,22,23	3.16	7 (38%)	26,32,35	0.99	2 (7%)
27	4AC	B1	1505	27	21,24,25	3.26	10 (47%)	29,34,37	1.06	4 (13%)
27	4AC	B1	2133	27	21,24,25	3.24	9 (42%)	29,34,37	1.04	4 (13%)
27	4AC	B1	1150	27	21,24,25	3.27	10 (47%)	29,34,37	1.08	4 (13%)
1	4AC	A1	945	1	21,24,25	3.30	9 (42%)	29,34,37	1.12	4 (13%)
1	4AC	A1	706	1	21,24,25	3.26	10 (47%)	29,34,37	1.03	4 (13%)
27	4AC	B1	116	27	21,24,25	3.24	10 (47%)	29,34,37	1.04	4 (13%)
27	4AC	B1	2454	27	21,24,25	3.29	10 (47%)	29,34,37	1.06	4 (13%)
27	4AC	B1	479	27	21,24,25	3.28	9 (42%)	29,34,37	1.10	4 (13%)
1	5MU	A1	1110	1	19,22,23	0.41	0	28,32,35	0.55	0
27	4AC	B1	715	27	21,24,25	3.26	10 (47%)	29,34,37	1.03	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	4AC	B1	1290	27	21,24,25	3.25	9 (42%)	29,34,37	1.02	4 (13%)
1	OMG	A1	507	1	18,26,27	2.59	8 (44%)	19,38,41	1.52	4 (21%)
1	4AC	A1	816	1	21,24,25	3.27	10 (47%)	29,34,37	1.05	4 (13%)
27	4AC	B1	1360	27	21,24,25	3.31	9 (42%)	29,34,37	1.48	5 (17%)
27	4AC	B1	1546	27	21,24,25	3.26	10 (47%)	29,34,37	1.06	4 (13%)
27	4AC	B1	1822	27	21,24,25	3.26	9 (42%)	29,34,37	1.08	4 (13%)
27	OMC	B1	2735	27	19,22,23	3.13	8 (42%)	26,31,34	0.73	0
27	4AC	B1	2792	27	21,24,25	3.24	10 (47%)	29,34,37	1.04	4 (13%)
1	OMG	A1	645	1	18,26,27	2.60	8 (44%)	19,38,41	1.46	4 (21%)
1	OMC	A1	1371	1	19,22,23	3.14	8 (42%)	26,31,34	0.72	0
27	OMG	B1	2540	27	18,26,27	2.60	8 (44%)	19,38,41	1.50	4 (21%)
27	4AC	B1	933	27	21,24,25	3.27	10 (47%)	29,34,37	1.09	4 (13%)
27	4AC	B1	979	27	21,24,25	3.26	9 (42%)	29,34,37	1.05	4 (13%)
27	OMG	B1	2684	27	18,26,27	2.61	8 (44%)	19,38,41	1.48	4 (21%)
1	OMU	A1	762	1	19,22,23	3.31	7 (36%)	26,31,34	1.70	5 (19%)
1	OMG	A1	459	1	18,26,27	2.59	8 (44%)	19,38,41	1.48	4 (21%)
1	OMC	A1	1364	1	19,22,23	3.13	8 (42%)	26,31,34	0.71	0
1	4AC	A1	367	1	21,24,25	3.24	10 (47%)	29,34,37	1.02	4 (13%)
28	4AC	B2	88	28	21,24,25	3.28	9 (42%)	29,34,37	1.06	4 (13%)
1	4AC	A1	5	1	21,24,25	3.27	9 (42%)	29,34,37	1.07	4 (13%)
1	OMG	A1	541	1	18,26,27	2.61	8 (44%)	19,38,41	1.98	6 (31%)
27	4AC	B1	1100	27	21,24,25	3.25	9 (42%)	29,34,37	1.04	4 (13%)
1	OMC	A1	1028	1	19,22,23	3.12	8 (42%)	26,31,34	0.72	0
27	4AC	B1	23	27	21,24,25	3.25	9 (42%)	29,34,37	1.06	4 (13%)
27	4AC	B1	1264	27	21,24,25	3.27	10 (47%)	29,34,37	1.06	4 (13%)
27	4AC	B1	1911	27	21,24,25	3.25	9 (42%)	29,34,37	1.03	4 (13%)
1	A2M	A1	361	1	18,25,26	0.63	1 (5%)	18,36,39	0.91	1 (5%)
27	OMG	B1	841	27	18,26,27	2.59	8 (44%)	19,38,41	1.49	4 (21%)
1	4AC	A1	836	1	21,24,25	3.26	10 (47%)	29,34,37	1.02	4 (13%)
1	4AC	A1	41	1	21,24,25	3.26	10 (47%)	29,34,37	1.41	6 (20%)
27	OMG	B1	920	27	18,26,27	2.61	8 (44%)	19,38,41	1.51	4 (21%)
27	5MU	B1	2401	27	19,22,23	0.41	0	28,32,35	0.71	0
27	4AC	B1	98	27	21,24,25	3.27	10 (47%)	29,34,37	1.03	4 (13%)
1	5MC	A1	466	1	18,22,23	3.12	7 (38%)	26,32,35	1.09	2 (7%)
27	OMG	B1	214	27	18,26,27	2.61	8 (44%)	19,38,41	1.55	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	4AC	B1	1374	27	21,24,25	3.30	10 (47%)	29,34,37	1.11	4 (13%)
27	4AC	B1	3020	27	21,24,25	3.27	9 (42%)	29,34,37	1.06	4 (13%)
1	5MC	A1	230	1	18,22,23	3.17	7 (38%)	26,32,35	0.99	2 (7%)
27	4AC	B1	2171	27	21,24,25	3.24	10 (47%)	29,34,37	1.23	6 (20%)
27	4AC	B1	1946	27	21,24,25	3.24	9 (42%)	29,34,37	1.42	6 (20%)
27	4AC	B1	2526	27	21,24,25	3.26	10 (47%)	29,34,37	1.27	6 (20%)
27	OMC	B1	2808	27	19,22,23	3.12	8 (42%)	26,31,34	0.72	0
1	4AC	A1	534	1	21,24,25	3.28	10 (47%)	29,34,37	1.05	4 (13%)
27	4AC	B1	1769	27	21,24,25	3.23	9 (42%)	29,34,37	1.02	3 (10%)
1	OMC	A1	117	1	19,22,23	3.11	8 (42%)	26,31,34	0.70	0
1	OMG	A1	668	1	18,26,27	2.61	8 (44%)	19,38,41	1.49	4 (21%)
27	4AC	B1	3011	27	21,24,25	3.27	9 (42%)	29,34,37	1.03	4 (13%)
27	4AC	B1	2213	27	21,24,25	3.24	9 (42%)	29,34,37	1.05	4 (13%)
27	OMG	B1	1965	27	18,26,27	2.60	8 (44%)	19,38,41	1.56	4 (21%)
27	LHH	B1	502	27	22,25,26	2.93	6 (27%)	29,35,38	1.33	2 (6%)
27	4AC	B1	953	27	21,24,25	3.26	10 (47%)	29,34,37	1.05	4 (13%)
27	4AC	B1	2602	27	21,24,25	3.25	10 (47%)	29,34,37	1.03	4 (13%)
1	4AC	A1	540	1	21,24,25	3.26	10 (47%)	29,34,37	1.04	4 (13%)
1	OMU	A1	1368	1	19,22,23	3.29	7 (36%)	26,31,34	1.72	5 (19%)
27	4AC	B1	434	27	21,24,25	3.25	10 (47%)	29,34,37	1.43	6 (20%)
27	OMG	B1	2180	27	18,26,27	2.60	8 (44%)	19,38,41	1.54	4 (21%)
27	4AC	B1	1052	27	21,24,25	3.28	9 (42%)	29,34,37	1.05	4 (13%)
1	4AC	A1	614	1	21,24,25	3.26	10 (47%)	29,34,37	1.05	4 (13%)
27	OMG	B1	55	27	18,26,27	2.59	8 (44%)	19,38,41	1.51	4 (21%)
27	4AC	B1	378	27	21,24,25	3.25	10 (47%)	29,34,37	1.43	6 (20%)
27	4AC	B1	2113	27	21,24,25	3.25	10 (47%)	29,34,37	1.04	4 (13%)
27	A2M	B1	940	27	18,25,26	4.26	7 (38%)	18,36,39	2.26	4 (22%)
1	OMC	A1	834	1	19,22,23	3.10	8 (42%)	26,31,34	0.66	0
27	4AC	B1	360	27	21,24,25	3.27	10 (47%)	29,34,37	1.04	4 (13%)
1	4AC	A1	1029	1	21,24,25	3.26	9 (42%)	29,34,37	1.05	4 (13%)
1	OMU	A1	775	1	19,22,23	3.29	7 (36%)	26,31,34	1.73	5 (19%)
27	4AC	B1	1442	27	21,24,25	3.24	10 (47%)	29,34,37	1.03	4 (13%)
27	5MC	B1	1977	27	18,22,23	3.18	7 (38%)	26,32,35	1.00	2 (7%)
27	4AC	B1	1107	27	21,24,25	3.22	10 (47%)	29,34,37	1.04	4 (13%)
27	OMG	B1	1557	27	18,26,27	2.60	8 (44%)	19,38,41	1.49	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4AC	A1	220	1	21,24,25	3.26	10 (47%)	29,34,37	1.03	4 (13%)
27	4AC	B1	80	27	21,24,25	3.26	10 (47%)	29,34,37	1.06	4 (13%)
1	A1I59	A1	1366	1	22,27,28	2.57	6 (27%)	29,39,42	1.07	2 (6%)
27	OMU	B1	926	27	19,22,23	3.32	7 (36%)	26,31,34	2.04	8 (30%)
27	4AC	B1	1501	27	21,24,25	3.28	9 (42%)	29,34,37	1.10	4 (13%)
27	4AC	B1	1885	27	21,24,25	3.25	10 (47%)	29,34,37	1.02	4 (13%)
28	4AC	B2	30	28	21,24,25	3.30	10 (47%)	29,34,37	1.06	4 (13%)
27	4AC	B1	1435	27	21,24,25	3.24	10 (47%)	29,34,37	1.06	4 (13%)
1	MA6	A1	1476	1	18,26,27	1.00	1 (5%)	19,38,41	4.37	3 (15%)
1	4AC	A1	141	1	21,24,25	3.30	9 (42%)	29,34,37	1.08	4 (13%)
27	A2M	B1	506	27	18,25,26	4.22	7 (38%)	18,36,39	2.28	4 (22%)
27	OMC	B1	501	27	19,22,23	3.12	8 (42%)	26,31,34	0.74	0
1	OMC	A1	1226	1	19,22,23	3.07	8 (42%)	26,31,34	0.72	0
1	4AC	A1	578	1	21,24,25	3.27	9 (42%)	29,34,37	1.29	6 (20%)
27	OMG	B1	2757	27	18,26,27	2.59	8 (44%)	19,38,41	1.59	5 (26%)
27	OMG	B1	2391	27	18,26,27	2.56	8 (44%)	19,38,41	1.53	5 (26%)
27	OMU	B1	454	27	19,22,23	3.32	7 (36%)	26,31,34	2.02	7 (26%)
1	OMG	A1	329	1	18,26,27	2.61	8 (44%)	19,38,41	1.58	5 (26%)
1	5MC	A1	927	1	18,22,23	3.21	7 (38%)	26,32,35	0.99	2 (7%)
1	4AC	A1	382	1	21,24,25	3.26	10 (47%)	29,34,37	1.02	4 (13%)
27	A2M	B1	2506	27	18,25,26	4.23	7 (38%)	18,36,39	2.25	4 (22%)
27	4AC	B1	1383	27	21,24,25	3.26	10 (47%)	29,34,37	1.07	4 (13%)
1	OMG	A1	1115	1	18,26,27	2.61	8 (44%)	19,38,41	1.53	4 (21%)
1	4AC	A1	87	1	21,24,25	3.28	9 (42%)	29,34,37	1.45	6 (20%)
27	4AC	B1	485	27	21,24,25	3.23	10 (47%)	29,34,37	1.02	3 (10%)
1	4SU	A1	756	1	18,21,22	3.89	8 (44%)	26,30,33	2.22	5 (19%)
27	5MC	B1	2067	27	18,22,23	3.20	7 (38%)	26,32,35	1.00	2 (7%)
27	4AC	B1	2809	27	21,24,25	3.26	10 (47%)	29,34,37	1.05	4 (13%)
27	OMC	B1	2119	27	19,22,23	3.10	8 (42%)	26,31,34	0.73	0
1	4AC	A1	636	1	21,24,25	3.27	9 (42%)	29,34,37	1.09	4 (13%)
27	4AC	B1	130	27	21,24,25	3.26	10 (47%)	29,34,37	1.03	4 (13%)
1	4AC	A1	1314	1	21,24,25	3.27	9 (42%)	29,34,37	1.04	4 (13%)
27	4AC	B1	3037	27	21,24,25	3.28	10 (47%)	29,34,37	1.04	4 (13%)
27	4AC	B1	732	27	21,24,25	3.27	9 (42%)	29,34,37	1.06	4 (13%)
27	5MU	B1	888	27	19,22,23	0.45	0	28,32,35	0.82	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	OMC	B1	1099	27	19,22,23	3.11	8 (42%)	26,31,34	0.69	0
27	4AC	B1	2844	27	21,24,25	3.26	10 (47%)	29,34,37	1.03	4 (13%)
1	OMG	A1	861	1	18,26,27	2.58	8 (44%)	19,38,41	1.50	4 (21%)
27	OMU	B1	2554	27	19,22,23	3.29	7 (36%)	26,31,34	1.69	4 (15%)
27	OMC	B1	1832	27	19,22,23	3.13	8 (42%)	26,31,34	0.69	0
27	4AC	B1	200	27	21,24,25	3.26	9 (42%)	29,34,37	1.04	4 (13%)
27	4AC	B1	866	27	21,24,25	3.26	10 (47%)	29,34,37	1.04	4 (13%)
28	4AC	B2	115	28	21,24,25	3.30	10 (47%)	29,34,37	1.41	6 (20%)
27	4AC	B1	1706	27	21,24,25	3.27	9 (42%)	29,34,37	1.05	4 (13%)
27	4AC	B1	950	27	21,24,25	3.24	10 (47%)	29,34,37	1.04	4 (13%)
1	A2M	A1	819	1	18,25,26	4.27	7 (38%)	18,36,39	2.27	4 (22%)
1	4AC	A1	719	1	21,24,25	3.24	9 (42%)	29,34,37	1.06	4 (13%)
27	4AC	B1	1649	27	21,24,25	3.28	9 (42%)	29,34,37	1.09	4 (13%)
1	5MC	A1	1362	1	18,22,23	3.19	7 (38%)	26,32,35	1.01	2 (7%)
1	5MC	A1	951	1	18,22,23	3.21	7 (38%)	26,32,35	1.06	2 (7%)
1	4AC	A1	216	1	21,24,25	3.30	10 (47%)	29,34,37	1.09	4 (13%)
27	4AC	B1	2469	27	21,24,25	3.25	10 (47%)	29,34,37	1.06	4 (13%)
1	4AC	A1	624	1	21,24,25	3.31	9 (42%)	29,34,37	1.13	4 (13%)
27	OMG	B1	2022	27	18,26,27	2.60	8 (44%)	19,38,41	1.53	5 (26%)
27	5MC	B1	2087	27	18,22,23	3.17	7 (38%)	26,32,35	0.99	2 (7%)
27	OMC	B1	2607	27	19,22,23	3.13	8 (42%)	26,31,34	0.72	0
27	5MC	B1	2617	27	18,22,23	3.19	7 (38%)	26,32,35	1.06	1 (3%)
27	4AC	B1	2968	27	21,24,25	3.25	10 (47%)	29,34,37	1.27	6 (20%)
1	5MC	A1	352	1	18,22,23	3.18	7 (38%)	26,32,35	0.99	2 (7%)
27	5MC	B1	336	27	18,22,23	3.17	7 (38%)	26,32,35	1.02	2 (7%)
27	OMG	B1	2984	27	18,26,27	2.59	8 (44%)	19,38,41	1.51	4 (21%)
27	4AC	B1	2429	27	21,24,25	3.25	10 (47%)	29,34,37	1.02	4 (13%)
27	4AC	B1	1751	27	21,24,25	3.28	10 (47%)	29,34,37	1.06	4 (13%)
1	4AC	A1	231	1	21,24,25	3.28	9 (42%)	29,34,37	1.07	4 (13%)
27	4AC	B1	344	27	21,24,25	3.29	9 (42%)	29,34,37	1.06	4 (13%)
1	MA6	A1	1475	1	18,26,27	0.98	1 (5%)	19,38,41	4.49	3 (15%)
1	OMG	A1	455	1	18,26,27	2.59	8 (44%)	19,38,41	1.54	5 (26%)
1	MA6	A1	1457	1	18,26,27	1.03	1 (5%)	19,38,41	4.23	3 (15%)
27	4AC	B1	19	27	21,24,25	3.28	9 (42%)	29,34,37	1.07	4 (13%)
27	4AC	B1	2821	27	21,24,25	3.29	9 (42%)	29,34,37	1.06	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	4AC	B1	1128	27	21,24,25	3.25	10 (47%)	29,34,37	1.02	4 (13%)
27	4AC	B1	162	27	21,24,25	3.28	10 (47%)	29,34,37	1.08	4 (13%)
27	4AC	B1	580	27	21,24,25	3.25	9 (42%)	29,34,37	1.02	4 (13%)
1	OMG	A1	1003	1	18,26,27	2.61	8 (44%)	19,38,41	1.52	4 (21%)
1	4AC	A1	307	1	21,24,25	3.24	10 (47%)	29,34,37	1.06	4 (13%)
1	5MC	A1	687	1	18,22,23	3.20	7 (38%)	26,32,35	0.98	2 (7%)
27	4AC	B1	1551	27	21,24,25	3.26	10 (47%)	29,34,37	1.04	4 (13%)
27	OMC	B1	2059	27	19,22,23	3.13	8 (42%)	26,31,34	0.76	0
1	4AC	A1	405	1	21,24,25	3.27	10 (47%)	29,34,37	1.05	4 (13%)
27	4AC	B1	1293	27	21,24,25	3.30	9 (42%)	29,34,37	1.34	6 (20%)
27	OMU	B1	1488	27	19,22,23	3.29	7 (36%)	26,31,34	1.69	4 (15%)
1	4AC	A1	691	1	21,24,25	3.28	10 (47%)	29,34,37	1.09	4 (13%)
27	OMG	B1	2028	27	18,26,27	2.59	8 (44%)	19,38,41	1.49	4 (21%)
27	OMG	B1	2562	27	18,26,27	2.60	8 (44%)	19,38,41	1.52	4 (21%)
1	OMC	A1	1194	1	19,22,23	3.12	8 (42%)	26,31,34	0.71	0
27	4AC	B1	1178	27	21,24,25	3.27	10 (47%)	29,34,37	1.05	4 (13%)
27	4AC	B1	2379	27	21,24,25	3.22	10 (47%)	29,34,37	1.03	3 (10%)
1	4AC	A1	291	1	21,24,25	3.25	10 (47%)	29,34,37	1.01	4 (13%)
1	4AC	A1	1181	1	21,24,25	3.26	10 (47%)	29,34,37	1.26	5 (17%)
1	5MC	A1	681	1	18,22,23	3.16	7 (38%)	26,32,35	1.20	4 (15%)
27	4AC	B1	227	27	21,24,25	3.29	10 (47%)	29,34,37	1.07	4 (13%)
27	4AC	B1	1061	27	21,24,25	3.27	9 (42%)	29,34,37	1.04	4 (13%)
27	4AC	B1	1846	27	21,24,25	3.28	10 (47%)	29,34,37	1.06	4 (13%)
27	4AC	B1	652	27	21,24,25	3.24	10 (47%)	29,34,37	1.06	4 (13%)
27	A2M	B1	857	27	18,25,26	4.21	7 (38%)	18,36,39	2.22	4 (22%)
27	4AC	B1	1743	27	21,24,25	3.29	9 (42%)	29,34,37	1.06	4 (13%)
1	OMU	A1	8	1	19,22,23	3.31	7 (36%)	26,31,34	1.78	6 (23%)

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	OMG	B1	856	27	-	2/5/27/28	0/3/3/3
27	4AC	B1	2492	27	-	0/11/29/30	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	4AC	B1	786	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	761	1	-	0/11/29/30	0/2/2/2
27	5MC	B1	1344	27	-	0/7/25/26	0/2/2/2
27	OMC	B1	1489	27	-	2/9/27/28	0/2/2/2
1	5MC	A1	863	1	-	0/7/25/26	0/2/2/2
27	4AC	B1	721	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	3006	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1579	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	808	27	-	0/5/27/28	0/3/3/3
27	4AC	B1	2020	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	527	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	856	1	-	0/11/29/30	0/2/2/2
27	OMG	B1	2365	27	-	0/5/27/28	0/3/3/3
1	4AC	A1	1254	1	-	0/11/29/30	0/2/2/2
1	LHH	A1	238	1	-	4/13/31/32	0/2/2/2
1	5MC	A1	473	1	-	0/7/25/26	0/2/2/2
27	OMG	B1	921	27	-	1/5/27/28	0/3/3/3
27	4AC	B1	1067	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1064	27	-	0/11/29/30	0/2/2/2
27	OMC	B1	1914	27	-	1/9/27/28	0/2/2/2
27	4AC	B1	1967	27	-	2/11/29/30	0/2/2/2
27	4AC	B1	2432	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	2749	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	839	1	-	2/11/29/30	0/2/2/2
1	G7M	A1	481	1	-	2/3/25/26	0/3/3/3
27	OMG	B1	2108	27	-	0/5/27/28	0/3/3/3
1	4AC	A1	1467	1	-	2/11/29/30	0/2/2/2
1	5MC	A1	1013	1	-	0/7/25/26	0/2/2/2
1	5MC	A1	17	1	-	2/7/25/26	0/2/2/2
1	4AC	A1	827	1	-	2/11/29/30	0/2/2/2
27	4SU	B1	2565	27	-	0/7/25/26	0/2/2/2
1	OMC	A1	1270	1	-	2/9/27/28	0/2/2/2
27	4AC	B1	1762	27	-	0/11/29/30	0/2/2/2
27	UR3	B1	2700	27	-	2/7/25/26	0/2/2/2
27	OMG	B1	530	27	-	0/5/27/28	0/3/3/3
27	OMC	B1	2557	27	-	2/9/27/28	0/2/2/2
27	4AC	B1	1608	27	-	2/11/29/30	0/2/2/2
27	4AC	B1	896	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	688	27	-	3/11/29/30	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	A1	467	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	1818	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	274	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	1639	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1345	27	-	0/11/29/30	0/2/2/2
27	LHH	B1	1439	27	-	2/13/31/32	0/2/2/2
1	OMU	A1	52	1	-	0/9/27/28	0/2/2/2
27	4AC	B1	337	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	419	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	1904	27	-	0/5/27/28	0/3/3/3
27	4AC	B1	2008	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	48	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	546	1	-	0/11/29/30	0/2/2/2
1	5MC	A1	1190	1	-	2/7/25/26	0/2/2/2
1	OMU	A1	1165	1	-	0/9/27/28	0/2/2/2
27	4AC	B1	1478	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	887	27	-	0/5/27/28	0/3/3/3
1	4AC	A1	499	1	-	2/11/29/30	0/2/2/2
1	4AC	A1	1227	1	-	0/11/29/30	0/2/2/2
1	4AC	A1	739	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	243	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	2850	27	-	0/11/29/30	0/2/2/2
27	A2M	B1	880	27	-	0/5/27/28	0/3/3/3
27	4AC	B1	2876	27	-	2/11/29/30	0/2/2/2
1	5MC	A1	1484	1	-	0/7/25/26	0/2/2/2
27	4AC	B1	1505	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	2133	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1150	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	945	1	-	0/11/29/30	0/2/2/2
1	4AC	A1	706	1	-	1/11/29/30	0/2/2/2
27	4AC	B1	116	27	-	2/11/29/30	0/2/2/2
27	4AC	B1	2454	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	479	27	-	3/11/29/30	0/2/2/2
1	5MU	A1	1110	1	-	0/7/25/26	0/2/2/2
27	4AC	B1	715	27	-	2/11/29/30	0/2/2/2
27	4AC	B1	1290	27	-	0/11/29/30	0/2/2/2
1	OMG	A1	507	1	-	0/5/27/28	0/3/3/3
1	4AC	A1	816	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	1360	27	-	2/11/29/30	0/2/2/2
27	4AC	B1	1546	27	-	0/11/29/30	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	4AC	B1	1822	27	-	0/11/29/30	0/2/2/2
27	OMC	B1	2735	27	-	0/9/27/28	0/2/2/2
27	4AC	B1	2792	27	-	0/11/29/30	0/2/2/2
1	OMG	A1	645	1	-	0/5/27/28	0/3/3/3
1	OMC	A1	1371	1	-	0/9/27/28	0/2/2/2
27	OMG	B1	2540	27	-	0/5/27/28	0/3/3/3
27	4AC	B1	933	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	979	27	-	3/11/29/30	0/2/2/2
27	OMG	B1	2684	27	-	0/5/27/28	0/3/3/3
1	OMU	A1	762	1	-	0/9/27/28	0/2/2/2
1	OMG	A1	459	1	-	0/5/27/28	0/3/3/3
1	OMC	A1	1364	1	-	0/9/27/28	0/2/2/2
1	4AC	A1	367	1	-	0/11/29/30	0/2/2/2
28	4AC	B2	88	28	-	0/11/29/30	0/2/2/2
1	4AC	A1	5	1	-	2/11/29/30	0/2/2/2
1	OMG	A1	541	1	-	2/5/27/28	0/3/3/3
27	4AC	B1	1100	27	-	0/11/29/30	0/2/2/2
1	OMC	A1	1028	1	-	0/9/27/28	0/2/2/2
27	4AC	B1	23	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1264	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1911	27	-	0/11/29/30	0/2/2/2
1	A2M	A1	361	1	-	2/5/27/28	0/3/3/3
27	OMG	B1	841	27	-	0/5/27/28	0/3/3/3
1	4AC	A1	836	1	-	0/11/29/30	0/2/2/2
1	4AC	A1	41	1	-	0/11/29/30	0/2/2/2
27	OMG	B1	920	27	-	0/5/27/28	0/3/3/3
27	5MU	B1	2401	27	-	3/7/25/26	0/2/2/2
27	4AC	B1	98	27	-	0/11/29/30	0/2/2/2
1	5MC	A1	466	1	-	3/7/25/26	0/2/2/2
27	OMG	B1	214	27	-	0/5/27/28	0/3/3/3
27	4AC	B1	1374	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	3020	27	-	0/11/29/30	0/2/2/2
1	5MC	A1	230	1	-	0/7/25/26	0/2/2/2
27	4AC	B1	2171	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1946	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	2526	27	-	0/11/29/30	0/2/2/2
27	OMC	B1	2808	27	-	0/9/27/28	0/2/2/2
1	4AC	A1	534	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	1769	27	-	0/11/29/30	0/2/2/2
1	OMC	A1	117	1	-	0/9/27/28	0/2/2/2
1	OMG	A1	668	1	-	0/5/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	4AC	B1	3011	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	2213	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	1965	27	-	0/5/27/28	0/3/3/3
27	LHH	B1	502	27	-	1/13/31/32	0/2/2/2
27	4AC	B1	953	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	2602	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	540	1	-	0/11/29/30	0/2/2/2
1	OMU	A1	1368	1	-	0/9/27/28	0/2/2/2
27	4AC	B1	434	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	2180	27	-	0/5/27/28	0/3/3/3
27	4AC	B1	1052	27	-	1/11/29/30	0/2/2/2
1	4AC	A1	614	1	-	0/11/29/30	0/2/2/2
27	OMG	B1	55	27	-	2/5/27/28	0/3/3/3
27	4AC	B1	378	27	-	1/11/29/30	0/2/2/2
27	4AC	B1	2113	27	-	0/11/29/30	0/2/2/2
27	A2M	B1	940	27	-	0/5/27/28	0/3/3/3
1	OMC	A1	834	1	-	0/9/27/28	0/2/2/2
27	4AC	B1	360	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	1029	1	-	0/11/29/30	0/2/2/2
1	OMU	A1	775	1	-	5/9/27/28	0/2/2/2
27	4AC	B1	1442	27	-	0/11/29/30	0/2/2/2
27	5MC	B1	1977	27	-	0/7/25/26	0/2/2/2
27	4AC	B1	1107	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	1557	27	-	4/5/27/28	0/3/3/3
1	4AC	A1	220	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	80	27	-	0/11/29/30	0/2/2/2
1	A1I59	A1	1366	1	-	1/11/33/34	0/2/2/2
27	OMU	B1	926	27	-	4/9/27/28	0/2/2/2
27	4AC	B1	1501	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1885	27	-	0/11/29/30	0/2/2/2
28	4AC	B2	30	28	-	0/11/29/30	0/2/2/2
27	4AC	B1	1435	27	-	0/11/29/30	0/2/2/2
1	MA6	A1	1476	1	-	2/7/29/30	0/3/3/3
1	4AC	A1	141	1	-	0/11/29/30	0/2/2/2
27	A2M	B1	506	27	-	0/5/27/28	0/3/3/3
27	OMC	B1	501	27	-	2/9/27/28	0/2/2/2
1	OMC	A1	1226	1	-	0/9/27/28	0/2/2/2
1	4AC	A1	578	1	-	0/11/29/30	0/2/2/2
27	OMG	B1	2757	27	-	0/5/27/28	0/3/3/3
27	OMG	B1	2391	27	-	3/5/27/28	0/3/3/3
27	OMU	B1	454	27	-	0/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	A1	329	1	-	3/5/27/28	0/3/3/3
1	5MC	A1	927	1	-	0/7/25/26	0/2/2/2
1	4AC	A1	382	1	-	0/11/29/30	0/2/2/2
27	A2M	B1	2506	27	-	0/5/27/28	0/3/3/3
27	4AC	B1	1383	27	-	2/11/29/30	0/2/2/2
1	OMG	A1	1115	1	-	0/5/27/28	0/3/3/3
1	4AC	A1	87	1	-	3/11/29/30	0/2/2/2
27	4AC	B1	485	27	-	0/11/29/30	0/2/2/2
1	4SU	A1	756	1	-	0/7/25/26	0/2/2/2
27	5MC	B1	2067	27	-	0/7/25/26	0/2/2/2
27	4AC	B1	2809	27	-	0/11/29/30	0/2/2/2
27	OMC	B1	2119	27	-	0/9/27/28	0/2/2/2
1	4AC	A1	636	1	-	1/11/29/30	0/2/2/2
27	4AC	B1	130	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	1314	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	3037	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	732	27	-	0/11/29/30	0/2/2/2
27	5MU	B1	888	27	-	0/7/25/26	0/2/2/2
27	OMC	B1	1099	27	-	0/9/27/28	0/2/2/2
27	4AC	B1	2844	27	-	0/11/29/30	0/2/2/2
1	OMG	A1	861	1	-	1/5/27/28	0/3/3/3
27	OMU	B1	2554	27	-	0/9/27/28	0/2/2/2
27	OMC	B1	1832	27	-	0/9/27/28	0/2/2/2
27	4AC	B1	200	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	866	27	-	0/11/29/30	0/2/2/2
28	4AC	B2	115	28	-	3/11/29/30	0/2/2/2
27	4AC	B1	1706	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	950	27	-	0/11/29/30	0/2/2/2
1	A2M	A1	819	1	-	2/5/27/28	0/3/3/3
1	4AC	A1	719	1	-	2/11/29/30	0/2/2/2
27	4AC	B1	1649	27	-	0/11/29/30	0/2/2/2
1	5MC	A1	1362	1	-	2/7/25/26	0/2/2/2
1	5MC	A1	951	1	-	1/7/25/26	0/2/2/2
1	4AC	A1	216	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	2469	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	624	1	-	0/11/29/30	0/2/2/2
27	OMG	B1	2022	27	-	1/5/27/28	0/3/3/3
27	5MC	B1	2087	27	-	0/7/25/26	0/2/2/2
27	OMC	B1	2607	27	-	2/9/27/28	0/2/2/2
27	5MC	B1	2617	27	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	4AC	B1	2968	27	-	0/11/29/30	0/2/2/2
1	5MC	A1	352	1	-	0/7/25/26	0/2/2/2
27	5MC	B1	336	27	-	0/7/25/26	0/2/2/2
27	OMG	B1	2984	27	-	0/5/27/28	0/3/3/3
27	4AC	B1	2429	27	-	3/11/29/30	0/2/2/2
27	4AC	B1	1751	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	231	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	344	27	-	2/11/29/30	0/2/2/2
1	MA6	A1	1475	1	-	0/7/29/30	0/3/3/3
1	OMG	A1	455	1	-	1/5/27/28	0/3/3/3
1	MA6	A1	1457	1	-	0/7/29/30	0/3/3/3
27	4AC	B1	19	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	2821	27	-	3/11/29/30	0/2/2/2
27	4AC	B1	1128	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	162	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	580	27	-	0/11/29/30	0/2/2/2
1	OMG	A1	1003	1	-	0/5/27/28	0/3/3/3
1	4AC	A1	307	1	-	0/11/29/30	0/2/2/2
1	5MC	A1	687	1	-	0/7/25/26	0/2/2/2
27	4AC	B1	1551	27	-	0/11/29/30	0/2/2/2
27	OMC	B1	2059	27	-	0/9/27/28	0/2/2/2
1	4AC	A1	405	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	1293	27	-	2/11/29/30	0/2/2/2
27	OMU	B1	1488	27	-	0/9/27/28	0/2/2/2
1	4AC	A1	691	1	-	2/11/29/30	0/2/2/2
27	OMG	B1	2028	27	-	1/5/27/28	0/3/3/3
27	OMG	B1	2562	27	-	0/5/27/28	0/3/3/3
1	OMC	A1	1194	1	-	0/9/27/28	0/2/2/2
27	4AC	B1	1178	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	2379	27	-	2/11/29/30	0/2/2/2
1	4AC	A1	291	1	-	0/11/29/30	0/2/2/2
1	4AC	A1	1181	1	-	0/11/29/30	0/2/2/2
1	5MC	A1	681	1	-	0/7/25/26	0/2/2/2
27	4AC	B1	227	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1061	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1846	27	-	1/11/29/30	0/2/2/2
27	4AC	B1	652	27	-	0/11/29/30	0/2/2/2
27	A2M	B1	857	27	-	2/5/27/28	0/3/3/3
27	4AC	B1	1743	27	-	0/11/29/30	0/2/2/2
1	OMU	A1	8	1	-	4/9/27/28	0/2/2/2

All (2073) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	819	A2M	O4'-C1'	15.43	1.62	1.41
27	B1	940	A2M	O4'-C1'	15.36	1.62	1.41
27	B1	880	A2M	O4'-C1'	15.27	1.62	1.41
27	B1	857	A2M	O4'-C1'	15.21	1.62	1.41
27	B1	506	A2M	O4'-C1'	15.18	1.62	1.41
27	B1	2506	A2M	O4'-C1'	15.14	1.62	1.41
1	A1	481	G7M	C8-N7	10.10	1.51	1.33
1	A1	481	G7M	C8-N9	9.96	1.51	1.33
1	A1	238	LHH	O2-C2	9.01	1.40	1.23
27	B1	502	LHH	O2-C2	8.89	1.40	1.23
27	B1	1439	LHH	O2-C2	8.87	1.40	1.23
1	A1	1366	A1I59	O2-C2	8.81	1.40	1.23
1	A1	756	4SU	C4-N3	8.78	1.47	1.37
27	B1	2565	4SU	C4-N3	8.69	1.46	1.37
27	B1	2700	UR3	C2-N1	8.48	1.50	1.38
27	B1	2617	5MC	C6-C5	8.04	1.47	1.34
1	A1	473	5MC	C6-C5	7.99	1.47	1.34
1	A1	863	5MC	C6-C5	7.98	1.47	1.34
1	A1	1013	5MC	C6-C5	7.97	1.47	1.34
1	A1	927	5MC	C6-C5	7.97	1.47	1.34
27	B1	2067	5MC	C6-C5	7.95	1.47	1.34
27	B1	1977	5MC	C6-C5	7.94	1.47	1.34
1	A1	1368	OMU	C2-N3	7.93	1.52	1.38
1	A1	1190	5MC	C6-C5	7.93	1.47	1.34
1	A1	1362	5MC	C6-C5	7.93	1.47	1.34
27	B1	454	OMU	C2-N3	7.93	1.52	1.38
1	A1	687	5MC	C6-C5	7.92	1.47	1.34
1	A1	230	5MC	C6-C5	7.91	1.47	1.34
27	B1	1344	5MC	C6-C5	7.90	1.47	1.34
1	A1	52	OMU	C2-N3	7.89	1.52	1.38
27	B1	336	5MC	C6-C5	7.88	1.47	1.34
1	A1	352	5MC	C6-C5	7.88	1.47	1.34
1	A1	17	5MC	C6-C5	7.87	1.47	1.34
27	B1	926	OMU	C2-N3	7.86	1.52	1.38
1	A1	681	5MC	C6-C5	7.85	1.47	1.34
1	A1	762	OMU	C2-N3	7.85	1.52	1.38
1	A1	1165	OMU	C2-N3	7.85	1.52	1.38
1	A1	1484	5MC	C6-C5	7.85	1.47	1.34
1	A1	775	OMU	C2-N3	7.83	1.51	1.38
27	B1	2087	5MC	C6-C5	7.83	1.47	1.34
1	A1	8	OMU	C2-N3	7.82	1.51	1.38
1	A1	951	5MC	C6-C5	7.80	1.47	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	926	OMU	C2-N1	7.80	1.51	1.38
27	B1	2554	OMU	C2-N3	7.79	1.51	1.38
27	B1	454	OMU	C2-N1	7.78	1.50	1.38
27	B1	1488	OMU	C2-N3	7.78	1.51	1.38
1	A1	8	OMU	C2-N1	7.70	1.50	1.38
1	A1	52	OMU	C2-N1	7.70	1.50	1.38
1	A1	466	5MC	C6-C5	7.68	1.47	1.34
1	A1	762	OMU	C2-N1	7.66	1.50	1.38
27	B1	2554	OMU	C2-N1	7.66	1.50	1.38
1	A1	775	OMU	C2-N1	7.64	1.50	1.38
27	B1	1488	OMU	C2-N1	7.62	1.50	1.38
1	A1	1165	OMU	C2-N1	7.61	1.50	1.38
1	A1	1368	OMU	C2-N1	7.55	1.50	1.38
1	A1	756	4SU	C2-N1	7.47	1.50	1.38
27	B1	501	OMC	C2-N3	7.44	1.51	1.36
27	B1	2565	4SU	C2-N1	7.42	1.50	1.38
1	A1	1028	OMC	C2-N3	7.37	1.51	1.36
27	B1	2557	OMC	C2-N3	7.37	1.51	1.36
27	B1	2059	OMC	C2-N3	7.37	1.51	1.36
27	B1	1832	OMC	C2-N3	7.37	1.51	1.36
27	B1	1099	OMC	C2-N3	7.36	1.51	1.36
1	A1	1270	OMC	C2-N3	7.36	1.51	1.36
27	B1	2735	OMC	C2-N3	7.35	1.51	1.36
1	A1	1371	OMC	C2-N3	7.35	1.51	1.36
1	A1	1194	OMC	C2-N3	7.34	1.51	1.36
27	B1	2808	OMC	C2-N3	7.33	1.51	1.36
1	A1	1364	OMC	C2-N3	7.32	1.51	1.36
1	A1	117	OMC	C2-N3	7.31	1.51	1.36
27	B1	1489	OMC	C2-N3	7.28	1.51	1.36
27	B1	2607	OMC	C2-N3	7.28	1.51	1.36
27	B1	1608	4AC	C4-N3	7.27	1.45	1.32
27	B1	2119	OMC	C2-N3	7.27	1.51	1.36
28	B2	30	4AC	C4-N3	7.26	1.45	1.32
1	A1	834	OMC	C2-N3	7.24	1.51	1.36
27	B1	1914	OMC	C2-N3	7.24	1.51	1.36
1	A1	624	4AC	C4-N3	7.23	1.45	1.32
1	A1	691	4AC	C4-N3	7.22	1.45	1.32
1	A1	1226	OMC	C2-N3	7.22	1.51	1.36
27	B1	1743	4AC	C4-N3	7.21	1.45	1.32
27	B1	344	4AC	C4-N3	7.20	1.45	1.32
27	B1	1374	4AC	C4-N3	7.20	1.45	1.32
27	B1	162	4AC	C4-N3	7.19	1.45	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B2	115	4AC	C4-N3	7.19	1.45	1.32
27	B1	419	4AC	C4-N3	7.18	1.45	1.32
27	B1	2454	4AC	C4-N3	7.18	1.45	1.32
1	A1	614	4AC	C4-N3	7.17	1.45	1.32
27	B1	1360	4AC	C4-N3	7.16	1.45	1.32
1	A1	761	4AC	C4-N3	7.16	1.45	1.32
1	A1	1181	4AC	C4-N3	7.16	1.45	1.32
27	B1	3037	4AC	C4-N3	7.15	1.45	1.32
1	A1	945	4AC	C4-N3	7.15	1.45	1.32
27	B1	3011	4AC	C4-N3	7.15	1.45	1.32
27	B1	227	4AC	C4-N3	7.15	1.45	1.32
27	B1	360	4AC	C4-N3	7.15	1.45	1.32
27	B1	1178	4AC	C4-N3	7.14	1.45	1.32
1	A1	216	4AC	C4-N3	7.14	1.45	1.32
1	A1	534	4AC	C4-N3	7.14	1.45	1.32
1	A1	141	4AC	C4-N3	7.14	1.45	1.32
27	B1	1293	4AC	C4-N3	7.14	1.45	1.32
27	B1	1579	4AC	C4-N3	7.13	1.45	1.32
27	B1	1501	4AC	C4-N3	7.13	1.45	1.32
1	A1	578	4AC	C4-N3	7.13	1.45	1.32
27	B1	80	4AC	C4-N3	7.13	1.45	1.32
27	B1	1751	4AC	C4-N3	7.13	1.45	1.32
27	B1	1150	4AC	C4-N3	7.13	1.45	1.32
1	A1	739	4AC	C4-N3	7.13	1.45	1.32
27	B1	715	4AC	C4-N3	7.12	1.45	1.32
1	A1	87	4AC	C4-N3	7.12	1.45	1.32
1	A1	231	4AC	C4-N3	7.12	1.45	1.32
27	B1	3020	4AC	C4-N3	7.12	1.45	1.32
27	B1	732	4AC	C4-N3	7.12	1.45	1.32
27	B1	19	4AC	C4-N3	7.12	1.45	1.32
28	B2	88	4AC	C4-N3	7.12	1.45	1.32
27	B1	866	4AC	C4-N3	7.11	1.45	1.32
27	B1	1061	4AC	C4-N3	7.11	1.45	1.32
27	B1	1264	4AC	C4-N3	7.11	1.45	1.32
27	B1	786	4AC	C4-N3	7.11	1.45	1.32
1	A1	827	4AC	C4-N3	7.11	1.45	1.32
27	B1	896	4AC	C4-N3	7.11	1.45	1.32
27	B1	1846	4AC	C4-N3	7.11	1.45	1.32
27	B1	1383	4AC	C4-N3	7.10	1.45	1.32
27	B1	1052	4AC	C4-N3	7.10	1.45	1.32
27	B1	1706	4AC	C4-N3	7.10	1.45	1.32
27	B1	979	4AC	C4-N3	7.10	1.45	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	2809	4AC	C4-N3	7.10	1.45	1.32
1	A1	816	4AC	C4-N3	7.09	1.45	1.32
27	B1	2526	4AC	C4-N3	7.09	1.45	1.32
27	B1	98	4AC	C4-N3	7.09	1.45	1.32
27	B1	688	4AC	C4-N3	7.09	1.45	1.32
27	B1	243	4AC	C4-N3	7.09	1.45	1.32
1	A1	274	4AC	C4-N3	7.09	1.45	1.32
1	A1	1467	4AC	C4-N3	7.09	1.45	1.32
27	B1	1649	4AC	C4-N3	7.08	1.45	1.32
27	B1	2821	4AC	C4-N3	7.08	1.45	1.32
1	A1	499	4AC	C4-N3	7.08	1.45	1.32
27	B1	2492	4AC	C4-N3	7.08	1.45	1.32
27	B1	2876	4AC	C4-N3	7.08	1.45	1.32
1	A1	1254	4AC	C4-N3	7.08	1.45	1.32
1	A1	836	4AC	C4-N3	7.08	1.45	1.32
1	A1	220	4AC	C4-N3	7.07	1.45	1.32
1	A1	1314	4AC	C4-N3	7.07	1.45	1.32
27	B1	953	4AC	C4-N3	7.07	1.45	1.32
27	B1	2844	4AC	C4-N3	7.07	1.45	1.32
27	B1	3006	4AC	C4-N3	7.07	1.45	1.32
27	B1	1546	4AC	C4-N3	7.07	1.45	1.32
27	B1	1639	4AC	C4-N3	7.06	1.45	1.32
27	B1	2469	4AC	C4-N3	7.06	1.45	1.32
27	B1	1505	4AC	C4-N3	7.06	1.45	1.32
27	B1	2432	4AC	C4-N3	7.06	1.45	1.32
1	A1	291	4AC	C4-N3	7.06	1.45	1.32
27	B1	527	4AC	C4-N3	7.06	1.45	1.32
1	A1	41	4AC	C4-N3	7.06	1.45	1.32
27	B1	479	4AC	C4-N3	7.05	1.45	1.32
1	A1	5	4AC	C4-N3	7.05	1.45	1.32
27	B1	2792	4AC	C4-N3	7.05	1.45	1.32
27	B1	2008	4AC	C4-N3	7.05	1.45	1.32
27	B1	2213	4AC	C4-N3	7.05	1.45	1.32
27	B1	1128	4AC	C4-N3	7.05	1.45	1.32
27	B1	1762	4AC	C4-N3	7.05	1.45	1.32
27	B1	337	4AC	C4-N3	7.04	1.45	1.32
27	B1	1100	4AC	C4-N3	7.04	1.45	1.32
27	B1	1818	4AC	C4-N3	7.04	1.45	1.32
1	A1	706	4AC	C4-N3	7.04	1.45	1.32
1	A1	546	4AC	C4-N3	7.04	1.45	1.32
27	B1	130	4AC	C4-N3	7.04	1.45	1.32
27	B1	1911	4AC	C4-N3	7.04	1.45	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	2429	4AC	C4-N3	7.04	1.45	1.32
1	A1	636	4AC	C4-N3	7.04	1.45	1.32
27	B1	200	4AC	C4-N3	7.04	1.45	1.32
27	B1	1551	4AC	C4-N3	7.04	1.45	1.32
27	B1	2602	4AC	C4-N3	7.04	1.45	1.32
27	B1	933	4AC	C4-N3	7.03	1.45	1.32
1	A1	839	4AC	C4-N3	7.03	1.45	1.32
1	A1	382	4AC	C4-N3	7.03	1.45	1.32
27	B1	2968	4AC	C4-N3	7.03	1.45	1.32
27	B1	950	4AC	C4-N3	7.02	1.45	1.32
27	B1	2171	4AC	C4-N3	7.02	1.45	1.32
27	B1	378	4AC	C4-N3	7.02	1.45	1.32
27	B1	580	4AC	C4-N3	7.02	1.45	1.32
1	A1	367	4AC	C4-N3	7.02	1.45	1.32
27	B1	23	4AC	C4-N3	7.02	1.45	1.32
27	B1	2113	4AC	C4-N3	7.02	1.45	1.32
1	A1	1029	4AC	C4-N3	7.02	1.45	1.32
1	A1	405	4AC	C4-N3	7.01	1.45	1.32
27	B1	1064	4AC	C4-N3	7.01	1.45	1.32
27	B1	1946	4AC	C4-N3	7.01	1.45	1.32
1	A1	540	4AC	C4-N3	7.01	1.45	1.32
27	B1	1442	4AC	C4-N3	7.01	1.45	1.32
27	B1	1885	4AC	C4-N3	7.01	1.45	1.32
27	B1	2850	4AC	C4-N3	7.00	1.45	1.32
27	B1	2749	4AC	C4-N3	7.00	1.45	1.32
1	A1	719	4AC	C4-N3	6.99	1.45	1.32
27	B1	1345	4AC	C4-N3	6.99	1.45	1.32
27	B1	434	4AC	C4-N3	6.99	1.45	1.32
27	B1	1435	4AC	C4-N3	6.98	1.45	1.32
27	B1	116	4AC	C4-N3	6.98	1.45	1.32
27	B1	2133	4AC	C4-N3	6.98	1.45	1.32
27	B1	1967	4AC	C4-N3	6.98	1.44	1.32
1	A1	856	4AC	C4-N3	6.97	1.44	1.32
27	B1	721	4AC	C4-N3	6.97	1.44	1.32
27	B1	2700	UR3	C6-C5	6.97	1.51	1.35
1	A1	307	4AC	C4-N3	6.97	1.44	1.32
27	B1	1290	4AC	C4-N3	6.96	1.44	1.32
27	B1	1822	4AC	C4-N3	6.96	1.44	1.32
27	B1	1478	4AC	C4-N3	6.96	1.44	1.32
27	B1	2020	4AC	C4-N3	6.96	1.44	1.32
27	B1	1067	4AC	C4-N3	6.96	1.44	1.32
27	B1	1107	4AC	C4-N3	6.94	1.44	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	48	4AC	C4-N3	6.93	1.44	1.32
27	B1	652	4AC	C4-N3	6.92	1.44	1.32
27	B1	1769	4AC	C4-N3	6.92	1.44	1.32
27	B1	2379	4AC	C4-N3	6.91	1.44	1.32
1	A1	467	4AC	C4-N3	6.81	1.44	1.32
27	B1	485	4AC	C4-N3	6.80	1.44	1.32
27	B1	2565	4SU	C2-N3	6.76	1.50	1.38
1	A1	756	4SU	C2-N3	6.71	1.49	1.38
1	A1	1227	4AC	C4-N3	6.68	1.44	1.32
27	B1	2059	OMC	C6-C5	6.67	1.50	1.35
27	B1	2735	OMC	C6-C5	6.66	1.50	1.35
1	A1	1371	OMC	C6-C5	6.64	1.50	1.35
27	B1	2607	OMC	C6-C5	6.62	1.50	1.35
1	A1	1270	OMC	C6-C5	6.62	1.50	1.35
1	A1	1364	OMC	C6-C5	6.62	1.50	1.35
27	B1	2808	OMC	C6-C5	6.62	1.50	1.35
27	B1	2119	OMC	C6-C5	6.61	1.50	1.35
27	B1	1099	OMC	C6-C5	6.61	1.50	1.35
1	A1	834	OMC	C6-C5	6.60	1.50	1.35
1	A1	238	LHH	C2-N3	6.60	1.49	1.36
1	A1	117	OMC	C6-C5	6.59	1.50	1.35
27	B1	1832	OMC	C6-C5	6.59	1.50	1.35
27	B1	1489	OMC	C6-C5	6.59	1.50	1.35
1	A1	1028	OMC	C6-C5	6.59	1.50	1.35
27	B1	2557	OMC	C6-C5	6.57	1.50	1.35
1	A1	1194	OMC	C6-C5	6.57	1.50	1.35
27	B1	1914	OMC	C6-C5	6.56	1.50	1.35
1	A1	1226	OMC	C6-C5	6.52	1.50	1.35
27	B1	501	OMC	C6-C5	6.50	1.50	1.35
27	B1	2506	A2M	O4'-C4'	-6.47	1.30	1.45
1	A1	856	4AC	C6-C5	6.42	1.50	1.35
27	B1	485	4AC	C6-C5	6.41	1.50	1.35
27	B1	2850	4AC	C6-C5	6.40	1.49	1.35
27	B1	1478	4AC	C6-C5	6.39	1.49	1.35
27	B1	2008	4AC	C6-C5	6.38	1.49	1.35
27	B1	1128	4AC	C6-C5	6.38	1.49	1.35
27	B1	2020	4AC	C6-C5	6.38	1.49	1.35
27	B1	1822	4AC	C6-C5	6.38	1.49	1.35
27	B1	506	A2M	O4'-C4'	-6.38	1.30	1.45
27	B1	1885	4AC	C6-C5	6.37	1.49	1.35
1	A1	5	4AC	C6-C5	6.37	1.49	1.35
27	B1	715	4AC	C6-C5	6.37	1.49	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	880	A2M	O4'-C4'	-6.37	1.30	1.45
1	A1	216	4AC	C6-C5	6.37	1.49	1.35
1	A1	1029	4AC	C6-C5	6.37	1.49	1.35
27	B1	1649	4AC	C6-C5	6.37	1.49	1.35
27	B1	2113	4AC	C6-C5	6.37	1.49	1.35
27	B1	1946	4AC	C6-C5	6.36	1.49	1.35
1	A1	546	4AC	C6-C5	6.36	1.49	1.35
1	A1	141	4AC	C6-C5	6.36	1.49	1.35
27	B1	1551	4AC	C6-C5	6.36	1.49	1.35
27	B1	1911	4AC	C6-C5	6.36	1.49	1.35
27	B1	1439	LHH	C2-N3	6.36	1.49	1.36
27	B1	1360	4AC	C6-C5	6.36	1.49	1.35
1	A1	8	OMU	C6-C5	6.35	1.49	1.35
27	B1	1290	4AC	C6-C5	6.35	1.49	1.35
27	B1	130	4AC	C6-C5	6.35	1.49	1.35
27	B1	1442	4AC	C6-C5	6.35	1.49	1.35
27	B1	2379	4AC	C6-C5	6.35	1.49	1.35
1	A1	1165	OMU	C6-C5	6.35	1.49	1.35
1	A1	405	4AC	C6-C5	6.35	1.49	1.35
1	A1	762	OMU	C6-C5	6.35	1.49	1.35
27	B1	721	4AC	C6-C5	6.35	1.49	1.35
1	A1	739	4AC	C6-C5	6.34	1.49	1.35
1	A1	1368	OMU	C6-C5	6.34	1.49	1.35
27	B1	2492	4AC	C6-C5	6.34	1.49	1.35
1	A1	274	4AC	C6-C5	6.34	1.49	1.35
27	B1	1107	4AC	C6-C5	6.34	1.49	1.35
1	A1	836	4AC	C6-C5	6.34	1.49	1.35
27	B1	1435	4AC	C6-C5	6.34	1.49	1.35
27	B1	1579	4AC	C6-C5	6.34	1.49	1.35
27	B1	940	A2M	O4'-C4'	-6.34	1.30	1.45
1	A1	706	4AC	C6-C5	6.34	1.49	1.35
27	B1	688	4AC	C6-C5	6.34	1.49	1.35
27	B1	3011	4AC	C6-C5	6.34	1.49	1.35
1	A1	231	4AC	C6-C5	6.34	1.49	1.35
27	B1	2133	4AC	C6-C5	6.33	1.49	1.35
27	B1	1264	4AC	C6-C5	6.33	1.49	1.35
27	B1	1178	4AC	C6-C5	6.33	1.49	1.35
27	B1	2429	4AC	C6-C5	6.33	1.49	1.35
27	B1	1706	4AC	C6-C5	6.33	1.49	1.35
1	A1	499	4AC	C6-C5	6.33	1.49	1.35
27	B1	162	4AC	C6-C5	6.33	1.49	1.35
27	B1	2821	4AC	C6-C5	6.33	1.49	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	652	4AC	C6-C5	6.33	1.49	1.35
27	B1	1639	4AC	C6-C5	6.33	1.49	1.35
27	B1	527	4AC	C6-C5	6.33	1.49	1.35
27	B1	866	4AC	C6-C5	6.33	1.49	1.35
27	B1	1067	4AC	C6-C5	6.33	1.49	1.35
27	B1	1293	4AC	C6-C5	6.33	1.49	1.35
27	B1	200	4AC	C6-C5	6.32	1.49	1.35
1	A1	775	OMU	C6-C5	6.32	1.49	1.35
1	A1	540	4AC	C6-C5	6.32	1.49	1.35
1	A1	1467	4AC	C6-C5	6.32	1.49	1.35
27	B1	580	4AC	C6-C5	6.32	1.49	1.35
27	B1	2749	4AC	C6-C5	6.32	1.49	1.35
27	B1	48	4AC	C6-C5	6.32	1.49	1.35
27	B1	2876	4AC	C6-C5	6.32	1.49	1.35
27	B1	1488	OMU	C6-C5	6.32	1.49	1.35
1	A1	534	4AC	C6-C5	6.32	1.49	1.35
27	B1	2432	4AC	C6-C5	6.32	1.49	1.35
27	B1	2454	4AC	C6-C5	6.32	1.49	1.35
27	B1	2809	4AC	C6-C5	6.31	1.49	1.35
1	A1	816	4AC	C6-C5	6.31	1.49	1.35
27	B1	1546	4AC	C6-C5	6.31	1.49	1.35
1	A1	307	4AC	C6-C5	6.31	1.49	1.35
27	B1	2968	4AC	C6-C5	6.31	1.49	1.35
27	B1	337	4AC	C6-C5	6.31	1.49	1.35
1	A1	41	4AC	C6-C5	6.31	1.49	1.35
27	B1	786	4AC	C6-C5	6.31	1.49	1.35
1	A1	52	OMU	C6-C5	6.31	1.49	1.35
28	B2	88	4AC	C6-C5	6.31	1.49	1.35
27	B1	19	4AC	C6-C5	6.31	1.49	1.35
27	B1	479	4AC	C6-C5	6.31	1.49	1.35
27	B1	1967	4AC	C6-C5	6.31	1.49	1.35
1	A1	827	4AC	C6-C5	6.30	1.49	1.35
27	B1	98	4AC	C6-C5	6.30	1.49	1.35
27	B1	116	4AC	C6-C5	6.30	1.49	1.35
27	B1	1769	4AC	C6-C5	6.30	1.49	1.35
1	A1	636	4AC	C6-C5	6.30	1.49	1.35
27	B1	1100	4AC	C6-C5	6.30	1.49	1.35
27	B1	1751	4AC	C6-C5	6.30	1.49	1.35
27	B1	2602	4AC	C6-C5	6.30	1.49	1.35
27	B1	378	4AC	C6-C5	6.30	1.49	1.35
27	B1	434	4AC	C6-C5	6.30	1.49	1.35
27	B1	2526	4AC	C6-C5	6.30	1.49	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	2844	4AC	C6-C5	6.30	1.49	1.35
27	B1	502	LHH	C2-N3	6.30	1.49	1.36
1	A1	291	4AC	C6-C5	6.30	1.49	1.35
27	B1	360	4AC	C6-C5	6.30	1.49	1.35
1	A1	382	4AC	C6-C5	6.30	1.49	1.35
1	A1	1314	4AC	C6-C5	6.30	1.49	1.35
27	B1	344	4AC	C6-C5	6.30	1.49	1.35
28	B2	115	4AC	C6-C5	6.30	1.49	1.35
28	B2	30	4AC	C6-C5	6.30	1.49	1.35
1	A1	220	4AC	C6-C5	6.30	1.49	1.35
1	A1	367	4AC	C6-C5	6.30	1.49	1.35
27	B1	23	4AC	C6-C5	6.29	1.49	1.35
27	B1	1150	4AC	C6-C5	6.29	1.49	1.35
27	B1	1505	4AC	C6-C5	6.29	1.49	1.35
1	A1	624	4AC	C2-N3	6.29	1.49	1.36
27	B1	1052	4AC	C6-C5	6.29	1.49	1.35
27	B1	2171	4AC	C6-C5	6.29	1.49	1.35
27	B1	2213	4AC	C6-C5	6.29	1.49	1.35
1	A1	839	4AC	C6-C5	6.29	1.49	1.35
27	B1	3020	4AC	C6-C5	6.28	1.49	1.35
1	A1	819	A2M	O4'-C4'	-6.28	1.31	1.45
27	B1	454	OMU	C6-C5	6.28	1.49	1.35
1	A1	945	4AC	C6-C5	6.28	1.49	1.35
27	B1	1818	4AC	C6-C5	6.28	1.49	1.35
1	A1	578	4AC	C6-C5	6.28	1.49	1.35
27	B1	896	4AC	C6-C5	6.28	1.49	1.35
1	A1	761	4AC	C6-C5	6.28	1.49	1.35
27	B1	243	4AC	C6-C5	6.28	1.49	1.35
27	B1	953	4AC	C6-C5	6.27	1.49	1.35
27	B1	1061	4AC	C6-C5	6.27	1.49	1.35
27	B1	2469	4AC	C6-C5	6.27	1.49	1.35
1	A1	691	4AC	C2-N3	6.27	1.49	1.36
27	B1	950	4AC	C6-C5	6.27	1.49	1.35
27	B1	2554	OMU	C6-C5	6.26	1.49	1.35
27	B1	926	OMU	C6-C5	6.26	1.49	1.35
1	A1	719	4AC	C6-C5	6.26	1.49	1.35
27	B1	1846	4AC	C6-C5	6.26	1.49	1.35
1	A1	945	4AC	C2-N3	6.26	1.49	1.36
27	B1	979	4AC	C6-C5	6.26	1.49	1.35
27	B1	80	4AC	C6-C5	6.26	1.49	1.35
27	B1	2792	4AC	C6-C5	6.26	1.49	1.35
1	A1	87	4AC	C6-C5	6.26	1.49	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	1345	4AC	C6-C5	6.26	1.49	1.35
27	B1	1374	4AC	C6-C5	6.26	1.49	1.35
27	B1	1762	4AC	C6-C5	6.26	1.49	1.35
27	B1	227	4AC	C6-C5	6.26	1.49	1.35
27	B1	1608	4AC	C2-N3	6.26	1.49	1.36
27	B1	419	4AC	C6-C5	6.26	1.49	1.35
27	B1	1743	4AC	C6-C5	6.26	1.49	1.35
1	A1	614	4AC	C6-C5	6.26	1.49	1.35
28	B2	30	4AC	C2-N3	6.26	1.49	1.36
27	B1	933	4AC	C6-C5	6.25	1.49	1.35
27	B1	1064	4AC	C6-C5	6.25	1.49	1.35
27	B1	3037	4AC	C6-C5	6.25	1.49	1.35
27	B1	3006	4AC	C6-C5	6.24	1.49	1.35
27	B1	1293	4AC	C2-N3	6.24	1.49	1.36
27	B1	1743	4AC	C2-N3	6.24	1.49	1.36
27	B1	1383	4AC	C6-C5	6.23	1.49	1.35
1	A1	756	4SU	C6-C5	6.23	1.49	1.35
1	A1	624	4AC	C6-C5	6.22	1.49	1.35
27	B1	1608	4AC	C6-C5	6.22	1.49	1.35
1	A1	87	4AC	C2-N3	6.22	1.49	1.36
1	A1	1254	4AC	C6-C5	6.21	1.49	1.35
27	B1	3006	4AC	C2-N3	6.21	1.49	1.36
27	B1	732	4AC	C6-C5	6.21	1.49	1.35
1	A1	739	4AC	C2-N3	6.21	1.48	1.36
27	B1	1501	4AC	C6-C5	6.21	1.49	1.35
27	B1	227	4AC	C2-N3	6.21	1.48	1.36
1	A1	1181	4AC	C2-N3	6.20	1.48	1.36
27	B1	1579	4AC	C2-N3	6.20	1.48	1.36
27	B1	1374	4AC	C2-N3	6.20	1.48	1.36
1	A1	1227	4AC	C6-C5	6.20	1.49	1.35
28	B2	115	4AC	C2-N3	6.20	1.48	1.36
27	B1	1501	4AC	C2-N3	6.19	1.48	1.36
1	A1	1181	4AC	C6-C5	6.19	1.49	1.35
1	A1	761	4AC	C2-N3	6.19	1.48	1.36
28	B2	88	4AC	C2-N3	6.18	1.48	1.36
27	B1	732	4AC	C2-N3	6.18	1.48	1.36
1	A1	216	4AC	C2-N3	6.18	1.48	1.36
27	B1	2565	4SU	C6-C5	6.17	1.49	1.35
27	B1	1639	4AC	C2-N3	6.17	1.48	1.36
1	A1	691	4AC	C6-C5	6.16	1.49	1.35
1	A1	636	4AC	C2-N3	6.16	1.48	1.36
1	A1	827	4AC	C2-N3	6.16	1.48	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	857	A2M	O4'-C4'	-6.16	1.31	1.45
27	B1	1649	4AC	C2-N3	6.16	1.48	1.36
1	A1	1254	4AC	C2-N3	6.16	1.48	1.36
1	A1	578	4AC	C2-N3	6.16	1.48	1.36
27	B1	360	4AC	C2-N3	6.15	1.48	1.36
27	B1	933	4AC	C2-N3	6.15	1.48	1.36
27	B1	1706	4AC	C2-N3	6.15	1.48	1.36
27	B1	2454	4AC	C2-N3	6.15	1.48	1.36
27	B1	3020	4AC	C2-N3	6.15	1.48	1.36
27	B1	3037	4AC	C2-N3	6.15	1.48	1.36
27	B1	2821	4AC	C2-N3	6.15	1.48	1.36
27	B1	344	4AC	C2-N3	6.15	1.48	1.36
1	A1	534	4AC	C2-N3	6.14	1.48	1.36
27	B1	2432	4AC	C2-N3	6.14	1.48	1.36
27	B1	1751	4AC	C2-N3	6.14	1.48	1.36
27	B1	2492	4AC	C2-N3	6.13	1.48	1.36
27	B1	950	4AC	C2-N3	6.13	1.48	1.36
27	B1	1052	4AC	C2-N3	6.13	1.48	1.36
1	A1	405	4AC	C2-N3	6.13	1.48	1.36
1	A1	141	4AC	C2-N3	6.12	1.48	1.36
27	B1	2844	4AC	C2-N3	6.12	1.48	1.36
1	A1	231	4AC	C2-N3	6.12	1.48	1.36
27	B1	1762	4AC	C2-N3	6.12	1.48	1.36
27	B1	19	4AC	C2-N3	6.12	1.48	1.36
27	B1	3011	4AC	C2-N3	6.12	1.48	1.36
27	B1	1178	4AC	C2-N3	6.11	1.48	1.36
27	B1	1846	4AC	C2-N3	6.11	1.48	1.36
27	B1	1150	4AC	C2-N3	6.11	1.48	1.36
1	A1	382	4AC	C2-N3	6.11	1.48	1.36
27	B1	2008	4AC	C2-N3	6.11	1.48	1.36
1	A1	546	4AC	C2-N3	6.11	1.48	1.36
27	B1	243	4AC	C2-N3	6.11	1.48	1.36
27	B1	479	4AC	C2-N3	6.10	1.48	1.36
27	B1	1064	4AC	C2-N3	6.10	1.48	1.36
27	B1	2876	4AC	C2-N3	6.10	1.48	1.36
27	B1	1546	4AC	C2-N3	6.10	1.48	1.36
1	A1	499	4AC	C2-N3	6.10	1.48	1.36
1	A1	220	4AC	C2-N3	6.10	1.48	1.36
27	B1	1345	4AC	C2-N3	6.10	1.48	1.36
1	A1	540	4AC	C2-N3	6.10	1.48	1.36
27	B1	1383	4AC	C2-N3	6.10	1.48	1.36
1	A1	5	4AC	C2-N3	6.10	1.48	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	614	4AC	C2-N3	6.10	1.48	1.36
27	B1	2429	4AC	C2-N3	6.10	1.48	1.36
27	B1	1264	4AC	C2-N3	6.10	1.48	1.36
27	B1	688	4AC	C2-N3	6.09	1.48	1.36
27	B1	1067	4AC	C2-N3	6.09	1.48	1.36
27	B1	434	4AC	C2-N3	6.09	1.48	1.36
1	A1	816	4AC	C2-N3	6.09	1.48	1.36
27	B1	98	4AC	C2-N3	6.08	1.48	1.36
1	A1	719	4AC	C2-N3	6.08	1.48	1.36
27	B1	953	4AC	C2-N3	6.08	1.48	1.36
27	B1	419	4AC	C2-N3	6.08	1.48	1.36
27	B1	896	4AC	C2-N3	6.08	1.48	1.36
27	B1	2809	4AC	C2-N3	6.08	1.48	1.36
27	B1	2792	4AC	C2-N3	6.08	1.48	1.36
27	B1	162	4AC	C2-N3	6.08	1.48	1.36
27	B1	80	4AC	C2-N3	6.07	1.48	1.36
27	B1	979	4AC	C2-N3	6.07	1.48	1.36
27	B1	1435	4AC	C2-N3	6.07	1.48	1.36
27	B1	527	4AC	C2-N3	6.07	1.48	1.36
1	A1	274	4AC	C2-N3	6.07	1.48	1.36
27	B1	378	4AC	C2-N3	6.07	1.48	1.36
1	A1	839	4AC	C2-N3	6.06	1.48	1.36
27	B1	337	4AC	C2-N3	6.06	1.48	1.36
1	A1	291	4AC	C2-N3	6.06	1.48	1.36
1	A1	307	4AC	C2-N3	6.06	1.48	1.36
27	B1	1061	4AC	C2-N3	6.06	1.48	1.36
27	B1	2968	4AC	C2-N3	6.06	1.48	1.36
1	A1	1314	4AC	C2-N3	6.06	1.48	1.36
27	B1	2749	4AC	C2-N3	6.06	1.48	1.36
27	B1	580	4AC	C2-N3	6.06	1.48	1.36
27	B1	200	4AC	C2-N3	6.05	1.48	1.36
27	B1	1360	4AC	C2-N3	6.05	1.48	1.36
27	B1	1822	4AC	C2-N3	6.05	1.48	1.36
27	B1	2469	4AC	C2-N3	6.05	1.48	1.36
1	A1	1029	4AC	C2-N3	6.05	1.48	1.36
27	B1	2020	4AC	C2-N3	6.05	1.48	1.36
27	B1	1885	4AC	C2-N3	6.05	1.48	1.36
27	B1	786	4AC	C2-N3	6.04	1.48	1.36
1	A1	367	4AC	C2-N3	6.04	1.48	1.36
27	B1	1290	4AC	C2-N3	6.04	1.48	1.36
27	B1	1818	4AC	C2-N3	6.04	1.48	1.36
1	A1	467	4AC	C6-C5	6.04	1.49	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	1128	4AC	C2-N3	6.04	1.48	1.36
27	B1	721	4AC	C2-N3	6.04	1.48	1.36
27	B1	1551	4AC	C2-N3	6.04	1.48	1.36
27	B1	2602	4AC	C2-N3	6.04	1.48	1.36
27	B1	2526	4AC	C2-N3	6.03	1.48	1.36
27	B1	715	4AC	C2-N3	6.03	1.48	1.36
27	B1	23	4AC	C2-N3	6.03	1.48	1.36
27	B1	1911	4AC	C2-N3	6.03	1.48	1.36
27	B1	1967	4AC	C2-N3	6.03	1.48	1.36
27	B1	652	4AC	C2-N3	6.03	1.48	1.36
27	B1	1100	4AC	C2-N3	6.02	1.48	1.36
27	B1	1505	4AC	C2-N3	6.02	1.48	1.36
27	B1	866	4AC	C2-N3	6.02	1.48	1.36
27	B1	116	4AC	C2-N3	6.02	1.48	1.36
27	B1	2171	4AC	C2-N3	6.02	1.48	1.36
1	A1	836	4AC	C2-N3	6.02	1.48	1.36
27	B1	130	4AC	C2-N3	6.02	1.48	1.36
1	A1	41	4AC	C2-N3	6.01	1.48	1.36
1	A1	1467	4AC	C2-N3	6.01	1.48	1.36
27	B1	1478	4AC	C2-N3	6.00	1.48	1.36
27	B1	1769	4AC	C2-N3	6.00	1.48	1.36
27	B1	2850	4AC	C2-N3	6.00	1.48	1.36
27	B1	2213	4AC	C2-N3	5.98	1.48	1.36
27	B1	2133	4AC	C2-N3	5.98	1.48	1.36
1	A1	856	4AC	C2-N3	5.98	1.48	1.36
27	B1	485	4AC	C2-N3	5.98	1.48	1.36
1	A1	706	4AC	C2-N3	5.96	1.48	1.36
27	B1	2700	UR3	C2-N3	5.96	1.50	1.39
27	B1	1442	4AC	C2-N3	5.95	1.48	1.36
27	B1	2113	4AC	C2-N3	5.95	1.48	1.36
27	B1	2379	4AC	C2-N3	5.94	1.48	1.36
27	B1	1107	4AC	C2-N3	5.94	1.48	1.36
1	A1	467	4AC	C2-N3	5.93	1.48	1.36
27	B1	48	4AC	C2-N3	5.92	1.48	1.36
27	B1	1946	4AC	C2-N3	5.92	1.48	1.36
1	A1	951	5MC	C4-N3	5.88	1.44	1.34
1	A1	927	5MC	C4-N3	5.85	1.44	1.34
1	A1	481	G7M	C2-N3	5.85	1.47	1.33
1	A1	951	5MC	C2-N3	5.84	1.48	1.36
1	A1	1362	5MC	C4-N3	5.83	1.44	1.34
1	A1	352	5MC	C4-N3	5.81	1.44	1.34
1	A1	687	5MC	C4-N3	5.80	1.43	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	2067	5MC	C4-N3	5.78	1.43	1.34
27	B1	2087	5MC	C4-N3	5.76	1.43	1.34
27	B1	336	5MC	C4-N3	5.76	1.43	1.34
27	B1	1344	5MC	C4-N3	5.74	1.43	1.34
1	A1	863	5MC	C4-N3	5.73	1.43	1.34
1	A1	230	5MC	C4-N3	5.73	1.43	1.34
1	A1	1013	5MC	C4-N3	5.72	1.43	1.34
1	A1	17	5MC	C4-N3	5.72	1.43	1.34
27	B1	1977	5MC	C4-N3	5.71	1.43	1.34
1	A1	1190	5MC	C4-N3	5.71	1.43	1.34
1	A1	1227	4AC	C2-N3	5.69	1.47	1.36
1	A1	681	5MC	C4-N3	5.69	1.43	1.34
1	A1	1484	5MC	C4-N3	5.69	1.43	1.34
1	A1	466	5MC	C4-N3	5.68	1.43	1.34
1	A1	473	5MC	C4-N3	5.68	1.43	1.34
1	A1	927	5MC	C2-N3	5.62	1.47	1.36
1	A1	687	5MC	C2-N3	5.62	1.47	1.36
27	B1	2617	5MC	C4-N3	5.62	1.43	1.34
27	B1	2067	5MC	C2-N3	5.62	1.47	1.36
1	A1	473	5MC	C2-N3	5.61	1.47	1.36
1	A1	1484	5MC	C2-N3	5.59	1.47	1.36
1	A1	645	OMG	C2-N3	5.58	1.46	1.33
1	A1	1362	5MC	C2-N3	5.57	1.47	1.36
1	A1	1013	5MC	C2-N3	5.57	1.47	1.36
1	A1	863	5MC	C2-N3	5.57	1.47	1.36
27	B1	1344	5MC	C2-N3	5.56	1.47	1.36
1	A1	230	5MC	C2-N3	5.56	1.47	1.36
1	A1	352	5MC	C2-N3	5.56	1.47	1.36
27	B1	2087	5MC	C2-N3	5.55	1.47	1.36
27	B1	336	5MC	C2-N3	5.55	1.47	1.36
1	A1	1190	5MC	C2-N3	5.54	1.47	1.36
27	B1	1977	5MC	C2-N3	5.54	1.47	1.36
1	A1	681	5MC	C2-N3	5.53	1.47	1.36
1	A1	466	5MC	C2-N3	5.52	1.47	1.36
27	B1	530	OMG	C2-N3	5.51	1.46	1.33
27	B1	920	OMG	C2-N3	5.49	1.46	1.33
1	A1	541	OMG	C2-N3	5.48	1.46	1.33
27	B1	2617	5MC	C2-N3	5.48	1.47	1.36
1	A1	17	5MC	C2-N3	5.48	1.47	1.36
1	A1	668	OMG	C2-N3	5.47	1.46	1.33
27	B1	887	OMG	C2-N3	5.47	1.46	1.33
27	B1	2684	OMG	C2-N3	5.46	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	2540	OMG	C2-N3	5.45	1.46	1.33
1	A1	1115	OMG	C2-N3	5.43	1.46	1.33
27	B1	1557	OMG	C2-N3	5.43	1.46	1.33
27	B1	2365	OMG	C2-N3	5.42	1.46	1.33
1	A1	459	OMG	C2-N3	5.42	1.46	1.33
27	B1	921	OMG	C2-N3	5.42	1.46	1.33
27	B1	55	OMG	C2-N3	5.41	1.46	1.33
27	B1	808	OMG	C2-N3	5.41	1.46	1.33
1	A1	1003	OMG	C2-N3	5.40	1.46	1.33
27	B1	841	OMG	C2-N3	5.40	1.46	1.33
27	B1	1904	OMG	C2-N3	5.39	1.46	1.33
27	B1	2562	OMG	C2-N3	5.38	1.46	1.33
27	B1	856	OMG	C2-N3	5.37	1.46	1.33
27	B1	2028	OMG	C2-N3	5.37	1.46	1.33
1	A1	507	OMG	C2-N3	5.35	1.46	1.33
27	B1	1965	OMG	C2-N3	5.35	1.46	1.33
27	B1	2984	OMG	C2-N3	5.35	1.46	1.33
27	B1	2180	OMG	C2-N3	5.32	1.46	1.33
1	A1	861	OMG	C2-N3	5.32	1.46	1.33
27	B1	214	OMG	C2-N3	5.32	1.46	1.33
1	A1	329	OMG	C2-N3	5.31	1.46	1.33
1	A1	455	OMG	C2-N3	5.30	1.46	1.33
27	B1	2022	OMG	C2-N3	5.29	1.46	1.33
27	B1	501	OMC	C4-N3	5.27	1.45	1.34
27	B1	2108	OMG	C2-N3	5.27	1.46	1.33
1	A1	1371	OMC	C4-N3	5.26	1.45	1.34
27	B1	2757	OMG	C2-N3	5.25	1.46	1.33
1	A1	1270	OMC	C4-N3	5.25	1.45	1.34
27	B1	2808	OMC	C4-N3	5.24	1.45	1.34
1	A1	1194	OMC	C4-N3	5.24	1.45	1.34
1	A1	1028	OMC	C4-N3	5.24	1.45	1.34
27	B1	1832	OMC	C4-N3	5.24	1.45	1.34
27	B1	2735	OMC	C4-N3	5.23	1.45	1.34
27	B1	2391	OMG	C2-N3	5.23	1.45	1.33
27	B1	2059	OMC	C4-N3	5.22	1.45	1.34
1	A1	1364	OMC	C4-N3	5.22	1.45	1.34
27	B1	2557	OMC	C4-N3	5.20	1.45	1.34
1	A1	117	OMC	C4-N3	5.20	1.45	1.34
27	B1	2607	OMC	C4-N3	5.19	1.44	1.34
27	B1	1099	OMC	C4-N3	5.19	1.44	1.34
1	A1	1226	OMC	C4-N3	5.19	1.44	1.34
1	A1	834	OMC	C4-N3	5.18	1.44	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	1489	OMC	C4-N3	5.16	1.44	1.34
27	B1	2119	OMC	C4-N3	5.16	1.44	1.34
27	B1	920	OMG	C4-N3	5.05	1.49	1.37
27	B1	530	OMG	C4-N3	5.05	1.49	1.37
1	A1	645	OMG	C4-N3	5.04	1.49	1.37
1	A1	541	OMG	C4-N3	5.04	1.49	1.37
27	B1	887	OMG	C4-N3	5.02	1.49	1.37
27	B1	2365	OMG	C4-N3	5.02	1.49	1.37
27	B1	2540	OMG	C4-N3	5.01	1.49	1.37
27	B1	2180	OMG	C4-N3	5.01	1.49	1.37
27	B1	841	OMG	C4-N3	5.00	1.49	1.37
1	A1	668	OMG	C4-N3	5.00	1.49	1.37
1	A1	459	OMG	C4-N3	4.99	1.49	1.37
27	B1	856	OMG	C4-N3	4.99	1.49	1.37
27	B1	2684	OMG	C4-N3	4.99	1.49	1.37
27	B1	2562	OMG	C4-N3	4.99	1.49	1.37
27	B1	1914	OMC	C4-N3	4.99	1.44	1.34
27	B1	808	OMG	C4-N3	4.98	1.49	1.37
27	B1	55	OMG	C4-N3	4.97	1.49	1.37
27	B1	1557	OMG	C4-N3	4.97	1.49	1.37
27	B1	2028	OMG	C4-N3	4.97	1.49	1.37
27	B1	1965	OMG	C4-N3	4.97	1.49	1.37
1	A1	1115	OMG	C4-N3	4.96	1.49	1.37
1	A1	861	OMG	C4-N3	4.96	1.49	1.37
27	B1	921	OMG	C4-N3	4.95	1.49	1.37
27	B1	214	OMG	C4-N3	4.94	1.49	1.37
1	A1	1003	OMG	C4-N3	4.94	1.49	1.37
27	B1	2984	OMG	C4-N3	4.94	1.49	1.37
1	A1	507	OMG	C4-N3	4.93	1.49	1.37
27	B1	1904	OMG	C4-N3	4.92	1.49	1.37
1	A1	455	OMG	C4-N3	4.92	1.49	1.37
27	B1	2108	OMG	C4-N3	4.92	1.49	1.37
1	A1	481	G7M	C6-N1	4.92	1.45	1.37
1	A1	329	OMG	C4-N3	4.91	1.49	1.37
27	B1	2022	OMG	C4-N3	4.90	1.49	1.37
27	B1	1360	4AC	C7-N4	4.88	1.46	1.37
27	B1	2391	OMG	C4-N3	4.85	1.49	1.37
1	A1	756	4SU	C5-C4	4.84	1.48	1.42
1	A1	1467	4AC	C7-N4	4.83	1.46	1.37
27	B1	921	OMG	C2-N2	4.83	1.45	1.34
27	B1	2757	OMG	C4-N3	4.82	1.49	1.37
27	B1	1965	OMG	C2-N2	4.81	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	1557	OMG	C2-N2	4.81	1.45	1.34
27	B1	2365	OMG	C2-N2	4.80	1.45	1.34
27	B1	920	OMG	C2-N2	4.80	1.45	1.34
27	B1	2684	OMG	C2-N2	4.80	1.45	1.34
27	B1	887	OMG	C2-N2	4.80	1.45	1.34
27	B1	530	OMG	C2-N2	4.80	1.45	1.34
27	B1	2180	OMG	C2-N2	4.80	1.45	1.34
1	A1	541	OMG	C2-N2	4.80	1.45	1.34
1	A1	668	OMG	C2-N2	4.80	1.45	1.34
27	B1	841	OMG	C2-N2	4.79	1.45	1.34
27	B1	2540	OMG	C2-N2	4.78	1.45	1.34
27	B1	214	OMG	C2-N2	4.78	1.45	1.34
1	A1	459	OMG	C2-N2	4.78	1.45	1.34
27	B1	2984	OMG	C2-N2	4.78	1.45	1.34
1	A1	329	OMG	C2-N2	4.77	1.45	1.34
1	A1	1115	OMG	C2-N2	4.77	1.45	1.34
27	B1	1374	4AC	C7-N4	4.77	1.46	1.37
27	B1	856	OMG	C2-N2	4.77	1.45	1.34
27	B1	2028	OMG	C2-N2	4.76	1.45	1.34
1	A1	624	4AC	C7-N4	4.76	1.46	1.37
27	B1	2565	4SU	C5-C4	4.76	1.48	1.42
27	B1	2022	OMG	C2-N2	4.76	1.45	1.34
27	B1	55	OMG	C2-N2	4.75	1.45	1.34
27	B1	2562	OMG	C2-N2	4.75	1.45	1.34
1	A1	645	OMG	C2-N2	4.75	1.45	1.34
1	A1	1003	OMG	C2-N2	4.75	1.45	1.34
1	A1	1366	A1I59	C4-N4	4.75	1.46	1.34
1	A1	861	OMG	C2-N2	4.75	1.45	1.34
1	A1	455	OMG	C2-N2	4.75	1.45	1.34
27	B1	1904	OMG	C2-N2	4.74	1.45	1.34
27	B1	2391	OMG	C2-N2	4.74	1.45	1.34
1	A1	481	G7M	C2-N2	4.74	1.45	1.34
1	A1	945	4AC	C7-N4	4.74	1.46	1.37
1	A1	507	OMG	C2-N2	4.73	1.45	1.34
1	A1	761	4AC	C7-N4	4.73	1.45	1.37
27	B1	502	LHH	C7-N4	4.73	1.45	1.37
27	B1	808	OMG	C2-N2	4.72	1.45	1.34
27	B1	1501	4AC	C7-N4	4.72	1.45	1.37
27	B1	1052	4AC	C7-N4	4.72	1.45	1.37
27	B1	1743	4AC	C7-N4	4.70	1.45	1.37
27	B1	227	4AC	C7-N4	4.70	1.45	1.37
27	B1	2757	OMG	C2-N2	4.69	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	1439	LHH	C7-N4	4.69	1.45	1.37
1	A1	216	4AC	C7-N4	4.69	1.45	1.37
27	B1	1751	4AC	C7-N4	4.68	1.45	1.37
1	A1	540	4AC	C7-N4	4.68	1.45	1.37
27	B1	2108	OMG	C2-N2	4.68	1.45	1.34
1	A1	141	4AC	C7-N4	4.68	1.45	1.37
27	B1	344	4AC	C7-N4	4.68	1.45	1.37
27	B1	1064	4AC	C7-N4	4.68	1.45	1.37
27	B1	1846	4AC	C7-N4	4.68	1.45	1.37
28	B2	88	4AC	C7-N4	4.68	1.45	1.37
27	B1	1293	4AC	C7-N4	4.68	1.45	1.37
28	B2	30	4AC	C7-N4	4.68	1.45	1.37
27	B1	1067	4AC	C7-N4	4.68	1.45	1.37
1	A1	827	4AC	C7-N4	4.67	1.45	1.37
27	B1	3006	4AC	C7-N4	4.67	1.45	1.37
28	B2	115	4AC	C7-N4	4.66	1.45	1.37
1	A1	614	4AC	C7-N4	4.66	1.45	1.37
27	B1	3037	4AC	C7-N4	4.66	1.45	1.37
27	B1	98	4AC	C7-N4	4.66	1.45	1.37
27	B1	732	4AC	C7-N4	4.66	1.45	1.37
1	A1	1254	4AC	C7-N4	4.66	1.45	1.37
27	B1	2526	4AC	C7-N4	4.66	1.45	1.37
1	A1	691	4AC	C7-N4	4.66	1.45	1.37
27	B1	1178	4AC	C7-N4	4.66	1.45	1.37
27	B1	1608	4AC	C7-N4	4.66	1.45	1.37
1	A1	87	4AC	C7-N4	4.65	1.45	1.37
1	A1	636	4AC	C7-N4	4.65	1.45	1.37
27	B1	162	4AC	C7-N4	4.65	1.45	1.37
27	B1	419	4AC	C7-N4	4.65	1.45	1.37
1	A1	534	4AC	C7-N4	4.65	1.45	1.37
27	B1	200	4AC	C7-N4	4.65	1.45	1.37
27	B1	1579	4AC	C7-N4	4.65	1.45	1.37
27	B1	786	4AC	C7-N4	4.65	1.45	1.37
27	B1	1706	4AC	C7-N4	4.65	1.45	1.37
27	B1	80	4AC	C7-N4	4.65	1.45	1.37
27	B1	1383	4AC	C7-N4	4.64	1.45	1.37
1	A1	719	4AC	C7-N4	4.64	1.45	1.37
27	B1	434	4AC	C7-N4	4.64	1.45	1.37
27	B1	2876	4AC	C7-N4	4.64	1.45	1.37
27	B1	2469	4AC	C7-N4	4.64	1.45	1.37
27	B1	1061	4AC	C7-N4	4.63	1.45	1.37
27	B1	360	4AC	C7-N4	4.63	1.45	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	231	4AC	C7-N4	4.63	1.45	1.37
27	B1	3020	4AC	C7-N4	4.63	1.45	1.37
27	B1	2492	4AC	C7-N4	4.63	1.45	1.37
27	B1	979	4AC	C7-N4	4.63	1.45	1.37
27	B1	2809	4AC	C7-N4	4.63	1.45	1.37
27	B1	1946	4AC	C7-N4	4.63	1.45	1.37
27	B1	2454	4AC	C7-N4	4.62	1.45	1.37
1	A1	546	4AC	C7-N4	4.62	1.45	1.37
1	A1	382	4AC	C7-N4	4.62	1.45	1.37
1	A1	220	4AC	C7-N4	4.62	1.45	1.37
1	A1	291	4AC	C7-N4	4.62	1.45	1.37
1	A1	816	4AC	C7-N4	4.62	1.45	1.37
27	B1	19	4AC	C7-N4	4.62	1.45	1.37
27	B1	1546	4AC	C7-N4	4.62	1.45	1.37
1	A1	41	4AC	C7-N4	4.62	1.45	1.37
1	A1	739	4AC	C7-N4	4.62	1.45	1.37
1	A1	274	4AC	C7-N4	4.62	1.45	1.37
27	B1	688	4AC	C7-N4	4.62	1.45	1.37
27	B1	1639	4AC	C7-N4	4.62	1.45	1.37
27	B1	1649	4AC	C7-N4	4.61	1.45	1.37
27	B1	23	4AC	C7-N4	4.61	1.45	1.37
27	B1	1360	4AC	C4-N4	4.61	1.46	1.39
27	B1	2432	4AC	C7-N4	4.61	1.45	1.37
27	B1	1150	4AC	C7-N4	4.61	1.45	1.37
27	B1	2844	4AC	C7-N4	4.61	1.45	1.37
27	B1	3011	4AC	C7-N4	4.61	1.45	1.37
1	A1	1181	4AC	C7-N4	4.61	1.45	1.37
27	B1	1505	4AC	C7-N4	4.61	1.45	1.37
27	B1	866	4AC	C7-N4	4.60	1.45	1.37
1	A1	578	4AC	C7-N4	4.60	1.45	1.37
27	B1	950	4AC	C7-N4	4.60	1.45	1.37
27	B1	2171	4AC	C7-N4	4.60	1.45	1.37
27	B1	933	4AC	C7-N4	4.60	1.45	1.37
27	B1	527	4AC	C7-N4	4.60	1.45	1.37
27	B1	1911	4AC	C7-N4	4.60	1.45	1.37
27	B1	2008	4AC	C7-N4	4.60	1.45	1.37
27	B1	1551	4AC	C7-N4	4.60	1.45	1.37
27	B1	479	4AC	C7-N4	4.59	1.45	1.37
1	A1	839	4AC	C7-N4	4.59	1.45	1.37
1	A1	405	4AC	C7-N4	4.59	1.45	1.37
27	B1	2850	4AC	C7-N4	4.59	1.45	1.37
27	B1	953	4AC	C7-N4	4.59	1.45	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	1818	4AC	C7-N4	4.59	1.45	1.37
27	B1	2133	4AC	C7-N4	4.59	1.45	1.37
1	A1	1314	4AC	C7-N4	4.59	1.45	1.37
27	B1	130	4AC	C7-N4	4.59	1.45	1.37
1	A1	1029	4AC	C7-N4	4.58	1.45	1.37
27	B1	2213	4AC	C7-N4	4.58	1.45	1.37
27	B1	580	4AC	C7-N4	4.58	1.45	1.37
27	B1	896	4AC	C7-N4	4.58	1.45	1.37
1	A1	499	4AC	C7-N4	4.58	1.45	1.37
27	B1	1128	4AC	C7-N4	4.58	1.45	1.37
1	A1	836	4AC	C7-N4	4.58	1.45	1.37
27	B1	1442	4AC	C7-N4	4.58	1.45	1.37
1	A1	307	4AC	C7-N4	4.57	1.45	1.37
27	B1	1264	4AC	C7-N4	4.57	1.45	1.37
27	B1	1885	4AC	C7-N4	4.57	1.45	1.37
27	B1	116	4AC	C7-N4	4.57	1.45	1.37
27	B1	243	4AC	C7-N4	4.57	1.45	1.37
27	B1	378	4AC	C7-N4	4.57	1.45	1.37
27	B1	652	4AC	C7-N4	4.57	1.45	1.37
27	B1	721	4AC	C7-N4	4.57	1.45	1.37
27	B1	2602	4AC	C7-N4	4.57	1.45	1.37
27	B1	1290	4AC	C7-N4	4.56	1.45	1.37
27	B1	1435	4AC	C7-N4	4.56	1.45	1.37
1	A1	5	4AC	C7-N4	4.56	1.45	1.37
27	B1	1762	4AC	C7-N4	4.55	1.45	1.37
27	B1	2020	4AC	C7-N4	4.55	1.45	1.37
27	B1	2821	4AC	C7-N4	4.55	1.45	1.37
27	B1	1100	4AC	C7-N4	4.55	1.45	1.37
27	B1	1345	4AC	C7-N4	4.55	1.45	1.37
1	A1	1467	4AC	C4-N4	4.55	1.46	1.39
27	B1	2792	4AC	C7-N4	4.55	1.45	1.37
27	B1	2113	4AC	C7-N4	4.55	1.45	1.37
27	B1	2429	4AC	C7-N4	4.54	1.45	1.37
1	A1	706	4AC	C7-N4	4.54	1.45	1.37
1	A1	367	4AC	C7-N4	4.54	1.45	1.37
27	B1	2968	4AC	C7-N4	4.54	1.45	1.37
27	B1	715	4AC	C7-N4	4.53	1.45	1.37
27	B1	337	4AC	C7-N4	4.52	1.45	1.37
1	A1	856	4AC	C7-N4	4.52	1.45	1.37
27	B1	2617	5MC	C2-N1	4.52	1.49	1.40
27	B1	1107	4AC	C7-N4	4.51	1.45	1.37
1	A1	951	5MC	C2-N1	4.51	1.49	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	2749	4AC	C7-N4	4.51	1.45	1.37
27	B1	1822	4AC	C7-N4	4.51	1.45	1.37
27	B1	1769	4AC	C7-N4	4.50	1.45	1.37
27	B1	2379	4AC	C7-N4	4.50	1.45	1.37
1	A1	467	4AC	C7-N4	4.50	1.45	1.37
27	B1	485	4AC	C7-N4	4.48	1.45	1.37
27	B1	1967	4AC	C7-N4	4.48	1.45	1.37
1	A1	1013	5MC	C2-N1	4.48	1.49	1.40
27	B1	1478	4AC	C7-N4	4.47	1.45	1.37
27	B1	502	LHH	C4-N4	4.45	1.46	1.39
1	A1	927	5MC	C2-N1	4.44	1.49	1.40
1	A1	1362	5MC	C2-N1	4.44	1.49	1.40
27	B1	48	4AC	C7-N4	4.43	1.45	1.37
27	B1	2067	5MC	C6-N1	4.42	1.45	1.38
1	A1	927	5MC	C6-N1	4.41	1.45	1.38
1	A1	238	LHH	C7-N4	4.40	1.45	1.37
1	A1	352	5MC	C2-N1	4.40	1.49	1.40
27	B1	1293	4AC	C4-N4	4.40	1.46	1.39
27	B1	2067	5MC	C2-N1	4.40	1.49	1.40
1	A1	466	5MC	C2-N1	4.39	1.49	1.40
1	A1	863	5MC	C2-N1	4.39	1.49	1.40
1	A1	473	5MC	C6-N1	4.39	1.45	1.38
1	A1	1371	OMC	C2-N1	4.39	1.49	1.40
27	B1	1914	OMC	C2-N1	4.39	1.49	1.40
27	B1	2087	5MC	C6-N1	4.38	1.45	1.38
27	B1	1977	5MC	C2-N1	4.38	1.49	1.40
1	A1	1190	5MC	C2-N1	4.38	1.49	1.40
1	A1	473	5MC	C2-N1	4.38	1.49	1.40
27	B1	336	5MC	C2-N1	4.38	1.49	1.40
27	B1	2087	5MC	C2-N1	4.38	1.49	1.40
1	A1	687	5MC	C6-N1	4.38	1.45	1.38
1	A1	352	5MC	C6-N1	4.37	1.45	1.38
1	A1	687	5MC	C2-N1	4.36	1.49	1.40
27	B1	1439	LHH	C4-N4	4.36	1.46	1.39
1	A1	1364	OMC	C2-N1	4.36	1.49	1.40
1	A1	1484	5MC	C2-N1	4.36	1.49	1.40
1	A1	1227	4AC	C7-N4	4.36	1.45	1.37
1	A1	238	LHH	C4-N3	4.36	1.40	1.32
27	B1	1178	4AC	C4-N4	4.36	1.46	1.39
27	B1	2557	OMC	C2-N1	4.36	1.49	1.40
1	A1	945	4AC	C4-N4	4.36	1.46	1.39
27	B1	2454	4AC	C4-N4	4.35	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	2607	OMC	C2-N1	4.35	1.49	1.40
1	A1	681	5MC	C6-N1	4.35	1.45	1.38
27	B1	1551	4AC	C4-N4	4.35	1.46	1.39
27	B1	1977	5MC	C6-N1	4.35	1.45	1.38
27	B1	1501	4AC	C4-N4	4.34	1.46	1.39
1	A1	230	5MC	C2-N1	4.34	1.49	1.40
27	B1	2059	OMC	C2-N1	4.34	1.49	1.40
27	B1	1344	5MC	C2-N1	4.34	1.49	1.40
1	A1	636	4AC	C4-N4	4.34	1.46	1.39
28	B2	88	4AC	C4-N4	4.34	1.46	1.39
27	B1	1489	OMC	C2-N1	4.34	1.49	1.40
27	B1	1374	4AC	C4-N4	4.33	1.46	1.39
1	A1	951	5MC	C6-N1	4.33	1.45	1.38
27	B1	3006	4AC	C4-N4	4.33	1.46	1.39
1	A1	1190	5MC	C6-N1	4.33	1.45	1.38
1	A1	1362	5MC	C6-N1	4.33	1.45	1.38
27	B1	2617	5MC	C6-N1	4.33	1.45	1.38
27	B1	1846	4AC	C4-N4	4.33	1.46	1.39
1	A1	816	4AC	C4-N4	4.33	1.46	1.39
1	A1	405	4AC	C4-N4	4.33	1.46	1.39
1	A1	17	5MC	C2-N1	4.33	1.49	1.40
27	B1	1832	OMC	C2-N1	4.33	1.49	1.40
1	A1	546	4AC	C4-N4	4.33	1.46	1.39
1	A1	739	4AC	C4-N4	4.32	1.46	1.39
27	B1	933	4AC	C4-N4	4.32	1.46	1.39
27	B1	652	4AC	C4-N4	4.32	1.46	1.39
27	B1	979	4AC	C4-N4	4.32	1.46	1.39
1	A1	863	5MC	C6-N1	4.32	1.45	1.38
1	A1	1013	5MC	C6-N1	4.32	1.45	1.38
27	B1	1067	4AC	C4-N4	4.32	1.46	1.39
1	A1	220	4AC	C4-N4	4.32	1.46	1.39
1	A1	624	4AC	C4-N4	4.32	1.46	1.39
27	B1	2735	OMC	C2-N1	4.31	1.49	1.40
1	A1	117	OMC	C2-N1	4.31	1.49	1.40
1	A1	1270	OMC	C2-N1	4.31	1.49	1.40
1	A1	5	4AC	C4-N4	4.31	1.46	1.39
27	B1	1383	4AC	C4-N4	4.31	1.46	1.39
1	A1	17	5MC	C6-N1	4.31	1.45	1.38
1	A1	578	4AC	C4-N4	4.31	1.46	1.39
1	A1	706	4AC	C4-N4	4.31	1.46	1.39
27	B1	19	4AC	C4-N4	4.31	1.46	1.39
27	B1	501	OMC	C2-N1	4.31	1.49	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	2808	OMC	C2-N1	4.31	1.49	1.40
27	B1	227	4AC	C4-N4	4.31	1.46	1.39
1	A1	1314	4AC	C4-N4	4.30	1.46	1.39
1	A1	87	4AC	C4-N4	4.30	1.46	1.39
27	B1	1579	4AC	C4-N4	4.30	1.46	1.39
1	A1	1194	OMC	C2-N1	4.30	1.49	1.40
27	B1	1099	OMC	C2-N1	4.30	1.49	1.40
27	B1	1608	4AC	C4-N4	4.30	1.46	1.39
27	B1	2113	4AC	C4-N4	4.30	1.46	1.39
27	B1	2008	4AC	C4-N4	4.30	1.46	1.39
1	A1	1029	4AC	C4-N4	4.29	1.46	1.39
27	B1	1290	4AC	C4-N4	4.29	1.46	1.39
27	B1	2432	4AC	C4-N4	4.29	1.46	1.39
1	A1	230	5MC	C6-N1	4.29	1.45	1.38
27	B1	2171	4AC	C4-N4	4.29	1.46	1.39
27	B1	3020	4AC	C4-N4	4.29	1.46	1.39
27	B1	2119	OMC	C2-N1	4.29	1.49	1.40
1	A1	141	4AC	C4-N4	4.29	1.46	1.39
27	B1	344	4AC	C4-N4	4.29	1.46	1.39
27	B1	2821	4AC	C4-N4	4.29	1.46	1.39
27	B1	715	4AC	C4-N4	4.29	1.46	1.39
1	A1	761	4AC	C4-N4	4.29	1.46	1.39
1	A1	1028	OMC	C2-N1	4.29	1.49	1.40
1	A1	41	4AC	C4-N4	4.29	1.46	1.39
1	A1	274	4AC	C4-N4	4.29	1.46	1.39
1	A1	681	5MC	C2-N1	4.29	1.49	1.40
27	B1	1107	4AC	C4-N4	4.29	1.46	1.39
27	B1	1264	4AC	C4-N4	4.29	1.46	1.39
28	B2	115	4AC	C4-N4	4.29	1.46	1.39
27	B1	2526	4AC	C4-N4	4.29	1.46	1.39
1	A1	1484	5MC	C6-N1	4.29	1.45	1.38
27	B1	580	4AC	C4-N4	4.29	1.46	1.39
27	B1	378	4AC	C4-N4	4.28	1.45	1.39
27	B1	23	4AC	C4-N4	4.28	1.45	1.39
27	B1	1435	4AC	C4-N4	4.28	1.45	1.39
1	A1	499	4AC	C4-N4	4.28	1.45	1.39
27	B1	98	4AC	C4-N4	4.28	1.45	1.39
27	B1	360	4AC	C4-N4	4.28	1.45	1.39
27	B1	479	4AC	C4-N4	4.28	1.45	1.39
1	A1	216	4AC	C4-N4	4.28	1.45	1.39
1	A1	382	4AC	C4-N4	4.28	1.45	1.39
27	B1	1818	4AC	C4-N4	4.28	1.45	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B2	30	4AC	C4-N4	4.28	1.45	1.39
27	B1	3037	4AC	C4-N4	4.27	1.45	1.39
27	B1	2492	4AC	C4-N4	4.27	1.45	1.39
27	B1	200	4AC	C4-N4	4.27	1.45	1.39
27	B1	130	4AC	C4-N4	4.27	1.45	1.39
27	B1	1946	4AC	C4-N4	4.27	1.45	1.39
27	B1	502	LHH	C4-N3	4.27	1.40	1.32
1	A1	839	4AC	C4-N4	4.27	1.45	1.39
27	B1	485	4AC	C4-N4	4.27	1.45	1.39
27	B1	2844	4AC	C4-N4	4.27	1.45	1.39
27	B1	1345	4AC	C4-N4	4.27	1.45	1.39
27	B1	2821	4AC	C2-N1	4.27	1.49	1.40
27	B1	2213	4AC	C4-N4	4.27	1.45	1.39
1	A1	540	4AC	C4-N4	4.26	1.45	1.39
27	B1	479	4AC	C2-N1	4.26	1.49	1.40
27	B1	336	5MC	C6-N1	4.26	1.45	1.38
1	A1	827	4AC	C4-N4	4.26	1.45	1.39
27	B1	1150	4AC	C4-N4	4.26	1.45	1.39
27	B1	1052	4AC	C4-N4	4.26	1.45	1.39
27	B1	732	4AC	C4-N4	4.26	1.45	1.39
27	B1	2020	4AC	C4-N4	4.26	1.45	1.39
1	A1	1254	4AC	C4-N4	4.26	1.45	1.39
27	B1	786	4AC	C4-N4	4.26	1.45	1.39
27	B1	2850	4AC	C4-N4	4.26	1.45	1.39
1	A1	624	4AC	C2-N1	4.26	1.49	1.40
27	B1	3011	4AC	C4-N4	4.26	1.45	1.39
27	B1	721	4AC	C4-N4	4.26	1.45	1.39
27	B1	2469	4AC	C4-N4	4.26	1.45	1.39
27	B1	419	4AC	C4-N4	4.26	1.45	1.39
27	B1	527	4AC	C4-N4	4.26	1.45	1.39
27	B1	1822	4AC	C4-N4	4.26	1.45	1.39
27	B1	337	4AC	C4-N4	4.25	1.45	1.39
27	B1	1546	4AC	C4-N4	4.25	1.45	1.39
1	A1	231	4AC	C4-N4	4.25	1.45	1.39
27	B1	950	4AC	C4-N4	4.25	1.45	1.39
27	B1	162	4AC	C4-N4	4.25	1.45	1.39
1	A1	719	4AC	C4-N4	4.25	1.45	1.39
27	B1	1064	4AC	C4-N4	4.25	1.45	1.39
27	B1	1743	4AC	C4-N4	4.25	1.45	1.39
27	B1	1061	4AC	C4-N4	4.25	1.45	1.39
27	B1	80	4AC	C4-N4	4.25	1.45	1.39
27	B1	1885	4AC	C4-N4	4.25	1.45	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	1344	5MC	C6-N1	4.24	1.45	1.38
27	B1	1706	4AC	C4-N4	4.24	1.45	1.39
1	A1	307	4AC	C4-N4	4.24	1.45	1.39
27	B1	1967	4AC	C4-N4	4.24	1.45	1.39
27	B1	2602	4AC	C4-N4	4.24	1.45	1.39
1	A1	836	4AC	C4-N4	4.23	1.45	1.39
27	B1	2968	4AC	C4-N4	4.23	1.45	1.39
27	B1	1762	4AC	C4-N4	4.23	1.45	1.39
27	B1	2876	4AC	C4-N4	4.23	1.45	1.39
1	A1	691	4AC	C4-N4	4.23	1.45	1.39
27	B1	1649	4AC	C4-N4	4.23	1.45	1.39
1	A1	534	4AC	C4-N4	4.23	1.45	1.39
27	B1	2379	4AC	C4-N4	4.23	1.45	1.39
27	B1	2749	4AC	C4-N4	4.23	1.45	1.39
27	B1	1911	4AC	C4-N4	4.22	1.45	1.39
1	A1	856	4AC	C4-N4	4.22	1.45	1.39
27	B1	1751	4AC	C4-N4	4.22	1.45	1.39
27	B1	688	4AC	C4-N4	4.22	1.45	1.39
1	A1	141	4AC	C2-N1	4.22	1.49	1.40
27	B1	1100	4AC	C4-N4	4.22	1.45	1.39
27	B1	953	4AC	C4-N4	4.22	1.45	1.39
27	B1	1639	4AC	C4-N4	4.22	1.45	1.39
27	B1	1439	LHH	C4-N3	4.21	1.40	1.32
27	B1	1505	4AC	C4-N4	4.21	1.45	1.39
27	B1	1769	4AC	C4-N4	4.21	1.45	1.39
27	B1	2133	4AC	C4-N4	4.21	1.45	1.39
1	A1	216	4AC	C5-C4	4.21	1.49	1.40
1	A1	367	4AC	C4-N4	4.20	1.45	1.39
27	B1	434	4AC	C4-N4	4.20	1.45	1.39
27	B1	2429	4AC	C4-N4	4.20	1.45	1.39
1	A1	756	4SU	C4-S4	-4.20	1.60	1.68
1	A1	834	OMC	C2-N1	4.20	1.49	1.40
27	B1	116	4AC	C4-N4	4.20	1.45	1.39
27	B1	243	4AC	C4-N4	4.20	1.45	1.39
1	A1	1165	OMU	C4-N3	4.20	1.46	1.38
1	A1	1226	OMC	C2-N1	4.20	1.49	1.40
27	B1	2792	4AC	C4-N4	4.20	1.45	1.39
1	A1	739	4AC	C2-N1	4.20	1.49	1.40
27	B1	1293	4AC	C2-N1	4.19	1.49	1.40
27	B1	896	4AC	C4-N4	4.19	1.45	1.39
1	A1	52	OMU	C4-N3	4.19	1.46	1.38
27	B1	1822	4AC	C2-N1	4.19	1.49	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	1374	4AC	C2-N1	4.19	1.49	1.40
1	A1	1181	4AC	C4-N4	4.19	1.45	1.39
1	A1	141	4AC	C5-C4	4.19	1.49	1.40
27	B1	1822	4AC	C5-C4	4.19	1.49	1.40
27	B1	2809	4AC	C4-N4	4.19	1.45	1.39
1	A1	691	4AC	C2-N1	4.18	1.49	1.40
27	B1	1442	4AC	C4-N4	4.18	1.45	1.39
1	A1	762	OMU	C4-N3	4.18	1.46	1.38
27	B1	1478	4AC	C4-N4	4.18	1.45	1.39
1	A1	945	4AC	C2-N1	4.18	1.49	1.40
1	A1	1254	4AC	C2-N1	4.18	1.49	1.40
1	A1	614	4AC	C4-N4	4.17	1.45	1.39
27	B1	2454	4AC	C2-N1	4.17	1.49	1.40
1	A1	466	5MC	C6-N1	4.17	1.45	1.38
27	B1	866	4AC	C4-N4	4.17	1.45	1.39
27	B1	1128	4AC	C4-N4	4.17	1.45	1.39
27	B1	1743	4AC	C2-N1	4.16	1.49	1.40
1	A1	481	G7M	C4-N3	4.16	1.47	1.37
1	A1	291	4AC	C4-N4	4.16	1.45	1.39
1	A1	1467	4AC	C5-C4	4.16	1.49	1.40
27	B1	1579	4AC	C2-N1	4.16	1.49	1.40
27	B1	2554	OMU	C4-N3	4.16	1.46	1.38
27	B1	344	4AC	C5-C4	4.16	1.49	1.40
1	A1	216	4AC	C2-N1	4.15	1.49	1.40
27	B1	227	4AC	C2-N1	4.15	1.49	1.40
27	B1	1505	4AC	C5-C4	4.15	1.49	1.40
27	B1	1846	4AC	C2-N1	4.15	1.49	1.40
27	B1	1061	4AC	C5-C4	4.15	1.49	1.40
27	B1	1150	4AC	C2-N1	4.15	1.49	1.40
27	B1	1501	4AC	C2-N1	4.15	1.49	1.40
1	A1	87	4AC	C2-N1	4.14	1.49	1.40
27	B1	1608	4AC	C2-N1	4.14	1.49	1.40
27	B1	1052	4AC	C2-N1	4.14	1.49	1.40
27	B1	1478	4AC	C5-C4	4.14	1.49	1.40
27	B1	3037	4AC	C2-N1	4.14	1.49	1.40
27	B1	1649	4AC	C5-C4	4.14	1.49	1.40
27	B1	2821	4AC	C5-C4	4.14	1.49	1.40
27	B1	337	4AC	C5-C4	4.14	1.49	1.40
1	A1	739	4AC	C5-C4	4.14	1.49	1.40
27	B1	1751	4AC	C2-N1	4.13	1.49	1.40
1	A1	546	4AC	C5-C4	4.13	1.49	1.40
27	B1	1100	4AC	C2-N1	4.13	1.49	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	1314	4AC	C5-C4	4.13	1.49	1.40
27	B1	926	OMU	C4-N3	4.13	1.46	1.38
27	B1	1360	4AC	C5-C4	4.13	1.49	1.40
27	B1	688	4AC	C2-N1	4.13	1.49	1.40
28	B2	115	4AC	C2-N1	4.13	1.49	1.40
27	B1	344	4AC	C2-N1	4.13	1.48	1.40
27	B1	1579	4AC	C5-C4	4.13	1.49	1.40
27	B1	2565	4SU	C4-S4	-4.13	1.60	1.68
1	A1	231	4AC	C2-N1	4.13	1.48	1.40
27	B1	454	OMU	C4-N3	4.13	1.46	1.38
27	B1	98	4AC	C5-C4	4.13	1.49	1.40
27	B1	652	4AC	C5-C4	4.13	1.49	1.40
27	B1	1885	4AC	C5-C4	4.13	1.49	1.40
27	B1	786	4AC	C5-C4	4.12	1.49	1.40
27	B1	2379	4AC	C5-C4	4.12	1.49	1.40
1	A1	499	4AC	C5-C4	4.12	1.49	1.40
27	B1	933	4AC	C2-N1	4.12	1.48	1.40
1	A1	499	4AC	C2-N1	4.12	1.48	1.40
1	A1	1181	4AC	C2-N1	4.12	1.48	1.40
1	A1	578	4AC	C2-N1	4.12	1.48	1.40
27	B1	3020	4AC	C2-N1	4.12	1.48	1.40
27	B1	162	4AC	C5-C4	4.12	1.49	1.40
1	A1	546	4AC	C2-N1	4.12	1.48	1.40
1	A1	761	4AC	C2-N1	4.12	1.48	1.40
1	A1	706	4AC	C5-C4	4.12	1.49	1.40
27	B1	3011	4AC	C2-N1	4.12	1.48	1.40
27	B1	2602	4AC	C5-C4	4.12	1.49	1.40
27	B1	1100	4AC	C5-C4	4.12	1.49	1.40
27	B1	2429	4AC	C5-C4	4.12	1.49	1.40
1	A1	534	4AC	C2-N1	4.12	1.48	1.40
27	B1	200	4AC	C5-C4	4.11	1.49	1.40
27	B1	527	4AC	C5-C4	4.11	1.49	1.40
1	A1	816	4AC	C2-N1	4.11	1.48	1.40
27	B1	2454	4AC	C5-C4	4.11	1.49	1.40
27	B1	98	4AC	C2-N1	4.11	1.48	1.40
27	B1	896	4AC	C2-N1	4.11	1.48	1.40
27	B1	337	4AC	C2-N1	4.11	1.48	1.40
28	B2	30	4AC	C2-N1	4.11	1.48	1.40
27	B1	80	4AC	C5-C4	4.11	1.49	1.40
1	A1	231	4AC	C5-C4	4.11	1.49	1.40
1	A1	1029	4AC	C5-C4	4.11	1.49	1.40
1	A1	856	4AC	C5-C4	4.11	1.49	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	19	4AC	C2-N1	4.11	1.48	1.40
27	B1	1505	4AC	C2-N1	4.11	1.48	1.40
1	A1	836	4AC	C2-N1	4.11	1.48	1.40
27	B1	1064	4AC	C2-N1	4.11	1.48	1.40
1	A1	1368	OMU	C4-N3	4.10	1.45	1.38
1	A1	1314	4AC	C2-N1	4.10	1.48	1.40
27	B1	2432	4AC	C2-N1	4.10	1.48	1.40
1	A1	827	4AC	C2-N1	4.10	1.48	1.40
27	B1	721	4AC	C5-C4	4.10	1.49	1.40
27	B1	48	4AC	C5-C4	4.10	1.49	1.40
27	B1	1639	4AC	C2-N1	4.10	1.48	1.40
27	B1	732	4AC	C2-N1	4.10	1.48	1.40
27	B1	1488	OMU	C4-N3	4.10	1.45	1.38
27	B1	896	4AC	C5-C4	4.10	1.49	1.40
1	A1	382	4AC	C5-C4	4.10	1.49	1.40
1	A1	5	4AC	C5-C4	4.10	1.49	1.40
27	B1	1128	4AC	C5-C4	4.10	1.49	1.40
1	A1	614	4AC	C2-N1	4.10	1.48	1.40
1	A1	827	4AC	C5-C4	4.10	1.49	1.40
27	B1	580	4AC	C5-C4	4.10	1.49	1.40
27	B1	2749	4AC	C5-C4	4.10	1.49	1.40
27	B1	2876	4AC	C2-N1	4.10	1.48	1.40
27	B1	1769	4AC	C2-N1	4.10	1.48	1.40
27	B1	485	4AC	C5-C4	4.10	1.49	1.40
27	B1	933	4AC	C5-C4	4.10	1.49	1.40
27	B1	2968	4AC	C5-C4	4.10	1.49	1.40
27	B1	48	4AC	C4-N4	4.10	1.45	1.39
27	B1	2020	4AC	C5-C4	4.09	1.49	1.40
27	B1	1061	4AC	C2-N1	4.09	1.48	1.40
27	B1	1264	4AC	C2-N1	4.09	1.48	1.40
27	B1	1639	4AC	C5-C4	4.09	1.49	1.40
27	B1	2876	4AC	C5-C4	4.09	1.49	1.40
1	A1	8	OMU	C4-N3	4.09	1.45	1.38
27	B1	130	4AC	C5-C4	4.09	1.49	1.40
27	B1	1264	4AC	C5-C4	4.09	1.49	1.40
27	B1	1706	4AC	C2-N1	4.09	1.48	1.40
27	B1	434	4AC	C5-C4	4.09	1.49	1.40
27	B1	2492	4AC	C2-N1	4.09	1.48	1.40
27	B1	1442	4AC	C5-C4	4.09	1.49	1.40
28	B2	88	4AC	C2-N1	4.09	1.48	1.40
1	A1	291	4AC	C5-C4	4.09	1.49	1.40
27	B1	2113	4AC	C5-C4	4.09	1.49	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	2492	4AC	C5-C4	4.09	1.49	1.40
27	B1	1649	4AC	C2-N1	4.09	1.48	1.40
27	B1	2133	4AC	C5-C4	4.09	1.49	1.40
1	A1	405	4AC	C2-N1	4.09	1.48	1.40
27	B1	1551	4AC	C5-C4	4.09	1.49	1.40
27	B1	866	4AC	C2-N1	4.09	1.48	1.40
27	B1	162	4AC	C2-N1	4.09	1.48	1.40
1	A1	534	4AC	C5-C4	4.09	1.49	1.40
1	A1	5	4AC	C2-N1	4.09	1.48	1.40
27	B1	1846	4AC	C5-C4	4.09	1.49	1.40
27	B1	2809	4AC	C5-C4	4.09	1.49	1.40
27	B1	866	4AC	C5-C4	4.08	1.49	1.40
27	B1	1911	4AC	C2-N1	4.08	1.48	1.40
27	B1	1383	4AC	C2-N1	4.08	1.48	1.40
1	A1	775	OMU	C4-N3	4.08	1.45	1.38
27	B1	3006	4AC	C2-N1	4.08	1.48	1.40
1	A1	405	4AC	C5-C4	4.08	1.49	1.40
1	A1	836	4AC	C5-C4	4.08	1.49	1.40
27	B1	953	4AC	C5-C4	4.08	1.49	1.40
1	A1	274	4AC	C2-N1	4.08	1.48	1.40
27	B1	378	4AC	C2-N1	4.08	1.48	1.40
1	A1	274	4AC	C5-C4	4.08	1.49	1.40
27	B1	1911	4AC	C5-C4	4.08	1.49	1.40
1	A1	367	4AC	C5-C4	4.08	1.49	1.40
27	B1	1608	4AC	C5-C4	4.08	1.49	1.40
27	B1	419	4AC	C2-N1	4.08	1.48	1.40
27	B1	479	4AC	C5-C4	4.08	1.49	1.40
27	B1	243	4AC	C5-C4	4.08	1.49	1.40
27	B1	2213	4AC	C5-C4	4.08	1.49	1.40
27	B1	2526	4AC	C2-N1	4.08	1.48	1.40
1	A1	945	4AC	C5-C4	4.07	1.49	1.40
27	B1	1345	4AC	C5-C4	4.07	1.49	1.40
1	A1	761	4AC	C5-C4	4.07	1.49	1.40
27	B1	3011	4AC	C5-C4	4.07	1.49	1.40
1	A1	636	4AC	C2-N1	4.07	1.48	1.40
27	B1	2008	4AC	C5-C4	4.07	1.49	1.40
1	A1	220	4AC	C5-C4	4.07	1.49	1.40
27	B1	953	4AC	C2-N1	4.07	1.48	1.40
27	B1	2809	4AC	C2-N1	4.07	1.48	1.40
27	B1	1290	4AC	C5-C4	4.07	1.49	1.40
27	B1	715	4AC	C5-C4	4.07	1.49	1.40
27	B1	1946	4AC	C5-C4	4.07	1.49	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B2	115	4AC	C5-C4	4.07	1.49	1.40
27	B1	2844	4AC	C2-N1	4.07	1.48	1.40
1	A1	41	4AC	C5-C4	4.07	1.49	1.40
1	A1	540	4AC	C5-C4	4.07	1.49	1.40
27	B1	527	4AC	C2-N1	4.07	1.48	1.40
27	B1	434	4AC	C2-N1	4.07	1.48	1.40
27	B1	2432	4AC	C5-C4	4.07	1.49	1.40
27	B1	360	4AC	C5-C4	4.07	1.49	1.40
27	B1	2469	4AC	C2-N1	4.07	1.48	1.40
27	B1	116	4AC	C2-N1	4.06	1.48	1.40
27	B1	227	4AC	C5-C4	4.06	1.49	1.40
27	B1	130	4AC	C2-N1	4.06	1.48	1.40
27	B1	1150	4AC	C5-C4	4.06	1.49	1.40
27	B1	2008	4AC	C2-N1	4.06	1.48	1.40
27	B1	116	4AC	C5-C4	4.06	1.49	1.40
27	B1	1052	4AC	C5-C4	4.06	1.49	1.40
27	B1	2850	4AC	C5-C4	4.06	1.49	1.40
27	B1	1751	4AC	C5-C4	4.06	1.49	1.40
27	B1	1290	4AC	C2-N1	4.06	1.48	1.40
27	B1	688	4AC	C5-C4	4.06	1.49	1.40
27	B1	2526	4AC	C5-C4	4.06	1.49	1.40
27	B1	3037	4AC	C5-C4	4.06	1.49	1.40
27	B1	3020	4AC	C5-C4	4.06	1.49	1.40
28	B2	30	4AC	C5-C4	4.06	1.49	1.40
27	B1	715	4AC	C2-N1	4.06	1.48	1.40
27	B1	1383	4AC	C5-C4	4.06	1.49	1.40
27	B1	2844	4AC	C5-C4	4.06	1.49	1.40
27	B1	1360	4AC	C2-N1	4.05	1.48	1.40
1	A1	816	4AC	C5-C4	4.05	1.49	1.40
27	B1	1374	4AC	C5-C4	4.05	1.49	1.40
27	B1	1546	4AC	C5-C4	4.05	1.49	1.40
27	B1	200	4AC	C2-N1	4.05	1.48	1.40
27	B1	2469	4AC	C5-C4	4.05	1.49	1.40
27	B1	2429	4AC	C2-N1	4.05	1.48	1.40
1	A1	382	4AC	C2-N1	4.05	1.48	1.40
27	B1	2133	4AC	C2-N1	4.05	1.48	1.40
27	B1	1706	4AC	C5-C4	4.05	1.49	1.40
27	B1	1546	4AC	C2-N1	4.05	1.48	1.40
1	A1	624	4AC	C5-C4	4.05	1.49	1.40
1	A1	614	4AC	C5-C4	4.05	1.49	1.40
27	B1	979	4AC	C2-N1	4.05	1.48	1.40
27	B1	786	4AC	C2-N1	4.05	1.48	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B2	88	4AC	C5-C4	4.05	1.49	1.40
27	B1	1551	4AC	C2-N1	4.05	1.48	1.40
1	A1	839	4AC	C5-C4	4.05	1.49	1.40
27	B1	19	4AC	C5-C4	4.05	1.49	1.40
1	A1	467	4AC	C2-N1	4.04	1.48	1.40
27	B1	2968	4AC	C2-N1	4.04	1.48	1.40
27	B1	80	4AC	C2-N1	4.04	1.48	1.40
27	B1	1967	4AC	C5-C4	4.04	1.49	1.40
27	B1	1435	4AC	C5-C4	4.04	1.49	1.40
27	B1	23	4AC	C2-N1	4.04	1.48	1.40
27	B1	1769	4AC	C5-C4	4.04	1.49	1.40
1	A1	307	4AC	C5-C4	4.04	1.49	1.40
27	B1	1762	4AC	C5-C4	4.04	1.49	1.40
1	A1	706	4AC	C2-N1	4.04	1.48	1.40
1	A1	367	4AC	C2-N1	4.04	1.48	1.40
27	B1	360	4AC	C2-N1	4.04	1.48	1.40
27	B1	1762	4AC	C2-N1	4.04	1.48	1.40
1	A1	220	4AC	C2-N1	4.04	1.48	1.40
1	A1	636	4AC	C5-C4	4.04	1.49	1.40
1	A1	839	4AC	C2-N1	4.03	1.48	1.40
27	B1	1178	4AC	C2-N1	4.03	1.48	1.40
27	B1	1064	4AC	C5-C4	4.03	1.49	1.40
27	B1	1501	4AC	C5-C4	4.03	1.49	1.40
1	A1	41	4AC	C2-N1	4.03	1.48	1.40
27	B1	580	4AC	C2-N1	4.03	1.48	1.40
1	A1	719	4AC	C5-C4	4.03	1.49	1.40
27	B1	243	4AC	C2-N1	4.03	1.48	1.40
27	B1	2020	4AC	C2-N1	4.03	1.48	1.40
27	B1	1067	4AC	C5-C4	4.03	1.49	1.40
27	B1	2792	4AC	C5-C4	4.03	1.49	1.40
1	A1	540	4AC	C2-N1	4.02	1.48	1.40
27	B1	2792	4AC	C2-N1	4.02	1.48	1.40
27	B1	1743	4AC	C5-C4	4.02	1.49	1.40
27	B1	1967	4AC	C2-N1	4.02	1.48	1.40
1	A1	87	4AC	C5-C4	4.02	1.49	1.40
1	A1	1227	4AC	C5-C4	4.02	1.49	1.40
1	A1	719	4AC	C2-N1	4.02	1.48	1.40
1	A1	238	LHH	C4-N4	4.02	1.45	1.39
1	A1	1254	4AC	C5-C4	4.02	1.49	1.40
27	B1	732	4AC	C5-C4	4.02	1.49	1.40
27	B1	1067	4AC	C2-N1	4.02	1.48	1.40
27	B1	23	4AC	C5-C4	4.02	1.49	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	2749	4AC	C2-N1	4.02	1.48	1.40
1	A1	578	4AC	C5-C4	4.02	1.49	1.40
27	B1	378	4AC	C5-C4	4.01	1.49	1.40
1	A1	307	4AC	C2-N1	4.01	1.48	1.40
27	B1	3006	4AC	C5-C4	4.01	1.49	1.40
27	B1	2850	4AC	C2-N1	4.01	1.48	1.40
27	B1	2213	4AC	C2-N1	4.01	1.48	1.40
1	A1	291	4AC	C2-N1	4.01	1.48	1.40
27	B1	2113	4AC	C2-N1	4.01	1.48	1.40
27	B1	2602	4AC	C2-N1	4.01	1.48	1.40
27	B1	652	4AC	C2-N1	4.01	1.48	1.40
27	B1	1178	4AC	C5-C4	4.01	1.49	1.40
27	B1	419	4AC	C5-C4	4.01	1.49	1.40
27	B1	1818	4AC	C2-N1	4.01	1.48	1.40
1	A1	1467	4AC	C2-N1	4.00	1.48	1.40
27	B1	48	4AC	C2-N1	4.00	1.48	1.40
27	B1	2171	4AC	C5-C4	4.00	1.49	1.40
1	A1	691	4AC	C5-C4	4.00	1.49	1.40
27	B1	1107	4AC	C5-C4	4.00	1.49	1.40
27	B1	721	4AC	C2-N1	4.00	1.48	1.40
27	B1	950	4AC	C5-C4	4.00	1.49	1.40
27	B1	1128	4AC	C2-N1	4.00	1.48	1.40
27	B1	1345	4AC	C2-N1	4.00	1.48	1.40
27	B1	1478	4AC	C2-N1	4.00	1.48	1.40
1	A1	1029	4AC	C2-N1	3.99	1.48	1.40
27	B1	979	4AC	C5-C4	3.99	1.49	1.40
1	A1	1181	4AC	C5-C4	3.99	1.49	1.40
27	B1	1818	4AC	C5-C4	3.99	1.49	1.40
27	B1	1107	4AC	C2-N1	3.98	1.48	1.40
1	A1	856	4AC	C2-N1	3.98	1.48	1.40
27	B1	1442	4AC	C2-N1	3.98	1.48	1.40
27	B1	1885	4AC	C2-N1	3.98	1.48	1.40
27	B1	2171	4AC	C2-N1	3.98	1.48	1.40
27	B1	1293	4AC	C5-C4	3.97	1.49	1.40
27	B1	950	4AC	C2-N1	3.97	1.48	1.40
27	B1	1435	4AC	C2-N1	3.97	1.48	1.40
1	A1	1227	4AC	C4-N4	3.96	1.45	1.39
27	B1	485	4AC	C2-N1	3.95	1.48	1.40
27	B1	2607	OMC	C4-N4	3.95	1.43	1.33
27	B1	2757	OMG	C6-N1	3.94	1.43	1.37
1	A1	1227	4AC	C2-N1	3.93	1.48	1.40
1	A1	1364	OMC	C4-N4	3.93	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	2735	OMC	C4-N4	3.92	1.43	1.33
1	A1	467	4AC	C4-N4	3.92	1.45	1.39
27	B1	1832	OMC	C4-N4	3.92	1.43	1.33
1	A1	1371	OMC	C4-N4	3.91	1.43	1.33
27	B1	2379	4AC	C2-N1	3.91	1.48	1.40
1	A1	467	4AC	C5-C4	3.91	1.49	1.40
27	B1	2022	OMG	C6-N1	3.90	1.43	1.37
1	A1	329	OMG	C6-N1	3.90	1.43	1.37
1	A1	834	OMC	C4-N4	3.89	1.43	1.33
1	A1	1270	OMC	C4-N4	3.89	1.43	1.33
27	B1	2557	OMC	C4-N4	3.89	1.43	1.33
1	A1	117	OMC	C4-N4	3.88	1.43	1.33
1	A1	1003	OMG	C6-N1	3.87	1.43	1.37
27	B1	2108	OMG	C6-N1	3.87	1.43	1.37
1	A1	1028	OMC	C4-N4	3.87	1.43	1.33
1	A1	455	OMG	C6-N1	3.87	1.43	1.37
1	A1	507	OMG	C6-N1	3.87	1.43	1.37
27	B1	2808	OMC	C4-N4	3.86	1.43	1.33
27	B1	2059	OMC	C4-N4	3.86	1.43	1.33
1	A1	1194	OMC	C4-N4	3.86	1.43	1.33
1	A1	1115	OMG	C6-N1	3.86	1.43	1.37
27	B1	1946	4AC	C2-N1	3.86	1.48	1.40
27	B1	1099	OMC	C4-N4	3.85	1.43	1.33
27	B1	501	OMC	C4-N4	3.84	1.43	1.33
27	B1	1489	OMC	C4-N4	3.84	1.43	1.33
27	B1	2119	OMC	C4-N4	3.84	1.42	1.33
27	B1	1914	OMC	C4-N4	3.82	1.42	1.33
1	A1	481	G7M	C2-N1	3.81	1.47	1.37
27	B1	1965	OMG	C6-N1	3.81	1.43	1.37
27	B1	214	OMG	C6-N1	3.80	1.43	1.37
1	A1	1226	OMC	C4-N4	3.80	1.42	1.33
27	B1	2684	OMG	C6-N1	3.80	1.43	1.37
27	B1	2984	OMG	C6-N1	3.78	1.43	1.37
27	B1	2562	OMG	C6-N1	3.77	1.43	1.37
27	B1	2028	OMG	C6-N1	3.77	1.43	1.37
27	B1	808	OMG	C6-N1	3.76	1.43	1.37
27	B1	887	OMG	C6-N1	3.75	1.43	1.37
27	B1	856	OMG	C6-N1	3.74	1.43	1.37
27	B1	1557	OMG	C6-N1	3.74	1.43	1.37
1	A1	668	OMG	C6-N1	3.73	1.43	1.37
1	A1	1366	A1I59	C6-C5	3.73	1.40	1.34
27	B1	2180	OMG	C6-N1	3.72	1.43	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	530	OMG	C6-N1	3.72	1.43	1.37
1	A1	541	OMG	C6-N1	3.72	1.43	1.37
1	A1	459	OMG	C6-N1	3.71	1.43	1.37
27	B1	2391	OMG	C6-N1	3.70	1.43	1.37
27	B1	2540	OMG	C6-N1	3.69	1.43	1.37
1	A1	861	OMG	C6-N1	3.69	1.43	1.37
27	B1	920	OMG	C6-N1	3.69	1.43	1.37
27	B1	1904	OMG	C6-N1	3.68	1.43	1.37
27	B1	841	OMG	C6-N1	3.67	1.43	1.37
27	B1	921	OMG	C6-N1	3.66	1.43	1.37
27	B1	2365	OMG	C6-N1	3.65	1.43	1.37
27	B1	55	OMG	C6-N1	3.62	1.43	1.37
1	A1	645	OMG	C6-N1	3.57	1.43	1.37
1	A1	1371	OMC	C6-N1	3.49	1.46	1.38
1	A1	1364	OMC	C6-N1	3.48	1.46	1.38
1	A1	1194	OMC	C6-N1	3.46	1.46	1.38
27	B1	2557	OMC	C6-N1	3.46	1.46	1.38
1	A1	1270	OMC	C6-N1	3.45	1.46	1.38
1	A1	1028	OMC	C6-N1	3.45	1.46	1.38
27	B1	2607	OMC	C6-N1	3.44	1.46	1.38
27	B1	1832	OMC	C6-N1	3.44	1.46	1.38
27	B1	2735	OMC	C6-N1	3.43	1.46	1.38
27	B1	2119	OMC	C6-N1	3.42	1.46	1.38
27	B1	1914	OMC	C6-N1	3.42	1.46	1.38
27	B1	2059	OMC	C6-N1	3.42	1.46	1.38
27	B1	2808	OMC	C6-N1	3.42	1.46	1.38
1	A1	834	OMC	C6-N1	3.40	1.46	1.38
1	A1	117	OMC	C6-N1	3.40	1.46	1.38
27	B1	501	OMC	C6-N1	3.39	1.46	1.38
27	B1	1099	OMC	C6-N1	3.39	1.46	1.38
27	B1	1489	OMC	C6-N1	3.37	1.46	1.38
1	A1	1366	A1I59	C2-N1	-3.34	1.32	1.40
1	A1	1226	OMC	C6-N1	3.32	1.46	1.38
27	B1	1946	4AC	C6-N1	3.29	1.45	1.38
28	B2	115	4AC	C6-N1	3.28	1.45	1.38
27	B1	1478	4AC	C6-N1	3.27	1.45	1.38
1	A1	546	4AC	C6-N1	3.25	1.45	1.38
1	A1	706	4AC	C6-N1	3.25	1.45	1.38
27	B1	485	4AC	C6-N1	3.25	1.45	1.38
27	B1	1551	4AC	C6-N1	3.24	1.45	1.38
1	A1	739	4AC	C6-N1	3.23	1.45	1.38
1	A1	1314	4AC	C6-N1	3.23	1.45	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	1061	4AC	C6-N1	3.23	1.45	1.38
27	B1	479	4AC	C6-N1	3.23	1.45	1.38
27	B1	2020	4AC	C6-N1	3.23	1.45	1.38
27	B1	2821	4AC	C6-N1	3.23	1.45	1.38
27	B1	200	4AC	C6-N1	3.23	1.45	1.38
27	B1	1822	4AC	C6-N1	3.22	1.45	1.38
27	B1	2008	4AC	C6-N1	3.22	1.45	1.38
27	B1	227	4AC	C6-N1	3.22	1.45	1.38
27	B1	2171	4AC	C6-N1	3.22	1.45	1.38
27	B1	344	4AC	C6-N1	3.22	1.45	1.38
27	B1	1967	4AC	C6-N1	3.22	1.45	1.38
27	B1	2809	4AC	C6-N1	3.22	1.45	1.38
1	A1	1029	4AC	C6-N1	3.22	1.45	1.38
27	B1	116	4AC	C6-N1	3.22	1.45	1.38
27	B1	2602	4AC	C6-N1	3.21	1.45	1.38
27	B1	130	4AC	C6-N1	3.21	1.45	1.38
27	B1	2492	4AC	C6-N1	3.21	1.45	1.38
27	B1	1264	4AC	C6-N1	3.21	1.45	1.38
27	B1	1290	4AC	C6-N1	3.21	1.45	1.38
27	B1	1383	4AC	C6-N1	3.21	1.45	1.38
27	B1	580	4AC	C6-N1	3.21	1.45	1.38
27	B1	434	4AC	C6-N1	3.21	1.45	1.38
27	B1	243	4AC	C6-N1	3.21	1.45	1.38
1	A1	839	4AC	C6-N1	3.21	1.45	1.38
27	B1	1128	4AC	C6-N1	3.20	1.45	1.38
27	B1	1846	4AC	C6-N1	3.20	1.45	1.38
27	B1	1546	4AC	C6-N1	3.20	1.45	1.38
27	B1	2133	4AC	C6-N1	3.20	1.45	1.38
1	A1	5	4AC	C6-N1	3.20	1.45	1.38
27	B1	1442	4AC	C6-N1	3.20	1.45	1.38
27	B1	715	4AC	C6-N1	3.20	1.45	1.38
27	B1	2429	4AC	C6-N1	3.20	1.45	1.38
27	B1	2526	4AC	C6-N1	3.20	1.45	1.38
1	A1	856	4AC	C6-N1	3.20	1.45	1.38
27	B1	786	4AC	C6-N1	3.20	1.45	1.38
1	A1	499	4AC	C6-N1	3.20	1.45	1.38
27	B1	721	4AC	C6-N1	3.20	1.45	1.38
27	B1	2968	4AC	C6-N1	3.20	1.45	1.38
27	B1	1374	4AC	C6-N1	3.20	1.45	1.38
27	B1	1911	4AC	C6-N1	3.20	1.45	1.38
27	B1	2876	4AC	C6-N1	3.20	1.45	1.38
1	A1	1254	4AC	C6-N1	3.19	1.45	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	836	4AC	C6-N1	3.19	1.45	1.38
27	B1	98	4AC	C6-N1	3.19	1.45	1.38
27	B1	1107	4AC	C6-N1	3.19	1.45	1.38
1	A1	41	4AC	C6-N1	3.19	1.45	1.38
27	B1	1360	4AC	C6-N1	3.19	1.45	1.38
1	A1	382	4AC	C6-N1	3.19	1.45	1.38
1	A1	274	4AC	C6-N1	3.19	1.45	1.38
27	B1	48	4AC	C6-N1	3.19	1.45	1.38
27	B1	337	4AC	C6-N1	3.19	1.45	1.38
27	B1	1505	4AC	C6-N1	3.19	1.45	1.38
27	B1	2454	4AC	C6-N1	3.19	1.45	1.38
27	B1	1067	4AC	C6-N1	3.19	1.45	1.38
27	B1	2379	4AC	C6-N1	3.19	1.45	1.38
1	A1	578	4AC	C6-N1	3.19	1.45	1.38
1	A1	636	4AC	C6-N1	3.19	1.45	1.38
1	A1	761	4AC	C6-N1	3.19	1.45	1.38
27	B1	162	4AC	C6-N1	3.19	1.45	1.38
27	B1	1100	4AC	C6-N1	3.19	1.45	1.38
1	A1	220	4AC	C6-N1	3.19	1.45	1.38
27	B1	1706	4AC	C6-N1	3.19	1.45	1.38
1	A1	405	4AC	C6-N1	3.19	1.45	1.38
27	B1	732	4AC	C6-N1	3.19	1.45	1.38
27	B1	1293	4AC	C6-N1	3.19	1.45	1.38
1	A1	141	4AC	C6-N1	3.18	1.45	1.38
27	B1	652	4AC	C6-N1	3.18	1.45	1.38
27	B1	527	4AC	C6-N1	3.18	1.45	1.38
27	B1	2850	4AC	C6-N1	3.18	1.45	1.38
1	A1	291	4AC	C6-N1	3.18	1.45	1.38
1	A1	1467	4AC	C6-N1	3.18	1.45	1.38
27	B1	23	4AC	C6-N1	3.18	1.45	1.38
27	B1	378	4AC	C6-N1	3.18	1.45	1.38
27	B1	2749	4AC	C6-N1	3.18	1.45	1.38
27	B1	1052	4AC	C6-N1	3.18	1.45	1.38
27	B1	2757	OMG	C5-C6	3.18	1.53	1.47
1	A1	1181	4AC	C6-N1	3.18	1.45	1.38
27	B1	688	4AC	C6-N1	3.17	1.45	1.38
27	B1	2113	4AC	C6-N1	3.17	1.45	1.38
27	B1	2700	UR3	O4-C4	-3.17	1.16	1.23
1	A1	329	OMG	C5-C6	3.17	1.53	1.47
1	A1	534	4AC	C6-N1	3.17	1.45	1.38
1	A1	816	4AC	C6-N1	3.17	1.45	1.38
27	B1	953	4AC	C6-N1	3.17	1.45	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	216	4AC	C6-N1	3.17	1.45	1.38
1	A1	819	A2M	C6-N6	3.17	1.45	1.34
1	A1	540	4AC	C6-N1	3.17	1.45	1.38
1	A1	367	4AC	C6-N1	3.17	1.45	1.38
27	B1	1769	4AC	C6-N1	3.17	1.45	1.38
27	B1	1751	4AC	C6-N1	3.17	1.45	1.38
27	B1	1639	4AC	C6-N1	3.16	1.45	1.38
27	B1	1885	4AC	C6-N1	3.16	1.45	1.38
27	B1	2432	4AC	C6-N1	3.16	1.45	1.38
27	B1	866	4AC	C6-N1	3.16	1.45	1.38
27	B1	1178	4AC	C6-N1	3.16	1.45	1.38
27	B1	1649	4AC	C6-N1	3.16	1.45	1.38
27	B1	896	4AC	C6-N1	3.16	1.45	1.38
27	B1	80	4AC	C6-N1	3.16	1.45	1.38
27	B1	1579	4AC	C6-N1	3.16	1.45	1.38
1	A1	231	4AC	C6-N1	3.16	1.45	1.38
27	B1	1818	4AC	C6-N1	3.16	1.45	1.38
1	A1	87	4AC	C6-N1	3.16	1.45	1.38
27	B1	1608	4AC	C6-N1	3.16	1.45	1.38
27	B1	2792	4AC	C6-N1	3.16	1.45	1.38
27	B1	1064	4AC	C6-N1	3.16	1.45	1.38
27	B1	933	4AC	C6-N1	3.15	1.45	1.38
1	A1	719	4AC	C6-N1	3.15	1.45	1.38
27	B1	857	A2M	C6-N6	3.15	1.45	1.34
27	B1	1762	4AC	C6-N1	3.15	1.45	1.38
27	B1	360	4AC	C6-N1	3.15	1.45	1.38
27	B1	1345	4AC	C6-N1	3.15	1.45	1.38
1	A1	1227	4AC	C6-N1	3.15	1.45	1.38
27	B1	2213	4AC	C6-N1	3.15	1.45	1.38
27	B1	950	4AC	C6-N1	3.14	1.45	1.38
27	B1	940	A2M	C6-N6	3.14	1.45	1.34
27	B1	506	A2M	C6-N6	3.14	1.45	1.34
27	B1	214	OMG	C5-C6	3.14	1.53	1.47
1	A1	307	4AC	C6-N1	3.14	1.45	1.38
1	A1	1003	OMG	C5-C6	3.14	1.53	1.47
27	B1	19	4AC	C6-N1	3.14	1.45	1.38
27	B1	1435	4AC	C6-N1	3.14	1.45	1.38
1	A1	945	4AC	C6-N1	3.14	1.45	1.38
27	B1	2469	4AC	C6-N1	3.14	1.45	1.38
27	B1	3011	4AC	C6-N1	3.14	1.45	1.38
1	A1	827	4AC	C6-N1	3.13	1.45	1.38
27	B1	3037	4AC	C6-N1	3.13	1.45	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	3006	4AC	C6-N1	3.13	1.45	1.38
27	B1	2562	OMG	C5-C6	3.13	1.53	1.47
27	B1	3020	4AC	C6-N1	3.12	1.45	1.38
1	A1	1115	OMG	C5-C6	3.12	1.53	1.47
27	B1	880	A2M	C6-N6	3.12	1.45	1.34
1	A1	614	4AC	C6-N1	3.12	1.45	1.38
27	B1	2506	A2M	C6-N6	3.12	1.45	1.34
27	B1	2180	OMG	C5-C6	3.12	1.53	1.47
27	B1	2844	4AC	C6-N1	3.12	1.45	1.38
27	B1	1743	4AC	C6-N1	3.12	1.45	1.38
28	B2	30	4AC	C6-N1	3.12	1.45	1.38
27	B1	856	OMG	C5-C6	3.12	1.53	1.47
27	B1	419	4AC	C6-N1	3.11	1.45	1.38
27	B1	1501	4AC	C6-N1	3.11	1.45	1.38
28	B2	88	4AC	C6-N1	3.11	1.45	1.38
27	B1	2022	OMG	C5-C6	3.11	1.53	1.47
27	B1	920	OMG	C5-C6	3.10	1.53	1.47
27	B1	979	4AC	C6-N1	3.10	1.45	1.38
1	A1	467	4AC	C6-N1	3.10	1.45	1.38
27	B1	1150	4AC	C6-N1	3.09	1.45	1.38
27	B1	2108	OMG	C5-C6	3.09	1.53	1.47
27	B1	1557	OMG	C5-C6	3.09	1.53	1.47
1	A1	668	OMG	C5-C6	3.08	1.53	1.47
1	A1	645	OMG	C5-C6	3.08	1.53	1.47
1	A1	624	4AC	C6-N1	3.08	1.45	1.38
27	B1	530	OMG	C5-C6	3.08	1.53	1.47
27	B1	808	OMG	C5-C6	3.08	1.53	1.47
27	B1	2028	OMG	C5-C6	3.08	1.53	1.47
27	B1	2365	OMG	C5-C6	3.08	1.53	1.47
1	A1	455	OMG	C5-C6	3.07	1.53	1.47
1	A1	691	4AC	C6-N1	3.07	1.45	1.38
1	A1	507	OMG	C5-C6	3.07	1.53	1.47
27	B1	1965	OMG	C5-C6	3.07	1.53	1.47
27	B1	887	OMG	C5-C6	3.06	1.53	1.47
27	B1	2684	OMG	C5-C6	3.06	1.53	1.47
1	A1	541	OMG	C5-C6	3.05	1.53	1.47
27	B1	2540	OMG	C5-C6	3.04	1.53	1.47
1	A1	459	OMG	C5-C6	3.02	1.53	1.47
27	B1	940	A2M	O3'-C3'	-3.02	1.35	1.43
27	B1	55	OMG	C5-C6	3.01	1.53	1.47
27	B1	841	OMG	C5-C6	3.01	1.53	1.47
27	B1	454	OMU	C6-N1	3.01	1.45	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	2984	OMG	C5-C6	3.00	1.53	1.47
27	B1	2506	A2M	O3'-C3'	-3.00	1.35	1.43
27	B1	921	OMG	C5-C6	3.00	1.53	1.47
27	B1	2391	OMG	C5-C6	2.99	1.53	1.47
1	A1	8	OMU	C6-N1	2.98	1.45	1.38
1	A1	775	OMU	C6-N1	2.97	1.45	1.38
27	B1	1488	OMU	C6-N1	2.97	1.45	1.38
1	A1	861	OMG	C5-C6	2.97	1.53	1.47
27	B1	1904	OMG	C5-C6	2.96	1.53	1.47
1	A1	52	OMU	C6-N1	2.96	1.45	1.38
1	A1	762	OMU	C6-N1	2.94	1.45	1.38
27	B1	926	OMU	C6-N1	2.94	1.45	1.38
1	A1	819	A2M	O3'-C3'	-2.94	1.36	1.43
27	B1	2087	5MC	CM5-C5	2.93	1.57	1.50
27	B1	880	A2M	O3'-C3'	-2.93	1.36	1.43
1	A1	681	5MC	CM5-C5	2.92	1.57	1.50
27	B1	2554	OMU	C6-N1	2.92	1.45	1.38
1	A1	951	5MC	CM5-C5	2.92	1.57	1.50
1	A1	687	5MC	CM5-C5	2.92	1.57	1.50
1	A1	1165	OMU	C6-N1	2.92	1.45	1.38
1	A1	1190	5MC	CM5-C5	2.92	1.57	1.50
1	A1	17	5MC	CM5-C5	2.91	1.57	1.50
27	B1	1344	5MC	CM5-C5	2.91	1.57	1.50
1	A1	473	5MC	CM5-C5	2.91	1.57	1.50
1	A1	1362	5MC	CM5-C5	2.91	1.57	1.50
1	A1	927	5MC	CM5-C5	2.90	1.57	1.50
1	A1	230	5MC	CM5-C5	2.90	1.57	1.50
27	B1	336	5MC	CM5-C5	2.90	1.57	1.50
27	B1	1977	5MC	CM5-C5	2.90	1.57	1.50
1	A1	1013	5MC	CM5-C5	2.90	1.57	1.50
1	A1	352	5MC	CM5-C5	2.89	1.57	1.50
27	B1	2067	5MC	CM5-C5	2.89	1.57	1.50
1	A1	863	5MC	CM5-C5	2.89	1.57	1.50
27	B1	506	A2M	O3'-C3'	-2.87	1.36	1.43
27	B1	2565	4SU	C6-N1	2.87	1.44	1.38
27	B1	926	OMU	O4-C4	-2.86	1.18	1.24
1	A1	756	4SU	C6-N1	2.86	1.44	1.38
1	A1	8	OMU	O4-C4	-2.86	1.19	1.24
1	A1	1484	5MC	CM5-C5	2.85	1.57	1.50
27	B1	857	A2M	O2'-C2'	2.85	1.49	1.42
27	B1	2022	OMG	C2-N1	2.84	1.44	1.37
1	A1	1368	OMU	C6-N1	2.84	1.44	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	775	OMU	O4-C4	-2.84	1.19	1.24
27	B1	1488	OMU	O4-C4	-2.84	1.19	1.24
27	B1	880	A2M	O2'-C2'	2.83	1.49	1.42
27	B1	2554	OMU	O4-C4	-2.83	1.19	1.24
1	A1	819	A2M	O2'-C2'	2.83	1.49	1.42
1	A1	455	OMG	C2-N1	2.83	1.44	1.37
27	B1	2617	5MC	CM5-C5	2.83	1.57	1.50
1	A1	8	OMU	C5-C4	2.83	1.49	1.43
27	B1	2506	A2M	O2'-C2'	2.83	1.49	1.42
1	A1	1165	OMU	C5-C4	2.83	1.49	1.43
27	B1	940	A2M	O2'-C2'	2.82	1.49	1.42
1	A1	466	5MC	CM5-C5	2.81	1.57	1.50
1	A1	775	OMU	C5-C4	2.81	1.49	1.43
1	A1	1366	A1I59	C1-C3	2.80	1.54	1.51
1	A1	762	OMU	O4-C4	-2.80	1.19	1.24
1	A1	1165	OMU	O4-C4	-2.79	1.19	1.24
27	B1	506	A2M	O2'-C2'	2.79	1.49	1.42
27	B1	2108	OMG	C2-N1	2.79	1.44	1.37
1	A1	762	OMU	C5-C4	2.79	1.49	1.43
1	A1	507	OMG	C2-N1	2.79	1.44	1.37
27	B1	1488	OMU	C5-C4	2.79	1.49	1.43
1	A1	861	OMG	C2-N1	2.78	1.44	1.37
27	B1	2028	OMG	C2-N1	2.78	1.44	1.37
27	B1	1557	OMG	C2-N1	2.78	1.44	1.37
1	A1	1368	OMU	O4-C4	-2.78	1.19	1.24
27	B1	920	OMG	C2-N1	2.78	1.44	1.37
27	B1	19	4AC	O2-C2	-2.77	1.18	1.23
27	B1	2391	OMG	C2-N1	2.77	1.44	1.37
27	B1	2684	OMG	C2-N1	2.77	1.44	1.37
27	B1	857	A2M	O3'-C3'	-2.77	1.36	1.43
27	B1	856	OMG	C2-N1	2.77	1.44	1.37
27	B1	454	OMU	O4-C4	-2.77	1.19	1.24
1	A1	52	OMU	C5-C4	2.77	1.49	1.43
27	B1	2984	OMG	C2-N1	2.77	1.44	1.37
27	B1	2554	OMU	C5-C4	2.77	1.49	1.43
1	A1	329	OMG	C2-N1	2.77	1.44	1.37
1	A1	541	OMG	C2-N1	2.77	1.44	1.37
1	A1	1003	OMG	C2-N1	2.77	1.44	1.37
27	B1	1965	OMG	C2-N1	2.76	1.44	1.37
1	A1	52	OMU	O4-C4	-2.76	1.19	1.24
1	A1	1368	OMU	C5-C4	2.76	1.49	1.43
27	B1	2757	OMG	C2-N1	2.76	1.44	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	2562	OMG	C2-N1	2.75	1.44	1.37
27	B1	2365	OMG	C2-N1	2.75	1.44	1.37
1	A1	1115	OMG	C2-N1	2.75	1.44	1.37
27	B1	214	OMG	C2-N1	2.75	1.44	1.37
27	B1	841	OMG	C2-N1	2.75	1.44	1.37
1	A1	668	OMG	C2-N1	2.74	1.44	1.37
27	B1	1904	OMG	C2-N1	2.74	1.44	1.37
27	B1	530	OMG	C2-N1	2.74	1.44	1.37
27	B1	926	OMU	C5-C4	2.74	1.49	1.43
1	A1	459	OMG	C2-N1	2.73	1.44	1.37
27	B1	55	OMG	C2-N1	2.73	1.44	1.37
27	B1	921	OMG	C2-N1	2.73	1.44	1.37
27	B1	485	4AC	O2-C2	-2.73	1.18	1.23
27	B1	2180	OMG	C2-N1	2.72	1.44	1.37
27	B1	2757	OMG	C5-C4	-2.72	1.36	1.43
27	B1	887	OMG	C2-N1	2.71	1.44	1.37
27	B1	214	OMG	C5-C4	-2.71	1.36	1.43
27	B1	688	4AC	O2-C2	-2.71	1.18	1.23
27	B1	2180	OMG	C5-C4	-2.71	1.36	1.43
1	A1	329	OMG	C5-C4	-2.70	1.36	1.43
1	A1	1013	5MC	C4-N4	2.70	1.41	1.34
27	B1	2108	OMG	C5-C4	-2.70	1.36	1.43
1	A1	1227	4AC	O2-C2	-2.70	1.18	1.23
27	B1	2540	OMG	C2-N1	2.70	1.44	1.37
27	B1	808	OMG	C2-N1	2.70	1.44	1.37
1	A1	1475	MA6	C5-C4	-2.70	1.33	1.40
27	B1	2792	4AC	O2-C2	-2.70	1.18	1.23
1	A1	951	5MC	C4-N4	2.69	1.41	1.34
27	B1	1769	4AC	O2-C2	-2.69	1.18	1.23
27	B1	227	4AC	O2-C2	-2.69	1.18	1.23
1	A1	645	OMG	C2-N1	2.69	1.44	1.37
27	B1	1914	OMC	O2-C2	-2.69	1.18	1.23
27	B1	940	A2M	C5-C4	-2.69	1.33	1.40
1	A1	861	OMG	C5-C4	-2.69	1.36	1.43
1	A1	1457	MA6	C5-C4	-2.69	1.33	1.40
27	B1	2700	UR3	C6-N1	2.69	1.44	1.38
27	B1	2557	OMC	O2-C2	-2.68	1.18	1.23
1	A1	927	5MC	C4-N4	2.68	1.41	1.34
27	B1	1904	OMG	C5-C4	-2.68	1.36	1.43
27	B1	454	OMU	C5-C4	2.68	1.49	1.43
27	B1	2607	OMC	O2-C2	-2.68	1.18	1.23
1	A1	473	5MC	C4-N4	2.68	1.41	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	1476	MA6	C5-C4	-2.68	1.33	1.40
27	B1	2749	4AC	O2-C2	-2.68	1.18	1.23
27	B1	378	4AC	O2-C2	-2.67	1.18	1.23
27	B1	1977	5MC	C4-N4	2.67	1.41	1.34
1	A1	41	4AC	O2-C2	-2.67	1.18	1.23
27	B1	2391	OMG	C5-C4	-2.67	1.36	1.43
27	B1	979	4AC	O2-C2	-2.67	1.18	1.23
27	B1	880	A2M	C5-C4	-2.67	1.33	1.40
27	B1	950	4AC	O2-C2	-2.67	1.18	1.23
1	A1	1484	5MC	C4-N4	2.67	1.41	1.34
27	B1	732	4AC	O2-C2	-2.67	1.18	1.23
1	A1	1190	5MC	C4-N4	2.67	1.41	1.34
27	B1	2067	5MC	C4-N4	2.67	1.41	1.34
27	B1	2876	4AC	O2-C2	-2.67	1.18	1.23
1	A1	1467	4AC	O2-C2	-2.66	1.18	1.23
27	B1	1967	4AC	O2-C2	-2.66	1.18	1.23
27	B1	336	5MC	C4-N4	2.66	1.41	1.34
27	B1	2562	OMG	C5-C4	-2.66	1.36	1.43
1	A1	1029	4AC	O2-C2	-2.66	1.18	1.23
27	B1	1107	4AC	O2-C2	-2.66	1.18	1.23
1	A1	87	4AC	O2-C2	-2.66	1.18	1.23
1	A1	455	OMG	C5-C4	-2.66	1.36	1.43
27	B1	2059	OMC	O2-C2	-2.66	1.18	1.23
27	B1	2119	OMC	O2-C2	-2.66	1.18	1.23
27	B1	933	4AC	O2-C2	-2.66	1.18	1.23
1	A1	1362	5MC	C4-N4	2.66	1.41	1.34
27	B1	1442	4AC	O2-C2	-2.66	1.18	1.23
27	B1	2850	4AC	O2-C2	-2.66	1.18	1.23
1	A1	481	G7M	C5-C6	2.65	1.52	1.45
1	A1	367	4AC	O2-C2	-2.65	1.18	1.23
27	B1	344	4AC	O2-C2	-2.65	1.18	1.23
27	B1	1762	4AC	O2-C2	-2.65	1.18	1.23
27	B1	1100	4AC	O2-C2	-2.65	1.18	1.23
27	B1	1818	4AC	O2-C2	-2.65	1.18	1.23
27	B1	48	4AC	O2-C2	-2.65	1.18	1.23
27	B1	2617	5MC	C4-N4	2.65	1.41	1.34
27	B1	501	OMC	O2-C2	-2.65	1.18	1.23
27	B1	2984	OMG	C5-C4	-2.65	1.36	1.43
27	B1	1546	4AC	O2-C2	-2.65	1.18	1.23
1	A1	687	5MC	C4-N4	2.65	1.41	1.34
1	A1	546	4AC	O2-C2	-2.65	1.18	1.23
27	B1	2022	OMG	C5-C4	-2.65	1.36	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	866	4AC	O2-C2	-2.65	1.18	1.23
27	B1	506	A2M	C5-C4	-2.65	1.33	1.40
27	B1	856	OMG	C5-C4	-2.65	1.36	1.43
27	B1	857	A2M	C5-C4	-2.65	1.33	1.40
1	A1	291	4AC	O2-C2	-2.65	1.18	1.23
27	B1	2379	4AC	O2-C2	-2.65	1.18	1.23
1	A1	1003	OMG	C5-C4	-2.65	1.36	1.43
1	A1	834	OMC	O2-C2	-2.64	1.18	1.23
1	A1	534	4AC	O2-C2	-2.64	1.18	1.23
27	B1	1639	4AC	O2-C2	-2.64	1.18	1.23
27	B1	1293	4AC	O2-C2	-2.64	1.18	1.23
27	B1	2844	4AC	O2-C2	-2.64	1.18	1.23
1	A1	863	5MC	C4-N4	2.64	1.41	1.34
27	B1	2133	4AC	O2-C2	-2.64	1.18	1.23
27	B1	953	4AC	O2-C2	-2.64	1.18	1.23
1	A1	719	4AC	O2-C2	-2.64	1.18	1.23
27	B1	1290	4AC	O2-C2	-2.64	1.18	1.23
27	B1	1832	OMC	O2-C2	-2.64	1.18	1.23
27	B1	3037	4AC	O2-C2	-2.64	1.18	1.23
27	B1	1946	4AC	O2-C2	-2.64	1.18	1.23
27	B1	1505	4AC	O2-C2	-2.64	1.18	1.23
27	B1	1706	4AC	O2-C2	-2.64	1.18	1.23
27	B1	2968	4AC	O2-C2	-2.64	1.18	1.23
27	B1	1501	4AC	O2-C2	-2.64	1.18	1.23
27	B1	419	4AC	O2-C2	-2.64	1.18	1.23
27	B1	1383	4AC	O2-C2	-2.64	1.18	1.23
27	B1	1885	4AC	O2-C2	-2.64	1.18	1.23
27	B1	1344	5MC	C4-N4	2.64	1.40	1.34
1	A1	614	4AC	O2-C2	-2.64	1.18	1.23
1	A1	230	5MC	C4-N4	2.64	1.40	1.34
27	B1	2506	A2M	C5-C4	-2.64	1.34	1.40
27	B1	200	4AC	O2-C2	-2.64	1.18	1.23
1	A1	1194	OMC	O2-C2	-2.64	1.18	1.23
1	A1	1181	4AC	O2-C2	-2.63	1.18	1.23
1	A1	17	5MC	C4-N4	2.63	1.40	1.34
27	B1	3011	4AC	O2-C2	-2.63	1.18	1.23
27	B1	360	4AC	O2-C2	-2.63	1.18	1.23
27	B1	2602	4AC	O2-C2	-2.63	1.18	1.23
27	B1	1965	OMG	C5-C4	-2.63	1.36	1.43
27	B1	921	OMG	C5-C4	-2.63	1.36	1.43
27	B1	23	4AC	O2-C2	-2.63	1.18	1.23
27	B1	1061	4AC	O2-C2	-2.63	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	1822	4AC	O2-C2	-2.63	1.18	1.23
27	B1	2171	4AC	O2-C2	-2.63	1.18	1.23
27	B1	2087	5MC	C4-N4	2.63	1.40	1.34
27	B1	1743	4AC	O2-C2	-2.63	1.18	1.23
1	A1	499	4AC	O2-C2	-2.63	1.18	1.23
27	B1	2113	4AC	O2-C2	-2.63	1.18	1.23
28	B2	115	4AC	O2-C2	-2.63	1.18	1.23
1	A1	839	4AC	O2-C2	-2.63	1.18	1.23
27	B1	2526	4AC	O2-C2	-2.63	1.18	1.23
27	B1	2700	UR3	C5-C4	2.63	1.50	1.43
1	A1	681	5MC	C4-N4	2.63	1.40	1.34
1	A1	836	4AC	O2-C2	-2.63	1.18	1.23
27	B1	1345	4AC	O2-C2	-2.63	1.18	1.23
27	B1	2735	OMC	O2-C2	-2.63	1.18	1.23
1	A1	1226	OMC	O2-C2	-2.63	1.18	1.23
1	A1	578	4AC	O2-C2	-2.63	1.18	1.23
1	A1	827	4AC	O2-C2	-2.63	1.18	1.23
1	A1	819	A2M	C5-C4	-2.63	1.34	1.40
27	B1	2808	OMC	O2-C2	-2.63	1.18	1.23
27	B1	580	4AC	O2-C2	-2.63	1.18	1.23
27	B1	721	4AC	O2-C2	-2.62	1.18	1.23
1	A1	382	4AC	O2-C2	-2.62	1.18	1.23
27	B1	434	4AC	O2-C2	-2.62	1.18	1.23
1	A1	231	4AC	O2-C2	-2.62	1.18	1.23
1	A1	706	4AC	O2-C2	-2.62	1.18	1.23
27	B1	479	4AC	O2-C2	-2.62	1.18	1.23
27	B1	1264	4AC	O2-C2	-2.62	1.18	1.23
1	A1	1115	OMG	C5-C4	-2.62	1.36	1.43
1	A1	540	4AC	O2-C2	-2.62	1.18	1.23
27	B1	2008	4AC	O2-C2	-2.62	1.18	1.23
27	B1	116	4AC	O2-C2	-2.62	1.18	1.23
27	B1	1435	4AC	O2-C2	-2.62	1.18	1.23
1	A1	691	4AC	O2-C2	-2.62	1.18	1.23
27	B1	130	4AC	O2-C2	-2.62	1.18	1.23
1	A1	507	OMG	C5-C4	-2.62	1.36	1.43
27	B1	1067	4AC	O2-C2	-2.62	1.18	1.23
27	B1	2821	4AC	O2-C2	-2.62	1.18	1.23
1	A1	307	4AC	O2-C2	-2.62	1.18	1.23
27	B1	527	4AC	O2-C2	-2.62	1.18	1.23
27	B1	1751	4AC	O2-C2	-2.62	1.18	1.23
27	B1	55	OMG	C5-C4	-2.62	1.36	1.43
27	B1	2432	4AC	O2-C2	-2.62	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	3020	4AC	O2-C2	-2.62	1.18	1.23
1	A1	141	4AC	O2-C2	-2.62	1.18	1.23
27	B1	1150	4AC	O2-C2	-2.62	1.18	1.23
27	B1	1551	4AC	O2-C2	-2.62	1.18	1.23
27	B1	98	4AC	O2-C2	-2.62	1.18	1.23
27	B1	1052	4AC	O2-C2	-2.62	1.18	1.23
27	B1	1846	4AC	O2-C2	-2.62	1.18	1.23
1	A1	274	4AC	O2-C2	-2.62	1.18	1.23
27	B1	1374	4AC	O2-C2	-2.62	1.18	1.23
27	B1	808	OMG	C5-C4	-2.61	1.36	1.43
1	A1	352	5MC	C4-N4	2.61	1.40	1.34
1	A1	739	4AC	O2-C2	-2.61	1.18	1.23
27	B1	1360	4AC	O2-C2	-2.61	1.18	1.23
27	B1	2429	4AC	O2-C2	-2.61	1.18	1.23
27	B1	3006	4AC	O2-C2	-2.61	1.18	1.23
1	A1	466	5MC	C4-N4	2.61	1.40	1.34
1	A1	624	4AC	O2-C2	-2.61	1.18	1.23
1	A1	816	4AC	O2-C2	-2.61	1.18	1.23
1	A1	1314	4AC	O2-C2	-2.61	1.18	1.23
1	A1	1254	4AC	O2-C2	-2.61	1.18	1.23
27	B1	715	4AC	O2-C2	-2.61	1.18	1.23
27	B1	1064	4AC	O2-C2	-2.61	1.18	1.23
1	A1	1028	OMC	O2-C2	-2.61	1.18	1.23
1	A1	1364	OMC	O2-C2	-2.61	1.18	1.23
27	B1	1911	4AC	O2-C2	-2.61	1.18	1.23
1	A1	856	4AC	O2-C2	-2.61	1.18	1.23
27	B1	2454	4AC	O2-C2	-2.61	1.18	1.23
1	A1	1371	OMC	O2-C2	-2.61	1.18	1.23
1	A1	945	4AC	O2-C2	-2.61	1.18	1.23
27	B1	1099	OMC	O2-C2	-2.61	1.18	1.23
27	B1	243	4AC	O2-C2	-2.61	1.18	1.23
1	A1	541	OMG	C5-C4	-2.60	1.36	1.43
27	B1	1478	4AC	O2-C2	-2.60	1.18	1.23
27	B1	2492	4AC	O2-C2	-2.60	1.18	1.23
27	B1	2213	4AC	O2-C2	-2.60	1.18	1.23
27	B1	2365	OMG	C5-C4	-2.60	1.36	1.43
27	B1	887	OMG	C5-C4	-2.60	1.36	1.43
27	B1	2028	OMG	C5-C4	-2.60	1.36	1.43
27	B1	896	4AC	O2-C2	-2.60	1.18	1.23
27	B1	1489	OMC	O2-C2	-2.60	1.18	1.23
27	B1	841	OMG	C5-C4	-2.60	1.36	1.43
27	B1	1608	4AC	O2-C2	-2.60	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	668	OMG	C5-C4	-2.60	1.36	1.43
27	B1	652	4AC	O2-C2	-2.60	1.18	1.23
27	B1	2540	OMG	C5-C4	-2.59	1.36	1.43
1	A1	1371	OMC	C5-C4	2.59	1.48	1.42
27	B1	1649	4AC	O2-C2	-2.59	1.18	1.23
27	B1	1128	4AC	O2-C2	-2.59	1.18	1.23
1	A1	216	4AC	O2-C2	-2.59	1.18	1.23
27	B1	1579	4AC	O2-C2	-2.59	1.18	1.23
1	A1	1270	OMC	O2-C2	-2.58	1.18	1.23
27	B1	2809	4AC	O2-C2	-2.58	1.18	1.23
27	B1	80	4AC	O2-C2	-2.58	1.18	1.23
27	B1	2607	OMC	C5-C4	2.58	1.48	1.42
1	A1	5	4AC	O2-C2	-2.58	1.18	1.23
1	A1	405	4AC	O2-C2	-2.58	1.18	1.23
1	A1	117	OMC	O2-C2	-2.58	1.18	1.23
27	B1	2469	4AC	O2-C2	-2.58	1.18	1.23
28	B2	88	4AC	O2-C2	-2.58	1.18	1.23
27	B1	162	4AC	O2-C2	-2.58	1.18	1.23
1	A1	459	OMG	C5-C4	-2.58	1.36	1.43
27	B1	337	4AC	O2-C2	-2.58	1.18	1.23
1	A1	467	4AC	O2-C2	-2.57	1.18	1.23
27	B1	1557	OMG	C5-C4	-2.57	1.36	1.43
27	B1	920	OMG	C5-C4	-2.57	1.36	1.43
1	A1	220	4AC	O2-C2	-2.57	1.18	1.23
27	B1	2020	4AC	O2-C2	-2.57	1.18	1.23
1	A1	636	4AC	O2-C2	-2.57	1.18	1.23
27	B1	2059	OMC	C5-C4	2.57	1.48	1.42
27	B1	786	4AC	O2-C2	-2.56	1.19	1.23
28	B2	30	4AC	O2-C2	-2.56	1.19	1.23
27	B1	2119	OMC	C5-C4	2.56	1.48	1.42
27	B1	2684	OMG	C5-C4	-2.56	1.36	1.43
1	A1	1194	OMC	C5-C4	2.55	1.48	1.42
1	A1	1028	OMC	C5-C4	2.55	1.48	1.42
27	B1	530	OMG	C5-C4	-2.55	1.36	1.43
1	A1	1364	OMC	C5-C4	2.55	1.48	1.42
1	A1	834	OMC	C5-C4	2.55	1.48	1.42
1	A1	761	4AC	O2-C2	-2.54	1.19	1.23
27	B1	1489	OMC	C5-C4	2.54	1.48	1.42
27	B1	1178	4AC	O2-C2	-2.54	1.19	1.23
27	B1	1832	OMC	C5-C4	2.53	1.48	1.42
27	B1	2735	OMC	C5-C4	2.53	1.48	1.42
27	B1	2557	OMC	C5-C4	2.53	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	117	OMC	C5-C4	2.51	1.48	1.42
1	A1	1366	A1I59	C6-N1	-2.51	1.33	1.38
27	B1	1914	OMC	C5-C4	2.51	1.48	1.42
1	A1	645	OMG	C5-C4	-2.51	1.36	1.43
1	A1	1270	OMC	C5-C4	2.50	1.48	1.42
27	B1	1099	OMC	C5-C4	2.50	1.48	1.42
27	B1	2808	OMC	C5-C4	2.49	1.48	1.42
27	B1	501	OMC	C5-C4	2.42	1.48	1.42
1	A1	1226	OMC	C5-C4	2.40	1.48	1.42
1	A1	481	G7M	C5-C4	2.39	1.43	1.39
27	B1	2700	UR3	O2-C2	-2.35	1.18	1.22
27	B1	2565	4SU	O2-C2	-2.32	1.18	1.23
27	B1	921	OMG	O6-C6	-2.30	1.18	1.23
1	A1	329	OMG	O6-C6	-2.29	1.18	1.23
1	A1	756	4SU	O2-C2	-2.29	1.18	1.23
27	B1	214	OMG	O6-C6	-2.28	1.18	1.23
27	B1	920	OMG	O6-C6	-2.27	1.18	1.23
27	B1	1904	OMG	O6-C6	-2.27	1.18	1.23
27	B1	2540	OMG	O6-C6	-2.26	1.18	1.23
27	B1	2984	OMG	O6-C6	-2.26	1.18	1.23
27	B1	856	OMG	O6-C6	-2.25	1.18	1.23
27	B1	55	OMG	O6-C6	-2.25	1.18	1.23
1	A1	1003	OMG	O6-C6	-2.25	1.18	1.23
1	A1	541	OMG	O6-C6	-2.25	1.18	1.23
1	A1	645	OMG	O6-C6	-2.25	1.18	1.23
27	B1	2180	OMG	O6-C6	-2.25	1.18	1.23
1	A1	861	OMG	O6-C6	-2.24	1.18	1.23
27	B1	2684	OMG	O6-C6	-2.24	1.18	1.23
27	B1	808	OMG	O6-C6	-2.24	1.18	1.23
27	B1	530	OMG	O6-C6	-2.23	1.18	1.23
27	B1	887	OMG	O6-C6	-2.23	1.18	1.23
1	A1	1115	OMG	O6-C6	-2.23	1.18	1.23
27	B1	2562	OMG	O6-C6	-2.23	1.18	1.23
27	B1	2022	OMG	O6-C6	-2.22	1.18	1.23
27	B1	2108	OMG	O6-C6	-2.22	1.18	1.23
27	B1	841	OMG	O6-C6	-2.22	1.18	1.23
1	A1	481	G7M	O6-C6	-2.21	1.18	1.23
1	A1	507	OMG	O6-C6	-2.21	1.18	1.23
27	B1	2391	OMG	O6-C6	-2.21	1.18	1.23
1	A1	459	OMG	O6-C6	-2.21	1.18	1.23
27	B1	2365	OMG	O6-C6	-2.20	1.18	1.23
1	A1	668	OMG	O6-C6	-2.20	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	1965	OMG	O6-C6	-2.20	1.18	1.23
27	B1	1557	OMG	O6-C6	-2.20	1.18	1.23
27	B1	2757	OMG	O6-C6	-2.20	1.18	1.23
1	A1	455	OMG	O6-C6	-2.19	1.18	1.23
27	B1	2028	OMG	O6-C6	-2.17	1.18	1.23
27	B1	857	A2M	C2-N3	2.15	1.35	1.32
1	A1	819	A2M	C2-N3	2.14	1.35	1.32
27	B1	1439	LHH	O7-C7	-2.08	1.18	1.23
27	B1	506	A2M	C2-N3	2.08	1.35	1.32
27	B1	2506	A2M	C2-N3	2.08	1.35	1.32
27	B1	502	LHH	O7-C7	-2.07	1.18	1.23
27	B1	940	A2M	C2-N3	2.07	1.35	1.32
27	B1	2113	4AC	O7-C7	-2.06	1.18	1.23
27	B1	1442	4AC	O7-C7	-2.06	1.18	1.23
27	B1	2171	4AC	O7-C7	-2.05	1.18	1.23
27	B1	1435	4AC	O7-C7	-2.05	1.18	1.23
27	B1	360	4AC	O7-C7	-2.05	1.18	1.23
1	A1	467	4AC	O7-C7	-2.05	1.18	1.23
27	B1	1546	4AC	O7-C7	-2.05	1.18	1.23
1	A1	706	4AC	O7-C7	-2.05	1.18	1.23
27	B1	485	4AC	O7-C7	-2.04	1.18	1.23
27	B1	652	4AC	O7-C7	-2.04	1.18	1.23
27	B1	1064	4AC	O7-C7	-2.04	1.18	1.23
1	A1	307	4AC	O7-C7	-2.04	1.18	1.23
27	B1	243	4AC	O7-C7	-2.04	1.18	1.23
27	B1	715	4AC	O7-C7	-2.04	1.18	1.23
27	B1	1128	4AC	O7-C7	-2.04	1.18	1.23
27	B1	1551	4AC	O7-C7	-2.04	1.18	1.23
1	A1	367	4AC	O7-C7	-2.04	1.18	1.23
27	B1	1505	4AC	O7-C7	-2.04	1.18	1.23
1	A1	816	4AC	O7-C7	-2.04	1.18	1.23
1	A1	405	4AC	O7-C7	-2.03	1.18	1.23
27	B1	162	4AC	O7-C7	-2.03	1.18	1.23
27	B1	1639	4AC	O7-C7	-2.03	1.18	1.23
27	B1	880	A2M	C2-N3	2.03	1.35	1.32
28	B2	30	4AC	O7-C7	-2.03	1.18	1.23
1	A1	836	4AC	O7-C7	-2.03	1.18	1.23
27	B1	950	4AC	O7-C7	-2.03	1.18	1.23
27	B1	2844	4AC	O7-C7	-2.03	1.18	1.23
1	A1	382	4AC	O7-C7	-2.03	1.18	1.23
1	A1	534	4AC	O7-C7	-2.03	1.18	1.23
27	B1	378	4AC	O7-C7	-2.03	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	933	4AC	O7-C7	-2.03	1.18	1.23
27	B1	1067	4AC	O7-C7	-2.03	1.18	1.23
27	B1	1846	4AC	O7-C7	-2.03	1.18	1.23
1	A1	1227	4AC	O7-C7	-2.03	1.18	1.23
27	B1	2809	4AC	O7-C7	-2.02	1.18	1.23
1	A1	291	4AC	O7-C7	-2.02	1.18	1.23
27	B1	1264	4AC	O7-C7	-2.02	1.18	1.23
27	B1	3037	4AC	O7-C7	-2.02	1.18	1.23
27	B1	1751	4AC	O7-C7	-2.02	1.18	1.23
27	B1	2008	4AC	O7-C7	-2.02	1.18	1.23
27	B1	2379	4AC	O7-C7	-2.02	1.18	1.23
27	B1	2876	4AC	O7-C7	-2.02	1.18	1.23
27	B1	2432	4AC	O7-C7	-2.02	1.18	1.23
27	B1	130	4AC	O7-C7	-2.02	1.18	1.23
27	B1	2020	4AC	O7-C7	-2.02	1.18	1.23
27	B1	2454	4AC	O7-C7	-2.02	1.18	1.23
1	A1	361	A2M	C8-N7	-2.02	1.31	1.34
1	A1	41	4AC	O7-C7	-2.02	1.18	1.23
27	B1	80	4AC	O7-C7	-2.02	1.18	1.23
27	B1	2749	4AC	O7-C7	-2.02	1.18	1.23
27	B1	2850	4AC	O7-C7	-2.02	1.18	1.23
27	B1	116	4AC	O7-C7	-2.01	1.18	1.23
27	B1	688	4AC	O7-C7	-2.01	1.18	1.23
27	B1	1478	4AC	O7-C7	-2.01	1.18	1.23
1	A1	856	4AC	O7-C7	-2.01	1.18	1.23
27	B1	866	4AC	O7-C7	-2.01	1.18	1.23
1	A1	540	4AC	O7-C7	-2.01	1.18	1.23
27	B1	1383	4AC	O7-C7	-2.01	1.18	1.23
27	B1	2792	4AC	O7-C7	-2.01	1.18	1.23
27	B1	98	4AC	O7-C7	-2.01	1.18	1.23
27	B1	337	4AC	O7-C7	-2.01	1.18	1.23
27	B1	2492	4AC	O7-C7	-2.01	1.18	1.23
27	B1	953	4AC	O7-C7	-2.01	1.18	1.23
27	B1	2469	4AC	O7-C7	-2.01	1.18	1.23
1	A1	238	LHH	O7-C7	-2.01	1.18	1.23
1	A1	827	4AC	O7-C7	-2.01	1.18	1.23
27	B1	1374	4AC	O7-C7	-2.01	1.18	1.23
27	B1	1885	4AC	O7-C7	-2.01	1.18	1.23
1	A1	1181	4AC	O7-C7	-2.01	1.18	1.23
27	B1	1150	4AC	O7-C7	-2.01	1.18	1.23
27	B1	1107	4AC	O7-C7	-2.01	1.18	1.23
27	B1	1178	4AC	O7-C7	-2.01	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	434	4AC	O7-C7	-2.01	1.18	1.23
1	A1	216	4AC	O7-C7	-2.00	1.18	1.23
1	A1	691	4AC	O7-C7	-2.00	1.18	1.23
1	A1	220	4AC	O7-C7	-2.00	1.18	1.23
27	B1	48	4AC	O7-C7	-2.00	1.18	1.23
27	B1	2602	4AC	O7-C7	-2.00	1.18	1.23
27	B1	227	4AC	O7-C7	-2.00	1.18	1.23
28	B2	115	4AC	O7-C7	-2.00	1.18	1.23
1	A1	614	4AC	O7-C7	-2.00	1.18	1.23
27	B1	2429	4AC	O7-C7	-2.00	1.18	1.23
27	B1	1762	4AC	O7-C7	-2.00	1.18	1.23
27	B1	2968	4AC	O7-C7	-2.00	1.18	1.23
27	B1	1818	4AC	O7-C7	-2.00	1.18	1.23
27	B1	1345	4AC	O7-C7	-2.00	1.18	1.23
27	B1	2526	4AC	O7-C7	-2.00	1.18	1.23

All (874) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	1475	MA6	N1-C6-N6	-13.53	102.81	117.06
1	A1	1476	MA6	N1-C6-N6	-13.49	102.85	117.06
1	A1	1475	MA6	C1'-N9-C4	12.76	149.06	126.64
1	A1	1457	MA6	C1'-N9-C4	12.36	148.36	126.64
1	A1	1457	MA6	N1-C6-N6	-12.27	104.14	117.06
1	A1	1476	MA6	C1'-N9-C4	11.90	147.54	126.64
27	B1	2565	4SU	C4-N3-C2	-7.84	119.73	127.34
1	A1	756	4SU	C4-N3-C2	-7.82	119.75	127.34
1	A1	238	LHH	C4-N3-C2	-5.69	112.37	120.12
1	A1	1476	MA6	N3-C2-N1	-5.60	119.93	128.68
1	A1	1457	MA6	N3-C2-N1	-5.54	120.01	128.68
1	A1	819	A2M	C1'-N9-C4	5.53	136.35	126.64
27	B1	506	A2M	C1'-N9-C4	5.52	136.34	126.64
27	B1	880	A2M	N3-C2-N1	-5.44	120.17	128.68
27	B1	940	A2M	N3-C2-N1	-5.44	120.17	128.68
1	A1	1475	MA6	N3-C2-N1	-5.44	120.18	128.68
27	B1	940	A2M	C1'-N9-C4	5.41	136.15	126.64
27	B1	857	A2M	N3-C2-N1	-5.41	120.23	128.68
27	B1	1439	LHH	C4-N3-C2	-5.39	112.78	120.12
27	B1	2506	A2M	N3-C2-N1	-5.39	120.26	128.68
1	A1	756	4SU	C5-C4-N3	5.38	119.68	114.69
27	B1	2565	4SU	C5-C4-N3	5.36	119.67	114.69
27	B1	506	A2M	N3-C2-N1	-5.35	120.32	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B1	2554	OMU	C4-N3-C2	-5.31	119.58	126.58
1	A1	775	OMU	C4-N3-C2	-5.31	119.58	126.58
1	A1	819	A2M	N3-C2-N1	-5.30	120.40	128.68
27	B1	2506	A2M	C1'-N9-C4	5.30	135.95	126.64
27	B1	880	A2M	C1'-N9-C4	5.28	135.92	126.64
27	B1	857	A2M	C1'-N9-C4	5.28	135.91	126.64
1	A1	8	OMU	C4-N3-C2	-5.26	119.64	126.58
27	B1	1488	OMU	C4-N3-C2	-5.23	119.68	126.58
1	A1	762	OMU	C4-N3-C2	-5.21	119.71	126.58
1	A1	1368	OMU	C4-N3-C2	-5.21	119.71	126.58
1	A1	1165	OMU	C4-N3-C2	-5.20	119.72	126.58
27	B1	1360	4AC	CM7-C7-N4	5.17	124.23	115.29
27	B1	926	OMU	C4-N3-C2	-5.15	119.78	126.58
27	B1	502	LHH	C4-N3-C2	-5.15	113.11	120.12
1	A1	52	OMU	C4-N3-C2	-5.11	119.84	126.58
1	A1	1467	4AC	CM7-C7-N4	5.08	124.08	115.29
27	B1	454	OMU	C4-N3-C2	-5.04	119.93	126.58
27	B1	2700	UR3	C4-N3-C2	-4.52	120.31	124.56
28	B2	115	4AC	O4'-C1'-N1	4.19	117.94	108.36
1	A1	775	OMU	N3-C2-N1	4.06	120.28	114.89
1	A1	1366	A1I59	C5-C6-N1	-4.03	118.18	123.38
1	A1	819	A2M	C5-C6-N6	-3.97	114.33	120.35
1	A1	541	OMG	O3'-C3'-C2'	3.93	122.33	111.17
27	B1	940	A2M	C5-C6-N6	-3.92	114.40	120.35
27	B1	857	A2M	C5-C6-N6	-3.91	114.42	120.35
1	A1	8	OMU	N3-C2-N1	3.91	120.08	114.89
27	B1	2565	4SU	N3-C2-N1	3.91	120.07	114.89
1	A1	756	4SU	N3-C2-N1	3.90	120.07	114.89
1	A1	1368	OMU	N3-C2-N1	3.89	120.06	114.89
27	B1	506	A2M	C5-C6-N6	-3.88	114.45	120.35
27	B1	926	OMU	O3'-C3'-C2'	3.88	122.18	111.17
27	B1	1488	OMU	N3-C2-N1	3.87	120.02	114.89
27	B1	454	OMU	O3'-C3'-C2'	3.84	122.07	111.17
27	B1	454	OMU	N3-C2-N1	3.83	119.98	114.89
27	B1	2506	A2M	C5-C6-N6	-3.83	114.54	120.35
1	A1	1165	OMU	N3-C2-N1	3.77	119.89	114.89
27	B1	434	4AC	O3'-C3'-C4'	3.77	121.95	111.05
1	A1	41	4AC	O3'-C3'-C4'	3.75	121.89	111.05
27	B1	378	4AC	O3'-C3'-C4'	3.74	121.87	111.05
27	B1	2554	OMU	N3-C2-N1	3.72	119.83	114.89
27	B1	880	A2M	C5-C6-N6	-3.71	114.71	120.35
27	B1	926	OMU	N3-C2-N1	3.70	119.80	114.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	87	4AC	O3'-C3'-C4'	3.68	121.69	111.05
1	A1	52	OMU	N3-C2-N1	3.67	119.77	114.89
1	A1	541	OMG	O3'-C3'-C4'	3.67	121.66	111.05
1	A1	762	OMU	N3-C2-N1	3.67	119.76	114.89
27	B1	1946	4AC	O3'-C3'-C4'	3.60	121.46	111.05
27	B1	454	OMU	O3'-C3'-C4'	3.55	121.31	111.05
27	B1	926	OMU	O3'-C3'-C4'	3.54	121.29	111.05
27	B1	808	OMG	C5-C6-N1	3.50	120.13	113.95
1	A1	329	OMG	C5-C6-N1	3.50	120.13	113.95
27	B1	2365	OMG	C5-C6-N1	3.48	120.10	113.95
1	A1	466	5MC	C5-C6-N1	-3.47	119.76	123.34
27	B1	856	OMG	C5-C6-N1	3.47	120.08	113.95
27	B1	2540	OMG	C5-C6-N1	3.47	120.08	113.95
27	B1	920	OMG	C5-C6-N1	3.46	120.06	113.95
27	B1	2562	OMG	C5-C6-N1	3.45	120.05	113.95
1	A1	541	OMG	C5-C6-N1	3.45	120.03	113.95
27	B1	887	OMG	C5-C6-N1	3.44	120.03	113.95
27	B1	2757	OMG	C5-C6-N1	3.44	120.02	113.95
1	A1	1115	OMG	C5-C6-N1	3.44	120.02	113.95
27	B1	2108	OMG	C5-C6-N1	3.44	120.02	113.95
27	B1	2180	OMG	C5-C6-N1	3.43	120.01	113.95
27	B1	841	OMG	C5-C6-N1	3.43	120.00	113.95
27	B1	2617	5MC	C5-C6-N1	-3.42	119.82	123.34
1	A1	668	OMG	C5-C6-N1	3.42	119.99	113.95
1	A1	1003	OMG	C5-C6-N1	3.42	119.98	113.95
27	B1	214	OMG	C5-C6-N1	3.41	119.97	113.95
27	B1	2391	OMG	C5-C6-N1	3.41	119.97	113.95
27	B1	2554	OMU	C5-C4-N3	3.40	119.93	114.84
27	B1	55	OMG	C5-C6-N1	3.40	119.96	113.95
1	A1	819	A2M	N6-C6-N1	3.40	125.64	118.57
27	B1	530	OMG	C5-C6-N1	3.40	119.96	113.95
1	A1	455	OMG	C5-C6-N1	3.40	119.96	113.95
27	B1	1904	OMG	C5-C6-N1	3.40	119.95	113.95
27	B1	940	A2M	N6-C6-N1	3.40	125.62	118.57
27	B1	921	OMG	C5-C6-N1	3.39	119.94	113.95
27	B1	2984	OMG	C5-C6-N1	3.39	119.94	113.95
27	B1	1557	OMG	C5-C6-N1	3.39	119.93	113.95
1	A1	756	4SU	C5-C4-S4	-3.38	120.11	124.47
27	B1	1965	OMG	C5-C6-N1	3.38	119.92	113.95
27	B1	2028	OMG	C5-C6-N1	3.38	119.92	113.95
1	A1	459	OMG	C5-C6-N1	3.38	119.92	113.95
1	A1	645	OMG	C5-C6-N1	3.38	119.91	113.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B1	2684	OMG	C5-C6-N1	3.37	119.91	113.95
27	B1	506	A2M	N6-C6-N1	3.37	125.57	118.57
27	B1	378	4AC	O3'-C3'-C2'	3.37	122.72	111.82
1	A1	507	OMG	C5-C6-N1	3.37	119.90	113.95
27	B1	2022	OMG	C5-C6-N1	3.36	119.89	113.95
1	A1	762	OMU	C5-C4-N3	3.36	119.86	114.84
27	B1	336	5MC	C5-C6-N1	-3.35	119.89	123.34
27	B1	2565	4SU	C5-C4-S4	-3.35	120.15	124.47
1	A1	861	OMG	C5-C6-N1	3.35	119.86	113.95
27	B1	926	OMU	C5-C4-N3	3.35	119.84	114.84
27	B1	857	A2M	N6-C6-N1	3.34	125.51	118.57
27	B1	434	4AC	O3'-C3'-C2'	3.33	122.61	111.82
1	A1	863	5MC	C5-C6-N1	-3.30	119.94	123.34
27	B1	1488	OMU	C5-C4-N3	3.30	119.78	114.84
1	A1	41	4AC	O3'-C3'-C2'	3.30	122.49	111.82
1	A1	8	OMU	C5-C4-N3	3.30	119.77	114.84
27	B1	2506	A2M	N6-C6-N1	3.29	125.39	118.57
1	A1	87	4AC	O3'-C3'-C2'	3.29	122.45	111.82
27	B1	880	A2M	N6-C6-N1	3.28	125.38	118.57
1	A1	52	OMU	C5-C4-N3	3.27	119.73	114.84
1	A1	1165	OMU	C5-C4-N3	3.25	119.70	114.84
27	B1	1946	4AC	O3'-C3'-C2'	3.23	122.27	111.82
1	A1	473	5MC	C5-C6-N1	-3.23	120.02	123.34
1	A1	775	OMU	C5-C4-N3	3.23	119.67	114.84
1	A1	352	5MC	C5-C6-N1	-3.23	120.02	123.34
1	A1	1362	5MC	C5-C6-N1	-3.22	120.02	123.34
1	A1	1368	OMU	C5-C4-N3	3.22	119.66	114.84
27	B1	2700	UR3	C1'-N1-C2	3.21	122.41	116.99
27	B1	454	OMU	C5-C4-N3	3.20	119.63	114.84
27	B1	1344	5MC	C5-C6-N1	-3.20	120.05	123.34
27	B1	1977	5MC	C5-C6-N1	-3.19	120.06	123.34
1	A1	687	5MC	C5-C6-N1	-3.17	120.08	123.34
1	A1	927	5MC	C5-C6-N1	-3.17	120.08	123.34
1	A1	1013	5MC	C5-C6-N1	-3.16	120.09	123.34
27	B1	2067	5MC	C5-C6-N1	-3.11	120.14	123.34
1	A1	1190	5MC	C5-C6-N1	-3.10	120.14	123.34
1	A1	230	5MC	C5-C6-N1	-3.09	120.16	123.34
1	A1	645	OMG	C2-N1-C6	-3.08	119.42	125.10
1	A1	17	5MC	C5-C6-N1	-3.04	120.21	123.34
1	A1	681	5MC	C5-C6-N1	-3.01	120.24	123.34
27	B1	808	OMG	C2-N1-C6	-3.01	119.56	125.10
1	A1	541	OMG	C2-N1-C6	-2.98	119.61	125.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B1	856	OMG	C2-N1-C6	-2.97	119.62	125.10
27	B1	2108	OMG	C2-N1-C6	-2.97	119.63	125.10
27	B1	2087	5MC	C5-C6-N1	-2.97	120.29	123.34
1	A1	1115	OMG	C2-N1-C6	-2.96	119.64	125.10
27	B1	2562	OMG	C2-N1-C6	-2.96	119.65	125.10
27	B1	920	OMG	C2-N1-C6	-2.96	119.65	125.10
27	B1	530	OMG	C2-N1-C6	-2.96	119.65	125.10
1	A1	668	OMG	C2-N1-C6	-2.96	119.66	125.10
27	B1	926	OMU	O4-C4-C5	-2.95	119.97	125.16
1	A1	455	OMG	C2-N1-C6	-2.95	119.66	125.10
1	A1	329	OMG	C2-N1-C6	-2.95	119.67	125.10
1	A1	1003	OMG	C2-N1-C6	-2.95	119.67	125.10
27	B1	887	OMG	C2-N1-C6	-2.94	119.67	125.10
27	B1	1557	OMG	C2-N1-C6	-2.94	119.67	125.10
1	A1	459	OMG	C2-N1-C6	-2.94	119.68	125.10
27	B1	2028	OMG	C2-N1-C6	-2.94	119.68	125.10
27	B1	2365	OMG	C2-N1-C6	-2.93	119.70	125.10
1	A1	507	OMG	C2-N1-C6	-2.93	119.70	125.10
27	B1	2540	OMG	C2-N1-C6	-2.93	119.70	125.10
1	A1	691	4AC	N4-C4-N3	2.93	118.77	113.85
27	B1	841	OMG	C2-N1-C6	-2.92	119.72	125.10
27	B1	2757	OMG	C2-N1-C6	-2.92	119.72	125.10
1	A1	624	4AC	N4-C4-N3	2.92	118.75	113.85
27	B1	2684	OMG	C2-N1-C6	-2.92	119.73	125.10
27	B1	2984	OMG	C2-N1-C6	-2.91	119.74	125.10
1	A1	52	OMU	O4-C4-C5	-2.91	120.04	125.16
27	B1	2022	OMG	C2-N1-C6	-2.88	119.79	125.10
27	B1	1293	4AC	O4'-C4'-C5'	2.88	118.85	109.37
1	A1	762	OMU	O4-C4-C5	-2.87	120.11	125.16
27	B1	856	OMG	C8-N7-C5	2.86	108.44	102.99
27	B1	2757	OMG	C8-N7-C5	2.86	108.44	102.99
27	B1	1608	4AC	O4'-C4'-C5'	2.86	118.77	109.37
1	A1	1181	4AC	O4'-C4'-C5'	2.86	118.77	109.37
1	A1	329	OMG	C8-N7-C5	2.86	108.43	102.99
27	B1	214	OMG	C2-N1-C6	-2.85	119.84	125.10
27	B1	214	OMG	C8-N7-C5	2.85	108.42	102.99
27	B1	2554	OMU	O4-C4-C5	-2.84	120.16	125.16
1	A1	481	G7M	C2-N1-C6	-2.83	119.88	125.10
27	B1	2391	OMG	C2-N1-C6	-2.83	119.88	125.10
1	A1	1165	OMU	O4-C4-C5	-2.83	120.18	125.16
1	A1	1115	OMG	C8-N7-C5	2.82	108.37	102.99
1	A1	1003	OMG	C8-N7-C5	2.82	108.37	102.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B1	1965	OMG	C2-N1-C6	-2.82	119.90	125.10
27	B1	2108	OMG	C8-N7-C5	2.82	108.36	102.99
27	B1	1374	4AC	N4-C4-N3	2.82	118.58	113.85
27	B1	921	OMG	C2-N1-C6	-2.81	119.92	125.10
27	B1	2180	OMG	C8-N7-C5	2.81	108.35	102.99
27	B1	1501	4AC	N4-C4-N3	2.81	118.57	113.85
1	A1	945	4AC	N4-C4-N3	2.81	118.56	113.85
27	B1	2180	OMG	C2-N1-C6	-2.80	119.93	125.10
27	B1	55	OMG	C2-N1-C6	-2.80	119.94	125.10
27	B1	2562	OMG	C8-N7-C5	2.80	108.33	102.99
27	B1	55	OMG	C8-N7-C5	2.80	108.32	102.99
27	B1	1557	OMG	C8-N7-C5	2.80	108.32	102.99
1	A1	1368	OMU	O4-C4-C5	-2.80	120.24	125.16
27	B1	2984	OMG	C8-N7-C5	2.80	108.32	102.99
27	B1	2022	OMG	C8-N7-C5	2.79	108.31	102.99
1	A1	541	OMG	C8-N7-C5	2.79	108.31	102.99
27	B1	454	OMU	O4-C4-C5	-2.79	120.25	125.16
27	B1	841	OMG	C8-N7-C5	2.79	108.30	102.99
1	A1	8	OMU	O4-C4-C5	-2.79	120.25	125.16
27	B1	1293	4AC	N4-C4-N3	2.79	118.53	113.85
27	B1	2968	4AC	O4'-C4'-C5'	2.79	118.55	109.37
27	B1	1488	OMU	O4-C4-C5	-2.79	120.26	125.16
1	A1	455	OMG	C8-N7-C5	2.79	108.30	102.99
27	B1	887	OMG	C8-N7-C5	2.79	108.30	102.99
27	B1	2540	OMG	C8-N7-C5	2.78	108.29	102.99
27	B1	1904	OMG	C2-N1-C6	-2.78	119.97	125.10
27	B1	921	OMG	C8-N7-C5	2.78	108.29	102.99
27	B1	808	OMG	C8-N7-C5	2.78	108.28	102.99
1	A1	861	OMG	C2-N1-C6	-2.78	119.98	125.10
27	B1	530	OMG	C8-N7-C5	2.78	108.28	102.99
27	B1	2365	OMG	C8-N7-C5	2.77	108.27	102.99
1	A1	668	OMG	C8-N7-C5	2.76	108.24	102.99
1	A1	861	OMG	C8-N7-C5	2.75	108.24	102.99
27	B1	920	OMG	C8-N7-C5	2.75	108.24	102.99
27	B1	2526	4AC	O4'-C4'-C5'	2.75	118.43	109.37
27	B1	2028	OMG	C8-N7-C5	2.75	108.23	102.99
1	A1	238	LHH	C5-C4-N4	-2.75	118.15	122.92
1	A1	578	4AC	O4'-C4'-C5'	2.75	118.41	109.37
27	B1	1293	4AC	C6-C5-C4	2.75	120.32	116.96
1	A1	645	OMG	C8-N7-C5	2.74	108.22	102.99
27	B1	732	4AC	N4-C4-N3	2.74	118.45	113.85
27	B1	2391	OMG	C8-N7-C5	2.74	108.21	102.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B1	1608	4AC	N4-C4-N3	2.74	118.45	113.85
27	B1	227	4AC	N4-C4-N3	2.72	118.42	113.85
27	B1	1360	4AC	C6-C5-C4	2.72	120.29	116.96
28	B2	30	4AC	N4-C4-N3	2.72	118.42	113.85
1	A1	459	OMG	C8-N7-C5	2.71	108.16	102.99
1	A1	1181	4AC	N4-C4-N3	2.71	118.41	113.85
1	A1	507	OMG	C8-N7-C5	2.71	108.15	102.99
27	B1	2684	OMG	C8-N7-C5	2.69	108.12	102.99
1	A1	1484	5MC	C5-C6-N1	-2.69	120.57	123.34
27	B1	1374	4AC	C6-C5-C4	2.69	120.26	116.96
28	B2	88	4AC	N4-C4-N3	2.69	118.37	113.85
27	B1	1743	4AC	N4-C4-N3	2.69	118.37	113.85
27	B1	1965	OMG	C8-N7-C5	2.69	108.11	102.99
27	B1	933	4AC	C6-C5-C4	2.69	120.25	116.96
27	B1	3006	4AC	N4-C4-N3	2.69	118.36	113.85
1	A1	775	OMU	O4-C4-C5	-2.68	120.45	125.16
1	A1	87	4AC	N4-C4-N3	2.68	118.35	113.85
1	A1	681	5MC	O4'-C4'-C5'	2.68	118.18	109.37
27	B1	1904	OMG	C8-N7-C5	2.68	108.09	102.99
27	B1	2557	OMC	C5'-C4'-C3'	2.67	125.20	115.18
27	B1	1579	4AC	C6-C5-C4	2.67	120.23	116.96
1	A1	1254	4AC	O4'-C4'-C5'	2.67	118.17	109.37
1	A1	231	4AC	C6-C5-C4	2.67	120.23	116.96
27	B1	1639	4AC	C6-C5-C4	2.67	120.23	116.96
27	B1	2557	OMC	O4'-C4'-C5'	2.67	118.14	109.37
1	A1	216	4AC	C6-C5-C4	2.66	120.22	116.96
1	A1	761	4AC	N4-C4-N3	2.66	118.31	113.85
1	A1	1467	4AC	C6-C5-C4	2.66	120.21	116.96
27	B1	1649	4AC	C6-C5-C4	2.65	120.21	116.96
27	B1	1822	4AC	C6-C5-C4	2.65	120.21	116.96
1	A1	578	4AC	N4-C4-N3	2.65	118.30	113.85
27	B1	19	4AC	C6-C5-C4	2.65	120.20	116.96
1	A1	945	4AC	C6-C5-C4	2.64	120.20	116.96
1	A1	827	4AC	C6-C5-C4	2.64	120.19	116.96
27	B1	3020	4AC	N4-C4-N3	2.64	118.29	113.85
27	B1	1150	4AC	C6-C5-C4	2.64	120.19	116.96
27	B1	2876	4AC	C6-C5-C4	2.64	120.19	116.96
1	A1	624	4AC	C6-C5-C4	2.64	120.19	116.96
1	A1	739	4AC	C6-C5-C4	2.63	120.18	116.96
1	A1	1254	4AC	N4-C4-N3	2.63	118.27	113.85
1	A1	719	4AC	N4-C4-N3	2.63	118.27	113.85
27	B1	2821	4AC	C6-C5-C4	2.63	120.18	116.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B1	950	4AC	N4-C4-N3	2.63	118.27	113.85
27	B1	2968	4AC	C5'-C4'-C3'	2.63	125.03	115.18
1	A1	1181	4AC	C5'-C4'-C3'	2.62	125.02	115.18
27	B1	2526	4AC	C5'-C4'-C3'	2.62	125.01	115.18
28	B2	115	4AC	C6-C5-C4	2.62	120.17	116.96
1	A1	761	4AC	C6-C5-C4	2.62	120.17	116.96
1	A1	546	4AC	C6-C5-C4	2.62	120.16	116.96
27	B1	227	4AC	C6-C5-C4	2.62	120.16	116.96
27	B1	527	4AC	C6-C5-C4	2.61	120.16	116.96
27	B1	2454	4AC	C6-C5-C4	2.61	120.16	116.96
27	B1	162	4AC	C6-C5-C4	2.61	120.16	116.96
27	B1	1383	4AC	N4-C4-N3	2.61	118.24	113.85
1	A1	614	4AC	N4-C4-N3	2.61	118.23	113.85
1	A1	534	4AC	N4-C4-N3	2.61	118.23	113.85
27	B1	479	4AC	C6-C5-C4	2.61	120.15	116.96
27	B1	933	4AC	N4-C4-N3	2.61	118.23	113.85
1	A1	5	4AC	C6-C5-C4	2.61	120.15	116.96
27	B1	3020	4AC	C6-C5-C4	2.60	120.15	116.96
1	A1	578	4AC	C5'-C4'-C3'	2.60	124.94	115.18
27	B1	1706	4AC	C6-C5-C4	2.60	120.14	116.96
1	A1	856	4AC	C6-C5-C4	2.60	120.14	116.96
27	B1	2526	4AC	N4-C4-N3	2.60	118.22	113.85
28	B2	115	4AC	N4-C4-N3	2.60	118.22	113.85
27	B1	866	4AC	C6-C5-C4	2.60	120.14	116.96
1	A1	141	4AC	C6-C5-C4	2.60	120.14	116.96
27	B1	1264	4AC	C6-C5-C4	2.60	120.14	116.96
1	A1	274	4AC	C6-C5-C4	2.60	120.14	116.96
27	B1	344	4AC	N4-C4-N3	2.60	118.21	113.85
27	B1	344	4AC	C6-C5-C4	2.59	120.13	116.96
27	B1	1505	4AC	C6-C5-C4	2.59	120.13	116.96
1	A1	816	4AC	C6-C5-C4	2.59	120.13	116.96
1	A1	1314	4AC	C6-C5-C4	2.59	120.13	116.96
27	B1	419	4AC	N4-C4-N3	2.59	118.20	113.85
27	B1	1064	4AC	N4-C4-N3	2.59	118.20	113.85
27	B1	80	4AC	C6-C5-C4	2.59	120.13	116.96
27	B1	19	4AC	N4-C4-N3	2.59	118.19	113.85
27	B1	1546	4AC	N4-C4-N3	2.59	118.19	113.85
1	A1	636	4AC	N4-C4-N3	2.58	118.19	113.85
27	B1	1100	4AC	C6-C5-C4	2.58	120.12	116.96
27	B1	1383	4AC	C6-C5-C4	2.58	120.12	116.96
27	B1	1064	4AC	C6-C5-C4	2.58	120.12	116.96
27	B1	652	4AC	C6-C5-C4	2.58	120.12	116.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	836	4AC	C6-C5-C4	2.58	120.12	116.96
27	B1	2379	4AC	C6-C5-C4	2.58	120.12	116.96
27	B1	688	4AC	C6-C5-C4	2.58	120.11	116.96
1	A1	540	4AC	C6-C5-C4	2.58	120.11	116.96
1	A1	578	4AC	C6-C5-C4	2.58	120.11	116.96
27	B1	360	4AC	C6-C5-C4	2.58	120.11	116.96
27	B1	1360	4AC	C5-C4-N3	-2.57	118.45	122.59
27	B1	1751	4AC	C6-C5-C4	2.57	120.11	116.96
1	A1	739	4AC	N4-C4-N3	2.57	118.17	113.85
27	B1	1052	4AC	C6-C5-C4	2.57	120.10	116.96
27	B1	337	4AC	C6-C5-C4	2.57	120.10	116.96
1	A1	534	4AC	C6-C5-C4	2.57	120.10	116.96
27	B1	1751	4AC	N4-C4-N3	2.56	118.16	113.85
27	B1	3037	4AC	N4-C4-N3	2.56	118.16	113.85
27	B1	360	4AC	N4-C4-N3	2.56	118.15	113.85
27	B1	979	4AC	N4-C4-N3	2.56	118.15	113.85
27	B1	2809	4AC	C6-C5-C4	2.56	120.09	116.96
1	A1	1254	4AC	C6-C5-C4	2.56	120.09	116.96
1	A1	499	4AC	C6-C5-C4	2.55	120.09	116.96
27	B1	434	4AC	C6-C5-C4	2.55	120.09	116.96
27	B1	786	4AC	C6-C5-C4	2.55	120.08	116.96
27	B1	2968	4AC	C6-C5-C4	2.55	120.08	116.96
27	B1	1052	4AC	N4-C4-N3	2.55	118.14	113.85
27	B1	1846	4AC	C6-C5-C4	2.55	120.08	116.96
27	B1	243	4AC	N4-C4-N3	2.55	118.14	113.85
1	A1	614	4AC	C6-C5-C4	2.55	120.08	116.96
27	B1	1608	4AC	C5'-C4'-C3'	2.55	124.72	115.18
27	B1	896	4AC	C6-C5-C4	2.55	120.08	116.96
1	A1	1254	4AC	C5'-C4'-C3'	2.54	124.72	115.18
1	A1	405	4AC	C6-C5-C4	2.54	120.07	116.96
27	B1	1501	4AC	C6-C5-C4	2.54	120.07	116.96
27	B1	1608	4AC	C6-C5-C4	2.54	120.07	116.96
1	A1	827	4AC	N4-C4-N3	2.54	118.12	113.85
27	B1	3011	4AC	C6-C5-C4	2.54	120.07	116.96
27	B1	3037	4AC	C6-C5-C4	2.54	120.07	116.96
27	B1	715	4AC	C6-C5-C4	2.54	120.06	116.96
27	B1	378	4AC	C6-C5-C4	2.54	120.06	116.96
27	B1	2171	4AC	O4'-C4'-C5'	2.54	117.72	109.37
1	A1	216	4AC	N4-C4-N3	2.53	118.11	113.85
27	B1	1435	4AC	C6-C5-C4	2.53	120.06	116.96
1	A1	839	4AC	C6-C5-C4	2.53	120.06	116.96
27	B1	1967	4AC	C6-C5-C4	2.53	120.06	116.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B1	2469	4AC	N4-C4-N3	2.53	118.10	113.85
27	B1	2844	4AC	N4-C4-N3	2.53	118.10	113.85
27	B1	2749	4AC	C6-C5-C4	2.53	120.05	116.96
27	B1	1178	4AC	N4-C4-N3	2.53	118.09	113.85
27	B1	1706	4AC	N4-C4-N3	2.53	118.09	113.85
27	B1	1846	4AC	N4-C4-N3	2.53	118.09	113.85
27	B1	1551	4AC	C6-C5-C4	2.52	120.05	116.96
27	B1	1885	4AC	C6-C5-C4	2.52	120.05	116.96
27	B1	1067	4AC	C6-C5-C4	2.52	120.05	116.96
27	B1	2469	4AC	C6-C5-C4	2.52	120.05	116.96
27	B1	1762	4AC	N4-C4-N3	2.52	118.09	113.85
27	B1	953	4AC	C6-C5-C4	2.52	120.05	116.96
1	A1	1029	4AC	C6-C5-C4	2.52	120.04	116.96
27	B1	2700	UR3	C6-N1-C2	-2.52	119.53	121.79
1	A1	636	4AC	C6-C5-C4	2.52	120.04	116.96
27	B1	1769	4AC	C6-C5-C4	2.52	120.04	116.96
27	B1	1293	4AC	C5'-C4'-C3'	2.52	124.61	115.18
27	B1	200	4AC	C6-C5-C4	2.52	120.04	116.96
27	B1	1061	4AC	C6-C5-C4	2.52	120.04	116.96
1	A1	87	4AC	C6-C5-C4	2.52	120.04	116.96
27	B1	162	4AC	N4-C4-N3	2.51	118.07	113.85
27	B1	2432	4AC	C6-C5-C4	2.51	120.04	116.96
27	B1	2008	4AC	C6-C5-C4	2.51	120.04	116.96
27	B1	378	4AC	N4-C4-N3	2.51	118.07	113.85
27	B1	1264	4AC	N4-C4-N3	2.51	118.07	113.85
27	B1	2020	4AC	C6-C5-C4	2.51	120.03	116.96
27	B1	2602	4AC	C6-C5-C4	2.51	120.03	116.96
27	B1	1911	4AC	C6-C5-C4	2.51	120.03	116.96
27	B1	1579	4AC	N4-C4-N3	2.51	118.06	113.85
27	B1	2454	4AC	N4-C4-N3	2.51	118.06	113.85
1	A1	307	4AC	C6-C5-C4	2.51	120.03	116.96
1	A1	499	4AC	N4-C4-N3	2.51	118.06	113.85
27	B1	1345	4AC	C6-C5-C4	2.50	120.03	116.96
1	A1	367	4AC	C6-C5-C4	2.50	120.02	116.96
27	B1	1150	4AC	N4-C4-N3	2.50	118.05	113.85
27	B1	80	4AC	N4-C4-N3	2.50	118.05	113.85
1	A1	291	4AC	C6-C5-C4	2.50	120.02	116.96
27	B1	1743	4AC	C6-C5-C4	2.50	120.02	116.96
27	B1	953	4AC	N4-C4-N3	2.50	118.05	113.85
1	A1	691	4AC	C6-C5-C4	2.50	120.02	116.96
27	B1	419	4AC	C6-C5-C4	2.50	120.02	116.96
27	B1	2171	4AC	N4-C4-N3	2.50	118.05	113.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	220	4AC	C6-C5-C4	2.50	120.02	116.96
27	B1	1818	4AC	N4-C4-N3	2.50	118.05	113.85
27	B1	1639	4AC	N4-C4-N3	2.50	118.04	113.85
27	B1	23	4AC	C6-C5-C4	2.50	120.02	116.96
27	B1	98	4AC	C6-C5-C4	2.50	120.02	116.96
27	B1	580	4AC	C6-C5-C4	2.50	120.02	116.96
27	B1	1290	4AC	C6-C5-C4	2.50	120.02	116.96
1	A1	1467	4AC	C5-C4-N3	-2.49	118.58	122.59
27	B1	1128	4AC	C6-C5-C4	2.49	120.01	116.96
27	B1	2792	4AC	C6-C5-C4	2.49	120.01	116.96
27	B1	527	4AC	N4-C4-N3	2.49	118.03	113.85
28	B2	88	4AC	C6-C5-C4	2.49	120.01	116.96
27	B1	732	4AC	C6-C5-C4	2.49	120.00	116.96
1	A1	540	4AC	N4-C4-N3	2.49	118.03	113.85
27	B1	116	4AC	C6-C5-C4	2.49	120.00	116.96
27	B1	2171	4AC	C5'-C4'-C3'	2.48	124.49	115.18
27	B1	2113	4AC	C6-C5-C4	2.48	120.00	116.96
27	B1	2133	4AC	C6-C5-C4	2.48	120.00	116.96
27	B1	2492	4AC	C6-C5-C4	2.48	120.00	116.96
27	B1	2526	4AC	C6-C5-C4	2.48	119.99	116.96
1	A1	706	4AC	C6-C5-C4	2.48	119.99	116.96
27	B1	2876	4AC	N4-C4-N3	2.47	118.01	113.85
27	B1	1818	4AC	C6-C5-C4	2.47	119.99	116.96
27	B1	479	4AC	N4-C4-N3	2.47	118.00	113.85
1	A1	231	4AC	N4-C4-N3	2.47	118.00	113.85
27	B1	1107	4AC	C6-C5-C4	2.47	119.98	116.96
27	B1	1478	4AC	C6-C5-C4	2.47	119.98	116.96
27	B1	1546	4AC	C6-C5-C4	2.47	119.98	116.96
27	B1	2844	4AC	C6-C5-C4	2.46	119.98	116.96
27	B1	2968	4AC	N4-C4-N3	2.46	117.99	113.85
1	A1	5	4AC	N4-C4-N3	2.46	117.99	113.85
1	A1	467	4AC	C6-C5-C4	2.46	119.97	116.96
27	B1	2492	4AC	N4-C4-N3	2.46	117.99	113.85
27	B1	950	4AC	C6-C5-C4	2.46	119.97	116.96
27	B1	1435	4AC	N4-C4-N3	2.46	117.98	113.85
1	A1	41	4AC	C6-C5-C4	2.46	119.97	116.96
27	B1	688	4AC	N4-C4-N3	2.46	117.98	113.85
27	B1	130	4AC	C6-C5-C4	2.46	119.97	116.96
27	B1	786	4AC	N4-C4-N3	2.46	117.98	113.85
1	A1	1181	4AC	C6-C5-C4	2.46	119.97	116.96
27	B1	926	OMU	C1'-N1-C2	2.46	122.02	117.57
27	B1	3011	4AC	N4-C4-N3	2.45	117.97	113.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B1	434	4AC	N4-C4-N3	2.45	117.97	113.85
27	B1	130	4AC	N4-C4-N3	2.45	117.97	113.85
1	A1	405	4AC	N4-C4-N3	2.45	117.97	113.85
27	B1	1442	4AC	C6-C5-C4	2.45	119.96	116.96
27	B1	243	4AC	C6-C5-C4	2.45	119.96	116.96
27	B1	1178	4AC	C6-C5-C4	2.45	119.96	116.96
27	B1	896	4AC	N4-C4-N3	2.45	117.96	113.85
27	B1	2821	4AC	N4-C4-N3	2.45	117.96	113.85
27	B1	2850	4AC	C6-C5-C4	2.44	119.95	116.96
1	A1	382	4AC	N4-C4-N3	2.44	117.95	113.85
27	B1	1946	4AC	C6-C5-C4	2.44	119.95	116.96
1	A1	681	5MC	C5'-C4'-C3'	2.44	124.33	115.18
1	A1	816	4AC	N4-C4-N3	2.44	117.95	113.85
1	A1	466	5MC	CM5-C5-C6	-2.44	119.59	122.85
27	B1	485	4AC	C6-C5-C4	2.44	119.94	116.96
27	B1	1946	4AC	N4-C4-N3	2.43	117.94	113.85
1	A1	141	4AC	N4-C4-N3	2.43	117.94	113.85
1	A1	382	4AC	C6-C5-C4	2.43	119.94	116.96
1	A1	546	4AC	N4-C4-N3	2.43	117.94	113.85
27	B1	98	4AC	N4-C4-N3	2.43	117.93	113.85
27	B1	200	4AC	N4-C4-N3	2.43	117.93	113.85
1	A1	951	5MC	C5-C6-N1	-2.43	120.84	123.34
27	B1	23	4AC	N4-C4-N3	2.43	117.93	113.85
27	B1	721	4AC	C6-C5-C4	2.42	119.93	116.96
27	B1	454	OMU	C1'-N1-C2	2.42	121.96	117.57
28	B2	30	4AC	C6-C5-C4	2.42	119.93	116.96
27	B1	866	4AC	N4-C4-N3	2.42	117.92	113.85
27	B1	2432	4AC	N4-C4-N3	2.42	117.92	113.85
27	B1	1061	4AC	N4-C4-N3	2.42	117.92	113.85
27	B1	2429	4AC	C6-C5-C4	2.42	119.92	116.96
1	A1	291	4AC	N4-C4-N3	2.42	117.92	113.85
27	B1	1345	4AC	N4-C4-N3	2.42	117.91	113.85
27	B1	1649	4AC	N4-C4-N3	2.42	117.91	113.85
1	A1	719	4AC	C6-C5-C4	2.42	119.92	116.96
27	B1	3006	4AC	C6-C5-C4	2.42	119.92	116.96
27	B1	116	4AC	N4-C4-N3	2.41	117.91	113.85
27	B1	1360	4AC	O7-C7-N4	-2.41	117.91	121.82
27	B1	1551	4AC	N4-C4-N3	2.41	117.90	113.85
27	B1	2792	4AC	N4-C4-N3	2.41	117.90	113.85
27	B1	2171	4AC	C6-C5-C4	2.41	119.91	116.96
1	A1	220	4AC	N4-C4-N3	2.41	117.89	113.85
27	B1	2213	4AC	N4-C4-N3	2.41	117.89	113.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	41	4AC	N4-C4-N3	2.40	117.89	113.85
27	B1	48	4AC	C6-C5-C4	2.40	119.90	116.96
1	A1	367	4AC	N4-C4-N3	2.40	117.88	113.85
1	A1	1029	4AC	N4-C4-N3	2.39	117.87	113.85
27	B1	2850	4AC	N4-C4-N3	2.39	117.87	113.85
27	B1	2213	4AC	C6-C5-C4	2.39	119.89	116.96
27	B1	979	4AC	C6-C5-C4	2.39	119.89	116.96
1	A1	274	4AC	N4-C4-N3	2.38	117.86	113.85
27	B1	1762	4AC	C6-C5-C4	2.38	119.88	116.96
1	A1	1467	4AC	O7-C7-N4	-2.38	117.96	121.82
27	B1	1946	4AC	C5-C4-N3	-2.38	118.76	122.59
1	A1	1314	4AC	N4-C4-N3	2.38	117.85	113.85
27	B1	485	4AC	CM7-C7-N4	2.38	119.41	115.29
27	B1	715	4AC	N4-C4-N3	2.38	117.84	113.85
27	B1	1067	4AC	C5-C4-N3	-2.38	118.77	122.59
27	B1	2749	4AC	N4-C4-N3	2.37	117.84	113.85
27	B1	1107	4AC	N4-C4-N3	2.37	117.82	113.85
27	B1	1100	4AC	N4-C4-N3	2.36	117.82	113.85
27	B1	1067	4AC	N4-C4-N3	2.36	117.82	113.85
27	B1	502	LHH	CM7-C7-N4	2.36	119.38	115.29
27	B1	2602	4AC	N4-C4-N3	2.36	117.81	113.85
27	B1	337	4AC	N4-C4-N3	2.35	117.81	113.85
1	A1	1227	4AC	C6-C5-C4	2.35	119.84	116.96
1	A1	839	4AC	N4-C4-N3	2.35	117.79	113.85
27	B1	2809	4AC	N4-C4-N3	2.34	117.78	113.85
1	A1	307	4AC	N4-C4-N3	2.34	117.78	113.85
27	B1	652	4AC	N4-C4-N3	2.34	117.78	113.85
27	B1	2113	4AC	N4-C4-N3	2.34	117.77	113.85
27	B1	1442	4AC	N4-C4-N3	2.34	117.77	113.85
27	B1	1107	4AC	C5-C4-N3	-2.34	118.83	122.59
1	A1	945	4AC	CM7-C7-N4	2.33	119.33	115.29
27	B1	1435	4AC	C5-C4-N3	-2.33	118.85	122.59
27	B1	721	4AC	N4-C4-N3	2.32	117.75	113.85
27	B1	1505	4AC	N4-C4-N3	2.32	117.75	113.85
27	B1	1293	4AC	C5-C4-N3	-2.31	118.87	122.59
27	B1	580	4AC	N4-C4-N3	2.31	117.74	113.85
27	B1	3006	4AC	C5-C4-N3	-2.31	118.87	122.59
1	A1	719	4AC	C5-C4-N3	-2.31	118.87	122.59
28	B2	30	4AC	C5-C4-N3	-2.31	118.88	122.59
27	B1	2008	4AC	N4-C4-N3	2.31	117.73	113.85
27	B1	1911	4AC	N4-C4-N3	2.30	117.72	113.85
27	B1	2133	4AC	N4-C4-N3	2.29	117.70	113.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	856	4AC	N4-C4-N3	2.29	117.69	113.85
27	B1	1264	4AC	C5-C4-N3	-2.28	118.93	122.59
27	B1	950	4AC	C5-C4-N3	-2.28	118.93	122.59
27	B1	1290	4AC	N4-C4-N3	2.27	117.67	113.85
27	B1	2429	4AC	N4-C4-N3	2.27	117.67	113.85
27	B1	530	OMG	O6-C6-C5	-2.27	119.93	124.37
1	A1	578	4AC	C5-C4-N3	-2.27	118.94	122.59
1	A1	636	4AC	C5-C4-N3	-2.27	118.94	122.59
1	A1	541	OMG	O6-C6-C5	-2.27	119.94	124.37
27	B1	1064	4AC	C5-C4-N3	-2.27	118.95	122.59
28	B2	115	4AC	C2'-C1'-N1	2.27	119.63	113.22
27	B1	1885	4AC	N4-C4-N3	2.26	117.65	113.85
27	B1	2020	4AC	N4-C4-N3	2.26	117.65	113.85
27	B1	2171	4AC	C5-C4-N3	-2.26	118.95	122.59
27	B1	1360	4AC	O7-C7-CM7	-2.26	117.86	122.06
1	A1	668	OMG	O6-C6-C5	-2.26	119.96	124.37
27	B1	1178	4AC	C5-C4-N3	-2.26	118.96	122.59
1	A1	5	4AC	C5-C4-N3	-2.25	118.97	122.59
1	A1	624	4AC	CM7-C7-N4	2.25	119.19	115.29
27	B1	841	OMG	O6-C6-C5	-2.25	119.97	124.37
1	A1	238	LHH	CM7-C7-N4	2.25	119.19	115.29
1	A1	307	4AC	C5-C4-N3	-2.25	118.97	122.59
27	B1	1374	4AC	C5-C4-N3	-2.25	118.97	122.59
27	B1	2850	4AC	C5-C4-N3	-2.25	118.97	122.59
27	B1	2540	OMG	O6-C6-C5	-2.25	119.98	124.37
27	B1	1293	4AC	CM7-C7-N4	2.25	119.18	115.29
27	B1	856	OMG	O6-C6-C5	-2.25	119.98	124.37
27	B1	2984	OMG	O6-C6-C5	-2.25	119.98	124.37
27	B1	808	OMG	O6-C6-C5	-2.25	119.98	124.37
27	B1	1478	4AC	C5-C4-N3	-2.25	118.98	122.59
1	A1	329	OMG	O6-C6-C5	-2.25	119.98	124.37
27	B1	2492	4AC	C5-C4-N3	-2.25	118.98	122.59
27	B1	1501	4AC	C5-C4-N3	-2.25	118.98	122.59
27	B1	527	4AC	C5-C4-N3	-2.24	118.98	122.59
27	B1	721	4AC	C5-C4-N3	-2.24	118.98	122.59
27	B1	887	OMG	O6-C6-C5	-2.24	119.99	124.37
1	A1	856	4AC	C5-C4-N3	-2.24	118.98	122.59
1	A1	459	OMG	O6-C6-C5	-2.24	120.00	124.37
1	A1	645	OMG	O6-C6-C5	-2.24	120.00	124.37
27	B1	1128	4AC	N4-C4-N3	2.24	117.61	113.85
1	A1	1003	OMG	O6-C6-C5	-2.24	120.00	124.37
27	B1	1769	4AC	N4-C4-N3	2.24	117.61	113.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B1	652	4AC	C5-C4-N3	-2.24	118.99	122.59
27	B1	1965	OMG	O6-C6-C5	-2.24	120.00	124.37
1	A1	945	4AC	C5-C4-N3	-2.24	118.99	122.59
27	B1	1822	4AC	N4-C4-N3	2.23	117.60	113.85
27	B1	130	4AC	C5-C4-N3	-2.23	119.00	122.59
27	B1	336	5MC	CM5-C5-C6	-2.23	119.86	122.85
27	B1	1818	4AC	C5-C4-N3	-2.23	119.00	122.59
27	B1	2968	4AC	C5-C4-N3	-2.23	119.00	122.59
27	B1	116	4AC	C5-C4-N3	-2.23	119.00	122.59
27	B1	1557	OMG	O6-C6-C5	-2.23	120.02	124.37
1	A1	382	4AC	C5-C4-N3	-2.23	119.00	122.59
27	B1	2492	4AC	CM7-C7-N4	2.23	119.15	115.29
27	B1	2365	OMG	O6-C6-C5	-2.23	120.02	124.37
1	A1	1115	OMG	O6-C6-C5	-2.23	120.02	124.37
27	B1	1546	4AC	C5-C4-N3	-2.23	119.01	122.59
27	B1	2684	OMG	O6-C6-C5	-2.22	120.03	124.37
27	B1	2113	4AC	C5-C4-N3	-2.22	119.02	122.59
27	B1	1374	4AC	CM7-C7-N4	2.22	119.14	115.29
27	B1	1551	4AC	C5-C4-N3	-2.22	119.02	122.59
27	B1	2028	OMG	O6-C6-C5	-2.22	120.04	124.37
27	B1	2391	OMG	O6-C6-C5	-2.22	120.04	124.37
27	B1	2432	4AC	C5-C4-N3	-2.22	119.02	122.59
27	B1	2526	4AC	C5-C4-N3	-2.22	119.03	122.59
1	A1	836	4AC	N4-C4-N3	2.22	117.57	113.85
27	B1	2749	4AC	C5-C4-N3	-2.22	119.03	122.59
27	B1	2757	OMG	O6-C6-C5	-2.21	120.05	124.37
27	B1	2108	OMG	O6-C6-C5	-2.21	120.05	124.37
27	B1	2213	4AC	C5-C4-N3	-2.21	119.03	122.59
27	B1	2562	OMG	O6-C6-C5	-2.21	120.06	124.37
1	A1	8	OMU	O2'-C2'-C1'	2.21	113.39	109.08
1	A1	455	OMG	O6-C6-C5	-2.21	120.06	124.37
27	B1	2757	OMG	N2-C2-N1	2.21	121.42	116.71
27	B1	1967	4AC	N4-C4-N3	2.21	117.56	113.85
1	A1	405	4AC	C5-C4-N3	-2.21	119.04	122.59
1	A1	1467	4AC	O7-C7-CM7	-2.21	117.96	122.06
27	B1	979	4AC	C5-C4-N3	-2.21	119.04	122.59
1	A1	827	4AC	C5-C4-N3	-2.21	119.04	122.59
27	B1	2020	4AC	C5-C4-N3	-2.20	119.05	122.59
27	B1	1579	4AC	CM7-C7-N4	2.20	119.10	115.29
1	A1	706	4AC	N4-C4-N3	2.20	117.55	113.85
27	B1	786	4AC	C5-C4-N3	-2.20	119.05	122.59
27	B1	888	5MU	C1'-N1-C2	2.20	121.56	117.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	546	4AC	C5-C4-N3	-2.20	119.05	122.59
28	B2	88	4AC	C5-C4-N3	-2.20	119.05	122.59
1	A1	507	OMG	O6-C6-C5	-2.20	120.08	124.37
1	A1	706	4AC	CM7-C7-N4	2.20	119.10	115.29
27	B1	419	4AC	CM7-C7-N4	2.20	119.10	115.29
27	B1	920	OMG	O6-C6-C5	-2.20	120.08	124.37
27	B1	1383	4AC	C5-C4-N3	-2.20	119.06	122.59
27	B1	2022	OMG	O6-C6-C5	-2.20	120.08	124.37
1	A1	614	4AC	C5-C4-N3	-2.19	119.06	122.59
1	A1	1362	5MC	CM5-C5-C6	-2.19	119.92	122.85
27	B1	732	4AC	C5-C4-N3	-2.19	119.06	122.59
1	A1	1314	4AC	C5-C4-N3	-2.19	119.07	122.59
1	A1	636	4AC	CM7-C7-N4	2.19	119.08	115.29
1	A1	761	4AC	CM7-C7-N4	2.19	119.08	115.29
27	B1	23	4AC	C5-C4-N3	-2.19	119.07	122.59
1	A1	534	4AC	C5-C4-N3	-2.19	119.07	122.59
1	A1	540	4AC	C5-C4-N3	-2.19	119.07	122.59
1	A1	624	4AC	C5-C4-N3	-2.19	119.07	122.59
27	B1	378	4AC	C5-C4-N3	-2.19	119.07	122.59
27	B1	715	4AC	C5-C4-N3	-2.19	119.07	122.59
27	B1	1706	4AC	C5-C4-N3	-2.19	119.07	122.59
27	B1	19	4AC	C5-C4-N3	-2.19	119.07	122.59
27	B1	2876	4AC	C5-C4-N3	-2.19	119.08	122.59
27	B1	580	4AC	C5-C4-N3	-2.18	119.08	122.59
27	B1	1478	4AC	N4-C4-N3	2.18	117.52	113.85
1	A1	951	5MC	CM5-C5-C6	-2.18	119.93	122.85
27	B1	1546	4AC	CM7-C7-N4	2.18	119.07	115.29
1	A1	1254	4AC	C5-C4-N3	-2.18	119.08	122.59
27	B1	2180	OMG	O6-C6-C5	-2.18	120.11	124.37
1	A1	863	5MC	CM5-C5-C6	-2.18	119.94	122.85
1	A1	761	4AC	C5-C4-N3	-2.18	119.08	122.59
27	B1	1846	4AC	C5-C4-N3	-2.18	119.08	122.59
1	A1	17	5MC	CM5-C5-C6	-2.18	119.94	122.85
1	A1	5	4AC	CM7-C7-N4	2.18	119.06	115.29
27	B1	1967	4AC	C5-C4-N3	-2.18	119.09	122.59
27	B1	953	4AC	C5-C4-N3	-2.18	119.09	122.59
27	B1	243	4AC	C5-C4-N3	-2.18	119.09	122.59
1	A1	861	OMG	O6-C6-C5	-2.17	120.12	124.37
1	A1	1029	4AC	C5-C4-N3	-2.17	119.09	122.59
27	B1	1762	4AC	CM7-C7-N4	2.17	119.06	115.29
27	B1	1846	4AC	CM7-C7-N4	2.17	119.06	115.29
27	B1	1608	4AC	CM7-C7-N4	2.17	119.05	115.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B1	162	4AC	C5-C4-N3	-2.17	119.09	122.59
27	B1	1751	4AC	C5-C4-N3	-2.17	119.10	122.59
1	A1	87	4AC	C5-C4-N3	-2.17	119.10	122.59
27	B1	162	4AC	CM7-C7-N4	2.17	119.05	115.29
27	B1	419	4AC	C5-C4-N3	-2.17	119.10	122.59
27	B1	360	4AC	C5-C4-N3	-2.17	119.10	122.59
27	B1	1052	4AC	C5-C4-N3	-2.17	119.10	122.59
27	B1	2429	4AC	C5-C4-N3	-2.17	119.10	122.59
27	B1	2565	4SU	O2-C2-N1	-2.17	119.90	122.79
1	A1	274	4AC	CM7-C7-N4	2.17	119.04	115.29
27	B1	485	4AC	C5-C4-N3	-2.17	119.11	122.59
27	B1	55	OMG	O6-C6-C5	-2.17	120.14	124.37
1	A1	41	4AC	C5-C4-N3	-2.17	119.11	122.59
1	A1	231	4AC	C5-C4-N3	-2.17	119.11	122.59
1	A1	578	4AC	CM7-C7-N4	2.17	119.04	115.29
27	B1	1579	4AC	C5-C4-N3	-2.17	119.11	122.59
1	A1	274	4AC	C5-C4-N3	-2.16	119.11	122.59
27	B1	200	4AC	C5-C4-N3	-2.16	119.11	122.59
27	B1	479	4AC	C5-C4-N3	-2.16	119.11	122.59
27	B1	1290	4AC	C5-C4-N3	-2.16	119.11	122.59
1	A1	839	4AC	C5-C4-N3	-2.16	119.11	122.59
27	B1	214	OMG	O6-C6-C5	-2.16	120.15	124.37
27	B1	2526	4AC	CM7-C7-N4	2.16	119.03	115.29
27	B1	1442	4AC	C5-C4-N3	-2.16	119.12	122.59
27	B1	1743	4AC	C5-C4-N3	-2.16	119.12	122.59
27	B1	1649	4AC	C5-C4-N3	-2.16	119.12	122.59
27	B1	1769	4AC	C5-C4-N3	-2.16	119.12	122.59
28	B2	115	4AC	C5-C4-N3	-2.16	119.12	122.59
27	B1	1885	4AC	C5-C4-N3	-2.15	119.13	122.59
1	A1	739	4AC	CM7-C7-N4	2.15	119.02	115.29
27	B1	1442	4AC	CM7-C7-N4	2.15	119.02	115.29
27	B1	23	4AC	CM7-C7-N4	2.15	119.02	115.29
27	B1	1608	4AC	C5-C4-N3	-2.15	119.13	122.59
27	B1	786	4AC	CM7-C7-N4	2.15	119.02	115.29
1	A1	216	4AC	C5-C4-N3	-2.15	119.13	122.59
27	B1	1344	5MC	CM5-C5-C6	-2.15	119.98	122.85
27	B1	1743	4AC	CM7-C7-N4	2.15	119.01	115.29
27	B1	3037	4AC	CM7-C7-N4	2.15	119.01	115.29
28	B2	88	4AC	CM7-C7-N4	2.15	119.01	115.29
27	B1	1911	4AC	C5-C4-N3	-2.15	119.14	122.59
27	B1	2087	5MC	CM5-C5-C6	-2.15	119.98	122.85
27	B1	926	OMU	C2'-C3'-C4'	2.15	106.66	101.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	87	4AC	CM7-C7-N4	2.15	119.01	115.29
27	B1	200	4AC	CM7-C7-N4	2.15	119.01	115.29
1	A1	816	4AC	C5-C4-N3	-2.15	119.14	122.59
1	A1	719	4AC	CM7-C7-N4	2.15	119.01	115.29
27	B1	866	4AC	C5-C4-N3	-2.15	119.14	122.59
27	B1	2469	4AC	C5-C4-N3	-2.15	119.14	122.59
27	B1	2602	4AC	C5-C4-N3	-2.15	119.14	122.59
27	B1	2454	4AC	CM7-C7-N4	2.15	119.00	115.29
28	B2	115	4AC	CM7-C7-N4	2.15	119.00	115.29
1	A1	706	4AC	C5-C4-N3	-2.15	119.14	122.59
1	A1	739	4AC	C5-C4-N3	-2.14	119.14	122.59
27	B1	344	4AC	CM7-C7-N4	2.14	119.00	115.29
27	B1	1100	4AC	C5-C4-N3	-2.14	119.15	122.59
27	B1	1977	5MC	CM5-C5-C6	-2.14	119.99	122.85
27	B1	979	4AC	CM7-C7-N4	2.14	119.00	115.29
27	B1	933	4AC	C5-C4-N3	-2.14	119.15	122.59
27	B1	2379	4AC	C5-C4-N3	-2.14	119.15	122.59
1	A1	775	OMU	O2-C2-N1	-2.14	119.94	122.79
27	B1	2379	4AC	N4-C4-N3	2.14	117.44	113.85
27	B1	1501	4AC	CM7-C7-N4	2.14	118.99	115.29
27	B1	3020	4AC	C5-C4-N3	-2.14	119.15	122.59
1	A1	1254	4AC	CM7-C7-N4	2.14	118.99	115.29
1	A1	467	4AC	N4-C4-N3	2.14	117.44	113.85
1	A1	499	4AC	C5-C4-N3	-2.13	119.16	122.59
27	B1	1762	4AC	C5-C4-N3	-2.13	119.16	122.59
1	A1	1368	OMU	O2-C2-N1	-2.13	119.95	122.79
27	B1	1904	OMG	O6-C6-C5	-2.13	120.21	124.37
27	B1	921	OMG	O6-C6-C5	-2.13	120.21	124.37
1	A1	405	4AC	CM7-C7-N4	2.13	118.98	115.29
27	B1	2454	4AC	C5-C4-N3	-2.13	119.16	122.59
1	A1	216	4AC	CM7-C7-N4	2.13	118.98	115.29
1	A1	291	4AC	C5-C4-N3	-2.13	119.16	122.59
27	B1	1639	4AC	C5-C4-N3	-2.13	119.16	122.59
27	B1	2133	4AC	C5-C4-N3	-2.13	119.17	122.59
1	A1	361	A2M	C5-C6-N6	2.13	123.59	120.35
27	B1	344	4AC	C5-C4-N3	-2.13	119.17	122.59
27	B1	688	4AC	C5-C4-N3	-2.13	119.17	122.59
27	B1	1345	4AC	C5-C4-N3	-2.13	119.17	122.59
27	B1	2821	4AC	C5-C4-N3	-2.13	119.17	122.59
27	B1	1264	4AC	CM7-C7-N4	2.13	118.97	115.29
28	B2	30	4AC	CM7-C7-N4	2.13	118.97	115.29
27	B1	2968	4AC	CM7-C7-N4	2.13	118.97	115.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	691	4AC	C5-C4-N3	-2.12	119.17	122.59
27	B1	479	4AC	CM7-C7-N4	2.12	118.97	115.29
27	B1	1067	4AC	CM7-C7-N4	2.12	118.97	115.29
1	A1	352	5MC	CM5-C5-C6	-2.12	120.01	122.85
27	B1	3037	4AC	C5-C4-N3	-2.12	119.18	122.59
27	B1	580	4AC	CM7-C7-N4	2.12	118.97	115.29
27	B1	2067	5MC	CM5-C5-C6	-2.12	120.02	122.85
27	B1	227	4AC	C5-C4-N3	-2.12	119.18	122.59
27	B1	2602	4AC	CM7-C7-N4	2.12	118.96	115.29
1	A1	1013	5MC	CM5-C5-C6	-2.12	120.02	122.85
1	A1	367	4AC	C5-C4-N3	-2.12	119.18	122.59
1	A1	534	4AC	CM7-C7-N4	2.12	118.96	115.29
27	B1	1435	4AC	CM7-C7-N4	2.12	118.96	115.29
27	B1	3020	4AC	CM7-C7-N4	2.12	118.96	115.29
27	B1	2844	4AC	C5-C4-N3	-2.12	119.19	122.59
1	A1	307	4AC	CM7-C7-N4	2.12	118.96	115.29
1	A1	540	4AC	CM7-C7-N4	2.12	118.96	115.29
1	A1	546	4AC	CM7-C7-N4	2.12	118.95	115.29
27	B1	1383	4AC	CM7-C7-N4	2.12	118.95	115.29
27	B1	1649	4AC	CM7-C7-N4	2.12	118.95	115.29
27	B1	2432	4AC	CM7-C7-N4	2.12	118.95	115.29
27	B1	3006	4AC	CM7-C7-N4	2.12	118.95	115.29
27	B1	2008	4AC	C5-C4-N3	-2.11	119.19	122.59
27	B1	1639	4AC	CM7-C7-N4	2.11	118.95	115.29
27	B1	2469	4AC	CM7-C7-N4	2.11	118.95	115.29
27	B1	1751	4AC	CM7-C7-N4	2.11	118.95	115.29
27	B1	19	4AC	CM7-C7-N4	2.11	118.95	115.29
27	B1	2792	4AC	C5-C4-N3	-2.11	119.20	122.59
27	B1	48	4AC	N4-C4-N3	2.11	117.40	113.85
27	B1	933	4AC	CM7-C7-N4	2.11	118.94	115.29
1	A1	220	4AC	C5-C4-N3	-2.11	119.20	122.59
27	B1	1061	4AC	C5-C4-N3	-2.11	119.20	122.59
1	A1	1029	4AC	CM7-C7-N4	2.11	118.94	115.29
27	B1	2213	4AC	CM7-C7-N4	2.11	118.94	115.29
1	A1	756	4SU	O2-C2-N1	-2.11	119.98	122.79
27	B1	434	4AC	C5-C4-N3	-2.11	119.20	122.59
27	B1	80	4AC	CM7-C7-N4	2.11	118.94	115.29
27	B1	1064	4AC	CM7-C7-N4	2.11	118.94	115.29
27	B1	2113	4AC	CM7-C7-N4	2.11	118.94	115.29
27	B1	1150	4AC	C5-C4-N3	-2.10	119.21	122.59
27	B1	1551	4AC	CM7-C7-N4	2.10	118.93	115.29
27	B1	337	4AC	C5-C4-N3	-2.10	119.21	122.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B1	1706	4AC	CM7-C7-N4	2.10	118.93	115.29
27	B1	688	4AC	CM7-C7-N4	2.10	118.93	115.29
27	B1	1128	4AC	C5-C4-N3	-2.10	119.21	122.59
27	B1	2850	4AC	CM7-C7-N4	2.10	118.93	115.29
27	B1	2391	OMG	N2-C2-N1	2.10	121.18	116.71
27	B1	732	4AC	CM7-C7-N4	2.10	118.92	115.29
1	A1	927	5MC	CM5-C5-C6	-2.10	120.05	122.85
1	A1	839	4AC	CM7-C7-N4	2.10	118.92	115.29
27	B1	360	4AC	CM7-C7-N4	2.10	118.92	115.29
27	B1	2809	4AC	C5-C4-N3	-2.10	119.22	122.59
27	B1	1822	4AC	C5-C4-N3	-2.09	119.22	122.59
1	A1	291	4AC	CM7-C7-N4	2.09	118.92	115.29
1	A1	499	4AC	CM7-C7-N4	2.09	118.92	115.29
27	B1	2008	4AC	CM7-C7-N4	2.09	118.92	115.29
27	B1	3011	4AC	C5-C4-N3	-2.09	119.22	122.59
27	B1	2020	4AC	CM7-C7-N4	2.09	118.91	115.29
27	B1	2876	4AC	CM7-C7-N4	2.09	118.91	115.29
27	B1	1052	4AC	CM7-C7-N4	2.09	118.91	115.29
27	B1	1885	4AC	CM7-C7-N4	2.09	118.91	115.29
27	B1	2171	4AC	CM7-C7-N4	2.09	118.91	115.29
1	A1	687	5MC	CM5-C5-C6	-2.09	120.06	122.85
27	B1	130	4AC	CM7-C7-N4	2.09	118.91	115.29
27	B1	2821	4AC	CM7-C7-N4	2.09	118.91	115.29
27	B1	715	4AC	CM7-C7-N4	2.09	118.91	115.29
1	A1	231	4AC	CM7-C7-N4	2.09	118.91	115.29
1	A1	614	4AC	CM7-C7-N4	2.09	118.91	115.29
27	B1	80	4AC	C5-C4-N3	-2.09	119.23	122.59
1	A1	856	4AC	CM7-C7-N4	2.09	118.90	115.29
27	B1	1061	4AC	CM7-C7-N4	2.09	118.90	115.29
27	B1	1505	4AC	C5-C4-N3	-2.09	119.24	122.59
27	B1	1818	4AC	CM7-C7-N4	2.09	118.90	115.29
1	A1	230	5MC	CM5-C5-C6	-2.09	120.06	122.85
1	A1	220	4AC	CM7-C7-N4	2.08	118.90	115.29
1	A1	827	4AC	CM7-C7-N4	2.08	118.90	115.29
27	B1	243	4AC	CM7-C7-N4	2.08	118.90	115.29
27	B1	2133	4AC	CM7-C7-N4	2.08	118.90	115.29
27	B1	1505	4AC	CM7-C7-N4	2.08	118.89	115.29
27	B1	2429	4AC	CM7-C7-N4	2.08	118.89	115.29
27	B1	866	4AC	CM7-C7-N4	2.08	118.89	115.29
27	B1	1178	4AC	CM7-C7-N4	2.08	118.89	115.29
27	B1	434	4AC	CM7-C7-N4	2.08	118.89	115.29
1	A1	836	4AC	C5-C4-N3	-2.08	119.25	122.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	1165	OMU	O2-C2-N1	-2.07	120.03	122.79
27	B1	1100	4AC	CM7-C7-N4	2.07	118.88	115.29
27	B1	652	4AC	CM7-C7-N4	2.07	118.88	115.29
27	B1	1290	4AC	CM7-C7-N4	2.07	118.88	115.29
27	B1	1822	4AC	CM7-C7-N4	2.07	118.88	115.29
27	B1	1439	LHH	O2-C2-N3	-2.07	118.96	122.33
27	B1	337	4AC	CM7-C7-N4	2.07	118.88	115.29
27	B1	98	4AC	C5-C4-N3	-2.07	119.26	122.59
27	B1	1478	4AC	CM7-C7-N4	2.07	118.87	115.29
27	B1	1911	4AC	CM7-C7-N4	2.07	118.87	115.29
1	A1	141	4AC	C5-C4-N3	-2.07	119.27	122.59
27	B1	98	4AC	CM7-C7-N4	2.06	118.86	115.29
27	B1	953	4AC	CM7-C7-N4	2.06	118.86	115.29
1	A1	1366	A1I59	O2-C2-N3	-2.06	118.97	122.33
27	B1	2792	4AC	CM7-C7-N4	2.06	118.86	115.29
1	A1	382	4AC	CM7-C7-N4	2.06	118.86	115.29
1	A1	816	4AC	CM7-C7-N4	2.06	118.86	115.29
27	B1	2809	4AC	CM7-C7-N4	2.06	118.86	115.29
27	B1	227	4AC	CM7-C7-N4	2.06	118.86	115.29
27	B1	1107	4AC	CM7-C7-N4	2.06	118.86	115.29
27	B1	3011	4AC	CM7-C7-N4	2.06	118.86	115.29
1	A1	1484	5MC	CM5-C5-C6	-2.06	120.10	122.85
27	B1	1128	4AC	CM7-C7-N4	2.06	118.85	115.29
27	B1	2749	4AC	CM7-C7-N4	2.06	118.85	115.29
27	B1	527	4AC	CM7-C7-N4	2.05	118.85	115.29
1	A1	141	4AC	CM7-C7-N4	2.05	118.85	115.29
27	B1	721	4AC	CM7-C7-N4	2.05	118.84	115.29
27	B1	2844	4AC	CM7-C7-N4	2.05	118.84	115.29
1	A1	1181	4AC	C5-C4-N3	-2.05	119.30	122.59
27	B1	1150	4AC	CM7-C7-N4	2.04	118.83	115.29
1	A1	41	4AC	CM7-C7-N4	2.04	118.83	115.29
1	A1	52	OMU	O2-C2-N1	-2.04	120.07	122.79
27	B1	1946	4AC	CM7-C7-N4	2.04	118.83	115.29
27	B1	896	4AC	C5-C4-N3	-2.04	119.31	122.59
27	B1	378	4AC	CM7-C7-N4	2.04	118.82	115.29
1	A1	1190	5MC	CM5-C5-C6	-2.03	120.14	122.85
1	A1	8	OMU	CM2-O2'-C2'	2.03	119.85	114.52
27	B1	116	4AC	CM7-C7-N4	2.03	118.80	115.29
1	A1	238	LHH	O2-C2-N3	-2.02	119.04	122.33
27	B1	48	4AC	C5-C4-N3	-2.02	119.34	122.59
1	A1	1314	4AC	CM7-C7-N4	2.02	118.79	115.29
1	A1	681	5MC	CM5-C5-C6	-2.02	120.15	122.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	691	4AC	CM7-C7-N4	2.02	118.79	115.29
1	A1	367	4AC	CM7-C7-N4	2.02	118.79	115.29
27	B1	950	4AC	CM7-C7-N4	2.02	118.79	115.29
1	A1	455	OMG	N2-C2-N1	2.01	121.00	116.71
1	A1	836	4AC	CM7-C7-N4	2.01	118.77	115.29
27	B1	1967	4AC	CM7-C7-N4	2.01	118.77	115.29
1	A1	329	OMG	N2-C2-N1	2.01	120.99	116.71
27	B1	2022	OMG	N2-C2-N1	2.01	120.98	116.71
1	A1	473	5MC	CM5-C5-C6	-2.00	120.17	122.85
1	A1	762	OMU	O2-C2-N1	-2.00	120.12	122.79
27	B1	1345	4AC	CM7-C7-N4	2.00	118.76	115.29

There are no chirality outliers.

All (138) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A1	8	OMU	C1'-C2'-O2'-CM2
1	A1	238	LHH	C5-C4-N4-C7
1	A1	238	LHH	N3-C4-N4-C7
1	A1	238	LHH	C3'-C4'-C5'-O5'
1	A1	238	LHH	O4'-C4'-C5'-O5'
1	A1	329	OMG	O4'-C4'-C5'-O5'
1	A1	329	OMG	C3'-C4'-C5'-O5'
1	A1	361	A2M	O4'-C4'-C5'-O5'
1	A1	466	5MC	C3'-C4'-C5'-O5'
1	A1	541	OMG	C3'-C4'-C5'-O5'
1	A1	819	A2M	O4'-C4'-C5'-O5'
1	A1	819	A2M	C3'-C4'-C5'-O5'
1	A1	951	5MC	C4'-C5'-O5'-P
1	A1	1270	OMC	C3'-C4'-C5'-O5'
1	A1	1270	OMC	O4'-C4'-C5'-O5'
1	A1	1476	MA6	O4'-C4'-C5'-O5'
1	A1	481	G7M	O4'-C4'-C5'-O5'
1	A1	827	4AC	O4'-C4'-C5'-O5'
1	A1	1366	A1I59	C3-C1-CM5-N5
27	B1	55	OMG	O4'-C4'-C5'-O5'
27	B1	55	OMG	C3'-C4'-C5'-O5'
27	B1	501	OMC	O4'-C4'-C5'-O5'
27	B1	856	OMG	O4'-C4'-C5'-O5'
27	B1	857	A2M	C3'-C4'-C5'-O5'
27	B1	979	4AC	O4'-C4'-C5'-O5'
27	B1	979	4AC	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	B1	1293	4AC	O4'-C4'-C5'-O5'
27	B1	1293	4AC	C3'-C4'-C5'-O5'
27	B1	1439	LHH	C3'-C4'-C5'-O5'
27	B1	1439	LHH	O4'-C4'-C5'-O5'
27	B1	1608	4AC	O4'-C4'-C5'-O5'
27	B1	1608	4AC	C3'-C4'-C5'-O5'
27	B1	2391	OMG	C4'-C5'-O5'-P
27	B1	2401	5MU	O4'-C1'-N1-C2
27	B1	2401	5MU	O4'-C1'-N1-C6
27	B1	2700	UR3	O4'-C1'-N1-C6
27	B1	2700	UR3	O4'-C1'-N1-C2
27	B1	2821	4AC	C3'-C4'-C5'-O5'
1	A1	17	5MC	O4'-C4'-C5'-O5'
1	A1	361	A2M	C3'-C4'-C5'-O5'
1	A1	1190	5MC	O4'-C4'-C5'-O5'
1	A1	1190	5MC	C3'-C4'-C5'-O5'
1	A1	1476	MA6	C3'-C4'-C5'-O5'
1	A1	481	G7M	C3'-C4'-C5'-O5'
1	A1	691	4AC	C3'-C4'-C5'-O5'
1	A1	827	4AC	C3'-C4'-C5'-O5'
27	B1	344	4AC	C3'-C4'-C5'-O5'
27	B1	501	OMC	C3'-C4'-C5'-O5'
27	B1	1383	4AC	O4'-C4'-C5'-O5'
27	B1	1557	OMG	O4'-C4'-C5'-O5'
27	B1	1557	OMG	C3'-C4'-C5'-O5'
27	B1	2821	4AC	O4'-C4'-C5'-O5'
1	A1	8	OMU	O4'-C4'-C5'-O5'
1	A1	17	5MC	C3'-C4'-C5'-O5'
1	A1	466	5MC	O4'-C4'-C5'-O5'
1	A1	541	OMG	O4'-C4'-C5'-O5'
1	A1	5	4AC	O4'-C4'-C5'-O5'
1	A1	691	4AC	O4'-C4'-C5'-O5'
1	A1	839	4AC	O4'-C4'-C5'-O5'
27	B1	116	4AC	O4'-C4'-C5'-O5'
27	B1	344	4AC	O4'-C4'-C5'-O5'
27	B1	688	4AC	O4'-C4'-C5'-O5'
27	B1	856	OMG	C3'-C4'-C5'-O5'
27	B1	857	A2M	O4'-C4'-C5'-O5'
27	B1	1383	4AC	C3'-C4'-C5'-O5'
27	B1	1489	OMC	C3'-C4'-C5'-O5'
27	B1	2391	OMG	C3'-C4'-C5'-O5'
27	B1	2429	4AC	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	B1	2429	4AC	C3'-C4'-C5'-O5'
28	B2	115	4AC	C3'-C4'-C5'-O5'
1	A1	775	OMU	C3'-C2'-O2'-CM2
1	A1	775	OMU	C2'-C1'-N1-C6
1	A1	87	4AC	O4'-C4'-C5'-O5'
27	B1	479	4AC	C3'-C4'-C5'-O5'
27	B1	1489	OMC	O4'-C4'-C5'-O5'
27	B1	1967	4AC	O4'-C4'-C5'-O5'
27	B1	2391	OMG	O4'-C4'-C5'-O5'
27	B1	2876	4AC	O4'-C4'-C5'-O5'
28	B2	115	4AC	O4'-C4'-C5'-O5'
27	B1	715	4AC	O4'-C4'-C5'-O5'
1	A1	499	4AC	C3'-C4'-C5'-O5'
27	B1	2607	OMC	O4'-C4'-C5'-O5'
1	A1	1467	4AC	O7-C7-N4-C4
1	A1	1467	4AC	CM7-C7-N4-C4
27	B1	1360	4AC	O7-C7-N4-C4
27	B1	1360	4AC	CM7-C7-N4-C4
1	A1	719	4AC	O4'-C4'-C5'-O5'
27	B1	2379	4AC	O4'-C4'-C5'-O5'
27	B1	2557	OMC	C4'-C5'-O5'-P
28	B2	115	4AC	C4'-C5'-O5'-P
1	A1	466	5MC	C4'-C5'-O5'-P
1	A1	5	4AC	C3'-C4'-C5'-O5'
27	B1	116	4AC	C3'-C4'-C5'-O5'
27	B1	2022	OMG	O4'-C4'-C5'-O5'
1	A1	775	OMU	C2'-C1'-N1-C2
1	A1	775	OMU	O4'-C1'-N1-C6
1	A1	1362	5MC	O4'-C4'-C5'-O5'
27	B1	479	4AC	O4'-C4'-C5'-O5'
27	B1	921	OMG	C3'-C4'-C5'-O5'
27	B1	1846	4AC	O4'-C4'-C5'-O5'
27	B1	926	OMU	O4'-C1'-N1-C6
27	B1	1557	OMG	C3'-C2'-O2'-CM2
1	A1	775	OMU	O4'-C1'-N1-C2
1	A1	839	4AC	C3'-C4'-C5'-O5'
27	B1	688	4AC	C3'-C4'-C5'-O5'
27	B1	2557	OMC	C3'-C4'-C5'-O5'
27	B1	926	OMU	C2'-C1'-N1-C2
27	B1	926	OMU	C2'-C1'-N1-C6
27	B1	2401	5MU	O4'-C4'-C5'-O5'
27	B1	926	OMU	O4'-C1'-N1-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	A1	499	4AC	O4'-C4'-C5'-O5'
27	B1	378	4AC	O4'-C4'-C5'-O5'
1	A1	455	OMG	O4'-C4'-C5'-O5'
1	A1	87	4AC	C3'-C4'-C5'-O5'
27	B1	715	4AC	C3'-C4'-C5'-O5'
27	B1	1967	4AC	C3'-C4'-C5'-O5'
27	B1	2876	4AC	C3'-C4'-C5'-O5'
27	B1	1557	OMG	C1'-C2'-O2'-CM2
1	A1	8	OMU	C2'-C1'-N1-C6
1	A1	329	OMG	C4'-C5'-O5'-P
1	A1	636	4AC	C2'-C1'-N1-C2
27	B1	479	4AC	C2'-C1'-N1-C2
27	B1	688	4AC	C2'-C1'-N1-C2
27	B1	1914	OMC	C2'-C1'-N1-C2
27	B1	2821	4AC	C2'-C1'-N1-C2
1	A1	1362	5MC	C3'-C4'-C5'-O5'
1	A1	8	OMU	O4'-C1'-N1-C6
1	A1	87	4AC	C2'-C1'-N1-C2
27	B1	979	4AC	C2'-C1'-N1-C2
27	B1	1052	4AC	C2'-C1'-N1-C2
1	A1	861	OMG	C4'-C5'-O5'-P
27	B1	2028	OMG	C4'-C5'-O5'-P
1	A1	706	4AC	O4'-C4'-C5'-O5'
1	A1	719	4AC	C3'-C4'-C5'-O5'
27	B1	2379	4AC	C3'-C4'-C5'-O5'
27	B1	2607	OMC	C3'-C4'-C5'-O5'
27	B1	502	LHH	N3-C4-N4-C7
27	B1	2429	4AC	C4'-C5'-O5'-P

There are no ring outliers.

176 monomers are involved in 268 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B1	856	OMG	1	0
27	B1	2492	4AC	4	0
27	B1	786	4AC	1	0
1	A1	761	4AC	1	0
27	B1	1489	OMC	2	0
27	B1	721	4AC	1	0
27	B1	3006	4AC	3	0
27	B1	1579	4AC	2	0
27	B1	2020	4AC	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B1	527	4AC	1	0
1	A1	856	4AC	1	0
1	A1	1254	4AC	1	0
27	B1	921	OMG	1	0
27	B1	1067	4AC	2	0
27	B1	1064	4AC	2	0
27	B1	1914	OMC	2	0
27	B1	1967	4AC	1	0
27	B1	2432	4AC	2	0
27	B1	2749	4AC	2	0
1	A1	839	4AC	2	0
1	A1	1467	4AC	2	0
1	A1	1013	5MC	1	0
1	A1	827	4AC	1	0
27	B1	1762	4AC	1	0
27	B1	530	OMG	1	0
27	B1	1608	4AC	1	0
27	B1	896	4AC	2	0
27	B1	688	4AC	1	0
1	A1	467	4AC	1	0
27	B1	1818	4AC	2	0
1	A1	274	4AC	1	0
27	B1	1639	4AC	1	0
27	B1	1345	4AC	1	0
1	A1	52	OMU	1	0
27	B1	337	4AC	3	0
27	B1	419	4AC	2	0
27	B1	2008	4AC	1	0
27	B1	48	4AC	2	0
1	A1	546	4AC	1	0
27	B1	1478	4AC	2	0
27	B1	887	OMG	1	0
1	A1	499	4AC	2	0
1	A1	1227	4AC	1	0
1	A1	739	4AC	1	0
27	B1	243	4AC	2	0
27	B1	2850	4AC	1	0
27	B1	2876	4AC	1	0
27	B1	1505	4AC	1	0
27	B1	2133	4AC	1	0
27	B1	1150	4AC	1	0
1	A1	945	4AC	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A1	706	4AC	2	0
27	B1	116	4AC	1	0
27	B1	2454	4AC	1	0
27	B1	479	4AC	1	0
27	B1	715	4AC	1	0
27	B1	1290	4AC	1	0
1	A1	507	OMG	1	0
1	A1	816	4AC	2	0
27	B1	1360	4AC	7	0
27	B1	1546	4AC	2	0
27	B1	1822	4AC	1	0
27	B1	2792	4AC	1	0
27	B1	933	4AC	2	0
27	B1	979	4AC	2	0
27	B1	2684	OMG	1	0
1	A1	1364	OMC	1	0
1	A1	367	4AC	1	0
28	B2	88	4AC	2	0
1	A1	5	4AC	1	0
1	A1	541	OMG	1	0
27	B1	1100	4AC	1	0
27	B1	23	4AC	1	0
27	B1	1264	4AC	1	0
27	B1	1911	4AC	1	0
1	A1	836	4AC	1	0
1	A1	41	4AC	1	0
27	B1	920	OMG	2	0
27	B1	2401	5MU	1	0
27	B1	98	4AC	1	0
27	B1	1374	4AC	3	0
27	B1	3020	4AC	1	0
27	B1	2171	4AC	2	0
27	B1	1946	4AC	1	0
27	B1	2526	4AC	1	0
1	A1	534	4AC	1	0
27	B1	1769	4AC	4	0
1	A1	668	OMG	1	0
27	B1	3011	4AC	1	0
27	B1	2213	4AC	2	0
27	B1	953	4AC	1	0
27	B1	2602	4AC	1	0
1	A1	540	4AC	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A1	1368	OMU	1	0
27	B1	434	4AC	1	0
27	B1	1052	4AC	3	0
1	A1	614	4AC	1	0
27	B1	55	OMG	1	0
27	B1	378	4AC	2	0
27	B1	2113	4AC	2	0
27	B1	360	4AC	1	0
1	A1	1029	4AC	1	0
1	A1	775	OMU	1	0
27	B1	1442	4AC	1	0
27	B1	1977	5MC	1	0
27	B1	1107	4AC	3	0
1	A1	220	4AC	2	0
27	B1	80	4AC	1	0
1	A1	1366	A1I59	2	0
27	B1	926	OMU	1	0
27	B1	1501	4AC	2	0
27	B1	1885	4AC	2	0
28	B2	30	4AC	3	0
27	B1	1435	4AC	2	0
1	A1	1476	MA6	3	0
1	A1	141	4AC	1	0
27	B1	506	A2M	1	0
1	A1	1226	OMC	1	0
1	A1	578	4AC	2	0
27	B1	454	OMU	1	0
1	A1	329	OMG	1	0
1	A1	382	4AC	1	0
27	B1	1383	4AC	1	0
1	A1	87	4AC	2	0
27	B1	485	4AC	3	0
27	B1	2067	5MC	1	0
27	B1	2809	4AC	2	0
1	A1	636	4AC	3	0
27	B1	130	4AC	1	0
1	A1	1314	4AC	4	0
27	B1	3037	4AC	2	0
27	B1	732	4AC	1	0
27	B1	888	5MU	1	0
27	B1	2844	4AC	2	0
27	B1	200	4AC	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B1	866	4AC	1	0
28	B2	115	4AC	2	0
27	B1	1706	4AC	1	0
27	B1	950	4AC	2	0
1	A1	719	4AC	2	0
27	B1	1649	4AC	1	0
1	A1	951	5MC	4	0
1	A1	216	4AC	1	0
27	B1	2469	4AC	1	0
1	A1	624	4AC	4	0
27	B1	2617	5MC	6	0
27	B1	2968	4AC	1	0
1	A1	352	5MC	1	0
27	B1	2429	4AC	2	0
27	B1	1751	4AC	1	0
1	A1	231	4AC	1	0
27	B1	344	4AC	1	0
1	A1	1475	MA6	3	0
1	A1	1457	MA6	2	0
27	B1	19	4AC	1	0
27	B1	2821	4AC	1	0
27	B1	1128	4AC	1	0
27	B1	162	4AC	1	0
27	B1	580	4AC	1	0
1	A1	307	4AC	2	0
27	B1	1551	4AC	1	0
1	A1	405	4AC	2	0
27	B1	1293	4AC	2	0
27	B1	1488	OMU	1	0
1	A1	691	4AC	4	0
27	B1	2562	OMG	2	0
27	B1	1178	4AC	2	0
27	B1	2379	4AC	2	0
1	A1	291	4AC	1	0
1	A1	1181	4AC	4	0
27	B1	227	4AC	1	0
27	B1	1061	4AC	1	0
27	B1	1846	4AC	2	0
27	B1	652	4AC	1	0
27	B1	857	A2M	1	0
27	B1	1743	4AC	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 13 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

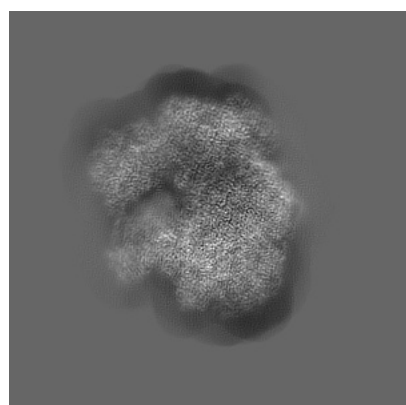
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53100. These allow visual inspection of the internal detail of the map and identification of artifacts.

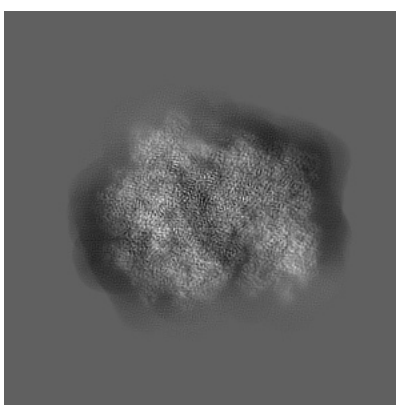
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

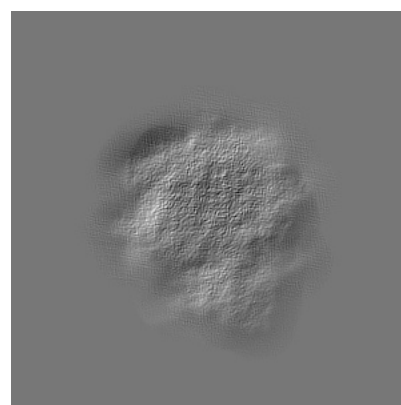
6.1.1 Primary map



X



Y

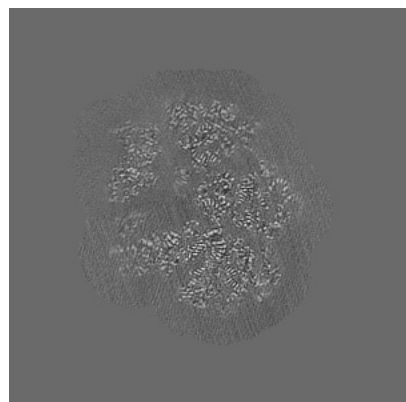


Z

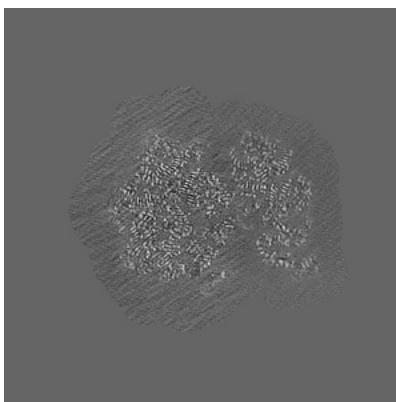
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

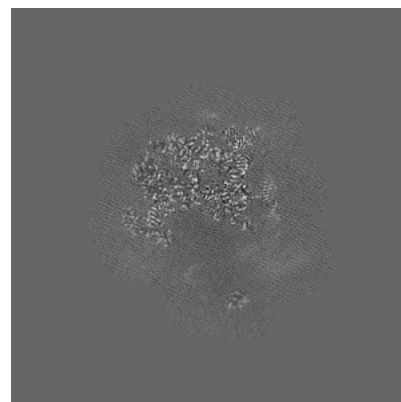
6.2.1 Primary map



X Index: 224



Y Index: 224

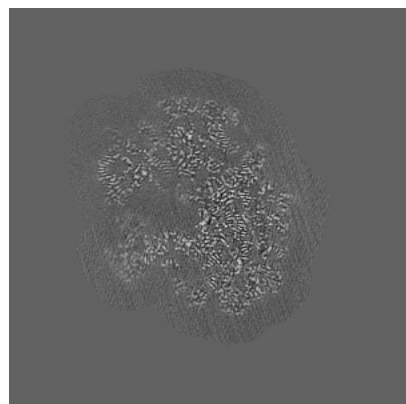


Z Index: 224

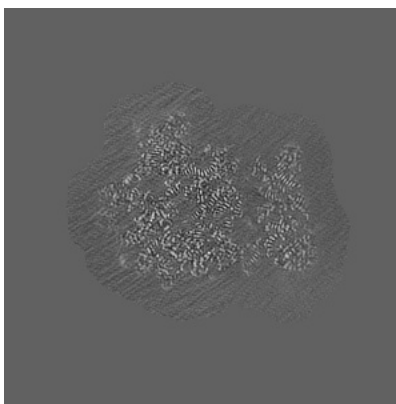
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

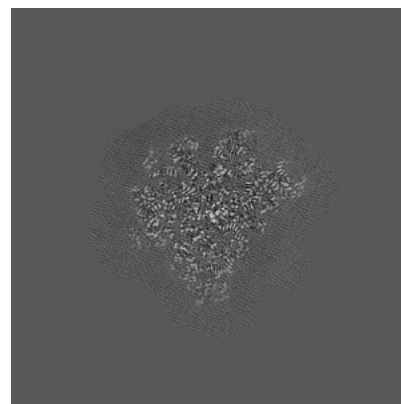
6.3.1 Primary map



X Index: 238



Y Index: 242

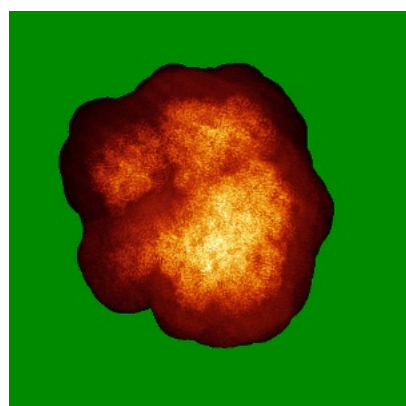


Z Index: 182

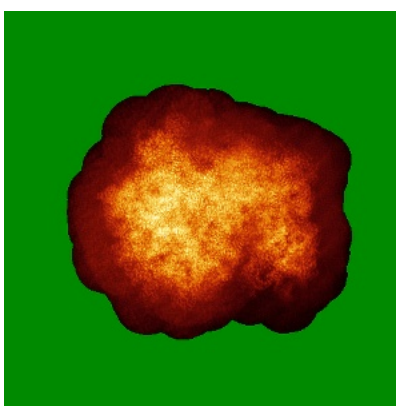
The images above show the largest variance slices of the map in three orthogonal directions.

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

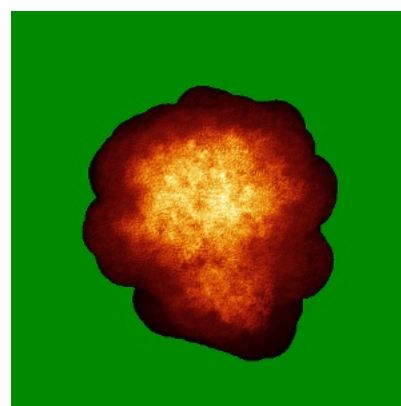
6.4.1 Primary map



X



Y

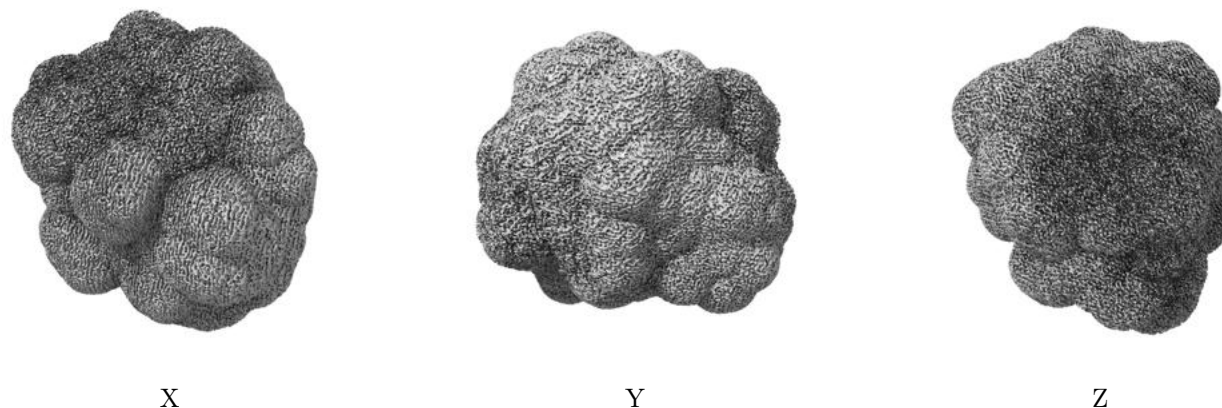


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.0083. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

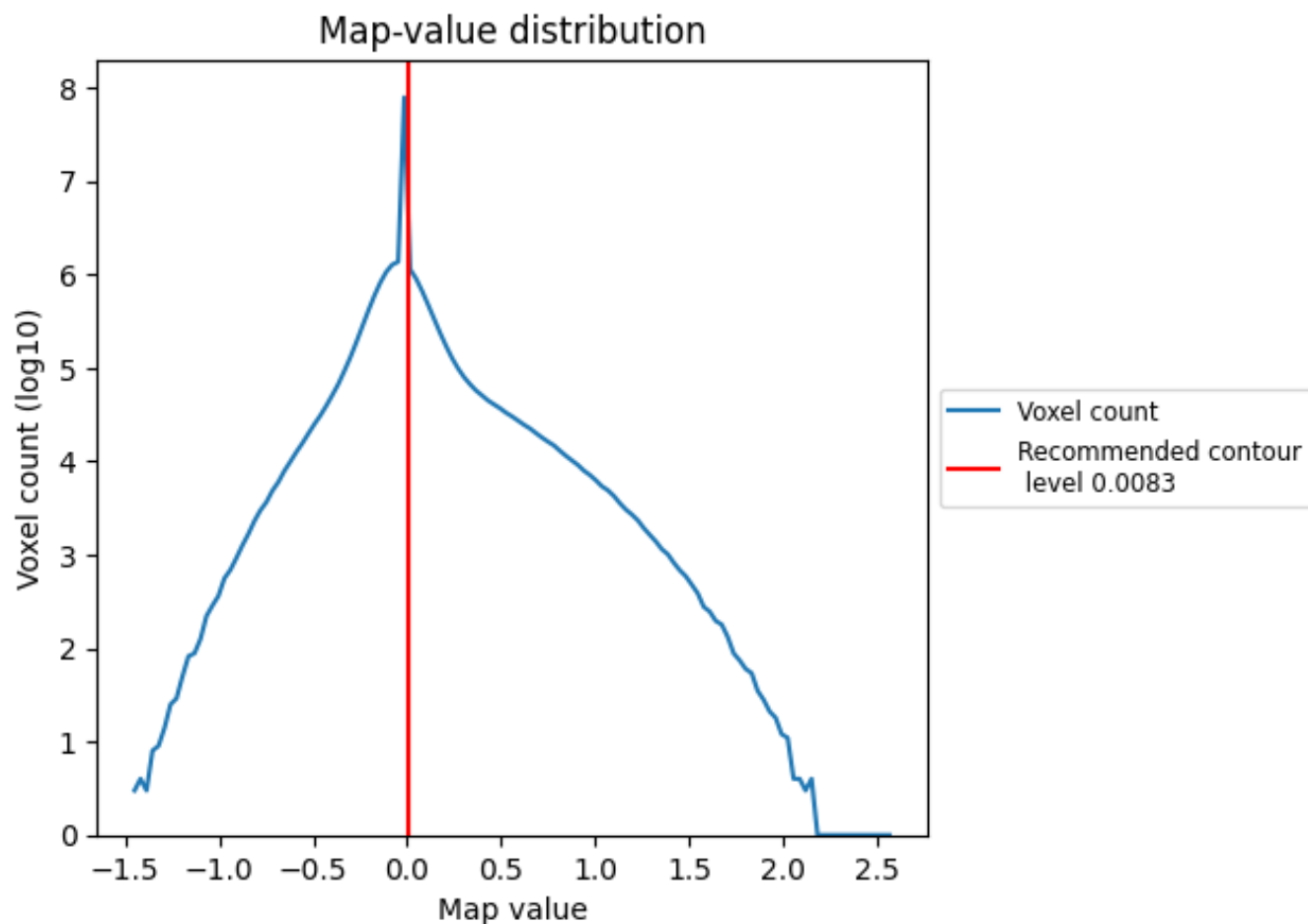
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

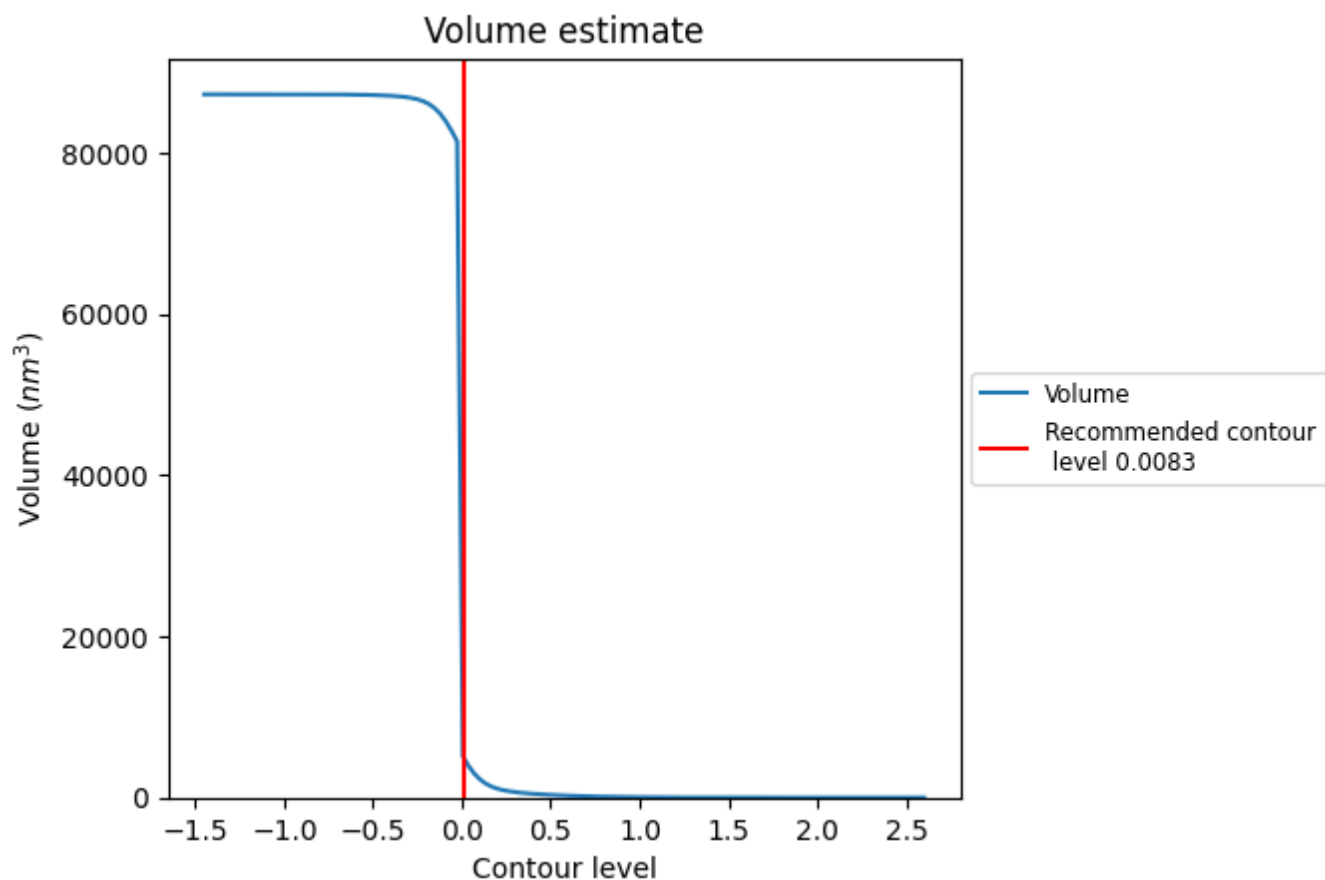
This section contains the results of statistical analysis of the map.

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.

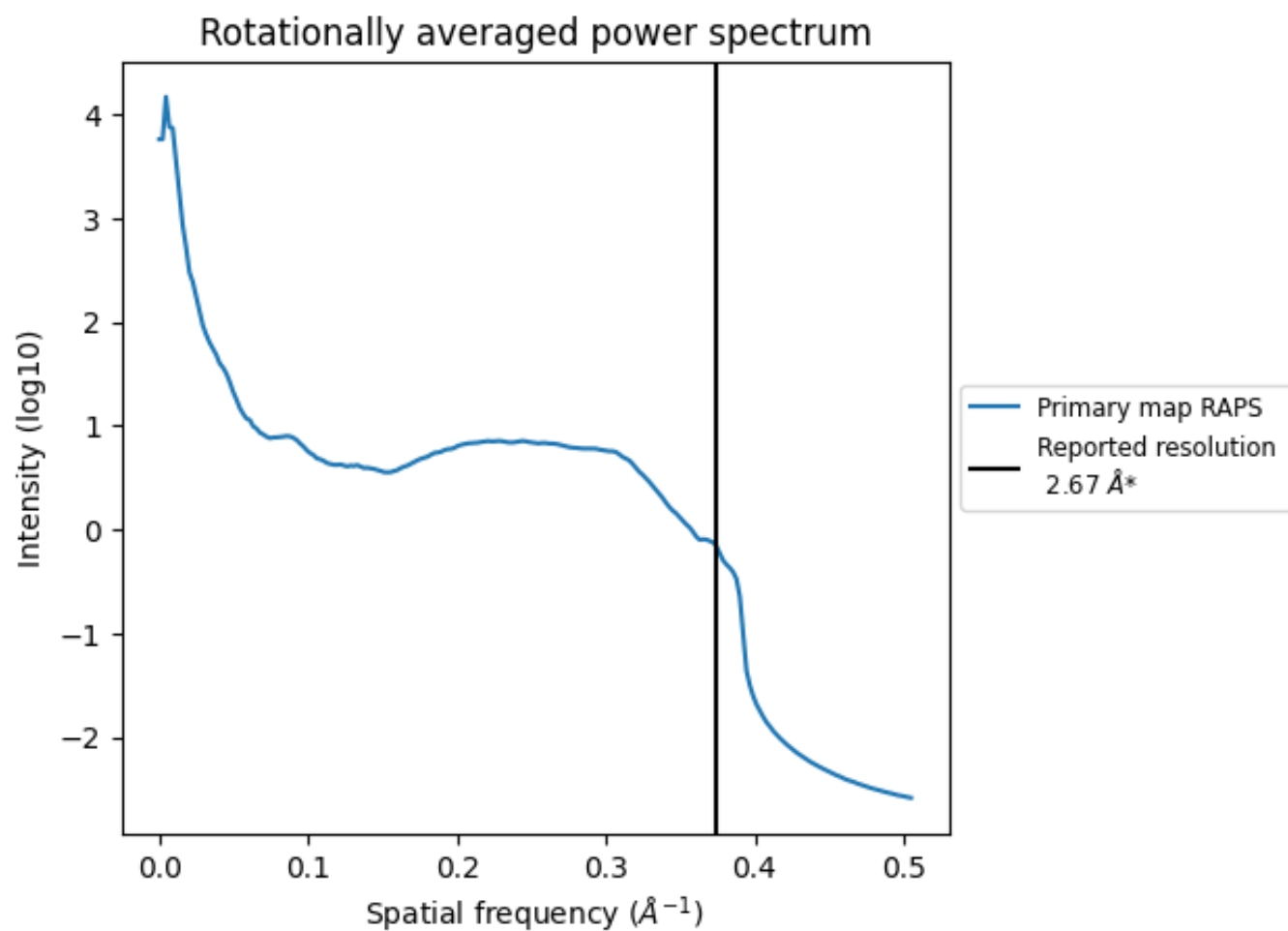
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5004 nm³; this corresponds to an approximate mass of 4520 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



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

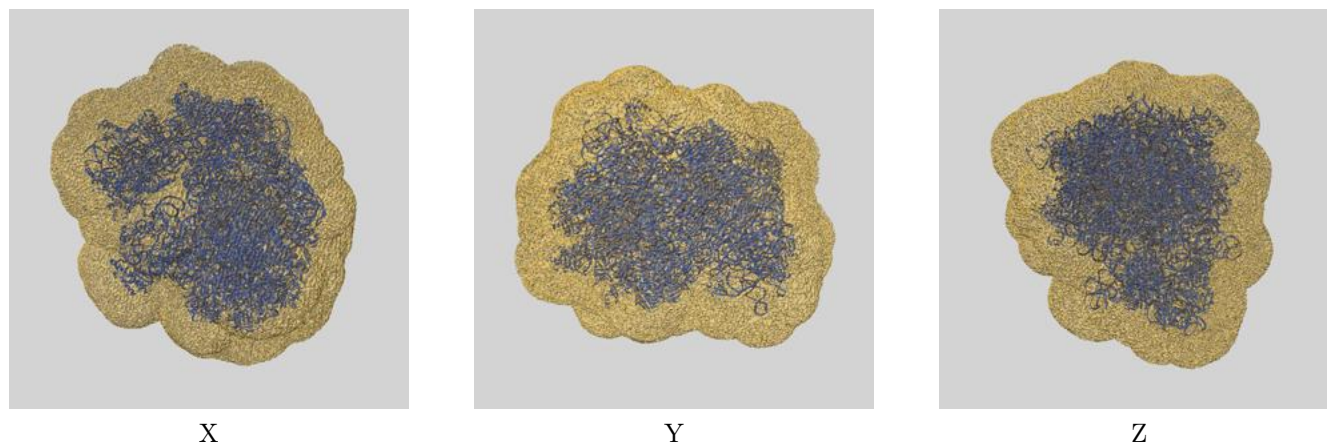
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

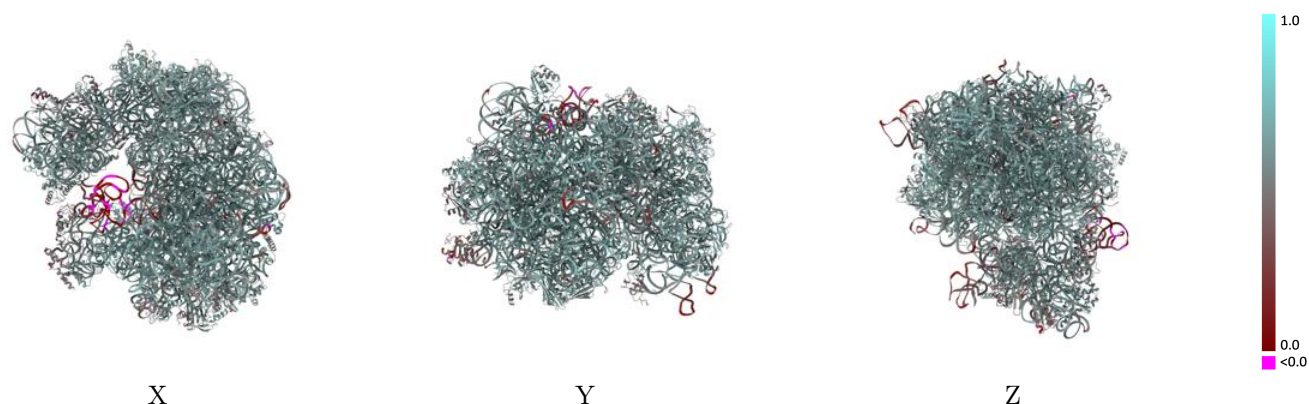
This section contains information regarding the fit between EMDB map EMD-53100 and PDB model 9QF6. Per-residue inclusion information can be found in section [3](#) on page [18](#).

9.1 Map-model overlay [i](#)



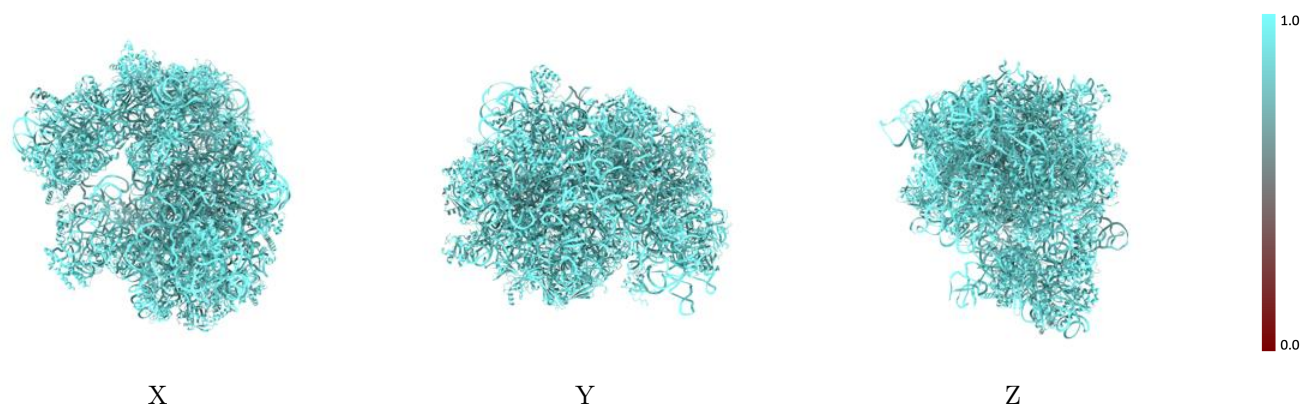
The images above show the 3D surface view of the map at the recommended contour level 0.0083 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



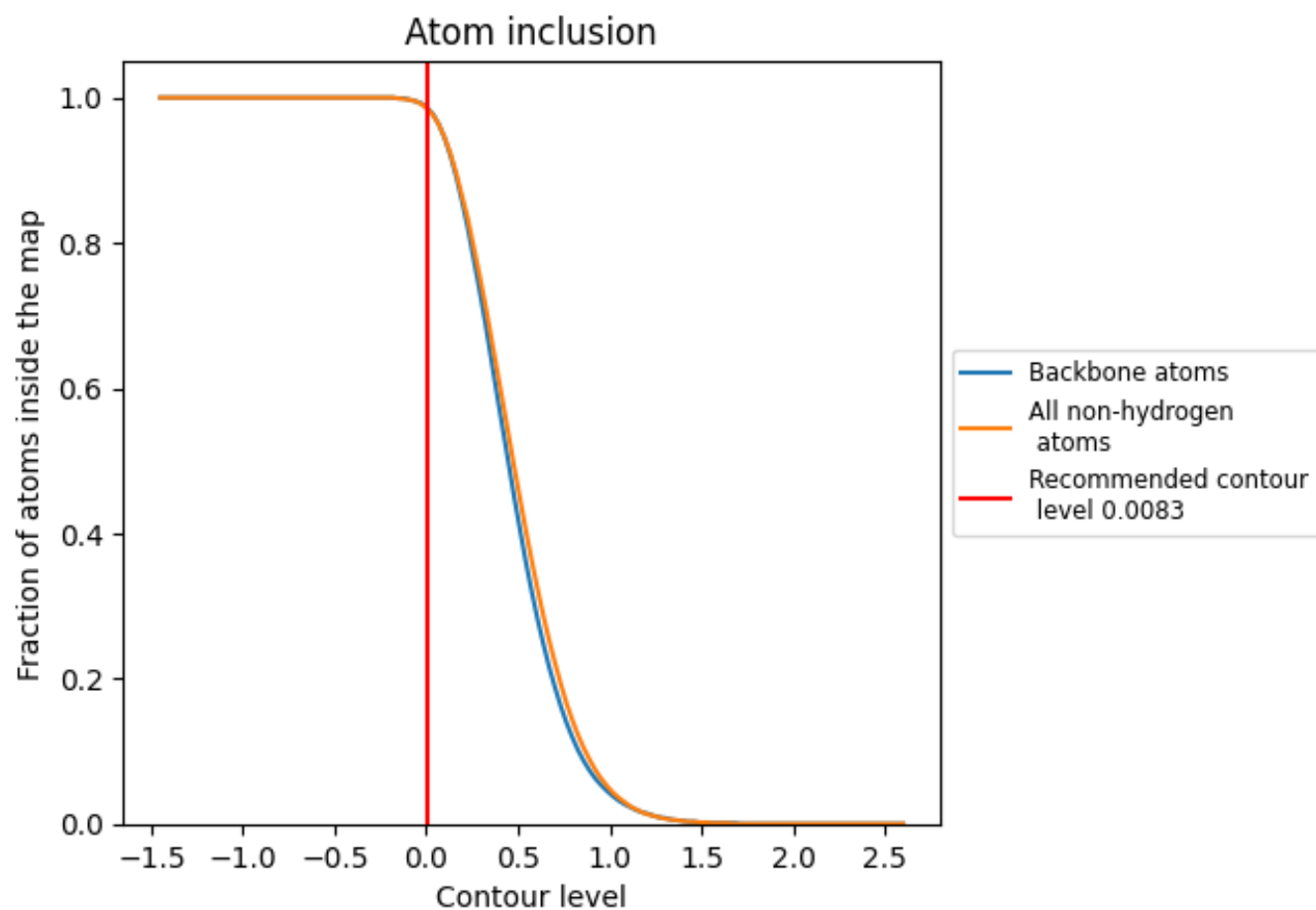
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0083).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

































































The table lists the average atom inclusion at the recommended contour level (0.0083) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9840	 0.5690
A1	 0.9880	 0.5630
Aa	 0.9810	 0.5580
Ab	 0.9620	 0.5110
Ac	 0.9730	 0.5520
Ad	 0.9910	 0.5850
Ae	 0.9900	 0.5930
Af	 0.9880	 0.5880
Ag	 0.9770	 0.5140
Ah	 0.9860	 0.5650
Ai	 0.9920	 0.6050
Aj	 0.9940	 0.5990
Ak	 0.9870	 0.5790
Al	 0.8880	 0.4620
Am	 0.9810	 0.5600
An	 0.9890	 0.6010
Ao	 0.9650	 0.5540
Ap	 0.9840	 0.5460
Aq	 0.9740	 0.5820
Ar	 0.9920	 0.6050
As	 0.9740	 0.5080
At	 0.9960	 0.5600
Au	 0.9850	 0.5780
Av	 0.9990	 0.5600
Aw	 0.9870	 0.5730
Ax	 0.9790	 0.5220
Az	 0.9860	 0.5780
B1	 0.9840	 0.5690
B2	 0.9930	 0.5440
BA	 0.9920	 0.6240
BB	 0.9900	 0.6090
BC	 0.9840	 0.5930
BD	 0.9480	 0.4400
BE	 0.9970	 0.5700
BF	 0.9960	 0.5660



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
BG	 0.8910	 0.3840
BH	 0.9920	 0.5980
BI	 0.9930	 0.6140
BJ	 0.9880	 0.6170
BK	 0.9780	 0.5220
BL	 0.9870	 0.5280
BM	 0.9920	 0.5460
BN	 0.9970	 0.6370
BO	 0.9970	 0.5240
BP	 0.9960	 0.5850
BQ	 0.9930	 0.5950
BR	 0.9990	 0.6280
BS	 0.9920	 0.6100
BT	 0.9940	 0.6050
BU	 0.9880	 0.5820
BV	 0.9900	 0.6100
BW	 0.9870	 0.5300
BX	 0.9930	 0.6070
BY	 0.9780	 0.5370
BZ	 0.9900	 0.5870
Ba	 0.9880	 0.6060
Bb	 0.9910	 0.6070
Bc	 0.9920	 0.6030
Bd	 0.9940	 0.6380
Be	 0.9850	 0.6060
Bf	 0.9930	 0.6160
Bg	 1.0000	 0.5950
Bh	 0.9840	 0.6080
Bi	 0.9960	 0.6220
Bj	 0.9870	 0.5520
Bk	 0.9980	 0.6030
Bl	 0.8800	 0.4330