



Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 02:20 am BST

PDB ID : 9F1C / pdb_00009f1c
EMDB ID : EMD-50125
Title : Mammalian quaternary complex of a translating 80S ribosome, NAC, MetAP1 and NatA/E
Authors : Yudin, D.; Scaiola, A.; Ban, N.
Deposited on : 2024-04-18
Resolution : 3.78 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

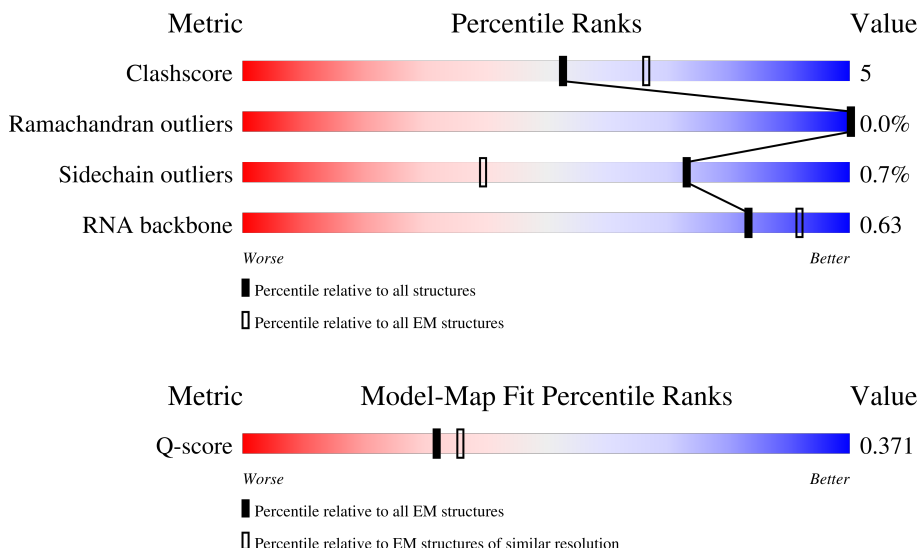
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.78 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10074 (3.28 - 4.27)

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	AH	3	100% 100%
2	Bb	245	6% 40% 56%
3	B7	120	72% 23%

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Mol	Chain	Length	Quality of chain
4	AT	76	
5	Ar	151	
6	B8	158	
7	BU	128	
8	As	145	
9	BA	257	
10	BV	140	
11	At	119	
12	BB	403	
13	BX	156	
14	Au	83	
15	BC	412	
16	BP	184	
17	BZ	136	
18	Aw	143	
19	BE	291	
20	B5	4808	
21	BQ	188	
22	Ba	148	
23	Ax	130	
24	BF	247	
25	BY	145	
26	BW	157	
27	AZ	294	
28	Ay	124	

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Mol	Chain	Length	Quality of chain
29	BG	266	
30	Av	130	
31	BR	196	
32	Aa	264	
33	Az	25	
34	BH	192	
35	BS	176	
36	Ab	293	
37	Bc	115	
38	BI	214	
39	B	297	
40	EA	386	
41	Ac	281	
42	Bd	125	
43	BJ	178	
44	Ct	238	
45	Ad	263	
46	Be	135	
47	BK	32	
48	Cu	162	
49	Ae	204	
50	Bf	110	
51	BL	211	
52	DA	403	
53	Af	249	

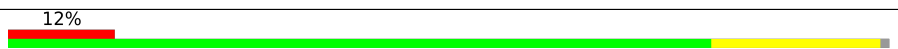
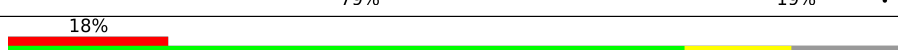
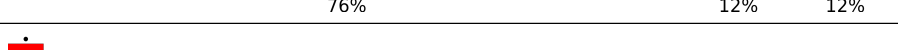
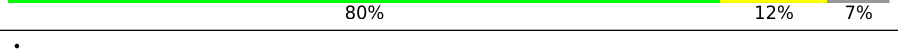
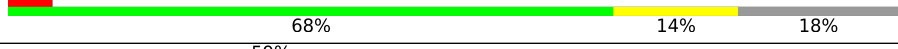
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Mol	Chain	Length	Quality of chain
54	Bg	117	
55	BM	218	
56	DB	915	
57	Ag	432	
58	Bh	123	
59	BN	204	
60	DC	235	
61	Ah	208	
62	Bi	105	
63	BO	203	
64	A2	1870	
65	Ai	194	
66	Bj	97	
67	AA	84	
68	Aj	165	
69	Bk	70	
70	AB	69	
71	Ak	158	
72	Bl	51	
73	AC	156	
74	Al	132	
75	Bm	128	
76	AD	133	
77	Am	151	
78	Bo	106	

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Mol	Chain	Length	Quality of chain
79	AE	115	
80	An	151	
81	Bp	92	
82	AF	317	
83	Ao	145	
84	Br	136	
85	AG	56	
86	Ap	172	
87	Bs	318	
88	BT	160	
89	Aq	135	
90	Bt	165	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
91	UNX	B5	5253	-	-	X	-
91	UNX	Be	205	-	-	X	-

2 Entry composition [i](#)

There are 98 unique types of molecules in this entry. The entry contains 236684 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 mRNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	AH	3	Total	C	O	P	0	0
			36	15	18	3		

- Molecule 2 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Bb	108	Total	C	N	O	S	0	0
			881	548	196	134	3		

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B7	119	Total	C	N	O	P	0	0
			2538	1131	451	837	119		

- Molecule 4 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AT	76	Total	C	N	O	P	0	0
			939	393	11	459	76		

- Molecule 5 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Ar	148	Total	C	N	O	S	0	0
			1217	763	245	208	1		

- Molecule 6 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B8	156	Total	C	N	O	P	0	0
			3319	1481	585	1097	156		

- Molecule 7 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BU	102	Total	C	N	O	S	0	0
			831	531	146	152	2		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BU	32	GLY	ARG	variant	UNP G1TSG1
BU	36	ALA	GLU	variant	UNP G1TSG1
BU	39	PHE	SER	variant	UNP G1TSG1
BU	54	GLY	ARG	variant	UNP G1TSG1
BU	97	ARG	HIS	variant	UNP G1TSG1

- Molecule 8 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	As	143	Total	C	N	O	S	0	0
			1113	698	214	198	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
As	119	GLY	TRP	variant	UNP G1TN62
As	142	ASN	LYS	variant	UNP G1TN62

- Molecule 9 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BA	253	Total	C	N	O	S	0	0
			1940	1214	396	324	6		

- Molecule 10 is a protein called Ribosomal protein L23.

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

- Molecule 11 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	At	104	Total	C	N	O	S	0	0
			822	514	156	148	4		

- Molecule 12 is a protein called Ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BB	398	Total	C	N	O	S	0	0
			3206	2042	605	546	13		

- Molecule 13 is a protein called Ribosomal_L23eN domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BX	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 14 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Au	83	Total	C	N	O	S	0	0
			640	394	117	124	5		

- Molecule 15 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BC	362	Total	C	N	O	S	0	0
			2886	1814	577	481	14		

- Molecule 16 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BP	159	Total	C	N	O	S	0	0
			1289	809	249	222	9		

- Molecule 17 is a protein called 60S ribosomal protein L27.

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

- Molecule 18 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Aw	141	Total	C	N	O	S	0	0
			1099	693	219	184	3		

- Molecule 19 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BE	243	Total	C	N	O	S	0	0
			1960	1258	378	321	3		

- Molecule 20 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	B5	3706	Total	C	N	O	P	0	0
			79525	35447	14532	25840	3706		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B5	3550	UY1	U	conflict	GB GBCN01009604.1

- Molecule 21 is a protein called Large ribosomal subunit protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BQ	187	Total	C	N	O	S	0	0
			1515	946	315	250	4		

- Molecule 22 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Ba	147	Total	C	N	O	S	0	0
			1163	734	239	186	4		

- Molecule 23 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Ax	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

- Molecule 24 is a protein called Ribosomal Protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BF	226	Total	C	N	O	S	0	0
			1886	1211	362	304	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BF	61	ARG	GLY	variant	UNP G1TUB1
BF	93	ARG	GLY	variant	UNP G1TUB1
BF	131	MET	VAL	variant	UNP G1TUB1
BF	153	ILE	VAL	variant	UNP G1TUB1

- Molecule 25 is a protein called Ribosomal protein L26.

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

- Molecule 26 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BW	121	Total	C	N	O	S	0	0
			991	619	202	166	4		

- Molecule 27 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AZ	221	Total	C	N	O	S	0	0
			1743	1107	305	323	8		

- Molecule 28 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Ay	85	Total	C	N	O	S	0	0
			683	439	128	115	1		

- Molecule 29 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BG	233	Total	C	N	O	S	0	0
			1877	1197	361	315	4		

- Molecule 30 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Av	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 31 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BR	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BR	38	ARG	CYS	variant	UNP G1TJR3
BR	64	ARG	GLN	variant	UNP G1TJR3
BR	94	THR	LYS	variant	UNP G1TJR3

- Molecule 32 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Aa	224	Total	C	N	O	S	0	0
			1815	1152	328	321	14		

- Molecule 33 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Az	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 34 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BH	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 35 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BS	176	Total	C	N	O	S	0	0
			1457	924	288	234	11		

- Molecule 36 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Ab	220	Total	C	N	O	S	0	0
			1706	1105	292	300	9		

- Molecule 37 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Bc	108	Total	C	N	O	S	0	0
			836	530	148	151	7		

- Molecule 38 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BI	213	Total	C	N	O	S	0	0
			1717	1086	332	285	14		

- Molecule 39 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	B	295	Total	C	N	O	S	0	0
			2398	1516	439	429	14		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	176	SER	GLY	variant	UNP G1SZF4
B	248	ARG	GLN	variant	UNP G1SZF4

- Molecule 40 is a protein called Methionine aminopeptidase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	EA	304	Total	C	N	O	S	13	0
			2445	1540	439	443	23		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EA	220	ASN	ASP	engineered mutation	UNP P53582

- Molecule 41 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Ac	225	Total	C	N	O	S	0	0
			1751	1116	315	313	7		

- Molecule 42 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Bd	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 43 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BJ	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 44 is a protein called Nascent polypeptide-associated complex subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Ct	116	Total	C	N	O	S	0	0
			904	566	165	169	4		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ct	-22	MET	-	initiating methionine	UNP Q13765
Ct	-21	GLY	-	expression tag	UNP Q13765
Ct	-20	SER	-	expression tag	UNP Q13765
Ct	-19	SER	-	expression tag	UNP Q13765
Ct	-18	HIS	-	expression tag	UNP Q13765
Ct	-17	HIS	-	expression tag	UNP Q13765
Ct	-16	HIS	-	expression tag	UNP Q13765
Ct	-15	HIS	-	expression tag	UNP Q13765
Ct	-14	HIS	-	expression tag	UNP Q13765
Ct	-13	HIS	-	expression tag	UNP Q13765
Ct	-12	SER	-	expression tag	UNP Q13765
Ct	-11	SER	-	expression tag	UNP Q13765
Ct	-10	GLY	-	expression tag	UNP Q13765
Ct	-9	LEU	-	expression tag	UNP Q13765
Ct	-8	GLU	-	expression tag	UNP Q13765
Ct	-7	VAL	-	expression tag	UNP Q13765
Ct	-6	LEU	-	expression tag	UNP Q13765
Ct	-5	PHE	-	expression tag	UNP Q13765
Ct	-4	GLN	-	expression tag	UNP Q13765

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Chain	Residue	Modelled	Actual	Comment	Reference
Ct	-3	GLY	-	expression tag	UNP Q13765
Ct	-2	PRO	-	expression tag	UNP Q13765
Ct	-1	SER	-	expression tag	UNP Q13765
Ct	0	GLY	-	expression tag	UNP Q13765

- Molecule 45 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Ad	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ad	25	GLY	SER	variant	UNP G1TK17
Ad	51	ARG	LYS	variant	UNP G1TK17
Ad	78	THR	ALA	variant	UNP G1TK17
Ad	156	VAL	MET	variant	UNP G1TK17

- Molecule 46 is a protein called Ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Be	130	Total	C	N	O	S	0	0
			1070	676	221	168	5		

- Molecule 47 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	BK	32	Total	C	N	O	0	0
			160	96	32	32		

- Molecule 48 is a protein called Transcription factor BTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Cu	106	Total	C	N	O	S	0	0
			821	514	153	151	3		

- Molecule 49 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Ae	191	Total	C	N	O	S	0	0
			1509	943	286	273	7		

- Molecule 50 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Bf	110	Total	C	N	O	S	0	0
			884	560	175	144	5		

- Molecule 51 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BL	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BL	74	ARG	HIS	variant	UNP G1TKB3
BL	190	ARG	HIS	variant	UNP G1TKB3

- Molecule 52 is a protein called Glutathione S-transferase class-mu 26 kDa isozyme,N-alpha-acetyltransferase 50.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	DA	155	Total	C	N	O	S	0	0
			1260	808	221	225	6		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DA	-15	GLY	-	linker	UNP P08515
DA	-14	SER	-	linker	UNP P08515
DA	-13	GLY	-	linker	UNP P08515
DA	-12	SER	-	linker	UNP P08515
DA	-11	GLY	-	linker	UNP P08515
DA	-10	SER	-	linker	UNP P08515
DA	-9	GLU	-	linker	UNP P08515
DA	-8	ASN	-	linker	UNP P08515
DA	-7	LEU	-	linker	UNP P08515
DA	-6	TYR	-	linker	UNP P08515
DA	-5	PHE	-	linker	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
DA	-4	GLN	-	linker	UNP P08515
DA	-3	GLY	-	linker	UNP P08515
DA	-2	ALA	-	linker	UNP P08515
DA	-1	MET	-	linker	UNP P08515
DA	0	VAL	-	linker	UNP P08515

- Molecule 53 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Af	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 54 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Bg	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 55 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BM	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 56 is a protein called N-alpha-acetyltransferase 15, NatA auxiliary subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	DB	837	Total	C	N	O	S	0	0
			6900	4391	1192	1276	41		

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DB	-48	MET	-	initiating methionine	UNP Q9BXJ9
DB	-47	GLY	-	expression tag	UNP Q9BXJ9
DB	-46	SER	-	expression tag	UNP Q9BXJ9
DB	-45	SER	-	expression tag	UNP Q9BXJ9
DB	-44	HIS	-	expression tag	UNP Q9BXJ9
DB	-43	HIS	-	expression tag	UNP Q9BXJ9
DB	-42	HIS	-	expression tag	UNP Q9BXJ9
DB	-41	HIS	-	expression tag	UNP Q9BXJ9

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Chain	Residue	Modelled	Actual	Comment	Reference
DB	-40	HIS	-	expression tag	UNP Q9BXJ9
DB	-39	HIS	-	expression tag	UNP Q9BXJ9
DB	-38	SER	-	expression tag	UNP Q9BXJ9
DB	-37	SER	-	expression tag	UNP Q9BXJ9
DB	-36	GLY	-	expression tag	UNP Q9BXJ9
DB	-35	LEU	-	expression tag	UNP Q9BXJ9
DB	-34	VAL	-	expression tag	UNP Q9BXJ9
DB	-33	PRO	-	expression tag	UNP Q9BXJ9
DB	-32	ARG	-	expression tag	UNP Q9BXJ9
DB	-31	GLY	-	expression tag	UNP Q9BXJ9
DB	-30	SER	-	expression tag	UNP Q9BXJ9
DB	-29	HIS	-	expression tag	UNP Q9BXJ9
DB	-28	MET	-	expression tag	UNP Q9BXJ9
DB	-27	ALA	-	expression tag	UNP Q9BXJ9
DB	-26	SER	-	expression tag	UNP Q9BXJ9
DB	-25	MET	-	expression tag	UNP Q9BXJ9
DB	-24	THR	-	expression tag	UNP Q9BXJ9
DB	-23	GLY	-	expression tag	UNP Q9BXJ9
DB	-22	GLY	-	expression tag	UNP Q9BXJ9
DB	-21	GLN	-	expression tag	UNP Q9BXJ9
DB	-20	GLN	-	expression tag	UNP Q9BXJ9
DB	-19	MET	-	expression tag	UNP Q9BXJ9
DB	-18	GLY	-	expression tag	UNP Q9BXJ9
DB	-17	ARG	-	expression tag	UNP Q9BXJ9
DB	-16	ALA	-	expression tag	UNP Q9BXJ9
DB	-15	ARG	-	expression tag	UNP Q9BXJ9
DB	-14	GLY	-	expression tag	UNP Q9BXJ9
DB	-13	ILE	-	expression tag	UNP Q9BXJ9
DB	-12	GLN	-	expression tag	UNP Q9BXJ9
DB	-11	ARG	-	expression tag	UNP Q9BXJ9
DB	-10	PRO	-	expression tag	UNP Q9BXJ9
DB	-9	THR	-	expression tag	UNP Q9BXJ9
DB	-8	SER	-	expression tag	UNP Q9BXJ9
DB	-7	THR	-	expression tag	UNP Q9BXJ9
DB	-6	SER	-	expression tag	UNP Q9BXJ9
DB	-5	SER	-	expression tag	UNP Q9BXJ9
DB	-4	LEU	-	expression tag	UNP Q9BXJ9
DB	-3	VAL	-	expression tag	UNP Q9BXJ9
DB	-2	ALA	-	expression tag	UNP Q9BXJ9
DB	-1	ALA	-	expression tag	UNP Q9BXJ9
DB	0	ALA	-	expression tag	UNP Q9BXJ9

- Molecule 57 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Ag	190	Total	C	N	O	S	0	0
			1529	975	281	272	1		

- Molecule 58 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Bh	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 59 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	BN	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 60 is a protein called N-alpha-acetyltransferase 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	DC	160	Total	C	N	O	S	0	0
			1295	815	234	235	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DC	24	GLN	GLU	engineered mutation	UNP P41227
DC	26	PHE	TYR	engineered mutation	UNP P41227

- Molecule 61 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Ah	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ah	47	ARG	GLY	variant	UNP G1TJW1

- Molecule 62 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Bi	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 63 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	BO	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

- Molecule 64 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	A2	1770	Total	C	N	O	P	0	0
			37833	16911	6781	12371	1770		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A2	1249	B8N	C	conflict	GB GBCT01000564.1
A2	1338	4AC	C	conflict	GB GBCT01000564.1
A2	1843	4AC	C	conflict	GB GBCT01000564.1

- Molecule 65 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Ai	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 66 is a protein called Ribosomal protein L37.

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

- Molecule 67 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	AA	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 68 is a protein called S10_ plectin domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Aj	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 69 is a protein called 60S ribosomal protein L38.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bk	24	LYS	ASN	variant	UNP G1U001

- Molecule 70 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	AB	63	Total	C	N	O	S	0	0
			495	302	98	93	2		

- Molecule 71 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Ak	154	Total	C	N	O	S	0	0
			1262	804	236	216	6		

- Molecule 72 is a protein called 60S ribosomal protein L39-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Bl	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 73 is a protein called Ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	AC	74	Total	C	N	O	S	0	0
			610	385	117	101	7		

- Molecule 74 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Al	124	Total	C	N	O	S	0	0
			958	600	170	179	9		

- Molecule 75 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Bm	52	Total	C	N	O	S	0	0
			432	269	90	67	6		

- Molecule 76 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	AD	57	Total	C	N	O	S	0	0
			457	282	101	73	1		

- Molecule 77 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Am	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 78 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Bo	105	Total	C	N	O	S	0	0
			863	543	175	139	6		

- Molecule 79 is a protein called Small ribosomal subunit protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	AE	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 80 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	An	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
An	138	IAS	ASP	conflict	UNP A0AAA9WYR1

- Molecule 81 is a protein called 60S ribosomal protein L37a.

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

- Molecule 82 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	AF	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 83 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Ao	128	Total	C	N	O	S	0	0
			1048	665	197	179	7		

- Molecule 84 is a protein called Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Br	126	Total	C	N	O	S	0	0
			1014	629	209	170	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Br	103	ARG	HIS	conflict	UNP G1U7L1

- Molecule 85 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	AG	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 86 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Ap	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 87 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	Bs	196	Total	C	N	O	S	0	0
			1507	959	263	276	9		

- Molecule 88 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	BT	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 89 is a protein called 40S ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
89	Aq	134	Total	C	N	O	S	0	0
			1080	678	201	197	4		

- Molecule 90 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
90	Bt	156	Total	C	N	O	S	0	0
			1178	733	221	220	4		

- Molecule 91 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

Mol	Chain	Residues	Atoms		AltConf
91	Bb	2	Total	X	0
			2	2	
91	B7	6	Total	X	0
			6	6	
91	AT	2	Total	X	0
			2	2	
91	Ar	1	Total	X	0
			1	1	
91	B8	6	Total	X	0
			6	6	
91	BA	3	Total	X	0
			3	3	
91	BB	1	Total	X	0
			1	1	
91	BP	1	Total	X	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
91	B5	186	Total 186	X 186	0
91	BQ	2	Total 2	X 2	0
91	BY	1	Total 1	X 1	0
91	BH	1	Total 1	X 1	0
91	BI	1	Total 1	X 1	0
91	Ad	1	Total 1	X 1	0
91	Be	4	Total 4	X 4	0
91	Bf	1	Total 1	X 1	0
91	BL	1	Total 1	X 1	0
91	BN	1	Total 1	X 1	0
91	A2	49	Total 49	X 49	0
91	Bj	1	Total 1	X 1	0
91	Ak	1	Total 1	X 1	0
91	Bo	1	Total 1	X 1	0
91	AE	1	Total 1	X 1	0
91	An	1	Total 1	X 1	0
91	BT	2	Total 2	X 2	0

- Molecule 92 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

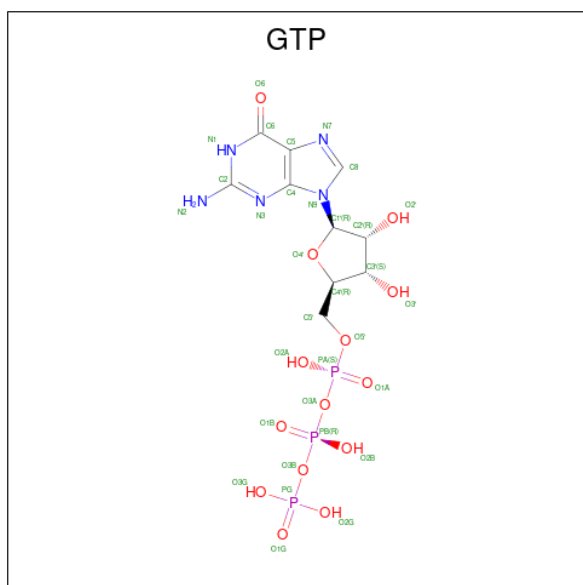
Mol	Chain	Residues	Atoms		AltConf
92	B7	9	Total 9	Mg 9	0
92	AT	2	Total 2	Mg 2	0

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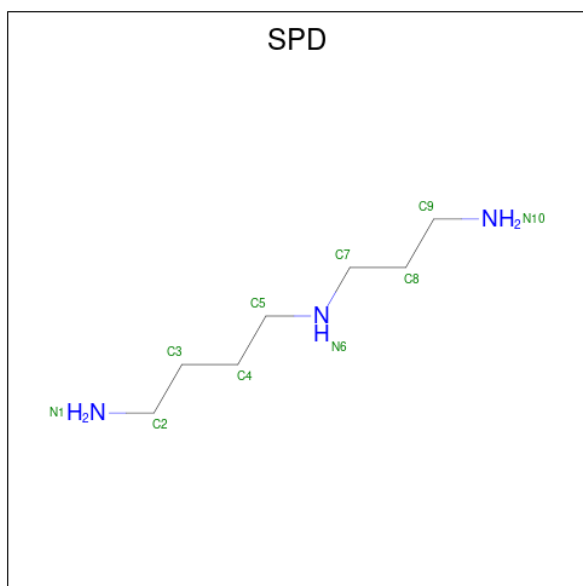
Mol	Chain	Residues	Atoms		AltConf
92	B8	8	Total 8	Mg 8	0
92	BV	1	Total 1	Mg 1	0
92	BB	1	Total 1	Mg 1	0
92	BP	1	Total 1	Mg 1	0
92	B5	282	Total 282	Mg 282	0
92	Ba	1	Total 1	Mg 1	0
92	BR	1	Total 1	Mg 1	0
92	BI	1	Total 1	Mg 1	0
92	Be	1	Total 1	Mg 1	0
92	A2	111	Total 111	Mg 111	0
92	Bj	1	Total 1	Mg 1	0

- Molecule 93 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
93	B7	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 94 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



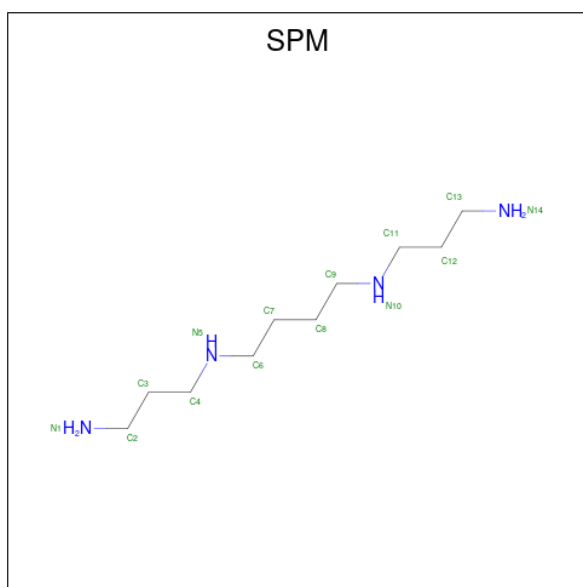
Mol	Chain	Residues	Atoms			AltConf
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	

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Mol	Chain	Residues	Atoms			AltConf
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	A2	1	Total	C	N	0
			10	7	3	
94	A2	1	Total	C	N	0
			10	7	3	
94	A2	1	Total	C	N	0
			10	7	3	
94	A2	1	Total	C	N	0
			10	7	3	
94	A2	1	Total	C	N	0
			10	7	3	
94	A2	1	Total	C	N	0
			10	7	3	

- Molecule 95 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).

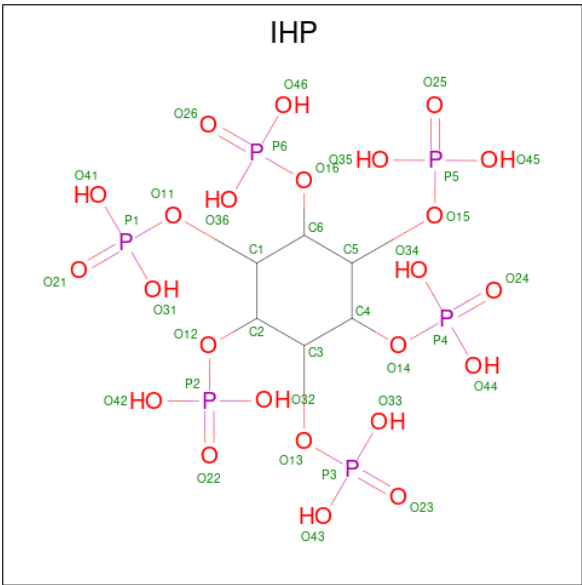


Mol	Chain	Residues	Atoms			AltConf
95	B5	1	Total	C	N	0
			14	10	4	
95	B5	1	Total	C	N	0
			14	10	4	
95	A2	1	Total	C	N	0
			14	10	4	

- Molecule 96 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
96	Bg	1	Total	Zn	0
			1	1	
96	Bj	1	Total	Zn	0
			1	1	
96	AC	1	Total	Zn	0
			1	1	
96	Bm	1	Total	Zn	0
			1	1	
96	Bo	1	Total	Zn	0
			1	1	
96	AE	1	Total	Zn	0
			1	1	
96	Bp	1	Total	Zn	0
			1	1	
96	AG	1	Total	Zn	0
			1	1	

- Molecule 97 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆).



Mol	Chain	Residues	Atoms				AltConf
97	DB	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 98 is water.

Mol	Chain	Residues	Atoms		AltConf
98	AH	3	Total	O	0
			3	3	
98	Bb	1	Total	O	0
			1	1	
98	B7	44	Total	O	0
			44	44	
98	AT	12	Total	O	0
			12	12	
98	Ar	2	Total	O	0
			2	2	
98	B8	47	Total	O	0
			47	47	
98	As	2	Total	O	0
			2	2	
98	BA	5	Total	O	0
			5	5	
98	BV	2	Total	O	0
			2	2	
98	At	1	Total	O	0
			1	1	
98	BB	6	Total	O	0
			6	6	

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Mol	Chain	Residues	Atoms		AltConf
98	BX	2	Total 2	O 2	0
98	BC	7	Total 7	O 7	0
98	BP	3	Total 3	O 3	0
98	Aw	5	Total 5	O 5	0
98	B5	1398	Total 1398	O 1398	0
98	Ba	8	Total 8	O 8	0
98	BR	5	Total 5	O 5	0
98	Aa	3	Total 3	O 3	0
98	BH	1	Total 1	O 1	0
98	Ab	1	Total 1	O 1	0
98	BI	2	Total 2	O 2	0
98	B	1	Total 1	O 1	0
98	Bd	1	Total 1	O 1	0
98	Ct	1	Total 1	O 1	0
98	Ad	1	Total 1	O 1	0
98	Be	4	Total 4	O 4	0
98	BL	2	Total 2	O 2	0
98	Af	1	Total 1	O 1	0
98	Bg	1	Total 1	O 1	0
98	BN	5	Total 5	O 5	0
98	A2	527	Total 527	O 527	0

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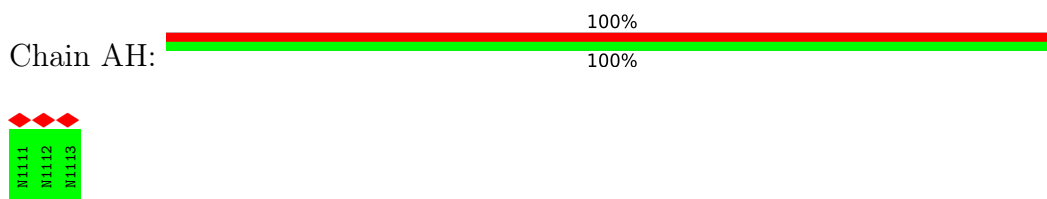
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Mol	Chain	Residues	Atoms		AltConf
98	Bj	5	Total 5	O 5	0
98	Ak	2	Total 2	O 2	0
98	Bl	2	Total 2	O 2	0
98	AE	1	Total 1	O 1	0
98	An	1	Total 1	O 1	0
98	Ap	2	Total 2	O 2	0

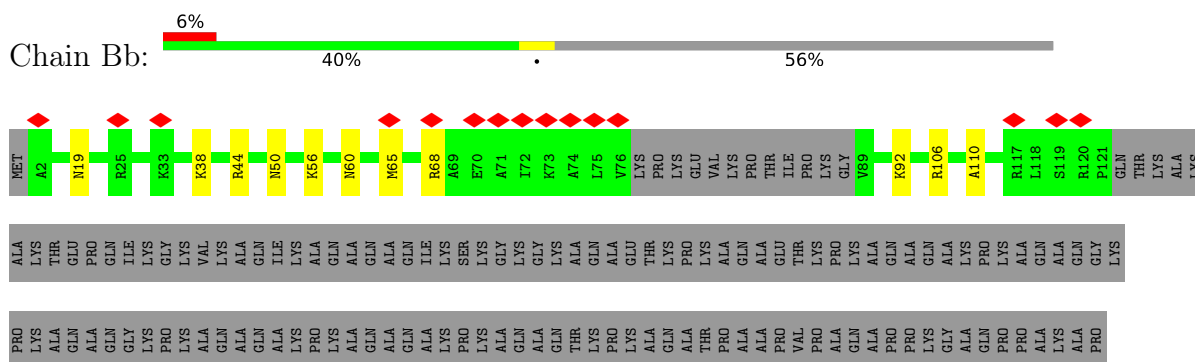
3 Residue-property plots

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.

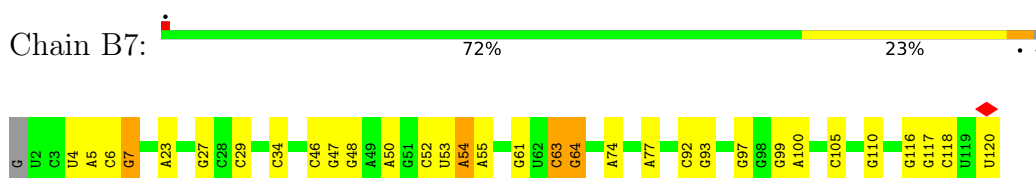
- Molecule 1: mRNA



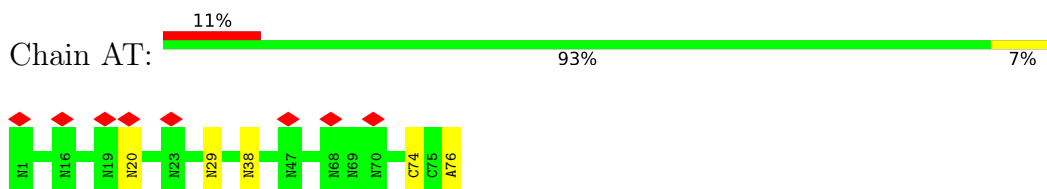
- Molecule 2: 60S ribosomal protein L29



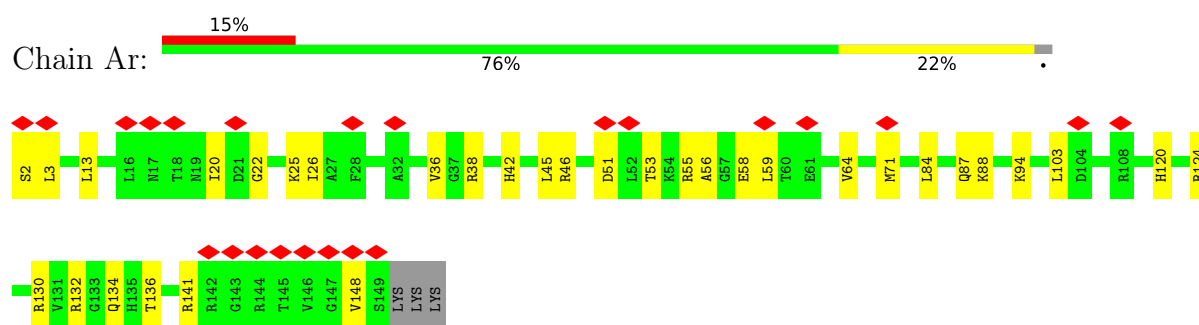
- Molecule 3: 5S rRNA



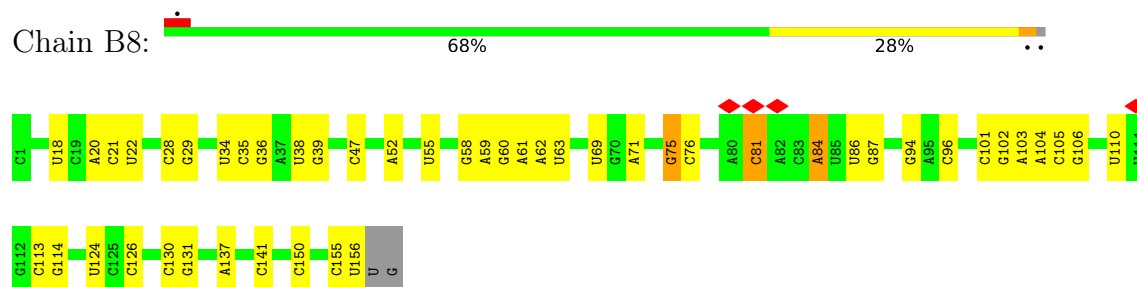
- Molecule 4: P-site tRNA



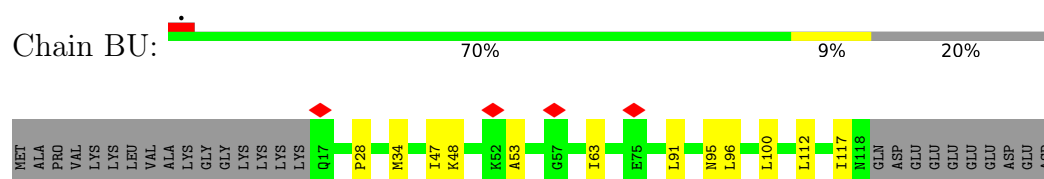
- Molecule 5: Small ribosomal subunit protein uS13



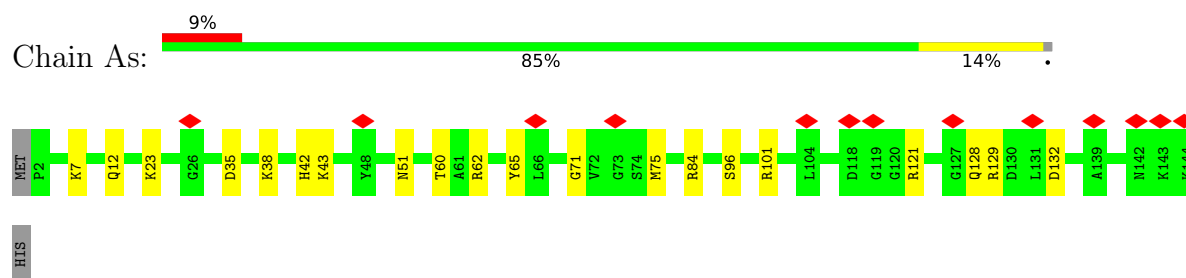
- Molecule 6: 5.8S rRNA



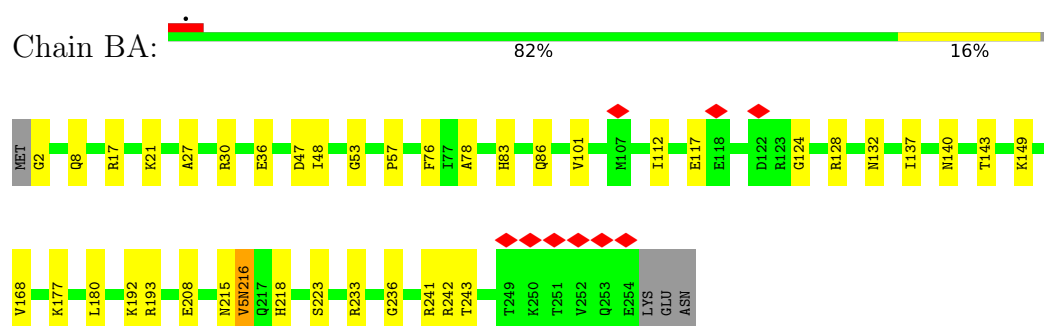
- Molecule 7: 60S ribosomal protein L22



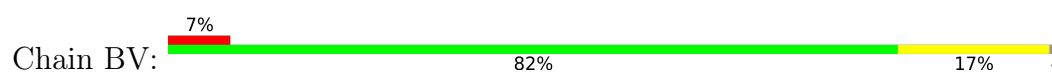
- Molecule 8: 40S ribosomal protein S19



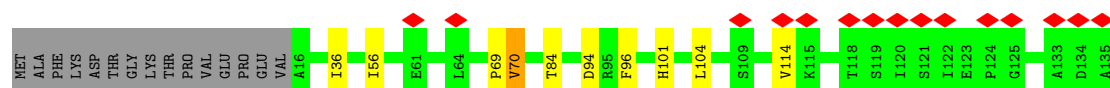
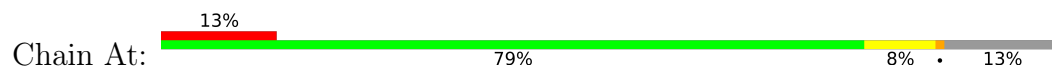
- Molecule 9: Large ribosomal subunit protein uL2



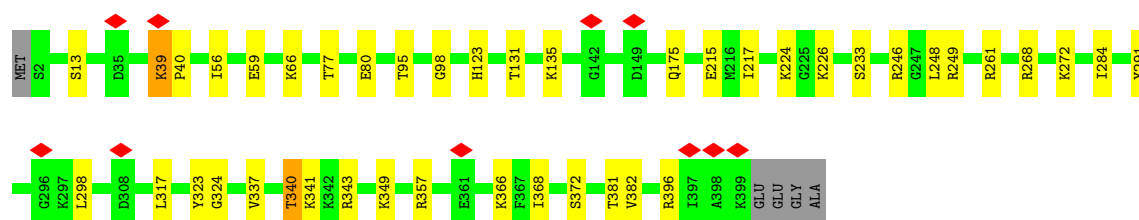
- Molecule 10: Ribosomal protein L23



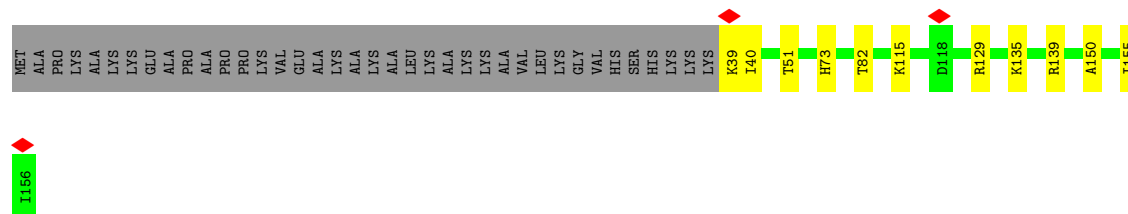
- Molecule 11: Small ribosomal subunit protein uS10



- Molecule 12: Ribosomal protein L3



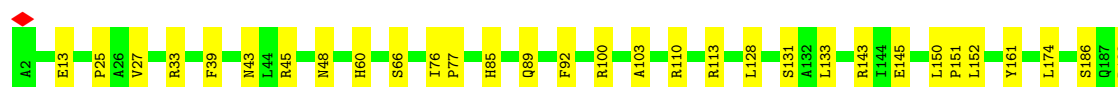
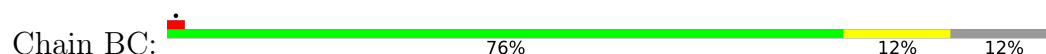
- Molecule 13: Ribosomal_L23eN domain-containing protein

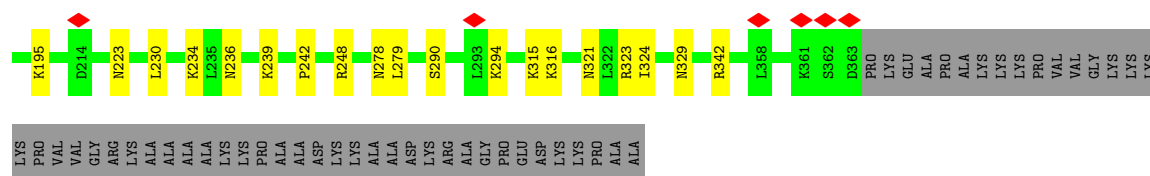


- Molecule 14: Small ribosomal subunit protein eS21

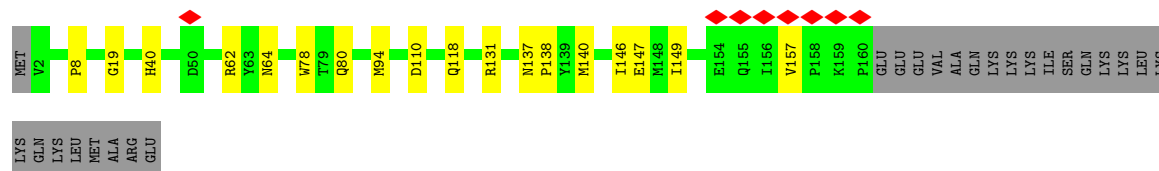
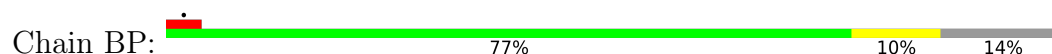


- Molecule 15: Large ribosomal subunit protein uL4

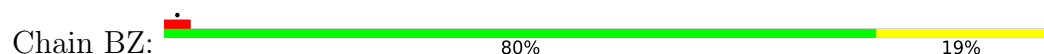




- Molecule 16: Large ribosomal subunit protein uL22



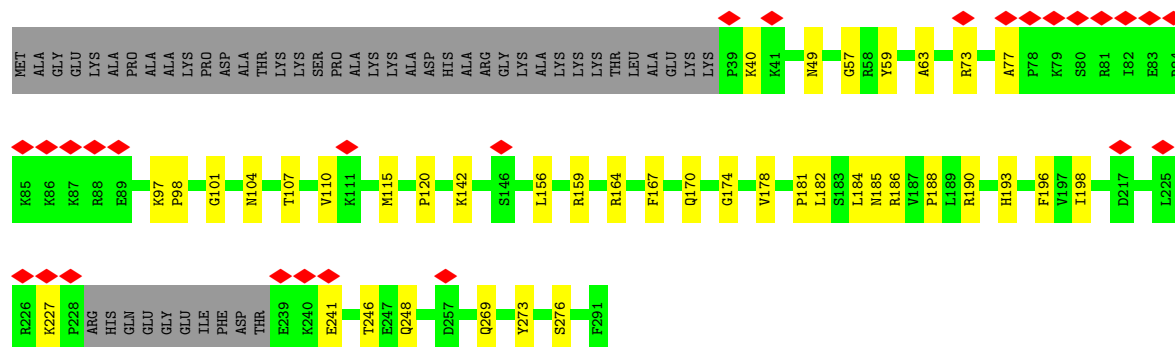
- Molecule 17: 60S ribosomal protein L27



- Molecule 18: 40S ribosomal protein S23

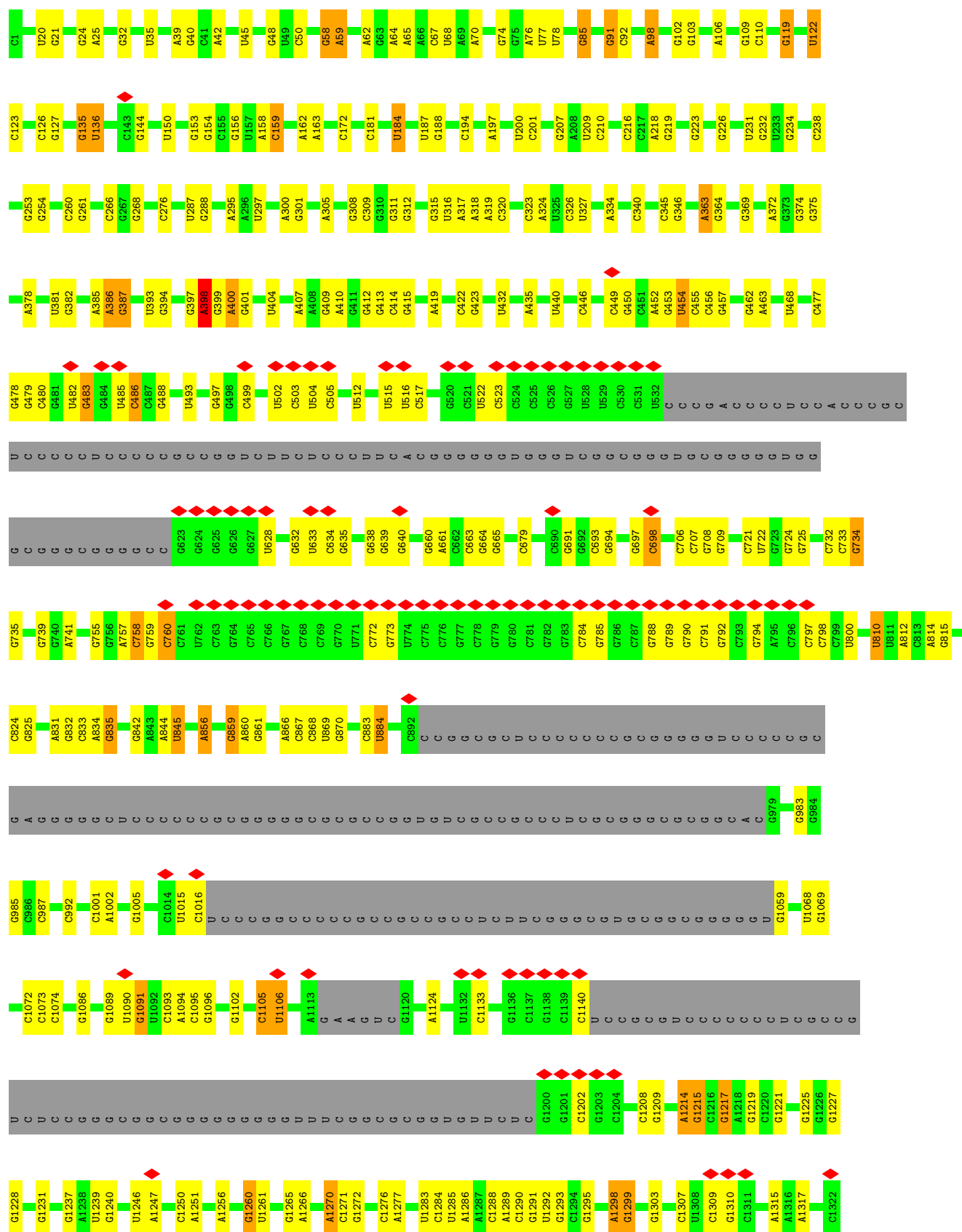


- Molecule 19: 60S ribosomal protein L6



- Molecule 20: 28S rRNA







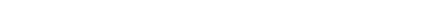


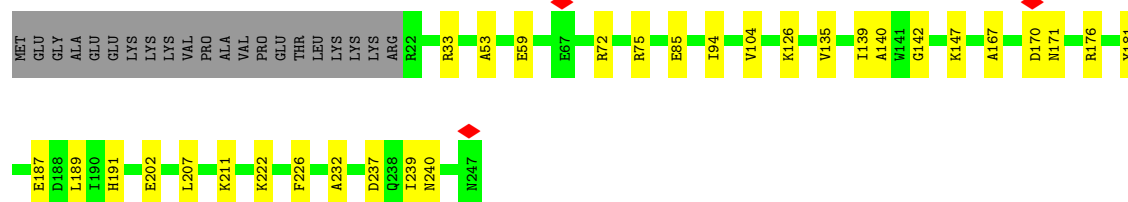


- [illegible]

- [illegible]

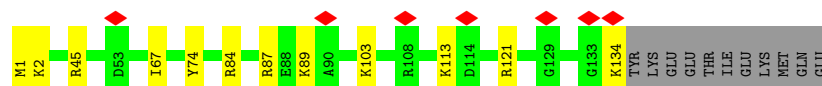
- WORLDWIDE
PDB
PROTEIN DATA BANK

Chain BF:  79% 13% 9%

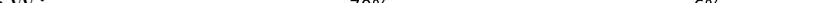


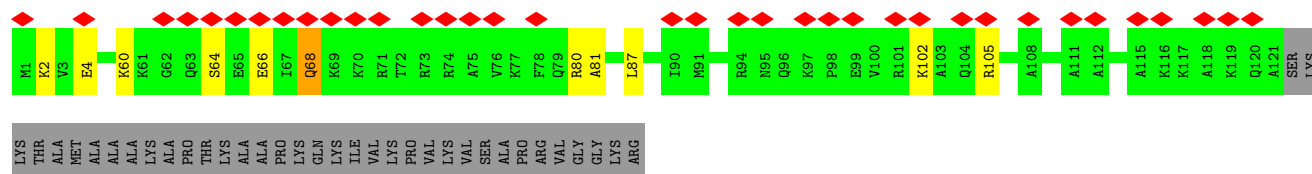
- Molecule 25: Ribosomal protein L26

Chain BY: 



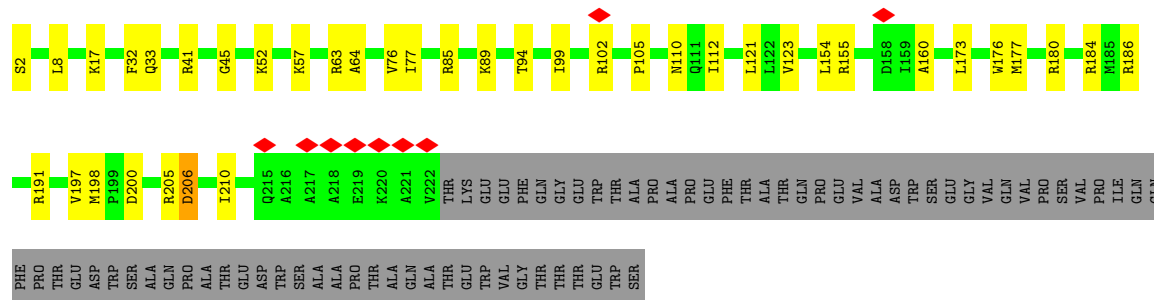
- Molecule 26: Ribosomal protein L24

Chain BW: 



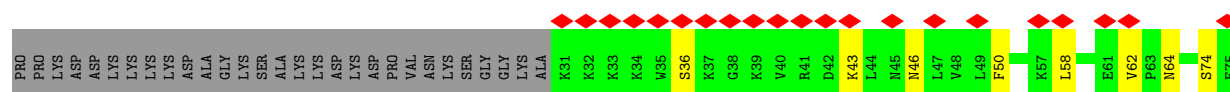
- Molecule 27: Small ribosomal subunit protein uS2

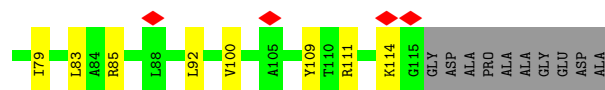
Chain AZ:



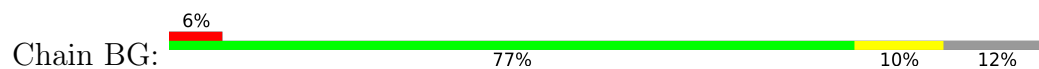
- Molecule 28: 40S ribosomal protein S25

Chain A: 20% 56% 13% 31%

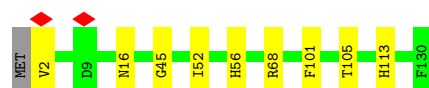




- Molecule 29: 60S ribosomal protein L7a



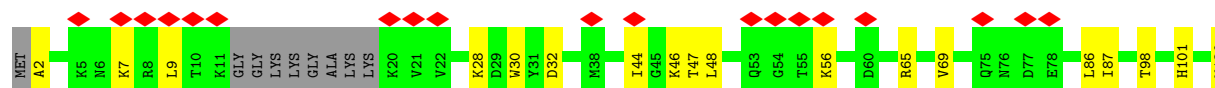
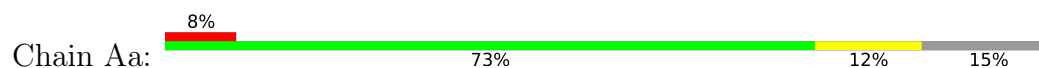
- Molecule 30: Ribosomal protein S15a



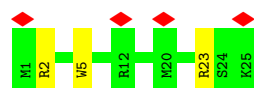
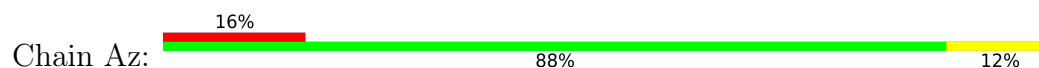
- Molecule 31: Ribosomal protein L19



- Molecule 32: 40S ribosomal protein S3a



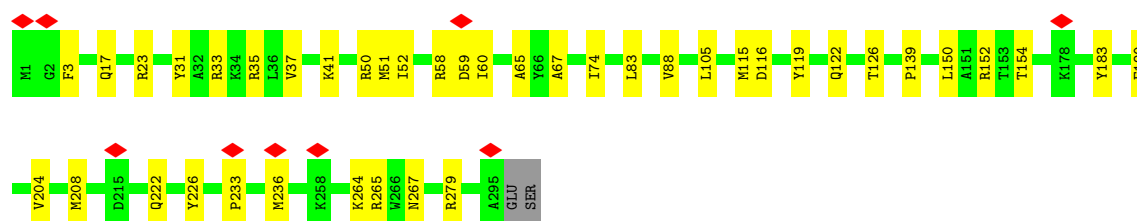
- Molecule 33: 60S ribosomal protein L41



- Molecule 34: 60S ribosomal protein L9

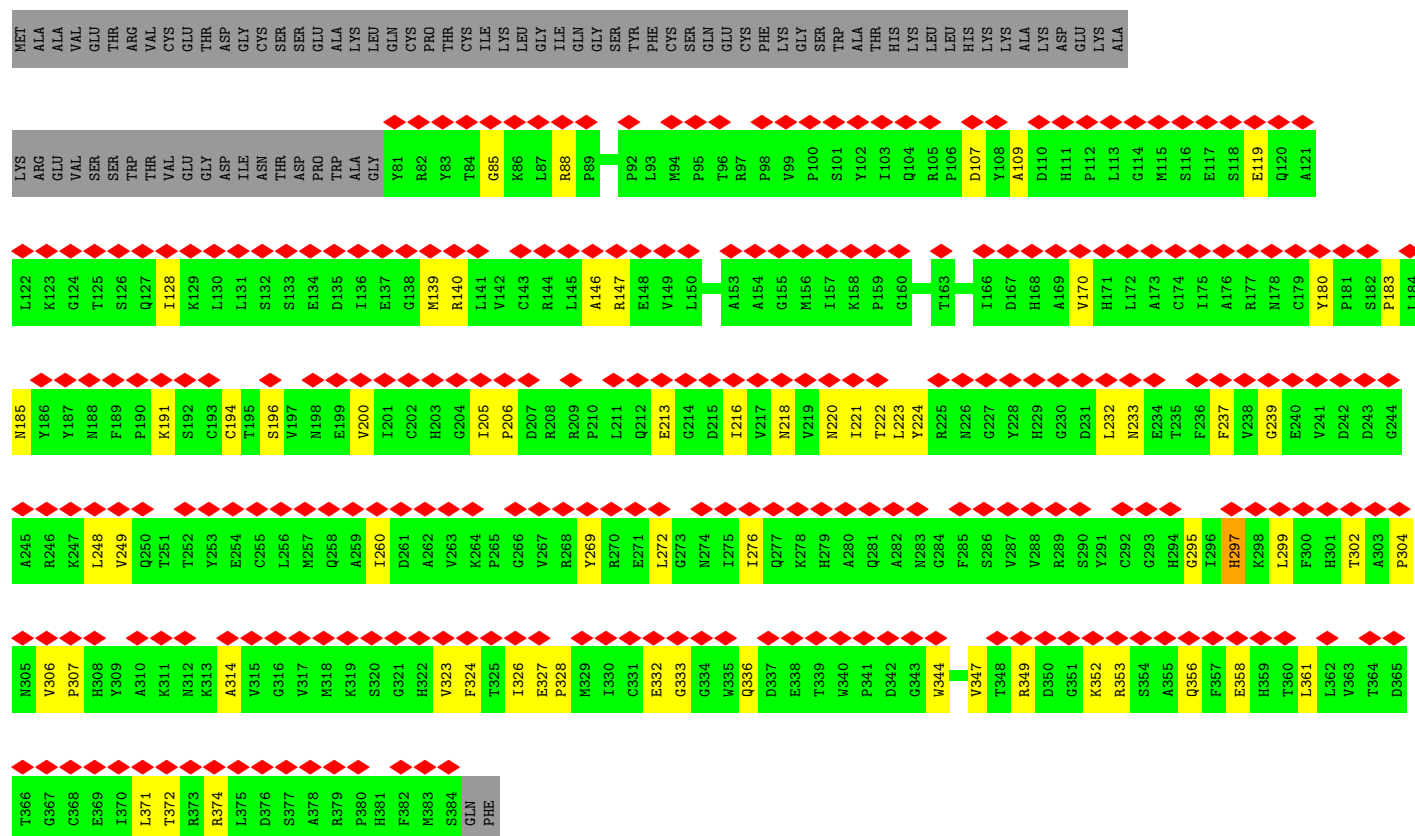


Chain B: 



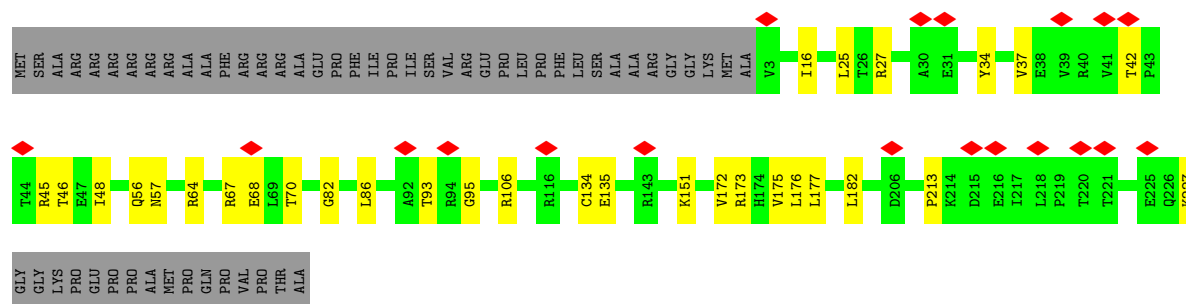
• Molecule 40: Methionine aminopeptidase 1

Chain EA: 

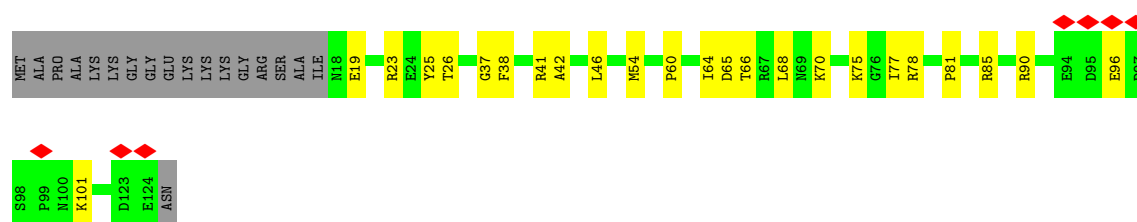


• Molecule 41: 40S ribosomal protein S3

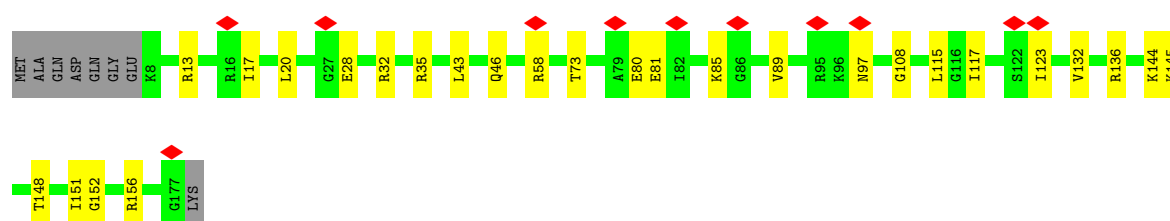
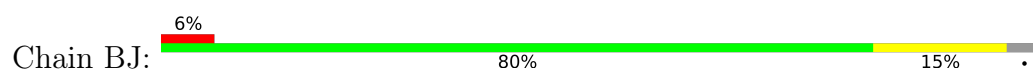
Chain Ac: 



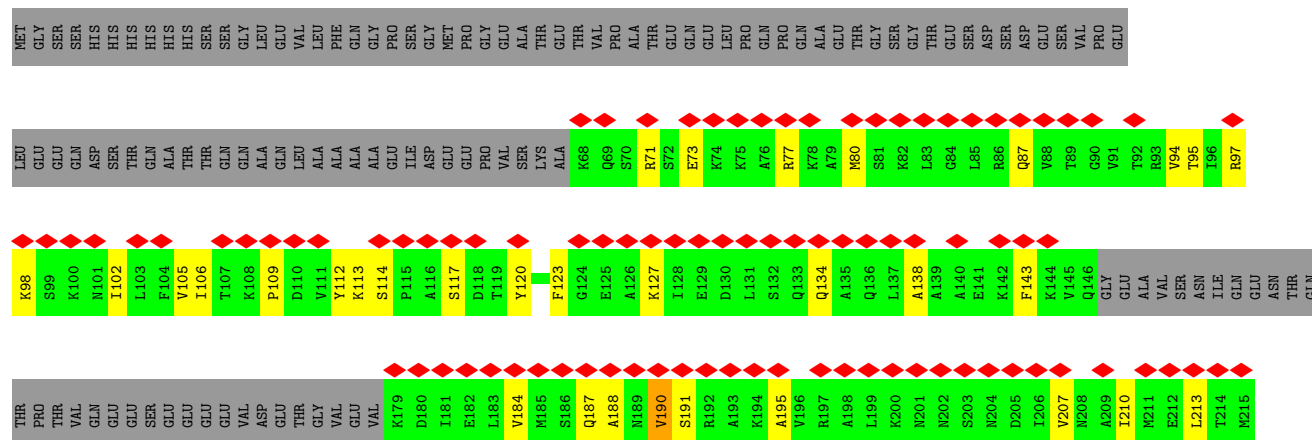
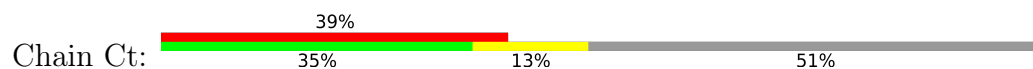
- Molecule 42: 60S ribosomal protein L31



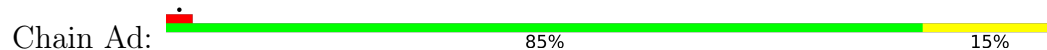
- Molecule 43: 60S ribosomal protein L11



- Molecule 44: Nascent polypeptide-associated complex subunit alpha

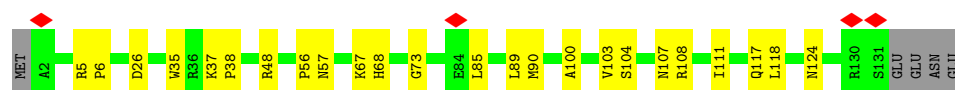


- Molecule 45: 40S ribosomal protein S4



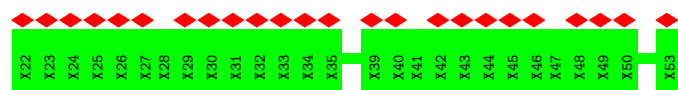
- Molecule 46: Ribosomal protein L32

Chain Be:  79% 18%



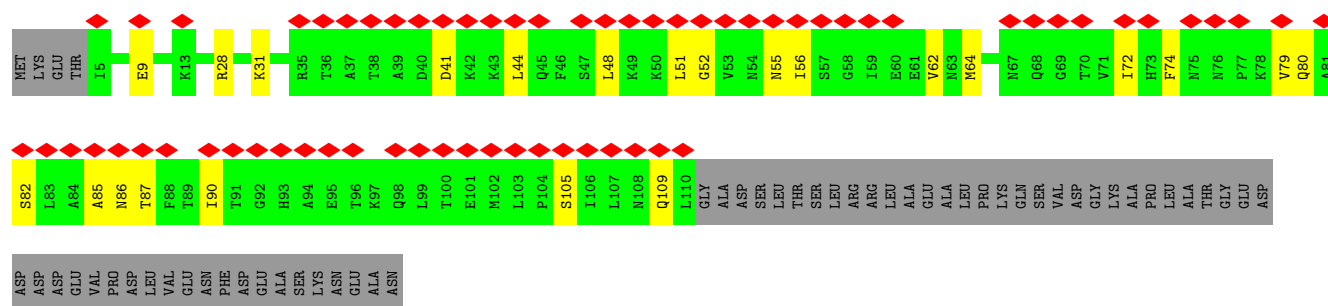
- Molecule 47: Nascent chain

Chain BK:  75% 100%



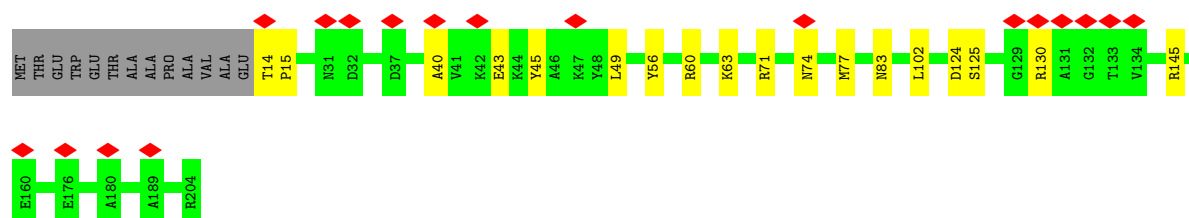
- Molecule 48: Transcription factor BTF3

Chain Cu:  41% 51% 14% 35%



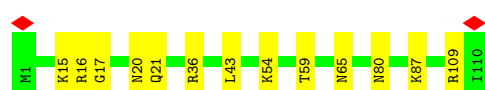
- Molecule 49: Ribosomal protein S5

Chain Ae:  9% 85% 9% 6%



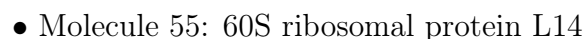
- Molecule 50: 60S ribosomal protein L35a

Chain Bf:  88% 12%

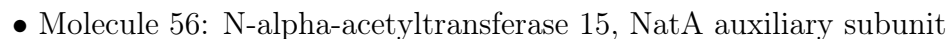


- Molecule 51: Large ribosomal subunit protein eL13

Chain BL:  6% 88% 12%

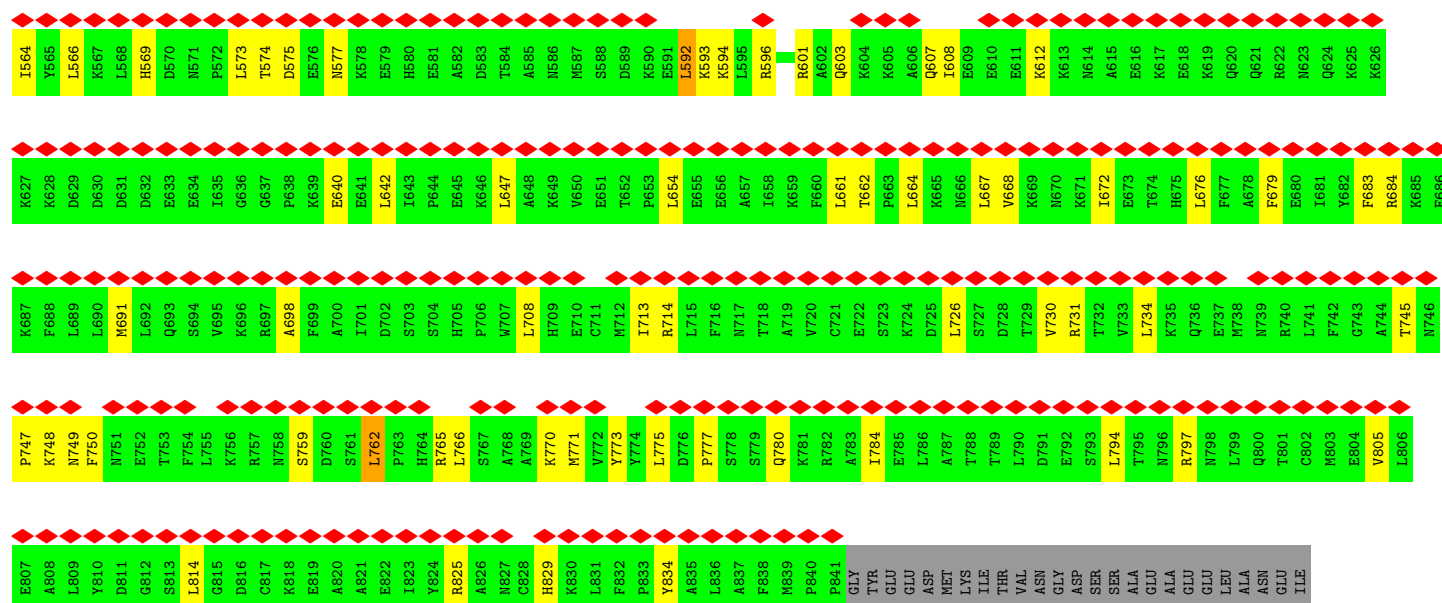


Frequency	Percentage
Daily	53%
Weekly	10%
Monthly	37%

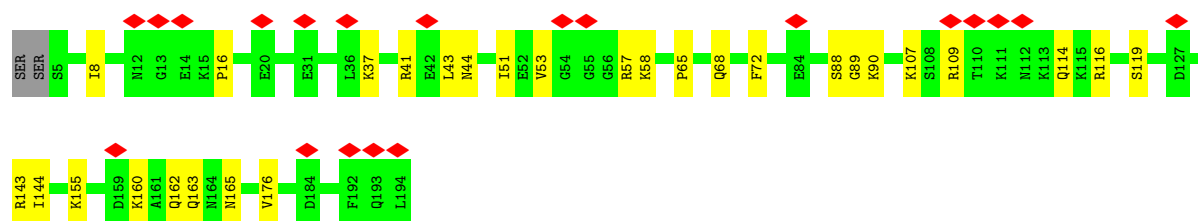
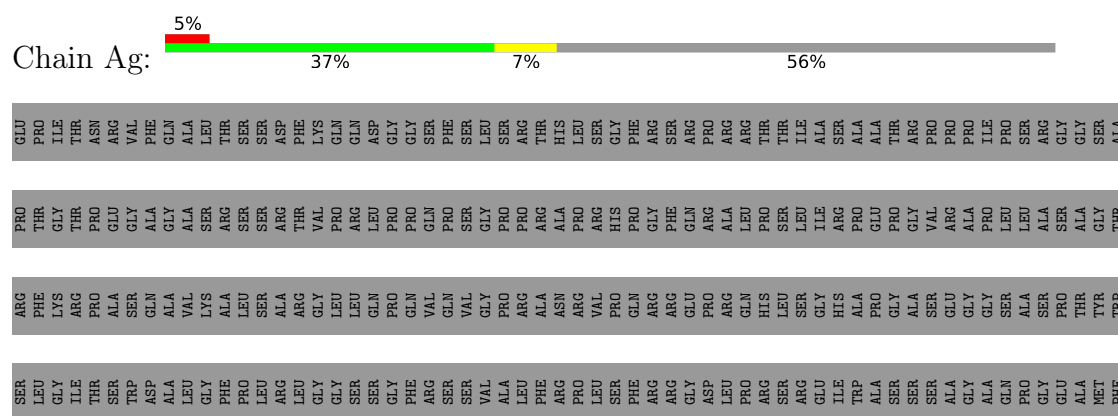


Device Type	Percentage
Smartphone	79%
Tablet	68%
Feature phone	22%
Smartwatch	9%

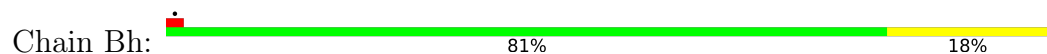




• Molecule 57: 40S ribosomal protein S7

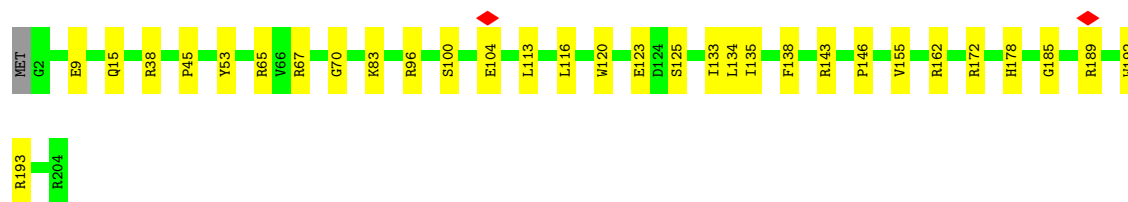


• Molecule 58: 60S ribosomal protein L35

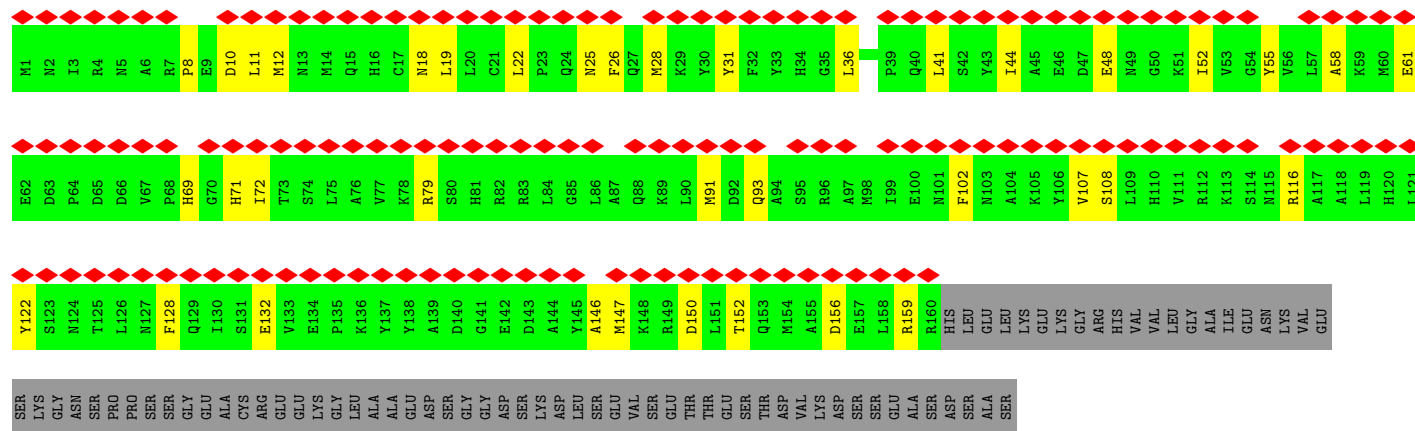


• Molecule 59: Ribosomal protein L15

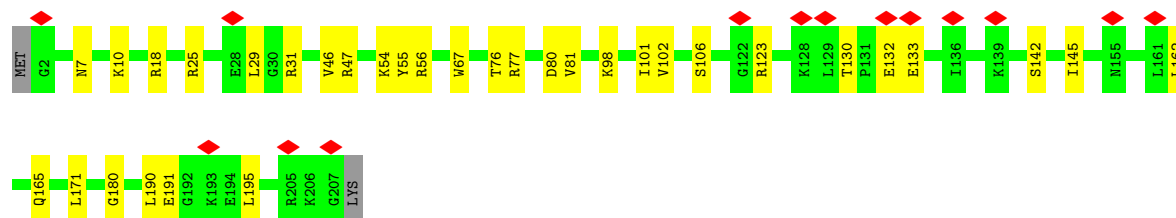
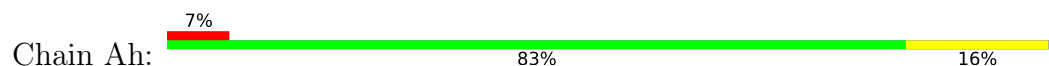




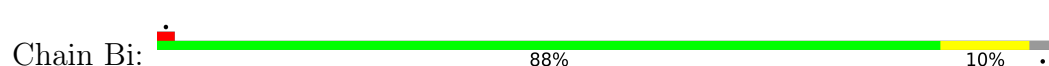
- Molecule 60: N-alpha-acetyltransferase 10



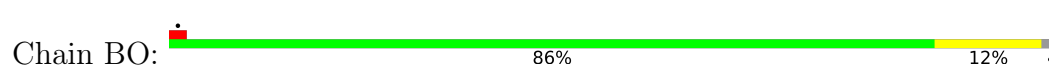
- Molecule 61: 40S ribosomal protein S8



- Molecule 62: 60S ribosomal protein L36

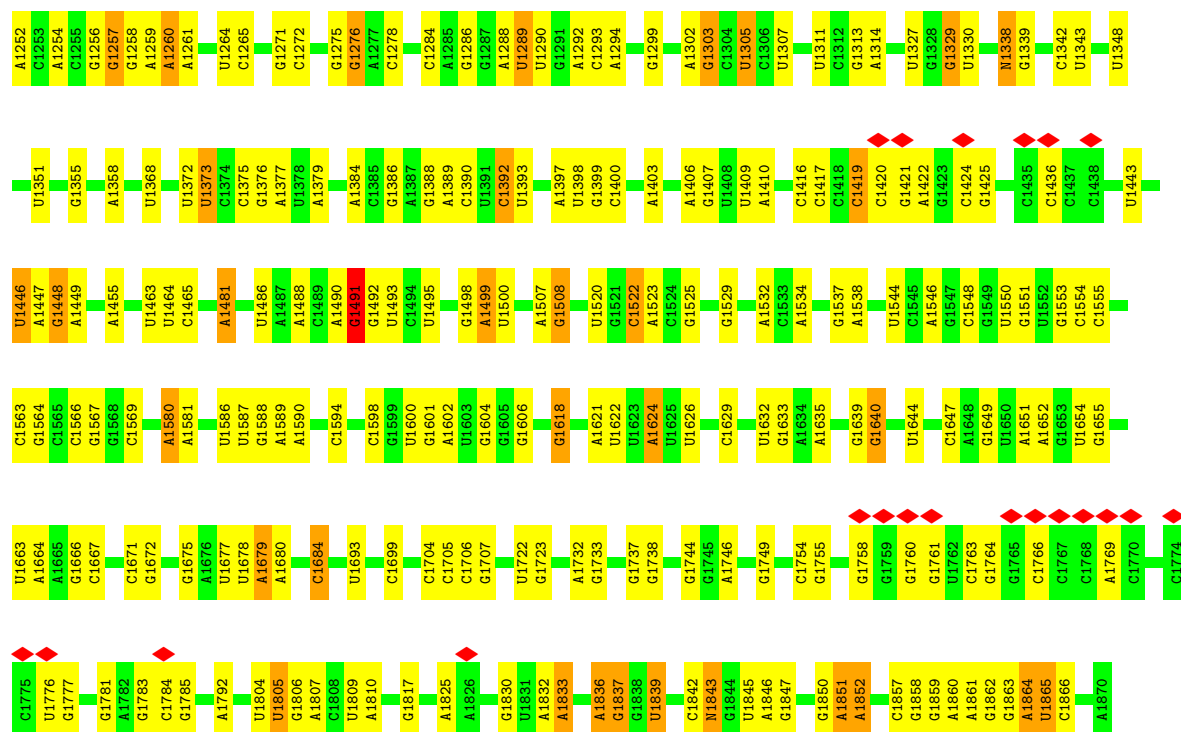


- Molecule 63: Large ribosomal subunit protein uL13

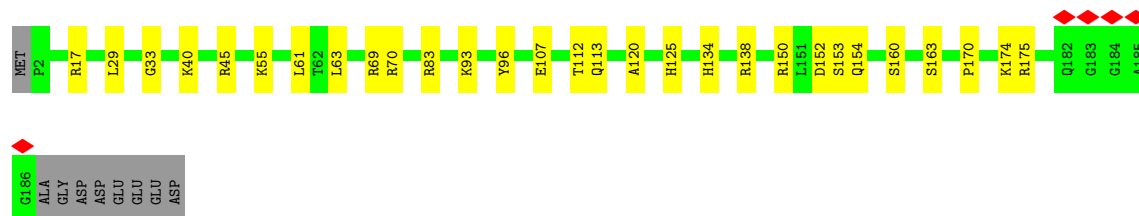
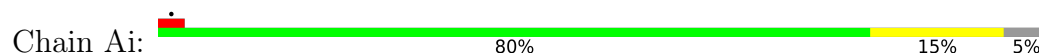


Chain A2:

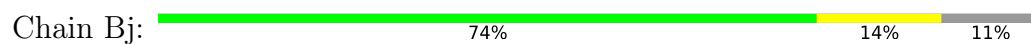




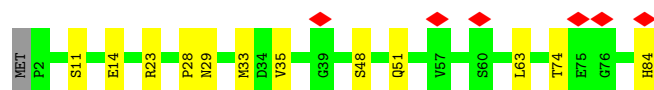
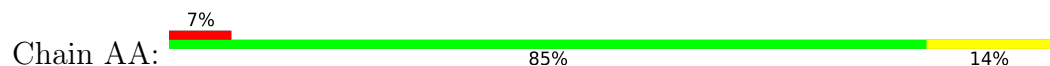
• Molecule 65: 40S ribosomal protein S9



• Molecule 66: Ribosomal protein L37

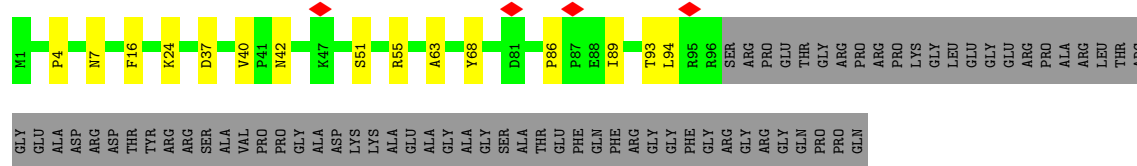


• Molecule 67: 40S ribosomal protein S27



• Molecule 68: S10_pectin domain-containing protein

Chain Aj: 



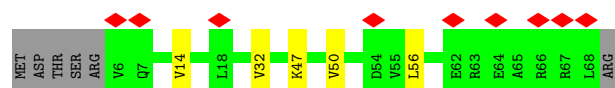
- Molecule 69: 60S ribosomal protein L38

Chain Bk: 



- Molecule 70: 40S ribosomal protein S28

Chain AB: 



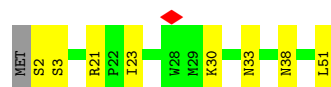
- Molecule 71: 40S ribosomal protein S11

Chain Ak: 



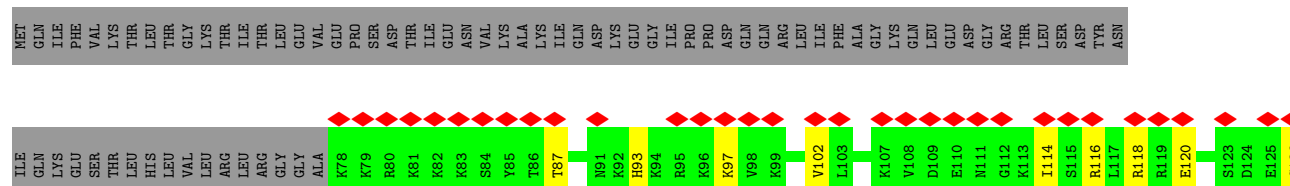
- Molecule 72: 60S ribosomal protein L39-like

Chain Bl: 



- Molecule 73: Ribosomal protein S27a

Chain AC: 



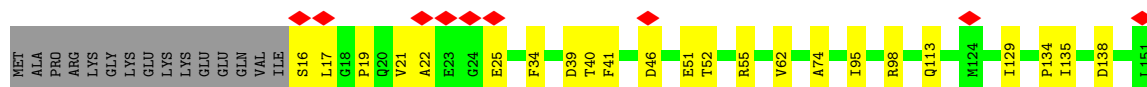
- Molecule 79: Small ribosomal subunit protein eS26

Chain AE: 

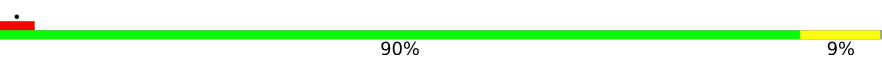


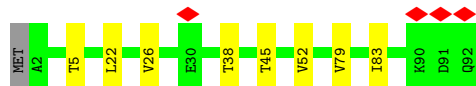
- Molecule 80: Small ribosomal subunit protein uS11

Chain An: 



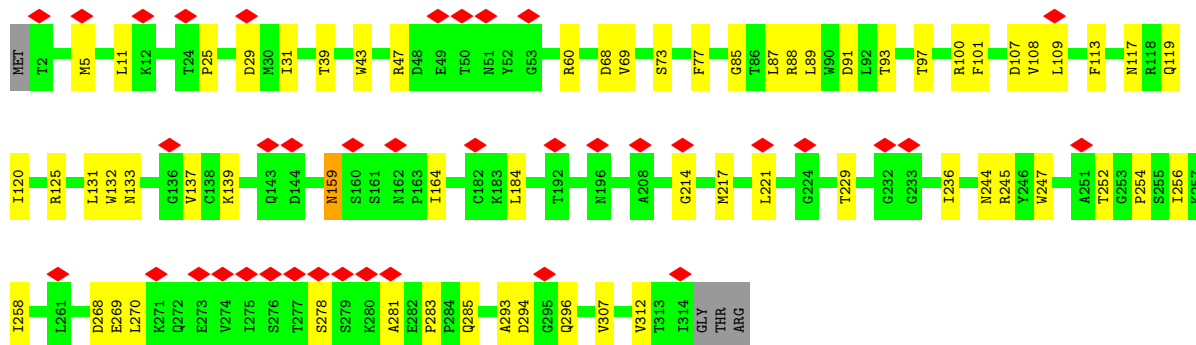
- Molecule 81: 60S ribosomal protein L37a

Chain Bp: 



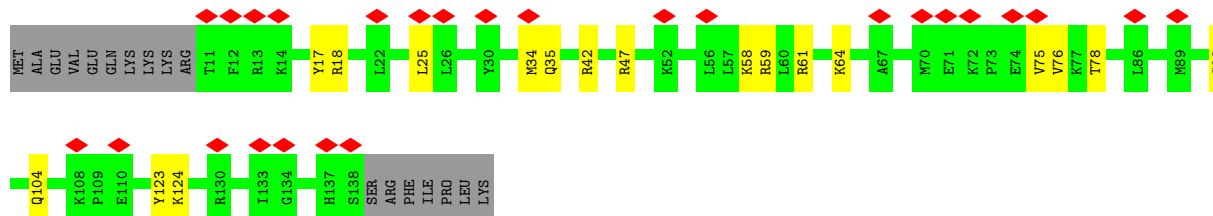
- Molecule 82: Small ribosomal subunit protein RACK1

Chain AF: 

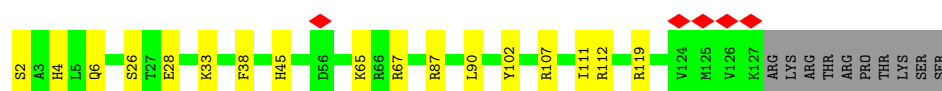


- Molecule 83: 40S ribosomal protein uS19

Chain Ao: 

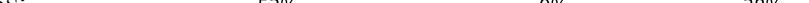


- Molecule 84: Large ribosomal subunit protein eL28



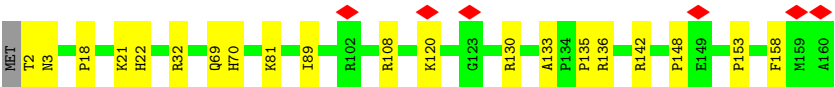
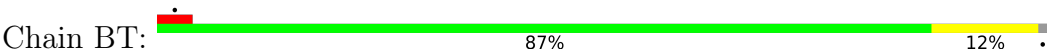
-
- | Category | Number of Genes |
|----------|-----------------|
| MET | 1 |
| G2 | 2 |
| Q16 | 3 |
| G17 | 4 |
| R22 | 5 |
| R27 | 6 |
| K33 | 7 |
| Y34 | 8 |
| N37 | 9 |
| R40 | 10 |
| R44 | 11 |
| F52 | 12 |
| I53 | 13 |
| K54 | 14 |
| L55 | 15 |
| D56 | 16 |

- [illegible]

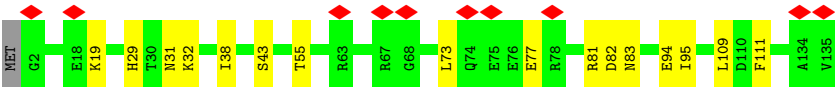
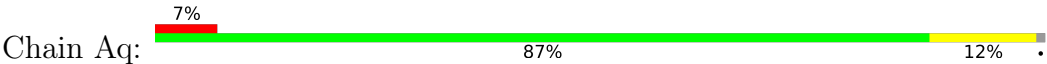
- Chain Bs: 

[illegible]

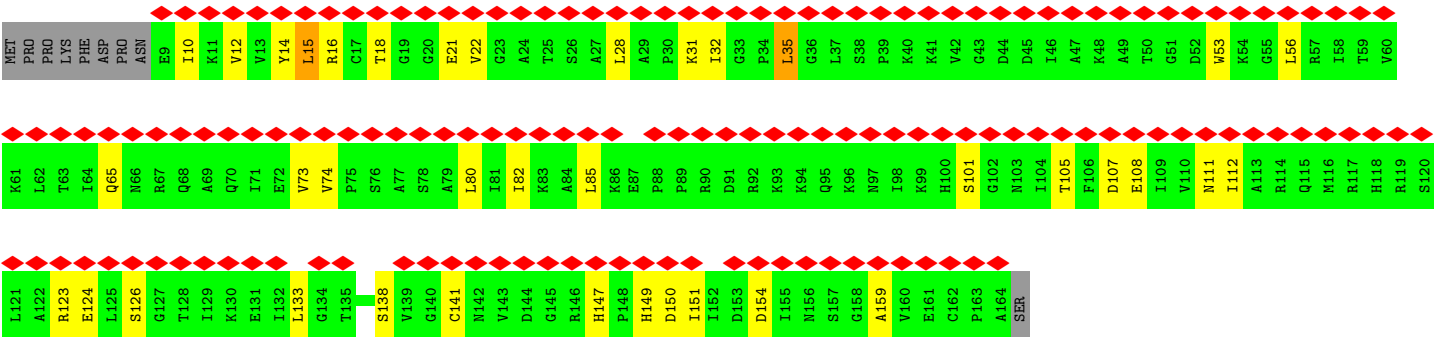
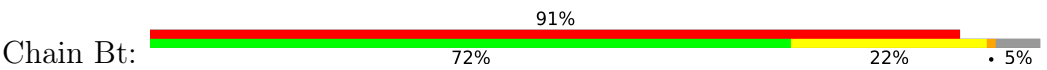
- 
- WORLDWIDE
PDB
PROTEIN DATA BANK



• Molecule 89: 40S ribosomal protein eS17



• Molecule 90: 60S ribosomal protein L12



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21864	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	OTHER	Depositor
Maximum map value	0.906	Depositor
Minimum map value	-0.490	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.175	Depositor
Map size (Å)	596.4, 596.4, 596.4	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, AYA, SPD, 4AC, OMC, SAC, IAS, A2M, MLZ, PSU, HY3, G7M, UNX, 1MA, 6MZ, MG, V5N, NMM, AME, ZN, OMG, OMU, 5MC, IHP, M3L, GTP, B8N, UY1, SPM, MA6, HIC

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	$\# Z > 5$
2	Bb	0.06	0/884	0.17	0/1169
3	B7	0.05	0/2835	0.08	0/4418
4	AT	0.27	0/68	0.35	0/103
5	Ar	0.06	0/1226	0.18	0/1643
6	B8	0.06	0/3635	0.11	0/5661
7	BU	0.08	0/845	0.21	0/1134
8	As	0.06	0/1119	0.18	0/1498
9	BA	0.08	0/1965	0.22	0/2633
10	BV	0.08	0/1048	0.21	0/1402
11	At	0.14	0/832	0.23	0/1117
12	BB	0.08	0/3261	0.20	0/4364
13	BX	0.07	0/984	0.19	0/1323
14	Au	0.06	0/636	0.18	0/852
15	BC	0.07	0/2932	0.18	0/3939
16	BP	0.07	0/1317	0.20	0/1768
17	BZ	0.06	0/1130	0.18	0/1507
18	Aw	0.07	0/1107	0.19	0/1475
19	BE	0.11	0/1998	0.22	0/2673
20	B5	0.10	2/86006 (0.0%)	0.12	0/134179
21	BQ	0.07	0/1539	0.20	0/2054
22	Ba	0.07	0/1179	0.18	0/1572
23	Ax	0.06	0/1032	0.17	0/1371
24	BF	0.07	0/1922	0.18	0/2563
25	BY	0.07	0/1132	0.20	0/1504
26	BW	0.06	0/1006	0.18	0/1334
27	AZ	0.07	0/1771	0.20	0/2406
28	Ay	0.07	0/691	0.19	0/922
29	BG	0.07	0/1908	0.19	0/2566
30	Av	0.08	0/1051	0.18	0/1406
31	BR	0.06	0/1524	0.16	0/2013
32	Aa	0.08	0/1841	0.20	0/2459

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Az	0.05	0/240	0.13	0/305
34	BH	0.07	0/1535	0.19	0/2063
35	BS	0.08	0/1497	0.19	0/2008
36	Ab	0.07	0/1742	0.20	0/2354
37	Bc	0.06	0/847	0.17	0/1134
38	BI	0.07	0/1756	0.18	0/2346
39	B	0.08	0/2444	0.20	0/3273
40	EA	0.07	0/2561	0.21	0/3473
41	Ac	0.07	0/1779	0.19	0/2395
42	Bd	0.08	0/903	0.20	0/1216
43	BJ	0.06	0/1385	0.18	0/1852
44	Ct	0.12	0/909	0.28	0/1214
45	Ad	0.07	0/2118	0.20	0/2849
46	Be	0.07	0/1088	0.21	0/1451
48	Cu	0.16	0/829	0.31	0/1112
49	Ae	0.07	0/1531	0.22	0/2059
50	Bf	0.08	0/903	0.20	0/1208
51	BL	0.07	0/1733	0.19	0/2316
52	DA	0.07	0/1284	0.21	0/1728
53	Af	0.06	0/1946	0.18	0/2590
54	Bg	0.06	0/916	0.19	0/1220
55	BM	0.07	0/1158	0.19	0/1547
56	DB	0.14	0/7038	0.29	0/9468
57	Ag	0.07	0/1552	0.19	0/2079
58	Bh	0.06	0/1021	0.15	0/1348
59	BN	0.07	0/1746	0.18	0/2338
60	DC	0.11	0/1323	0.25	0/1783
61	Ah	0.07	0/1715	0.19	0/2287
62	Bi	0.06	0/841	0.18	0/1112
63	BO	0.08	0/1662	0.19	0/2222
64	A2	0.13	2/40342 (0.0%)	0.12	0/62877
65	Ai	0.06	0/1550	0.18	0/2069
66	Bj	0.07	0/720	0.20	0/952
67	AA	0.06	0/665	0.19	0/891
68	Aj	0.07	0/834	0.20	0/1125
69	Bk	0.07	0/575	0.18	0/761
70	AB	0.06	0/497	0.17	0/666
71	Ak	0.07	0/1284	0.19	0/1717
72	Bl	0.08	0/459	0.19	0/608
73	AC	0.06	0/622	0.19	0/822
74	Al	0.07	0/968	0.21	0/1296
75	Bm	0.07	0/426	0.21	0/564
76	AD	0.06	0/462	0.18	0/607

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
77	Am	0.06	0/1232	0.17	0/1656
78	Bo	0.08	0/866	0.19	0/1141
79	AE	0.17	0/828	0.23	0/1109
80	An	0.11	0/1020	0.22	0/1366
81	Bp	0.07	0/718	0.20	0/953
82	AF	0.07	0/2493	0.21	0/3394
83	Ao	0.06	0/1069	0.18	0/1429
84	Br	0.07	0/1020	0.21	0/1366
85	AG	0.06	0/470	0.18	0/623
86	Ap	0.08	0/1142	0.25	0/1528
87	Bs	0.07	0/1530	0.20	0/2064
88	BT	0.07	0/1326	0.19	0/1770
89	Aq	0.06	0/1094	0.18	0/1469
90	Bt	0.07	0/1193	0.22	0/1609
All	All	0.10	4/243831 (0.0%)	0.16	0/355810

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	A2	1679	A2M	O3'-P	5.06	1.61	1.56
20	B5	2258	OMU	O3'-P	5.05	1.61	1.56
64	A2	485	A2M	O3'-P	5.02	1.61	1.56
20	B5	4269	A2M	O3'-P	5.01	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
78	Bo	53	MLZ	Mainchain

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	AH	36	0	25	0	0
2	Bb	881	0	957	13	0
3	B7	2538	0	1283	20	0
4	AT	939	0	617	4	0
5	Ar	1217	0	1279	21	0
6	B8	3319	0	1684	28	0
7	BU	831	0	852	5	0
8	As	1113	0	1145	17	0
9	BA	1940	0	2029	32	0
10	BV	1034	0	1096	16	0
11	At	822	0	887	7	0
12	BB	3206	0	3352	34	0
13	BX	967	0	1040	8	0
14	Au	640	0	633	10	0
15	BC	2886	0	3057	36	0
16	BP	1289	0	1329	11	0
17	BZ	1107	0	1182	15	0
18	Aw	1099	0	1162	4	0
19	BE	1960	0	2153	26	0
20	B5	79525	0	40256	667	0
21	BQ	1515	0	1634	21	0
22	Ba	1163	0	1202	17	0
23	Ax	1015	0	1086	15	0
24	BF	1886	0	2008	24	0
25	BY	1115	0	1205	11	0
26	BW	991	0	1048	7	0
27	AZ	1743	0	1748	25	0
28	Ay	683	0	761	12	0
29	BG	1877	0	2023	17	0
30	Av	1034	0	1080	7	0
31	BR	1508	0	1664	8	0
32	Aa	1815	0	1908	22	0
33	Az	239	0	289	2	0
34	BH	1516	0	1597	17	0
35	BS	1457	0	1492	15	0
36	Ab	1706	0	1796	19	0
37	Bc	836	0	888	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BI	1717	0	1764	21	0
39	B	2398	0	2428	30	0
40	EA	2445	0	2407	36	0
41	Ac	1751	0	1846	22	0
42	Bd	888	0	930	14	0
43	BJ	1362	0	1399	18	0
44	Ct	904	0	968	26	0
45	Ad	2076	0	2177	25	0
46	Be	1070	0	1164	17	0
47	BK	160	0	37	0	0
48	Cu	821	0	867	18	0
49	Ae	1509	0	1563	16	0
50	Bf	884	0	922	8	0
51	BL	1702	0	1820	15	0
52	DA	1260	0	1282	19	0
53	Af	1923	0	2089	35	0
54	Bg	906	0	998	10	0
55	BM	1137	0	1211	15	0
56	DB	6900	0	6944	151	0
57	Ag	1529	0	1627	17	0
58	Bh	1013	0	1147	20	0
59	BN	1701	0	1749	23	0
60	DC	1295	0	1267	26	0
61	Ah	1686	0	1772	22	0
62	Bi	830	0	916	8	0
63	BO	1630	0	1778	19	0
64	A2	37833	0	19167	355	0
65	Ai	1525	0	1640	19	0
66	Bj	705	0	737	13	0
67	AA	651	0	672	8	0
68	Aj	810	0	836	12	0
69	Bk	569	0	637	7	0
70	AB	495	0	523	2	0
71	Ak	1262	0	1335	11	0
72	Bl	447	0	479	6	0
73	AC	610	0	634	13	0
74	Al	958	0	993	15	0
75	Bm	432	0	470	3	0
76	AD	457	0	502	9	0
77	Am	1208	0	1293	11	0
78	Bo	863	0	929	10	0
79	AE	814	0	863	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	An	1016	0	1038	16	0
81	Bp	708	0	756	6	0
82	AF	2436	0	2393	37	0
83	Ao	1048	0	1093	12	0
84	Br	1014	0	1083	12	0
85	AG	459	0	448	11	0
86	Ap	1124	0	1193	19	0
87	Bs	1507	0	1564	18	0
88	BT	1298	0	1365	21	0
89	Aq	1080	0	1135	10	0
90	Bt	1178	0	1235	22	0
91	A2	49	0	0	2	0
91	AE	1	0	0	0	0
91	AT	2	0	0	0	0
91	Ad	1	0	0	0	0
91	Ak	1	0	0	0	0
91	An	1	0	0	0	0
91	Ar	1	0	0	0	0
91	B5	186	0	0	6	0
91	B7	6	0	0	1	0
91	B8	6	0	0	0	0
91	BA	3	0	0	0	0
91	BB	1	0	0	0	0
91	BH	1	0	0	0	0
91	BI	1	0	0	0	0
91	BL	1	0	0	0	0
91	BN	1	0	0	0	0
91	BP	1	0	0	0	0
91	BQ	2	0	0	0	0
91	BT	2	0	0	0	0
91	BY	1	0	0	0	0
91	Bb	2	0	0	0	0
91	Be	4	0	0	2	0
91	Bf	1	0	0	0	0
91	Bj	1	0	0	0	0
91	Bo	1	0	0	0	0
92	A2	111	0	0	0	0
92	AT	2	0	0	0	0
92	B5	282	0	0	0	0
92	B7	9	0	0	0	0
92	B8	8	0	0	0	0
92	BB	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
92	BI	1	0	0	0	0
92	BP	1	0	0	0	0
92	BR	1	0	0	0	0
92	BV	1	0	0	0	0
92	Ba	1	0	0	0	0
92	Be	1	0	0	0	0
92	Bj	1	0	0	0	0
93	B7	32	0	11	0	0
94	A2	80	0	152	5	0
94	B5	220	0	418	17	0
95	A2	14	0	26	4	0
95	B5	28	0	51	2	0
96	AC	1	0	0	0	0
96	AE	1	0	0	0	0
96	AG	1	0	0	0	0
96	Bg	1	0	0	0	0
96	Bj	1	0	0	0	0
96	Bm	1	0	0	0	0
96	Bo	1	0	0	0	0
96	Bp	1	0	0	0	0
97	DB	36	0	6	2	0
98	A2	527	0	0	25	0
98	AE	1	0	0	0	0
98	AH	3	0	0	0	0
98	AT	12	0	0	0	0
98	Aa	3	0	0	0	0
98	Ab	1	0	0	0	0
98	Ad	1	0	0	0	0
98	Af	1	0	0	0	0
98	Ak	2	0	0	0	0
98	An	1	0	0	0	0
98	Ap	2	0	0	0	0
98	Ar	2	0	0	0	0
98	As	2	0	0	0	0
98	At	1	0	0	0	0
98	Aw	5	0	0	1	0
98	B	1	0	0	0	0
98	B5	1398	0	0	58	0
98	B7	44	0	0	2	0
98	B8	47	0	0	1	0
98	BA	5	0	0	0	0
98	BB	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
98	BC	7	0	0	0	0
98	BH	1	0	0	0	0
98	BI	2	0	0	0	0
98	BL	2	0	0	0	0
98	BN	5	0	0	0	0
98	BP	3	0	0	0	0
98	BR	5	0	0	0	0
98	BV	2	0	0	0	0
98	BX	2	0	0	0	0
98	Ba	8	0	0	1	0
98	Bb	1	0	0	0	0
98	Bd	1	0	0	0	0
98	Be	4	0	0	0	0
98	Bg	1	0	0	0	0
98	Bj	5	0	0	0	0
98	Bl	2	0	0	0	0
98	Ct	1	0	0	0	0
All	All	236684	0	178196	2069	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (2069) 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)
91:B7:210:UNX:UNK	98:B7:306:HOH:O	1.57	0.85
91:B5:5113:UNX:UNK	98:B5:5788:HOH:O	1.57	0.85
91:A2:1979:UNX:UNK	98:A2:2108:HOH:O	1.57	0.85
98:B5:6310:HOH:O	91:Be:205:UNX:UNK	1.60	0.82
30:Av:2:VAL:N	64:A2:1092:C:HO2'	1.78	0.81
98:B5:5800:HOH:O	91:Be:205:UNX:UNK	1.63	0.78
45:Ad:125:LYS:H	45:Ad:142:HIS:HD2	1.33	0.76
20:B5:4436:G:C8	98:B5:5557:HOH:O	2.39	0.76
20:B5:394:G:OP2	44:Ct:71:ARG:NH1	2.19	0.75
64:A2:1131:G:OP2	64:A2:1131:G:N2	2.18	0.75
20:B5:1899:A:H1'	87:Bs:63:LYS:HD3	1.70	0.74
20:B5:2697:G:P	91:B5:5253:UNX:UNK	2.09	0.73
52:DA:45:LEU:HB3	52:DA:61:CYS:HB2	1.69	0.73
64:A2:228:C:H42	64:A2:902:G:H1'	1.54	0.72
64:A2:1397:A:O2'	64:A2:1399:G:N7	2.22	0.72
52:DA:142:ILE:HG22	52:DA:144:PRO:HD2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B5:2697:G:OP1	91:B5:5253:UNX:UNK	1.71	0.72
20:B5:1810:A2M:HM'2	20:B5:1811:G:H5'	1.73	0.71
56:DB:188:GLU:HB3	56:DB:533:ILE:HD12	1.73	0.71
86:Ap:97:GLN:HB2	86:Ap:105:LYS:HG3	1.72	0.71
91:B5:5228:UNX:UNK	98:B5:5941:HOH:O	1.72	0.70
20:B5:1676:A:P	98:B5:5531:HOH:O	2.49	0.70
20:B5:2635:C:P	98:B5:5536:HOH:O	2.49	0.70
64:A2:577:A2M:HM'2	64:A2:578:U:H5'	1.73	0.70
64:A2:43:U:P	98:A2:2273:HOH:O	2.50	0.69
10:BV:69:LYS:HG2	10:BV:71:GLU:HG2	1.74	0.69
80:An:34:PHE:HB3	80:An:41:PHE:HB2	1.75	0.69
8:As:101:ARG:NH2	64:A2:1567:G:N7	2.40	0.69
20:B5:3978:U:O4	78:Bo:8:ARG:NH2	2.26	0.69
39:B:83:LEU:HB3	39:B:88:VAL:HB	1.74	0.69
64:A2:1260:A:H1'	64:A2:1265:C:H42	1.58	0.69
64:A2:1491:OMG:HM22	64:A2:1492:G:H5'	1.74	0.68
2:Bb:106:ARG:NH2	20:B5:1391:C:O2'	2.25	0.68
19:BE:227:LYS:HE2	19:BE:241:GLU:H	1.57	0.68
44:Ct:98:LYS:HB2	44:Ct:102:ILE:HB	1.74	0.68
20:B5:2696:C:O3'	91:B5:5253:UNX:UNK	1.74	0.68
20:B5:3557:A2M:HM'2	20:B5:3558:C:H5'	1.76	0.68
20:B5:1476:C:P	98:B5:5528:HOH:O	2.52	0.68
20:B5:4279:A:P	98:B5:5765:HOH:O	2.51	0.68
49:Ae:60:ARG:HD2	64:A2:1680:A:H2'	1.76	0.68
64:A2:165:G:H2'	64:A2:166:A2M:H8	1.75	0.68
64:A2:869:G:OP2	64:A2:869:G:N2	2.23	0.68
20:B5:1809:C:H2'	20:B5:1810:A2M:H8	1.76	0.68
12:BB:268:ARG:NH2	20:B5:3628:C:O2'	2.27	0.68
20:B5:2688:A:P	98:B5:5521:HOH:O	2.51	0.68
20:B5:3373:U:OP2	20:B5:3378:A:N6	2.27	0.68
34:BH:23:ARG:HE	34:BH:39:ASN:HA	1.58	0.67
56:DB:762:LEU:HD12	56:DB:797:ARG:HG2	1.76	0.67
79:AE:44:ILE:O	80:An:113:GLN:NE2	2.28	0.67
56:DB:330:ARG:HG2	56:DB:386:LYS:HZ3	1.60	0.67
64:A2:1286:G:H22	74:Al:57:ASP:HB2	1.60	0.67
20:B5:3561:G:H2'	20:B5:3562:A2M:H8	1.75	0.67
55:BM:40:GLY:HA3	55:BM:45:VAL:HB	1.75	0.67
19:BE:115:MET:O	84:Br:87:ARG:NH1	2.28	0.67
64:A2:1830:G:H1'	64:A2:1851:MA6:H2	1.77	0.67
87:Bs:65:ILE:HG23	87:Bs:75:LEU:HB3	1.76	0.67
64:A2:1604:G:P	98:A2:2117:HOH:O	2.53	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B5:308:G:N2	20:B5:308:G:OP2	2.28	0.66
20:B5:1908:G:H4'	87:Bs:36:GLY:HA2	1.75	0.66
20:B5:2704:OMC:HM22	20:B5:2705:G:H5'	1.76	0.66
95:B5:4947:SPM:H22	21:BQ:11:ARG:HB3	1.77	0.66
27:AZ:94:THR:HG23	27:AZ:186:ARG:HH12	1.60	0.66
64:A2:1675:G:N7	86:Ap:17:LYS:NZ	2.43	0.66
10:BV:15:ARG:NH2	20:B5:4416:C:O2'	2.28	0.66
40:EA:109:ALA:O	40:EA:185:ASN:ND2	2.28	0.66
20:B5:1922:A:H1'	20:B5:1949:A:H4'	1.76	0.66
24:BF:237:ASP:O	24:BF:240:ASN:ND2	2.29	0.66
20:B5:1635:G:P	98:B5:5537:HOH:O	2.52	0.66
82:AF:247:TRP:HB3	82:AF:258:ILE:HD11	1.77	0.66
20:B5:1237:G:OP2	20:B5:1237:G:N2	2.21	0.66
20:B5:4194:G:C8	98:B5:5746:HOH:O	2.48	0.66
52:DA:54:ILE:HB	56:DB:407:LEU:HD21	1.78	0.66
48:Cu:52:GLY:H	48:Cu:82:SER:HB2	1.60	0.66
21:BQ:16:LYS:O	21:BQ:33:ARG:NH2	2.29	0.66
44:Ct:97:ARG:NH2	48:Cu:105:SER:O	2.28	0.66
64:A2:513:A2M:HM'2	64:A2:514:G:H5'	1.78	0.66
8:As:7:LYS:HB3	86:Ap:37:ARG:HG2	1.77	0.66
56:DB:441:ASP:O	56:DB:445:ASN:ND2	2.28	0.66
20:B5:1399:G:OP2	20:B5:1399:G:N2	2.27	0.65
20:B5:1567:G:O6	91:B5:5211:UNX:UNK	1.56	0.65
56:DB:277:LEU:HD11	56:DB:301:LEU:HD21	1.78	0.65
82:AF:119:GLN:HB3	82:AF:131:LEU:HD11	1.78	0.65
20:B5:4480:A:H61	20:B5:4704:U:H3	1.44	0.65
87:Bs:39:GLN:HE22	87:Bs:106:LYS:HA	1.62	0.65
20:B5:3540:OMC:HM22	20:B5:3541:G:H5'	1.79	0.65
20:B5:2548:G:O6	31:BR:46:LYS:NZ	2.29	0.65
61:Ah:101:ILE:HD12	61:Ah:190:LEU:HD11	1.78	0.65
20:B5:308:G:H2'	62:Bi:41:ARG:HH12	1.62	0.65
20:B5:4103:G:P	98:B5:5518:HOH:O	2.53	0.65
64:A2:1220:C:P	98:A2:2139:HOH:O	2.55	0.65
12:BB:246:ARG:NH2	20:B5:4304:U:OP2	2.30	0.65
20:B5:3958:A:N1	88:BT:3:ASN:ND2	2.42	0.65
64:A2:1289:OMU:OP2	73:AC:97:LYS:NZ	2.30	0.65
20:B5:410:A:HO2'	20:B5:414:C:HO2'	1.44	0.65
20:B5:1550:G:P	98:B5:5940:HOH:O	2.54	0.65
20:B5:3478:A:P	98:B5:5524:HOH:O	2.54	0.65
20:B5:4174:A:P	98:B5:5917:HOH:O	2.55	0.65
41:Ac:177:LEU:HD13	41:Ac:182:LEU:HD13	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Ae:130:ARG:HD2	64:A2:1684:C:H5'	1.78	0.65
29:BG:103:ARG:NH2	29:BG:192:ARG:O	2.29	0.65
64:A2:905:A:O2'	71:Ak:48:LYS:NZ	2.29	0.65
15:BC:143:ARG:NH1	20:B5:2143:A:N7	2.45	0.65
15:BC:223:ASN:ND2	20:B5:223:G:N3	2.45	0.64
22:Ba:24:LYS:HD2	22:Ba:26:ARG:HH21	1.62	0.64
82:AF:77:PHE:HB3	82:AF:89:LEU:HD11	1.78	0.64
56:DB:794:LEU:HD13	56:DB:797:ARG:HH22	1.61	0.64
64:A2:976:G:OP1	80:An:98:ARG:NH1	2.30	0.64
20:B5:1937:A:N3	20:B5:1958:C:O2'	2.30	0.64
56:DB:353:LEU:HB3	56:DB:373:LEU:HG	1.79	0.64
20:B5:1489:A2M:OP2	98:B5:5539:HOH:O	2.15	0.64
43:BJ:35:ARG:NH1	43:BJ:123:ILE:O	2.31	0.64
56:DB:80:HIS:CE1	56:DB:109:TRP:HB2	2.32	0.64
64:A2:1678:U:H2'	64:A2:1679:A2M:H8	1.79	0.64
40:EA:326:ILE:HG22	40:EA:328:PRO:HD3	1.79	0.64
53:Af:13:GLN:NE2	64:A2:153:G:N3	2.44	0.64
20:B5:435:A:O2'	46:Be:26:ASP:OD2	2.15	0.64
20:B5:2267:OMG:HM22	20:B5:2268:U:H5''	1.80	0.64
20:B5:3421:G:O2'	20:B5:3550:UY1:OP2	2.15	0.64
20:B5:679:C:O2'	56:DB:593:LYS:NZ	2.29	0.64
25:BY:67:ILE:O	25:BY:84:ARG:NH2	2.31	0.64
56:DB:254:ASN:HB2	56:DB:260:TYR:HE2	1.63	0.64
64:A2:94:G:P	98:A2:2102:HOH:O	2.53	0.64
21:BQ:119:LYS:HE3	21:BQ:121:LEU:HD21	1.80	0.64
26:BW:80:ARG:NH2	53:Af:129:VAL:O	2.31	0.64
14:Au:38:GLU:HA	27:AZ:63:ARG:HH21	1.63	0.64
43:BJ:43:LEU:HD13	43:BJ:117:ILE:HD11	1.78	0.64
40:EA:183:PRO:HD3	40:EA:222:THR:HB	1.80	0.64
64:A2:1805:OMU:O4	91:A2:1943:UNX:UNK	1.79	0.64
53:Af:2:LYS:HG2	53:Af:17:GLU:HG2	1.80	0.63
56:DB:148:ARG:NH2	56:DB:189:TYR:OH	2.30	0.63
64:A2:1386:G:P	98:A2:2106:HOH:O	2.55	0.63
64:A2:671:A:OP2	98:A2:2107:HOH:O	2.15	0.63
8:As:12:GLN:HE22	64:A2:1594:C:H1'	1.64	0.63
20:B5:1674:U:H5'	94:B5:5066:SPD:H41	1.80	0.63
20:B5:1789:A:OP2	51:BL:5:ARG:NH2	2.31	0.63
64:A2:1031:A:H2'	64:A2:1032:A2M:H8	1.79	0.63
64:A2:1227:G:N1	64:A2:1640:G7M:OP2	2.27	0.63
20:B5:85:G:N2	20:B5:98:A:OP2	2.29	0.63
20:B5:3985:A:P	98:B5:5818:HOH:O	2.56	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:AZ:17:LYS:HB3	27:AZ:173:LEU:HD11	1.80	0.63
45:Ad:100:ARG:HB2	45:Ad:114:ILE:HD13	1.80	0.63
20:B5:24:G:N7	66:Bj:46:LYS:NZ	2.46	0.63
56:DB:513:ARG:NH1	56:DB:640:GLU:O	2.31	0.63
74:Al:89:VAL:HG11	74:Al:109:VAL:HG11	1.81	0.63
20:B5:1504:G:OP1	98:B5:5540:HOH:O	2.16	0.63
20:B5:4639:C:O2'	20:B5:4641:C:OP2	2.17	0.63
45:Ad:44:LEU:HD21	45:Ad:72:ILE:HD11	1.81	0.63
53:Af:2:LYS:HB3	53:Af:15:LEU:HD11	1.79	0.63
12:BB:357:ARG:HE	20:B5:4361:C:H5''	1.63	0.63
41:Ac:213:PRO:HG3	89:Aq:19:LYS:HB3	1.81	0.63
56:DB:354:LYS:HG3	56:DB:373:LEU:HD21	1.81	0.63
20:B5:1869:U:OP2	63:BO:49:ARG:NH1	2.31	0.62
20:B5:2205:U:H2'	20:B5:2206:A2M:H8	1.81	0.62
45:Ad:11:ARG:HA	45:Ad:28:ALA:HB2	1.79	0.62
74:Al:79:VAL:HG11	74:Al:85:LEU:HB2	1.81	0.62
40:EA:260:ILE:HG12	40:EA:361[A]:LEU:HD11	1.80	0.62
64:A2:1392:OMC:HM22	64:A2:1393:U:H5'	1.80	0.62
20:B5:734:G:OP2	55:BM:71:LYS:NZ	2.33	0.62
20:B5:2250:G:N2	72:Bl:51:LEU:OXT	2.32	0.62
82:AF:60:ARG:HE	86:Ap:97:GLN:HE22	1.48	0.62
24:BF:85:GLU:OE2	88:BT:136:ARG:NH1	2.32	0.62
44:Ct:187:GLN:HE22	56:DB:77:LEU:HD13	1.64	0.62
20:B5:1888:U:OP1	34:BH:64:ARG:NH1	2.32	0.62
64:A2:1216:C:H42	64:A2:1221:A:H61	1.46	0.62
12:BB:396:ARG:NH2	20:B5:4779:U:OP2	2.33	0.62
20:B5:1915:G:N3	90:Bt:138:SER:OG	2.33	0.62
3:B7:6:C:H4'	39:B:52:ILE:HD13	1.82	0.62
20:B5:1741:A:H5''	20:B5:1742:G:H5'	1.82	0.62
20:B5:3676:OMG:HN1	20:B5:3797:U:H3	1.47	0.62
68:Aj:51:SER:OG	68:Aj:55:ARG:NH1	2.33	0.62
20:B5:4163:C:P	98:B5:5617:HOH:O	2.57	0.62
27:AZ:198:MET:HG2	27:AZ:200:ASP:H	1.65	0.62
29:BG:58:PRO:HD2	29:BG:61:ILE:HD12	1.80	0.62
56:DB:118:ARG:NH2	56:DB:147:GLN:OE1	2.33	0.62
59:BN:53:TYR:HB2	59:BN:133:ILE:HD13	1.81	0.62
20:B5:4640:G:H1	20:B5:4659:C:H42	1.48	0.61
60:DC:10:ASP:HB3	60:DC:52:ILE:HD11	1.80	0.61
73:AC:116:ARG:NH1	73:AC:120:GLU:OE2	2.33	0.61
51:BL:43:ALA:HB1	51:BL:149:GLN:HE22	1.65	0.61
64:A2:664:C:P	98:A2:2162:HOH:O	2.58	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:AA:84:HIS:OXT	77:Am:19:ARG:NH1	2.33	0.61
78:Bo:36:GLN:OE1	78:Bo:39:ARG:NH2	2.34	0.61
12:BB:317:LEU:HD22	12:BB:382:VAL:HG13	1.81	0.61
36:Ab:187:ARG:NH1	64:A2:1143:G:OP1	2.31	0.61
38:BI:38:ARG:HD2	38:BI:41:ALA:HB2	1.81	0.61
44:Ct:188:ALA:HB2	44:Ct:210:ILE:HG23	1.83	0.61
64:A2:90:G:OP2	94:A2:1908:SPD:N10	2.34	0.61
89:Aq:29:HIS:HA	89:Aq:32:LYS:HE2	1.82	0.61
20:B5:4638:G:N2	20:B5:4661:C:O2	2.33	0.61
73:AC:126:CYS:HB3	73:AC:143:LYS:HD3	1.82	0.61
9:BA:132:ASN:ND2	20:B5:3415:C:OP1	2.34	0.61
43:BJ:144:LYS:O	43:BJ:148:THR:OG1	2.19	0.61
11:At:94:ASP:OD2	85:AG:44:ARG:NH1	2.32	0.61
20:B5:399:G:H2'	20:B5:400:A2M:H8	1.83	0.61
20:B5:4287:G:N2	20:B5:4290:A:OP2	2.34	0.61
24:BF:104:VAL:HG13	24:BF:135:VAL:HG12	1.81	0.61
38:BI:54:SER:HB2	38:BI:135:ILE:HD11	1.82	0.61
44:Ct:80:MET:HE2	48:Cu:44:LEU:HD23	1.82	0.61
64:A2:121:OMU:HM22	64:A2:122:G:H5'	1.82	0.61
64:A2:1355:G:N2	64:A2:1358:A:OP2	2.32	0.61
7:BU:48:LYS:HG2	7:BU:53:ALA:HB2	1.81	0.61
13:BX:82:THR:HG22	13:BX:155:ILE:HG23	1.82	0.61
20:B5:4744:G:N2	20:B5:4780:G:O2'	2.33	0.61
48:Cu:62:VAL:HG11	48:Cu:90:ILE:HD13	1.83	0.61
50:Bf:43:LEU:O	50:Bf:109:ARG:NH1	2.33	0.61
56:DB:137:ARG:HH11	56:DB:157:ALA:HB2	1.66	0.61
20:B5:2194:OMC:HM22	20:B5:2195:U:H5'	1.82	0.61
20:B5:4764:C:O2'	20:B5:4767:G:N3	2.33	0.61
64:A2:142:C:N4	64:A2:330:G:OP1	2.30	0.61
76:AD:109:ARG:O	76:AD:113:ASN:ND2	2.33	0.61
20:B5:4366:OMU:OP2	20:B5:4416:C:N4	2.34	0.61
59:BN:116:LEU:HD22	59:BN:135:ILE:HD11	1.83	0.61
64:A2:1049:G:N7	98:A2:2178:HOH:O	2.31	0.61
87:Bs:48:ARG:HD3	90:Bt:123:ARG:HG2	1.82	0.61
86:Ap:101:ASP:OD1	86:Ap:102:GLU:N	2.34	0.60
29:BG:185:LYS:O	29:BG:189:ARG:NH2	2.34	0.60
52:DA:10:ASP:OD1	52:DA:47:LYS:NZ	2.34	0.60
53:Af:2:LYS:NZ	64:A2:156:G:OP1	2.34	0.60
56:DB:608:ILE:HG22	56:DB:612:LYS:HE3	1.84	0.60
64:A2:642:A:OP1	65:Ai:40:LYS:NZ	2.31	0.60
12:BB:224:LYS:HG2	12:BB:340:THR:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B5:1260:OMG:HM22	20:B5:1261:U:H5'	1.83	0.60
20:B5:4202:OMC:HM22	20:B5:4203:PSU:H5''	1.83	0.60
82:AF:236:ILE:HG12	82:AF:252:THR:HG22	1.83	0.60
20:B5:1829:G:OP2	20:B5:1829:G:N2	2.32	0.60
20:B5:3909:U:H5'	20:B5:3910:C:H5''	1.83	0.60
35:BS:173:ASN:ND2	35:BS:175:PHE:O	2.34	0.60
59:BN:96:ARG:HH21	59:BN:100:SER:HG	1.50	0.60
82:AF:11:LEU:HB2	82:AF:307:VAL:HB	1.82	0.60
27:AZ:41:ARG:HE	27:AZ:45:GLY:HA2	1.66	0.60
43:BJ:13:ARG:O	43:BJ:136:ARG:NH1	2.35	0.60
53:Af:162:LEU:HD11	53:Af:172:LYS:HG3	1.83	0.60
57:Ag:107:LYS:O	57:Ag:109:ARG:NH2	2.34	0.60
65:Ai:170:PRO:O	65:Ai:175:ARG:NH1	2.33	0.60
87:Bs:47:LEU:HB3	87:Bs:51:ALA:HB3	1.83	0.60
20:B5:1415:C:H5''	21:BQ:144:LYS:HG2	1.83	0.60
40:EA:139:MET:HE2	40:EA:323:VAL:HG11	1.83	0.60
20:B5:2298:G:N2	20:B5:2312:C:O2	2.35	0.60
74:Al:11:VAL:HG13	74:Al:13:ASP:H	1.65	0.60
39:B:17:GLN:NE2	88:BT:22:HIS:O	2.35	0.60
42:Bd:64:ILE:HG23	42:Bd:68:LEU:HD23	1.83	0.60
20:B5:3644:U:OP1	98:B5:5544:HOH:O	2.16	0.60
56:DB:423:ASN:HB3	56:DB:426:GLU:HB2	1.84	0.60
82:AF:87:LEU:HB2	82:AF:101:PHE:HB2	1.84	0.60
20:B5:70:A:OP2	22:Ba:64:LYS:NZ	2.34	0.60
36:Ab:207:ALA:HB2	64:A2:4:C:H4'	1.84	0.60
40:EA:180:TYR:HB3	40:EA:224:TYR:HB3	1.83	0.59
64:A2:75:G:O2'	64:A2:77:A:OP1	2.20	0.59
20:B5:103:G:N7	98:B5:5726:HOH:O	2.32	0.59
20:B5:393:U:H5''	44:Ct:71:ARG:HH22	1.65	0.59
20:B5:4061:A:OP1	88:BT:69:GLN:NE2	2.35	0.59
26:BW:66:GLU:HG3	26:BW:68:GLN:HE22	1.67	0.59
61:Ah:47:ARG:NH2	64:A2:447:G:OP2	2.32	0.59
64:A2:1264:U:O2	85:AG:16:GLN:NE2	2.33	0.59
74:Al:75:ASN:N	74:Al:75:ASN:OD1	2.34	0.59
20:B5:106:A:P	98:B5:5526:HOH:O	2.58	0.59
20:B5:4282:OMC:HM22	20:B5:4283:C:H5'	1.84	0.59
32:Aa:28:LYS:HB3	32:Aa:48:LEU:HD11	1.84	0.59
45:Ad:31:PRO:HG3	45:Ad:43:PRO:HG3	1.84	0.59
56:DB:270:PRO:HG2	56:DB:276:ARG:HG2	1.83	0.59
77:Am:136:PRO:HG2	77:Am:139:TRP:HB2	1.82	0.59
20:B5:755:G:H1	20:B5:800:U:H3	1.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BR:44:LEU:HD22	31:BR:49:LEU:HD12	1.84	0.59
20:B5:3619:OMC:HM22	20:B5:3620:G:H5'	1.83	0.59
20:B5:68:U:OP1	59:BN:178:HIS:ND1	2.32	0.59
20:B5:1924:G:H1'	20:B5:1942:G:H2'	1.85	0.59
20:B5:4218:G:O2'	75:Bm:100:TYR:O	2.21	0.59
16:BP:138:PRO:HB3	16:BP:140:MET:HE2	1.84	0.59
40:EA:233:ASN:H	40:EA:358:GLU:HB3	1.68	0.59
20:B5:375:G:OP2	66:Bj:52:LYS:NZ	2.35	0.59
20:B5:1423:C:OP1	22:Ba:132:ARG:NH2	2.36	0.59
41:Ac:16:ILE:HG21	85:AG:22:ARG:HH11	1.67	0.59
64:A2:831:A:OP2	64:A2:847:G:N2	2.35	0.59
64:A2:1529:G:O2'	64:A2:1667:C:OP1	2.18	0.59
82:AF:244:ASN:ND2	82:AF:294:ASP:O	2.36	0.59
12:BB:246:ARG:NH1	20:B5:4271:C:OP1	2.35	0.59
20:B5:4307:C:P	98:B5:5718:HOH:O	2.61	0.59
30:Av:45:GLY:O	30:Av:68:ARG:NH2	2.36	0.59
65:Ai:93:LYS:HB2	65:Ai:96:TYR:HD2	1.68	0.59
10:BV:106:VAL:HG12	10:BV:112:MET:HA	1.85	0.59
49:Ae:56:TYR:HB3	49:Ae:63:LYS:HA	1.84	0.59
64:A2:1390:C:OP1	89:Aq:43:SER:OG	2.19	0.59
87:Bs:32:ALA:O	87:Bs:85:ASN:ND2	2.36	0.59
9:BA:2:GLY:N	20:B5:3651:C:OP1	2.36	0.58
20:B5:1772:G:OP1	88:BT:120:LYS:NZ	2.34	0.58
64:A2:1651:A:H5''	86:Ap:139:ALA:HB2	1.84	0.58
6:B8:81:C:HO2'	58:Bh:2:ALA:N	2.01	0.58
20:B5:4416:C:O2'	20:B5:4418:A:OP2	2.21	0.58
64:A2:678:G:N1	64:A2:1028:A:OP2	2.27	0.58
64:A2:1548:C:N4	64:A2:1587:U:O4	2.35	0.58
64:A2:1839:U:P	98:A2:2105:HOH:O	2.61	0.58
10:BV:13:LYS:HB3	10:BV:128:LEU:HD11	1.85	0.58
12:BB:175:GLN:NE2	20:B5:4724:U:OP1	2.37	0.58
16:BP:118:GLN:NE2	16:BP:147:GLU:OE2	2.36	0.58
20:B5:2507:G:H4'	20:B5:2520:G:H4'	1.85	0.58
20:B5:3585:PSU:O2'	20:B5:4718:A:N3	2.36	0.58
34:BH:141:LYS:NZ	34:BH:142:ASP:OD2	2.35	0.58
54:Bg:5:LEU:HD21	54:Bg:30:ILE:HG22	1.86	0.58
64:A2:49:C:H2'	64:A2:473:C:H41	1.67	0.58
64:A2:445:G:H4'	94:A2:1908:SPD:H91	1.84	0.58
6:B8:86:U:OP2	25:BY:113:LYS:NZ	2.35	0.58
20:B5:3541:G:OP2	20:B5:3541:G:N2	2.29	0.58
26:BW:80:ARG:NH1	64:A2:167:G:O2'	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:Ac:42:THR:OG1	41:Ac:45:ARG:O	2.18	0.58
60:DC:72:ILE:HG13	60:DC:91:MET:HE1	1.85	0.58
64:A2:894:U:H2'	64:A2:895:G:H8	1.67	0.58
2:Bb:56:LYS:O	2:Bb:60:ASN:ND2	2.33	0.58
15:BC:342:ARG:NH2	20:B5:845:U:OP1	2.35	0.58
53:Af:159:ARG:HB3	53:Af:171:THR:HB	1.85	0.58
64:A2:1544:U:H5''	86:Ap:37:ARG:HH12	1.69	0.58
87:Bs:19:GLN:NE2	87:Bs:23:ASP:OD2	2.36	0.58
8:As:121:ARG:NH1	64:A2:1564:G:OP1	2.36	0.58
20:B5:327:U:O2'	62:Bi:30:ARG:NH1	2.36	0.58
20:B5:3469:A:P	98:B5:5530:HOH:O	2.62	0.58
95:B5:4947:SPM:N5	21:BQ:8:ASN:O	2.35	0.58
26:BW:2:LYS:NZ	26:BW:4:GLU:OE2	2.35	0.58
64:A2:1261:A:P	98:A2:2143:HOH:O	2.61	0.58
82:AF:120:ILE:HB	82:AF:132:TRP:HB2	1.86	0.58
16:BP:8:PRO:HG3	16:BP:149:ILE:HD13	1.86	0.58
20:B5:1924:G:N2	20:B5:1924:G:OP1	2.36	0.58
20:B5:4122:A:O2'	22:Ba:42:ARG:NH1	2.36	0.58
20:B5:4124:A:P	98:B5:5505:HOH:O	2.55	0.58
41:Ac:27:ARG:NH2	64:A2:1499:A:OP2	2.35	0.58
86:Ap:53:GLU:OE1	86:Ap:85:ARG:NH2	2.35	0.58
20:B5:1093:C:H2'	20:B5:1094:A:H8	1.67	0.58
20:B5:1980:A:N7	20:B5:4180:C:O2'	2.36	0.58
20:B5:2250:G:N2	20:B5:2250:G:OP2	2.33	0.58
64:A2:191:A:H62	64:A2:208:G:H21	1.52	0.58
82:AF:217:MET:HG2	82:AF:229:THR:HG22	1.86	0.58
56:DB:726:LEU:HB2	56:DB:731:ARG:CZ	2.33	0.58
12:BB:261:ARG:HB2	63:BO:64:THR:HG21	1.85	0.58
20:B5:3539:A:OP1	33:Az:23:ARG:NH2	2.37	0.58
45:Ad:49:ARG:NH2	64:A2:497:C:OP1	2.37	0.58
20:B5:3450:A2M:HM'2	20:B5:3451:A:H5'	1.86	0.57
41:Ac:45:ARG:NH2	41:Ac:82:GLY:O	2.37	0.57
64:A2:1018:U:OP1	77:Am:62:GLN:NE2	2.37	0.57
64:A2:1551:G:H3'	64:A2:1580:A:H61	1.69	0.57
64:A2:1839:U:P	98:A2:2126:HOH:O	2.61	0.57
71:Ak:135:SER:O	71:Ak:139:ARG:NH1	2.37	0.57
80:An:95:ILE:HB	80:An:129:ILE:HG12	1.86	0.57
19:BE:49:ASN:HD21	19:BE:57:GLY:HA3	1.69	0.57
20:B5:364:G:O6	66:Bj:55:ARG:NH2	2.30	0.57
20:B5:1624:A:N3	20:B5:1791:U:O2'	2.35	0.57
20:B5:4440:G:OP1	20:B5:4440:G:N2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B5:3805:A:N1	20:B5:3917:C:N4	2.51	0.57
27:AZ:206:ASP:OD1	27:AZ:206:ASP:N	2.36	0.57
56:DB:69:VAL:HG21	56:DB:89:LEU:HD11	1.87	0.57
56:DB:748:LYS:HG2	56:DB:775:LEU:HD13	1.85	0.57
9:BA:21:LYS:HG2	20:B5:1496:C:H5''	1.86	0.57
20:B5:3476:OMG:HM22	20:B5:3477:U:H5'	1.85	0.57
64:A2:1508:G:N2	73:AC:87:THR:O	2.36	0.57
64:A2:1148:C:OP1	79:AE:6:ARG:NH1	2.36	0.57
90:Bt:10:ILE:HG12	90:Bt:65:GLN:HG2	1.86	0.57
9:BA:101:VAL:HG22	9:BA:165:VAL:HG22	1.87	0.57
20:B5:2431:C:OP1	20:B5:2611:C:O2'	2.21	0.57
20:B5:4390:G:N7	98:B5:5727:HOH:O	2.32	0.57
84:Br:90:LEU:HD22	84:Br:111:ILE:HG23	1.86	0.57
9:BA:241:ARG:NH1	20:B5:3391:G:OP1	2.37	0.57
10:BV:85:ARG:NH1	10:BV:99:GLU:O	2.38	0.57
18:Aw:18:ARG:NH1	64:A2:360:U:OP2	2.36	0.57
64:A2:166:A2M:HM'2	64:A2:167:G:H5'	1.87	0.57
3:B7:52:C:O2'	3:B7:54:A:N7	2.37	0.57
20:B5:454:U:H1'	46:Be:5:ARG:HE	1.69	0.57
20:B5:1805:U:OP1	38:BI:4:ARG:NH1	2.37	0.57
64:A2:852:C:H5''	64:A2:853:G:H5'	1.87	0.57
64:A2:1842:C:H2'	64:A2:1843:4AC:H6	1.87	0.57
89:Aq:94:GLU:HG2	89:Aq:95:ILE:HG13	1.87	0.57
5:Ar:36:VAL:HG21	5:Ar:71:MET:HE3	1.87	0.57
20:B5:4268:G:O2'	20:B5:4271:C:OP2	2.21	0.57
32:Aa:7:LYS:NZ	64:A2:966:U:OP1	2.34	0.57
38:BI:57:TYR:OH	38:BI:128:ARG:NH2	2.38	0.57
57:Ag:114:GLN:NE2	64:A2:875:G:N3	2.50	0.57
64:A2:1448:OMG:HM22	64:A2:1449:A:H5'	1.87	0.57
79:AE:51:ARG:NH1	79:AE:55:GLU:OE2	2.37	0.57
20:B5:92:C:OP1	94:B5:5359:SPD:N10	2.38	0.57
20:B5:135:G:N2	58:Bh:95:LEU:O	2.35	0.57
27:AZ:76:VAL:HG12	27:AZ:123:VAL:HB	1.87	0.57
27:AZ:184:ARG:HD3	27:AZ:191:ARG:HG2	1.87	0.57
28:Ay:85:ARG:NH2	64:A2:1598:C:OP2	2.36	0.57
39:B:37:VAL:HB	39:B:67:ALA:HB2	1.87	0.57
64:A2:1087:G:OP2	79:AE:12:LYS:NZ	2.36	0.57
20:B5:3642:C:O2'	20:B5:3942:OMG:N2	2.39	0.56
20:B5:4383:OMG:HM22	20:B5:4384:U:H5'	1.86	0.56
41:Ac:106:ARG:HG3	41:Ac:175:VAL:HB	1.87	0.56
64:A2:518:OMC:HM22	64:A2:519:G:H5'	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:A2:753:G:O2'	64:A2:754:C:O2	2.23	0.56
77:Am:99:ARG:NH2	77:Am:119:GLU:OE2	2.38	0.56
20:B5:432:U:H1'	94:B5:5159:SPD:HN6	1.70	0.56
20:B5:4632:A:OP1	63:BO:188:LYS:NZ	2.38	0.56
24:BF:85:GLU:HB2	88:BT:135:PRO:HB3	1.86	0.56
38:BI:33:ILE:O	38:BI:69:ARG:NH1	2.38	0.56
56:DB:193:LEU:O	56:DB:197:ASN:ND2	2.38	0.56
56:DB:549:ARG:HB2	56:DB:667:LEU:HD12	1.87	0.56
57:Ag:143:ARG:HB2	57:Ag:155:LYS:HB2	1.87	0.56
7:BU:91:LEU:HD22	7:BU:96:LEU:HD11	1.87	0.56
9:BA:215:ASN:ND2	20:B5:4292:A:N7	2.53	0.56
20:B5:1005:G:OP1	88:BT:142:ARG:NH1	2.35	0.56
20:B5:1412:G:O2'	21:BQ:75:ARG:NH2	2.36	0.56
32:Aa:44:ILE:HD12	32:Aa:69:VAL:HG21	1.87	0.56
38:BI:48:LEU:HB2	38:BI:142:LEU:HD23	1.86	0.56
44:Ct:98:LYS:HE2	48:Cu:56:ILE:HG21	1.87	0.56
53:Af:21:GLU:OE1	53:Af:25:ARG:NH2	2.39	0.56
60:DC:150:ASP:OD2	60:DC:152:THR:OG1	2.14	0.56
79:AE:44:ILE:HD12	79:AE:65:PRO:HG2	1.87	0.56
6:B8:141:C:OP1	59:BN:38:ARG:NH1	2.38	0.56
12:BB:343:ARG:NH1	20:B5:4715:U:O2	2.38	0.56
20:B5:74:G:H5''	51:BL:59:VAL:HB	1.88	0.56
20:B5:1741:A:N3	88:BT:130:ARG:NH2	2.50	0.56
20:B5:2363:C:H1'	20:B5:2483:G:H21	1.70	0.56
28:Ay:46:ASN:ND2	64:A2:1600:U:OP2	2.36	0.56
64:A2:1618:G:N1	64:A2:1621:A:OP2	2.37	0.56
6:B8:52:A:OP1	72:Bl:21:ARG:NH1	2.38	0.56
20:B5:194:C:O2	25:BY:121:ARG:NH2	2.38	0.56
20:B5:1994:G:O5'	63:BO:130:LYS:NZ	2.38	0.56
27:AZ:155:ARG:NH2	64:A2:1138:U:O2'	2.38	0.56
49:Ae:63:LYS:NZ	64:A2:1679:A2M:OP2	2.33	0.56
55:BM:29:ASP:OD1	55:BM:30:VAL:N	2.39	0.56
56:DB:148:ARG:HA	56:DB:151:TRP:HD1	1.71	0.56
82:AF:256:ILE:HB	82:AF:270:LEU:HB2	1.88	0.56
20:B5:3492:A2M:N1	64:A2:1825:A:O2'	2.31	0.56
36:Ab:194:ARG:NH1	64:A2:1157:U:O4	2.38	0.56
64:A2:105:PSU:OP1	94:A2:1935:SPD:N10	2.37	0.56
64:A2:747:C:O2	64:A2:797:G:N2	2.39	0.56
64:A2:1034:G:N1	64:A2:1081:A:O2'	2.32	0.56
64:A2:1400:C:OP1	82:AF:100:ARG:NH2	2.38	0.56
64:A2:1704:OMC:HM22	64:A2:1705:C:H5'	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B8:38:U:O2'	58:Bh:86:LYS:NZ	2.36	0.56
64:A2:510:OMG:HM22	64:A2:511:G:H5'	1.87	0.56
12:BB:131:THR:O	12:BB:135:LYS:NZ	2.39	0.56
20:B5:741:A:N6	20:B5:810:U:O2	2.38	0.56
20:B5:3942:OMG:HM22	20:B5:3943:G:H5'	1.88	0.56
64:A2:437:OMG:OP2	64:A2:472:G:O2'	2.24	0.56
11:At:101:HIS:ND1	64:A2:1448:OMG:OP1	2.39	0.56
20:B5:381:U:H4'	20:B5:415:G:H5'	1.87	0.56
20:B5:1493:U:H2'	20:B5:1494:G:H8	1.69	0.56
20:B5:1611:U:OP2	22:Ba:26:ARG:NH2	2.31	0.56
20:B5:1772:G:N2	20:B5:1774:G:O4'	2.38	0.56
15:BC:60:HIS:HA	15:BC:92:PHE:HE1	1.71	0.56
20:B5:2444:A:N6	20:B5:2587:A:OP2	2.38	0.56
20:B5:2602:G:O2'	20:B5:2605:G:N2	2.38	0.56
31:BR:12:SER:OG	31:BR:17:CYS:O	2.23	0.56
20:B5:2362:U:O2'	20:B5:2373:U:O2	2.24	0.55
40:EA:276:ILE:HD13	40:EA:328:PRO:HB3	1.87	0.55
64:A2:1089:U:OP1	95:A2:1939:SPM:N14	2.39	0.55
68:Aj:24:LYS:O	68:Aj:42:ASN:ND2	2.36	0.55
90:Bt:105:THR:HG22	90:Bt:107:ASP:H	1.72	0.55
5:Ar:22:GLY:HA2	5:Ar:56:ALA:HB3	1.88	0.55
14:Au:38:GLU:OE2	14:Au:51:LYS:NZ	2.37	0.55
15:BC:45:ARG:O	15:BC:48:ASN:ND2	2.40	0.55
20:B5:375:G:N7	66:Bj:56:ARG:NH2	2.55	0.55
20:B5:2243:G:H21	54:Bg:6:THR:HG22	1.72	0.55
27:AZ:33:GLN:HB3	27:AZ:154:LEU:HD12	1.88	0.55
32:Aa:56:LYS:NZ	64:A2:953:G:OP1	2.40	0.55
39:B:65:ALA:HB2	39:B:74:ILE:HD13	1.89	0.55
63:BO:125:LYS:HG2	63:BO:129:LEU:HD12	1.88	0.55
64:A2:1419:C:O2'	64:A2:1421:G:OP2	2.24	0.55
8:As:84:ARG:NH2	64:A2:1532:A:OP1	2.39	0.55
12:BB:13:SER:HB2	20:B5:4368:A:H4'	1.88	0.55
20:B5:1757:G:N2	20:B5:1757:G:OP2	2.39	0.55
20:B5:1838:G:O2'	46:Be:57:ASN:OD1	2.25	0.55
49:Ae:124:ASP:OD1	49:Ae:125:SER:N	2.39	0.55
56:DB:592:LEU:HB3	56:DB:596:ARG:HH21	1.71	0.55
20:B5:1921:G:N2	20:B5:1948:A:O2'	2.32	0.55
20:B5:4018:G:N2	20:B5:4018:G:OP2	2.39	0.55
60:DC:12:MET:HA	60:DC:28:MET:HE1	1.88	0.55
64:A2:62:G:H1'	64:A2:172:OMU:HM23	1.88	0.55
17:BZ:121:ARG:O	17:BZ:124:THR:OG1	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B5:856:A:H1'	20:B5:2015:G:H5''	1.88	0.55
20:B5:2620:G:H5''	20:B5:2621:G:H5'	1.87	0.55
23:Ax:87:PRO:HD2	23:Ax:90:ARG:HD2	1.88	0.55
6:B8:81:C:O2'	58:Bh:2:ALA:N	2.39	0.55
8:As:101:ARG:NH1	64:A2:1566:C:OP2	2.38	0.55
17:BZ:76:ASN:OD1	17:BZ:77:TYR:N	2.39	0.55
20:B5:4138:OMG:HM21	20:B5:4140:A:H2'	1.88	0.55
28:Ay:111:ARG:HD2	28:Ay:114:LYS:HE3	1.88	0.55
53:Af:85:ARG:O	53:Af:87:ARG:NH1	2.39	0.55
64:A2:926:G:H1	64:A2:1018:U:H3	1.52	0.55
22:Ba:103:VAL:HB	22:Ba:108:TYR:HB2	1.89	0.55
38:BI:61:SER:HA	38:BI:126:VAL:HG12	1.89	0.55
38:BI:66:GLU:OE2	38:BI:69:ARG:NH2	2.40	0.55
40:EA:196:SER:HB2	40:EA:218:ASN:HB3	1.89	0.55
51:BL:109:SER:O	51:BL:113:ASN:ND2	2.34	0.55
65:Ai:138:ARG:NH1	65:Ai:153:SER:OG	2.39	0.55
65:Ai:170:PRO:HB3	65:Ai:174:LYS:HE3	1.88	0.55
67:AA:11:SER:OG	67:AA:14:GLU:OE1	2.24	0.55
20:B5:2007:C:OP1	50:Bf:15:LYS:NZ	2.39	0.55
20:B5:3518:U:OP1	20:B5:4296:G:O2'	2.23	0.55
48:Cu:48:LEU:HA	48:Cu:51:LEU:HB2	1.89	0.55
64:A2:437:OMG:HM22	64:A2:438:G:H5'	1.89	0.55
82:AF:39:THR:HG22	82:AF:60:ARG:HG2	1.89	0.55
20:B5:2647:OMC:HM22	20:B5:2648:C:H5'	1.87	0.55
27:AZ:102:ARG:HH12	27:AZ:105:PRO:HD3	1.71	0.55
56:DB:254:ASN:OD1	60:DC:93:GLN:NE2	2.40	0.55
56:DB:330:ARG:HA	56:DB:333:TYR:CD2	2.42	0.55
54:Bg:64:LEU:HD23	54:Bg:67:LEU:HD12	1.89	0.55
87:Bs:68:HIS:HB3	87:Bs:75:LEU:HD22	1.88	0.55
20:B5:2338:U:H2'	20:B5:2339:G:H8	1.73	0.54
49:Ae:125:SER:O	70:AB:47:LYS:NZ	2.40	0.54
89:Aq:77:GLU:OE2	89:Aq:81:ARG:NH2	2.40	0.54
20:B5:253:G:H2'	20:B5:254:G:H8	1.73	0.54
20:B5:4052:OMU:HM22	20:B5:4053:A:H5'	1.89	0.54
35:BS:95:ARG:NH2	35:BS:112:ASP:OD2	2.40	0.54
53:Af:148:SER:N	53:Af:151:ASP:OD2	2.41	0.54
53:Af:159:ARG:NH2	64:A2:78:C:OP1	2.40	0.54
64:A2:1289:OMU:HM22	64:A2:1290:U:H5'	1.90	0.54
8:As:38:LYS:NZ	64:A2:1629:C:OP1	2.33	0.54
20:B5:4273:G:OP2	20:B5:4273:G:N2	2.36	0.54
39:B:41:LYS:NZ	88:BT:32:ARG:O	2.29	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:AC:126:CYS:HB2	73:AC:130:VAL:HB	1.90	0.54
82:AF:133:ASN:HD21	82:AF:137:VAL:HB	1.72	0.54
83:Ao:58:LYS:HG2	83:Ao:61:ARG:HH22	1.72	0.54
5:Ar:13:LEU:HB2	5:Ar:20:ILE:HB	1.88	0.54
20:B5:172:C:O2	58:Bh:112:ARG:NH1	2.40	0.54
94:B5:5159:SPD:H101	63:BO:91:LYS:HD3	1.72	0.54
53:Af:98:ARG:NH2	53:Af:103:ASP:OD1	2.41	0.54
56:DB:330:ARG:HA	56:DB:333:TYR:HD2	1.71	0.54
56:DB:538:TYR:HE1	60:DC:36:LEU:HB3	1.71	0.54
9:BA:36:GLU:OE1	9:BA:163:ARG:NH1	2.36	0.54
20:B5:407:A:O2'	20:B5:410:A:OP1	2.23	0.54
29:BG:166:LEU:HD21	59:BN:45:PRO:HG2	1.89	0.54
48:Cu:62:VAL:HB	48:Cu:74:PHE:HB2	1.90	0.54
86:Ap:129:SER:O	86:Ap:131:LYS:NZ	2.37	0.54
3:B7:6:C:O2'	39:B:50:ARG:NH2	2.40	0.54
15:BC:13:GLU:OE1	15:BC:161:TYR:OH	2.26	0.54
20:B5:67:C:OP2	20:B5:312:G:N2	2.40	0.54
20:B5:480:C:OP1	84:Br:67:ARG:NH1	2.40	0.54
20:B5:1265:G:O6	98:B5:5541:HOH:O	2.16	0.54
20:B5:1694:C:O2	39:B:3:PHE:N	2.39	0.54
20:B5:2194:OMC:P	98:B5:5529:HOH:O	2.65	0.54
20:B5:4366:OMU:HM22	20:B5:4367:C:H5'	1.89	0.54
36:Ab:183:LYS:HD3	36:Ab:194:ARG:HH21	1.72	0.54
56:DB:569:HIS:HB2	56:DB:684:ARG:HH11	1.72	0.54
5:Ar:141:ARG:NH2	64:A2:1525:G:N7	2.53	0.54
20:B5:3850:G:O3'	54:Bg:90:ARG:NH2	2.40	0.54
64:A2:430:C:O2'	64:A2:812:A:N1	2.40	0.54
71:Ak:119:ASP:O	71:Ak:147:LYS:NZ	2.39	0.54
24:BF:170:ASP:OD1	24:BF:171:ASN:N	2.41	0.54
27:AZ:177:MET:SD	27:AZ:180:ARG:NH2	2.81	0.54
56:DB:545:GLU:HA	56:DB:548:LEU:HG	1.89	0.54
64:A2:64:A:H2	64:A2:83:A:H62	1.55	0.54
64:A2:355:OMU:HM22	64:A2:356:G:H5'	1.89	0.54
64:A2:614:G:N2	64:A2:627:G:OP1	2.38	0.54
20:B5:238:C:OP2	25:BY:45:ARG:NH2	2.41	0.54
20:B5:1284:OMC:HM22	20:B5:1285:U:H5'	1.89	0.54
20:B5:4506:C:OP2	63:BO:171:LYS:NZ	2.37	0.54
56:DB:513:ARG:HH22	56:DB:640:GLU:HB2	1.73	0.54
3:B7:105:C:OP2	38:BI:203:ARG:NH1	2.40	0.54
8:As:129:ARG:NH1	64:A2:1417:C:OP1	2.40	0.54
20:B5:1395:U:OP2	24:BF:33:ARG:NH2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BH:186:THR:O	34:BH:189:GLN:NE2	2.41	0.54
45:Ad:134:LYS:NZ	64:A2:127:C:O2	2.35	0.54
53:Af:172:LYS:HD3	64:A2:65:C:H4'	1.90	0.54
64:A2:1481:A:O2'	85:AG:56:ASP:OXT	2.26	0.54
20:B5:2207:OMG:HM22	20:B5:2208:OMC:H5''	1.90	0.53
27:AZ:176:TRP:HE1	27:AZ:197:VAL:HG23	1.73	0.53
36:Ab:196:ILE:HB	36:Ab:223:TYR:HB2	1.89	0.53
52:DA:6:ILE:HG12	52:DA:51:PHE:HD1	1.73	0.53
64:A2:1329:OMG:HM22	64:A2:1330:U:H5'	1.90	0.53
14:Au:15:ARG:NH1	14:Au:33:GLN:OE1	2.38	0.53
15:BC:239:LYS:O	15:BC:248:ARG:NH1	2.34	0.53
18:Aw:93:PHE:O	18:Aw:140:ARG:NH1	2.41	0.53
20:B5:3651:C:H2'	20:B5:3652:PSU:H6	1.73	0.53
89:Aq:31:ASN:ND2	89:Aq:55:THR:OG1	2.38	0.53
20:B5:468:U:OP1	56:DB:601:ARG:NH2	2.41	0.53
20:B5:2260:A:H2'	20:B5:2261:A:H8	1.73	0.53
35:BS:127:MET:HG2	88:BT:153:PRO:HB2	1.91	0.53
37:Bc:8:LYS:NZ	64:A2:1009:A:OP2	2.29	0.53
52:DA:74:ILE:HG13	52:DA:111:LEU:HB3	1.90	0.53
64:A2:191:A:H3'	64:A2:192:C:H5''	1.89	0.53
64:A2:469:A2M:HM'2	64:A2:470:A:H5'	1.91	0.53
3:B7:77:A:H62	3:B7:99:G:H21	1.56	0.53
14:Au:43:THR:OG1	14:Au:45:ARG:NH1	2.39	0.53
20:B5:835:G:OP1	55:BM:23:LYS:NZ	2.37	0.53
20:B5:1095:C:H2'	20:B5:1096:G:H8	1.73	0.53
20:B5:2206:A2M:HM'2	20:B5:2207:OMG:H5'	1.90	0.53
20:B5:2658:A2M:HM'2	20:B5:2659:G:H5'	1.90	0.53
23:Ax:48:TYR:HA	64:A2:840:C:H42	1.73	0.53
30:Av:56:HIS:HB3	77:Am:20:ARG:HH21	1.74	0.53
41:Ac:70:THR:HG22	41:Ac:86:LEU:HD13	1.90	0.53
56:DB:56:LEU:HB3	56:DB:61:LYS:HB2	1.91	0.53
56:DB:592:LEU:HD22	56:DB:596:ARG:HE	1.73	0.53
84:Br:26:SER:OG	84:Br:28:GLU:OE1	2.22	0.53
85:AG:17:GLY:O	85:AG:27:ARG:NH1	2.41	0.53
12:BB:215:GLU:OE2	12:BB:349:LYS:NZ	2.39	0.53
12:BB:340:THR:OG1	12:BB:341:LYS:N	2.40	0.53
14:Au:15:ARG:HA	36:Ab:259:THR:HG21	1.89	0.53
19:BE:164:ARG:O	19:BE:185:ASN:ND2	2.41	0.53
20:B5:35:U:O2'	20:B5:1606:G:N3	2.40	0.53
20:B5:1528:G:OP1	31:BR:92:LYS:NZ	2.41	0.53
20:B5:2221:G:N2	20:B5:2224:A:OP2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B5:4516:G:H5''	63:BO:176:ARG:HD3	1.90	0.53
52:DA:16:ILE:HD13	52:DA:40:LEU:HD21	1.90	0.53
70:AB:32:VAL:HG11	70:AB:56:LEU:HD12	1.91	0.53
83:Ao:59:ARG:HH11	83:Ao:76:VAL:HG13	1.74	0.53
2:Bb:106:ARG:HH22	20:B5:1391:C:HO2'	1.56	0.53
20:B5:3378:A:N6	98:B5:5546:HOH:O	2.40	0.53
20:B5:3562:A2M:HM'2	20:B5:3563:U:H5'	1.91	0.53
20:B5:3669:C:H1'	59:BN:125:SER:HB3	1.89	0.53
23:Ax:57:VAL:HB	23:Ax:60:PHE:HE2	1.74	0.53
35:BS:76:LYS:NZ	35:BS:100:LEU:O	2.38	0.53
52:DA:64:ASP:OD2	52:DA:110:TYR:OH	2.25	0.53
56:DB:745:THR:HB	56:DB:749:ASN:HD22	1.73	0.53
57:Ag:65:PRO:HD2	57:Ag:68:GLN:HE21	1.73	0.53
64:A2:1276:G:N2	64:A2:1507:A:OP2	2.38	0.53
3:B7:92:C:H2'	3:B7:93:G:H8	1.72	0.53
16:BP:64:ASN:ND2	16:BP:80:GLN:OE1	2.41	0.53
56:DB:210:LEU:HD12	56:DB:237:LEU:HD12	1.90	0.53
20:B5:721:C:OP1	24:BF:72:ARG:NH2	2.41	0.53
20:B5:2649:A:O2'	94:B5:5010:SPD:N1	2.42	0.53
24:BF:189:LEU:HD21	24:BF:207:LEU:HD21	1.90	0.53
44:Ct:114:SER:OG	44:Ct:117:SER:O	2.24	0.53
44:Ct:184:VAL:HG13	44:Ct:210:ILE:HG12	1.90	0.53
56:DB:134:ARG:NH2	56:DB:158:TYR:HA	2.23	0.53
15:BC:323:ARG:HB2	20:B5:1225:G:H5'	1.91	0.53
19:BE:40:LYS:HB2	20:B5:883:C:H4'	1.90	0.53
20:B5:992:C:OP1	20:B5:1106:U:O2'	2.27	0.53
20:B5:4166:PSU:O2	20:B5:4221:G:N2	2.42	0.53
94:B5:5297:SPD:H102	35:BS:166:ARG:HB3	1.73	0.53
21:BQ:122:THR:OG1	21:BQ:124:ASP:OD1	2.17	0.53
35:BS:99:ASP:OD1	35:BS:100:LEU:N	2.41	0.53
38:BI:87:ILE:HG12	38:BI:138:ILE:HG12	1.91	0.53
64:A2:463:OMC:HM22	64:A2:464:C:H5'	1.91	0.53
19:BE:77:ALA:HB2	20:B5:1217:G:H4'	1.91	0.53
20:B5:48:G:OP1	59:BN:192:TRP:NE1	2.36	0.53
20:B5:859:G:O2'	20:B5:2106:A:N6	2.41	0.53
20:B5:3634:A:OP2	98:B5:5549:HOH:O	2.19	0.53
56:DB:226:VAL:HG12	56:DB:230:LYS:HE2	1.91	0.53
15:BC:234:LYS:HD2	20:B5:1317:A:H2	1.74	0.52
20:B5:1256:A:N6	98:B5:5829:HOH:O	2.39	0.52
20:B5:2127:G:OP1	22:Ba:7:LYS:NZ	2.38	0.52
53:Af:135:PRO:HG2	53:Af:141:ILE:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:Af:170:ARG:NH1	64:A2:71:G:O6	2.42	0.52
56:DB:79:SER:OG	56:DB:82:CYS:SG	2.60	0.52
64:A2:865:A:H2'	64:A2:866:A:H8	1.74	0.52
75:Bm:94:MET:HG2	75:Bm:105:PRO:HA	1.91	0.52
20:B5:2712:U:O2'	20:B5:2724:A:N7	2.42	0.52
20:B5:3351:G:H22	20:B5:3356:A:H1'	1.74	0.52
20:B5:3610:C:OP1	20:B5:4146:G:O2'	2.25	0.52
20:B5:4194:G:H5''	20:B5:4195:A:H5''	1.91	0.52
27:AZ:85:ARG:NH2	89:Aq:82:ASP:O	2.41	0.52
56:DB:418:TYR:HB3	56:DB:423:ASN:HB2	1.91	0.52
32:Aa:179:ASN:ND2	32:Aa:183:GLU:OE1	2.42	0.52
34:BH:137:SER:HB2	34:BH:145:VAL:HG23	1.90	0.52
64:A2:1021:A:N7	77:Am:70:LYS:NZ	2.56	0.52
20:B5:1888:U:H5'	34:BH:65:LYS:HE2	1.90	0.52
22:Ba:14:HIS:ND1	98:Ba:403:HOH:O	2.34	0.52
42:Bd:38:PHE:HB3	42:Bd:78:ARG:HG2	1.90	0.52
78:Bo:34:TYR:O	78:Bo:39:ARG:NH1	2.41	0.52
13:BX:51:THR:O	20:B5:2318:G:N2	2.26	0.52
20:B5:4332:G:N7	98:B5:5762:HOH:O	2.34	0.52
20:B5:4610:C:N4	35:BS:171:ARG:O	2.43	0.52
42:Bd:54:MET:HE3	42:Bd:60:PRO:HA	1.91	0.52
56:DB:128:ARG:NH2	56:DB:545:GLU:HB3	2.25	0.52
56:DB:192:LEU:HG	56:DB:533:ILE:HG21	1.91	0.52
74:Al:25:ALA:O	74:Al:30:GLY:N	2.39	0.52
90:Bt:32:ILE:HB	90:Bt:35:LEU:HD11	1.90	0.52
5:Ar:3:LEU:HB3	28:Ay:50:PHE:HD2	1.74	0.52
6:B8:126:C:O2'	20:B5:2336:G:O2'	2.25	0.52
20:B5:2161:G:N2	20:B5:2164:G:OP2	2.38	0.52
39:B:208:MET:HE3	39:B:233:PRO:HG3	1.90	0.52
56:DB:91:ARG:HH22	56:DB:120:LEU:HA	1.74	0.52
56:DB:535:LEU:HD23	56:DB:538:TYR:HD2	1.75	0.52
64:A2:1288:A:H62	64:A2:1313:G:H21	1.56	0.52
64:A2:1865:U:OP2	79:AE:4:LYS:NZ	2.35	0.52
66:Bj:21:ARG:NH2	66:Bj:37:CYS:O	2.43	0.52
17:BZ:111:ARG:NH1	20:B5:2420:C:OP1	2.42	0.52
19:BE:182:LEU:HD12	19:BE:186:ARG:HA	1.92	0.52
20:B5:4073:C:OP1	88:BT:70:HIS:NE2	2.43	0.52
20:B5:4429:U:OP2	20:B5:4452:G:N1	2.35	0.52
52:DA:115:ILE:HD13	52:DA:146:ASP:HB2	1.92	0.52
58:Bh:4:ILE:HD12	58:Bh:53:SER:HB3	1.91	0.52
83:Ao:64:LYS:HZ2	83:Ao:92:SER:HG	1.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Aw:26:GLN:NE2	98:Aw:201:HOH:O	2.42	0.52
20:B5:1923:A:N7	20:B5:1949:A:O2'	2.40	0.52
20:B5:2208:OMC:HM21	20:B5:2671:U:H2'	1.91	0.52
20:B5:2370:A:OP1	31:BR:38:ARG:NH2	2.41	0.52
40:EA:216:ILE:HD11	40:EA:353:ARG:HB3	1.91	0.52
63:BO:54:TYR:OH	63:BO:73:PHE:O	2.27	0.52
64:A2:1809:U:H2'	64:A2:1810:A:H8	1.74	0.52
77:Am:83:ASP:OD1	77:Am:83:ASP:N	2.43	0.52
9:BA:27:ALA:O	9:BA:128:ARG:NH1	2.42	0.52
9:BA:117:GLU:O	9:BA:162:ASN:ND2	2.40	0.52
20:B5:2249:G:N7	72:Bl:2:SER:N	2.58	0.52
20:B5:2623:C:H2'	20:B5:2624:G:H8	1.74	0.52
15:BC:110:ARG:NH1	20:B5:1463:A:OP1	2.43	0.52
41:Ac:151:LYS:NZ	64:A2:1486:U:OP1	2.43	0.52
64:A2:54:A:H3'	64:A2:452:G:H22	1.74	0.52
78:Bo:59:LYS:NZ	78:Bo:61:LYS:O	2.40	0.52
12:BB:95:THR:HG22	20:B5:4649:A:H4'	1.92	0.51
20:B5:1842:G:OP1	50:Bf:87:LYS:NZ	2.27	0.51
20:B5:3374:A:OP1	98:B5:5552:HOH:O	2.19	0.51
34:BH:113:GLU:HG2	34:BH:125:ARG:HG2	1.92	0.51
53:Af:196:LYS:NZ	64:A2:126:G:O6	2.34	0.51
55:BM:24:LEU:HB2	55:BM:43:THR:HG21	1.91	0.51
64:A2:1292:A:O2'	73:AC:145:CYS:SG	2.61	0.51
64:A2:1388:G:P	98:A2:2112:HOH:O	2.67	0.51
9:BA:208:GLU:OE1	20:B5:1584:G:N1	2.41	0.51
20:B5:136:U:O4	58:Bh:79:LYS:NZ	2.37	0.51
64:A2:99:A2M:HM'2	64:A2:100:U:H5'	1.92	0.51
64:A2:1804:U:H2'	64:A2:1805:OMU:H6	1.92	0.51
67:AA:23:ARG:HH22	67:AA:29:ASN:HD21	1.58	0.51
9:BA:137:ILE:HD11	9:BA:149:LYS:HB2	1.92	0.51
16:BP:94:MET:HE1	16:BP:146:ILE:HB	1.93	0.51
19:BE:59:TYR:HB3	19:BE:63:ALA:HB3	1.91	0.51
20:B5:150:U:N3	29:BG:162:ASP:O	2.36	0.51
55:BM:5:ARG:NE	55:BM:59:ASP:OD1	2.43	0.51
56:DB:825:ARG:O	56:DB:829:HIS:ND1	2.43	0.51
64:A2:655:A:N6	98:A2:2249:HOH:O	2.43	0.51
64:A2:1080:C:O2'	64:A2:1183:A:N1	2.41	0.51
64:A2:1861:A:N7	79:AE:34:LYS:NZ	2.58	0.51
64:A2:1864:A:OP2	79:AE:4:LYS:NZ	2.42	0.51
7:BU:28:PRO:HB2	7:BU:34:MET:HG2	1.92	0.51
20:B5:374:G:OP2	66:Bj:56:ARG:NH1	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B5:483:G:O2'	20:B5:486:C:OP2	2.28	0.51
20:B5:1759:C:H5'	39:B:139:PRO:HB3	1.92	0.51
20:B5:3449:A:OP2	20:B5:3467:G:N2	2.44	0.51
20:B5:3580:U:H2'	20:B5:3581:A:H8	1.75	0.51
23:Ax:7:ILE:HG22	23:Ax:27:VAL:HG22	1.92	0.51
32:Aa:32:ASP:OD1	32:Aa:46:LYS:NZ	2.42	0.51
45:Ad:240:ARG:NH2	64:A2:845:U:OP1	2.44	0.51
57:Ag:119:SER:O	64:A2:914:A:N6	2.42	0.51
64:A2:292:G:N2	71:Ak:40:ILE:O	2.44	0.51
64:A2:1209:A:O2'	64:A2:1836:A:N7	2.37	0.51
7:BU:100:LEU:HD13	7:BU:112:LEU:HD23	1.91	0.51
20:B5:2422:G:N2	20:B5:2425:A:OP2	2.38	0.51
20:B5:3936:U:OP1	94:B5:5276:SPD:N10	2.43	0.51
34:BH:120:GLU:OE1	34:BH:124:ARG:NH2	2.42	0.51
44:Ct:94:VAL:HG23	44:Ct:109:PRO:HG3	1.93	0.51
65:Ai:120:ALA:O	65:Ai:125:HIS:ND1	2.38	0.51
68:Aj:63:ALA:HB3	68:Aj:68:TYR:HE2	1.74	0.51
15:BC:316:LYS:HB2	15:BC:324:ILE:HG13	1.93	0.51
40:EA:170[A]:VAL:HG11	40:EA:221:ILE:HD12	1.92	0.51
42:Bd:65:ASP:OD1	42:Bd:66:THR:N	2.43	0.51
64:A2:1555:C:O2	68:Aj:24:LYS:NZ	2.38	0.51
78:Bo:26:TYR:HB3	78:Bo:67:VAL:HB	1.92	0.51
82:AF:214:GLY:HA2	82:AF:236:ILE:HG13	1.93	0.51
87:Bs:30:VAL:HG21	87:Bs:187:LEU:HD13	1.92	0.51
3:B7:23:A:N3	3:B7:118:C:O2'	2.43	0.51
20:B5:2122:A:O2'	46:Be:48:ARG:NH2	2.43	0.51
41:Ac:67:ARG:NE	68:Aj:93:THR:O	2.43	0.51
64:A2:27:A2M:HM'2	64:A2:28:U:H5'	1.93	0.51
64:A2:1805:OMU:HM22	64:A2:1806:G:H5'	1.91	0.51
82:AF:133:ASN:HB3	82:AF:139:LYS:HE3	1.93	0.51
20:B5:311:G:H2'	20:B5:312:G:H8	1.76	0.51
20:B5:788:G:H2'	20:B5:789:G:H8	1.76	0.51
20:B5:1915:G:N2	90:Bt:138:SER:O	2.41	0.51
40:EA:213:GLU:HG3	40:EA:239:GLY:HA3	1.92	0.51
44:Ct:97:ARG:HE	48:Cu:109:GLN:NE2	2.07	0.51
53:Af:56:ASN:HD22	53:Af:62:PRO:HA	1.76	0.51
72:Bl:23:ILE:HG23	72:Bl:38:ASN:HB2	1.91	0.51
5:Ar:136:THR:OG1	64:A2:1522:C:OP2	2.29	0.51
12:BB:95:THR:OG1	12:BB:98:GLY:O	2.20	0.51
20:B5:632:G:H5''	20:B5:633:U:H5'	1.93	0.51
20:B5:1935:C:H42	20:B5:1939:G:H22	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B5:2492:G:N7	98:B5:5774:HOH:O	2.35	0.51
20:B5:4445:U:H1'	20:B5:4446:A:H5''	1.92	0.51
29:BG:83:PHE:HA	29:BG:183:ILE:HD13	1.93	0.51
29:BG:154:LEU:HB3	29:BG:204:PHE:HB2	1.92	0.51
90:Bt:147:HIS:HD2	90:Bt:149:HIS:HB2	1.75	0.51
20:B5:40:G:N2	20:B5:4126:A:N7	2.58	0.51
20:B5:478:G:H2'	20:B5:479:G:H8	1.75	0.51
20:B5:2257:G:H2'	20:B5:2258:OMU:H6	1.92	0.51
40:EA:307:PRO:HD2	40:EA:314:ALA:HB2	1.93	0.51
85:AG:22:ARG:HH21	85:AG:37:ASN:HB2	1.76	0.51
3:B7:27:G:O6	39:B:58:ARG:NH2	2.37	0.50
20:B5:1015:U:H3	20:B5:1086:G:H1	1.57	0.50
20:B5:2363:C:H2'	20:B5:2364:G:H8	1.76	0.50
48:Cu:48:LEU:HD23	48:Cu:51:LEU:HD12	1.94	0.50
49:Ae:49:LEU:HD12	86:Ap:50:LYS:HG2	1.92	0.50
82:AF:91:ASP:OD2	82:AF:93:THR:OG1	2.25	0.50
3:B7:63:C:H5'	3:B7:64:G:H5''	1.94	0.50
7:BU:47:ILE:HD12	7:BU:63:ILE:HD11	1.94	0.50
20:B5:345:C:H2'	20:B5:346:G:H8	1.74	0.50
20:B5:369:G:N2	20:B5:372:A:OP2	2.38	0.50
20:B5:2178:C:H2'	20:B5:2179:G:H8	1.77	0.50
32:Aa:150:ILE:HG12	64:A2:1125:C:H5''	1.92	0.50
40:EA:194:CYS:HB2	40:EA:220:ASN:HB3	1.92	0.50
40:EA:218:ASN:ND2	40:EA:356:GLN:O	2.45	0.50
49:Ae:63:LYS:HD2	49:Ae:71:ARG:HH12	1.76	0.50
58:Bh:80:PRO:HD2	58:Bh:83:LEU:HD12	1.92	0.50
64:A2:832:G:H2'	64:A2:833:G:H8	1.76	0.50
12:BB:56:ILE:HG22	12:BB:368:ILE:HA	1.93	0.50
20:B5:1394:U:O2'	24:BF:33:ARG:NE	2.37	0.50
20:B5:2161:G:N7	98:B5:5776:HOH:O	2.35	0.50
20:B5:4297:U:H2'	20:B5:4298:PSU:H6	1.77	0.50
53:Af:121:ILE:N	53:Af:125:THR:OG1	2.43	0.50
56:DB:794:LEU:HD13	56:DB:797:ARG:NH2	2.26	0.50
64:A2:660:G:O2'	64:A2:663:G:O2'	2.28	0.50
67:AA:35:VAL:HG21	67:AA:63:LEU:HD13	1.93	0.50
86:Ap:112:LEU:HD22	86:Ap:119:LEU:HD13	1.93	0.50
12:BB:343:ARG:HH12	20:B5:4715:U:H1'	1.75	0.50
20:B5:1539:G:N7	94:B5:5377:SPD:N10	2.59	0.50
45:Ad:124:CYS:HB3	45:Ad:141:THR:HB	1.94	0.50
49:Ae:74:ASN:HA	49:Ae:77:MET:HE2	1.92	0.50
64:A2:1598:C:H4'	64:A2:1604:G:C6	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:Aj:4:PRO:HB2	68:Aj:7:ASN:HD22	1.77	0.50
71:Ak:111:VAL:HG22	71:Ak:140:PHE:HB2	1.93	0.50
20:B5:394:G:N2	20:B5:397:G:OP2	2.34	0.50
39:B:122:GLN:NE2	39:B:126:THR:OG1	2.44	0.50
43:BJ:46:GLN:NE2	43:BJ:73:THR:O	2.41	0.50
48:Cu:64:MET:HB2	48:Cu:72:ILE:HB	1.94	0.50
56:DB:190:SER:HB2	56:DB:220:ILE:HA	1.93	0.50
56:DB:484:CYS:HA	60:DC:19:LEU:HD13	1.92	0.50
64:A2:1546:A:H4'	86:Ap:74:GLY:HA2	1.93	0.50
19:BE:164:ARG:NH1	19:BE:276:SER:OG	2.43	0.50
20:B5:1536:G:N7	98:B5:5772:HOH:O	2.35	0.50
20:B5:2012:C:H5''	24:BF:211:LYS:HB3	1.94	0.50
28:Ay:74:SER:OG	28:Ay:79:ILE:O	2.23	0.50
45:Ad:108:ARG:NH2	64:A2:847:G:N7	2.59	0.50
57:Ag:162:GLN:OE1	57:Ag:165:ASN:ND2	2.44	0.50
20:B5:1834:G:O2'	20:B5:1846:A:N3	2.42	0.50
20:B5:3962:G:P	98:B5:5752:HOH:O	2.69	0.50
40:EA:147:ARG:HD2	40:EA:374:ARG:HG2	1.92	0.50
64:A2:1141:G:HO2'	64:A2:1152:G:HO2'	1.58	0.50
12:BB:80:GLU:OE1	12:BB:323:TYR:OH	2.28	0.50
18:Aw:91:LEU:HB3	76:AD:83:VAL:HG11	1.94	0.50
19:BE:170:GLN:HE21	19:BE:174:GLY:HA2	1.75	0.50
20:B5:404:U:O3'	25:BY:87:ARG:NH2	2.41	0.50
20:B5:422:C:H2'	20:B5:423:G:H8	1.77	0.50
20:B5:1776:A:OP1	88:BT:108:ARG:NH1	2.44	0.50
61:Ah:67:TRP:NE1	61:Ah:191:GLU:OE2	2.33	0.50
77:Am:130:LYS:NZ	77:Am:139:TRP:O	2.39	0.50
4:AT:38:N:O2'	64:A2:1059:A:OP1	2.29	0.50
17:BZ:25:ILE:HA	17:BZ:43:VAL:HG12	1.93	0.50
20:B5:1458:A:H4'	20:B5:1459:G:H5'	1.93	0.50
20:B5:1853:C:H4'	63:BO:89:PRO:HD3	1.94	0.50
20:B5:1955:C:H2'	20:B5:1956:A:H8	1.76	0.50
20:B5:4769:U:H2'	20:B5:4770:G:H8	1.75	0.50
28:Ay:79:ILE:HB	28:Ay:83:LEU:HD23	1.94	0.50
40:EA:327:GLU:HB2	40:EA:356:GLN:HE21	1.77	0.50
45:Ad:87:MET:HE2	45:Ad:123:LEU:HB2	1.94	0.50
51:BL:91:ALA:HB1	51:BL:96:ILE:HB	1.92	0.50
56:DB:184:LYS:HG2	56:DB:189:TYR:CZ	2.47	0.50
57:Ag:160:LYS:HA	57:Ag:163:GLN:HB2	1.94	0.50
58:Bh:104:THR:HG23	59:BN:146:PRO:HB2	1.94	0.50
60:DC:41:LEU:HB3	60:DC:58:ALA:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:Ah:55:TYR:OH	64:A2:310:G:OP2	2.29	0.50
64:A2:1532:A:H4'	64:A2:1606:G:H4'	1.93	0.50
64:A2:1663:U:O4	64:A2:1664:A:N6	2.43	0.50
64:A2:1758:G:H1	64:A2:1776:U:H3	1.60	0.50
67:AA:28:PRO:HG3	77:Am:17:PRO:HG3	1.94	0.50
82:AF:73:SER:OG	82:AF:117:ASN:OD1	2.25	0.50
19:BE:181:PRO:HD2	19:BE:184:LEU:HD12	1.93	0.49
20:B5:664:G:H2'	20:B5:665:G:H8	1.77	0.49
20:B5:1341:A:HO2'	20:B5:1422:C:HO2'	1.57	0.49
20:B5:4222:C:O2	34:BH:173:ARG:NH2	2.45	0.49
20:B5:4331:U:H2'	20:B5:4332:G:C8	2.47	0.49
35:BS:29:ARG:HB2	88:BT:148:PRO:HB2	1.92	0.49
52:DA:90:THR:HG23	52:DA:127:PHE:HZ	1.78	0.49
82:AF:88:ARG:HH11	82:AF:97:THR:HG21	1.77	0.49
5:Ar:88:LYS:NZ	83:Ao:35:GLN:O	2.36	0.49
6:B8:36:G:C5	58:Bh:89:ARG:HD3	2.47	0.49
6:B8:71:A:N1	6:B8:84:A:O2'	2.41	0.49
9:BA:223:SER:OG	20:B5:3480:A:O2'	2.25	0.49
12:BB:233:SER:OG	12:BB:272:LYS:NZ	2.42	0.49
19:BE:159:ARG:NH1	20:B5:4679:C:OP1	2.46	0.49
20:B5:207:G:H21	20:B5:232:G:H21	1.59	0.49
20:B5:3603:A:P	98:B5:5535:HOH:O	2.69	0.49
20:B5:4151:G:OP2	38:BI:7:ARG:NH2	2.45	0.49
20:B5:4269:A2M:H5''	20:B5:4270:G:H5'	1.94	0.49
56:DB:103:TYR:HB3	56:DB:120:LEU:HD11	1.94	0.49
56:DB:473:THR:OG1	56:DB:478:ASN:OD1	2.27	0.49
56:DB:569:HIS:CE1	56:DB:654:LEU:HG	2.47	0.49
64:A2:944:U:O2'	80:An:135:ILE:O	2.30	0.49
82:AF:5:MET:HG2	82:AF:312:VAL:HG22	1.93	0.49
86:Ap:86:GLN:HG2	86:Ap:90:LYS:HE2	1.93	0.49
4:AT:20:N:OP1	43:BJ:58:ARG:NH2	2.38	0.49
15:BC:278:ASN:OD1	15:BC:279:LEU:N	2.45	0.49
20:B5:4057:A:H2'	20:B5:4058:PSU:H6	1.77	0.49
20:B5:4135:C:H2'	20:B5:4136:A:H8	1.78	0.49
57:Ag:8:ILE:HD13	57:Ag:16:PRO:HB3	1.94	0.49
64:A2:1088:A:OP1	79:AE:3:LYS:NZ	2.44	0.49
64:A2:1260:A:N6	64:A2:1520:U:OP1	2.45	0.49
64:A2:1809:U:H2'	64:A2:1810:A:C8	2.48	0.49
65:Ai:113:GLN:OE1	65:Ai:154:GLN:NE2	2.42	0.49
9:BA:30:ARG:HG3	9:BA:76:PHE:HZ	1.77	0.49
20:B5:1524:U:H2'	20:B5:1525:G:H8	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B5:3425:U:OP2	98:B5:5553:HOH:O	2.20	0.49
20:B5:4350:G:N2	20:B5:4353:A:OP2	2.44	0.49
31:BR:176:ARG:NH2	64:A2:910:G:OP1	2.45	0.49
39:B:31:TYR:O	39:B:35:ARG:NH1	2.45	0.49
42:Bd:19:GLU:O	42:Bd:90:ARG:NE	2.46	0.49
54:Bg:60:ARG:HB2	54:Bg:63:VAL:HG23	1.95	0.49
56:DB:191:GLU:HB3	56:DB:195:TYR:CZ	2.48	0.49
73:AC:114:ILE:HD12	74:Al:71:GLU:HG2	1.95	0.49
20:B5:158:A:N1	20:B5:276:C:O2'	2.39	0.49
20:B5:1326:G:H2'	20:B5:1327:G:H8	1.78	0.49
48:Cu:28:ARG:HH11	48:Cu:31:LYS:HG3	1.78	0.49
61:Ah:80:ASP:OD1	61:Ah:81:VAL:N	2.46	0.49
15:BC:150:LEU:HD12	15:BC:151:PRO:HA	1.95	0.49
20:B5:4507:G:OP1	63:BO:117:ARG:NH2	2.46	0.49
32:Aa:179:ASN:HB3	32:Aa:183:GLU:HB2	1.93	0.49
32:Aa:189:ILE:HB	32:Aa:190:PRO:HD3	1.94	0.49
38:BI:49:CYS:SG	38:BI:51:HIS:NE2	2.85	0.49
39:B:267:ASN:OD1	39:B:267:ASN:N	2.45	0.49
49:Ae:71:ARG:NH2	64:A2:1678:U:OP1	2.45	0.49
56:DB:773:TYR:CE1	56:DB:780:GLN:HA	2.47	0.49
57:Ag:43:LEU:HB3	57:Ag:72:PHE:CE2	2.48	0.49
64:A2:521:A:O2'	64:A2:826:A:N3	2.41	0.49
82:AF:107:ASP:HB2	82:AF:125:ARG:HH11	1.76	0.49
2:Bb:68:ARG:NH1	20:B5:1769:G:H4'	2.28	0.49
36:Ab:191:VAL:HG11	36:Ab:236:PHE:HA	1.95	0.49
36:Ab:232:THR:HG22	36:Ab:235:ASN:H	1.78	0.49
38:BI:53:VAL:HG11	88:BT:158:PHE:HZ	1.78	0.49
39:B:150:LEU:HD22	43:BJ:145:LYS:HE3	1.94	0.49
56:DB:114:LEU:HD13	56:DB:144:ARG:HH21	1.78	0.49
64:A2:875:G:H2'	64:A2:876:A:H8	1.77	0.49
20:B5:300:A:H2'	20:B5:301:G:H8	1.78	0.49
20:B5:1943:U:H2'	20:B5:1944:G:C8	2.48	0.49
48:Cu:41:ASP:HA	48:Cu:44:LEU:HD12	1.95	0.49
19:BE:97:LYS:HD2	19:BE:110:VAL:HG21	1.95	0.49
20:B5:345:C:H2'	20:B5:346:G:C8	2.48	0.49
20:B5:398:A2M:H8	20:B5:398:A2M:O5'	2.13	0.49
20:B5:2745:G:OP2	20:B5:3328:A:N6	2.44	0.49
35:BS:69:GLU:HG2	35:BS:101:THR:HG22	1.95	0.49
44:Ct:134:GLN:O	44:Ct:138:ALA:N	2.37	0.49
56:DB:170:ILE:HG23	56:DB:174:PHE:CZ	2.47	0.49
56:DB:401:ILE:HA	56:DB:410:LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:A2:220:U:H2'	64:A2:221:A:H8	1.78	0.49
64:A2:1240:U:H5''	83:Ao:124:LYS:HD3	1.94	0.49
87:Bs:30:VAL:HG12	87:Bs:189:ILE:HA	1.94	0.49
20:B5:3924:A:H2'	20:B5:3925:G:H8	1.78	0.49
26:BW:81:ALA:HB2	26:BW:87:LEU:HB2	1.95	0.49
36:Ab:131:GLY:HA3	36:Ab:216:MET:HB3	1.95	0.49
63:BO:130:LYS:HB2	63:BO:133:ARG:HG2	1.93	0.49
64:A2:35:C:H2'	64:A2:36:PSU:H6	1.78	0.49
64:A2:953:G:H21	80:An:52:THR:HG21	1.78	0.49
82:AF:29:ASP:OD1	82:AF:47:ARG:NH1	2.40	0.49
2:Bb:50:ASN:HD21	20:B5:1766:C:H1'	1.77	0.48
6:B8:155:C:OP1	29:BG:89:ARG:NH2	2.45	0.48
10:BV:69:LYS:NZ	10:BV:71:GLU:OE2	2.37	0.48
20:B5:119:G:O4'	29:BG:132:ARG:NH2	2.46	0.48
20:B5:1250:C:H2'	20:B5:1251:A:H8	1.77	0.48
45:Ad:85:GLY:N	45:Ad:88:ASP:OD2	2.35	0.48
45:Ad:143:ASP:OD1	45:Ad:143:ASP:N	2.46	0.48
50:Bf:36:ARG:HB2	50:Bf:80:ASN:HA	1.94	0.48
64:A2:21:U:O2'	65:Ai:17:ARG:O	2.30	0.48
64:A2:954:C:O2	80:An:55:ARG:NH1	2.43	0.48
90:Bt:82:ILE:HA	90:Bt:85:LEU:HD12	1.94	0.48
20:B5:3524:OMG:HM22	20:B5:3525:U:H5'	1.95	0.48
24:BF:126:LYS:HB2	88:BT:133:ALA:HB3	1.95	0.48
28:Ay:92:LEU:HD22	28:Ay:109:TYR:HE1	1.77	0.48
40:EA:205:ILE:HD11	40:EA:344:TRP:HB2	1.95	0.48
46:Be:117:GLN:O	84:Br:119:ARG:NH2	2.45	0.48
64:A2:867:PSU:H2'	64:A2:868:OMG:H8	1.78	0.48
64:A2:1311:U:H5''	73:AC:130:VAL:HG13	1.95	0.48
72:Bl:30:LYS:HB2	72:Bl:33:ASN:HB2	1.94	0.48
9:BA:140:ASN:ND2	9:BA:143:THR:OG1	2.47	0.48
20:B5:1001:C:H2'	20:B5:1002:A:H8	1.78	0.48
20:B5:1341:A:O2'	20:B5:1422:C:O2'	2.24	0.48
56:DB:418:TYR:O	56:DB:422:GLY:N	2.47	0.48
56:DB:418:TYR:O	56:DB:423:ASN:N	2.42	0.48
60:DC:132:GLU:HB3	60:DC:146:ALA:HB3	1.95	0.48
9:BA:57:PRO:HG2	9:BA:78:ALA:HB3	1.94	0.48
20:B5:1631:C:H41	20:B5:4124:A:H5''	1.78	0.48
20:B5:1846:A:H4'	24:BF:222:LYS:HE3	1.95	0.48
20:B5:3997:A:H5''	43:BJ:108:GLY:HA3	1.95	0.48
20:B5:4745:U:H4'	20:B5:4746:A:H5'	1.96	0.48
40:EA:85:GLY:O	40:EA:88:ARG:NH1	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:Ac:93:THR:HG22	41:Ac:95:GLY:H	1.78	0.48
42:Bd:26:THR:HG1	42:Bd:85:ARG:HH11	1.60	0.48
51:BL:129:ARG:NH1	58:Bh:116:LEU:O	2.47	0.48
52:DA:18:GLN:HE21	56:DB:437:LEU:HB3	1.77	0.48
61:Ah:7:ASN:HD22	64:A2:387:C:H5'	1.78	0.48
65:Ai:33:GLY:HA3	76:AD:112:TYR:CG	2.48	0.48
71:Ak:147:LYS:HD2	71:Ak:151:THR:HG21	1.96	0.48
90:Bt:154:ASP:HB3	90:Bt:159:ALA:HB3	1.95	0.48
6:B8:84:A:O4'	58:Bh:3:LYS:NZ	2.46	0.48
8:As:96:SER:OG	64:A2:1569:C:OP1	2.30	0.48
20:B5:419:A:N3	20:B5:1276:C:O2'	2.45	0.48
20:B5:3377:U:OP2	98:B5:5552:HOH:O	2.20	0.48
39:B:119:TYR:OH	39:B:139:PRO:O	2.29	0.48
53:Af:102:VAL:HG13	53:Af:106:LEU:HD12	1.94	0.48
56:DB:56:LEU:HD22	56:DB:61:LYS:HD2	1.95	0.48
56:DB:112:ASP:HB3	56:DB:143:LEU:HD11	1.96	0.48
56:DB:331:SER:HB3	60:DC:48:GLU:HG3	1.96	0.48
61:Ah:98:LYS:HB3	64:A2:378:G:H5'	1.95	0.48
64:A2:522:A:OP1	65:Ai:45:ARG:NH1	2.42	0.48
64:A2:1009:A:H2'	64:A2:1010:A:H8	1.78	0.48
69:Bk:26:LYS:NZ	69:Bk:28:ASN:OD1	2.46	0.48
82:AF:245:ARG:NH2	82:AF:296:GLN:OE1	2.47	0.48
19:BE:188:PRO:HG3	20:B5:4677:A:H1'	1.96	0.48
20:B5:363:A:N7	20:B5:378:A:N6	2.62	0.48
20:B5:1760:G:H4'	20:B5:1761:U:H5''	1.95	0.48
20:B5:2624:G:O2'	72:Bl:3:SER:O	2.31	0.48
20:B5:3965:A:H5''	88:BT:2:THR:HG22	1.95	0.48
21:BQ:67:ILE:HG12	21:BQ:98:LEU:HD11	1.96	0.48
39:B:152:ARG:HG3	39:B:154:THR:HG23	1.95	0.48
65:Ai:107:GLU:HA	65:Ai:112:THR:HG21	1.96	0.48
71:Ak:78:THR:HG22	71:Ak:79:LYS:HG3	1.94	0.48
20:B5:638:G:OP2	51:BL:162:LYS:NZ	2.41	0.48
20:B5:2360:A:O2'	54:Bg:66:ARG:NH1	2.46	0.48
20:B5:4037:G:H5'	20:B5:4039:PSU:C6	2.49	0.48
24:BF:181:TYR:CZ	24:BF:202:GLU:HG2	2.49	0.48
45:Ad:104:ASP:OD1	45:Ad:108:ARG:N	2.35	0.48
56:DB:326:PHE:CZ	56:DB:379:TYR:HA	2.49	0.48
56:DB:713:ILE:HB	56:DB:771:MET:HE2	1.94	0.48
64:A2:26:U:H2'	64:A2:27:A2M:H8	1.95	0.48
71:Ak:18:GLN:HG2	71:Ak:33:LEU:HD21	1.94	0.48
20:B5:2302:G:N2	20:B5:2305:C:OP2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:AZ:32:PHE:CD1	64:A2:1098:G:H4'	2.49	0.48
32:Aa:86:LEU:HB3	32:Aa:98:THR:HB	1.96	0.48
36:Ab:121:ARG:NH1	36:Ab:121:ARG:O	2.47	0.48
36:Ab:253:PRO:HA	36:Ab:256:TRP:CE2	2.48	0.48
40:EA:295:GLY:HA2	40:EA:324:PHE:HA	1.95	0.48
53:Af:49:VAL:HG23	53:Af:114:VAL:HB	1.96	0.48
79:AE:59:PHE:HB2	79:AE:62:TYR:HB2	1.96	0.48
19:BE:190:ARG:NH2	20:B5:4680:G:O3'	2.47	0.48
20:B5:3863:G:H2'	20:B5:3864:G:H8	1.78	0.48
20:B5:4330:A:H62	20:B5:4464:G:H21	1.62	0.48
53:Af:57:ASP:OD1	53:Af:61:PHE:N	2.47	0.48
56:DB:566:LEU:O	56:DB:684:ARG:NH1	2.35	0.48
56:DB:573:LEU:O	56:DB:574:THR:OG1	2.27	0.48
57:Ag:57:ARG:NH2	57:Ag:89:GLY:O	2.46	0.48
64:A2:381:G:N1	64:A2:384:G:OP2	2.38	0.48
64:A2:631:U:O2	64:A2:631:U:H2'	2.14	0.48
6:B8:75:OMG:OP2	25:BY:74:TYR:OH	2.26	0.48
9:BA:117:GLU:HG2	9:BA:124:GLY:H	1.79	0.48
17:BZ:95:VAL:HG13	17:BZ:96:VAL:HG23	1.96	0.48
20:B5:62:A:OP1	59:BN:172:ARG:NH1	2.44	0.48
36:Ab:192:LEU:HB3	36:Ab:227:ARG:HG2	1.96	0.48
40:EA:272:LEU:HD12	40:EA:306:VAL:HG11	1.95	0.48
53:Af:103:ASP:OD2	53:Af:105:ASN:ND2	2.40	0.48
17:BZ:11:VAL:HG12	17:BZ:82:PRO:HA	1.95	0.47
17:BZ:36:ARG:NH1	17:BZ:38:TYR:OH	2.40	0.47
17:BZ:90:PRO:O	17:BZ:117:LYS:NZ	2.47	0.47
20:B5:1290:C:H2'	20:B5:1291:G:H8	1.79	0.47
27:AZ:89:LYS:NZ	89:Aq:83:ASN:OD1	2.47	0.47
64:A2:1180:G:N2	64:A2:1183:A:OP2	2.47	0.47
64:A2:1286:G:H1	74:Al:57:ASP:H	1.61	0.47
64:A2:1299:G:H4'	83:Ao:78:THR:HA	1.94	0.47
76:AD:91:LEU:HD23	76:AD:91:LEU:H	1.79	0.47
9:BA:17:ARG:NH1	20:B5:2293:G:OP1	2.47	0.47
12:BB:39:LYS:HG2	12:BB:40:PRO:HD2	1.96	0.47
13:BX:73:HIS:CD2	13:BX:115:LYS:HD3	2.49	0.47
19:BE:269:GLN:HG2	20:B5:4669:C:H5''	1.96	0.47
20:B5:58:G:H4'	20:B5:59:A:H4'	1.96	0.47
20:B5:1648:U:OP1	21:BQ:143:ARG:NH2	2.44	0.47
20:B5:2239:A:OP1	94:B5:5010:SPD:N1	2.47	0.47
20:B5:2312:C:O2	20:B5:2312:C:H2'	2.13	0.47
20:B5:3678:G:H1	20:B5:3795:U:H3	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Ax:84:LYS:O	45:Ad:63:LYS:NZ	2.42	0.47
38:BI:42:LYS:HB2	38:BI:45:GLU:HG3	1.96	0.47
5:Ar:26:ILE:HG13	5:Ar:45:LEU:HD21	1.96	0.47
8:As:42:HIS:HE2	8:As:43:LYS:HE2	1.80	0.47
20:B5:2447:C:H2'	20:B5:2448:G:H8	1.79	0.47
20:B5:2615:C:O3'	69:Bk:17:ARG:NH2	2.47	0.47
20:B5:3941:G:O2'	20:B5:4188:PSU:OP1	2.26	0.47
44:Ct:87:GLN:HG2	44:Ct:112:TYR:CE2	2.50	0.47
56:DB:124:GLN:HB3	56:DB:133:TYR:HE1	1.79	0.47
56:DB:333:TYR:HD1	56:DB:339:VAL:HG22	1.79	0.47
69:Bk:13:LEU:HD23	69:Bk:16:ARG:HH21	1.80	0.47
14:Au:82:ASN:O	27:AZ:52:LYS:NZ	2.41	0.47
20:B5:2146:C:H5''	46:Be:104:SER:HB3	1.95	0.47
21:BQ:178:ARG:H	22:Ba:51:GLY:HA2	1.78	0.47
50:Bf:16:ARG:HB3	50:Bf:21:GLN:HG3	1.95	0.47
64:A2:1744:G:H21	64:A2:1792:A:H62	1.63	0.47
64:A2:1766:C:H1'	64:A2:1769:A:H61	1.79	0.47
78:Bo:74:GLU:HB3	78:Bo:77:CYS:HB3	1.97	0.47
86:Ap:24:HIS:HE1	86:Ap:26:LYS:HD3	1.78	0.47
5:Ar:25:LYS:HD2	5:Ar:55:ARG:HD3	1.95	0.47
20:B5:1877:C:N3	98:B5:5773:HOH:O	2.35	0.47
20:B5:2540:A:N7	98:B5:5785:HOH:O	2.36	0.47
22:Ba:83:SER:OG	22:Ba:86:THR:OG1	2.30	0.47
56:DB:171:LEU:HD13	56:DB:196:GLN:HG2	1.97	0.47
56:DB:593:LYS:HE3	56:DB:593:LYS:HB3	1.74	0.47
64:A2:1166:G:OP2	64:A2:1166:G:N2	2.29	0.47
17:BZ:87:VAL:HG12	17:BZ:89:ILE:HG13	1.96	0.47
20:B5:1437:G:OP2	20:B5:1437:G:N2	2.38	0.47
20:B5:3545:A:N3	20:B5:4284:G:O2'	2.41	0.47
20:B5:4068:G:N2	20:B5:4071:A:OP2	2.47	0.47
28:Ay:58:LEU:HD12	28:Ay:62:VAL:HG21	1.95	0.47
34:BH:37:ASP:OD2	34:BH:39:ASN:ND2	2.48	0.47
40:EA:140:ARG:HG2	40:EA:371:LEU:HD22	1.95	0.47
52:DA:28:PRO:O	52:DA:141:ARG:NH2	2.47	0.47
56:DB:421:ALA:HB1	56:DB:834:TYR:HB2	1.96	0.47
20:B5:253:G:H2'	20:B5:254:G:C8	2.49	0.47
20:B5:758:C:O2'	20:B5:760:C:N4	2.39	0.47
20:B5:1611:U:H2'	20:B5:1612:G:H8	1.80	0.47
20:B5:1688:A:H2'	20:B5:1689:G:C8	2.50	0.47
20:B5:1712:U:H2'	20:B5:1713:C:C6	2.50	0.47
20:B5:2300:G:OP1	59:BN:65:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Ax:12:PHE:HZ	23:Ax:21:LYS:HD3	1.79	0.47
23:Ax:29:HIS:ND1	23:Ax:29:HIS:O	2.48	0.47
24:BF:142:GLY:HA3	24:BF:239:ILE:HB	1.97	0.47
27:AZ:77:ILE:HD11	27:AZ:99:ILE:HD12	1.95	0.47
30:Av:16:ASN:ND2	64:A2:1095:C:O2	2.48	0.47
40:EA:333:GLY:HA3	40:EA:352:LYS:HD2	1.96	0.47
42:Bd:75:LYS:HE2	42:Bd:81:PRO:HG3	1.96	0.47
43:BJ:20:LEU:HD13	43:BJ:132:VAL:HG22	1.97	0.47
44:Ct:113:LYS:HE2	44:Ct:120:TYR:CE2	2.50	0.47
52:DA:45:LEU:HD13	52:DA:72:LEU:HD11	1.96	0.47
55:BM:7:VAL:HG11	55:BM:52:PHE:HE1	1.80	0.47
56:DB:496:LYS:HE2	56:DB:504:ALA:HB1	1.95	0.47
56:DB:541:LEU:HD12	60:DC:36:LEU:HD21	1.95	0.47
61:Ah:165:GLN:HE22	61:Ah:195:LEU:HD11	1.80	0.47
64:A2:159:A2M:H8	64:A2:159:A2M:O5'	2.15	0.47
64:A2:526:A:H2'	64:A2:527:A:H8	1.80	0.47
64:A2:1649:G:C5	86:Ap:17:LYS:HE2	2.50	0.47
64:A2:1763:C:H2'	64:A2:1764:G:C8	2.50	0.47
65:Ai:152:ASP:OD1	65:Ai:152:ASP:N	2.47	0.47
86:Ap:117:ARG:HE	86:Ap:121:VAL:HG21	1.79	0.47
13:BX:139:ARG:NH1	20:B5:2376:C:OP1	2.47	0.47
20:B5:1907:G:H4'	87:Bs:34:ASN:HD22	1.80	0.47
22:Ba:84:GLU:OE2	22:Ba:87:ARG:NH2	2.47	0.47
28:Ay:36:SER:HB3	64:A2:1639:G:H4'	1.97	0.47
36:Ab:128:VAL:HG11	36:Ab:155:ILE:HG12	1.97	0.47
43:BJ:17:ILE:HD12	43:BJ:80:GLU:HG2	1.97	0.47
44:Ct:95:THR:HG21	48:Cu:109:GLN:HB3	1.96	0.47
58:Bh:66:LYS:NZ	58:Bh:82:ASP:OD2	2.47	0.47
64:A2:27:A2M:OP2	98:A2:2113:HOH:O	2.20	0.47
64:A2:1246:G:O2'	64:A2:1493:U:OP1	2.32	0.47
73:AC:102:VAL:HG21	74:Al:35:ILE:HG21	1.96	0.47
20:B5:4508:G:H2'	20:B5:4509:A:C8	2.50	0.47
22:Ba:14:HIS:O	22:Ba:16:SER:N	2.48	0.47
39:B:183:TYR:HA	39:B:190:PHE:HA	1.97	0.47
64:A2:678:G:H21	64:A2:1029:A:H62	1.63	0.47
64:A2:929:G:H1	64:A2:1014:U:H3	1.63	0.47
64:A2:1271:G:O2'	64:A2:1302:A:N7	2.47	0.47
64:A2:1284:C:O2'	64:A2:1314:A:N1	2.41	0.47
64:A2:1846:A:H2'	64:A2:1847:G:C8	2.50	0.47
82:AF:278:SER:HB2	82:AF:281:ALA:HB3	1.97	0.47
83:Ao:17:TYR:HB3	83:Ao:25:LEU:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
90:Bt:80:LEU:HD13	90:Bt:112:ILE:HG23	1.96	0.47
3:B7:55:A:O2'	43:BJ:151:ILE:O	2.29	0.47
19:BE:156:LEU:HD11	19:BE:198:ILE:HG13	1.96	0.47
20:B5:3386:G:O2'	20:B5:3425:U:OP1	2.33	0.47
20:B5:4026:A:OP2	39:B:23:ARG:NH2	2.48	0.47
20:B5:4331:U:H2'	20:B5:4332:G:H8	1.80	0.47
20:B5:4340:U:H2'	20:B5:4341:G:H8	1.80	0.47
56:DB:794:LEU:H	56:DB:797:ARG:HH12	1.63	0.47
59:BN:189:ARG:HG2	59:BN:193:ARG:HH11	1.80	0.47
62:Bi:99:LYS:HG2	62:Bi:103:LYS:HE2	1.97	0.47
66:Bj:2:THR:O	66:Bj:7:SER:OG	2.25	0.47
68:Aj:37:ASP:OD1	68:Aj:37:ASP:N	2.46	0.47
20:B5:184:U:H3	20:B5:253:G:H1	1.63	0.46
20:B5:287:U:H2'	20:B5:288:G:C8	2.51	0.46
20:B5:4295:G:H2'	20:B5:4296:G:H8	1.80	0.46
42:Bd:37:GLY:O	42:Bd:41:ARG:HG3	2.15	0.46
64:A2:1618:G:H3'	83:Ao:47:ARG:HH22	1.80	0.46
6:B8:60:G:O6	58:Bh:62:ASN:ND2	2.40	0.46
16:BP:40:HIS:NE2	16:BP:110:ASP:O	2.37	0.46
20:B5:1546:U:OP2	20:B5:2699:C:O2'	2.31	0.46
20:B5:1678:G:N3	20:B5:1681:A:N6	2.63	0.46
20:B5:3966:6MZ:OP1	88:BT:2:THR:N	2.47	0.46
20:B5:4714:G:O2'	20:B5:4716:A:N6	2.46	0.46
56:DB:770:LYS:HG2	56:DB:814:LEU:HD21	1.98	0.46
60:DC:156:ASP:OD1	60:DC:159:ARG:NH1	2.48	0.46
61:Ah:10:LYS:NZ	64:A2:371:G:O2'	2.48	0.46
64:A2:103:A:H61	64:A2:356:G:H2'	1.80	0.46
64:A2:1388:G:O5'	98:A2:2112:HOH:O	2.20	0.46
64:A2:1624:A:OP2	94:A2:1901:SPD:N1	2.49	0.46
12:BB:224:LYS:HE3	12:BB:340:THR:HB	1.97	0.46
13:BX:39:LYS:HB3	13:BX:40:ILE:H	1.54	0.46
14:Au:43:THR:HG1	14:Au:45:ARG:HH11	1.58	0.46
15:BC:152:LEU:HD21	15:BC:174:LEU:HD13	1.96	0.46
20:B5:91:G:OP1	78:Bo:44:LYS:NZ	2.38	0.46
22:Ba:89:ASN:OD1	22:Ba:92:LYS:NZ	2.49	0.46
32:Aa:155:TYR:OH	64:A2:990:C:OP2	2.26	0.46
9:BA:193:ARG:NH2	20:B5:3410:G:OP2	2.42	0.46
19:BE:120:PRO:O	84:Br:112:ARG:NH1	2.48	0.46
20:B5:184:U:H3	20:B5:253:G:H22	1.63	0.46
20:B5:382:G:H4'	20:B5:407:A:N1	2.30	0.46
20:B5:1334:G:N2	20:B5:1337:G:OP2	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B5:3432:C:H2'	20:B5:3478:A:H61	1.79	0.46
20:B5:4699:G:H2'	20:B5:4700:G:C8	2.50	0.46
43:BJ:81:GLU:OE2	43:BJ:85:LYS:NZ	2.37	0.46
61:Ah:130:THR:OG1	61:Ah:132:GLU:OE1	2.33	0.46
63:BO:10:ASP:OD2	63:BO:37:ARG:NH2	2.47	0.46
64:A2:42:A:O3'	98:A2:2114:HOH:O	2.21	0.46
64:A2:1229:A:O2'	64:A2:1635:A:N3	2.43	0.46
64:A2:1760:G:H2'	64:A2:1761:G:H8	1.80	0.46
87:Bs:125:ALA:HA	87:Bs:154:ILE:HB	1.98	0.46
20:B5:679:C:H2'	56:DB:594:LYS:HE2	1.98	0.46
20:B5:842:G:H3'	24:BF:147:LYS:HD2	1.97	0.46
20:B5:1757:G:O2'	20:B5:1759:C:OP2	2.27	0.46
20:B5:1789:A:N3	20:B5:2126:G:O2'	2.48	0.46
20:B5:3975:U:H4'	78:Bo:89:LYS:HE2	1.98	0.46
27:AZ:77:ILE:HG13	27:AZ:99:ILE:HB	1.97	0.46
37:Bc:4:ALA:O	37:Bc:7:THR:OG1	2.28	0.46
39:B:59:ASP:OD1	39:B:60:ILE:N	2.48	0.46
44:Ct:94:VAL:HB	44:Ct:106:ILE:HB	1.96	0.46
56:DB:171:LEU:O	56:DB:196:GLN:NE2	2.49	0.46
56:DB:178:GLN:O	56:DB:189:TYR:OH	2.31	0.46
64:A2:1051:A:H62	64:A2:1069:G:H21	1.64	0.46
64:A2:1832:A:H2'	64:A2:1833:6MZ:H8	1.97	0.46
74:Al:49:LEU:HB3	74:Al:111:VAL:HB	1.97	0.46
2:Bb:92:LYS:HD2	20:B5:1105:C:C5	2.50	0.46
5:Ar:132:ARG:HB2	5:Ar:134:GLN:HE22	1.80	0.46
15:BC:60:HIS:NE2	15:BC:100:ARG:HD3	2.31	0.46
20:B5:1564:U:O4	94:B5:5377:SPD:N6	2.48	0.46
20:B5:1653:C:O2'	24:BF:176:ARG:NH2	2.48	0.46
20:B5:2577:U:H2'	20:B5:2578:G:C8	2.50	0.46
21:BQ:178:ARG:N	22:Ba:51:GLY:HA2	2.31	0.46
40:EA:128:ILE:HG23	40:EA:304:PRO:HD3	1.97	0.46
44:Ct:73:GLU:OE2	48:Cu:86:ASN:ND2	2.47	0.46
52:DA:7:GLU:OE2	60:DC:116:ARG:NH2	2.49	0.46
56:DB:213:LEU:O	56:DB:217:GLU:HG3	2.16	0.46
56:DB:730:VAL:O	56:DB:734:LEU:HG	2.15	0.46
61:Ah:10:LYS:O	61:Ah:18:ARG:NH1	2.49	0.46
64:A2:1303:G:N1	64:A2:1307:U:O4	2.49	0.46
90:Bt:101:SER:HA	90:Bt:141:CYS:HA	1.98	0.46
12:BB:317:LEU:HB2	12:BB:372:SER:HB2	1.98	0.46
20:B5:639:G:H2'	20:B5:640:G:H8	1.81	0.46
20:B5:788:G:H2'	20:B5:789:G:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B5:1610:C:O2	20:B5:4136:A:O2'	2.30	0.46
32:Aa:146:ARG:NH1	64:A2:1123:A:N3	2.64	0.46
56:DB:98:GLU:HA	56:DB:101:LYS:HD2	1.98	0.46
59:BN:138:PHE:HA	59:BN:143:ARG:HE	1.81	0.46
64:A2:5:U:H2'	64:A2:6:G:H8	1.79	0.46
64:A2:1222:G:O2'	64:A2:1677:U:O2	2.30	0.46
74:Al:37:GLU:HA	74:Al:40:LYS:HD2	1.97	0.46
88:BT:18:PRO:HG2	88:BT:21:LYS:HB2	1.97	0.46
6:B8:21:C:N4	6:B8:22:U:O4	2.49	0.46
6:B8:47:C:H1'	6:B8:61:A:H2'	1.97	0.46
20:B5:722:U:OP1	24:BF:75:ARG:NH2	2.49	0.46
20:B5:3587:C:H2'	20:B5:3588:A:H8	1.81	0.46
40:EA:233:ASN:ND2	40:EA:358:GLU:OE1	2.48	0.46
41:Ac:25:LEU:HD12	41:Ac:37:VAL:HG11	1.97	0.46
44:Ct:73:GLU:HG2	48:Cu:85:ALA:O	2.15	0.46
64:A2:1338:4AC:H2'	64:A2:1339:G:C8	2.51	0.46
64:A2:1754:C:H2'	64:A2:1755:G:H8	1.81	0.46
66:Bj:28:HIS:HE1	66:Bj:30:GLN:HB2	1.81	0.46
20:B5:757:A:N6	20:B5:759:G:O6	2.49	0.46
20:B5:2106:A:OP1	84:Br:107:ARG:NH2	2.49	0.46
20:B5:2210:A:OP1	98:B5:5554:HOH:O	2.20	0.46
34:BH:111:LEU:HD11	34:BH:125:ARG:HB3	1.98	0.46
35:BS:112:ASP:OD1	35:BS:116:ARG:NH1	2.43	0.46
40:EA:119:GLU:HG2	40:EA:299:LEU:HB3	1.97	0.46
51:BL:80:GLU:CD	51:BL:102:ARG:HH12	2.24	0.46
56:DB:766:LEU:HD21	56:DB:805:VAL:HG22	1.98	0.46
64:A2:1222:G:H2'	64:A2:1223:G:H8	1.81	0.46
3:B7:47:G:H21	39:B:222:GLN:HE22	1.64	0.46
20:B5:45:U:O4	59:BN:83:LYS:NZ	2.49	0.46
20:B5:1068:U:H2'	20:B5:1069:G:C8	2.50	0.46
20:B5:1879:G:H22	20:B5:4180:C:H5''	1.81	0.46
20:B5:4486:G:H2'	20:B5:4489:G:H5'	1.97	0.46
40:EA:248:LEU:HD22	40:EA:332:GLU:HG3	1.98	0.46
64:A2:928:C:O2	67:AA:51:GLN:NE2	2.49	0.46
64:A2:984:A:OP1	64:A2:1074:U:O2'	2.27	0.46
64:A2:1376:G:H2'	64:A2:1377:A:H8	1.81	0.46
64:A2:1590:A:N3	64:A2:1654:U:O2'	2.48	0.46
90:Bt:18:THR:OG1	90:Bt:21:GLU:O	2.26	0.46
15:BC:321:ASN:ND2	20:B5:709:G:OP1	2.41	0.45
20:B5:158:A:H5''	20:B5:159:C:H2'	1.98	0.45
20:B5:1307:C:OP2	51:BL:39:ARG:NH2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B5:3882:G:H2'	20:B5:3883:G:H8	1.81	0.45
20:B5:4283:C:H2'	20:B5:4284:G:C8	2.51	0.45
60:DC:128:PHE:HB3	60:DC:147:MET:HE2	1.98	0.45
64:A2:823:PSU:HN3	64:A2:827:A:H62	1.64	0.45
64:A2:1256:G:O3'	85:AG:40:ARG:NH2	2.48	0.45
71:Ak:57:ASP:HB3	71:Ak:60:CYS:HB2	1.98	0.45
20:B5:135:G:N7	58:Bh:97:LYS:HE3	2.31	0.45
20:B5:733:C:H4'	55:BM:69:ARG:HH21	1.82	0.45
20:B5:1858:G:H22	94:B5:5297:SPD:H101	1.64	0.45
20:B5:1859:C:H3'	20:B5:1860:C:H5''	1.99	0.45
20:B5:2384:G:H2'	20:B5:2385:G:C8	2.51	0.45
20:B5:4646:G:N2	20:B5:4652:G:H2'	2.31	0.45
21:BQ:88:ASP:HB2	21:BQ:109:ALA:HB2	1.98	0.45
51:BL:130:LYS:HB3	51:BL:133:ALA:HB3	1.98	0.45
56:DB:159:HIS:CE1	56:DB:167:ALA:HB1	2.52	0.45
64:A2:583:U:H2'	64:A2:584:A:H5''	1.99	0.45
64:A2:675:C:OP1	95:A2:1939:SPM:H112	2.16	0.45
82:AF:25:PRO:HA	82:AF:293:ALA:HB2	1.98	0.45
10:BV:131:ARG:O	10:BV:134:SER:OG	2.30	0.45
19:BE:193:HIS:HB3	19:BE:196:PHE:HD1	1.82	0.45
20:B5:734:G:H2'	20:B5:735:G:H8	1.82	0.45
36:Ab:102:LEU:HD22	36:Ab:130:ILE:HG12	1.97	0.45
56:DB:201:ARG:NH2	56:DB:229:THR:HB	2.31	0.45
56:DB:550:GLN:HG2	56:DB:668:VAL:HG23	1.97	0.45
77:Am:40:LEU:HD12	77:Am:50:ILE:HG23	1.98	0.45
20:B5:1290:C:H2'	20:B5:1291:G:C8	2.51	0.45
20:B5:2207:OMG:N7	98:B5:5784:HOH:O	2.36	0.45
24:BF:53:ALA:HB2	24:BF:187:GLU:HG3	1.99	0.45
42:Bd:26:THR:OG1	42:Bd:85:ARG:NH1	2.46	0.45
44:Ct:190:VAL:HG21	44:Ct:213:LEU:HB3	1.97	0.45
56:DB:225:ALA:HB1	56:DB:536:ARG:HH12	1.80	0.45
56:DB:773:TYR:HE1	56:DB:780:GLN:HA	1.81	0.45
64:A2:616:C:O2'	76:AD:82:ARG:NE	2.45	0.45
90:Bt:108:GLU:HA	90:Bt:111:ASN:HD21	1.81	0.45
12:BB:217:ILE:HD13	12:BB:284:ILE:HD11	1.98	0.45
14:Au:1:AME:HT23	14:Au:1:AME:HA	1.51	0.45
16:BP:78:TRP:CD1	16:BP:80:GLN:H	2.34	0.45
20:B5:231:U:O2	25:BY:103:LYS:NZ	2.48	0.45
20:B5:305:A:P	59:BN:15:GLN:HE22	2.40	0.45
20:B5:1621:C:O2'	20:B5:1643:G:OP1	2.33	0.45
20:B5:2601:G:O2'	20:B5:2608:A:N3	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Aa:30:TRP:CG	80:An:19:PRO:HB3	2.51	0.45
46:Be:90:MET:HG3	84:Br:33:LYS:HA	1.97	0.45
52:DA:51:PHE:O	52:DA:54:ILE:HG12	2.16	0.45
56:DB:679:PHE:HB3	56:DB:691:MET:HE1	1.99	0.45
64:A2:1056:A:N7	98:A2:2220:HOH:O	2.36	0.45
64:A2:1399:G:O2'	82:AF:88:ARG:NH2	2.42	0.45
64:A2:1763:C:H2'	64:A2:1764:G:H8	1.80	0.45
90:Bt:53:TRP:HD1	90:Bt:56:LEU:HB2	1.81	0.45
90:Bt:133:LEU:HD11	90:Bt:151:ILE:HG13	1.98	0.45
5:Ar:51:ASP:OD2	5:Ar:53:THR:OG1	2.34	0.45
5:Ar:88:LYS:O	83:Ao:18:ARG:NH1	2.50	0.45
19:BE:101:GLY:HA3	19:BE:104:ASN:HB2	1.99	0.45
20:B5:2399:G:H2'	20:B5:2400:G:H8	1.81	0.45
20:B5:2577:U:H2'	20:B5:2578:G:H8	1.81	0.45
20:B5:4020:A:H2'	20:B5:4021:G:C8	2.52	0.45
20:B5:4323:U:H2'	20:B5:4324:G:C8	2.51	0.45
20:B5:4663:C:O2	20:B5:4665:C:N4	2.49	0.45
27:AZ:52:LYS:HB2	89:Aq:109:LEU:HD13	1.98	0.45
34:BH:92:MET:HE2	34:BH:179:ILE:HG22	1.99	0.45
64:A2:445:G:N2	64:A2:448:A:OP2	2.48	0.45
15:BC:25:PRO:HB2	15:BC:27:VAL:HG12	1.98	0.45
15:BC:76:ILE:HD12	15:BC:77:PRO:HD2	1.99	0.45
17:BZ:30:ASP:O	17:BZ:39:SER:OG	2.32	0.45
20:B5:1299:G:OP1	21:BQ:108:ARG:NH2	2.43	0.45
20:B5:2232:A:H5'	42:Bd:70:LYS:HE2	1.97	0.45
20:B5:4135:C:H2'	20:B5:4136:A:C8	2.51	0.45
20:B5:4345:A:N1	20:B5:4356:A:H5''	2.31	0.45
36:Ab:118:ALA:HB1	64:A2:1488:A:H1'	1.99	0.45
38:BI:171:TRP:HB2	38:BI:178:ALA:HA	1.98	0.45
60:DC:18:ASN:HD21	60:DC:26:PHE:H	1.65	0.45
12:BB:226:LYS:NZ	20:B5:4414:U:OP1	2.47	0.45
20:B5:1449:U:H2'	20:B5:1450:G:H8	1.82	0.45
20:B5:1823:C:H2'	20:B5:1824:G:H8	1.80	0.45
30:Av:68:ARG:HD2	36:Ab:256:TRP:CG	2.52	0.45
32:Aa:2:ALA:N	80:An:62:VAL:O	2.48	0.45
39:B:37:VAL:HG12	39:B:50:ARG:HD3	1.99	0.45
55:BM:27:ILE:HD13	55:BM:38:VAL:HG12	1.99	0.45
56:DB:134:ARG:HB3	56:DB:138:TYR:CZ	2.52	0.45
56:DB:507:LYS:HA	56:DB:510:GLU:HB2	1.97	0.45
64:A2:1342:C:N3	98:A2:2213:HOH:O	2.36	0.45
80:An:46:ASP:N	80:An:46:ASP:OD1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:AF:164:ILE:HD11	82:AF:221:LEU:HD13	1.99	0.45
86:Ap:16:LYS:HG3	86:Ap:17:LYS:H	1.82	0.45
2:Bb:38:LYS:HE2	20:B5:1755:C:H4'	1.98	0.45
3:B7:29:C:O2'	3:B7:50:A:N1	2.46	0.45
3:B7:97:G:N7	98:B7:311:HOH:O	2.36	0.45
6:B8:96:C:H5''	58:Bh:66:LYS:HG2	1.99	0.45
13:BX:82:THR:HG21	58:Bh:37:THR:HG22	1.99	0.45
15:BC:294:LYS:NZ	20:B5:2028:G:OP2	2.48	0.45
19:BE:142:LYS:NZ	20:B5:706:C:OP1	2.40	0.45
20:B5:1698:G:H2'	20:B5:1699:G:H8	1.82	0.45
20:B5:4049:C:H3'	20:B5:4051:G:H21	1.82	0.45
46:Be:67:LYS:HG2	46:Be:68:HIS:CD2	2.52	0.45
56:DB:326:PHE:CZ	56:DB:382:GLN:HB2	2.52	0.45
57:Ag:37:LYS:O	57:Ag:41:ARG:HG3	2.17	0.45
63:BO:18:ARG:CZ	63:BO:128:ARG:HH21	2.30	0.45
86:Ap:34:VAL:HG22	86:Ap:70:VAL:HB	1.98	0.45
13:BX:129:ARG:HD3	13:BX:135:LYS:HE3	1.98	0.45
20:B5:1292:U:H2'	20:B5:1293:G:H8	1.82	0.45
20:B5:2318:G:H4'	20:B5:2319:G:H8	1.80	0.45
20:B5:3455:A:H2'	20:B5:3456:A2M:H8	1.97	0.45
44:Ct:195:ALA:HA	44:Ct:213:LEU:HD11	1.99	0.45
45:Ad:112:HIS:NE2	45:Ad:237:SER:O	2.50	0.45
53:Af:198:ARG:NH2	64:A2:126:G:OP2	2.44	0.45
56:DB:575:ASP:O	56:DB:577:ASN:ND2	2.50	0.45
64:A2:1338:4AC:H2'	64:A2:1339:G:H8	1.82	0.45
64:A2:1588:G:OP1	64:A2:1588:G:N2	2.45	0.45
6:B8:130:C:H2'	6:B8:131:G:H8	1.82	0.44
13:BX:150:ALA:HB1	13:BX:155:ILE:HB	1.99	0.44
19:BE:273:TYR:OH	55:BM:106:ASP:OD2	2.34	0.44
20:B5:1980:A:H62	20:B5:4180:C:H1'	1.82	0.44
20:B5:2332:C:H4'	20:B5:2333:U:H5	1.82	0.44
20:B5:3631:OMG:HM22	20:B5:3632:G:H5'	1.99	0.44
20:B5:3850:G:N1	54:Bg:98:GLU:OE2	2.36	0.44
42:Bd:42:ALA:HB3	42:Bd:77:ILE:HG13	1.98	0.44
53:Af:164:LYS:HG2	53:Af:165:GLU:H	1.82	0.44
64:A2:527:A:H5'	76:AD:105:ARG:HH21	1.82	0.44
64:A2:1563:C:H2'	64:A2:1564:G:H8	1.83	0.44
15:BC:316:LYS:NZ	20:B5:1225:G:OP1	2.48	0.44
20:B5:697:G:N2	20:B5:698:C:O2	2.50	0.44
20:B5:2204:G:O2'	20:B5:3591:G:O6	2.31	0.44
20:B5:2486:G:H1	20:B5:2534:U:H3	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B5:3808:C:H2'	20:B5:3809:G:H8	1.83	0.44
24:BF:226:PHE:N	24:BF:232:ALA:O	2.51	0.44
43:BJ:35:ARG:HD2	43:BJ:123:ILE:HA	1.99	0.44
46:Be:6:PRO:HG3	46:Be:73:GLY:HA3	1.99	0.44
56:DB:158:TYR:HB3	56:DB:167:ALA:HB2	1.99	0.44
60:DC:122:TYR:HB3	60:DC:128:PHE:HB2	1.99	0.44
64:A2:1481:A:H5'	86:Ap:131:LYS:HE2	1.99	0.44
76:AD:102:ARG:HD3	76:AD:106:ALA:HB1	1.98	0.44
19:BE:98:PRO:HA	19:BE:107:THR:HA	1.98	0.44
20:B5:1227:G:N1	20:B5:2015:G:OP1	2.44	0.44
20:B5:4426:G:H2'	20:B5:4427:A:C8	2.52	0.44
34:BH:26:ILE:HG13	34:BH:35:ARG:HG2	1.98	0.44
34:BH:41:ILE:HG22	34:BH:43:VAL:HG13	1.98	0.44
39:B:51:MET:HE3	39:B:105:LEU:HD23	1.99	0.44
41:Ac:64:ARG:HD2	68:Aj:94:LEU:HD21	1.99	0.44
45:Ad:151:ASP:HB3	45:Ad:154:ILE:HG13	1.99	0.44
52:DA:17:LYS:HG2	56:DB:436:ALA:HB1	1.99	0.44
64:A2:949:C:H2'	64:A2:950:G:H8	1.81	0.44
64:A2:1754:C:O2	64:A2:1781:G:N2	2.51	0.44
3:B7:7:G:O5'	39:B:33:ARG:NH1	2.51	0.44
3:B7:48:G:OP1	39:B:226:TYR:OH	2.25	0.44
20:B5:2146:C:OP1	46:Be:107:ASN:ND2	2.49	0.44
27:AZ:57:LYS:NZ	27:AZ:160:ALA:O	2.41	0.44
51:BL:135:LYS:N	51:BL:138:ASP:OD2	2.47	0.44
60:DC:8:PRO:HA	60:DC:11:LEU:HG	1.98	0.44
74:Al:32:ALA:HB1	74:Al:37:GLU:HG2	1.99	0.44
82:AF:254:PRO:HB3	82:AF:283:PRO:HB2	2.00	0.44
5:Ar:46:ARG:HG2	8:As:35:ASP:HB2	1.99	0.44
10:BV:31:ASN:ND2	10:BV:115:SER:OG	2.49	0.44
12:BB:123:HIS:ND1	20:B5:4727:U:OP2	2.50	0.44
16:BP:62:ARG:NH1	20:B5:423:G:OP1	2.43	0.44
20:B5:663:C:H2'	20:B5:664:G:C8	2.53	0.44
20:B5:663:C:H2'	20:B5:664:G:H8	1.82	0.44
20:B5:1717:C:H2'	20:B5:1718:PSU:H6	1.83	0.44
20:B5:1980:A:N6	20:B5:4180:C:O2	2.51	0.44
20:B5:2688:A:H61	20:B5:3575:C:H42	1.66	0.44
20:B5:3339:U:H2'	20:B5:3340:A:H8	1.83	0.44
20:B5:3380:A:H1'	20:B5:3517:A2M:N6	2.33	0.44
20:B5:4020:A:H2'	20:B5:4021:G:H8	1.83	0.44
20:B5:4450:C:H2'	20:B5:4451:A:C8	2.53	0.44
20:B5:4609:G:H5''	55:BM:91:TRP:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BS:80:ILE:HG12	35:BS:129:VAL:HG22	2.00	0.44
40:EA:191:LYS:HG3	40:EA:206:PRO:HD2	1.98	0.44
53:Af:53:SER:HB2	64:A2:165:G:H4'	1.99	0.44
53:Af:174:PRO:HB3	64:A2:65:C:C6	2.52	0.44
56:DB:431:MET:HB3	56:DB:448:CYS:SG	2.57	0.44
60:DC:122:TYR:O	60:DC:128:PHE:N	2.46	0.44
64:A2:920:A:O2'	94:A2:1921:SPD:N1	2.49	0.44
64:A2:1376:G:H2'	64:A2:1377:A:C8	2.53	0.44
82:AF:87:LEU:HD21	82:AF:108:VAL:HG11	1.99	0.44
82:AF:159:ASN:HD22	82:AF:159:ASN:H	1.64	0.44
90:Bt:14:TYR:O	90:Bt:31:LYS:NZ	2.50	0.44
2:Bb:65:MET:HA	2:Bb:68:ARG:HH12	1.82	0.44
8:As:65:TYR:HE1	8:As:128:GLN:HG3	1.83	0.44
20:B5:2662:U:OP1	98:B5:5558:HOH:O	2.21	0.44
20:B5:4323:U:H2'	20:B5:4324:G:H8	1.83	0.44
32:Aa:87:ILE:HG22	32:Aa:101:HIS:HB2	1.99	0.44
56:DB:117:LEU:HB2	56:DB:140:LEU:HD21	2.00	0.44
56:DB:134:ARG:NH2	56:DB:161:LEU:HB2	2.33	0.44
56:DB:543:LYS:O	56:DB:547:VAL:HG23	2.17	0.44
64:A2:564:G:O2'	64:A2:565:A:H8	2.01	0.44
64:A2:935:G:H22	64:A2:1009:A:H2	1.66	0.44
17:BZ:38:TYR:HB3	20:B5:2499:U:H5''	2.00	0.44
20:B5:287:U:H2'	20:B5:288:G:H8	1.81	0.44
20:B5:456:C:H2'	20:B5:457:G:C8	2.53	0.44
20:B5:3432:C:O2'	20:B5:3506:A:N3	2.41	0.44
23:Ax:104:ARG:NH2	64:A2:508:G:OP2	2.51	0.44
38:BI:101:LYS:NZ	38:BI:102:MET:O	2.42	0.44
50:Bf:17:GLY:N	50:Bf:20:ASN:O	2.42	0.44
56:DB:291:LEU:HB3	56:DB:295:ARG:CZ	2.47	0.44
64:A2:1389:A:N6	98:A2:2253:HOH:O	2.44	0.44
64:A2:1859:G:H2'	64:A2:1860:A:H8	1.82	0.44
69:Bk:12:LEU:HB3	69:Bk:16:ARG:NH1	2.33	0.44
75:Bm:112:LYS:HB3	75:Bm:114:LYS:HG2	2.00	0.44
84:Br:38:PHE:O	84:Br:45:HIS:NE2	2.36	0.44
9:BA:128:ARG:NH2	20:B5:3413:G:OP2	2.50	0.44
20:B5:1208:C:H2'	20:B5:1209:G:H8	1.83	0.44
20:B5:1682:A:N1	20:B5:1728:C:O2'	2.48	0.44
20:B5:4043:G:H2'	20:B5:4044:A:H8	1.82	0.44
20:B5:4269:A2M:OP1	98:B5:5562:HOH:O	2.21	0.44
29:BG:110:LYS:HG3	29:BG:113:ARG:HH21	1.82	0.44
39:B:264:LYS:NZ	39:B:265:ARG:O	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:Ag:58:LYS:HB2	57:Ag:90:LYS:HG2	2.00	0.44
64:A2:983:G:H2'	64:A2:984:A:C8	2.53	0.44
82:AF:31:ILE:HG13	82:AF:43:TRP:HB2	2.00	0.44
6:B8:106:G:H4'	6:B8:137:A:H5'	2.00	0.44
14:AU:34:MET:HE2	27:AZ:64:ALA:HB1	1.98	0.44
20:B5:1697:G:H2'	20:B5:1698:G:H8	1.83	0.44
20:B5:2399:G:H2'	20:B5:2400:G:C8	2.53	0.44
20:B5:2544:U:H2'	20:B5:2545:C:C6	2.53	0.44
20:B5:4336:A2M:HM'2	20:B5:4337:U:H5'	2.00	0.44
20:B5:4495:U:H5''	50:Bf:54:LYS:HE3	2.00	0.44
32:Aa:146:ARG:HB2	32:Aa:149:GLN:HB2	1.99	0.44
56:DB:69:VAL:O	56:DB:86:TYR:OH	2.20	0.44
56:DB:708:LEU:HD23	56:DB:708:LEU:HA	1.89	0.44
64:A2:398:G:OP2	71:Ak:108:ASN:ND2	2.51	0.44
64:A2:1550:U:OP1	85:AG:34:TYR:OH	2.33	0.44
15:BC:242:PRO:HB2	20:B5:2140:G:H4'	2.00	0.43
20:B5:1758:G:O2'	39:B:115:MET:SD	2.74	0.43
20:B5:2652:G:O2'	20:B5:4390:G:OP1	2.33	0.43
20:B5:3334:C:H2'	20:B5:3335:G:C8	2.52	0.43
41:Ac:48:ILE:HB	41:Ac:86:LEU:HG	2.00	0.43
42:Bd:96:GLU:O	42:Bd:101:LYS:NZ	2.50	0.43
56:DB:258:TRP:CZ3	56:DB:296:LEU:HG	2.53	0.43
56:DB:338:LYS:O	56:DB:342:ILE:HG13	2.18	0.43
56:DB:447:LYS:O	56:DB:451:TYR:HD1	2.01	0.43
56:DB:496:LYS:NZ	56:DB:560:ILE:O	2.43	0.43
64:A2:412:G:H2'	64:A2:413:G:H8	1.83	0.43
64:A2:562:A:O2'	65:Ai:134:HIS:NE2	2.51	0.43
83:Ao:75:VAL:HG21	83:Ao:104:GLN:HG2	1.99	0.43
10:BV:45:ILE:HG21	10:BV:53:PRO:HB3	2.00	0.43
10:BV:51:ARG:NH1	20:B5:4366:OMU:OP1	2.50	0.43
12:BB:59:GLU:HB2	12:BB:366:LYS:HE3	2.00	0.43
15:BC:85:HIS:O	15:BC:89:GLN:NE2	2.51	0.43
20:B5:2450:C:H2'	20:B5:2451:G:C8	2.54	0.43
20:B5:2542:C:N4	98:B5:5824:HOH:O	2.51	0.43
20:B5:2667:OMC:HM22	20:B5:2668:A:H5'	2.00	0.43
20:B5:4140:A:N7	98:B5:5781:HOH:O	2.35	0.43
20:B5:4367:C:H2'	20:B5:4368:A:H8	1.83	0.43
45:Ad:19:MET:HG3	64:A2:847:G:H2'	1.99	0.43
56:DB:672:ILE:HG23	56:DB:698:ALA:HB1	2.00	0.43
56:DB:759:SER:O	56:DB:765:ARG:NE	2.51	0.43
60:DC:18:ASN:ND2	60:DC:31:TYR:OH	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:DC:61:GLU:OE1	60:DC:69:HIS:NE2	2.41	0.43
64:A2:99:A2M:H8	64:A2:99:A2M:O5'	2.18	0.43
80:An:22:ALA:N	80:An:25:GLU:OE2	2.47	0.43
84:Br:65:LYS:O	84:Br:102:TYR:OH	2.30	0.43
90:Bt:124:GLU:HG3	90:Bt:126:SER:H	1.82	0.43
11:At:70:VAL:HG13	11:At:104:LEU:HB2	2.01	0.43
20:B5:385:A:H4'	20:B5:386:A:H5'	1.99	0.43
20:B5:4050:A:OP2	88:BT:81:LYS:NZ	2.48	0.43
20:B5:4166:PSU:OP2	20:B5:4167:C:N4	2.51	0.43
20:B5:4445:U:H4'	20:B5:4446:A:OP1	2.18	0.43
20:B5:4508:G:H2'	20:B5:4509:A:H8	1.83	0.43
41:Ac:56:GLN:NE2	41:Ac:57:ASN:OD1	2.51	0.43
41:Ac:172:VAL:O	41:Ac:173:ARG:NH1	2.43	0.43
56:DB:541:LEU:HD23	56:DB:541:LEU:HA	1.87	0.43
83:Ao:34:MET:HB3	83:Ao:42:ARG:HG3	2.00	0.43
2:Bb:65:MET:HG2	2:Bb:68:ARG:HH22	1.83	0.43
8:As:132:ASP:OD2	64:A2:1416:C:O2'	2.27	0.43
9:BA:112:ILE:H	81:Bp:83:ILE:HD11	1.84	0.43
20:B5:226:G:OP2	25:BY:1:MET:N	2.43	0.43
20:B5:4488:A:H2'	20:B5:4689:U:H3	1.83	0.43
56:DB:80:HIS:NE2	56:DB:109:TRP:HB2	2.32	0.43
61:Ah:54:LYS:HE3	64:A2:382:C:H5''	2.01	0.43
64:A2:116:OMU:HM22	64:A2:117:C:H5'	2.00	0.43
64:A2:925:G:H5'	77:Am:4:MET:HE3	2.01	0.43
64:A2:945:A:H5''	80:An:134:PRO:HB3	2.00	0.43
6:B8:58:G:N7	66:Bj:63:ARG:NH2	2.52	0.43
15:BC:186:SER:O	15:BC:188:ARG:NH1	2.51	0.43
20:B5:1815:U:H2'	20:B5:1816:G:C8	2.53	0.43
20:B5:2293:G:O6	98:B5:5559:HOH:O	2.21	0.43
56:DB:408:ILE:HD12	60:DC:79:ARG:HH22	1.83	0.43
56:DB:469:THR:HB	56:DB:478:ASN:HD22	1.84	0.43
59:BN:155:VAL:O	59:BN:162:ARG:NH2	2.36	0.43
64:A2:597:U:O2'	64:A2:646:C:O2	2.35	0.43
65:Ai:83:ARG:HH21	65:Ai:150:ARG:NH1	2.15	0.43
74:Al:11:VAL:HG21	74:Al:16:THR:HG21	2.00	0.43
78:Bo:12:CYS:HB3	78:Bo:15:CYS:HB2	2.00	0.43
8:As:60:THR:HG23	8:As:75:MET:HE2	1.99	0.43
20:B5:387:G:OP2	25:BY:89:LYS:NZ	2.45	0.43
20:B5:1697:G:H2'	20:B5:1698:G:C8	2.53	0.43
20:B5:1898:U:H1'	20:B5:1900:G:C2	2.53	0.43
20:B5:2501:G:O2'	20:B5:2518:G:N2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Ba:75:LEU:HD22	22:Ba:117:LEU:HD11	1.99	0.43
46:Be:35:TRP:CZ2	46:Be:56:PRO:HD2	2.54	0.43
61:Ah:106:SER:HB3	61:Ah:171:LEU:HG	2.01	0.43
64:A2:1076:C:H2'	64:A2:1077:G:H8	1.82	0.43
64:A2:1373:U:OP1	64:A2:1386:G:N2	2.39	0.43
5:Ar:84:LEU:O	5:Ar:87:GLN:NE2	2.38	0.43
20:B5:2365:G:OP2	54:Bg:29:ARG:NH2	2.48	0.43
20:B5:3852:G:N2	29:BG:43:GLN:O	2.51	0.43
20:B5:4166:PSU:H2'	20:B5:4166:PSU:O4	2.19	0.43
23:Ax:117:VAL:HG11	23:Ax:125:VAL:HG21	2.00	0.43
51:BL:172:GLU:HG3	62:Bi:3:LEU:HD22	2.01	0.43
52:DA:137:ASN:HA	52:DA:145:ALA:HB1	2.01	0.43
61:Ah:56:ARG:NH1	61:Ah:180:GLY:O	2.52	0.43
64:A2:1008:C:H2'	64:A2:1009:A:C8	2.53	0.43
87:Bs:82:ILE:HG23	87:Bs:86:VAL:HG21	2.01	0.43
9:BA:53:GLY:O	9:BA:192:LYS:NZ	2.50	0.43
20:B5:477:C:H2'	20:B5:478:G:H8	1.84	0.43
20:B5:707:C:H2'	20:B5:708:G:H8	1.83	0.43
20:B5:1611:U:OP1	98:B5:5560:HOH:O	2.21	0.43
20:B5:4043:G:H22	20:B5:4059:A:H2	1.67	0.43
20:B5:4050:A:OP2	20:B5:4051:G:N2	2.52	0.43
20:B5:4086:U:O2	94:B5:5359:SPD:N10	2.52	0.43
27:AZ:205:ARG:HH21	27:AZ:210:ILE:HA	1.83	0.43
32:Aa:30:TRP:CE2	32:Aa:48:LEU:HD13	2.54	0.43
33:Az:2:ARG:HD3	33:Az:5:TRP:NE1	2.33	0.43
45:Ad:12:VAL:O	64:A2:813:A:O2'	2.30	0.43
56:DB:538:TYR:CD1	60:DC:36:LEU:HD22	2.53	0.43
64:A2:115:U:H2'	64:A2:116:OMU:H6	2.00	0.43
64:A2:1845:U:H2'	64:A2:1846:A:C8	2.54	0.43
2:Bb:110:ALA:HB1	20:B5:1215:G:H5''	2.01	0.43
3:B7:116:G:H2'	3:B7:117:G:H8	1.83	0.43
8:As:62:ARG:NH2	64:A2:1544:U:OP2	2.32	0.43
9:BA:242:ARG:NH2	9:BA:243:THR:O	2.51	0.43
12:BB:317:LEU:HD21	12:BB:381:THR:HA	2.01	0.43
15:BC:33:ARG:NH1	20:B5:1295:G:OP1	2.44	0.43
20:B5:478:G:H2'	20:B5:479:G:C8	2.52	0.43
20:B5:3537:U:H2'	20:B5:3538:G:H8	1.83	0.43
20:B5:3652:PSU:P	98:B5:5506:HOH:O	2.67	0.43
20:B5:4194:G:C8	98:B5:5522:HOH:O	2.58	0.43
20:B5:4792:U:H3'	20:B5:4793:C:C6	2.54	0.43
23:Ax:25:ILE:HD13	23:Ax:44:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:Bh:31:LEU:HB3	58:Bh:47:ILE:HG12	2.01	0.43
64:A2:389:U:H2'	64:A2:390:A:H8	1.84	0.43
64:A2:1293:C:N3	73:AC:138:ARG:NH2	2.66	0.43
64:A2:1446:PSU:O2	64:A2:1447:A:N6	2.52	0.43
64:A2:1837:G:N2	98:A2:2276:HOH:O	2.52	0.43
66:Bj:28:HIS:CE1	66:Bj:30:GLN:HB2	2.54	0.43
89:Aq:109:LEU:HG	89:Aq:111:PHE:HD2	1.84	0.43
15:BC:39:PHE:O	15:BC:43:ASN:ND2	2.36	0.43
15:BC:329:ASN:ND2	24:BF:187:GLU:OE2	2.52	0.43
16:BP:131:ARG:HG3	16:BP:137:ASN:ND2	2.34	0.43
20:B5:153:G:H2'	20:B5:154:G:H8	1.83	0.43
20:B5:1595:C:OP2	98:B5:5556:HOH:O	2.20	0.43
20:B5:1898:U:O4'	20:B5:1964:A:N6	2.52	0.43
20:B5:4364:OMG:HM22	20:B5:4365:U:H5'	2.01	0.43
94:B5:5318:SPD:N6	59:BN:70:GLY:O	2.51	0.43
44:Ct:143:PHE:CE2	56:DB:173:GLU:HB3	2.54	0.43
46:Be:89:LEU:HD13	46:Be:118:LEU:HD22	2.01	0.43
48:Cu:55:ASN:ND2	48:Cu:80:GLN:HG2	2.34	0.43
56:DB:444:ILE:HG22	56:DB:448:CYS:SG	2.59	0.43
64:A2:1305:U:H5''	73:AC:93:HIS:HB2	2.01	0.43
80:An:16:SER:OG	80:An:17:LEU:N	2.51	0.43
6:B8:124:U:O4	6:B8:126:C:N4	2.52	0.42
20:B5:462:G:H2'	20:B5:463:A:C8	2.54	0.42
20:B5:1601:A:O2'	66:Bj:49:TRP:O	2.37	0.42
20:B5:4065:C:H2'	20:B5:4066:G:H8	1.82	0.42
23:Ax:23:MET:N	23:Ax:23:MET:SD	2.92	0.42
36:Ab:168:GLY:N	36:Ab:179:THR:O	2.39	0.42
64:A2:120:U:H2'	64:A2:121:OMU:H6	2.01	0.42
64:A2:1537:G:H2'	64:A2:1538:A:C8	2.54	0.42
64:A2:1857:C:H2'	64:A2:1858:G:H8	1.84	0.42
5:Ar:38:ARG:O	5:Ar:42:HIS:ND1	2.35	0.42
9:BA:233:ARG:HB2	20:B5:3930:G:H5'	2.01	0.42
10:BV:21:PRO:HA	10:BV:54:ALA:HA	2.00	0.42
15:BC:128:LEU:O	15:BC:131:SER:OG	2.36	0.42
20:B5:2142:G:H3'	20:B5:2143:A:H5''	2.01	0.42
20:B5:2239:A:N7	20:B5:2657:C:H2'	2.33	0.42
20:B5:4046:U:H4'	88:BT:89:ILE:HG22	2.00	0.42
28:Ay:43:LYS:HE3	64:A2:1601:G:H4'	2.01	0.42
29:BG:81:ASN:ND2	29:BG:238:GLY:HA3	2.34	0.42
36:Ab:169:TYR:OH	36:Ab:175:GLY:O	2.30	0.42
56:DB:175:ARG:HG3	56:DB:196:GLN:NE2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:DB:642:LEU:HB3	56:DB:647:LEU:HD11	2.01	0.42
61:Ah:31:ARG:NH2	64:A2:382:C:OP2	2.52	0.42
64:A2:62:G:O2'	64:A2:172:OMU:OP1	2.36	0.42
64:A2:240:G:H2'	64:A2:241:G:C8	2.55	0.42
64:A2:1118:C:O2'	64:A2:1119:C:O4'	2.37	0.42
64:A2:1706:C:H2'	64:A2:1707:G:C8	2.54	0.42
68:Aj:16:PHE:HE2	68:Aj:89:ILE:HG22	1.84	0.42
5:Ar:55:ARG:HB2	5:Ar:58:GLU:HG3	2.01	0.42
6:B8:20:A:OP1	98:B8:301:HOH:O	2.21	0.42
15:BC:230:LEU:HD21	15:BC:236:ASN:H	1.85	0.42
20:B5:3450:A2M:H8	20:B5:3450:A2M:O5'	2.18	0.42
21:BQ:124:ASP:OD1	21:BQ:125:GLN:N	2.52	0.42
21:BQ:130:SER:OG	21:BQ:134:ARG:N	2.52	0.42
32:Aa:47:THR:OG1	32:Aa:65:ARG:NH1	2.52	0.42
39:B:204:VAL:HB	39:B:236:MET:HE1	1.99	0.42
48:Cu:82:SER:OG	48:Cu:87:THR:OG1	2.24	0.42
49:Ae:145:ARG:NH1	64:A2:1221:A:O2'	2.51	0.42
56:DB:90:GLN:HB3	56:DB:95:LYS:HB2	1.99	0.42
56:DB:156:ILE:HD11	56:DB:535:LEU:HD22	2.02	0.42
61:Ah:76:THR:OG1	61:Ah:77:ARG:N	2.49	0.42
64:A2:1105:G:H2'	64:A2:1106:G:H8	1.84	0.42
11:At:96:PHE:HB3	85:AG:52:PHE:HB3	2.01	0.42
12:BB:291:TYR:HB3	12:BB:298:LEU:HD11	2.02	0.42
20:B5:318:A:H2'	20:B5:319:A:H8	1.84	0.42
20:B5:2450:C:H2'	20:B5:2451:G:H8	1.84	0.42
20:B5:2662:U:P	98:B5:5558:HOH:O	2.77	0.42
20:B5:4324:G:H2'	20:B5:4325:PSU:H6	1.85	0.42
40:EA:232:LEU:HD13	40:EA:372:THR:HB	2.01	0.42
50:Bf:59:THR:OG1	50:Bf:65:ASN:OD1	2.37	0.42
57:Ag:44:ASN:OD1	57:Ag:68:GLN:NE2	2.37	0.42
61:Ah:25:ARG:NH2	64:A2:434:A:OP1	2.49	0.42
63:BO:125:LYS:HE3	63:BO:125:LYS:HB3	1.90	0.42
64:A2:383:C:H2'	64:A2:384:G:H8	1.85	0.42
64:A2:1049:G:OP2	98:A2:2115:HOH:O	2.21	0.42
64:A2:1288:A:H62	64:A2:1313:G:N2	2.17	0.42
64:A2:1817:G:N7	98:A2:2225:HOH:O	2.37	0.42
65:Ai:160:SER:HB3	65:Ai:163:SER:HB2	2.00	0.42
87:Bs:58:ASN:O	87:Bs:62:ARG:HG3	2.19	0.42
20:B5:1271:C:H2'	20:B5:1272:G:C8	2.55	0.42
20:B5:1509:A:OP1	81:Bp:5:THR:OG1	2.34	0.42
20:B5:1696:U:H2'	20:B5:1697:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B5:1701:C:H2'	20:B5:1702:C:C6	2.55	0.42
20:B5:2654:G:N2	20:B5:2657:C:OP2	2.37	0.42
20:B5:3456:A2M:HM'2	20:B5:3457:G:H5'	1.99	0.42
20:B5:3908:C:H5	29:BG:73:ARG:HH12	1.68	0.42
20:B5:4674:C:N4	20:B5:4675:G:O6	2.52	0.42
38:BI:187:GLU:HG3	38:BI:189:ARG:HG3	2.01	0.42
40:EA:200:VAL:HG22	40:EA:347:VAL:HG12	2.00	0.42
56:DB:125:ILE:HA	56:DB:133:TYR:CZ	2.55	0.42
61:Ah:81:VAL:HG22	61:Ah:102:VAL:HG12	2.02	0.42
69:Bk:12:LEU:HB3	69:Bk:16:ARG:HH12	1.85	0.42
90:Bt:15:LEU:HD22	90:Bt:16:ARG:H	1.84	0.42
6:B8:28:C:H2'	6:B8:29:G:H8	1.85	0.42
9:BA:216:V5N:O2	9:BA:218:HIS:ND1	2.42	0.42
12:BB:324:GLY:HA2	20:B5:4790:C:H4'	2.00	0.42
20:B5:1942:G:N2	20:B5:1943:U:O4	2.51	0.42
20:B5:2630:A2M:H8	20:B5:2630:A2M:H2'	1.82	0.42
20:B5:3941:G:OP1	20:B5:3967:C:O2'	2.28	0.42
45:Ad:55:ALA:HB1	45:Ad:60:GLU:HB2	2.01	0.42
56:DB:441:ASP:HB3	56:DB:443:PHE:HD1	1.84	0.42
64:A2:673:A:C2	95:A2:1939:SPM:H72	2.55	0.42
74:Al:72:HIS:CD2	74:Al:74:ILE:HD11	2.55	0.42
87:Bs:143:ILE:HG12	87:Bs:160:LEU:HD21	2.02	0.42
4:AT:29:N:H4'	5:Ar:148:VAL:HG11	2.02	0.42
5:Ar:124:ARG:NE	5:Ar:130:ARG:O	2.32	0.42
11:At:56:ILE:HD11	11:At:69:PRO:HD3	2.01	0.42
20:B5:1283:U:OP1	22:Ba:8:THR:OG1	2.37	0.42
20:B5:1335:A:P	21:BQ:181:ARG:HH22	2.42	0.42
20:B5:3676:OMG:HM22	20:B5:3677:A:H5'	2.01	0.42
20:B5:3843:G:H4'	20:B5:3844:C:H5'	2.02	0.42
29:BG:102:TYR:OH	29:BG:211:ASP:OD2	2.37	0.42
51:BL:81:LEU:HD12	51:BL:86:ILE:HB	2.01	0.42
56:DB:37:LEU:HD22	56:DB:43:ALA:HA	2.02	0.42
59:BN:96:ARG:NH1	59:BN:104:GLU:OE1	2.53	0.42
64:A2:412:G:H2'	64:A2:413:G:C8	2.55	0.42
64:A2:485:A2M:O5'	64:A2:485:A2M:H8	2.20	0.42
64:A2:1100:G:H22	64:A2:1134:A:H2	1.66	0.42
64:A2:1846:A:H2'	64:A2:1847:G:H8	1.85	0.42
9:BA:180:LEU:HD21	81:Bp:22:LEU:HB3	2.01	0.42
10:BV:89:ARG:HB2	10:BV:95:PHE:CE2	2.54	0.42
15:BC:66:SER:HA	15:BC:77:PRO:HA	2.00	0.42
15:BC:143:ARG:HE	15:BC:145:GLU:CD	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:BC:315:LYS:HD2	24:BF:167:ALA:HB1	2.00	0.42
20:B5:62:A:N3	20:B5:77:U:O2'	2.48	0.42
20:B5:784:C:H2'	20:B5:785:G:H8	1.84	0.42
20:B5:1298:A:H62	20:B5:1457:G:HO2'	1.58	0.42
20:B5:1333:U:OP1	20:B5:1452:A:O2'	2.26	0.42
20:B5:1458:A:H62	21:BQ:87:THR:HG21	1.83	0.42
20:B5:3618:G:OP2	63:BO:90:HIS:NE2	2.51	0.42
20:B5:4432:G:H21	34:BH:163:GLN:HE22	1.68	0.42
21:BQ:177:ALA:O	21:BQ:184:ARG:HB2	2.19	0.42
28:Ay:100:VAL:HG21	49:Ae:102:LEU:HD21	2.01	0.42
38:BI:141:LYS:HD2	38:BI:143:GLN:HE22	1.84	0.42
43:BJ:35:ARG:HB3	43:BJ:123:ILE:HG23	2.02	0.42
53:Af:44:GLU:HB3	53:Af:119:LYS:HD3	2.02	0.42
56:DB:52:LYS:O	56:DB:55:THR:OG1	2.35	0.42
60:DC:44:ILE:HA	60:DC:55:TYR:HA	2.02	0.42
61:Ah:162:LEU:HD11	61:Ah:191:GLU:HG2	2.02	0.42
63:BO:108:ILE:HD12	63:BO:160:ARG:CZ	2.50	0.42
64:A2:16:G:H21	64:A2:1196:A:H62	1.67	0.42
64:A2:1030:G:N7	98:A2:2224:HOH:O	2.37	0.42
64:A2:1090:G:H4'	95:A2:1939:SPM:H111	2.01	0.42
64:A2:1259:A:O5'	98:A2:2116:HOH:O	2.22	0.42
90:Bt:28:LEU:O	90:Bt:32:ILE:HG12	2.20	0.42
15:BC:290:SER:HB3	84:Br:4:HIS:HE1	1.85	0.42
20:B5:2350:A:H3'	20:B5:2351:PSU:H6	1.84	0.42
20:B5:3455:A:OP2	62:Bi:68:ARG:NH2	2.47	0.42
20:B5:4693:G:H2'	20:B5:4694:A:C8	2.55	0.42
56:DB:555:PHE:HB3	56:DB:559:ARG:NE	2.34	0.42
56:DB:714:ARG:HG3	56:DB:771:MET:HE1	2.00	0.42
64:A2:5:U:H2'	64:A2:6:G:C8	2.54	0.42
64:A2:640:C:H2'	64:A2:641:A:C8	2.55	0.42
82:AF:68:ASP:OD1	82:AF:69:VAL:N	2.53	0.42
82:AF:85:GLY:HA2	82:AF:108:VAL:HG23	2.02	0.42
2:Bb:44:ARG:NH1	20:B5:1420:G:OP1	2.53	0.42
9:BA:8:GLN:HA	20:B5:3399:C:H4'	2.02	0.42
10:BV:13:LYS:HD2	10:BV:128:LEU:HD21	2.02	0.42
10:BV:37:LEU:HB3	10:BV:63:ALA:HB1	2.02	0.42
20:B5:78:U:H5''	59:BN:185:GLY:HA2	2.01	0.42
20:B5:1089:G:H2'	20:B5:1091:G:C8	2.55	0.42
20:B5:1688:A:H2'	20:B5:1689:G:H8	1.84	0.42
20:B5:1922:A:H3'	20:B5:1926:C:H41	1.85	0.42
20:B5:3854:C:H5''	20:B5:3855:A:H5''	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B5:4282:OMC:P	98:B5:5534:HOH:O	2.78	0.42
20:B5:4450:C:H2'	20:B5:4451:A:H8	1.85	0.42
53:Af:87:ARG:NH2	64:A2:163:U:OP2	2.53	0.42
53:Af:162:LEU:HD12	53:Af:170:ARG:HD2	2.02	0.42
56:DB:661:LEU:HD23	56:DB:664:LEU:HD12	2.02	0.42
57:Ag:51:ILE:HD11	57:Ag:176:VAL:HG22	2.00	0.42
64:A2:836:C:H2'	64:A2:838:A:N3	2.35	0.42
67:AA:33:MET:HE2	67:AA:48:SER:HA	2.02	0.42
90:Bt:53:TRP:CD1	90:Bt:56:LEU:HB2	2.55	0.42
9:BA:236:GLY:N	20:B5:3419:A:O2'	2.53	0.41
20:B5:2557:G:H2'	20:B5:2558:G:H8	1.84	0.41
20:B5:3863:G:H2'	20:B5:3864:G:C8	2.55	0.41
20:B5:4012:G:N3	20:B5:4012:G:H2'	2.35	0.41
20:B5:4381:A:OP1	20:B5:4382:PSU:O2'	2.35	0.41
21:BQ:133:GLY:O	21:BQ:136:THR:OG1	2.34	0.41
23:Ax:21:LYS:HB2	23:Ax:75:ILE:HB	2.02	0.41
25:BY:2:LYS:HE3	25:BY:2:LYS:HB3	1.87	0.41
27:AZ:110:ASN:OD1	64:A2:1351:U:O2'	2.31	0.41
32:Aa:120:MET:HE2	32:Aa:142:PHE:HE1	1.84	0.41
44:Ct:190:VAL:HG12	44:Ct:191:SER:H	1.83	0.41
46:Be:85:LEU:HD22	46:Be:111:ILE:HG23	2.02	0.41
49:Ae:14:THR:HB	49:Ae:15:PRO:HD3	2.00	0.41
53:Af:31:ARG:NH1	64:A2:1746:A:O3'	2.51	0.41
56:DB:57:ASN:ND2	56:DB:89:LEU:HD22	2.35	0.41
56:DB:73:LEU:HB3	56:DB:77:LEU:HD23	2.02	0.41
56:DB:496:LYS:HG2	56:DB:564:ILE:HD11	2.02	0.41
64:A2:875:G:H2'	64:A2:876:A:C8	2.55	0.41
87:Bs:85:ASN:OD1	87:Bs:85:ASN:N	2.46	0.41
87:Bs:94:ASP:OD2	87:Bs:97:GLU:N	2.52	0.41
2:Bb:19:ASN:ND2	20:B5:1641:C:OP1	2.45	0.41
15:BC:103:ALA:HA	20:B5:1472:G:H22	1.85	0.41
15:BC:113:ARG:HD2	20:B5:1463:A:H5''	2.02	0.41
19:BE:73:ARG:HD3	20:B5:884:U:C5	2.55	0.41
20:B5:122:U:H2'	20:B5:123:C:C6	2.55	0.41
20:B5:295:A:C2	20:B5:317:A:H1'	2.55	0.41
20:B5:2128:A:H2'	20:B5:2129:G:C8	2.56	0.41
20:B5:2128:A:H2'	20:B5:2129:G:H8	1.85	0.41
20:B5:2329:G:H2'	20:B5:2330:G:C8	2.55	0.41
20:B5:3519:G:H21	20:B5:3521:C:H42	1.68	0.41
20:B5:3665:G:H2'	20:B5:3666:G:H8	1.85	0.41
20:B5:3972:G:H2'	20:B5:3973:OMU:H6	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:BJ:89:VAL:HG21	43:BJ:115:LEU:HD23	2.02	0.41
56:DB:296:LEU:N	56:DB:297:PRO:HD2	2.35	0.41
64:A2:197:U:H2'	64:A2:198:U:C6	2.56	0.41
64:A2:462:U:H2'	64:A2:463:OMC:H6	1.85	0.41
64:A2:640:C:OP1	76:AD:114:ARG:NH2	2.53	0.41
64:A2:865:A:H2'	64:A2:866:A:C8	2.53	0.41
74:Al:55:ASN:OD1	74:Al:55:ASN:N	2.52	0.41
80:An:40:THR:HG21	80:An:74:ALA:HB2	2.01	0.41
90:Bt:147:HIS:NE2	90:Bt:150:ASP:OD1	2.54	0.41
9:BA:47:ASP:OD1	9:BA:48:ILE:N	2.54	0.41
11:At:36:ILE:HG12	11:At:114:VAL:HG21	2.03	0.41
20:B5:156:G:OP2	58:Bh:106:LYS:NZ	2.52	0.41
20:B5:477:C:H2'	20:B5:478:G:C8	2.55	0.41
20:B5:1208:C:H2'	20:B5:1209:G:C8	2.55	0.41
20:B5:1489:A2M:N3	66:Bj:11:ARG:HB2	2.35	0.41
20:B5:1729:U:C5	94:B5:5066:SPD:H72	2.55	0.41
20:B5:2244:A2M:HM'2	20:B5:2245:G:O5'	2.19	0.41
20:B5:3992:G:H2'	20:B5:3993:G:H8	1.86	0.41
94:B5:5257:SPD:H21	21:BQ:181:ARG:HB3	2.02	0.41
24:BF:59:GLU:OE1	24:BF:191:HIS:NE2	2.53	0.41
24:BF:94:ILE:HD13	24:BF:140:ALA:HB2	2.02	0.41
28:Ay:64:ASN:HD22	28:Ay:114:LYS:HE2	1.86	0.41
29:BG:159:HIS:CD2	29:BG:185:LYS:HG2	2.56	0.41
32:Aa:147:ASN:OD1	32:Aa:148:ASN:N	2.52	0.41
38:BI:38:ARG:NH2	38:BI:83:ASP:O	2.40	0.41
45:Ad:80:ILE:HG13	45:Ad:81:THR:HG23	2.03	0.41
54:Bg:41:ALA:O	54:Bg:52:ARG:NH1	2.52	0.41
55:BM:36:ALA:HB2	55:BM:52:PHE:CZ	2.55	0.41
59:BN:120:TRP:HE1	59:BN:123:GLU:HB3	1.85	0.41
64:A2:668:U:O4	64:A2:1144:A:N6	2.53	0.41
64:A2:1671:C:H2'	64:A2:1672:G:C8	2.55	0.41
67:AA:23:ARG:HH12	67:AA:29:ASN:HD21	1.67	0.41
3:B7:34:C:N3	3:B7:46:C:O2'	2.51	0.41
5:Ar:59:LEU:HD23	5:Ar:64:VAL:HG22	2.03	0.41
19:BE:246:THR:HG22	19:BE:248:GLN:H	1.85	0.41
20:B5:311:G:H2'	20:B5:312:G:C8	2.54	0.41
20:B5:1487:G:N2	20:B5:1592:A:OP2	2.33	0.41
20:B5:1698:G:H2'	20:B5:1699:G:C8	2.56	0.41
20:B5:2245:G:H1'	54:Bg:12:SER:HB3	2.02	0.41
20:B5:2387:G:H4'	20:B5:2389:G:N7	2.35	0.41
20:B5:2539:A:H62	69:Bk:35:LYS:NZ	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B5:2613:C:H2'	20:B5:2614:G:H8	1.84	0.41
20:B5:3834:G:H1'	20:B5:3835:G:C8	2.55	0.41
20:B5:4340:U:H2'	20:B5:4341:G:C8	2.55	0.41
22:Ba:71:PRO:HG2	22:Ba:108:TYR:HA	2.01	0.41
23:Ax:120:THR:OG1	64:A2:151:C:OP1	2.24	0.41
26:BW:102:LYS:HG2	26:BW:105:ARG:NH2	2.35	0.41
40:EA:269:TYR:HB3	40:EA:306:VAL:HG22	2.02	0.41
49:Ae:83:ASN:HD22	64:A2:1652:A:H1'	1.84	0.41
56:DB:326:PHE:O	56:DB:330:ARG:HG3	2.21	0.41
61:Ah:56:ARG:NH2	64:A2:381:G:OP1	2.54	0.41
64:A2:509:A:H2'	64:A2:510:OMG:O4'	2.21	0.41
64:A2:521:A:H2'	64:A2:522:A:H8	1.84	0.41
64:A2:1014:U:OP1	64:A2:1130:G:O2'	2.38	0.41
64:A2:1256:G:OP1	64:A2:1257:G:O2'	2.28	0.41
64:A2:1375:C:O2'	64:A2:1465:C:O2	2.33	0.41
64:A2:1806:G:H2'	64:A2:1807:A:C8	2.55	0.41
6:B8:101:C:O2'	66:Bj:20:ARG:O	2.33	0.41
20:B5:126:C:OP1	58:Bh:78:TYR:OH	2.39	0.41
20:B5:1939:G:O2'	20:B5:1940:G:N7	2.51	0.41
20:B5:3817:G:H2'	20:B5:3818:G:C8	2.56	0.41
20:B5:4283:C:H2'	20:B5:4284:G:H8	1.86	0.41
20:B5:4666:G:N2	20:B5:4666:G:OP2	2.54	0.41
26:BW:60:LYS:O	26:BW:64:SER:OG	2.32	0.41
44:Ct:207:VAL:HG13	56:DB:73:LEU:HD12	2.01	0.41
46:Be:104:SER:O	46:Be:108:ARG:HG3	2.20	0.41
56:DB:496:LYS:HZ3	56:DB:564:ILE:HD12	1.86	0.41
73:AC:118:ARG:NH1	73:AC:134:SER:OG	2.54	0.41
6:B8:75:OMG:HM22	6:B8:76:C:H5'	2.02	0.41
20:B5:664:G:H2'	20:B5:665:G:C8	2.54	0.41
20:B5:772:C:H2'	20:B5:773:G:H8	1.86	0.41
40:EA:146:ALA:HA	40:EA:223:LEU:HD13	2.03	0.41
40:EA:336:GLN:HB3	40:EA:349:ARG:HD3	2.01	0.41
44:Ct:77:ARG:HH21	44:Ct:123:PHE:HB3	1.85	0.41
55:BM:108:ASP:HB3	63:BO:199:HIS:CD2	2.56	0.41
64:A2:1865:U:H3'	79:AE:5:ARG:HH21	1.85	0.41
80:An:39:ASP:OD1	80:An:40:THR:N	2.53	0.41
6:B8:28:C:O2'	20:B5:1315:A:N1	2.52	0.41
20:B5:32:G:H21	20:B5:50:C:H5	1.69	0.41
20:B5:260:C:H2'	20:B5:261:G:H8	1.85	0.41
20:B5:1089:G:H2'	20:B5:1091:G:H8	1.86	0.41
20:B5:1285:U:H2'	20:B5:1286:A:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B5:1726:A:H4'	94:B5:5066:SPD:H21	2.01	0.41
20:B5:4667:C:H4'	55:BM:117:LYS:HE2	2.03	0.41
34:BH:59:LYS:HE2	34:BH:66:GLU:HB3	2.02	0.41
48:Cu:79:VAL:HG22	48:Cu:90:ILE:HG23	2.02	0.41
56:DB:676:LEU:HA	56:DB:679:PHE:CD2	2.56	0.41
61:Ah:123:ARG:NH1	61:Ah:133:GLU:OE1	2.40	0.41
64:A2:192:C:H4'	64:A2:192:C:OP1	2.20	0.41
64:A2:1632:U:O4	64:A2:1633:G:N1	2.54	0.41
64:A2:1857:C:H2'	64:A2:1858:G:C8	2.55	0.41
65:Ai:29:LEU:HD23	76:AD:116:PHE:HE2	1.85	0.41
5:Ar:120:HIS:CE1	5:Ar:124:ARG:HD2	2.55	0.41
16:BP:19:GLY:N	16:BP:146:ILE:O	2.53	0.41
20:B5:772:C:H2'	20:B5:773:G:C8	2.56	0.41
20:B5:1250:C:H2'	20:B5:1251:A:C8	2.56	0.41
20:B5:2323:G:H2'	20:B5:2324:G:H8	1.85	0.41
20:B5:3680:C:H2'	20:B5:3681:A:O4'	2.21	0.41
20:B5:4758:A:H2'	20:B5:4759:G:C8	2.56	0.41
32:Aa:123:ALA:HB2	32:Aa:165:ARG:HG3	2.03	0.41
35:BS:74:ARG:HH21	35:BS:76:LYS:HD3	1.85	0.41
41:Ac:68:GLU:HG3	68:Aj:93:THR:HG21	2.03	0.41
46:Be:37:LYS:HD2	46:Be:38:PRO:HD2	2.03	0.41
56:DB:482:MET:HE2	60:DC:25:ASN:HB2	2.03	0.41
64:A2:1222:G:H2'	64:A2:1223:G:C8	2.56	0.41
69:Bk:26:LYS:HB2	69:Bk:69:LEU:HD12	2.02	0.41
85:AG:33:LYS:HE2	85:AG:34:TYR:CZ	2.56	0.41
4:AT:74:C:H3'	38:BI:110:ARG:HH22	1.86	0.41
6:B8:102:G:OP2	6:B8:104:A:O2'	2.35	0.41
9:BA:83:HIS:CE1	9:BA:86:GLN:HB2	2.56	0.41
9:BA:168:VAL:HG13	81:Bp:79:VAL:HG11	2.03	0.41
10:BV:19:GLY:O	20:B5:2689:G:O2'	2.35	0.41
11:At:94:ASP:OD1	85:AG:54:LYS:NZ	2.40	0.41
15:BC:195:LYS:NZ	20:B5:2177:C:OP2	2.51	0.41
19:BE:167:PHE:HA	19:BE:178:VAL:HG12	2.03	0.41
20:B5:102:G:N7	98:B5:5802:HOH:O	2.37	0.41
20:B5:1016:C:O2'	20:B5:1059:G:O4'	2.38	0.41
20:B5:1524:U:H2'	20:B5:1525:G:C8	2.55	0.41
20:B5:1548:A:H5''	20:B5:2682:U:H5''	2.03	0.41
20:B5:1984:G:O6	20:B5:3602:C:O2'	2.37	0.41
20:B5:2216:C:H5'	42:Bd:46:LEU:HD22	2.03	0.41
20:B5:2383:C:H2'	20:B5:2384:G:C8	2.55	0.41
20:B5:2739:G:OP1	31:BR:136:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B5:3517:A2M:HM'1	20:B5:4283:C:H1'	2.03	0.41
20:B5:4006:U:H2'	20:B5:4007:C:C6	2.56	0.41
20:B5:4156:G:H2'	20:B5:4157:G:H8	1.85	0.41
20:B5:4269:A2M:HM'3	20:B5:4305:A:N7	2.36	0.41
23:Ax:80:ASP:OD1	23:Ax:81:TYR:N	2.53	0.41
35:BS:162:GLN:HB3	63:BO:122:ALA:HA	2.03	0.41
40:EA:297:HIS:CE1	40:EA:302:THR:HG21	2.56	0.41
41:Ac:34:TYR:CE1	41:Ac:37:VAL:HG13	2.56	0.41
42:Bd:23:ARG:NE	42:Bd:25:TYR:OH	2.43	0.41
46:Be:124:ASN:OD1	46:Be:124:ASN:N	2.54	0.41
51:BL:87:HIS:HB3	51:BL:90:VAL:HG23	2.02	0.41
52:DA:90:THR:HG23	52:DA:127:PHE:CZ	2.56	0.41
53:Af:137:ARG:HD3	53:Af:178:ARG:NH2	2.36	0.41
55:BM:88:ALA:O	55:BM:93:LYS:NZ	2.53	0.41
56:DB:56:LEU:HB2	56:DB:65:ALA:HB2	2.02	0.41
56:DB:175:ARG:CZ	56:DB:193:LEU:HD23	2.51	0.41
56:DB:187:TYR:HE2	60:DC:102:PHE:HA	1.86	0.41
56:DB:326:PHE:O	56:DB:330:ARG:N	2.53	0.41
56:DB:794:LEU:H	56:DB:797:ARG:NH1	2.18	0.41
59:BN:9:GLU:HB2	62:Bi:44:ILE:HG13	2.03	0.41
60:DC:71:HIS:ND1	60:DC:108:SER:O	2.50	0.41
62:Bi:70:LEU:HD21	62:Bi:80:HIS:HE1	1.86	0.41
64:A2:643:U:H4'	64:A2:645:OMG:H4'	2.03	0.41
64:A2:700:C:H2'	64:A2:701:G:C8	2.56	0.41
64:A2:1093:G:H2'	64:A2:1094:A:H8	1.86	0.41
64:A2:1294:A:N3	73:AC:138:ARG:NH1	2.68	0.41
64:A2:1373:U:P	64:A2:1386:G:H22	2.42	0.41
65:Ai:63:LEU:HD11	65:Ai:69:ARG:NH2	2.36	0.41
79:AE:33:ASP:OD1	79:AE:33:ASP:N	2.53	0.41
9:BA:30:ARG:NH1	9:BA:36:GLU:OE2	2.51	0.41
10:BV:14:PHE:HE2	12:BB:66:LYS:HB2	1.86	0.41
15:BC:133:LEU:HD13	84:Br:6:GLN:HE21	1.86	0.41
20:B5:162:A:H2'	20:B5:163:A:C8	2.55	0.41
20:B5:320:C:OP1	62:Bi:84:LYS:NZ	2.33	0.41
20:B5:1288:C:H2'	20:B5:1289:A:C8	2.56	0.41
20:B5:1868:A:C8	20:B5:1871:A:H1'	2.56	0.41
20:B5:2301:C:H5''	59:BN:67:ARG:HD2	2.03	0.41
20:B5:3996:G:OP1	43:BJ:97:ASN:ND2	2.54	0.41
20:B5:4099:PSU:H5'	20:B5:4100:U:H5'	2.02	0.41
20:B5:4297:U:H2'	20:B5:4298:PSU:C6	2.56	0.41
20:B5:4511:A:C2	34:BH:60:TRP:HD1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B5:4805:U:H2'	20:B5:4806:U:C6	2.56	0.41
25:BY:134:LYS:HE3	25:BY:134:LYS:HB3	1.94	0.41
29:BG:137:ARG:HA	29:BG:137:ARG:HH11	1.85	0.41
41:Ac:134:CYS:SG	41:Ac:135:GLU:N	2.94	0.41
44:Ct:105:VAL:HB	44:Ct:127:LYS:HD2	2.02	0.41
46:Be:100:ALA:HB3	46:Be:103:VAL:HG23	2.03	0.41
49:Ae:43:GLU:H	49:Ae:43:GLU:CD	2.28	0.41
53:Af:15:LEU:HD22	64:A2:155:G:H4'	2.01	0.41
56:DB:292:VAL:N	56:DB:293:PRO:HD2	2.36	0.41
57:Ag:88:SER:OG	57:Ag:89:GLY:N	2.52	0.41
57:Ag:116:ARG:NH2	64:A2:689:U:OP1	2.54	0.41
64:A2:445:G:N2	64:A2:447:G:H3'	2.36	0.41
64:A2:656:A:H4'	64:A2:657:G:H3'	2.03	0.41
64:A2:867:PSU:H2'	64:A2:868:OMG:C8	2.55	0.41
64:A2:1732:A:H2'	64:A2:1733:G:C8	2.55	0.41
82:AF:109:LEU:HD21	82:AF:125:ARG:CZ	2.50	0.41
8:As:23:LYS:HZ1	8:As:51:ASN:HB3	1.85	0.40
8:As:71:GLY:O	8:As:75:MET:HG2	2.21	0.40
12:BB:224:LYS:NZ	20:B5:4413:C:OP1	2.36	0.40
14:Au:39:VAL:HG11	27:AZ:8:LEU:HD11	2.03	0.40
16:BP:40:HIS:CE1	16:BP:157:VAL:HB	2.56	0.40
17:BZ:22:LYS:NZ	17:BZ:129:TRP:O	2.48	0.40
20:B5:522:U:H2'	20:B5:523:C:C6	2.57	0.40
20:B5:693:C:H2'	20:B5:694:G:H8	1.85	0.40
20:B5:1214:A:H61	20:B5:2054:G:H21	1.69	0.40
20:B5:1276:C:H2'	20:B5:1277:A:C8	2.56	0.40
20:B5:2727:G:H2'	20:B5:2728:A:C8	2.56	0.40
20:B5:2727:G:H2'	20:B5:2728:A:H8	1.86	0.40
20:B5:3557:A2M:O5'	20:B5:3557:A2M:H8	2.20	0.40
20:B5:3640:A:N7	20:B5:4195:A:N6	2.69	0.40
35:BS:127:MET:HA	88:BT:153:PRO:HD2	2.03	0.40
36:Ab:252:THR:OG1	36:Ab:254:ASP:OD1	2.33	0.40
37:Bc:99:PRO:HG3	37:Bc:105:ILE:HG13	2.04	0.40
41:Ac:176:LEU:HD13	64:A2:1500:U:H4'	2.02	0.40
49:Ae:40:ALA:HB1	49:Ae:45:TYR:CG	2.55	0.40
53:Af:164:LYS:NZ	64:A2:68:A:OP2	2.39	0.40
64:A2:1040:C:H2'	64:A2:1041:G:H8	1.86	0.40
65:Ai:61:LEU:HA	65:Ai:70:ARG:HH12	1.86	0.40
2:Bb:65:MET:HA	2:Bb:68:ARG:NH1	2.36	0.40
3:B7:74:A:N1	3:B7:100:A:H5''	2.36	0.40
20:B5:400:A2M:HM'2	20:B5:401:G:O5'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B5:1943:U:H3	20:B5:1954:U:H3	1.67	0.40
20:B5:2517:A:OP2	37:Bc:31:TYR:N	2.51	0.40
20:B5:2687:A:O2'	20:B5:4377:G:H4'	2.21	0.40
20:B5:4381:A:H3'	20:B5:4382:PSU:H4'	2.03	0.40
23:Ax:51:THR:OG1	23:Ax:53:ASP:OD1	2.29	0.40
24:BF:135:VAL:HG23	24:BF:139:ILE:HD13	2.02	0.40
37:Bc:17:ARG:HB3	37:Bc:104:ILE:HB	2.03	0.40
40:EA:107:ASP:N	40:EA:107:ASP:OD1	2.54	0.40
41:Ac:227:LYS:HD2	82:AF:184:LEU:HD23	2.02	0.40
45:Ad:211:LYS:NZ	45:Ad:215:GLY:O	2.45	0.40
51:BL:150:LEU:HD23	51:BL:154:VAL:HG22	2.02	0.40
53:Af:92:ARG:O	64:A2:454:C:O2'	2.32	0.40
56:DB:603:GLN:O	56:DB:607:GLN:HG3	2.21	0.40
59:BN:113:LEU:HB2	59:BN:134:LEU:HD23	2.03	0.40
61:Ah:142:SER:HB3	61:Ah:145:ILE:HG12	2.02	0.40
64:A2:1104:C:H2'	64:A2:1105:G:C8	2.57	0.40
64:A2:1737:G:H2'	64:A2:1738:G:C8	2.56	0.40
65:Ai:134:HIS:HD1	65:Ai:163:SER:HG	1.62	0.40
78:Bo:69:ARG:HG3	78:Bo:82:MET:HE1	2.04	0.40
82:AF:254:PRO:HD3	82:AF:285:GLN:HG3	2.02	0.40
90:Bt:147:HIS:CD2	90:Bt:149:HIS:HB2	2.55	0.40
20:B5:20:U:H3'	20:B5:21:G:H8	1.86	0.40
20:B5:1479:A2M:HM'2	20:B5:1480:A:O5'	2.21	0.40
20:B5:1635:G:P	98:B5:6097:HOH:O	2.80	0.40
20:B5:1968:A:H2'	20:B5:1969:A:C8	2.57	0.40
20:B5:3870:U:H3	20:B5:3887:G:H1	1.69	0.40
20:B5:3952:C:O2'	20:B5:4081:C:O2'	2.34	0.40
20:B5:4041:U:H2'	20:B5:4042:PSU:H6	1.86	0.40
30:Av:101:PHE:HA	30:Av:113:HIS:CE1	2.57	0.40
31:BR:139:MET:HG2	31:BR:143:HIS:CE1	2.57	0.40
39:B:116:ASP:OD1	39:B:116:ASP:N	2.52	0.40
43:BJ:152:GLY:O	43:BJ:156:ARG:HG3	2.21	0.40
45:Ad:126:VAL:HG22	45:Ad:139:LEU:HD21	2.04	0.40
45:Ad:186:GLY:HA3	64:A2:810:A:OP1	2.22	0.40
52:DA:8:LEU:HG	52:DA:91:LYS:HE3	2.03	0.40
56:DB:280:TYR:CE1	56:DB:296:LEU:HD13	2.55	0.40
56:DB:435:GLN:HE21	56:DB:448:CYS:HB2	1.86	0.40
56:DB:747:PRO:HA	56:DB:750:PHE:CD2	2.56	0.40
64:A2:282:C:N4	64:A2:892:G:O4'	2.55	0.40
64:A2:468:G:H2'	64:A2:469:A2M:H8	2.04	0.40
64:A2:1050:A:OP2	64:A2:1069:G:N1	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:A2:1760:G:H2'	64:A2:1761:G:C8	2.56	0.40
3:B7:61:G:O2'	39:B:279:ARG:NH1	2.52	0.40
6:B8:18:U:O2	20:B5:2152:G:O2'	2.39	0.40
12:BB:248:LEU:HD12	12:BB:249:ARG:HG3	2.04	0.40
17:BZ:125:GLY:HA3	29:BG:30:PRO:HB2	2.04	0.40
20:B5:260:C:H2'	20:B5:261:G:C8	2.57	0.40
20:B5:1285:U:H2'	20:B5:1286:A:C8	2.56	0.40
20:B5:1739:U:H2'	20:B5:1740:A:H8	1.86	0.40
20:B5:3601:OMC:C4	94:B5:5159:SPD:H52	2.57	0.40
30:Av:52:ILE:HB	57:Ag:144:ILE:HB	2.04	0.40
32:Aa:28:LYS:NZ	80:An:51:GLU:OE1	2.53	0.40
37:Bc:4:ALA:O	37:Bc:8:LYS:HG2	2.22	0.40
38:BI:36:LEU:HD22	38:BI:69:ARG:HD2	2.04	0.40
40:EA:237:PHE:HE1	40:EA:249:VAL:HG21	1.87	0.40
41:Ac:34:TYR:HE1	41:Ac:37:VAL:HG13	1.86	0.40
53:Af:126:ASP:OD1	53:Af:126:ASP:N	2.54	0.40
56:DB:448:CYS:O	56:DB:452:MET:HG2	2.21	0.40
97:DB:901:IHP:O25	97:DB:901:IHP:H4	2.21	0.40
64:A2:1409:U:H2'	64:A2:1410:A:C8	2.56	0.40
71:Ak:61:PRO:HD3	71:Ak:141:ASN:HD21	1.86	0.40
81:Bp:38:THR:HA	81:Bp:45:THR:HA	2.03	0.40
82:AF:268:ASP:OD1	82:AF:269:GLU:N	2.54	0.40
3:B7:4:U:H2'	3:B7:5:A:H8	1.86	0.40
5:Ar:124:ARG:NH1	83:Ao:123:TYR:OH	2.55	0.40
6:B8:113:C:OP2	20:B5:2621:G:N2	2.55	0.40
9:BA:177:LYS:HG3	81:Bp:26:VAL:HG23	2.04	0.40
12:BB:77:THR:HG21	12:BB:337:VAL:HG22	2.04	0.40
17:BZ:50:PRO:HD3	17:BZ:68:ILE:HG12	2.04	0.40
17:BZ:51:ARG:HB2	17:BZ:65:ARG:HB3	2.03	0.40
20:B5:323:C:H2'	20:B5:324:A:C8	2.56	0.40
20:B5:422:C:H2'	20:B5:423:G:C8	2.55	0.40
20:B5:1298:A:OP1	21:BQ:108:ARG:NH2	2.42	0.40
20:B5:1695:U:H2'	20:B5:1696:U:C6	2.57	0.40
20:B5:2451:G:H2'	20:B5:2452:G:H8	1.86	0.40
35:BS:141:ALA:O	35:BS:144:GLN:HG2	2.20	0.40
43:BJ:28:GLU:OE2	43:BJ:32:ARG:NH1	2.55	0.40
45:Ad:62:LYS:HE3	45:Ad:62:LYS:HB3	1.94	0.40
56:DB:556:LYS:NZ	97:DB:901:IHP:O42	2.54	0.40
56:DB:777:PRO:O	56:DB:780:GLN:HG3	2.20	0.40
64:A2:17:C:H2'	64:A2:18:C:C6	2.57	0.40
64:A2:653:U:H2'	64:A2:654:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:A2:1278:C:OP1	68:Aj:51:SER:OG	2.34	0.40
64:A2:1776:U:H2'	64:A2:1777:G:H8	1.86	0.40
68:Aj:86:PRO:HG2	68:Aj:89:ILE:HG13	2.04	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	Bb	103/245 (42%)	99 (96%)	4 (4%)	0	100	100
5	Ar	146/151 (97%)	144 (99%)	2 (1%)	0	100	100
7	BU	100/128 (78%)	99 (99%)	1 (1%)	0	100	100
8	As	140/145 (97%)	140 (100%)	0	0	100	100
9	BA	250/257 (97%)	241 (96%)	9 (4%)	0	100	100
10	BV	137/140 (98%)	136 (99%)	1 (1%)	0	100	100
11	At	102/119 (86%)	101 (99%)	1 (1%)	0	100	100
12	BB	395/403 (98%)	391 (99%)	4 (1%)	0	100	100
13	BX	116/156 (74%)	115 (99%)	1 (1%)	0	100	100
14	Au	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
15	BC	360/412 (87%)	356 (99%)	4 (1%)	0	100	100
16	BP	157/184 (85%)	156 (99%)	1 (1%)	0	100	100
17	BZ	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
18	Aw	138/143 (96%)	137 (99%)	1 (1%)	0	100	100
19	BE	239/291 (82%)	235 (98%)	4 (2%)	0	100	100
21	BQ	185/188 (98%)	183 (99%)	2 (1%)	0	100	100
22	Ba	144/148 (97%)	139 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	Ax	123/130 (95%)	123 (100%)	0	0	100	100
24	BF	224/247 (91%)	219 (98%)	5 (2%)	0	100	100
25	BY	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
26	BW	119/157 (76%)	119 (100%)	0	0	100	100
27	AZ	219/294 (74%)	216 (99%)	3 (1%)	0	100	100
28	Ay	83/124 (67%)	81 (98%)	2 (2%)	0	100	100
29	BG	229/266 (86%)	226 (99%)	3 (1%)	0	100	100
30	Av	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
31	BR	178/196 (91%)	178 (100%)	0	0	100	100
32	Aa	220/264 (83%)	218 (99%)	2 (1%)	0	100	100
33	Az	23/25 (92%)	23 (100%)	0	0	100	100
34	BH	188/192 (98%)	188 (100%)	0	0	100	100
35	BS	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
36	Ab	218/293 (74%)	217 (100%)	1 (0%)	0	100	100
37	Bc	106/115 (92%)	106 (100%)	0	0	100	100
38	BI	211/214 (99%)	209 (99%)	2 (1%)	0	100	100
39	B	293/297 (99%)	289 (99%)	4 (1%)	0	100	100
40	EA	315/386 (82%)	310 (98%)	4 (1%)	1 (0%)	36	67
41	Ac	223/281 (79%)	221 (99%)	2 (1%)	0	100	100
42	Bd	105/125 (84%)	105 (100%)	0	0	100	100
43	BJ	168/178 (94%)	167 (99%)	1 (1%)	0	100	100
44	Ct	112/238 (47%)	108 (96%)	4 (4%)	0	100	100
45	Ad	260/263 (99%)	258 (99%)	2 (1%)	0	100	100
46	Be	128/135 (95%)	127 (99%)	1 (1%)	0	100	100
48	Cu	104/162 (64%)	99 (95%)	5 (5%)	0	100	100
49	Ae	189/204 (93%)	188 (100%)	1 (0%)	0	100	100
50	Bf	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
51	BL	208/211 (99%)	205 (99%)	3 (1%)	0	100	100
52	DA	153/403 (38%)	152 (99%)	1 (1%)	0	100	100
53	Af	235/249 (94%)	234 (100%)	1 (0%)	0	100	100
54	Bg	112/117 (96%)	111 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	BM	136/218 (62%)	134 (98%)	2 (2%)	0	100	100
56	DB	835/915 (91%)	821 (98%)	14 (2%)	0	100	100
57	Ag	188/432 (44%)	185 (98%)	3 (2%)	0	100	100
58	Bh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
59	BN	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
60	DC	158/235 (67%)	156 (99%)	2 (1%)	0	100	100
61	Ah	204/208 (98%)	200 (98%)	4 (2%)	0	100	100
62	Bi	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
63	BO	197/203 (97%)	196 (100%)	1 (0%)	0	100	100
65	Ai	183/194 (94%)	181 (99%)	2 (1%)	0	100	100
66	Bj	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
67	AA	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
68	Aj	94/165 (57%)	91 (97%)	3 (3%)	0	100	100
69	Bk	67/70 (96%)	67 (100%)	0	0	100	100
70	AB	61/69 (88%)	61 (100%)	0	0	100	100
71	Ak	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
72	Bl	48/51 (94%)	48 (100%)	0	0	100	100
73	AC	72/156 (46%)	70 (97%)	2 (3%)	0	100	100
74	Al	122/132 (92%)	120 (98%)	2 (2%)	0	100	100
75	Bm	49/128 (38%)	49 (100%)	0	0	100	100
76	AD	55/133 (41%)	55 (100%)	0	0	100	100
77	Am	148/151 (98%)	147 (99%)	1 (1%)	0	100	100
78	Bo	102/106 (96%)	102 (100%)	0	0	100	100
79	AE	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
80	An	132/151 (87%)	130 (98%)	2 (2%)	0	100	100
81	Bp	89/92 (97%)	88 (99%)	1 (1%)	0	100	100
82	AF	311/317 (98%)	305 (98%)	6 (2%)	0	100	100
83	Ao	126/145 (87%)	124 (98%)	2 (2%)	0	100	100
84	Br	124/136 (91%)	123 (99%)	1 (1%)	0	100	100
85	AG	53/56 (95%)	53 (100%)	0	0	100	100
86	Ap	139/172 (81%)	133 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
87	Bs	194/318 (61%)	190 (98%)	4 (2%)	0	100	100
88	BT	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
89	Aq	132/135 (98%)	132 (100%)	0	0	100	100
90	Bt	154/165 (93%)	153 (99%)	1 (1%)	0	100	100
All	All	13380/15955 (84%)	13211 (99%)	168 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
40	EA	297	HIS

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	Bb	87/183 (48%)	87 (100%)	0	100	100
5	Ar	127/130 (98%)	125 (98%)	2 (2%)	55	68
7	BU	91/113 (80%)	89 (98%)	2 (2%)	45	63
8	As	112/114 (98%)	112 (100%)	0	100	100
9	BA	194/198 (98%)	194 (100%)	0	100	100
10	BV	106/107 (99%)	106 (100%)	0	100	100
11	At	94/107 (88%)	92 (98%)	2 (2%)	47	63
12	BB	344/347 (99%)	342 (99%)	2 (1%)	78	79
13	BX	106/134 (79%)	106 (100%)	0	100	100
14	Au	67/67 (100%)	66 (98%)	1 (2%)	57	69
15	BC	302/336 (90%)	302 (100%)	0	100	100
16	BP	140/163 (86%)	140 (100%)	0	100	100
17	BZ	117/118 (99%)	117 (100%)	0	100	100
18	Aw	112/114 (98%)	110 (98%)	2 (2%)	51	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	BE	216/251 (86%)	216 (100%)	0	100	100
21	BQ	164/165 (99%)	162 (99%)	2 (1%)	63	71
22	Ba	118/119 (99%)	118 (100%)	0	100	100
23	Ax	107/112 (96%)	106 (99%)	1 (1%)	70	74
24	BF	197/215 (92%)	197 (100%)	0	100	100
25	BY	124/135 (92%)	124 (100%)	0	100	100
26	BW	100/126 (79%)	99 (99%)	1 (1%)	68	74
27	AZ	182/242 (75%)	179 (98%)	3 (2%)	55	68
28	Ay	75/102 (74%)	75 (100%)	0	100	100
29	BG	199/223 (89%)	196 (98%)	3 (2%)	57	69
30	Av	112/113 (99%)	111 (99%)	1 (1%)	70	74
31	BR	159/175 (91%)	159 (100%)	0	100	100
32	Aa	203/231 (88%)	201 (99%)	2 (1%)	68	74
33	Az	24/24 (100%)	24 (100%)	0	100	100
34	BH	169/171 (99%)	169 (100%)	0	100	100
35	BS	154/154 (100%)	154 (100%)	0	100	100
36	Ab	185/223 (83%)	184 (100%)	1 (0%)	81	81
37	Bc	92/98 (94%)	91 (99%)	1 (1%)	65	73
38	BI	180/181 (99%)	178 (99%)	2 (1%)	65	73
39	B	247/250 (99%)	247 (100%)	0	100	100
40	EA	274/330 (83%)	274 (100%)	0	100	100
41	Ac	189/232 (82%)	188 (100%)	1 (0%)	81	81
42	Bd	98/110 (89%)	98 (100%)	0	100	100
43	BJ	143/149 (96%)	143 (100%)	0	100	100
44	Ct	100/202 (50%)	99 (99%)	1 (1%)	68	74
45	Ad	224/225 (100%)	224 (100%)	0	100	100
46	Be	116/121 (96%)	116 (100%)	0	100	100
48	Cu	90/136 (66%)	89 (99%)	1 (1%)	65	73
49	Ae	161/170 (95%)	161 (100%)	0	100	100
50	Bf	89/89 (100%)	89 (100%)	0	100	100
51	BL	175/176 (99%)	174 (99%)	1 (1%)	78	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	DA	137/355 (39%)	135 (98%)	2 (2%)	57	69
53	Af	207/218 (95%)	206 (100%)	1 (0%)	81	81
54	Bg	98/100 (98%)	98 (100%)	0	100	100
55	BM	117/161 (73%)	117 (100%)	0	100	100
56	DB	746/806 (93%)	731 (98%)	15 (2%)	48	64
57	Ag	170/360 (47%)	169 (99%)	1 (1%)	78	79
58	Bh	109/110 (99%)	109 (100%)	0	100	100
59	BN	171/172 (99%)	171 (100%)	0	100	100
60	DC	136/202 (67%)	134 (98%)	2 (2%)	57	69
61	Ah	178/180 (99%)	176 (99%)	2 (1%)	65	73
62	Bi	86/89 (97%)	86 (100%)	0	100	100
63	BO	171/173 (99%)	169 (99%)	2 (1%)	63	71
65	Ai	161/168 (96%)	160 (99%)	1 (1%)	78	79
66	Bj	73/80 (91%)	73 (100%)	0	100	100
67	AA	75/76 (99%)	74 (99%)	1 (1%)	61	71
68	Aj	87/136 (64%)	86 (99%)	1 (1%)	65	73
69	Bk	64/65 (98%)	63 (98%)	1 (2%)	55	68
70	AB	56/62 (90%)	54 (96%)	2 (4%)	31	53
71	Ak	139/142 (98%)	138 (99%)	1 (1%)	76	77
72	Bl	47/48 (98%)	47 (100%)	0	100	100
73	AC	67/140 (48%)	67 (100%)	0	100	100
74	Al	104/108 (96%)	102 (98%)	2 (2%)	50	65
75	Bm	47/115 (41%)	47 (100%)	0	100	100
76	AD	47/106 (44%)	47 (100%)	0	100	100
77	Am	130/131 (99%)	130 (100%)	0	100	100
78	Bo	92/93 (99%)	92 (100%)	0	100	100
79	AE	88/98 (90%)	86 (98%)	2 (2%)	44	62
80	An	105/118 (89%)	104 (99%)	1 (1%)	68	74
81	Bp	74/75 (99%)	73 (99%)	1 (1%)	59	70
82	AF	272/275 (99%)	270 (99%)	2 (1%)	76	77
83	Ao	114/130 (88%)	114 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
84	Br	109/119 (92%)	109 (100%)	0	100	100
85	AG	48/49 (98%)	48 (100%)	0	100	100
86	Ap	117/140 (84%)	117 (100%)	0	100	100
87	Bs	164/258 (64%)	163 (99%)	1 (1%)	78	79
88	BT	139/140 (99%)	139 (100%)	0	100	100
89	Aq	120/121 (99%)	118 (98%)	2 (2%)	53	67
90	Bt	128/137 (93%)	122 (95%)	6 (5%)	23	47
All	All	11658/13537 (86%)	11577 (99%)	81 (1%)	73	77

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	Ar	94	LYS
5	Ar	103	LEU
7	BU	95	ASN
7	BU	117	ILE
11	At	70	VAL
11	At	84	THR
12	BB	39	LYS
12	BB	340	THR
14	Au	42	VAL
18	Aw	105	PHE
18	Aw	125	VAL
21	BQ	82	VAL
21	BQ	115	LYS
23	Ax	7	ILE
26	BW	68	GLN
27	AZ	112	ILE
27	AZ	121	LEU
27	AZ	206	ASP
29	BG	106	THR
29	BG	159	HIS
29	BG	220	GLU
30	Av	105	THR
32	Aa	9	LEU
32	Aa	178	THR
36	Ab	121	ARG
37	Bc	94	LEU
38	BI	31	ILE
38	BI	129	VAL

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Mol	Chain	Res	Type
41	Ac	46	THR
44	Ct	190	VAL
48	Cu	9	GLU
51	BL	115	GLN
52	DA	22	LEU
52	DA	74	ILE
53	Af	44	GLU
56	DB	120	LEU
56	DB	141	LEU
56	DB	170	ILE
56	DB	210	LEU
56	DB	296	LEU
56	DB	373	LEU
56	DB	401	ILE
56	DB	444	ILE
56	DB	534	THR
56	DB	547	VAL
56	DB	592	LEU
56	DB	662	THR
56	DB	683	PHE
56	DB	762	LEU
56	DB	784	ILE
57	Ag	53	VAL
60	DC	22	LEU
60	DC	107	VAL
61	Ah	29	LEU
61	Ah	46	VAL
63	BO	126	VAL
63	BO	174	LEU
65	Ai	55	LYS
67	AA	74	THR
68	Aj	40	VAL
69	Bk	36	VAL
70	AB	14	VAL
70	AB	50	VAL
71	Ak	76	VAL
74	Al	75	ASN
74	Al	104	VAL
79	AE	40	VAL
79	AE	75	VAL
80	An	21	VAL
81	Bp	52	VAL

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Mol	Chain	Res	Type
82	AF	113	PHE
82	AF	159	ASN
87	Bs	78	LEU
89	Aq	38	ILE
89	Aq	73	LEU
90	Bt	12	VAL
90	Bt	15	LEU
90	Bt	22	VAL
90	Bt	35	LEU
90	Bt	73	VAL
90	Bt	74	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (157) such sidechains are listed below:

Mol	Chain	Res	Type
2	Bb	50	ASN
7	BU	17	GLN
7	BU	118	ASN
8	As	12	GLN
9	BA	97	ASN
9	BA	140	ASN
9	BA	205	ASN
11	At	97	GLN
12	BB	184	GLN
12	BB	289	GLN
13	BX	111	GLN
14	Au	2	GLN
15	BC	48	ASN
15	BC	50	GLN
15	BC	61	GLN
15	BC	89	GLN
15	BC	119	GLN
15	BC	212	ASN
15	BC	276	ASN
15	BC	299	GLN
15	BC	310	HIS
15	BC	329	ASN
16	BP	75	GLN
16	BP	120	ASN
17	BZ	127	ASN
19	BE	131	HIS
19	BE	269	GLN

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Mol	Chain	Res	Type
21	BQ	125	GLN
22	Ba	14	HIS
22	Ba	19	HIS
22	Ba	28	HIS
22	Ba	34	ASN
22	Ba	60	HIS
23	Ax	89	HIS
24	BF	57	HIS
24	BF	204	ASN
25	BY	61	HIS
26	BW	68	GLN
26	BW	120	GLN
27	AZ	113	GLN
27	AZ	169	HIS
28	Ay	64	ASN
28	Ay	112	ASN
29	BG	64	GLN
29	BG	81	ASN
29	BG	141	ASN
30	Av	82	GLN
30	Av	91	ASN
31	BR	40	GLN
32	Aa	76	ASN
32	Aa	186	ASN
34	BH	39	ASN
36	Ab	178	HIS
37	Bc	40	GLN
38	BI	59	GLN
38	BI	73	ASN
38	BI	163	GLN
39	B	111	ASN
39	B	122	GLN
39	B	202	GLN
39	B	275	GLN
39	B	282	GLN
40	EA	218	ASN
40	EA	233	ASN
40	EA	258	GLN
40	EA	281	GLN
41	Ac	4	GLN
41	Ac	145	GLN
42	Bd	116	ASN

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Mol	Chain	Res	Type
43	BJ	97	ASN
44	Ct	202	ASN
45	Ad	98	ASN
45	Ad	142	HIS
45	Ad	157	ASN
46	Be	34	ASN
46	Be	68	HIS
48	Cu	15	GLN
49	Ae	65	GLN
49	Ae	118	ASN
50	Bf	21	GLN
50	Bf	56	ASN
51	BL	19	GLN
51	BL	149	GLN
52	DA	18	GLN
52	DA	24	GLN
52	DA	52	ASN
52	DA	65	HIS
53	Af	56	ASN
53	Af	163	ASN
54	Bg	114	GLN
55	BM	33	GLN
55	BM	34	ASN
55	BM	125	ASN
56	DB	196	GLN
56	DB	219	GLN
56	DB	251	GLN
56	DB	362	ASN
56	DB	377	GLN
56	DB	456	ASN
56	DB	526	HIS
56	DB	551	HIS
56	DB	569	HIS
56	DB	577	ASN
56	DB	597	ASN
56	DB	603	GLN
56	DB	705	HIS
56	DB	749	ASN
56	DB	764	HIS
56	DB	798	ASN
57	Ag	91	HIS
59	BN	37	HIS

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Mol	Chain	Res	Type
59	BN	117	ASN
60	DC	18	ASN
60	DC	25	ASN
60	DC	93	GLN
60	DC	153	GLN
61	Ah	7	ASN
61	Ah	167	GLN
63	BO	167	HIS
63	BO	180	GLN
66	Bj	30	GLN
66	Bj	66	HIS
67	AA	29	ASN
67	AA	51	GLN
68	Aj	50	GLN
68	Aj	77	GLN
69	Bk	58	GLN
71	Ak	11	GLN
71	Ak	18	GLN
71	Ak	108	ASN
72	Bl	25	GLN
74	Al	72	HIS
76	AD	89	GLN
77	Am	36	GLN
77	Am	58	HIS
78	Bo	102	GLN
79	AE	72	HIS
82	AF	159	ASN
82	AF	196	ASN
82	AF	222	ASN
83	Ao	137	HIS
84	Br	4	HIS
84	Br	6	GLN
85	AG	3	HIS
86	Ap	11	GLN
86	Ap	24	HIS
86	Ap	80	GLN
86	Ap	97	GLN
86	Ap	114	GLN
87	Bs	34	ASN
87	Bs	39	GLN
87	Bs	41	GLN
87	Bs	190	GLN

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Mol	Chain	Res	Type
89	Aq	31	ASN
89	Aq	74	GLN
90	Bt	70	GLN
90	Bt	100	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AH	0/3	-	-
20	B5	3694/4808 (76%)	433 (11%)	2 (0%)
3	B7	118/120 (98%)	7 (5%)	0
4	AT	2/76 (2%)	1 (50%)	0
6	B8	155/158 (98%)	16 (10%)	0
64	A2	1764/1870 (94%)	211 (11%)	0
All	All	5733/7035 (81%)	668 (11%)	2 (0%)

All (668) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	B7	7	G
3	B7	53	U
3	B7	54	A
3	B7	63	C
3	B7	64	G
3	B7	110	G
3	B7	120	U
4	AT	76	A
6	B8	34	U
6	B8	35	C
6	B8	39	G
6	B8	59	A
6	B8	62	A
6	B8	63	U
6	B8	81	C
6	B8	84	A
6	B8	87	G
6	B8	94	G
6	B8	103	A
6	B8	105	C
6	B8	110	U
6	B8	114	G

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Mol	Chain	Res	Type
6	B8	150	C
6	B8	156	U
20	B5	25	A
20	B5	39	A
20	B5	42	A
20	B5	58	G
20	B5	59	A
20	B5	64	A
20	B5	65	A
20	B5	76	A
20	B5	85	G
20	B5	91	G
20	B5	98	A
20	B5	109	G
20	B5	110	C
20	B5	119	G
20	B5	122	U
20	B5	127	G
20	B5	135	G
20	B5	136	U
20	B5	144	G
20	B5	159	C
20	B5	181	C
20	B5	184	U
20	B5	187	U
20	B5	188	G
20	B5	197	A
20	B5	200	U
20	B5	201	C
20	B5	209	U
20	B5	210	C
20	B5	216	C
20	B5	218	A
20	B5	219	G
20	B5	234	G
20	B5	266	C
20	B5	268	G
20	B5	297	U
20	B5	309	C
20	B5	315	G
20	B5	316	U
20	B5	326	C

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Mol	Chain	Res	Type
20	B5	334	A
20	B5	340	C
20	B5	363	A
20	B5	386	A
20	B5	387	G
20	B5	398	A2M
20	B5	409	G
20	B5	412	G
20	B5	413	G
20	B5	440	U
20	B5	446	C
20	B5	449	C
20	B5	450	G
20	B5	452	A
20	B5	453	G
20	B5	454	U
20	B5	455	C
20	B5	482	U
20	B5	483	G
20	B5	485	U
20	B5	486	C
20	B5	488	G
20	B5	493	U
20	B5	497	G
20	B5	499	C
20	B5	502	U
20	B5	503	C
20	B5	504	U
20	B5	505	C
20	B5	512	U
20	B5	515	U
20	B5	516	U
20	B5	517	C
20	B5	628	U
20	B5	634	C
20	B5	635	G
20	B5	660	G
20	B5	661	A
20	B5	691	G
20	B5	698	C
20	B5	724	G
20	B5	725	G

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Mol	Chain	Res	Type
20	B5	732	C
20	B5	734	G
20	B5	739	G
20	B5	758	C
20	B5	760	C
20	B5	790	G
20	B5	791	C
20	B5	792	G
20	B5	794	G
20	B5	797	C
20	B5	798	C
20	B5	810	U
20	B5	812	A
20	B5	814	A
20	B5	815	G
20	B5	824	C
20	B5	825	G
20	B5	831	A
20	B5	832	G
20	B5	833	C
20	B5	834	A
20	B5	835	G
20	B5	844	A
20	B5	845	U
20	B5	856	A
20	B5	859	G
20	B5	860	A
20	B5	861	G
20	B5	866	A
20	B5	867	C
20	B5	868	C
20	B5	869	U
20	B5	870	G
20	B5	884	U
20	B5	983	G
20	B5	985	G
20	B5	987	C
20	B5	1072	C
20	B5	1073	C
20	B5	1074	C
20	B5	1090	U
20	B5	1091	G

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Mol	Chain	Res	Type
20	B5	1102	G
20	B5	1105	C
20	B5	1106	U
20	B5	1124	A
20	B5	1133	C
20	B5	1140	C
20	B5	1202	C
20	B5	1214	A
20	B5	1215	G
20	B5	1217	G
20	B5	1219	G
20	B5	1221	G
20	B5	1228	G
20	B5	1231	G
20	B5	1239	U
20	B5	1240	G
20	B5	1246	U
20	B5	1247	A
20	B5	1270	A2M
20	B5	1298	A
20	B5	1299	G
20	B5	1303	G
20	B5	1309	C
20	B5	1310	G
20	B5	1323	C
20	B5	1331	A
20	B5	1341	A
20	B5	1351	G
20	B5	1362	C
20	B5	1375	A
20	B5	1391	C
20	B5	1393	C
20	B5	1452	A
20	B5	1453	G
20	B5	1457	G
20	B5	1459	G
20	B5	1469	U
20	B5	1489	A2M
20	B5	1502	A
20	B5	1521	C
20	B5	1533	U
20	B5	1546	U

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Mol	Chain	Res	Type
20	B5	1551	U
20	B5	1568	A
20	B5	1579	G
20	B5	1580	OMG
20	B5	1586	A
20	B5	1588	G
20	B5	1589	A
20	B5	1605	A
20	B5	1609	G
20	B5	1616	C
20	B5	1631	C
20	B5	1632	PSU
20	B5	1653	C
20	B5	1657	C
20	B5	1658	C
20	B5	1704	A
20	B5	1705	A
20	B5	1726	A
20	B5	1743	A
20	B5	1754	G
20	B5	1774	G
20	B5	1775	G
20	B5	1776	A
20	B5	1781	G
20	B5	1794	G
20	B5	1808	G
20	B5	1836	A
20	B5	1857	U
20	B5	1859	C
20	B5	1860	C
20	B5	1861	G
20	B5	1870	C
20	B5	1871	A
20	B5	1879	G
20	B5	1887	G
20	B5	1898	U
20	B5	1899	A
20	B5	1900	G
20	B5	1913	U
20	B5	1922	A
20	B5	1923	A
20	B5	1924	G

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Mol	Chain	Res	Type
20	B5	1925	U
20	B5	1926	C
20	B5	1936	U
20	B5	1940	G
20	B5	1942	G
20	B5	1943	U
20	B5	1963	G
20	B5	1965	A
20	B5	1973	G
20	B5	1985	G
20	B5	1987	U
20	B5	1994	G
20	B5	1995	G
20	B5	2008	A
20	B5	2023	U
20	B5	2032	G
20	B5	2034	A
20	B5	2037	G
20	B5	2041	G
20	B5	2044	A
20	B5	2045	G
20	B5	2046	A
20	B5	2101	C
20	B5	2132	C
20	B5	2143	A
20	B5	2144	G
20	B5	2156	A
20	B5	2174	G
20	B5	2191	G
20	B5	2194	OMC
20	B5	2203	A
20	B5	2238	A
20	B5	2253	C
20	B5	2264	G
20	B5	2268	U
20	B5	2332	C
20	B5	2333	U
20	B5	2334	C
20	B5	2349	G
20	B5	2356	A
20	B5	2372	A
20	B5	2380	A

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Mol	Chain	Res	Type
20	B5	2387	G
20	B5	2388	U
20	B5	2390	G
20	B5	2409	G
20	B5	2430	A
20	B5	2432	C
20	B5	2444	A
20	B5	2470	C
20	B5	2496	C
20	B5	2503	A
20	B5	2530	U
20	B5	2537	G
20	B5	2538	A
20	B5	2539	A
20	B5	2551	U
20	B5	2552	C
20	B5	2553	C
20	B5	2554	G
20	B5	2586	A
20	B5	2606	U
20	B5	2612	U
20	B5	2630	A2M
20	B5	2631	U
20	B5	2633	U
20	B5	2641	A
20	B5	2657	C
20	B5	2669	U
20	B5	2670	G
20	B5	2672	U
20	B5	2678	A
20	B5	2698	G
20	B5	2745	G
20	B5	3329	G
20	B5	3350	C
20	B5	3358	G
20	B5	3367	A
20	B5	3380	A
20	B5	3385	A
20	B5	3394	A
20	B5	3396	G
20	B5	3428	C
20	B5	3443	A

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Mol	Chain	Res	Type
20	B5	3444	A
20	B5	3485	G
20	B5	3492	A2M
20	B5	3493	C
20	B5	3498	A
20	B5	3508	G
20	B5	3509	G
20	B5	3516	A
20	B5	3543	G
20	B5	3546	U
20	B5	3549	A
20	B5	3551	G
20	B5	3570	U
20	B5	3571	G
20	B5	3572	U
20	B5	3600	G
20	B5	3609	A
20	B5	3610	C
20	B5	3611	G
20	B5	3629	G
20	B5	3633	A
20	B5	3638	A
20	B5	3639	G
20	B5	3640	A
20	B5	3647	U
20	B5	3670	G
20	B5	3671	G
20	B5	3804	G
20	B5	3823	G
20	B5	3824	C
20	B5	3825	G
20	B5	3832	G
20	B5	3833	A
20	B5	3834	G
20	B5	3847	C
20	B5	3849	G
20	B5	3850	G
20	B5	3855	A
20	B5	3869	G
20	B5	3875	C
20	B5	3891	C
20	B5	3892	G

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Mol	Chain	Res	Type
20	B5	3904	C
20	B5	3908	C
20	B5	3916	A
20	B5	3929	G
20	B5	3930	G
20	B5	3937	G
20	B5	3949	A
20	B5	3975	U
20	B5	3979	A
20	B5	3997	A
20	B5	4000	G
20	B5	4012	G
20	B5	4014	A
20	B5	4017	A
20	B5	4019	A
20	B5	4027	A
20	B5	4051	G
20	B5	4052	OMU
20	B5	4060	C
20	B5	4076	G
20	B5	4078	C
20	B5	4096	C
20	B5	4100	U
20	B5	4119	G
20	B5	4123	G
20	B5	4124	A
20	B5	4133	C
20	B5	4140	A
20	B5	4167	C
20	B5	4168	A
20	B5	4183	U
20	B5	4190	C
20	B5	4194	G
20	B5	4210	A
20	B5	4212	C
20	B5	4221	G
20	B5	4258	U
20	B5	4259	A
20	B5	4294	A
20	B5	4306	C
20	B5	4321	G
20	B5	4336	A2M

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Mol	Chain	Res	Type
20	B5	4381	A
20	B5	4382	PSU
20	B5	4383	OMG
20	B5	4402	A
20	B5	4416	C
20	B5	4437	A
20	B5	4446	A
20	B5	4454	A
20	B5	4455	U
20	B5	4465	G
20	B5	4475	A
20	B5	4476	C
20	B5	4477	G
20	B5	4478	G
20	B5	4486	G
20	B5	4487	A
20	B5	4488	A
20	B5	4489	G
20	B5	4490	G
20	B5	4492	G
20	B5	4498	G
20	B5	4501	G
20	B5	4504	C
20	B5	4506	C
20	B5	4512	G
20	B5	4518	C
20	B5	4609	G
20	B5	4610	C
20	B5	4614	G
20	B5	4616	G
20	B5	4621	U
20	B5	4622	C
20	B5	4634	U
20	B5	4638	G
20	B5	4639	C
20	B5	4640	G
20	B5	4644	C
20	B5	4645	C
20	B5	4646	G
20	B5	4649	A
20	B5	4651	G
20	B5	4655	G

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Mol	Chain	Res	Type
20	B5	4658	G
20	B5	4674	C
20	B5	4705	A
20	B5	4715	U
20	B5	4728	U
20	B5	4729	C
20	B5	4753	A
20	B5	4756	G
20	B5	4761	U
20	B5	4762	C
20	B5	4763	C
20	B5	4780	G
20	B5	4789	C
20	B5	4801	G
20	B5	4808	U
64	A2	3	C
64	A2	26	U
64	A2	33	G
64	A2	41	G
64	A2	44	U
64	A2	46	A
64	A2	56	G
64	A2	67	C
64	A2	68	A
64	A2	73	C
64	A2	74	G
64	A2	77	A
64	A2	79	A
64	A2	103	A
64	A2	113	G
64	A2	115	U
64	A2	126	G
64	A2	130	G
64	A2	143	U
64	A2	147	A
64	A2	155	G
64	A2	162	C
64	A2	168	C
64	A2	178	C
64	A2	180	G
64	A2	184	G
64	A2	188	C

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Mol	Chain	Res	Type
64	A2	192	C
64	A2	226	A
64	A2	282	C
64	A2	295	U
64	A2	306	U
64	A2	310	G
64	A2	313	G
64	A2	320	C
64	A2	324	C
64	A2	325	U
64	A2	327	C
64	A2	328	G
64	A2	336	G
64	A2	348	G
64	A2	363	C
64	A2	365	A
64	A2	369	U
64	A2	370	C
64	A2	386	G
64	A2	387	C
64	A2	401	C
64	A2	410	C
64	A2	439	G
64	A2	449	A
64	A2	451	C
64	A2	465	A
64	A2	466	A
64	A2	472	G
64	A2	473	C
64	A2	474	A
64	A2	475	G
64	A2	483	G
64	A2	488	U
64	A2	493	C
64	A2	494	A
64	A2	509	A
64	A2	526	A
64	A2	549	C
64	A2	561	A
64	A2	565	A
64	A2	569	C
64	A2	584	A

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Mol	Chain	Res	Type
64	A2	590	G
64	A2	592	U
64	A2	607	G
64	A2	609	C
64	A2	615	C
64	A2	618	G
64	A2	629	A
64	A2	644	A
64	A2	645	OMG
64	A2	661	C
64	A2	669	A2M
64	A2	670	A
64	A2	672	A
64	A2	673	A
64	A2	674	G
64	A2	733	U
64	A2	734	C
64	A2	747	C
64	A2	748	U
64	A2	754	C
64	A2	755	G
64	A2	756	C
64	A2	798	C
64	A2	799	G
64	A2	812	A
64	A2	822	G
64	A2	823	PSU
64	A2	831	A
64	A2	832	G
64	A2	837	G
64	A2	838	A
64	A2	839	G
64	A2	840	C
64	A2	841	C
64	A2	842	G
64	A2	848	A
64	A2	871	A
64	A2	873	A
64	A2	879	G
64	A2	886	U
64	A2	892	G
64	A2	914	A

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Mol	Chain	Res	Type
64	A2	915	U
64	A2	921	A
64	A2	923	A
64	A2	934	G
64	A2	944	U
64	A2	956	A
64	A2	972	G
64	A2	991	A
64	A2	993	A
64	A2	1000	G
64	A2	1003	U
64	A2	1024	A
64	A2	1061	A
64	A2	1062	U
64	A2	1063	A
64	A2	1084	A
64	A2	1086	C
64	A2	1116	U
64	A2	1117	C
64	A2	1118	C
64	A2	1119	C
64	A2	1122	G
64	A2	1134	A
64	A2	1145	A
64	A2	1154	C
64	A2	1155	U
64	A2	1196	A
64	A2	1208	G
64	A2	1216	C
64	A2	1217	C
64	A2	1225	G
64	A2	1243	U
64	A2	1252	A
64	A2	1254	A
64	A2	1257	G
64	A2	1258	G
64	A2	1260	A
64	A2	1272	C
64	A2	1275	G
64	A2	1276	G
64	A2	1303	G
64	A2	1305	U

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Mol	Chain	Res	Type
64	A2	1343	U
64	A2	1372	U
64	A2	1373	U
64	A2	1379	A
64	A2	1398	U
64	A2	1403	A
64	A2	1406	A
64	A2	1407	G
64	A2	1419	C
64	A2	1420	C
64	A2	1422	A
64	A2	1424	C
64	A2	1425	G
64	A2	1436	C
64	A2	1455	A
64	A2	1463	U
64	A2	1464	U
64	A2	1481	A
64	A2	1490	A
64	A2	1491	OMG
64	A2	1495	U
64	A2	1498	G
64	A2	1499	A
64	A2	1508	G
64	A2	1522	C
64	A2	1523	A
64	A2	1534	A
64	A2	1553	G
64	A2	1554	C
64	A2	1580	A
64	A2	1581	A
64	A2	1586	U
64	A2	1589	A
64	A2	1602	A
64	A2	1618	G
64	A2	1622	U
64	A2	1624	A
64	A2	1647	C
64	A2	1655	G
64	A2	1666	G
64	A2	1684	C
64	A2	1699	C

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Mol	Chain	Res	Type
64	A2	1722	U
64	A2	1723	G
64	A2	1749	G
64	A2	1783	G
64	A2	1784	C
64	A2	1785	G
64	A2	1836	A
64	A2	1837	G
64	A2	1839	U
64	A2	1850	G
64	A2	1852	MA6
64	A2	1862	G
64	A2	1863	G
64	A2	1864	A
64	A2	1865	U
64	A2	1866	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	B5	1588	G
20	B5	4445	U

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

223 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	$\# Z > 2$
20	OMC	B5	2208	92,20	19,22,23	0.81	0	26,31,34	0.84	0
64	OMU	A2	355	64	19,22,23	1.22	3 (15%)	26,31,34	1.69	4 (15%)
64	PSU	A2	1348	64	18,21,22	1.33	2 (11%)	22,30,33	1.86	3 (13%)
64	OMC	A2	174	92,64	19,22,23	0.81	0	26,31,34	0.80	0
64	PSU	A2	1057	64	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	PSU	B5	4740	20	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
64	4AC	A2	1338	64	21,24,25	1.07	1 (4%)	29,34,37	1.15	3 (10%)
20	OMC	B5	2194	92,20	19,22,23	0.82	0	26,31,34	0.85	0
64	PSU	A2	650	64	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
12	HIC	BB	245	12	10,11,12	0.62	0	8,14,16	0.39	0
20	PSU	B5	4435	20	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
20	PSU	B5	4382	20	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
20	OMU	B5	3973	20	19,22,23	1.21	2 (10%)	26,31,34	1.69	4 (15%)
20	PSU	B5	4166	20	18,21,22	1.40	3 (16%)	22,30,33	1.81	4 (18%)
64	PSU	A2	816	64	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
20	OMU	B5	2258	20	19,22,23	1.21	2 (10%)	26,31,34	1.67	4 (15%)
64	PSU	A2	1239	64	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
20	PSU	B5	1721	20	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
64	OMU	A2	116	64	19,22,23	1.20	2 (10%)	26,31,34	1.70	4 (15%)
20	5MC	B5	3514	92,20	18,22,23	0.97	2 (11%)	26,32,35	1.15	3 (11%)
20	UR3	B5	4276	20	19,22,23	0.99	0	26,32,35	1.42	1 (3%)
20	OMG	B5	4138	20	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
64	PSU	A2	36	64	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
64	A2M	A2	591	64	22,25,26	1.48	4 (18%)	31,36,39	2.23	7 (22%)
64	OMG	A2	1329	64	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
20	A2M	B5	3599	20	22,25,26	1.47	4 (18%)	31,36,39	2.15	10 (32%)
64	OMU	A2	1289	64	19,22,23	1.22	3 (15%)	26,31,34	1.67	5 (19%)
20	A2M	B5	4336	20	22,25,26	1.46	4 (18%)	31,36,39	2.11	10 (32%)
20	OMG	B5	3476	20	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
15	AYA	BC	2	15	6,7,8	0.70	0	5,8,10	0.39	0
20	PSU	B5	3427	20	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
20	PSU	B5	4298	20	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
20	OMG	B5	3974	20	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
64	OMG	A2	684	64	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
20	OMC	B5	3540	20	19,22,23	0.82	0	26,31,34	0.80	0
20	PSU	B5	1491	20	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
20	OMG	B5	4116	20	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
64	PSU	A2	1233	64	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
20	PSU	B5	2475	20	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
75	M3L	Bm	98	75	10,11,12	0.83	0	9,14,16	0.52	0
64	A2M	A2	166	64	22,25,26	1.47	4 (18%)	31,36,39	2.13	10 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
64	OMU	A2	628	64	19,22,23	1.18	2 (10%)	26,31,34	1.73	5 (19%)
20	OMG	B5	4240	20	23,26,27	1.21	3 (13%)	33,38,41	1.94	6 (18%)
64	A2M	A2	669	92,64	22,25,26	1.47	4 (18%)	31,36,39	2.14	10 (32%)
64	A2M	A2	513	64	22,25,26	1.47	4 (18%)	31,36,39	2.14	9 (29%)
64	A2M	A2	577	64	22,25,26	1.46	4 (18%)	31,36,39	2.12	10 (32%)
20	PSU	B5	3576	20	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
64	PSU	A2	1368	64	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
27	SAC	AZ	2	27	7,8,9	0.54	0	8,9,11	0.87	1 (12%)
64	PSU	A2	119	64	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
20	OMG	B5	4364	20	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
20	A2M	B5	1270	20	22,25,26	1.45	4 (18%)	31,36,39	2.08	9 (29%)
20	A2M	B5	3456	20	22,25,26	1.46	4 (18%)	31,36,39	2.13	10 (32%)
64	OMC	A2	463	64	19,22,23	0.83	0	26,31,34	0.88	1 (3%)
20	A2M	B5	400	20	22,25,26	1.47	4 (18%)	31,36,39	2.10	9 (29%)
20	OMU	B5	2680	20	19,22,23	1.20	2 (10%)	26,31,34	1.70	5 (19%)
20	PSU	B5	4749	20	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
20	PSU	B5	3554	20	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
20	6MZ	B5	3966	20	22,25,26	1.45	4 (18%)	30,36,39	2.19	9 (30%)
20	PSU	B5	3585	92,20	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
20	OMC	B5	3601	20	19,22,23	0.81	0	26,31,34	0.81	0
64	OMU	A2	1327	92,64	19,22,23	1.19	2 (10%)	26,31,34	1.71	5 (19%)
20	PSU	B5	4217	20	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
20	A2M	B5	2244	92,20	22,25,26	1.46	4 (18%)	31,36,39	2.11	10 (32%)
20	PSU	B5	3502	20	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
64	OMC	A2	1392	64	19,22,23	0.82	0	26,31,34	0.86	1 (3%)
20	PSU	B5	1537	20	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
6	OMG	B8	75	6	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
64	OMC	A2	518	64	19,22,23	0.82	0	26,31,34	0.87	1 (3%)
20	OMG	B5	1580	20	23,26,27	1.21	3 (13%)	33,38,41	1.92	6 (18%)
22	V5N	Ba	39	22	9,11,12	2.06	2 (22%)	9,14,16	1.68	2 (22%)
64	PSU	A2	1046	64	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
64	PSU	A2	218	64	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
20	PSU	B5	3500	20	18,21,22	1.33	2 (11%)	22,30,33	1.85	3 (13%)
20	OMG	B5	3676	20	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
20	OMG	B5	3524	20	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	A2M	B5	3562	20	22,25,26	1.46	4 (18%)	31,36,39	2.12	9 (29%)
64	PSU	A2	109	64	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
20	OMG	B5	2267	20	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
20	PSU	B5	4169	20	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
20	OMG	B5	3942	20,4	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
64	PSU	A2	407	64	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
64	PSU	A2	1175	64	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
20	OMG	B5	1477	20	23,26,27	1.21	3 (13%)	33,38,41	1.94	6 (18%)
64	A2M	A2	469	64	22,25,26	1.47	4 (18%)	31,36,39	2.10	10 (32%)
64	PSU	A2	1446	64	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
20	OMG	B5	2719	20	23,26,27	1.21	3 (13%)	33,38,41	1.98	6 (18%)
64	MA6	A2	1852	64	23,26,27	2.23	5 (21%)	34,38,41	3.69	14 (41%)
64	PSU	A2	1178	64	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
8	NMM	As	67	8	9,11,12	0.59	0	6,12,14	0.45	0
64	PSU	A2	802	64	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
20	OMG	B5	4245	20	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
20	OMG	B5	2207	20	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
64	PSU	A2	823	64	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
20	OMC	B5	2265	92,20	19,22,23	0.82	0	26,31,34	0.86	1 (3%)
20	UY1	B5	3550	20	19,22,23	1.40	3 (15%)	22,31,34	1.85	5 (22%)
78	MLZ	Bo	53	78	8,9,10	0.49	0	4,9,11	0.13	0
80	IAS	An	138	80	6,7,8	1.07	0	6,8,10	1.33	1 (16%)
20	OMC	B5	2647	20	19,22,23	0.83	0	26,31,34	0.84	0
20	PSU	B5	3490	20	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
20	OMU	B5	4366	20	19,22,23	1.21	2 (10%)	26,31,34	1.71	4 (15%)
64	OMG	A2	645	64	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
20	PSU	B5	4058	20	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
64	PSU	A2	1005	64	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
20	5MC	B5	4193	20	18,22,23	0.99	2 (11%)	26,32,35	1.17	2 (7%)
20	OMC	B5	1284	20	19,22,23	0.82	0	26,31,34	0.82	0
20	OMG	B5	4369	20	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
64	PSU	A2	687	64	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
64	A2M	A2	1032	64	22,25,26	1.46	4 (18%)	31,36,39	2.11	10 (32%)
20	A2M	B5	3517	20	22,25,26	1.44	4 (18%)	31,36,39	2.17	11 (35%)
20	PSU	B5	4107	20	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	A2M	B5	3492	20,64	22,25,26	1.47	4 (18%)	31,36,39	2.17	10 (32%)
20	PSU	B5	4322	20	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
20	PSU	B5	4045	20	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
20	PSU	B5	1632	20	18,21,22	1.36	2 (11%)	22,30,33	1.85	4 (18%)
64	A2M	A2	485	64	22,25,26	1.47	4 (18%)	31,36,39	2.11	9 (29%)
20	PSU	B5	4419	20	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
20	PSU	B5	4325	20	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
5	SAC	Ar	2	5	7,8,9	0.52	0	8,9,11	0.90	1 (12%)
20	1MA	B5	1266	92,20	21,25,26	1.39	4 (19%)	31,37,40	1.71	5 (16%)
20	A2M	B5	2206	92,20	22,25,26	1.47	4 (18%)	31,36,39	2.13	9 (29%)
20	OMC	B5	4282	92,20	19,22,23	0.82	0	26,31,34	0.87	1 (3%)
20	PSU	B5	4177	20	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
20	PSU	B5	4099	20	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
64	PSU	A2	864	64	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
20	OMC	B5	3573	20	19,22,23	0.81	0	26,31,34	0.87	1 (3%)
64	OMU	A2	121	64	19,22,23	1.21	3 (15%)	26,31,34	1.69	4 (15%)
64	4AC	A2	1843	64	21,24,25	1.09	2 (9%)	29,34,37	1.23	3 (10%)
20	A2M	B5	4317	20	22,25,26	1.47	4 (18%)	31,36,39	2.15	9 (29%)
20	PSU	B5	4042	20	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
64	OMU	A2	172	64	19,22,23	1.20	3 (15%)	26,31,34	1.70	4 (15%)
64	PSU	A2	1082	64	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
20	PSU	B5	3466	20	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
20	PSU	B5	3616	20	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
64	OMG	A2	1448	64	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
20	PSU	B5	4149	20	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
20	A2M	B5	1479	20	22,25,26	1.46	4 (18%)	31,36,39	2.12	9 (29%)
20	OMU	B5	4052	20	19,22,23	1.22	3 (15%)	26,31,34	1.69	4 (15%)
18	HY3	Aw	62	18	6,8,9	1.99	1 (16%)	5,10,12	1.10	1 (20%)
20	PSU	B5	1720	20	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
20	OMC	B5	1820	92,20	19,22,23	0.80	0	26,31,34	0.79	0
64	PSU	A2	610	64	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
64	A2M	A2	159	64	22,25,26	1.47	4 (18%)	31,36,39	2.15	9 (29%)
64	OMG	A2	868	64	23,26,27	1.18	3 (13%)	33,38,41	1.92	5 (15%)
64	PSU	A2	682	64	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
20	OMU	B5	3657	20	19,22,23	1.21	2 (10%)	26,31,34	1.71	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	PSU	B5	3462	20	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
20	PSU	B5	3494	20	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
20	PSU	B5	4278	20	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
20	A2M	B5	1489	92,20	22,25,26	1.45	4 (18%)	31,36,39	2.10	9 (29%)
20	OMG	B5	4383	20	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
64	PSU	A2	1626	64	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
20	PSU	B5	4203	20	18,21,22	1.36	2 (11%)	22,30,33	1.83	3 (13%)
20	PSU	B5	4374	20	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
64	A2M	A2	1384	64	22,25,26	1.47	4 (18%)	31,36,39	2.11	10 (32%)
20	A2M	B5	4269	92,20	22,25,26	1.46	4 (18%)	31,36,39	2.12	10 (32%)
64	OMU	A2	429	64	19,22,23	1.21	3 (15%)	26,31,34	1.67	4 (15%)
64	PSU	A2	867	64	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
20	OMC	B5	2667	20	19,22,23	0.81	0	26,31,34	0.82	0
64	PSU	A2	573	64	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
6	PSU	B8	55	6	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
20	A2M	B5	3450	20	22,25,26	1.47	4 (18%)	31,36,39	2.09	9 (29%)
64	PSU	A2	105	64	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
20	OMC	B5	4202	20	19,22,23	0.82	0	26,31,34	0.81	0
20	PSU	B5	3652	92,20	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)
20	OMU	B5	4244	20	19,22,23	1.20	2 (10%)	26,31,34	1.68	5 (19%)
64	PSU	A2	1047	64	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
20	A2M	B5	1810	92,20	22,25,26	1.47	4 (18%)	31,36,39	2.15	10 (32%)
20	PSU	B5	4267	92,20	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
64	PSU	A2	967	64	18,21,22	1.37	2 (11%)	22,30,33	1.85	3 (13%)
64	PSU	A2	93	64	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
20	A2M	B5	3557	20	22,25,26	1.46	4 (18%)	31,36,39	2.14	10 (32%)
64	OMG	A2	437	64	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
64	PSU	A2	210	64	18,21,22	1.35	2 (11%)	22,30,33	1.82	3 (13%)
64	A2M	A2	99	92,64	22,25,26	1.46	4 (18%)	31,36,39	2.12	9 (29%)
20	PSU	B5	3447	20	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
64	G7M	A2	1640	64	23,26,27	3.15	9 (39%)	35,39,42	3.32	13 (37%)
20	A2M	B5	2658	92,20	22,25,26	1.46	4 (18%)	31,36,39	2.12	9 (29%)
20	PSU	B5	3496	20	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
20	PSU	B5	3583	20	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
20	PSU	B5	1683	20	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	OMC	B5	2704	20	19,22,23	0.82	0	26,31,34	0.82	0
64	PSU	A2	1644	92,64	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
64	6MZ	A2	1833	92,64	22,25,26	1.45	4 (18%)	30,36,39	2.17	9 (30%)
20	PSU	B5	1731	20	18,21,22	1.35	2 (11%)	22,30,33	1.89	4 (18%)
20	PSU	B5	1801	20	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
20	OMC	B5	3619	20	19,22,23	0.81	0	26,31,34	0.84	0
20	PSU	B5	4039	20	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
20	PSU	B5	4711	20	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
64	A2M	A2	27	92,64	22,25,26	1.46	4 (18%)	31,36,39	2.10	9 (29%)
64	PSU	A2	652	64	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
20	A2M	B5	398	20	22,25,26	1.46	4 (18%)	31,36,39	2.19	10 (32%)
20	PSU	B5	2351	20	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
20	PSU	B5	3371	20	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
64	PSU	A2	815	64	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
6	PSU	B8	69	6	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
64	MA6	A2	1851	64	23,26,27	2.27	5 (21%)	34,38,41	3.68	14 (41%)
20	PSU	B5	1638	20	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
20	PSU	B5	1799	20	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
64	OMG	A2	602	64	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
64	A2M	A2	1679	64	22,25,26	1.45	4 (18%)	31,36,39	2.24	10 (32%)
64	OMG	A2	510	92,64	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
20	A2M	B5	2630	92,20	22,25,26	1.46	4 (18%)	31,36,39	2.17	9 (29%)
64	PSU	A2	1693	64	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
2	MLZ	Bb	5	2	8,9,10	0.49	0	4,9,11	0.14	0
64	B8N	A2	1249	64	24,29,30	1.33	3 (12%)	29,42,45	1.30	3 (10%)
20	OMG	B5	1260	20	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
9	V5N	BA	216	9	9,11,12	2.06	2 (22%)	9,14,16	1.72	2 (22%)
20	PSU	B5	3369	20	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
20	OMG	B5	3359	20	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
64	PSU	A2	1245	64	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
64	OMG	A2	1491	92,64	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
64	OMU	A2	1443	92,64	19,22,23	1.23	3 (15%)	26,31,34	1.69	5 (19%)
64	OMC	A2	1704	64	19,22,23	0.80	0	26,31,34	0.79	0
64	OMU	A2	1805	64	19,22,23	1.22	3 (15%)	26,31,34	1.69	5 (19%)
20	OMC	B5	3433	20	19,22,23	0.79	0	26,31,34	0.75	0
20	PSU	B5	1718	20	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	AME	Au	1	14	9,10,11	0.47	0	9,11,13	0.87	1 (11%)
20	PSU	B5	4246	20	18,21,22	1.34	2 (11%)	22,30,33	1.92	4 (18%)
20	OMG	B5	3631	20	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
84	SAC	Br	2	84	7,8,9	0.53	0	8,9,11	0.83	1 (12%)
64	PSU	A2	34	64	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
20	PSU	B5	4188	20	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)

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
20	OMC	B5	2208	92,20	-	0/9/27/28	0/2/2/2
64	OMU	A2	355	64	-	0/9/27/28	0/2/2/2
64	PSU	A2	1348	64	-	0/7/25/26	0/2/2/2
64	OMC	A2	174	92,64	-	0/9/27/28	0/2/2/2
64	PSU	A2	1057	64	-	0/7/25/26	0/2/2/2
20	PSU	B5	4740	20	-	0/7/25/26	0/2/2/2
64	4AC	A2	1338	64	-	3/11/29/30	0/2/2/2
20	OMC	B5	2194	92,20	-	1/9/27/28	0/2/2/2
64	PSU	A2	650	64	-	0/7/25/26	0/2/2/2
12	HIC	BB	245	12	-	2/5/6/8	0/1/1/1
20	PSU	B5	4435	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	4382	20	-	4/7/25/26	0/2/2/2
20	OMU	B5	3973	20	-	0/9/27/28	0/2/2/2
20	PSU	B5	4166	20	-	3/7/25/26	0/2/2/2
64	PSU	A2	816	64	-	0/7/25/26	0/2/2/2
20	OMU	B5	2258	20	-	0/9/27/28	0/2/2/2
64	PSU	A2	1239	64	-	0/7/25/26	0/2/2/2
20	PSU	B5	1721	20	-	0/7/25/26	0/2/2/2
64	OMU	A2	116	64	-	0/9/27/28	0/2/2/2
20	5MC	B5	3514	92,20	-	0/7/25/26	0/2/2/2
20	UR3	B5	4276	20	-	0/7/25/26	0/2/2/2
20	OMG	B5	4138	20	-	0/9/27/28	0/3/3/3
64	PSU	A2	36	64	-	0/7/25/26	0/2/2/2
64	A2M	A2	591	64	-	4/9/27/28	0/3/3/3
64	OMG	A2	1329	64	-	0/9/27/28	0/3/3/3
20	A2M	B5	3599	20	-	1/9/27/28	0/3/3/3
64	OMU	A2	1289	64	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	A2M	B5	4336	20	-	1/9/27/28	0/3/3/3
20	OMG	B5	3476	20	-	1/9/27/28	0/3/3/3
15	AYA	BC	2	15	-	3/4/6/8	-
20	PSU	B5	3427	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	4298	20	-	0/7/25/26	0/2/2/2
20	OMG	B5	3974	20	-	0/9/27/28	0/3/3/3
64	OMG	A2	684	64	-	0/9/27/28	0/3/3/3
20	OMC	B5	3540	20	-	0/9/27/28	0/2/2/2
20	PSU	B5	1491	20	-	0/7/25/26	0/2/2/2
20	OMG	B5	4116	20	-	0/9/27/28	0/3/3/3
64	PSU	A2	1233	64	-	0/7/25/26	0/2/2/2
20	PSU	B5	2475	20	-	0/7/25/26	0/2/2/2
75	M3L	Bm	98	75	-	0/9/10/12	-
64	A2M	A2	166	64	-	0/9/27/28	0/3/3/3
64	OMU	A2	628	64	-	4/9/27/28	0/2/2/2
20	OMG	B5	4240	20	-	0/9/27/28	0/3/3/3
64	A2M	A2	669	92,64	-	2/9/27/28	0/3/3/3
64	A2M	A2	513	64	-	2/9/27/28	0/3/3/3
64	A2M	A2	577	64	-	2/9/27/28	0/3/3/3
20	PSU	B5	3576	20	-	1/7/25/26	0/2/2/2
64	PSU	A2	1368	64	-	0/7/25/26	0/2/2/2
27	SAC	AZ	2	27	-	2/7/8/10	-
64	PSU	A2	119	64	-	0/7/25/26	0/2/2/2
20	OMG	B5	4364	20	-	1/9/27/28	0/3/3/3
20	A2M	B5	1270	20	-	0/9/27/28	0/3/3/3
20	A2M	B5	3456	20	-	0/9/27/28	0/3/3/3
64	OMC	A2	463	64	-	0/9/27/28	0/2/2/2
20	A2M	B5	400	20	-	0/9/27/28	0/3/3/3
20	OMU	B5	2680	20	-	1/9/27/28	0/2/2/2
20	PSU	B5	4749	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	3554	20	-	0/7/25/26	0/2/2/2
20	6MZ	B5	3966	20	-	0/9/27/28	0/3/3/3
20	PSU	B5	3585	92,20	-	0/7/25/26	0/2/2/2
20	OMC	B5	3601	20	-	0/9/27/28	0/2/2/2
64	OMU	A2	1327	92,64	-	0/9/27/28	0/2/2/2
20	PSU	B5	4217	20	-	0/7/25/26	0/2/2/2
20	A2M	B5	2244	92,20	-	0/9/27/28	0/3/3/3
20	PSU	B5	3502	20	-	0/7/25/26	0/2/2/2
64	OMC	A2	1392	64	-	0/9/27/28	0/2/2/2
20	PSU	B5	1537	20	-	0/7/25/26	0/2/2/2
6	OMG	B8	75	6	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
64	OMC	A2	518	64	-	0/9/27/28	0/2/2/2
20	OMG	B5	1580	20	-	0/9/27/28	0/3/3/3
22	V5N	Ba	39	22	-	1/9/10/12	0/1/1/1
64	PSU	A2	1046	64	-	0/7/25/26	0/2/2/2
64	PSU	A2	218	64	-	0/7/25/26	0/2/2/2
20	PSU	B5	3500	20	-	0/7/25/26	0/2/2/2
20	OMG	B5	3676	20	-	0/9/27/28	0/3/3/3
20	OMG	B5	3524	20	-	0/9/27/28	0/3/3/3
20	A2M	B5	3562	20	-	0/9/27/28	0/3/3/3
64	PSU	A2	109	64	-	0/7/25/26	0/2/2/2
20	OMG	B5	2267	20	-	0/9/27/28	0/3/3/3
20	PSU	B5	4169	20	-	0/7/25/26	0/2/2/2
20	OMG	B5	3942	20,4	-	0/9/27/28	0/3/3/3
64	PSU	A2	407	64	-	0/7/25/26	0/2/2/2
64	PSU	A2	1175	64	-	0/7/25/26	0/2/2/2
20	OMG	B5	1477	20	-	0/9/27/28	0/3/3/3
64	A2M	A2	469	64	-	2/9/27/28	0/3/3/3
64	PSU	A2	1446	64	-	0/7/25/26	0/2/2/2
20	OMG	B5	2719	20	-	0/9/27/28	0/3/3/3
64	MA6	A2	1852	64	-	4/11/29/30	0/3/3/3
64	PSU	A2	1178	64	-	0/7/25/26	0/2/2/2
8	NMM	As	67	8	-	0/9/11/13	-
64	PSU	A2	802	64	-	0/7/25/26	0/2/2/2
20	OMG	B5	4245	20	-	0/9/27/28	0/3/3/3
20	OMG	B5	2207	20	-	2/9/27/28	0/3/3/3
64	PSU	A2	823	64	-	0/7/25/26	0/2/2/2
20	OMC	B5	2265	92,20	-	0/9/27/28	0/2/2/2
20	UY1	B5	3550	20	-	1/9/27/28	0/2/2/2
78	MLZ	Bo	53	78	-	1/7/8/10	-
80	IAS	An	138	80	-	2/7/7/8	-
20	OMC	B5	2647	20	-	0/9/27/28	0/2/2/2
20	PSU	B5	3490	20	-	0/7/25/26	0/2/2/2
20	OMU	B5	4366	20	-	0/9/27/28	0/2/2/2
64	OMG	A2	645	64	-	3/9/27/28	0/3/3/3
20	PSU	B5	4058	20	-	0/7/25/26	0/2/2/2
64	PSU	A2	1005	64	-	0/7/25/26	0/2/2/2
20	5MC	B5	4193	20	-	4/7/25/26	0/2/2/2
20	OMC	B5	1284	20	-	0/9/27/28	0/2/2/2
20	OMG	B5	4369	20	-	0/9/27/28	0/3/3/3
64	PSU	A2	687	64	-	0/7/25/26	0/2/2/2
64	A2M	A2	1032	64	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	A2M	B5	3517	20	-	2/9/27/28	0/3/3/3
20	PSU	B5	4107	20	-	0/7/25/26	0/2/2/2
20	A2M	B5	3492	20,64	-	1/9/27/28	0/3/3/3
20	PSU	B5	4322	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	4045	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	1632	20	-	0/7/25/26	0/2/2/2
64	A2M	A2	485	64	-	0/9/27/28	0/3/3/3
20	PSU	B5	4419	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	4325	20	-	0/7/25/26	0/2/2/2
5	SAC	Ar	2	5	-	0/7/8/10	-
20	1MA	B5	1266	92,20	-	0/7/25/26	0/3/3/3
20	A2M	B5	2206	92,20	-	0/9/27/28	0/3/3/3
20	OMC	B5	4282	92,20	-	0/9/27/28	0/2/2/2
20	PSU	B5	4177	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	4099	20	-	0/7/25/26	0/2/2/2
64	PSU	A2	864	64	-	0/7/25/26	0/2/2/2
20	OMC	B5	3573	20	-	0/9/27/28	0/2/2/2
64	OMU	A2	121	64	-	0/9/27/28	0/2/2/2
64	4AC	A2	1843	64	-	4/11/29/30	0/2/2/2
20	A2M	B5	4317	20	-	0/9/27/28	0/3/3/3
20	PSU	B5	4042	20	-	0/7/25/26	0/2/2/2
64	OMU	A2	172	64	-	0/9/27/28	0/2/2/2
64	PSU	A2	1082	64	-	0/7/25/26	0/2/2/2
20	PSU	B5	3466	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	3616	20	-	0/7/25/26	0/2/2/2
64	OMG	A2	1448	64	-	3/9/27/28	0/3/3/3
20	PSU	B5	4149	20	-	0/7/25/26	0/2/2/2
20	A2M	B5	1479	20	-	0/9/27/28	0/3/3/3
20	OMU	B5	4052	20	-	1/9/27/28	0/2/2/2
18	HY3	Aw	62	18	-	1/1/12/14	0/1/1/1
20	PSU	B5	1720	20	-	0/7/25/26	0/2/2/2
20	OMC	B5	1820	92,20	-	0/9/27/28	0/2/2/2
64	PSU	A2	610	64	-	0/7/25/26	0/2/2/2
64	A2M	A2	159	64	-	0/9/27/28	0/3/3/3
64	OMG	A2	868	64	-	1/9/27/28	0/3/3/3
64	PSU	A2	682	64	-	0/7/25/26	0/2/2/2
20	OMU	B5	3657	20	-	1/9/27/28	0/2/2/2
20	PSU	B5	3462	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	3494	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	4278	20	-	0/7/25/26	0/2/2/2
20	A2M	B5	1489	92,20	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	OMG	B5	4383	20	-	1/9/27/28	0/3/3/3
64	PSU	A2	1626	64	-	0/7/25/26	0/2/2/2
20	PSU	B5	4203	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	4374	20	-	0/7/25/26	0/2/2/2
64	A2M	A2	1384	64	-	0/9/27/28	0/3/3/3
20	A2M	B5	4269	92,20	-	0/9/27/28	0/3/3/3
64	OMU	A2	429	64	-	4/9/27/28	0/2/2/2
64	PSU	A2	867	64	-	0/7/25/26	0/2/2/2
20	OMC	B5	2667	20	-	1/9/27/28	0/2/2/2
64	PSU	A2	573	64	-	0/7/25/26	0/2/2/2
6	PSU	B8	55	6	-	0/7/25/26	0/2/2/2
20	A2M	B5	3450	20	-	0/9/27/28	0/3/3/3
64	PSU	A2	105	64	-	0/7/25/26	0/2/2/2
20	OMC	B5	4202	20	-	0/9/27/28	0/2/2/2
20	PSU	B5	3652	92,20	-	0/7/25/26	0/2/2/2
20	OMU	B5	4244	20	-	0/9/27/28	0/2/2/2
64	PSU	A2	1047	64	-	0/7/25/26	0/2/2/2
20	A2M	B5	1810	92,20	-	0/9/27/28	0/3/3/3
20	PSU	B5	4267	92,20	-	0/7/25/26	0/2/2/2
64	PSU	A2	967	64	-	0/7/25/26	0/2/2/2
64	PSU	A2	93	64	-	0/7/25/26	0/2/2/2
20	A2M	B5	3557	20	-	0/9/27/28	0/3/3/3
64	OMG	A2	437	64	-	0/9/27/28	0/3/3/3
64	PSU	A2	210	64	-	0/7/25/26	0/2/2/2
64	A2M	A2	99	92,64	-	1/9/27/28	0/3/3/3
20	PSU	B5	3447	20	-	0/7/25/26	0/2/2/2
64	G7M	A2	1640	64	-	2/7/25/26	0/3/3/3
20	A2M	B5	2658	92,20	-	0/9/27/28	0/3/3/3
20	PSU	B5	3496	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	3583	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	1683	20	-	0/7/25/26	0/2/2/2
20	OMC	B5	2704	20	-	0/9/27/28	0/2/2/2
64	PSU	A2	1644	92,64	-	0/7/25/26	0/2/2/2
64	6MZ	A2	1833	92,64	-	0/9/27/28	0/3/3/3
20	PSU	B5	1731	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	1801	20	-	0/7/25/26	0/2/2/2
20	OMC	B5	3619	20	-	2/9/27/28	0/2/2/2
20	PSU	B5	4039	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	4711	20	-	0/7/25/26	0/2/2/2
64	A2M	A2	27	92,64	-	3/9/27/28	0/3/3/3
64	PSU	A2	652	64	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	A2M	B5	398	20	-	2/9/27/28	0/3/3/3
20	PSU	B5	2351	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	3371	20	-	0/7/25/26	0/2/2/2
64	PSU	A2	815	64	-	0/7/25/26	0/2/2/2
6	PSU	B8	69	6	-	0/7/25/26	0/2/2/2
64	MA6	A2	1851	64	-	3/11/29/30	0/3/3/3
20	PSU	B5	1638	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	1799	20	-	0/7/25/26	0/2/2/2
64	OMG	A2	602	64	-	0/9/27/28	0/3/3/3
64	A2M	A2	1679	64	-	1/9/27/28	0/3/3/3
64	OMG	A2	510	92,64	-	1/9/27/28	0/3/3/3
20	A2M	B5	2630	92,20	-	3/9/27/28	0/3/3/3
64	PSU	A2	1693	64	-	0/7/25/26	0/2/2/2
2	MLZ	Bb	5	2	-	2/7/8/10	-
64	B8N	A2	1249	64	-	4/16/34/35	0/2/2/2
20	OMG	B5	1260	20	-	0/9/27/28	0/3/3/3
9	V5N	BA	216	9	-	3/9/10/12	0/1/1/1
20	PSU	B5	3369	20	-	0/7/25/26	0/2/2/2
20	OMG	B5	3359	20	-	0/9/27/28	0/3/3/3
64	PSU	A2	1245	64	-	0/7/25/26	0/2/2/2
64	OMG	A2	1491	92,64	-	0/9/27/28	0/3/3/3
64	OMU	A2	1443	92,64	-	0/9/27/28	0/2/2/2
64	OMC	A2	1704	64	-	1/9/27/28	0/2/2/2
64	OMU	A2	1805	64	-	0/9/27/28	0/2/2/2
20	OMC	B5	3433	20	-	4/9/27/28	0/2/2/2
20	PSU	B5	1718	20	-	0/7/25/26	0/2/2/2
14	AME	Au	1	14	-	2/9/10/12	-
20	PSU	B5	4246	20	-	2/7/25/26	0/2/2/2
20	OMG	B5	3631	20	-	1/9/27/28	0/3/3/3
84	SAC	Br	2	84	-	1/7/8/10	-
64	PSU	A2	34	64	-	0/7/25/26	0/2/2/2
20	PSU	B5	4188	20	-	0/7/25/26	0/2/2/2

All (506) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	A2	1640	G7M	C4-N9	7.96	1.58	1.38
64	A2	1640	G7M	O6-C6	7.64	1.38	1.23
64	A2	1851	MA6	C5-N7	6.86	1.52	1.39
64	A2	1852	MA6	C5-N7	6.68	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	A2	1640	G7M	C5-C4	6.23	1.54	1.38
64	A2	1851	MA6	C8-N9	-5.39	1.27	1.37
64	A2	1852	MA6	C8-N9	-5.35	1.28	1.37
9	BA	216	V5N	CG-ND1	-4.89	1.33	1.37
22	Ba	39	V5N	CG-ND1	-4.86	1.33	1.37
64	A2	591	A2M	C5-C4	4.67	1.47	1.39
20	B5	3492	A2M	C5-C4	4.56	1.47	1.39
64	A2	513	A2M	C5-C4	4.56	1.47	1.39
64	A2	159	A2M	C5-C4	4.55	1.47	1.39
20	B5	2658	A2M	C5-C4	4.53	1.47	1.39
20	B5	400	A2M	C5-C4	4.52	1.47	1.39
64	A2	1833	6MZ	C5-C4	4.52	1.47	1.39
20	B5	4317	A2M	C5-C4	4.52	1.47	1.39
64	A2	669	A2M	C5-C4	4.51	1.47	1.39
64	A2	485	A2M	C5-C4	4.51	1.47	1.39
20	B5	1479	A2M	C5-C4	4.51	1.47	1.39
64	A2	166	A2M	C5-C4	4.51	1.47	1.39
20	B5	3966	6MZ	C5-C4	4.50	1.47	1.39
64	A2	469	A2M	C5-C4	4.50	1.47	1.39
64	A2	577	A2M	C5-C4	4.50	1.47	1.39
20	B5	3450	A2M	C5-C4	4.50	1.47	1.39
20	B5	2630	A2M	C5-C4	4.50	1.47	1.39
20	B5	3599	A2M	C5-C4	4.50	1.47	1.39
18	Aw	62	HY3	C3-CA	-4.49	1.50	1.55
20	B5	398	A2M	C5-C4	4.49	1.47	1.39
20	B5	2206	A2M	C5-C4	4.49	1.47	1.39
20	B5	4336	A2M	C5-C4	4.49	1.47	1.39
64	A2	99	A2M	C5-C4	4.49	1.47	1.39
20	B5	1810	A2M	C5-C4	4.49	1.47	1.39
20	B5	3562	A2M	C5-C4	4.48	1.47	1.39
64	A2	1384	A2M	C5-C4	4.48	1.47	1.39
64	A2	27	A2M	C5-C4	4.48	1.47	1.39
64	A2	1640	G7M	C2-N2	4.48	1.44	1.34
20	B5	2244	A2M	C5-C4	4.47	1.47	1.39
20	B5	3557	A2M	C5-C4	4.47	1.47	1.39
20	B5	4269	A2M	C5-C4	4.47	1.47	1.39
64	A2	1032	A2M	C5-C4	4.46	1.47	1.39
64	A2	1679	A2M	C5-C4	4.44	1.47	1.39
20	B5	1270	A2M	C5-C4	4.44	1.47	1.39
20	B5	3456	A2M	C5-C4	4.43	1.47	1.39
20	B5	1489	A2M	C5-C4	4.42	1.47	1.39
20	B5	3517	A2M	C5-C4	4.38	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	A2	1640	G7M	C2-N1	3.87	1.47	1.37
20	B5	3550	UY1	C6-C5	3.71	1.39	1.35
64	A2	1851	MA6	C4-N9	-3.71	1.29	1.37
64	A2	1852	MA6	C4-N9	-3.60	1.29	1.37
64	A2	1640	G7M	C2-N3	3.35	1.41	1.33
20	B5	4166	PSU	C6-C5	3.31	1.39	1.35
20	B5	1632	PSU	C6-C5	3.29	1.39	1.35
64	A2	967	PSU	C6-C5	3.28	1.39	1.35
64	A2	34	PSU	C6-C5	3.21	1.39	1.35
20	B5	1721	PSU	C6-C5	3.21	1.39	1.35
64	A2	218	PSU	C6-C5	3.21	1.39	1.35
64	A2	210	PSU	C6-C5	3.20	1.39	1.35
20	B5	3585	PSU	C6-C5	3.20	1.39	1.35
64	A2	1626	PSU	C6-C5	3.20	1.39	1.35
20	B5	3494	PSU	C6-C5	3.19	1.39	1.35
64	A2	1851	MA6	C5-C4	3.19	1.45	1.39
20	B5	4203	PSU	C6-C5	3.18	1.39	1.35
20	B5	3462	PSU	C6-C5	3.18	1.39	1.35
64	A2	573	PSU	C6-C5	3.18	1.39	1.35
64	A2	823	PSU	C6-C5	3.18	1.39	1.35
20	B5	3466	PSU	C6-C5	3.18	1.39	1.35
64	A2	867	PSU	C6-C5	3.17	1.39	1.35
20	B5	4169	PSU	C6-C5	3.17	1.39	1.35
20	B5	1266	1MA	C6-N6	3.17	1.35	1.28
64	A2	1057	PSU	C6-C5	3.17	1.39	1.35
64	A2	1249	B8N	C6-C5	3.17	1.39	1.34
64	A2	1852	MA6	C5-C4	3.17	1.44	1.39
20	B5	4322	PSU	C6-C5	3.16	1.39	1.35
20	B5	4382	PSU	C6-C5	3.16	1.39	1.35
20	B5	4149	PSU	C6-C5	3.16	1.39	1.35
64	A2	1233	PSU	C6-C5	3.16	1.39	1.35
20	B5	3496	PSU	C6-C5	3.16	1.39	1.35
20	B5	4107	PSU	C6-C5	3.16	1.39	1.35
64	A2	1046	PSU	C6-C5	3.16	1.39	1.35
20	B5	3490	PSU	C6-C5	3.15	1.39	1.35
20	B5	4278	PSU	C6-C5	3.15	1.39	1.35
64	A2	1693	PSU	C6-C5	3.15	1.39	1.35
20	B5	4711	PSU	C6-C5	3.15	1.39	1.35
64	A2	407	PSU	C6-C5	3.15	1.39	1.35
64	A2	109	PSU	C6-C5	3.15	1.39	1.35
64	A2	1368	PSU	C6-C5	3.15	1.39	1.35
64	A2	682	PSU	C6-C5	3.15	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B8	69	PSU	C6-C5	3.14	1.39	1.35
20	B5	2475	PSU	C6-C5	3.14	1.39	1.35
64	A2	816	PSU	C6-C5	3.14	1.39	1.35
20	B5	1799	PSU	C6-C5	3.14	1.39	1.35
64	A2	815	PSU	C6-C5	3.14	1.39	1.35
20	B5	1266	1MA	C5-C4	3.14	1.47	1.38
20	B5	4099	PSU	C6-C5	3.14	1.39	1.35
20	B5	4435	PSU	C6-C5	3.14	1.39	1.35
64	A2	1446	PSU	C6-C5	3.14	1.39	1.35
20	B5	3583	PSU	C6-C5	3.13	1.39	1.35
20	B5	4042	PSU	C6-C5	3.13	1.39	1.35
64	A2	650	PSU	C6-C5	3.13	1.39	1.35
20	B5	2719	OMG	C5-C4	3.13	1.47	1.38
64	A2	1239	PSU	C6-C5	3.13	1.39	1.35
20	B5	1720	PSU	C6-C5	3.13	1.39	1.35
64	A2	802	PSU	C6-C5	3.13	1.39	1.35
64	A2	1082	PSU	C6-C5	3.13	1.39	1.35
64	A2	1178	PSU	C6-C5	3.13	1.39	1.35
20	B5	3524	OMG	C5-C4	3.13	1.47	1.38
64	A2	1491	OMG	C5-C4	3.12	1.47	1.38
20	B5	3427	PSU	C6-C5	3.12	1.39	1.35
20	B5	3576	PSU	C6-C5	3.12	1.39	1.35
20	B5	1580	OMG	C5-C4	3.12	1.47	1.38
64	A2	610	PSU	C6-C5	3.12	1.39	1.35
20	B5	3371	PSU	C6-C5	3.12	1.39	1.35
20	B5	3652	PSU	C6-C5	3.12	1.39	1.35
20	B5	1718	PSU	C6-C5	3.12	1.39	1.35
20	B5	4325	PSU	C6-C5	3.12	1.39	1.35
20	B5	4188	PSU	C6-C5	3.11	1.39	1.35
64	A2	687	PSU	C6-C5	3.11	1.39	1.35
20	B5	3502	PSU	C6-C5	3.11	1.38	1.35
20	B5	4246	PSU	C6-C5	3.11	1.38	1.35
20	B5	3554	PSU	C6-C5	3.11	1.38	1.35
20	B5	4740	PSU	C6-C5	3.11	1.38	1.35
64	A2	437	OMG	C5-C4	3.11	1.47	1.38
64	A2	105	PSU	C6-C5	3.11	1.38	1.35
64	A2	1245	PSU	C6-C5	3.11	1.38	1.35
20	B5	3616	PSU	C6-C5	3.11	1.38	1.35
64	A2	864	PSU	C6-C5	3.11	1.38	1.35
64	A2	1005	PSU	C6-C5	3.11	1.38	1.35
20	B5	1731	PSU	C6-C5	3.11	1.38	1.35
20	B5	3447	PSU	C6-C5	3.11	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B5	4419	PSU	C6-C5	3.11	1.38	1.35
20	B5	3369	PSU	C6-C5	3.11	1.38	1.35
20	B5	4245	OMG	C5-C4	3.11	1.47	1.38
64	A2	36	PSU	C6-C5	3.10	1.38	1.35
64	A2	119	PSU	C6-C5	3.10	1.38	1.35
64	A2	602	OMG	C5-C4	3.10	1.47	1.38
64	A2	652	PSU	C6-C5	3.10	1.38	1.35
20	B5	4369	OMG	C5-C4	3.10	1.47	1.38
20	B5	1801	PSU	C6-C5	3.10	1.38	1.35
20	B5	4217	PSU	C6-C5	3.10	1.38	1.35
20	B5	3359	OMG	C5-C4	3.10	1.47	1.38
20	B5	4240	OMG	C5-C4	3.10	1.47	1.38
20	B5	3676	OMG	C5-C4	3.10	1.47	1.38
64	A2	1175	PSU	C6-C5	3.10	1.38	1.35
20	B5	1537	PSU	C6-C5	3.09	1.38	1.35
20	B5	1477	OMG	C5-C4	3.09	1.47	1.38
20	B5	2207	OMG	C5-C4	3.09	1.47	1.38
6	B8	55	PSU	C6-C5	3.09	1.38	1.35
64	A2	93	PSU	C6-C5	3.09	1.38	1.35
64	A2	510	OMG	C5-C4	3.09	1.47	1.38
64	A2	645	OMG	C5-C4	3.09	1.47	1.38
20	B5	2267	OMG	C5-C4	3.09	1.47	1.38
20	B5	4177	PSU	C6-C5	3.09	1.38	1.35
64	A2	1329	OMG	C5-C4	3.08	1.47	1.38
64	A2	1448	OMG	C5-C4	3.08	1.47	1.38
20	B5	3942	OMG	C5-C4	3.08	1.47	1.38
20	B5	4058	PSU	C6-C5	3.08	1.38	1.35
64	A2	1047	PSU	C6-C5	3.08	1.38	1.35
64	A2	868	OMG	C5-C4	3.08	1.47	1.38
20	B5	4138	OMG	C5-C4	3.08	1.47	1.38
20	B5	4364	OMG	C5-C4	3.08	1.47	1.38
20	B5	4045	PSU	C6-C5	3.07	1.38	1.35
64	A2	1348	PSU	C6-C5	3.07	1.38	1.35
64	A2	1249	B8N	C4-N3	-3.07	1.34	1.40
20	B5	3476	OMG	C5-C4	3.07	1.47	1.38
20	B5	4383	OMG	C5-C4	3.07	1.47	1.38
20	B5	4267	PSU	C6-C5	3.06	1.38	1.35
20	B5	2351	PSU	C6-C5	3.06	1.38	1.35
64	A2	684	OMG	C5-C4	3.06	1.47	1.38
20	B5	1638	PSU	C6-C5	3.06	1.38	1.35
20	B5	1683	PSU	C6-C5	3.06	1.38	1.35
20	B5	4374	PSU	C6-C5	3.06	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B5	3500	PSU	C6-C5	3.06	1.38	1.35
6	B8	75	OMG	C5-C4	3.06	1.47	1.38
20	B5	4116	OMG	C5-C4	3.06	1.47	1.38
20	B5	3974	OMG	C5-C4	3.05	1.47	1.38
20	B5	3631	OMG	C5-C4	3.05	1.47	1.38
20	B5	1491	PSU	C6-C5	3.05	1.38	1.35
20	B5	4039	PSU	C6-C5	3.04	1.38	1.35
64	A2	1644	PSU	C6-C5	3.04	1.38	1.35
20	B5	4749	PSU	C6-C5	3.03	1.38	1.35
20	B5	1260	OMG	C5-C4	3.03	1.47	1.38
20	B5	4298	PSU	C6-C5	3.01	1.38	1.35
64	A2	1851	MA6	C6-N6	2.99	1.45	1.36
64	A2	1843	4AC	C4-N4	-2.94	1.35	1.39
64	A2	1852	MA6	C6-N6	2.89	1.45	1.36
20	B5	4193	5MC	C6-C5	2.86	1.39	1.34
64	A2	1338	4AC	C4-N4	-2.84	1.35	1.39
20	B5	3550	UY1	C2-N1	2.81	1.40	1.36
20	B5	3514	5MC	C6-C5	2.79	1.39	1.34
22	Ba	39	V5N	CD2-NE2	-2.79	1.33	1.37
9	BA	216	V5N	CD2-NE2	-2.77	1.33	1.37
20	B5	1731	PSU	C4-N3	-2.72	1.33	1.38
20	B5	3652	PSU	C4-N3	-2.72	1.33	1.38
64	A2	1679	A2M	C5-C6	2.72	1.48	1.41
20	B5	1491	PSU	C4-N3	-2.71	1.33	1.38
20	B5	3599	A2M	C5-C6	2.70	1.48	1.41
64	A2	1082	PSU	C4-N3	-2.70	1.33	1.38
64	A2	159	A2M	C5-C6	2.70	1.48	1.41
64	A2	469	A2M	C5-C6	2.70	1.48	1.41
64	A2	166	A2M	C5-C6	2.69	1.48	1.41
64	A2	610	PSU	C4-N3	-2.69	1.33	1.38
20	B5	3369	PSU	C4-N3	-2.69	1.33	1.38
20	B5	3456	A2M	C5-C6	2.69	1.48	1.41
20	B5	4336	A2M	C5-C6	2.69	1.48	1.41
64	A2	591	A2M	C5-C6	2.69	1.48	1.41
20	B5	4317	A2M	C5-C6	2.68	1.48	1.41
64	A2	1384	A2M	C5-C6	2.68	1.48	1.41
64	A2	513	A2M	C5-C6	2.68	1.48	1.41
20	B5	3616	PSU	C4-N3	-2.68	1.33	1.38
20	B5	4169	PSU	C4-N3	-2.68	1.33	1.38
20	B5	3427	PSU	C4-N3	-2.68	1.33	1.38
64	A2	577	A2M	C5-C6	2.68	1.48	1.41
20	B5	2351	PSU	C4-N3	-2.68	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B5	2244	A2M	C5-C6	2.68	1.48	1.41
20	B5	398	A2M	C5-C6	2.67	1.48	1.41
20	B5	3492	A2M	C5-C6	2.67	1.48	1.41
64	A2	485	A2M	C5-C6	2.67	1.48	1.41
20	B5	4042	PSU	C4-N3	-2.67	1.33	1.38
64	A2	27	A2M	C5-C6	2.67	1.48	1.41
20	B5	1721	PSU	C4-N3	-2.67	1.33	1.38
64	A2	1644	PSU	C4-N3	-2.67	1.33	1.38
20	B5	2630	A2M	C5-C6	2.67	1.48	1.41
20	B5	4278	PSU	C4-N3	-2.66	1.33	1.38
20	B5	3576	PSU	C4-N3	-2.66	1.33	1.38
64	A2	218	PSU	C4-N3	-2.66	1.33	1.38
20	B5	1720	PSU	C4-N3	-2.66	1.33	1.38
20	B5	4267	PSU	C4-N3	-2.66	1.33	1.38
20	B5	1799	PSU	C4-N3	-2.66	1.33	1.38
20	B5	1683	PSU	C4-N3	-2.66	1.33	1.38
64	A2	119	PSU	C4-N3	-2.66	1.33	1.38
20	B5	4269	A2M	C5-C6	2.66	1.48	1.41
20	B5	3562	A2M	C5-C6	2.66	1.48	1.41
64	A2	669	A2M	C5-C6	2.66	1.48	1.41
64	A2	687	PSU	C4-N3	-2.66	1.33	1.38
64	A2	1032	A2M	C5-C6	2.66	1.48	1.41
20	B5	1718	PSU	C4-N3	-2.66	1.33	1.38
20	B5	3450	A2M	C5-C6	2.66	1.48	1.41
20	B5	3447	PSU	C4-N3	-2.66	1.33	1.38
64	A2	1368	PSU	C4-N3	-2.65	1.33	1.38
20	B5	3371	PSU	C4-N3	-2.65	1.33	1.38
20	B5	3583	PSU	C4-N3	-2.65	1.33	1.38
20	B5	4419	PSU	C4-N3	-2.65	1.33	1.38
64	A2	682	PSU	C4-N3	-2.65	1.33	1.38
20	B5	2658	A2M	C5-C6	2.65	1.48	1.41
20	B5	3466	PSU	C4-N3	-2.65	1.33	1.38
20	B5	1270	A2M	C5-C6	2.65	1.48	1.41
20	B5	4217	PSU	C4-N3	-2.65	1.33	1.38
6	B8	55	PSU	C4-N3	-2.65	1.33	1.38
20	B5	4246	PSU	C4-N3	-2.65	1.33	1.38
20	B5	2206	A2M	C5-C6	2.65	1.48	1.41
20	B5	400	A2M	C5-C6	2.65	1.48	1.41
20	B5	4435	PSU	C4-N3	-2.65	1.33	1.38
64	A2	823	PSU	C4-N3	-2.65	1.33	1.38
20	B5	4298	PSU	C4-N3	-2.65	1.33	1.38
20	B5	4374	PSU	C4-N3	-2.65	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B5	1479	A2M	C5-C6	2.65	1.48	1.41
20	B5	2475	PSU	C4-N3	-2.65	1.33	1.38
20	B5	4107	PSU	C4-N3	-2.65	1.33	1.38
20	B5	1638	PSU	C4-N3	-2.65	1.33	1.38
20	B5	1801	PSU	C4-N3	-2.65	1.33	1.38
20	B5	4177	PSU	C4-N3	-2.65	1.33	1.38
20	B5	1489	A2M	C5-C6	2.65	1.48	1.41
64	A2	1233	PSU	C4-N3	-2.65	1.33	1.38
20	B5	3554	PSU	C4-N3	-2.65	1.33	1.38
64	A2	105	PSU	C4-N3	-2.65	1.33	1.38
20	B5	3490	PSU	C4-N3	-2.64	1.33	1.38
64	A2	816	PSU	C4-N3	-2.64	1.33	1.38
64	A2	652	PSU	C4-N3	-2.64	1.33	1.38
64	A2	650	PSU	C4-N3	-2.64	1.33	1.38
20	B5	1537	PSU	C4-N3	-2.64	1.33	1.38
64	A2	1348	PSU	C4-N3	-2.64	1.33	1.38
64	A2	93	PSU	C4-N3	-2.64	1.33	1.38
64	A2	573	PSU	C4-N3	-2.64	1.33	1.38
64	A2	1693	PSU	C4-N3	-2.64	1.33	1.38
20	B5	4039	PSU	C4-N3	-2.64	1.33	1.38
64	A2	1175	PSU	C4-N3	-2.64	1.33	1.38
64	A2	815	PSU	C4-N3	-2.63	1.33	1.38
64	A2	1047	PSU	C4-N3	-2.63	1.33	1.38
64	A2	99	A2M	C5-C6	2.63	1.48	1.41
20	B5	3462	PSU	C4-N3	-2.63	1.34	1.38
20	B5	1810	A2M	C5-C6	2.63	1.48	1.41
20	B5	4749	PSU	C4-N3	-2.63	1.34	1.38
64	A2	1057	PSU	C4-N3	-2.63	1.34	1.38
20	B5	4203	PSU	C4-N3	-2.63	1.34	1.38
20	B5	3500	PSU	C4-N3	-2.63	1.34	1.38
20	B5	4058	PSU	C4-N3	-2.63	1.34	1.38
20	B5	4188	PSU	C4-N3	-2.62	1.34	1.38
64	A2	1005	PSU	C4-N3	-2.62	1.34	1.38
64	A2	1239	PSU	C4-N3	-2.62	1.34	1.38
20	B5	3557	A2M	C5-C6	2.62	1.48	1.41
20	B5	4325	PSU	C4-N3	-2.62	1.34	1.38
20	B5	4149	PSU	C4-N3	-2.62	1.34	1.38
64	A2	1178	PSU	C4-N3	-2.62	1.34	1.38
20	B5	4099	PSU	C4-N3	-2.62	1.34	1.38
64	A2	1245	PSU	C4-N3	-2.62	1.34	1.38
64	A2	407	PSU	C4-N3	-2.62	1.34	1.38
64	A2	967	PSU	C4-N3	-2.62	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	A2	36	PSU	C4-N3	-2.62	1.34	1.38
64	A2	867	PSU	C4-N3	-2.61	1.34	1.38
20	B5	3502	PSU	C4-N3	-2.61	1.34	1.38
20	B5	4740	PSU	C4-N3	-2.61	1.34	1.38
64	A2	1446	PSU	C4-N3	-2.61	1.34	1.38
6	B8	69	PSU	C4-N3	-2.61	1.34	1.38
20	B5	4382	PSU	C4-N3	-2.61	1.34	1.38
64	A2	864	PSU	C4-N3	-2.61	1.34	1.38
64	A2	210	PSU	C4-N3	-2.61	1.34	1.38
20	B5	3517	A2M	C5-C6	2.61	1.48	1.41
20	B5	4322	PSU	C4-N3	-2.60	1.34	1.38
20	B5	4045	PSU	C4-N3	-2.60	1.34	1.38
20	B5	4711	PSU	C4-N3	-2.60	1.34	1.38
64	A2	34	PSU	C4-N3	-2.60	1.34	1.38
64	A2	1046	PSU	C4-N3	-2.60	1.34	1.38
20	B5	3496	PSU	C4-N3	-2.60	1.34	1.38
64	A2	1626	PSU	C4-N3	-2.59	1.34	1.38
20	B5	3585	PSU	C4-N3	-2.59	1.34	1.38
20	B5	3494	PSU	C4-N3	-2.59	1.34	1.38
64	A2	802	PSU	C4-N3	-2.59	1.34	1.38
20	B5	1632	PSU	C4-N3	-2.59	1.34	1.38
64	A2	109	PSU	C4-N3	-2.58	1.34	1.38
20	B5	3657	OMU	C4-N3	-2.56	1.34	1.38
20	B5	2719	OMG	C6-N1	-2.55	1.34	1.38
64	A2	510	OMG	C6-N1	-2.53	1.34	1.38
20	B5	4240	OMG	C6-N1	-2.52	1.34	1.38
64	A2	1327	OMU	C4-N3	-2.52	1.34	1.38
20	B5	1477	OMG	C6-N1	-2.52	1.34	1.38
64	A2	1249	B8N	C2-N3	-2.52	1.34	1.38
20	B5	3966	6MZ	C5-C6	2.51	1.48	1.41
20	B5	3524	OMG	C6-N1	-2.51	1.34	1.38
64	A2	429	OMU	C4-N3	-2.51	1.34	1.38
64	A2	645	OMG	C6-N1	-2.51	1.34	1.38
64	A2	1491	OMG	C6-N1	-2.51	1.34	1.38
20	B5	4052	OMU	C4-N3	-2.51	1.34	1.38
64	A2	355	OMU	C4-N3	-2.51	1.34	1.38
64	A2	1443	OMU	C4-N3	-2.50	1.34	1.38
20	B5	4166	PSU	C4-N3	-2.50	1.34	1.38
20	B5	4369	OMG	C6-N1	-2.50	1.34	1.38
20	B5	1260	OMG	C6-N1	-2.50	1.34	1.38
64	A2	172	OMU	C4-N3	-2.50	1.34	1.38
20	B5	3942	OMG	C6-N1	-2.50	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B5	2258	OMU	C4-N3	-2.50	1.34	1.38
20	B5	4383	OMG	C6-N1	-2.50	1.34	1.38
20	B5	4244	OMU	C4-N3	-2.50	1.34	1.38
20	B5	2207	OMG	C6-N1	-2.49	1.34	1.38
20	B5	3359	OMG	C6-N1	-2.49	1.34	1.38
20	B5	2267	OMG	C6-N1	-2.48	1.34	1.38
6	B8	75	OMG	C6-N1	-2.48	1.34	1.38
20	B5	3973	OMU	C4-N3	-2.48	1.34	1.38
20	B5	4138	OMG	C6-N1	-2.48	1.34	1.38
64	A2	684	OMG	C6-N1	-2.48	1.34	1.38
64	A2	116	OMU	C4-N3	-2.48	1.34	1.38
64	A2	1289	OMU	C4-N3	-2.47	1.34	1.38
64	A2	1448	OMG	C6-N1	-2.47	1.34	1.38
64	A2	166	A2M	C8-N7	2.47	1.36	1.31
20	B5	1810	A2M	C8-N7	2.47	1.36	1.31
20	B5	1580	OMG	C6-N1	-2.47	1.34	1.38
20	B5	4116	OMG	C6-N1	-2.47	1.34	1.38
64	A2	669	A2M	C8-N7	2.47	1.36	1.31
64	A2	1329	OMG	C6-N1	-2.47	1.34	1.38
20	B5	4366	OMU	C4-N3	-2.47	1.34	1.38
64	A2	1805	OMU	C4-N3	-2.46	1.34	1.38
64	A2	1833	6MZ	C5-C6	2.46	1.48	1.41
20	B5	2680	OMU	C4-N3	-2.46	1.34	1.38
20	B5	3631	OMG	C6-N1	-2.45	1.34	1.38
20	B5	3676	OMG	C6-N1	-2.45	1.34	1.38
20	B5	3974	OMG	C6-N1	-2.45	1.34	1.38
20	B5	4245	OMG	C6-N1	-2.45	1.34	1.38
64	A2	437	OMG	C6-N1	-2.45	1.34	1.38
64	A2	1679	A2M	C8-N7	2.45	1.36	1.31
64	A2	27	A2M	C8-N7	2.44	1.36	1.31
64	A2	1384	A2M	C8-N7	2.44	1.36	1.31
20	B5	4364	OMG	C6-N1	-2.44	1.34	1.38
64	A2	513	A2M	C8-N7	2.44	1.36	1.31
64	A2	602	OMG	C6-N1	-2.44	1.34	1.38
20	B5	3456	A2M	C8-N7	2.43	1.36	1.31
64	A2	628	OMU	C4-N3	-2.43	1.34	1.38
64	A2	121	OMU	C4-N3	-2.43	1.34	1.38
20	B5	3476	OMG	C6-N1	-2.43	1.34	1.38
20	B5	3492	A2M	C8-N7	2.43	1.36	1.31
20	B5	2244	A2M	C8-N7	2.43	1.36	1.31
20	B5	3599	A2M	C8-N7	2.43	1.36	1.31
64	A2	1032	A2M	C8-N7	2.43	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B5	3450	A2M	C8-N7	2.42	1.36	1.31
20	B5	3517	A2M	C8-N7	2.42	1.36	1.31
20	B5	4317	A2M	C8-N7	2.42	1.36	1.31
20	B5	1479	A2M	C8-N7	2.41	1.36	1.31
20	B5	3557	A2M	C8-N7	2.41	1.36	1.31
20	B5	3966	6MZ	C8-N7	2.41	1.36	1.31
20	B5	1270	A2M	C8-N7	2.41	1.36	1.31
64	A2	469	A2M	C8-N7	2.40	1.36	1.31
20	B5	1489	A2M	C8-N7	2.40	1.36	1.31
20	B5	4336	A2M	C8-N7	2.40	1.36	1.31
64	A2	485	A2M	C8-N7	2.40	1.36	1.31
64	A2	159	A2M	C8-N7	2.40	1.36	1.31
20	B5	2206	A2M	C8-N7	2.39	1.36	1.31
20	B5	400	A2M	C8-N7	2.39	1.36	1.31
20	B5	4269	A2M	C8-N7	2.39	1.36	1.31
64	A2	577	A2M	C8-N7	2.39	1.36	1.31
20	B5	3562	A2M	C8-N7	2.39	1.36	1.31
20	B5	398	A2M	C8-N7	2.38	1.36	1.31
64	A2	868	OMG	C6-N1	-2.38	1.34	1.38
20	B5	1266	1MA	C2-N3	2.37	1.35	1.30
20	B5	2630	A2M	C8-N7	2.36	1.36	1.31
64	A2	99	A2M	C8-N7	2.36	1.36	1.31
20	B5	2658	A2M	C8-N7	2.36	1.36	1.31
64	A2	1640	G7M	C5-N7	2.35	1.41	1.39
64	A2	591	A2M	C8-N7	2.30	1.36	1.31
20	B5	3514	5MC	C6-N1	-2.30	1.34	1.38
64	A2	1833	6MZ	C8-N7	2.30	1.36	1.31
64	A2	591	A2M	C5-N7	-2.29	1.34	1.39
64	A2	1833	6MZ	C5-N7	-2.28	1.34	1.39
20	B5	2206	A2M	C5-N7	-2.24	1.34	1.39
64	A2	1640	G7M	C4-N3	2.24	1.39	1.34
64	A2	485	A2M	C5-N7	-2.23	1.34	1.39
64	A2	99	A2M	C5-N7	-2.23	1.34	1.39
20	B5	400	A2M	C5-N7	-2.23	1.34	1.39
20	B5	1266	1MA	C5-N7	-2.23	1.34	1.39
20	B5	3562	A2M	C5-N7	-2.22	1.34	1.39
20	B5	1580	OMG	C5-N7	-2.22	1.34	1.39
20	B5	3966	6MZ	C5-N7	-2.22	1.34	1.39
20	B5	2658	A2M	C5-N7	-2.21	1.34	1.39
20	B5	4138	OMG	C5-N7	-2.21	1.34	1.39
20	B5	2267	OMG	C5-N7	-2.21	1.34	1.39
20	B5	2630	A2M	C5-N7	-2.21	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B5	1479	A2M	C5-N7	-2.20	1.34	1.39
20	B5	4269	A2M	C5-N7	-2.20	1.34	1.39
64	A2	159	A2M	C5-N7	-2.20	1.34	1.39
20	B5	4336	A2M	C5-N7	-2.20	1.34	1.39
64	A2	1032	A2M	C5-N7	-2.20	1.34	1.39
20	B5	4193	5MC	C6-N1	-2.19	1.34	1.38
20	B5	2719	OMG	C5-N7	-2.19	1.34	1.39
20	B5	2244	A2M	C5-N7	-2.19	1.34	1.39
20	B5	3942	OMG	C5-N7	-2.19	1.34	1.39
20	B5	4317	A2M	C5-N7	-2.19	1.34	1.39
64	A2	1443	OMU	C2-N1	2.19	1.42	1.38
20	B5	4116	OMG	C5-N7	-2.18	1.34	1.39
64	A2	1289	OMU	C2-N1	2.18	1.42	1.38
20	B5	3550	UY1	C6-N1	-2.18	1.32	1.36
20	B5	4240	OMG	C5-N7	-2.18	1.34	1.39
20	B5	3599	A2M	C5-N7	-2.18	1.34	1.39
64	A2	669	A2M	C5-N7	-2.18	1.34	1.39
20	B5	1810	A2M	C5-N7	-2.18	1.34	1.39
20	B5	3456	A2M	C5-N7	-2.17	1.34	1.39
20	B5	1477	OMG	C5-N7	-2.17	1.34	1.39
20	B5	3974	OMG	C5-N7	-2.17	1.34	1.39
64	A2	1805	OMU	C2-N1	2.17	1.41	1.38
64	A2	1491	OMG	C5-N7	-2.17	1.34	1.39
20	B5	398	A2M	C5-N7	-2.17	1.34	1.39
64	A2	355	OMU	C2-N3	-2.17	1.34	1.38
20	B5	3524	OMG	C5-N7	-2.17	1.34	1.39
64	A2	1384	A2M	C5-N7	-2.17	1.34	1.39
20	B5	3476	OMG	C5-N7	-2.17	1.34	1.39
20	B5	3492	A2M	C5-N7	-2.17	1.34	1.39
64	A2	469	A2M	C5-N7	-2.16	1.34	1.39
20	B5	3557	A2M	C5-N7	-2.16	1.34	1.39
6	B8	75	OMG	C5-N7	-2.16	1.34	1.39
20	B5	3517	A2M	C5-N7	-2.16	1.34	1.39
20	B5	1260	OMG	C5-N7	-2.16	1.34	1.39
20	B5	1270	A2M	C5-N7	-2.16	1.34	1.39
20	B5	3450	A2M	C5-N7	-2.16	1.34	1.39
20	B5	4245	OMG	C5-N7	-2.16	1.34	1.39
64	A2	437	OMG	C5-N7	-2.16	1.34	1.39
64	A2	1448	OMG	C5-N7	-2.15	1.34	1.39
20	B5	3973	OMU	C2-N3	-2.15	1.34	1.38
64	A2	628	OMU	C2-N3	-2.15	1.34	1.38
64	A2	121	OMU	C2-N3	-2.15	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B5	3359	OMG	C5-N7	-2.15	1.34	1.39
20	B5	4366	OMU	C2-N3	-2.15	1.34	1.38
20	B5	4383	OMG	C5-N7	-2.14	1.34	1.39
20	B5	2207	OMG	C5-N7	-2.14	1.34	1.39
20	B5	4364	OMG	C5-N7	-2.14	1.34	1.39
20	B5	4369	OMG	C5-N7	-2.14	1.34	1.39
64	A2	684	OMG	C5-N7	-2.14	1.34	1.39
20	B5	1489	A2M	C5-N7	-2.14	1.35	1.39
64	A2	513	A2M	C5-N7	-2.14	1.35	1.39
64	A2	510	OMG	C5-N7	-2.14	1.34	1.39
64	A2	1327	OMU	C2-N3	-2.13	1.34	1.38
64	A2	166	A2M	C5-N7	-2.13	1.35	1.39
64	A2	27	A2M	C5-N7	-2.12	1.35	1.39
64	A2	429	OMU	C2-N3	-2.12	1.34	1.38
64	A2	602	OMG	C5-N7	-2.12	1.35	1.39
64	A2	577	A2M	C5-N7	-2.12	1.35	1.39
20	B5	3676	OMG	C5-N7	-2.12	1.35	1.39
20	B5	4052	OMU	C2-N3	-2.11	1.34	1.38
20	B5	2680	OMU	C2-N3	-2.11	1.34	1.38
20	B5	2258	OMU	C2-N3	-2.11	1.34	1.38
64	A2	1443	OMU	C2-N3	-2.11	1.34	1.38
20	B5	3631	OMG	C5-N7	-2.11	1.35	1.39
64	A2	1329	OMG	C5-N7	-2.10	1.35	1.39
64	A2	172	OMU	C2-N3	-2.10	1.34	1.38
64	A2	1805	OMU	C2-N3	-2.10	1.34	1.38
64	A2	645	OMG	C5-N7	-2.09	1.35	1.39
20	B5	3657	OMU	C2-N3	-2.09	1.34	1.38
64	A2	1289	OMU	C2-N3	-2.09	1.34	1.38
64	A2	1843	4AC	C7-N4	-2.09	1.33	1.37
20	B5	4244	OMU	C2-N3	-2.09	1.34	1.38
64	A2	429	OMU	C2-N1	2.09	1.41	1.38
64	A2	1679	A2M	C5-N7	-2.09	1.35	1.39
64	A2	116	OMU	C2-N3	-2.08	1.34	1.38
20	B5	4166	PSU	C4-C5	2.07	1.50	1.44
20	B5	4052	OMU	C2-N1	2.04	1.41	1.38
64	A2	355	OMU	C2-N1	2.04	1.41	1.38
64	A2	1640	G7M	C6-N1	2.04	1.42	1.38
64	A2	868	OMG	C5-N7	-2.04	1.35	1.39
64	A2	172	OMU	C2-N1	2.02	1.41	1.38
64	A2	121	OMU	C2-N1	2.01	1.41	1.38

All (960) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	A2	1851	MA6	C4-N9-C8	14.65	121.60	105.73
64	A2	1852	MA6	C4-N9-C8	14.48	121.42	105.73
64	A2	1640	G7M	C8-N7-C5	11.43	122.07	107.78
64	A2	1852	MA6	N3-C4-N9	7.10	138.77	127.08
64	A2	591	A2M	C5-C4-N3	-7.01	117.60	126.75
64	A2	1851	MA6	N3-C4-N9	6.67	138.07	127.08
64	A2	1640	G7M	N9-C4-N3	6.64	139.27	125.94
20	B5	2719	OMG	C5-C4-N3	-6.44	118.02	128.46
20	B5	2658	A2M	C5-C4-N3	-6.41	118.39	126.75
64	A2	1640	G7M	C6-C5-N7	6.38	139.96	132.25
64	A2	1833	6MZ	C5-C4-N3	-6.37	118.44	126.75
20	B5	1479	A2M	C5-C4-N3	-6.32	118.51	126.75
64	A2	513	A2M	C5-C4-N3	-6.29	118.54	126.75
20	B5	2206	A2M	C5-C4-N3	-6.29	118.54	126.75
64	A2	166	A2M	C5-C4-N3	-6.26	118.58	126.75
20	B5	3450	A2M	C5-C4-N3	-6.25	118.59	126.75
64	A2	485	A2M	C5-C4-N3	-6.25	118.59	126.75
64	A2	99	A2M	C5-C4-N3	-6.24	118.61	126.75
20	B5	3524	OMG	C5-C4-N3	-6.24	118.34	128.46
64	A2	159	A2M	C5-C4-N3	-6.23	118.62	126.75
20	B5	3966	6MZ	C5-C4-N3	-6.22	118.63	126.75
64	A2	1491	OMG	C5-C4-N3	-6.20	118.40	128.46
20	B5	4317	A2M	C5-C4-N3	-6.19	118.67	126.75
20	B5	3562	A2M	C5-C4-N3	-6.17	118.70	126.75
64	A2	1032	A2M	C5-C4-N3	-6.17	118.70	126.75
20	B5	1477	OMG	C5-C4-N3	-6.17	118.45	128.46
20	B5	4138	OMG	C5-C4-N3	-6.17	118.45	128.46
64	A2	469	A2M	C5-C4-N3	-6.17	118.70	126.75
20	B5	1489	A2M	C5-C4-N3	-6.17	118.70	126.75
20	B5	4269	A2M	C5-C4-N3	-6.16	118.71	126.75
64	A2	577	A2M	C5-C4-N3	-6.16	118.71	126.75
64	A2	669	A2M	C5-C4-N3	-6.16	118.71	126.75
20	B5	400	A2M	C5-C4-N3	-6.16	118.72	126.75
20	B5	1270	A2M	C5-C4-N3	-6.16	118.72	126.75
20	B5	4245	OMG	C5-C4-N3	-6.15	118.49	128.46
64	A2	1384	A2M	C5-C4-N3	-6.15	118.73	126.75
64	A2	27	A2M	C5-C4-N3	-6.14	118.74	126.75
20	B5	1810	A2M	C5-C4-N3	-6.14	118.74	126.75
20	B5	4336	A2M	C5-C4-N3	-6.14	118.74	126.75
20	B5	2207	OMG	C5-C4-N3	-6.14	118.50	128.46
64	A2	1640	G7M	CN7-N7-C5	-6.14	119.14	126.77
20	B5	2244	A2M	C5-C4-N3	-6.14	118.74	126.75
20	B5	3359	OMG	C5-C4-N3	-6.13	118.51	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B5	3599	A2M	C5-C4-N3	-6.13	118.76	126.75
20	B5	4364	OMG	C5-C4-N3	-6.12	118.53	128.46
20	B5	2630	A2M	C5-C4-N3	-6.11	118.78	126.75
64	A2	645	OMG	C5-C4-N3	-6.11	118.55	128.46
64	A2	437	OMG	C5-C4-N3	-6.11	118.56	128.46
64	A2	510	OMG	C5-C4-N3	-6.10	118.57	128.46
20	B5	1580	OMG	C5-C4-N3	-6.09	118.57	128.46
20	B5	2267	OMG	C5-C4-N3	-6.09	118.57	128.46
20	B5	4246	PSU	N1-C2-N3	6.09	122.03	115.13
20	B5	398	A2M	C5-C4-N3	-6.09	118.80	126.75
20	B5	3517	A2M	C5-C4-N3	-6.09	118.81	126.75
20	B5	4116	OMG	C5-C4-N3	-6.08	118.59	128.46
20	B5	4383	OMG	C5-C4-N3	-6.08	118.60	128.46
64	A2	1448	OMG	C5-C4-N3	-6.08	118.60	128.46
20	B5	4240	OMG	C5-C4-N3	-6.07	118.61	128.46
20	B5	3942	OMG	C5-C4-N3	-6.06	118.62	128.46
20	B5	3476	OMG	C5-C4-N3	-6.06	118.63	128.46
20	B5	3557	A2M	C5-C4-N3	-6.06	118.85	126.75
20	B5	4369	OMG	C5-C4-N3	-6.05	118.65	128.46
20	B5	3974	OMG	C5-C4-N3	-6.05	118.65	128.46
20	B5	3492	A2M	C5-C4-N3	-6.04	118.87	126.75
6	B8	75	OMG	C5-C4-N3	-6.04	118.66	128.46
20	B5	3494	PSU	N1-C2-N3	6.04	121.97	115.13
64	A2	682	PSU	N1-C2-N3	6.03	121.97	115.13
20	B5	3456	A2M	C5-C4-N3	-6.03	118.88	126.75
20	B5	3631	OMG	C5-C4-N3	-6.03	118.68	128.46
64	A2	1329	OMG	C5-C4-N3	-6.03	118.68	128.46
64	A2	602	OMG	C5-C4-N3	-6.02	118.70	128.46
64	A2	684	OMG	C5-C4-N3	-6.02	118.70	128.46
20	B5	3676	OMG	C5-C4-N3	-6.01	118.70	128.46
64	A2	1178	PSU	N1-C2-N3	6.01	121.94	115.13
20	B5	4267	PSU	N1-C2-N3	6.00	121.93	115.13
64	A2	610	PSU	N1-C2-N3	6.00	121.93	115.13
20	B5	1260	OMG	C5-C4-N3	-6.00	118.72	128.46
20	B5	1638	PSU	N1-C2-N3	6.00	121.93	115.13
64	A2	1047	PSU	N1-C2-N3	6.00	121.93	115.13
64	A2	1679	A2M	C5-C4-N3	-5.99	118.93	126.75
20	B5	1491	PSU	N1-C2-N3	5.99	121.92	115.13
64	A2	802	PSU	N1-C2-N3	5.99	121.92	115.13
64	A2	1057	PSU	N1-C2-N3	5.99	121.92	115.13
64	A2	407	PSU	N1-C2-N3	5.99	121.91	115.13
20	B5	3616	PSU	N1-C2-N3	5.98	121.91	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	A2	1446	PSU	N1-C2-N3	5.98	121.91	115.13
20	B5	4298	PSU	N1-C2-N3	5.98	121.91	115.13
64	A2	1644	PSU	N1-C2-N3	5.98	121.91	115.13
20	B5	1721	PSU	N1-C2-N3	5.98	121.90	115.13
20	B5	1731	PSU	N1-C2-N3	5.97	121.90	115.13
6	B8	55	PSU	N1-C2-N3	5.97	121.90	115.13
64	A2	652	PSU	N1-C2-N3	5.97	121.90	115.13
64	A2	1239	PSU	N1-C2-N3	5.97	121.89	115.13
20	B5	3576	PSU	N1-C2-N3	5.97	121.89	115.13
64	A2	1245	PSU	N1-C2-N3	5.97	121.89	115.13
20	B5	3369	PSU	N1-C2-N3	5.97	121.89	115.13
20	B5	3502	PSU	N1-C2-N3	5.97	121.89	115.13
20	B5	3447	PSU	N1-C2-N3	5.96	121.89	115.13
64	A2	650	PSU	N1-C2-N3	5.96	121.89	115.13
64	A2	105	PSU	N1-C2-N3	5.96	121.89	115.13
20	B5	4217	PSU	N1-C2-N3	5.96	121.88	115.13
64	A2	815	PSU	N1-C2-N3	5.96	121.88	115.13
64	A2	1005	PSU	N1-C2-N3	5.96	121.88	115.13
64	A2	1852	MA6	C5-C4-N3	-5.96	118.98	126.75
20	B5	4058	PSU	N1-C2-N3	5.96	121.88	115.13
20	B5	4278	PSU	N1-C2-N3	5.95	121.88	115.13
64	A2	867	PSU	N1-C2-N3	5.95	121.88	115.13
64	A2	1175	PSU	N1-C2-N3	5.95	121.88	115.13
64	A2	1626	PSU	N1-C2-N3	5.95	121.87	115.13
20	B5	1801	PSU	N1-C2-N3	5.95	121.87	115.13
20	B5	1720	PSU	N1-C2-N3	5.95	121.87	115.13
20	B5	4042	PSU	N1-C2-N3	5.95	121.87	115.13
20	B5	1683	PSU	N1-C2-N3	5.95	121.87	115.13
20	B5	4382	PSU	N1-C2-N3	5.95	121.87	115.13
64	A2	816	PSU	N1-C2-N3	5.95	121.87	115.13
64	A2	93	PSU	N1-C2-N3	5.95	121.87	115.13
20	B5	1799	PSU	N1-C2-N3	5.94	121.86	115.13
20	B5	3371	PSU	N1-C2-N3	5.94	121.86	115.13
20	B5	4749	PSU	N1-C2-N3	5.94	121.86	115.13
20	B5	3490	PSU	N1-C2-N3	5.94	121.86	115.13
64	A2	864	PSU	N1-C2-N3	5.93	121.85	115.13
20	B5	3462	PSU	N1-C2-N3	5.93	121.85	115.13
64	A2	573	PSU	N1-C2-N3	5.93	121.85	115.13
20	B5	4169	PSU	N1-C2-N3	5.93	121.85	115.13
20	B5	4177	PSU	N1-C2-N3	5.93	121.85	115.13
20	B5	3652	PSU	N1-C2-N3	5.93	121.85	115.13
64	A2	1851	MA6	N9-C8-N7	-5.93	105.81	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	A2	1368	PSU	N1-C2-N3	5.92	121.84	115.13
20	B5	4374	PSU	N1-C2-N3	5.92	121.84	115.13
20	B5	1718	PSU	N1-C2-N3	5.92	121.84	115.13
64	A2	218	PSU	N1-C2-N3	5.92	121.84	115.13
20	B5	4435	PSU	N1-C2-N3	5.92	121.84	115.13
64	A2	34	PSU	N1-C2-N3	5.92	121.84	115.13
20	B5	4045	PSU	N1-C2-N3	5.92	121.83	115.13
64	A2	967	PSU	N1-C2-N3	5.91	121.83	115.13
20	B5	3496	PSU	N1-C2-N3	5.91	121.83	115.13
20	B5	2351	PSU	N1-C2-N3	5.91	121.83	115.13
20	B5	3585	PSU	N1-C2-N3	5.91	121.83	115.13
64	A2	1082	PSU	N1-C2-N3	5.91	121.83	115.13
20	B5	4740	PSU	N1-C2-N3	5.91	121.82	115.13
20	B5	4099	PSU	N1-C2-N3	5.91	121.82	115.13
20	B5	4419	PSU	N1-C2-N3	5.91	121.82	115.13
64	A2	119	PSU	N1-C2-N3	5.91	121.82	115.13
20	B5	2475	PSU	N1-C2-N3	5.90	121.82	115.13
20	B5	3466	PSU	N1-C2-N3	5.90	121.82	115.13
20	B5	4325	PSU	N1-C2-N3	5.90	121.81	115.13
64	A2	1233	PSU	N1-C2-N3	5.90	121.81	115.13
64	A2	687	PSU	N1-C2-N3	5.90	121.81	115.13
64	A2	823	PSU	N1-C2-N3	5.89	121.81	115.13
20	B5	3583	PSU	N1-C2-N3	5.89	121.81	115.13
64	A2	1046	PSU	N1-C2-N3	5.89	121.81	115.13
64	A2	109	PSU	N1-C2-N3	5.89	121.81	115.13
20	B5	3427	PSU	N1-C2-N3	5.89	121.80	115.13
20	B5	4322	PSU	N1-C2-N3	5.89	121.80	115.13
20	B5	4711	PSU	N1-C2-N3	5.89	121.80	115.13
64	A2	36	PSU	N1-C2-N3	5.89	121.80	115.13
20	B5	4039	PSU	N1-C2-N3	5.88	121.80	115.13
20	B5	4149	PSU	N1-C2-N3	5.88	121.80	115.13
20	B5	1537	PSU	N1-C2-N3	5.88	121.79	115.13
20	B5	4107	PSU	N1-C2-N3	5.88	121.79	115.13
64	A2	1693	PSU	N1-C2-N3	5.87	121.78	115.13
6	B8	69	PSU	N1-C2-N3	5.86	121.77	115.13
20	B5	3500	PSU	N1-C2-N3	5.86	121.77	115.13
20	B5	3554	PSU	N1-C2-N3	5.86	121.77	115.13
64	A2	1348	PSU	N1-C2-N3	5.86	121.76	115.13
64	A2	868	OMG	C5-C4-N3	-5.85	118.97	128.46
20	B5	4276	UR3	C4-N3-C2	-5.84	119.06	124.56
20	B5	4188	PSU	N1-C2-N3	5.82	121.73	115.13
64	A2	210	PSU	N1-C2-N3	5.81	121.72	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B5	1632	PSU	N1-C2-N3	5.81	121.71	115.13
20	B5	4203	PSU	N1-C2-N3	5.81	121.71	115.13
64	A2	1851	MA6	C4-C5-N7	-5.79	103.57	110.62
64	A2	1852	MA6	N9-C8-N7	-5.67	106.15	113.91
64	A2	1851	MA6	C5-C4-N3	-5.67	119.35	126.75
20	B5	4166	PSU	N1-C2-N3	5.65	121.54	115.13
20	B5	1266	1MA	C5-C4-N3	-5.58	118.94	127.26
64	A2	591	A2M	N3-C4-N9	5.54	136.21	127.08
64	A2	1852	MA6	C4-C5-N7	-5.37	104.08	110.62
20	B5	3550	UY1	C4-N3-C2	-5.12	118.96	126.34
20	B5	2719	OMG	C2-N3-C4	5.07	121.33	112.30
64	A2	1833	6MZ	N3-C4-N9	5.06	135.42	127.08
20	B5	2658	A2M	N3-C4-N9	4.97	135.27	127.08
20	B5	2207	OMG	C2-N3-C4	4.93	121.08	112.30
20	B5	3524	OMG	C2-N3-C4	4.92	121.07	112.30
20	B5	4245	OMG	C2-N3-C4	4.90	121.03	112.30
20	B5	4138	OMG	C2-N3-C4	4.90	121.03	112.30
20	B5	3676	OMG	C2-N3-C4	4.89	121.02	112.30
20	B5	3631	OMG	C2-N3-C4	4.89	121.02	112.30
64	A2	645	OMG	C2-N3-C4	4.88	121.00	112.30
64	A2	602	OMG	C2-N3-C4	4.88	121.00	112.30
20	B5	4364	OMG	C2-N3-C4	4.88	121.00	112.30
64	A2	513	A2M	N3-C4-N9	4.88	135.12	127.08
64	A2	437	OMG	C2-N3-C4	4.87	120.98	112.30
20	B5	3476	OMG	C2-N3-C4	4.87	120.98	112.30
20	B5	4369	OMG	C2-N3-C4	4.87	120.98	112.30
20	B5	3359	OMG	C2-N3-C4	4.87	120.97	112.30
20	B5	4383	OMG	C2-N3-C4	4.87	120.97	112.30
64	A2	166	A2M	N3-C4-N9	4.87	135.10	127.08
64	A2	1491	OMG	C2-N3-C4	4.87	120.97	112.30
20	B5	1479	A2M	N3-C4-N9	4.87	135.10	127.08
20	B5	1260	OMG	C2-N3-C4	4.86	120.97	112.30
20	B5	2719	OMG	N9-C4-N3	4.86	135.70	125.94
20	B5	1477	OMG	C2-N3-C4	4.86	120.96	112.30
20	B5	4116	OMG	C2-N3-C4	4.86	120.96	112.30
20	B5	2206	A2M	N3-C4-N9	4.85	135.08	127.08
20	B5	4240	OMG	C2-N3-C4	4.85	120.95	112.30
64	A2	1448	OMG	C2-N3-C4	4.85	120.95	112.30
64	A2	1640	G7M	C2-N3-C4	4.85	120.94	112.30
20	B5	2267	OMG	C2-N3-C4	4.85	120.94	112.30
20	B5	3966	6MZ	N3-C4-N9	4.85	135.06	127.08
64	A2	510	OMG	C2-N3-C4	4.84	120.93	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	A2	868	OMG	C2-N3-C4	4.84	120.93	112.30
20	B5	3974	OMG	C2-N3-C4	4.84	120.92	112.30
20	B5	3562	A2M	N3-C4-N9	4.84	135.05	127.08
64	A2	159	A2M	N3-C4-N9	4.84	135.05	127.08
64	A2	99	A2M	N3-C4-N9	4.83	135.05	127.08
64	A2	1329	OMG	C2-N3-C4	4.83	120.91	112.30
20	B5	3942	OMG	C2-N3-C4	4.83	120.91	112.30
6	B8	75	OMG	C2-N3-C4	4.83	120.90	112.30
20	B5	1580	OMG	C2-N3-C4	4.82	120.90	112.30
64	A2	485	A2M	N3-C4-N9	4.82	135.02	127.08
64	A2	684	OMG	C2-N3-C4	4.81	120.87	112.30
20	B5	3450	A2M	N3-C4-N9	4.81	135.00	127.08
20	B5	4317	A2M	N3-C4-N9	4.80	134.99	127.08
20	B5	3599	A2M	N3-C4-N9	4.79	134.98	127.08
20	B5	400	A2M	N3-C4-N9	4.79	134.98	127.08
64	A2	577	A2M	N3-C4-N9	4.79	134.98	127.08
20	B5	2630	A2M	N3-C4-N9	4.78	134.97	127.08
64	A2	1032	A2M	N3-C4-N9	4.78	134.96	127.08
20	B5	1489	A2M	N3-C4-N9	4.78	134.95	127.08
64	A2	669	A2M	N3-C4-N9	4.77	134.95	127.08
20	B5	3492	A2M	N3-C4-N9	4.77	134.94	127.08
64	A2	469	A2M	N3-C4-N9	4.77	134.94	127.08
20	B5	4336	A2M	N3-C4-N9	4.76	134.93	127.08
20	B5	398	A2M	N3-C4-N9	4.76	134.92	127.08
64	A2	1384	A2M	N3-C4-N9	4.76	134.92	127.08
20	B5	1270	A2M	N3-C4-N9	4.75	134.91	127.08
20	B5	4269	A2M	N3-C4-N9	4.75	134.91	127.08
20	B5	1266	1MA	C2-N3-C4	4.75	121.75	112.41
20	B5	2244	A2M	N3-C4-N9	4.74	134.90	127.08
20	B5	3557	A2M	N3-C4-N9	4.74	134.90	127.08
20	B5	3517	A2M	N3-C4-N9	4.74	134.90	127.08
20	B5	3456	A2M	N3-C4-N9	4.74	134.89	127.08
64	A2	27	A2M	N3-C4-N9	4.72	134.86	127.08
20	B5	1810	A2M	N3-C4-N9	4.72	134.86	127.08
20	B5	3524	OMG	N9-C4-N3	4.70	135.38	125.94
64	A2	1491	OMG	N9-C4-N3	4.67	135.31	125.94
20	B5	1580	OMG	N9-C4-N3	4.63	135.23	125.94
20	B5	1477	OMG	N9-C4-N3	4.63	135.23	125.94
64	A2	1679	A2M	N3-C4-N9	4.61	134.68	127.08
64	A2	437	OMG	N9-C4-N3	4.61	135.20	125.94
20	B5	4138	OMG	N9-C4-N3	4.60	135.17	125.94
64	A2	628	OMU	C4-N3-C2	-4.60	120.52	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B5	2267	OMG	N9-C4-N3	4.59	135.16	125.94
20	B5	3359	OMG	N9-C4-N3	4.58	135.13	125.94
64	A2	1640	G7M	C5-C4-N3	-4.56	119.40	128.15
20	B5	4245	OMG	N9-C4-N3	4.55	135.08	125.94
20	B5	3942	OMG	N9-C4-N3	4.54	135.06	125.94
20	B5	4240	OMG	N9-C4-N3	4.54	135.06	125.94
64	A2	510	OMG	N9-C4-N3	4.53	135.03	125.94
20	B5	4364	OMG	N9-C4-N3	4.53	135.03	125.94
64	A2	1843	4AC	N4-C4-N3	4.52	121.44	113.85
6	B8	75	OMG	N9-C4-N3	4.52	135.02	125.94
20	B5	4116	OMG	N9-C4-N3	4.51	135.00	125.94
64	A2	1327	OMU	C4-N3-C2	-4.51	120.63	126.58
64	A2	645	OMG	N9-C4-N3	4.51	134.99	125.94
20	B5	3657	OMU	C4-N3-C2	-4.50	120.64	126.58
20	B5	2207	OMG	N9-C4-N3	4.50	134.98	125.94
20	B5	2680	OMU	C4-N3-C2	-4.50	120.64	126.58
20	B5	4383	OMG	N9-C4-N3	4.49	134.95	125.94
64	A2	1448	OMG	N9-C4-N3	4.49	134.95	125.94
64	A2	684	OMG	N9-C4-N3	4.49	134.94	125.94
20	B5	3476	OMG	N9-C4-N3	4.48	134.94	125.94
64	A2	116	OMU	C4-N3-C2	-4.45	120.72	126.58
20	B5	3676	OMG	N9-C4-N3	4.45	134.87	125.94
20	B5	3974	OMG	N9-C4-N3	4.45	134.87	125.94
20	B5	4366	OMU	C4-N3-C2	-4.44	120.72	126.58
20	B5	3631	OMG	N9-C4-N3	4.44	134.86	125.94
20	B5	3973	OMU	C4-N3-C2	-4.43	120.73	126.58
64	A2	172	OMU	C4-N3-C2	-4.43	120.74	126.58
20	B5	4369	OMG	N9-C4-N3	4.42	134.82	125.94
20	B5	1260	OMG	N9-C4-N3	4.42	134.82	125.94
64	A2	1329	OMG	N9-C4-N3	4.42	134.81	125.94
64	A2	1679	A2M	C2'-C1'-N9	-4.42	106.09	113.53
20	B5	398	A2M	C2'-C1'-N9	-4.42	106.10	113.53
20	B5	4052	OMU	C4-N3-C2	-4.41	120.77	126.58
20	B5	4244	OMU	C4-N3-C2	-4.39	120.78	126.58
64	A2	355	OMU	C4-N3-C2	-4.37	120.82	126.58
64	A2	121	OMU	C4-N3-C2	-4.35	120.84	126.58
64	A2	602	OMG	N9-C4-N3	4.35	134.68	125.94
20	B5	2258	OMU	C4-N3-C2	-4.34	120.86	126.58
64	A2	429	OMU	C4-N3-C2	-4.31	120.90	126.58
64	A2	1443	OMU	C4-N3-C2	-4.29	120.92	126.58
64	A2	1289	OMU	C4-N3-C2	-4.28	120.94	126.58
64	A2	1805	OMU	C4-N3-C2	-4.26	120.96	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	A2	628	OMU	N3-C2-N1	4.26	120.54	114.89
20	B5	3657	OMU	N3-C2-N1	4.19	120.45	114.89
64	A2	868	OMG	N9-C4-N3	4.18	134.34	125.94
64	A2	591	A2M	C2-N3-C4	4.18	121.63	111.75
64	A2	1338	4AC	N4-C4-N3	4.13	120.78	113.85
20	B5	4366	OMU	N3-C2-N1	4.12	120.36	114.89
64	A2	1327	OMU	N3-C2-N1	4.12	120.36	114.89
20	B5	3550	UY1	N1-C2-N3	4.11	119.78	115.13
20	B5	3973	OMU	N3-C2-N1	4.10	120.33	114.89
64	A2	1851	MA6	N1-C2-N3	-4.09	122.20	128.60
64	A2	116	OMU	N3-C2-N1	4.09	120.32	114.89
20	B5	2258	OMU	N3-C2-N1	4.07	120.29	114.89
20	B5	2680	OMU	N3-C2-N1	4.05	120.27	114.89
20	B5	4244	OMU	N3-C2-N1	4.05	120.26	114.89
64	A2	429	OMU	N3-C2-N1	4.04	120.25	114.89
64	A2	1852	MA6	N1-C2-N3	-4.04	122.28	128.60
20	B5	4052	OMU	N3-C2-N1	4.04	120.25	114.89
64	A2	355	OMU	N3-C2-N1	4.04	120.25	114.89
64	A2	1805	OMU	N3-C2-N1	4.03	120.23	114.89
64	A2	1851	MA6	C2-N1-C6	4.02	121.24	111.75
20	B5	4246	PSU	C4-N3-C2	-4.01	120.57	126.34
64	A2	1443	OMU	N3-C2-N1	4.00	120.20	114.89
20	B5	1801	PSU	C4-N3-C2	-3.98	120.60	126.34
64	A2	121	OMU	N3-C2-N1	3.98	120.17	114.89
64	A2	172	OMU	N3-C2-N1	3.97	120.17	114.89
20	B5	4217	PSU	C4-N3-C2	-3.96	120.63	126.34
64	A2	1289	OMU	N3-C2-N1	3.96	120.15	114.89
64	A2	1178	PSU	C4-N3-C2	-3.96	120.63	126.34
64	A2	407	PSU	C4-N3-C2	-3.95	120.65	126.34
20	B5	1683	PSU	C4-N3-C2	-3.94	120.66	126.34
20	B5	1489	A2M	C2-N3-C4	3.94	121.06	111.75
20	B5	2658	A2M	C2-N3-C4	3.93	121.05	111.75
20	B5	1731	PSU	C4-N3-C2	-3.93	120.68	126.34
20	B5	1491	PSU	C4-N3-C2	-3.93	120.68	126.34
64	A2	650	PSU	C4-N3-C2	-3.92	120.68	126.34
64	A2	864	PSU	C4-N3-C2	-3.92	120.68	126.34
64	A2	105	PSU	C4-N3-C2	-3.92	120.69	126.34
64	A2	166	A2M	C2-N3-C4	3.92	121.01	111.75
20	B5	3616	PSU	C4-N3-C2	-3.92	120.69	126.34
64	A2	1640	G7M	CN7-N7-C8	-3.92	118.79	124.84
64	A2	513	A2M	C2-N3-C4	3.91	121.00	111.75
6	B8	55	PSU	C4-N3-C2	-3.91	120.70	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	A2	682	PSU	C4-N3-C2	-3.91	120.71	126.34
64	A2	610	PSU	C4-N3-C2	-3.91	120.71	126.34
20	B5	4267	PSU	C4-N3-C2	-3.90	120.71	126.34
20	B5	1799	PSU	C4-N3-C2	-3.90	120.72	126.34
64	A2	1679	A2M	C2-N3-C4	3.90	120.97	111.75
64	A2	218	PSU	C4-N3-C2	-3.90	120.72	126.34
20	B5	1720	PSU	C4-N3-C2	-3.90	120.72	126.34
64	A2	1446	PSU	C4-N3-C2	-3.90	120.72	126.34
64	A2	1175	PSU	C4-N3-C2	-3.89	120.73	126.34
20	B5	4749	PSU	C4-N3-C2	-3.89	120.73	126.34
64	A2	1082	PSU	C4-N3-C2	-3.89	120.74	126.34
64	A2	815	PSU	C4-N3-C2	-3.89	120.74	126.34
20	B5	4107	PSU	C4-N3-C2	-3.88	120.74	126.34
20	B5	4325	PSU	C4-N3-C2	-3.88	120.74	126.34
20	B5	1638	PSU	C4-N3-C2	-3.88	120.75	126.34
64	A2	119	PSU	C4-N3-C2	-3.88	120.75	126.34
64	A2	1047	PSU	C4-N3-C2	-3.88	120.75	126.34
64	A2	1644	PSU	C4-N3-C2	-3.88	120.75	126.34
64	A2	1348	PSU	C4-N3-C2	-3.88	120.75	126.34
20	B5	1718	PSU	C4-N3-C2	-3.88	120.75	126.34
64	A2	1239	PSU	C4-N3-C2	-3.88	120.75	126.34
20	B5	1479	A2M	C2-N3-C4	3.88	120.91	111.75
64	A2	1368	PSU	C4-N3-C2	-3.88	120.75	126.34
20	B5	2351	PSU	C4-N3-C2	-3.88	120.75	126.34
20	B5	4042	PSU	C4-N3-C2	-3.87	120.76	126.34
20	B5	3502	PSU	C4-N3-C2	-3.87	120.76	126.34
20	B5	4336	A2M	C2-N3-C4	3.87	120.89	111.75
64	A2	802	PSU	C4-N3-C2	-3.87	120.77	126.34
64	A2	867	PSU	C4-N3-C2	-3.86	120.77	126.34
64	A2	1693	PSU	C4-N3-C2	-3.86	120.77	126.34
20	B5	4177	PSU	C4-N3-C2	-3.86	120.78	126.34
20	B5	2206	A2M	C2-N3-C4	3.86	120.87	111.75
20	B5	3369	PSU	C4-N3-C2	-3.86	120.78	126.34
20	B5	4298	PSU	C4-N3-C2	-3.86	120.78	126.34
20	B5	4169	PSU	C4-N3-C2	-3.86	120.78	126.34
64	A2	27	A2M	C2-N3-C4	3.86	120.86	111.75
20	B5	4058	PSU	C4-N3-C2	-3.86	120.78	126.34
64	A2	1046	PSU	C4-N3-C2	-3.86	120.78	126.34
64	A2	159	A2M	C2-N3-C4	3.86	120.86	111.75
64	A2	485	A2M	C2-N3-C4	3.86	120.86	111.75
20	B5	3456	A2M	C2-N3-C4	3.86	120.86	111.75
64	A2	1852	MA6	C2-N1-C6	3.86	120.86	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B5	3599	A2M	C2-N3-C4	3.85	120.86	111.75
64	A2	1005	PSU	C4-N3-C2	-3.85	120.79	126.34
20	B5	3562	A2M	C2-N3-C4	3.85	120.85	111.75
20	B5	1810	A2M	C2-N3-C4	3.85	120.85	111.75
64	A2	469	A2M	C2-N3-C4	3.85	120.84	111.75
20	B5	4193	5MC	C5-C6-N1	-3.85	119.38	123.34
64	A2	1057	PSU	C4-N3-C2	-3.85	120.79	126.34
64	A2	1384	A2M	C2-N3-C4	3.85	120.84	111.75
20	B5	3554	PSU	C4-N3-C2	-3.85	120.80	126.34
64	A2	1032	A2M	C2-N3-C4	3.85	120.84	111.75
20	B5	1721	PSU	C4-N3-C2	-3.85	120.80	126.34
20	B5	1270	A2M	C2-N3-C4	3.85	120.84	111.75
20	B5	4317	A2M	C2-N3-C4	3.84	120.83	111.75
20	B5	3576	PSU	C4-N3-C2	-3.84	120.80	126.34
64	A2	669	A2M	C2-N3-C4	3.84	120.83	111.75
20	B5	3462	PSU	C4-N3-C2	-3.84	120.80	126.34
64	A2	1233	PSU	C4-N3-C2	-3.84	120.80	126.34
20	B5	3517	A2M	C2-N3-C4	3.84	120.83	111.75
20	B5	4435	PSU	C4-N3-C2	-3.84	120.80	126.34
64	A2	1245	PSU	C4-N3-C2	-3.84	120.81	126.34
64	A2	816	PSU	C4-N3-C2	-3.84	120.81	126.34
20	B5	4269	A2M	C2-N3-C4	3.84	120.81	111.75
20	B5	2244	A2M	C2-N3-C4	3.84	120.81	111.75
20	B5	3447	PSU	C4-N3-C2	-3.84	120.81	126.34
64	A2	99	A2M	C2-N3-C4	3.84	120.81	111.75
20	B5	3966	6MZ	C2-N3-C4	3.84	120.81	111.75
64	A2	93	PSU	C4-N3-C2	-3.83	120.82	126.34
64	A2	652	PSU	C4-N3-C2	-3.83	120.82	126.34
20	B5	3490	PSU	C4-N3-C2	-3.83	120.82	126.34
64	A2	36	PSU	C4-N3-C2	-3.83	120.82	126.34
64	A2	109	PSU	C4-N3-C2	-3.83	120.82	126.34
20	B5	4045	PSU	C4-N3-C2	-3.83	120.82	126.34
64	A2	573	PSU	C4-N3-C2	-3.83	120.83	126.34
20	B5	3450	A2M	C2-N3-C4	3.83	120.79	111.75
64	A2	1626	PSU	C4-N3-C2	-3.82	120.83	126.34
20	B5	3496	PSU	C4-N3-C2	-3.82	120.83	126.34
20	B5	398	A2M	C2-N3-C4	3.82	120.78	111.75
64	A2	1833	6MZ	C2-N3-C4	3.82	120.78	111.75
20	B5	3427	PSU	C4-N3-C2	-3.82	120.83	126.34
64	A2	577	A2M	C2-N3-C4	3.82	120.78	111.75
6	B8	69	PSU	C4-N3-C2	-3.82	120.83	126.34
20	B5	4099	PSU	C4-N3-C2	-3.82	120.83	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B5	4374	PSU	C4-N3-C2	-3.82	120.83	126.34
64	A2	34	PSU	C4-N3-C2	-3.82	120.83	126.34
20	B5	4149	PSU	C4-N3-C2	-3.82	120.84	126.34
20	B5	3494	PSU	C4-N3-C2	-3.82	120.84	126.34
20	B5	3500	PSU	C4-N3-C2	-3.82	120.84	126.34
20	B5	3557	A2M	C2-N3-C4	3.81	120.76	111.75
20	B5	4419	PSU	C4-N3-C2	-3.81	120.85	126.34
20	B5	3466	PSU	C4-N3-C2	-3.81	120.86	126.34
20	B5	2630	A2M	C2-N3-C4	3.80	120.73	111.75
20	B5	4322	PSU	C4-N3-C2	-3.80	120.86	126.34
20	B5	3583	PSU	C4-N3-C2	-3.80	120.86	126.34
20	B5	4711	PSU	C4-N3-C2	-3.80	120.86	126.34
20	B5	400	A2M	C2-N3-C4	3.80	120.72	111.75
20	B5	4039	PSU	C4-N3-C2	-3.80	120.87	126.34
64	A2	687	PSU	C4-N3-C2	-3.80	120.87	126.34
20	B5	4188	PSU	C4-N3-C2	-3.79	120.88	126.34
20	B5	3492	A2M	C2-N3-C4	3.79	120.70	111.75
20	B5	4740	PSU	C4-N3-C2	-3.78	120.89	126.34
20	B5	4278	PSU	C4-N3-C2	-3.78	120.90	126.34
64	A2	1640	G7M	C5-C6-N1	3.77	119.67	111.79
20	B5	4382	PSU	C4-N3-C2	-3.77	120.90	126.34
64	A2	823	PSU	C4-N3-C2	-3.77	120.90	126.34
20	B5	3371	PSU	C4-N3-C2	-3.77	120.91	126.34
20	B5	1810	A2M	C2'-C1'-N9	-3.76	107.19	113.53
64	A2	967	PSU	C4-N3-C2	-3.76	120.92	126.34
20	B5	3652	PSU	C4-N3-C2	-3.75	120.93	126.34
20	B5	2475	PSU	C4-N3-C2	-3.74	120.94	126.34
20	B5	4203	PSU	C4-N3-C2	-3.74	120.95	126.34
20	B5	1537	PSU	C4-N3-C2	-3.74	120.96	126.34
64	A2	210	PSU	C4-N3-C2	-3.72	120.97	126.34
20	B5	3557	A2M	C2'-C1'-N9	-3.72	107.26	113.53
20	B5	3585	PSU	C4-N3-C2	-3.72	120.98	126.34
20	B5	1632	PSU	C4-N3-C2	-3.71	120.99	126.34
64	A2	1640	G7M	C4-C5-N7	-3.67	101.66	107.67
64	A2	1640	G7M	N9-C8-N7	-3.63	103.23	112.21
20	B5	2680	OMU	C5-C4-N3	3.61	120.25	114.84
64	A2	172	OMU	C5-C4-N3	3.61	120.25	114.84
64	A2	116	OMU	C5-C4-N3	3.59	120.21	114.84
64	A2	1327	OMU	C5-C4-N3	3.59	120.21	114.84
20	B5	4052	OMU	C5-C4-N3	3.58	120.20	114.84
64	A2	628	OMU	C5-C4-N3	3.56	120.17	114.84
64	A2	355	OMU	C5-C4-N3	3.55	120.16	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B5	4244	OMU	C5-C4-N3	3.54	120.13	114.84
20	B5	3973	OMU	C5-C4-N3	3.54	120.13	114.84
64	A2	1289	OMU	C5-C4-N3	3.54	120.13	114.84
20	B5	3657	OMU	C5-C4-N3	3.53	120.12	114.84
64	A2	429	OMU	C5-C4-N3	3.53	120.12	114.84
20	B5	4366	OMU	C5-C4-N3	3.52	120.11	114.84
64	A2	99	A2M	C2'-C1'-N9	-3.52	107.61	113.53
64	A2	121	OMU	C5-C4-N3	3.52	120.10	114.84
64	A2	1443	OMU	C5-C4-N3	3.51	120.09	114.84
6	B8	55	PSU	O2-C2-N1	-3.50	118.94	122.79
64	A2	1805	OMU	C5-C4-N3	3.50	120.07	114.84
20	B5	4298	PSU	O2-C2-N1	-3.49	118.95	122.79
64	A2	1851	MA6	C4-N9-C1'	-3.48	118.30	126.59
20	B5	1638	PSU	O2-C2-N1	-3.48	118.96	122.79
20	B5	2258	OMU	C5-C4-N3	3.48	120.04	114.84
64	A2	1175	PSU	O2-C2-N1	-3.47	118.97	122.79
64	A2	868	OMG	C6-C5-N7	3.47	136.70	130.25
20	B5	3576	PSU	O2-C2-N1	-3.47	118.97	122.79
20	B5	4382	PSU	O2-C2-N1	-3.46	118.98	122.79
20	B5	4435	PSU	O2-C2-N1	-3.45	118.99	122.79
64	A2	1239	PSU	O2-C2-N1	-3.45	119.00	122.79
64	A2	1852	MA6	C2-N3-C4	3.44	119.89	111.75
20	B5	4419	PSU	O2-C2-N1	-3.44	119.00	122.79
20	B5	3369	PSU	O2-C2-N1	-3.44	119.00	122.79
20	B5	4267	PSU	O2-C2-N1	-3.44	119.00	122.79
64	A2	652	PSU	O2-C2-N1	-3.43	119.01	122.79
9	BA	216	V5N	CD2-CG-ND1	3.43	110.21	105.71
64	A2	1233	PSU	O2-C2-N1	-3.43	119.02	122.79
64	A2	1057	PSU	O2-C2-N1	-3.43	119.02	122.79
64	A2	1644	PSU	O2-C2-N1	-3.43	119.02	122.79
20	B5	4374	PSU	O2-C2-N1	-3.42	119.02	122.79
64	A2	1446	PSU	O2-C2-N1	-3.42	119.03	122.79
20	B5	3494	PSU	O2-C2-N1	-3.42	119.03	122.79
64	A2	1178	PSU	O2-C2-N1	-3.42	119.03	122.79
20	B5	1491	PSU	O2-C2-N1	-3.42	119.03	122.79
64	A2	1851	MA6	C6-C5-N7	3.41	139.01	133.28
20	B5	1721	PSU	O2-C2-N1	-3.41	119.04	122.79
20	B5	4749	PSU	O2-C2-N1	-3.41	119.04	122.79
64	A2	802	PSU	O2-C2-N1	-3.41	119.04	122.79
20	B5	3496	PSU	O2-C2-N1	-3.40	119.04	122.79
64	A2	867	PSU	O2-C2-N1	-3.40	119.04	122.79
20	B5	3585	PSU	O2-C2-N1	-3.40	119.05	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	A2	1851	MA6	C2-N3-C4	3.40	119.78	111.75
64	A2	1005	PSU	O2-C2-N1	-3.40	119.05	122.79
64	A2	1626	PSU	O2-C2-N1	-3.40	119.05	122.79
20	B5	3514	5MC	C5-C6-N1	-3.40	119.84	123.34
20	B5	2475	PSU	O2-C2-N1	-3.39	119.05	122.79
64	A2	815	PSU	O2-C2-N1	-3.39	119.06	122.79
64	A2	573	PSU	O2-C2-N1	-3.39	119.06	122.79
20	B5	4188	PSU	O2-C2-N1	-3.39	119.06	122.79
22	Ba	39	V5N	CD2-CG-ND1	3.39	110.16	105.71
20	B5	4169	PSU	O2-C2-N1	-3.39	119.06	122.79
20	B5	4149	PSU	O2-C2-N1	-3.39	119.06	122.79
20	B5	1683	PSU	O2-C2-N1	-3.39	119.06	122.79
20	B5	4042	PSU	O2-C2-N1	-3.39	119.06	122.79
64	A2	1852	MA6	C1'-N9-C8	-3.39	119.49	127.14
20	B5	3462	PSU	O2-C2-N1	-3.38	119.06	122.79
20	B5	4278	PSU	O2-C2-N1	-3.38	119.07	122.79
20	B5	3447	PSU	O2-C2-N1	-3.38	119.07	122.79
20	B5	1718	PSU	O2-C2-N1	-3.38	119.07	122.79
64	A2	682	PSU	O2-C2-N1	-3.38	119.07	122.79
64	A2	1245	PSU	O2-C2-N1	-3.38	119.07	122.79
20	B5	1266	1MA	N9-C4-N3	3.38	134.81	126.94
64	A2	1047	PSU	O2-C2-N1	-3.38	119.07	122.79
20	B5	4058	PSU	O2-C2-N1	-3.38	119.07	122.79
20	B5	3490	PSU	O2-C2-N1	-3.37	119.08	122.79
20	B5	4107	PSU	O2-C2-N1	-3.37	119.08	122.79
64	A2	650	PSU	O2-C2-N1	-3.37	119.08	122.79
20	B5	1720	PSU	O2-C2-N1	-3.37	119.08	122.79
20	B5	4039	PSU	O2-C2-N1	-3.37	119.08	122.79
64	A2	1679	A2M	C4-C5-N7	-3.36	106.52	110.62
64	A2	218	PSU	O2-C2-N1	-3.36	119.09	122.79
64	A2	687	PSU	O2-C2-N1	-3.36	119.09	122.79
20	B5	3616	PSU	O2-C2-N1	-3.36	119.09	122.79
20	B5	3652	PSU	O2-C2-N1	-3.36	119.09	122.79
64	A2	407	PSU	O2-C2-N1	-3.36	119.09	122.79
20	B5	4246	PSU	O2-C2-N1	-3.36	119.09	122.79
64	A2	109	PSU	O2-C2-N1	-3.36	119.10	122.79
20	B5	4045	PSU	O2-C2-N1	-3.35	119.10	122.79
64	A2	610	PSU	O2-C2-N1	-3.35	119.10	122.79
64	A2	823	PSU	O2-C2-N1	-3.35	119.10	122.79
20	B5	3502	PSU	O2-C2-N1	-3.35	119.10	122.79
20	B5	4322	PSU	O2-C2-N1	-3.35	119.10	122.79
64	A2	967	PSU	O2-C2-N1	-3.35	119.10	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B5	4711	PSU	O2-C2-N1	-3.35	119.10	122.79
20	B5	1799	PSU	O2-C2-N1	-3.35	119.11	122.79
20	B5	4740	PSU	O2-C2-N1	-3.35	119.11	122.79
20	B5	1801	PSU	O2-C2-N1	-3.35	119.11	122.79
20	B5	3500	PSU	O2-C2-N1	-3.34	119.11	122.79
20	B5	1731	PSU	O2-C2-N1	-3.34	119.11	122.79
20	B5	1489	A2M	C4-C5-N7	-3.34	106.55	110.62
64	A2	1368	PSU	O2-C2-N1	-3.34	119.11	122.79
20	B5	4177	PSU	O2-C2-N1	-3.34	119.12	122.79
64	A2	105	PSU	O2-C2-N1	-3.34	119.12	122.79
20	B5	3562	A2M	C2'-C1'-N9	-3.34	107.92	113.53
64	A2	36	PSU	O2-C2-N1	-3.33	119.12	122.79
20	B5	3583	PSU	O2-C2-N1	-3.33	119.12	122.79
64	A2	816	PSU	O2-C2-N1	-3.33	119.12	122.79
20	B5	4336	A2M	C4-C5-N7	-3.33	106.56	110.62
20	B5	4217	PSU	O2-C2-N1	-3.33	119.12	122.79
64	A2	93	PSU	O2-C2-N1	-3.33	119.12	122.79
20	B5	3456	A2M	C2'-C1'-N9	-3.32	107.93	113.53
20	B5	3427	PSU	O2-C2-N1	-3.32	119.13	122.79
20	B5	4325	PSU	O2-C2-N1	-3.32	119.13	122.79
64	A2	1693	PSU	O2-C2-N1	-3.32	119.13	122.79
64	A2	513	A2M	C4-C5-N7	-3.32	106.58	110.62
64	A2	577	A2M	C4-C5-N7	-3.32	106.58	110.62
64	A2	159	A2M	C4-C5-N7	-3.32	106.58	110.62
64	A2	119	PSU	O2-C2-N1	-3.32	119.14	122.79
20	B5	1810	A2M	C4-C5-N7	-3.31	106.58	110.62
64	A2	34	PSU	O2-C2-N1	-3.31	119.14	122.79
64	A2	27	A2M	C4-C5-N7	-3.31	106.58	110.62
64	A2	864	PSU	O2-C2-N1	-3.31	119.14	122.79
6	B8	69	PSU	O2-C2-N1	-3.31	119.14	122.79
20	B5	1537	PSU	O2-C2-N1	-3.31	119.14	122.79
20	B5	2206	A2M	C4-C5-N7	-3.31	106.59	110.62
20	B5	3966	6MZ	C6-C5-N7	3.31	135.97	132.39
64	A2	1348	PSU	O2-C2-N1	-3.31	119.15	122.79
20	B5	4269	A2M	C4-C5-N7	-3.31	106.59	110.62
20	B5	3966	6MZ	C9-N6-C6	-3.31	120.03	122.87
64	A2	602	OMG	C6-C5-N7	3.30	136.39	130.25
64	A2	669	A2M	C4-C5-N7	-3.30	106.59	110.62
20	B5	3371	PSU	O2-C2-N1	-3.30	119.16	122.79
20	B5	1479	A2M	C4-C5-N7	-3.30	106.60	110.62
20	B5	3450	A2M	C4-C5-N7	-3.30	106.60	110.62
64	A2	469	A2M	C4-C5-N7	-3.30	106.60	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	A2	485	A2M	C4-C5-N7	-3.30	106.60	110.62
64	A2	1046	PSU	O2-C2-N1	-3.30	119.16	122.79
20	B5	3554	PSU	O2-C2-N1	-3.30	119.16	122.79
20	B5	4317	A2M	C4-C5-N7	-3.29	106.61	110.62
20	B5	4099	PSU	O2-C2-N1	-3.29	119.17	122.79
20	B5	3466	PSU	O2-C2-N1	-3.29	119.17	122.79
20	B5	4203	PSU	O2-C2-N1	-3.29	119.17	122.79
64	A2	577	A2M	C2'-C1'-N9	-3.28	108.00	113.53
20	B5	4166	PSU	C4-N3-C2	-3.28	121.61	126.34
20	B5	4369	OMG	C6-C5-N7	3.28	136.35	130.25
20	B5	2630	A2M	C2'-C1'-N9	-3.28	108.01	113.53
64	A2	1679	A2M	N3-C2-N1	-3.28	123.48	128.60
20	B5	1270	A2M	C4-C5-N7	-3.27	106.63	110.62
20	B5	2244	A2M	C4-C5-N7	-3.27	106.63	110.62
20	B5	3676	OMG	C6-C5-N7	3.27	136.34	130.25
64	A2	1384	A2M	C4-C5-N7	-3.27	106.63	110.62
20	B5	3517	A2M	C4-C5-N7	-3.27	106.64	110.62
20	B5	4166	PSU	O2-C2-N1	-3.27	119.19	122.79
20	B5	2351	PSU	O2-C2-N1	-3.26	119.21	122.79
20	B5	398	A2M	C4-C5-N7	-3.25	106.66	110.62
20	B5	3599	A2M	C4-C5-N7	-3.25	106.66	110.62
64	A2	1032	A2M	C4-C5-N7	-3.25	106.66	110.62
20	B5	400	A2M	C4-C5-N7	-3.25	106.66	110.62
20	B5	2206	A2M	C2'-C1'-N9	-3.25	108.05	113.53
20	B5	1632	PSU	O2-C2-N1	-3.25	119.21	122.79
20	B5	2658	A2M	C4-C5-N7	-3.25	106.66	110.62
64	A2	1329	OMG	C6-C5-N7	3.24	136.28	130.25
20	B5	3966	6MZ	C4-C5-N7	-3.24	106.67	110.62
64	A2	166	A2M	C4-C5-N7	-3.24	106.67	110.62
64	A2	1082	PSU	O2-C2-N1	-3.24	119.22	122.79
20	B5	3631	OMG	C6-C5-N7	3.24	136.27	130.25
64	A2	645	OMG	C6-C5-N7	3.24	136.27	130.25
20	B5	1489	A2M	N3-C2-N1	-3.23	123.54	128.60
20	B5	1260	OMG	C6-C5-N7	3.23	136.26	130.25
20	B5	4383	OMG	C6-C5-N7	3.23	136.25	130.25
20	B5	2207	OMG	C6-C5-N7	3.23	136.25	130.25
64	A2	210	PSU	O2-C2-N1	-3.22	119.24	122.79
64	A2	99	A2M	C4-C5-N7	-3.22	106.70	110.62
20	B5	3557	A2M	C4-C5-N7	-3.22	106.70	110.62
20	B5	3974	OMG	C6-C5-N7	3.20	136.21	130.25
20	B5	3492	A2M	C4-C5-N7	-3.20	106.72	110.62
20	B5	3456	A2M	C4-C5-N7	-3.20	106.72	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B5	3562	A2M	C4-C5-N7	-3.19	106.73	110.62
64	A2	1448	OMG	C6-C5-N7	3.19	136.18	130.25
20	B5	3456	A2M	N3-C2-N1	-3.18	123.63	128.60
64	A2	166	A2M	N3-C2-N1	-3.18	123.63	128.60
64	A2	1640	G7M	O6-C6-C5	-3.18	120.89	128.06
64	A2	591	A2M	N3-C2-N1	-3.17	123.64	128.60
20	B5	2630	A2M	C4-C5-N7	-3.17	106.76	110.62
64	A2	684	OMG	C6-C5-N7	3.17	136.14	130.25
20	B5	3476	OMG	C6-C5-N7	3.17	136.13	130.25
20	B5	4317	A2M	C2'-C1'-N9	-3.17	108.20	113.53
20	B5	4336	A2M	N3-C2-N1	-3.16	123.66	128.60
20	B5	4116	OMG	C6-C5-N7	3.16	136.13	130.25
64	A2	591	A2M	C4-C5-N7	-3.16	106.77	110.62
20	B5	4245	OMG	C6-C5-N7	3.16	136.13	130.25
20	B5	4364	OMG	C6-C5-N7	3.16	136.13	130.25
20	B5	1810	A2M	N3-C2-N1	-3.16	123.66	128.60
64	A2	27	A2M	N3-C2-N1	-3.16	123.66	128.60
6	B8	75	OMG	C6-C5-N7	3.16	136.12	130.25
64	A2	1032	A2M	N3-C2-N1	-3.15	123.67	128.60
20	B5	3517	A2M	N3-C2-N1	-3.15	123.67	128.60
20	B5	3557	A2M	N3-C2-N1	-3.15	123.67	128.60
64	A2	510	OMG	C6-C5-N7	3.15	136.11	130.25
20	B5	4240	OMG	C6-C5-N7	3.15	136.11	130.25
64	A2	1852	MA6	C4-N9-C1'	-3.15	119.09	126.59
64	A2	1249	B8N	C4-N3-C2	-3.14	121.48	125.46
64	A2	1833	6MZ	C4-C5-N7	-3.14	106.79	110.62
20	B5	3599	A2M	N3-C2-N1	-3.14	123.69	128.60
64	A2	513	A2M	N3-C2-N1	-3.14	123.69	128.60
20	B5	3492	A2M	N3-C2-N1	-3.14	123.69	128.60
20	B5	1270	A2M	N3-C2-N1	-3.13	123.71	128.60
64	A2	1384	A2M	N3-C2-N1	-3.13	123.71	128.60
20	B5	3562	A2M	N3-C2-N1	-3.13	123.71	128.60
20	B5	398	A2M	N3-C2-N1	-3.12	123.72	128.60
64	A2	437	OMG	C6-C5-N7	3.12	136.06	130.25
20	B5	3599	A2M	C2'-C1'-N9	-3.12	108.27	113.53
20	B5	2658	A2M	N3-C2-N1	-3.12	123.73	128.60
64	A2	1851	MA6	C1'-N9-C8	-3.11	120.10	127.14
20	B5	2244	A2M	N3-C2-N1	-3.11	123.73	128.60
64	A2	469	A2M	N3-C2-N1	-3.11	123.73	128.60
20	B5	3359	OMG	C6-C5-N7	3.11	136.04	130.25
64	A2	669	A2M	N3-C2-N1	-3.11	123.74	128.60
20	B5	2244	A2M	C2'-C1'-N9	-3.11	108.30	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B5	4317	A2M	N3-C2-N1	-3.10	123.75	128.60
20	B5	4269	A2M	N3-C2-N1	-3.10	123.75	128.60
20	B5	3942	OMG	C6-C5-N7	3.09	136.00	130.25
64	A2	99	A2M	N3-C2-N1	-3.09	123.77	128.60
64	A2	1032	A2M	C2'-C1'-N9	-3.09	108.33	113.53
64	A2	485	A2M	N3-C2-N1	-3.09	123.78	128.60
20	B5	4138	OMG	C6-C5-N7	3.08	135.98	130.25
20	B5	2267	OMG	C6-C5-N7	3.08	135.98	130.25
64	A2	159	A2M	N3-C2-N1	-3.08	123.79	128.60
20	B5	2630	A2M	N3-C2-N1	-3.08	123.79	128.60
64	A2	577	A2M	N3-C2-N1	-3.07	123.79	128.60
20	B5	1479	A2M	N3-C2-N1	-3.07	123.80	128.60
20	B5	1477	OMG	C6-C5-N7	3.07	135.96	130.25
20	B5	3966	6MZ	N1-C2-N3	-3.07	123.80	128.60
20	B5	3524	OMG	C6-C5-N7	3.06	135.95	130.25
20	B5	1580	OMG	C6-C5-N7	3.06	135.94	130.25
20	B5	4269	A2M	C2'-C1'-N9	-3.06	108.38	113.53
64	A2	1491	OMG	C6-C5-N7	3.06	135.93	130.25
20	B5	3492	A2M	C2'-C1'-N9	-3.05	108.39	113.53
20	B5	2206	A2M	N3-C2-N1	-3.05	123.83	128.60
20	B5	400	A2M	N3-C2-N1	-3.04	123.85	128.60
64	A2	1852	MA6	C5-C4-N9	-3.04	102.25	105.78
20	B5	3450	A2M	N3-C2-N1	-3.03	123.86	128.60
64	A2	159	A2M	C2'-C1'-N9	-3.02	108.44	113.53
64	A2	1640	G7M	C2-N1-C6	-3.02	119.59	125.10
20	B5	2680	OMU	O4-C4-C5	-3.02	119.85	125.16
64	A2	172	OMU	O4-C4-C5	-3.01	119.87	125.16
64	A2	116	OMU	O4-C4-C5	-3.00	119.88	125.16
64	A2	121	OMU	O4-C4-C5	-3.00	119.89	125.16
64	A2	1833	6MZ	N1-C2-N3	-2.99	123.93	128.60
64	A2	1289	OMU	O4-C4-C5	-2.99	119.91	125.16
64	A2	355	OMU	O4-C4-C5	-2.98	119.92	125.16
64	A2	1327	OMU	O4-C4-C5	-2.98	119.92	125.16
64	A2	27	A2M	C2'-C1'-N9	-2.98	108.52	113.53
20	B5	4244	OMU	O4-C4-C5	-2.98	119.92	125.16
20	B5	3973	OMU	O4-C4-C5	-2.97	119.94	125.16
20	B5	400	A2M	C2'-C1'-N9	-2.96	108.54	113.53
64	A2	429	OMU	O4-C4-C5	-2.96	119.96	125.16
64	A2	1833	6MZ	C6-C5-N7	2.95	135.59	132.39
64	A2	628	OMU	O4-C4-C5	-2.95	119.97	125.16
20	B5	2719	OMG	C6-C5-N7	2.95	135.73	130.25
64	A2	1805	OMU	O4-C4-C5	-2.94	120.00	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B5	4366	OMU	O4-C4-C5	-2.93	120.00	125.16
64	A2	1852	MA6	C5-C6-N6	-2.93	120.19	125.30
20	B5	4052	OMU	O4-C4-C5	-2.93	120.01	125.16
64	A2	1852	MA6	C6-C5-N7	2.92	138.19	133.28
64	A2	1443	OMU	O4-C4-C5	-2.92	120.03	125.16
20	B5	2258	OMU	O4-C4-C5	-2.91	120.04	125.16
20	B5	3657	OMU	O4-C4-C5	-2.90	120.06	125.16
64	A2	1249	B8N	N3-C2-N1	2.87	120.81	116.76
64	A2	1384	A2M	C2'-C1'-N9	-2.84	108.75	113.53
64	A2	469	A2M	C2'-C1'-N9	-2.81	108.81	113.53
20	B5	4336	A2M	C5-N7-C8	2.80	107.49	103.51
64	A2	159	A2M	C5-N7-C8	2.80	107.49	103.51
64	A2	1679	A2M	C5-N7-C8	2.80	107.48	103.51
64	A2	577	A2M	C5-N7-C8	2.79	107.47	103.51
20	B5	3517	A2M	C5-N7-C8	2.79	107.47	103.51
64	A2	1833	6MZ	C9-N6-C6	-2.78	120.47	122.87
64	A2	513	A2M	C5-N7-C8	2.78	107.45	103.51
64	A2	469	A2M	C5-N7-C8	2.77	107.45	103.51
20	B5	1489	A2M	C5-N7-C8	2.77	107.45	103.51
20	B5	4269	A2M	C5-N7-C8	2.77	107.44	103.51
64	A2	485	A2M	C5-N7-C8	2.77	107.44	103.51
20	B5	2206	A2M	C5-N7-C8	2.76	107.43	103.51
64	A2	669	A2M	C5-N7-C8	2.75	107.42	103.51
20	B5	3456	A2M	C5-N7-C8	2.75	107.42	103.51
64	A2	1851	MA6	C5-C4-N9	-2.75	102.58	105.78
64	A2	166	A2M	C2'-C1'-N9	-2.75	108.90	113.53
20	B5	1479	A2M	C5-N7-C8	2.75	107.42	103.51
20	B5	3599	A2M	C5-N7-C8	2.75	107.41	103.51
64	A2	166	A2M	C5-N7-C8	2.74	107.40	103.51
64	A2	868	OMG	C4-C5-N7	-2.74	106.39	110.72
20	B5	2244	A2M	C5-N7-C8	2.74	107.40	103.51
64	A2	513	A2M	C2'-C1'-N9	-2.73	108.93	113.53
64	A2	1032	A2M	C5-N7-C8	2.73	107.38	103.51
20	B5	3492	A2M	C5-N7-C8	2.73	107.38	103.51
20	B5	398	A2M	C5-N7-C8	2.72	107.38	103.51
20	B5	1810	A2M	C5-N7-C8	2.72	107.38	103.51
64	A2	1384	A2M	C5-N7-C8	2.72	107.37	103.51
20	B5	4317	A2M	C5-N7-C8	2.72	107.37	103.51
20	B5	2658	A2M	C5-N7-C8	2.72	107.37	103.51
20	B5	3966	6MZ	C5-N7-C8	2.71	107.36	103.51
20	B5	3450	A2M	C5-N7-C8	2.71	107.36	103.51
20	B5	3557	A2M	C5-N7-C8	2.71	107.36	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	A2	27	A2M	C5-N7-C8	2.71	107.36	103.51
20	B5	400	A2M	C5-N7-C8	2.71	107.35	103.51
64	A2	591	A2M	C5-N7-C8	2.71	107.35	103.51
64	A2	602	OMG	C4-C5-N7	-2.70	106.44	110.72
64	A2	1833	6MZ	C5-N7-C8	2.70	107.34	103.51
20	B5	1270	A2M	C5-N7-C8	2.70	107.34	103.51
20	B5	3562	A2M	C5-N7-C8	2.69	107.34	103.51
20	B5	4369	OMG	C4-C5-N7	-2.69	106.47	110.72
20	B5	3456	A2M	C4-N9-C8	2.68	108.64	105.73
20	B5	3517	A2M	C4-N9-C8	2.68	108.64	105.73
20	B5	3450	A2M	C2'-C1'-N9	-2.67	109.03	113.53
64	A2	1329	OMG	C4-C5-N7	-2.67	106.50	110.72
64	A2	1679	A2M	C4-N9-C8	2.67	108.62	105.73
64	A2	645	OMG	C4-C5-N7	-2.66	106.51	110.72
20	B5	2207	OMG	C4-C5-N7	-2.66	106.51	110.72
20	B5	4336	A2M	C2'-C1'-N9	-2.66	109.05	113.53
64	A2	99	A2M	C5-N7-C8	2.66	107.29	103.51
20	B5	2630	A2M	C5-N7-C8	2.66	107.28	103.51
20	B5	3974	OMG	C4-C5-N7	-2.64	106.54	110.72
80	An	138	IAS	OD1-CG-CB	-2.64	117.74	125.43
64	A2	1448	OMG	C4-C5-N7	-2.64	106.55	110.72
20	B5	3676	OMG	C4-C5-N7	-2.64	106.55	110.72
20	B5	4383	OMG	C4-C5-N7	-2.64	106.55	110.72
20	B5	3557	A2M	C4-N9-C8	2.63	108.58	105.73
20	B5	3599	A2M	C4-N9-C8	2.63	108.58	105.73
20	B5	4364	OMG	C4-C5-N7	-2.63	106.56	110.72
20	B5	1260	OMG	C4-C5-N7	-2.62	106.57	110.72
20	B5	4245	OMG	C4-C5-N7	-2.62	106.57	110.72
20	B5	3492	A2M	C4-N9-C8	2.62	108.57	105.73
20	B5	1489	A2M	C4-N9-C8	2.62	108.57	105.73
20	B5	4116	OMG	C4-C5-N7	-2.60	106.60	110.72
20	B5	3631	OMG	C4-C5-N7	-2.60	106.60	110.72
20	B5	4166	PSU	C6-C5-C4	-2.60	116.38	118.20
20	B5	3359	OMG	C4-C5-N7	-2.60	106.61	110.72
64	A2	510	OMG	C4-C5-N7	-2.60	106.61	110.72
64	A2	669	A2M	C4-N9-C8	2.59	108.54	105.73
20	B5	3476	OMG	C4-C5-N7	-2.59	106.62	110.72
20	B5	4138	OMG	C4-C5-N7	-2.59	106.63	110.72
64	A2	577	A2M	C4-N9-C8	2.58	108.53	105.73
64	A2	684	OMG	C4-C5-N7	-2.58	106.64	110.72
20	B5	398	A2M	C4-N9-C8	2.58	108.52	105.73
20	B5	1477	OMG	C4-C5-N7	-2.58	106.64	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B5	4336	A2M	C4-N9-C8	2.57	108.52	105.73
20	B5	3514	5MC	C5-C4-N3	-2.57	118.90	121.67
20	B5	4240	OMG	C4-C5-N7	-2.57	106.66	110.72
64	A2	1491	OMG	C4-C5-N7	-2.57	106.66	110.72
20	B5	1266	1MA	C4-C5-N7	-2.56	106.66	110.72
64	A2	437	OMG	C4-C5-N7	-2.56	106.67	110.72
6	B8	75	OMG	C4-C5-N7	-2.56	106.67	110.72
20	B5	3524	OMG	C4-C5-N7	-2.55	106.69	110.72
64	A2	1384	A2M	C4-N9-C8	2.54	108.48	105.73
20	B5	1810	A2M	C4-N9-C8	2.54	108.48	105.73
20	B5	2719	OMG	C4-C5-N7	-2.54	106.71	110.72
20	B5	3942	OMG	C4-C5-N7	-2.53	106.71	110.72
20	B5	2267	OMG	C4-C5-N7	-2.53	106.71	110.72
20	B5	1270	A2M	C4-N9-C8	2.53	108.47	105.73
20	B5	4317	A2M	C4-N9-C8	2.53	108.47	105.73
20	B5	1580	OMG	C4-C5-N7	-2.53	106.72	110.72
64	A2	1032	A2M	C4-N9-C8	2.52	108.46	105.73
20	B5	3517	A2M	O4'-C1'-N9	2.52	113.02	108.06
20	B5	3562	A2M	C4-N9-C8	2.51	108.45	105.73
64	A2	513	A2M	C4-N9-C8	2.51	108.44	105.73
20	B5	3966	6MZ	C4-N9-C8	2.50	108.44	105.73
20	B5	2244	A2M	C4-N9-C8	2.50	108.44	105.73
64	A2	166	A2M	C4-N9-C8	2.50	108.44	105.73
14	Au	1	AME	O-C-CA	-2.50	118.22	124.78
20	B5	4269	A2M	C4-N9-C8	2.49	108.43	105.73
64	A2	1833	6MZ	C4-N9-C8	2.49	108.43	105.73
64	A2	27	A2M	C4-N9-C8	2.48	108.42	105.73
64	A2	469	A2M	C4-N9-C8	2.48	108.42	105.73
20	B5	400	A2M	C4-N9-C8	2.48	108.41	105.73
64	A2	159	A2M	C4-N9-C8	2.47	108.41	105.73
20	B5	2630	A2M	C4-N9-C8	2.47	108.40	105.73
20	B5	2206	A2M	C4-N9-C8	2.45	108.38	105.73
20	B5	4193	5MC	C5-C4-N3	-2.44	119.04	121.67
9	BA	216	V5N	O-C-CA	-2.44	118.39	124.78
5	Ar	2	SAC	O-C-CA	-2.43	118.41	124.78
64	A2	1679	A2M	C6-C5-N7	2.42	136.53	132.02
20	B5	3450	A2M	C4-N9-C8	2.42	108.35	105.73
64	A2	485	A2M	C2'-C1'-N9	-2.41	109.47	113.53
64	A2	1843	4AC	C5-C4-N4	-2.40	118.75	122.92
64	A2	99	A2M	C4-N9-C8	2.40	108.33	105.73
20	B5	1479	A2M	C4-N9-C8	2.40	108.33	105.73
20	B5	2658	A2M	C2'-C1'-N9	-2.39	109.50	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	A2	485	A2M	C4-N9-C8	2.39	108.32	105.73
64	A2	1338	4AC	C6-C5-C4	2.38	119.87	116.96
20	B5	3550	UY1	CM2-O2'-C2'	-2.37	108.29	114.52
64	A2	628	OMU	O2-C2-N1	-2.37	119.63	122.79
27	AZ	2	SAC	O-C-CA	-2.37	118.57	124.78
20	B5	3550	UY1	C6-C5-C4	2.35	119.84	118.20
20	B5	2658	A2M	C4-N9-C8	2.34	108.26	105.73
20	B5	1489	A2M	C6-C5-N7	2.33	136.36	132.02
20	B5	3517	A2M	C2'-C1'-N9	-2.32	109.62	113.53
64	A2	1443	OMU	C1'-N1-C2	2.31	121.75	117.57
20	B5	3550	UY1	O2-C2-N1	-2.27	120.29	122.79
20	B5	4336	A2M	C6-C5-N7	2.26	136.22	132.02
20	B5	3517	A2M	C6-C5-N7	2.25	136.21	132.02
64	A2	1852	MA6	N1-C6-N6	2.25	119.54	117.08
22	Ba	39	V5N	O-C-CA	-2.24	118.90	124.78
64	A2	1843	4AC	C6-C5-C4	2.24	119.70	116.96
84	Br	2	SAC	O-C-CA	-2.23	118.93	124.78
20	B5	1810	A2M	C6-C5-N7	2.23	136.17	132.02
64	A2	669	A2M	C6-C5-N7	2.23	136.17	132.02
20	B5	3456	A2M	C6-C5-N7	2.22	136.16	132.02
64	A2	1249	B8N	C5-C4-N3	2.22	120.29	116.17
64	A2	27	A2M	C6-C5-N7	2.21	136.14	132.02
64	A2	469	A2M	C6-C5-N7	2.21	136.13	132.02
18	Aw	62	HY3	O-C-CA	-2.20	118.68	124.83
64	A2	1327	OMU	O2-C2-N1	-2.20	119.86	122.79
64	A2	1384	A2M	C6-C5-N7	2.20	136.12	132.02
20	B5	2244	A2M	C6-C5-N7	2.19	136.10	132.02
20	B5	4269	A2M	C6-C5-N7	2.19	136.10	132.02
64	A2	513	A2M	C6-C5-N7	2.19	136.09	132.02
20	B5	398	A2M	C6-C5-N7	2.18	136.09	132.02
20	B5	3599	A2M	C6-C5-N7	2.18	136.09	132.02
64	A2	463	OMC	O2-C2-N3	-2.18	118.79	122.33
64	A2	577	A2M	C6-C5-N7	2.18	136.08	132.02
20	B5	2267	OMG	O6-C6-C5	-2.17	120.85	126.60
64	A2	166	A2M	C6-C5-N7	2.17	136.06	132.02
20	B5	1270	A2M	C6-C5-N7	2.17	136.06	132.02
64	A2	159	A2M	C6-C5-N7	2.16	136.05	132.02
20	B5	3557	A2M	C6-C5-N7	2.16	136.04	132.02
20	B5	3517	A2M	N9-C8-N7	-2.16	110.96	113.91
20	B5	4317	A2M	C6-C5-N7	2.15	136.03	132.02
6	B8	75	OMG	O6-C6-C5	-2.15	120.90	126.60
20	B5	2719	OMG	O6-C6-C5	-2.15	120.90	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	A2	1032	A2M	C6-C5-N7	2.15	136.02	132.02
20	B5	1580	OMG	O6-C6-C5	-2.15	120.91	126.60
20	B5	3942	OMG	O6-C6-C5	-2.14	120.91	126.60
20	B5	400	A2M	C6-C5-N7	2.14	136.01	132.02
20	B5	1479	A2M	C6-C5-N7	2.14	136.01	132.02
64	A2	1805	OMU	C1'-N1-C2	2.14	121.45	117.57
20	B5	3492	A2M	C6-C5-N7	2.14	136.01	132.02
20	B5	2206	A2M	C6-C5-N7	2.14	136.00	132.02
20	B5	3514	5MC	O2-C2-N3	-2.14	118.86	122.33
64	A2	1679	A2M	N9-C8-N7	-2.14	110.99	113.91
20	B5	3456	A2M	N9-C8-N7	-2.13	110.99	113.91
64	A2	485	A2M	C6-C5-N7	2.13	135.99	132.02
64	A2	1448	OMG	O6-C6-C5	-2.13	120.94	126.60
20	B5	4240	OMG	O6-C6-C5	-2.13	120.95	126.60
64	A2	1491	OMG	O6-C6-C5	-2.13	120.95	126.60
20	B5	3562	A2M	C6-C5-N7	2.13	135.98	132.02
20	B5	3359	OMG	O6-C6-C5	-2.13	120.96	126.60
64	A2	437	OMG	O6-C6-C5	-2.13	120.96	126.60
20	B5	3573	OMC	O2-C2-N3	-2.12	118.88	122.33
64	A2	669	A2M	C2'-C1'-N9	-2.12	109.96	113.53
20	B5	3450	A2M	C6-C5-N7	2.12	135.97	132.02
64	A2	1289	OMU	C1'-N1-C2	2.12	121.41	117.57
20	B5	2630	A2M	C6-C5-N7	2.12	135.96	132.02
20	B5	1479	A2M	C2'-C1'-N9	-2.12	109.97	113.53
64	A2	510	OMG	O6-C6-C5	-2.11	120.99	126.60
64	A2	684	OMG	O6-C6-C5	-2.11	120.99	126.60
64	A2	591	A2M	C4-N9-C8	2.11	108.02	105.73
20	B5	1477	OMG	O6-C6-C5	-2.11	121.00	126.60
64	A2	645	OMG	O6-C6-C5	-2.11	121.01	126.60
20	B5	3631	OMG	O6-C6-C5	-2.10	121.02	126.60
20	B5	4245	OMG	O6-C6-C5	-2.10	121.02	126.60
20	B5	4364	OMG	O6-C6-C5	-2.10	121.04	126.60
20	B5	3524	OMG	O6-C6-C5	-2.10	121.04	126.60
20	B5	3476	OMG	O6-C6-C5	-2.09	121.04	126.60
20	B5	3676	OMG	O6-C6-C5	-2.09	121.05	126.60
20	B5	2207	OMG	O6-C6-C5	-2.09	121.05	126.60
20	B5	3974	OMG	O6-C6-C5	-2.09	121.06	126.60
20	B5	4116	OMG	O6-C6-C5	-2.09	121.06	126.60
20	B5	3657	OMU	O2-C2-N1	-2.09	120.01	122.79
20	B5	4383	OMG	O6-C6-C5	-2.09	121.06	126.60
20	B5	1260	OMG	O6-C6-C5	-2.08	121.07	126.60
20	B5	2658	A2M	C6-C5-N7	2.08	135.90	132.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	A2	1640	G7M	C5-C4-N9	-2.08	101.33	105.89
20	B5	2265	OMC	O2-C2-N3	-2.08	118.95	122.33
20	B5	4138	OMG	O6-C6-C5	-2.08	121.08	126.60
64	A2	99	A2M	C6-C5-N7	2.08	135.89	132.02
64	A2	1392	OMC	O2-C2-N3	-2.07	118.97	122.33
64	A2	518	OMC	O2-C2-N3	-2.07	118.97	122.33
20	B5	3599	A2M	N9-C8-N7	-2.06	111.09	113.91
20	B5	1489	A2M	N9-C8-N7	-2.06	111.09	113.91
20	B5	4336	A2M	N9-C8-N7	-2.06	111.09	113.91
64	A2	1851	MA6	C5-N7-C8	2.06	106.44	103.51
64	A2	1851	MA6	C5-C6-N6	-2.05	121.72	125.30
64	A2	669	A2M	N9-C8-N7	-2.05	111.11	113.91
20	B5	4282	OMC	O2-C2-N3	-2.05	119.00	122.33
20	B5	3557	A2M	N9-C8-N7	-2.05	111.11	113.91
64	A2	577	A2M	N9-C8-N7	-2.05	111.11	113.91
20	B5	1632	PSU	O4'-C1'-C2'	2.04	108.03	105.14
64	A2	1329	OMG	O6-C6-C5	-2.04	121.18	126.60
64	A2	602	OMG	O6-C6-C5	-2.03	121.21	126.60
64	A2	1338	4AC	C5-C4-N4	-2.03	119.39	122.92
20	B5	3492	A2M	N9-C8-N7	-2.03	111.14	113.91
20	B5	1270	A2M	C2'-C1'-N9	-2.03	110.12	113.53
64	A2	1032	A2M	N9-C8-N7	-2.02	111.15	113.91
20	B5	2680	OMU	O2-C2-N1	-2.02	120.10	122.79
20	B5	4269	A2M	N9-C8-N7	-2.02	111.15	113.91
20	B5	4244	OMU	O2-C2-N1	-2.02	120.10	122.79
20	B5	4369	OMG	O6-C6-C5	-2.02	121.25	126.60
20	B5	4246	PSU	C5-C6-N1	-2.02	119.08	122.11
20	B5	1810	A2M	N9-C8-N7	-2.02	111.16	113.91
64	A2	1384	A2M	N9-C8-N7	-2.01	111.16	113.91
20	B5	398	A2M	N9-C8-N7	-2.01	111.17	113.91
20	B5	1266	1MA	C6-C5-N7	2.01	135.85	132.20
20	B5	1731	PSU	C5-C6-N1	-2.01	119.10	122.11
20	B5	2244	A2M	N9-C8-N7	-2.00	111.17	113.91
64	A2	469	A2M	N9-C8-N7	-2.00	111.17	113.91
64	A2	166	A2M	N9-C8-N7	-2.00	111.17	113.91

There are no chirality outliers.

All (118) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	BA	216	V5N	O-C-CA-CB
15	BC	2	AYA	C-CA-N-CT

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Mol	Chain	Res	Type	Atoms
20	B5	3433	OMC	C2'-C1'-N1-C2
20	B5	3433	OMC	C2'-C1'-N1-C6
20	B5	4166	PSU	C2'-C1'-C5-C4
20	B5	4166	PSU	C2'-C1'-C5-C6
20	B5	4193	5MC	C2'-C1'-N1-C2
20	B5	4193	5MC	C2'-C1'-N1-C6
20	B5	4336	A2M	C4'-C5'-O5'-P
20	B5	4382	PSU	O4'-C1'-C5-C4
20	B5	4382	PSU	O4'-C1'-C5-C6
20	B5	4382	PSU	C3'-C4'-C5'-O5'
64	A2	429	OMU	C2'-C1'-N1-C2
64	A2	429	OMU	C2'-C1'-N1-C6
64	A2	513	A2M	C3'-C4'-C5'-O5'
64	A2	628	OMU	C2'-C1'-N1-C2
64	A2	628	OMU	C2'-C1'-N1-C6
64	A2	669	A2M	O4'-C4'-C5'-O5'
64	A2	1448	OMG	C3'-C4'-C5'-O5'
64	A2	1851	MA6	C5-C6-N6-C9
64	A2	1851	MA6	C5-C6-N6-C10
64	A2	1852	MA6	C5-C6-N6-C9
78	Bo	53	MLZ	O-C-CA-CB
64	A2	1249	B8N	N34-C33-C34-O35
64	A2	1338	4AC	N3-C4-N4-C7
64	A2	1338	4AC	O7-C7-N4-C4
64	A2	1338	4AC	CM7-C7-N4-C4
64	A2	1843	4AC	N3-C4-N4-C7
64	A2	1843	4AC	C5-C4-N4-C7
64	A2	1843	4AC	O7-C7-N4-C4
64	A2	1843	4AC	CM7-C7-N4-C4
15	BC	2	AYA	OT-CT-N-CA
15	BC	2	AYA	CM-CT-N-CA
64	A2	429	OMU	O4'-C1'-N1-C2
20	B5	398	A2M	O4'-C4'-C5'-O5'
20	B5	1489	A2M	O4'-C4'-C5'-O5'
20	B5	3517	A2M	O4'-C4'-C5'-O5'
64	A2	513	A2M	O4'-C4'-C5'-O5'
64	A2	645	OMG	O4'-C4'-C5'-O5'
64	A2	645	OMG	C3'-C4'-C5'-O5'
14	Au	1	AME	CT2-CT1-N-CA
14	Au	1	AME	OT-CT1-N-CA
64	A2	1249	B8N	N34-C33-C34-O36
20	B5	398	A2M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
20	B5	2207	OMG	O4'-C4'-C5'-O5'
20	B5	3517	A2M	C3'-C4'-C5'-O5'
64	A2	27	A2M	O4'-C4'-C5'-O5'
64	A2	669	A2M	C3'-C4'-C5'-O5'
64	A2	1851	MA6	N1-C6-N6-C9
64	A2	1852	MA6	N1-C6-N6-C9
64	A2	429	OMU	O4'-C1'-N1-C6
20	B5	1489	A2M	C3'-C4'-C5'-O5'
20	B5	4382	PSU	O4'-C4'-C5'-O5'
64	A2	27	A2M	C3'-C4'-C5'-O5'
64	A2	1448	OMG	O4'-C4'-C5'-O5'
20	B5	2207	OMG	C3'-C4'-C5'-O5'
64	A2	1852	MA6	C5-C6-N6-C10
12	BB	245	HIC	CA-CB-CG-CD2
12	BB	245	HIC	CA-CB-CG-ND1
64	A2	591	A2M	C3'-C4'-C5'-O5'
64	A2	1640	G7M	O4'-C4'-C5'-O5'
20	B5	2630	A2M	C2'-C1'-N9-C8
20	B5	3433	OMC	O4'-C1'-N1-C6
64	A2	628	OMU	O4'-C1'-N1-C6
64	A2	1249	B8N	C32-C33-C34-O36
20	B5	3576	PSU	C4'-C5'-O5'-P
20	B5	3619	OMC	C4'-C5'-O5'-P
64	A2	469	A2M	O4'-C4'-C5'-O5'
64	A2	1640	G7M	C3'-C4'-C5'-O5'
64	A2	591	A2M	C2'-C1'-N9-C4
64	A2	591	A2M	C2'-C1'-N9-C8
27	AZ	2	SAC	C-CA-N-C1A
27	AZ	2	SAC	CB-CA-N-C1A
20	B5	3476	OMG	C3'-C2'-O2'-CM2
20	B5	3619	OMC	C3'-C2'-O2'-CM2
20	B5	3657	OMU	C3'-C2'-O2'-CM2
64	A2	510	OMG	C3'-C2'-O2'-CM2
80	An	138	IAS	C-CA-CB-CG
20	B5	4246	PSU	C4'-C5'-O5'-P
2	Bb	5	MLZ	N-CA-CB-CG
64	A2	577	A2M	C3'-C4'-C5'-O5'
64	A2	1249	B8N	C32-C33-C34-O35
20	B5	3433	OMC	O4'-C1'-N1-C2
64	A2	628	OMU	O4'-C1'-N1-C2
64	A2	1852	MA6	C4'-C5'-O5'-P
64	A2	645	OMG	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
9	BA	216	V5N	O2-CB-CG-CD2
22	Ba	39	V5N	O2-CB-CG-CD2
64	A2	99	A2M	O4'-C4'-C5'-O5'
20	B5	3631	OMG	C3'-C2'-O2'-CM2
20	B5	4052	OMU	C3'-C2'-O2'-CM2
64	A2	868	OMG	C3'-C2'-O2'-CM2
64	A2	1448	OMG	C3'-C2'-O2'-CM2
20	B5	4193	5MC	O4'-C1'-N1-C6
20	B5	2630	A2M	C2'-C1'-N9-C4
20	B5	3550	UY1	C4'-C5'-O5'-P
20	B5	4166	PSU	O4'-C1'-C5-C4
20	B5	2667	OMC	C3'-C2'-O2'-CM2
20	B5	2680	OMU	C3'-C2'-O2'-CM2
20	B5	4383	OMG	C3'-C2'-O2'-CM2
64	A2	27	A2M	C3'-C2'-O2'-CM'
64	A2	1679	A2M	C3'-C2'-O2'-CM'
20	B5	2194	OMC	O4'-C4'-C5'-O5'
64	A2	577	A2M	O4'-C4'-C5'-O5'
2	Bb	5	MLZ	C-CA-CB-CG
20	B5	3599	A2M	C1'-C2'-O2'-CM'
20	B5	2630	A2M	O4'-C1'-N9-C8
64	A2	591	A2M	O4'-C1'-N9-C8
20	B5	4193	5MC	O4'-C1'-N1-C2
18	Aw	62	HY3	O-C-CA-C3
20	B5	3492	A2M	O4'-C4'-C5'-O5'
20	B5	4246	PSU	C3'-C4'-C5'-O5'
80	An	138	IAS	N-CA-CB-CG
84	Br	2	SAC	C-CA-N-C1A
20	B5	4364	OMG	C3'-C2'-O2'-CM2
64	A2	1704	OMC	C3'-C2'-O2'-CM2
64	A2	469	A2M	C3'-C4'-C5'-O5'
9	BA	216	V5N	CA-CB-CG-ND1

There are no ring outliers.

99 monomers are involved in 139 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B5	2208	OMC	2	0
64	A2	355	OMU	1	0
64	A2	1338	4AC	2	0
20	B5	2194	OMC	2	0
20	B5	4382	PSU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B5	3973	OMU	1	0
20	B5	4166	PSU	3	0
20	B5	2258	OMU	1	0
64	A2	116	OMU	2	0
20	B5	4138	OMG	1	0
64	A2	36	PSU	1	0
64	A2	1329	OMG	1	0
64	A2	1289	OMU	2	0
20	B5	4336	A2M	1	0
20	B5	3476	OMG	1	0
20	B5	4298	PSU	2	0
20	B5	3540	OMC	1	0
64	A2	166	A2M	2	0
64	A2	513	A2M	1	0
64	A2	577	A2M	1	0
20	B5	4364	OMG	1	0
20	B5	3456	A2M	2	0
64	A2	463	OMC	2	0
20	B5	400	A2M	2	0
20	B5	3966	6MZ	1	0
20	B5	3585	PSU	1	0
20	B5	3601	OMC	1	0
20	B5	2244	A2M	1	0
64	A2	1392	OMC	1	0
6	B8	75	OMG	2	0
64	A2	518	OMC	1	0
20	B5	3676	OMG	2	0
20	B5	3524	OMG	1	0
20	B5	3562	A2M	2	0
20	B5	2267	OMG	1	0
20	B5	3942	OMG	2	0
64	A2	469	A2M	2	0
64	A2	1446	PSU	1	0
20	B5	2207	OMG	3	0
64	A2	823	PSU	1	0
20	B5	3550	UY1	1	0
20	B5	2647	OMC	1	0
20	B5	4366	OMU	3	0
64	A2	645	OMG	1	0
20	B5	4058	PSU	1	0
20	B5	1284	OMC	1	0
64	A2	1032	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B5	3517	A2M	2	0
20	B5	3492	A2M	1	0
64	A2	485	A2M	1	0
20	B5	4325	PSU	1	0
20	B5	2206	A2M	2	0
20	B5	4282	OMC	2	0
20	B5	4099	PSU	1	0
64	A2	121	OMU	2	0
64	A2	1843	4AC	1	0
20	B5	4042	PSU	1	0
64	A2	172	OMU	2	0
64	A2	1448	OMG	2	0
20	B5	1479	A2M	1	0
20	B5	4052	OMU	1	0
64	A2	159	A2M	1	0
64	A2	868	OMG	2	0
20	B5	1489	A2M	2	0
20	B5	4383	OMG	1	0
20	B5	4203	PSU	1	0
20	B5	4269	A2M	3	0
64	A2	867	PSU	2	0
20	B5	2667	OMC	1	0
20	B5	3450	A2M	2	0
64	A2	105	PSU	1	0
20	B5	4202	OMC	1	0
20	B5	3652	PSU	2	0
20	B5	1810	A2M	2	0
20	B5	3557	A2M	2	0
64	A2	437	OMG	2	0
64	A2	99	A2M	2	0
64	A2	1640	G7M	1	0
20	B5	2658	A2M	1	0
20	B5	2704	OMC	1	0
64	A2	1833	6MZ	1	0
20	B5	3619	OMC	1	0
20	B5	4039	PSU	1	0
64	A2	27	A2M	3	0
20	B5	398	A2M	1	0
20	B5	2351	PSU	1	0
64	A2	1851	MA6	1	0
64	A2	1679	A2M	2	0
64	A2	510	OMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B5	2630	A2M	1	0
20	B5	1260	OMG	1	0
9	BA	216	V5N	1	0
64	A2	1491	OMG	1	0
64	A2	1704	OMC	1	0
64	A2	1805	OMU	3	0
20	B5	1718	PSU	1	0
14	Au	1	AME	1	0
20	B5	3631	OMG	1	0
20	B5	4188	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 740 ligands modelled in this entry, 277 are unknown and 428 are monoatomic - leaving 35 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
94	SPD	B5	4989	-	9,9,9	0.15	0	8,8,8	0.20	0
94	SPD	B5	5084	-	9,9,9	0.15	0	8,8,8	0.20	0
94	SPD	B5	5159	-	9,9,9	0.15	0	8,8,8	0.16	0
94	SPD	B5	5297	-	9,9,9	0.16	0	8,8,8	0.18	0
94	SPD	A2	2056	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	A2	2063	-	9,9,9	0.16	0	8,8,8	0.17	0
95	SPM	B5	5203	-	13,13,13	0.15	0	12,12,12	0.14	0
93	GTP	B7	212	3	30,34,34	0.50	0	46,54,54	0.54	0
94	SPD	B5	5101	-	9,9,9	0.15	0	8,8,8	0.17	0
95	SPM	A2	1939	-	13,13,13	0.14	0	12,12,12	0.17	0
94	SPD	B5	5318	-	9,9,9	0.16	0	8,8,8	0.17	0
94	SPD	B5	5359	-	9,9,9	0.15	0	8,8,8	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
94	SPD	B5	5237	-	9,9,9	0.16	0	8,8,8	0.18	0
94	SPD	B5	5216	-	9,9,9	0.15	0	8,8,8	0.15	0
94	SPD	B5	5122	-	9,9,9	0.15	0	8,8,8	0.19	0
94	SPD	B5	5010	-	9,9,9	0.16	0	8,8,8	0.19	0
94	SPD	B5	4968	-	9,9,9	0.15	0	8,8,8	0.17	0
94	SPD	A2	1935	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	B5	4926	-	9,9,9	0.15	0	8,8,8	0.18	0
97	IHP	DB	901	-	36,36,36	1.55	6 (16%)	54,60,60	1.13	4 (7%)
94	SPD	B5	5140	-	9,9,9	0.16	0	8,8,8	0.18	0
94	SPD	B5	5066	-	9,9,9	0.15	0	8,8,8	0.19	0
94	SPD	B5	5338	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	B5	5377	-	9,9,9	0.16	0	8,8,8	0.18	0
94	SPD	A2	1928	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	B5	5046	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	A2	1921	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	A2	1901	-	9,9,9	0.16	0	8,8,8	0.19	0
94	SPD	A2	1915	-	9,9,9	0.16	0	8,8,8	0.18	0
94	SPD	A2	1908	-	9,9,9	0.15	0	8,8,8	0.19	0
94	SPD	B5	4905	-	9,9,9	0.15	0	8,8,8	0.19	0
94	SPD	B5	5276	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	B5	5027	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	B5	5257	-	9,9,9	0.16	0	8,8,8	0.17	0
95	SPM	B5	4947	-	13,13,13	0.15	0	12,12,12	0.19	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
94	SPD	B5	4989	-	-	0/7/7/7	-
94	SPD	B5	5084	-	-	0/7/7/7	-
94	SPD	B5	5159	-	-	1/7/7/7	-
94	SPD	B5	5297	-	-	1/7/7/7	-
94	SPD	A2	2056	-	-	1/7/7/7	-
94	SPD	A2	2063	-	-	0/7/7/7	-
95	SPM	B5	5203	-	-	0/11/11/11	-
93	GTP	B7	212	3	-	0/22/38/38	0/3/3/3
94	SPD	B5	5101	-	-	0/7/7/7	-
95	SPM	A2	1939	-	-	1/11/11/11	-
94	SPD	B5	5318	-	-	1/7/7/7	-
94	SPD	B5	5359	-	-	0/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
94	SPD	B5	5237	-	-	1/7/7/7	-
94	SPD	B5	5216	-	-	1/7/7/7	-
94	SPD	B5	5122	-	-	1/7/7/7	-
94	SPD	B5	5010	-	-	0/7/7/7	-
94	SPD	B5	4968	-	-	0/7/7/7	-
94	SPD	A2	1935	-	-	0/7/7/7	-
94	SPD	B5	4926	-	-	0/7/7/7	-
97	IHP	DB	901	-	-	8/30/54/54	0/1/1/1
94	SPD	B5	5140	-	-	0/7/7/7	-
94	SPD	B5	5066	-	-	0/7/7/7	-
94	SPD	B5	5338	-	-	0/7/7/7	-
94	SPD	B5	5377	-	-	0/7/7/7	-
94	SPD	A2	1928	-	-	1/7/7/7	-
94	SPD	B5	5046	-	-	0/7/7/7	-
94	SPD	A2	1921	-	-	0/7/7/7	-
94	SPD	A2	1901	-	-	0/7/7/7	-
94	SPD	A2	1915	-	-	0/7/7/7	-
94	SPD	A2	1908	-	-	0/7/7/7	-
94	SPD	B5	4905	-	-	1/7/7/7	-
94	SPD	B5	5276	-	-	0/7/7/7	-
94	SPD	B5	5027	-	-	0/7/7/7	-
94	SPD	B5	5257	-	-	1/7/7/7	-
95	SPM	B5	4947	-	-	1/11/11/11	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
97	DB	901	IHP	P2-O12	3.53	1.66	1.59
97	DB	901	IHP	P5-O15	3.45	1.65	1.59
97	DB	901	IHP	P1-O11	3.25	1.65	1.59
97	DB	901	IHP	P6-O16	3.22	1.65	1.59
97	DB	901	IHP	P3-O13	3.20	1.65	1.59
97	DB	901	IHP	P4-O14	3.19	1.65	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
97	DB	901	IHP	C6-C5-C4	4.29	119.80	110.41
97	DB	901	IHP	C5-C4-C3	3.60	118.29	110.41
97	DB	901	IHP	C5-C6-C1	3.58	118.24	110.41
97	DB	901	IHP	C4-C3-C2	2.22	115.27	110.41

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
97	DB	901	IHP	C1-C2-O12-P2
97	DB	901	IHP	C4-C5-O15-P5
97	DB	901	IHP	C4-O14-P4-O34
95	A2	1939	SPM	C8-C9-N10-C11
97	DB	901	IHP	C4-O14-P4-O24
97	DB	901	IHP	C2-O12-P2-O32
94	B5	5237	SPD	C2-C3-C4-C5
94	B5	5159	SPD	C2-C3-C4-C5
94	A2	1928	SPD	C2-C3-C4-C5
94	B5	5216	SPD	C2-C3-C4-C5
97	DB	901	IHP	C6-C1-O11-P1
97	DB	901	IHP	C2-O12-P2-O42
97	DB	901	IHP	C5-O15-P5-O45
94	A2	2056	SPD	C2-C3-C4-C5
94	B5	5257	SPD	C2-C3-C4-C5
94	B5	5297	SPD	C2-C3-C4-C5
94	B5	5122	SPD	C2-C3-C4-C5
94	B5	5318	SPD	C2-C3-C4-C5
94	B5	4905	SPD	C4-C5-N6-C7
95	B5	4947	SPM	C6-C7-C8-C9

There are no ring outliers.

16 monomers are involved in 30 short contacts:

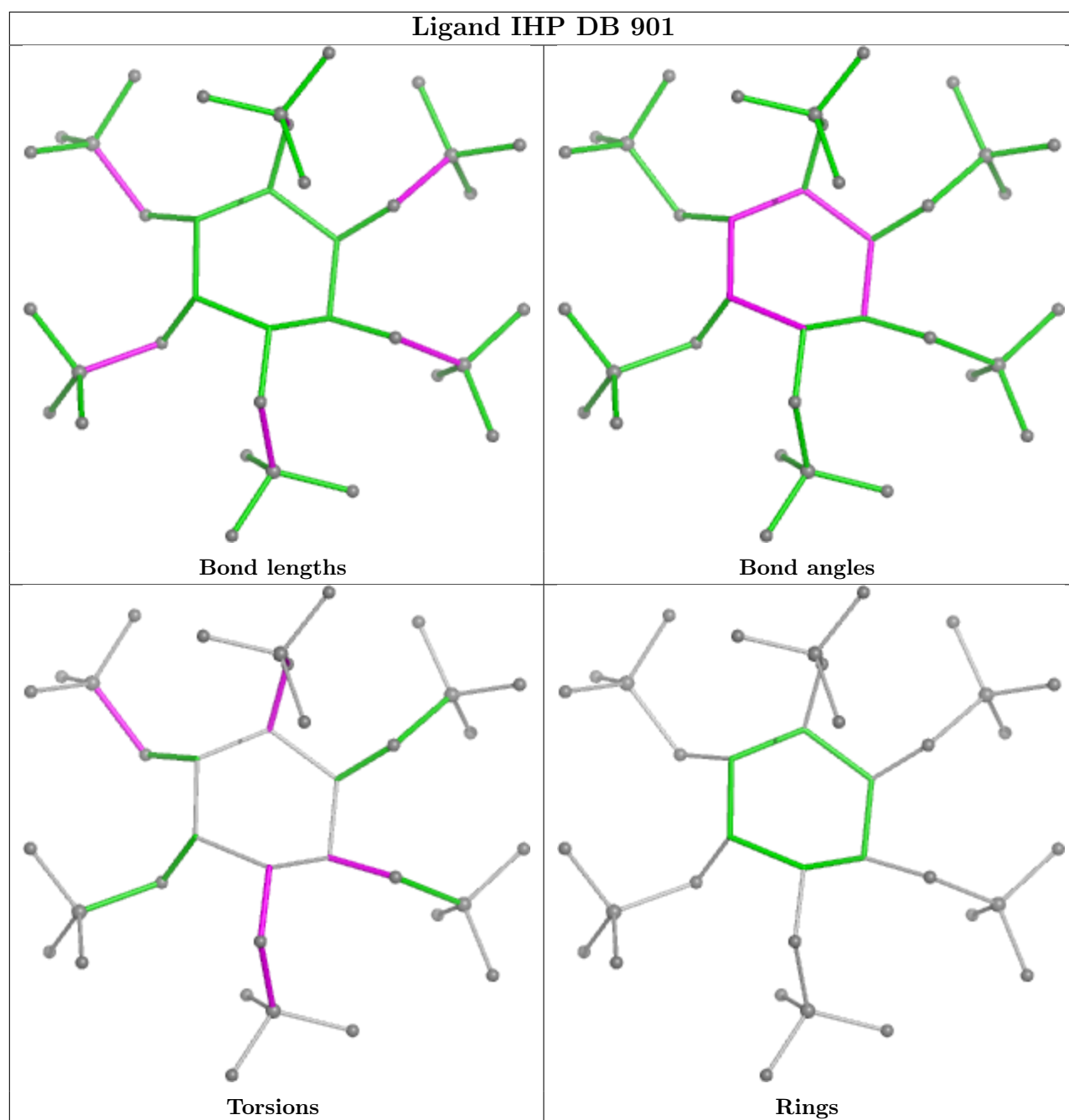
Mol	Chain	Res	Type	Clashes	Symm-Clashes
94	B5	5159	SPD	3	0
94	B5	5297	SPD	2	0
95	A2	1939	SPM	4	0
94	B5	5318	SPD	1	0
94	B5	5359	SPD	2	0
94	B5	5010	SPD	2	0
94	A2	1935	SPD	1	0
97	DB	901	IHP	2	0
94	B5	5066	SPD	3	0
94	B5	5377	SPD	2	0
94	A2	1921	SPD	1	0
94	A2	1901	SPD	1	0
94	A2	1908	SPD	2	0
94	B5	5276	SPD	1	0
94	B5	5257	SPD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
95	B5	4947	SPM	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

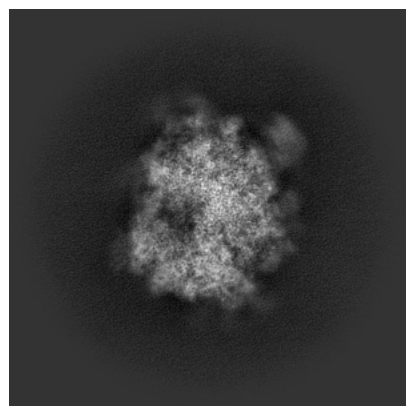
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50125. These allow visual inspection of the internal detail of the map and identification of artifacts.

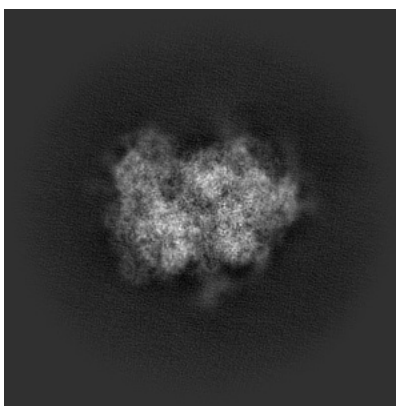
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

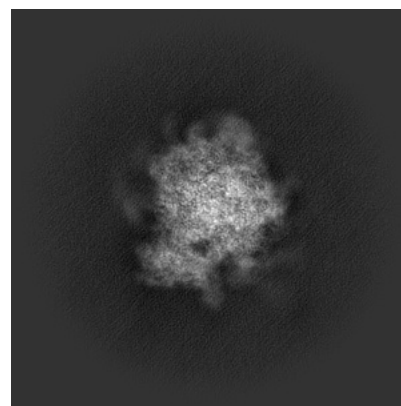
6.1.1 Primary map



X

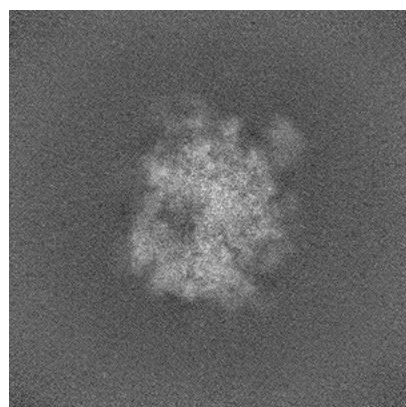


Y

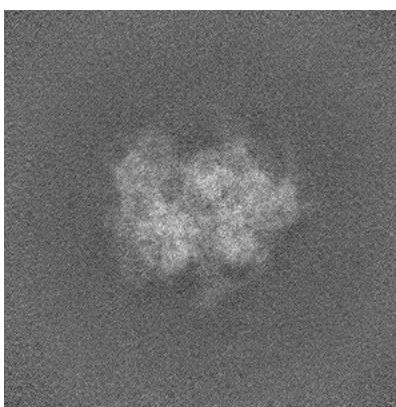


Z

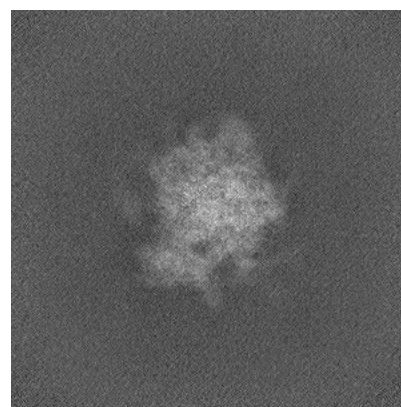
6.1.2 Raw map



X



Y

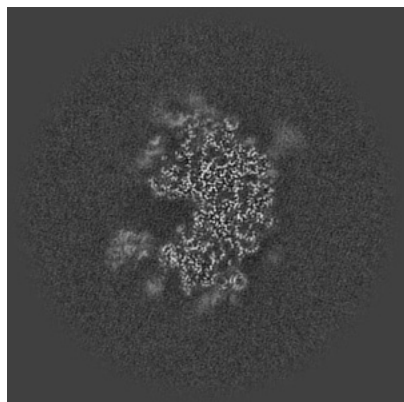


Z

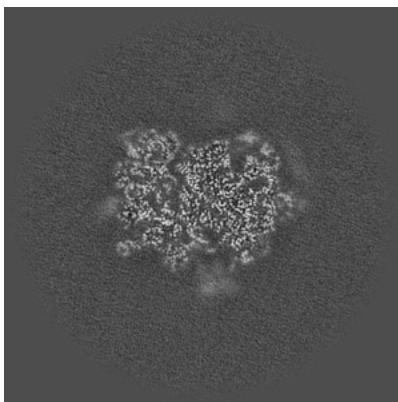
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

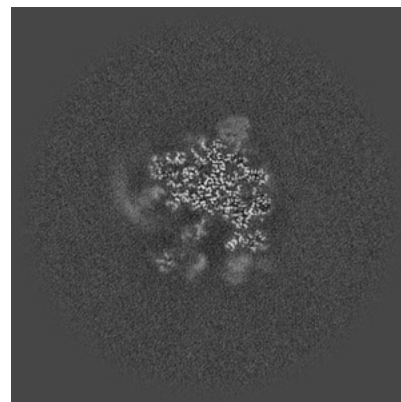
6.2.1 Primary map



X Index: 280

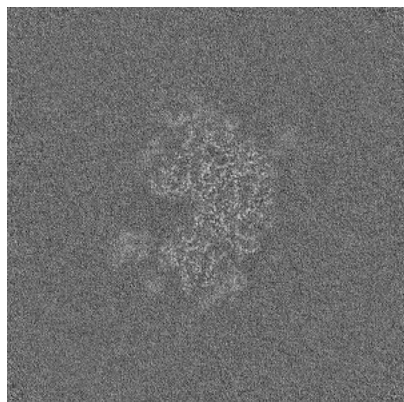


Y Index: 280

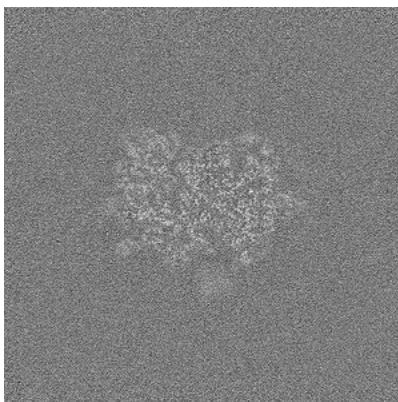


Z Index: 280

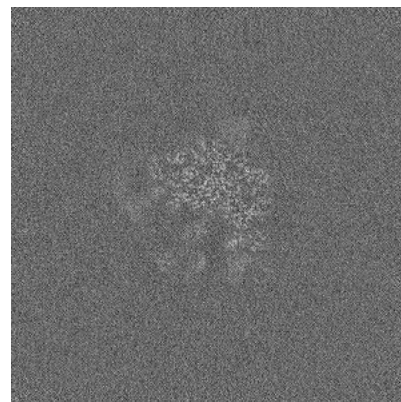
6.2.2 Raw map



X Index: 280



Y Index: 280

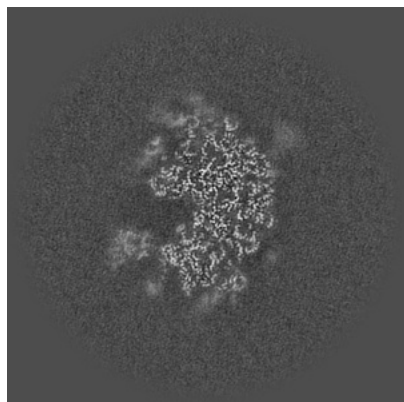


Z Index: 280

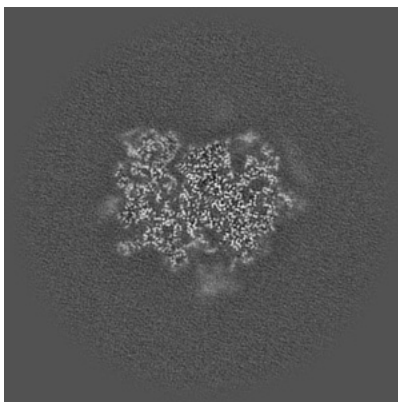
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

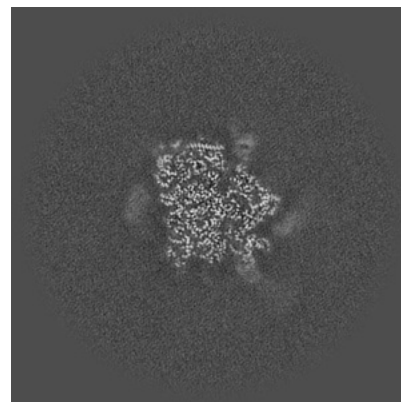
6.3.1 Primary map



X Index: 279

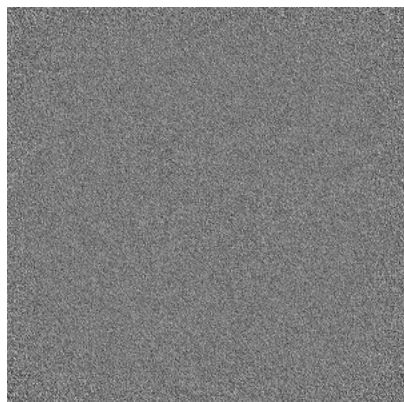


Y Index: 281

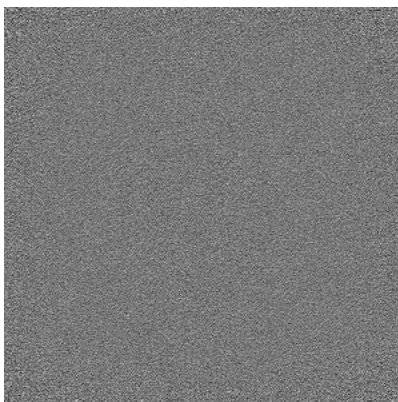


Z Index: 309

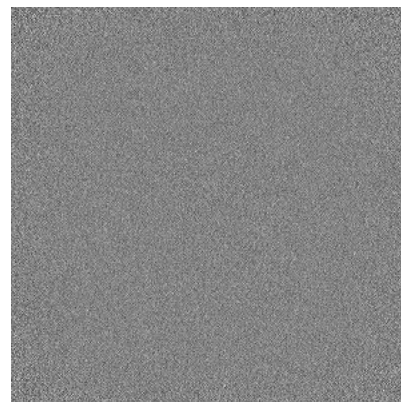
6.3.2 Raw map



X Index: 0



Y Index: 0

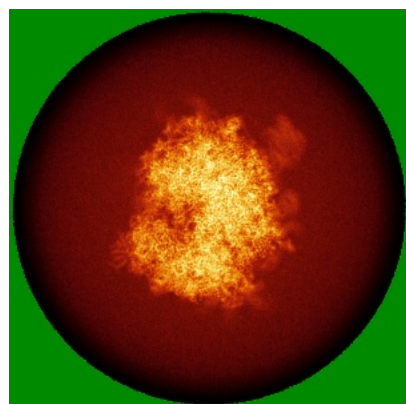


Z Index: 0

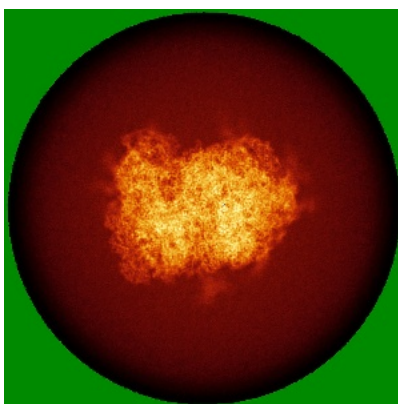
The images above show the largest variance slices of the map in three orthogonal directions.

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

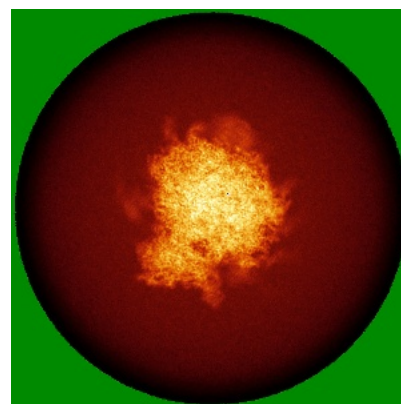
6.4.1 Primary map



X

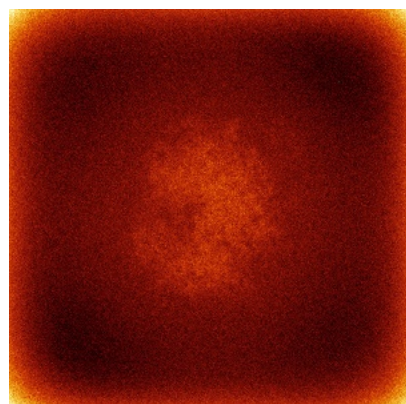


Y

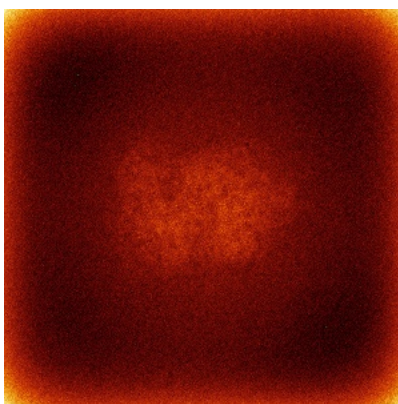


Z

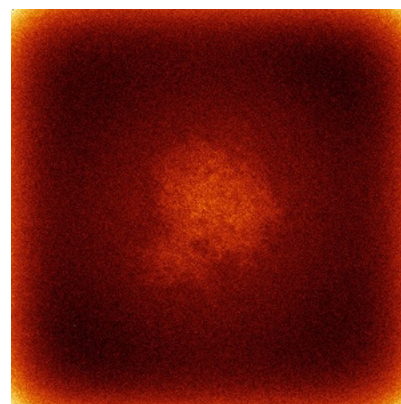
6.4.2 Raw map



X



Y

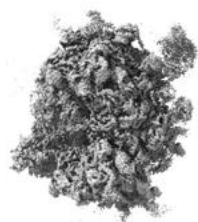


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



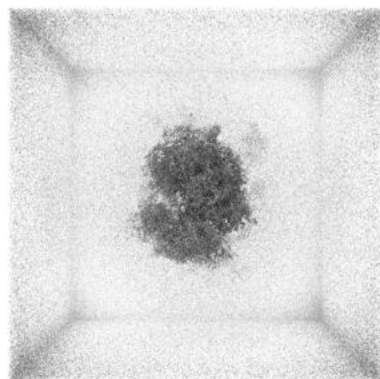
Y



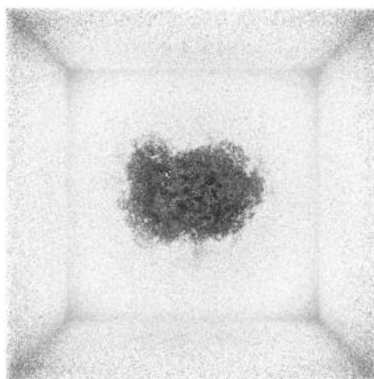
Z

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

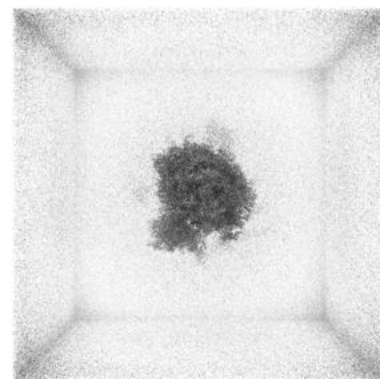
6.5.2 Raw map



X



Y



Z

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

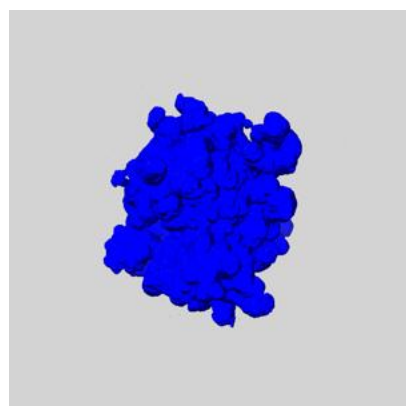
6.6 Mask visualisation [i](#)

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

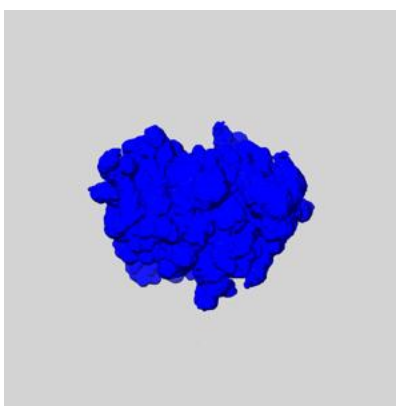
A mask typically either:

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

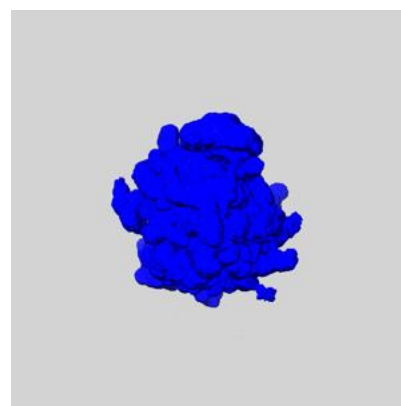
6.6.1 emd_50125_msk_1.map [i](#)



X

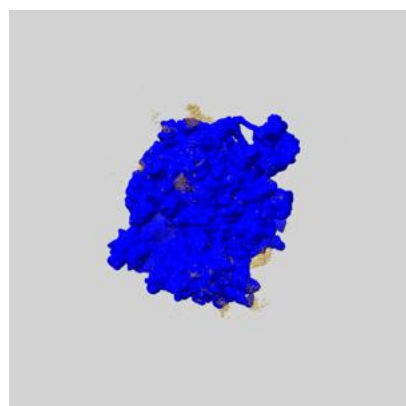


Y

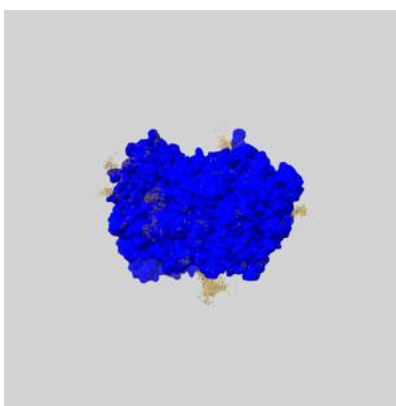


Z

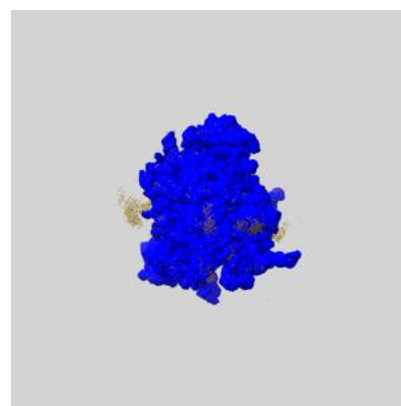
6.6.2 emd_50125_msk_2.map [i](#)



X



Y

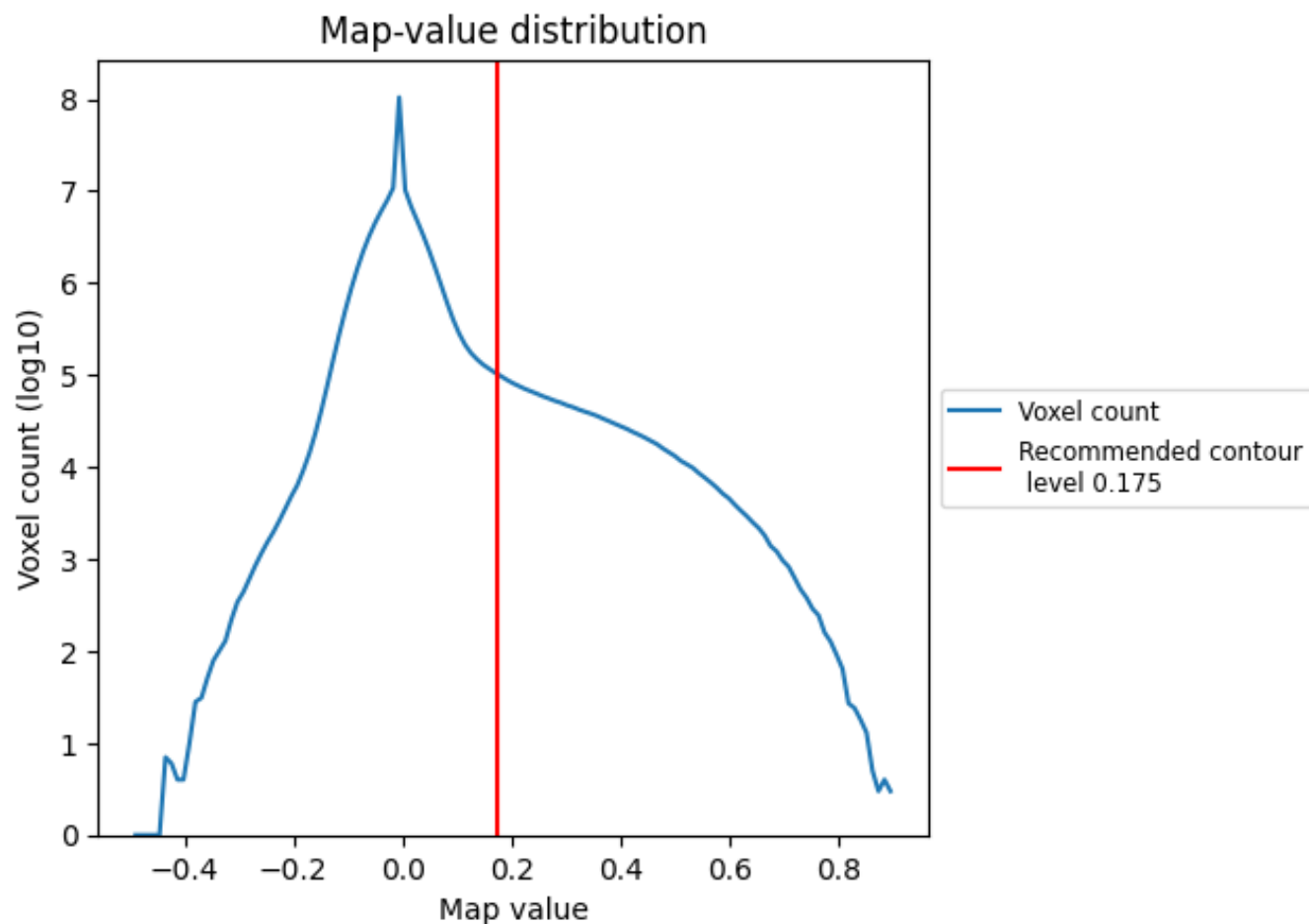


Z

7 Map analysis [i](#)

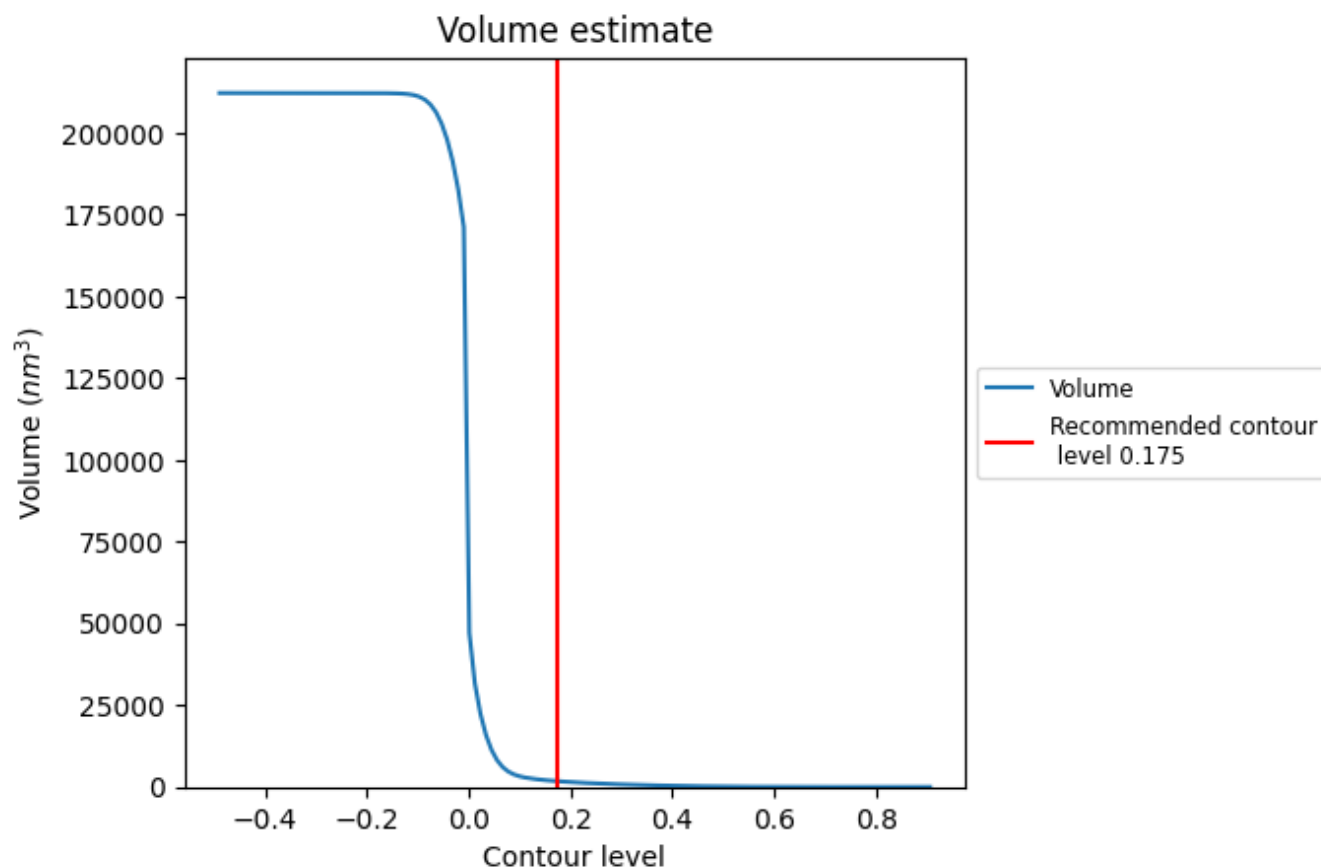
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

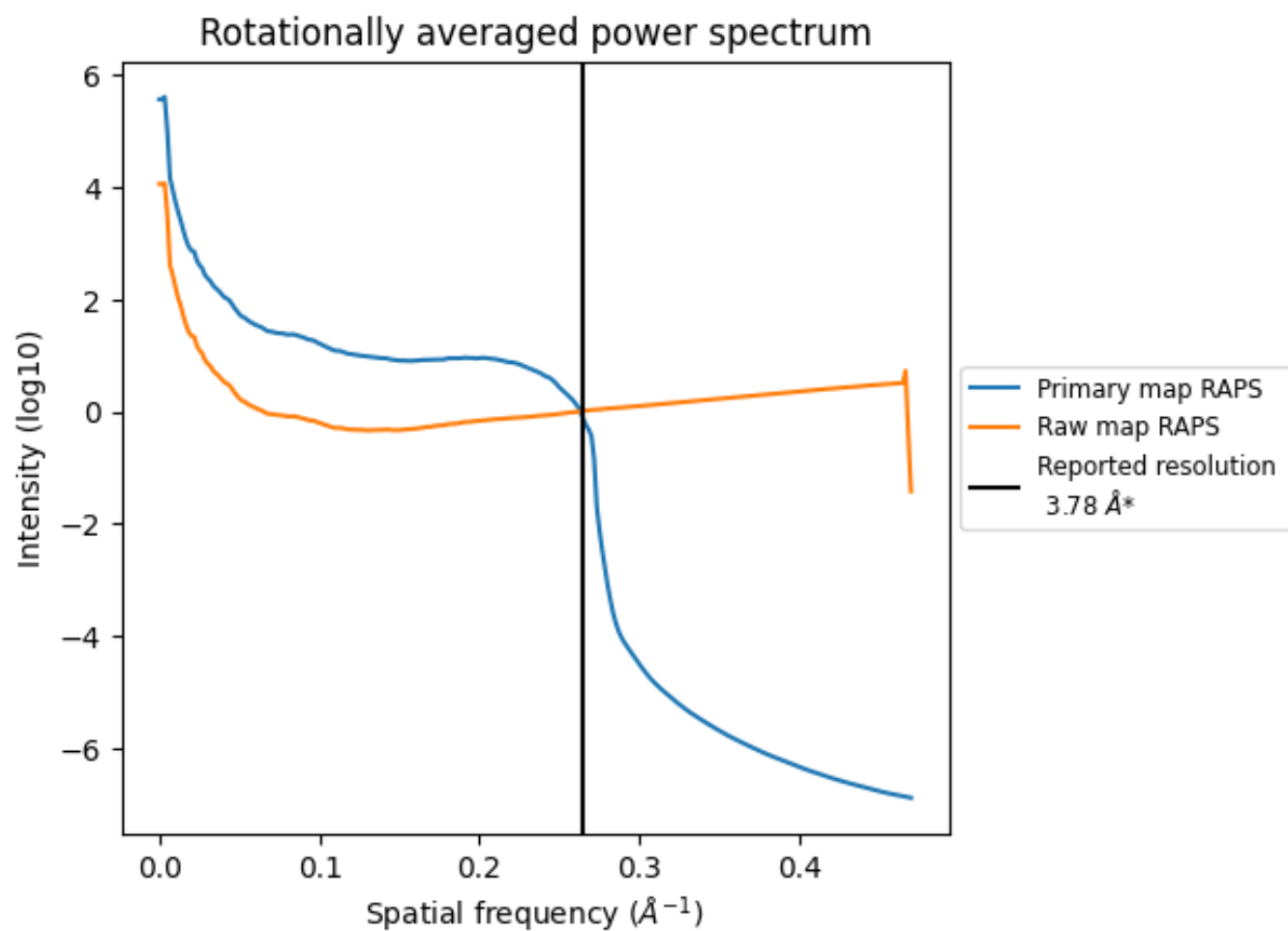
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1752 nm³; this corresponds to an approximate mass of 1582 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 ⓘ

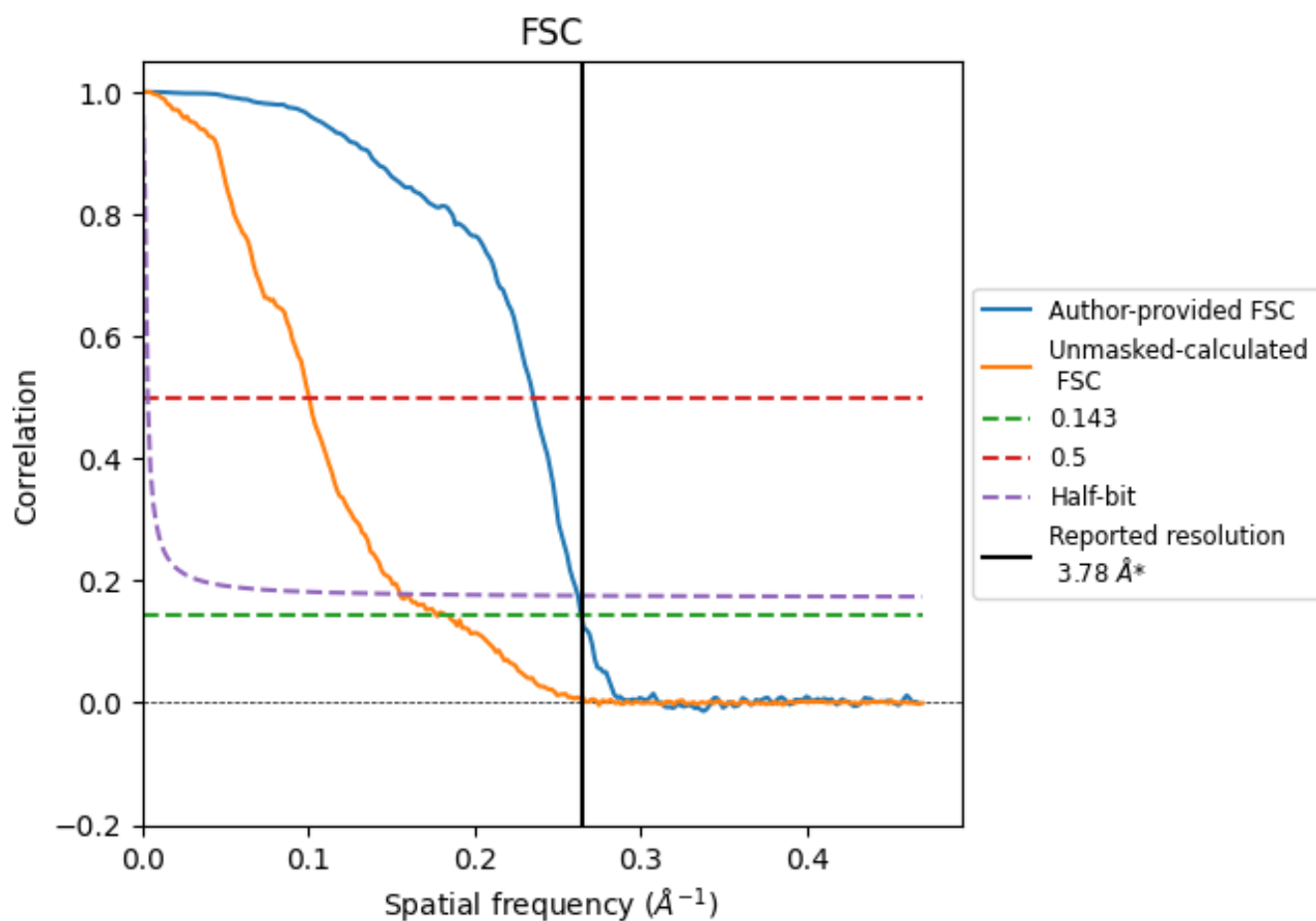


*Reported resolution corresponds to spatial frequency of 0.265 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.265 Å⁻¹

8.2 Resolution estimates [i](#)

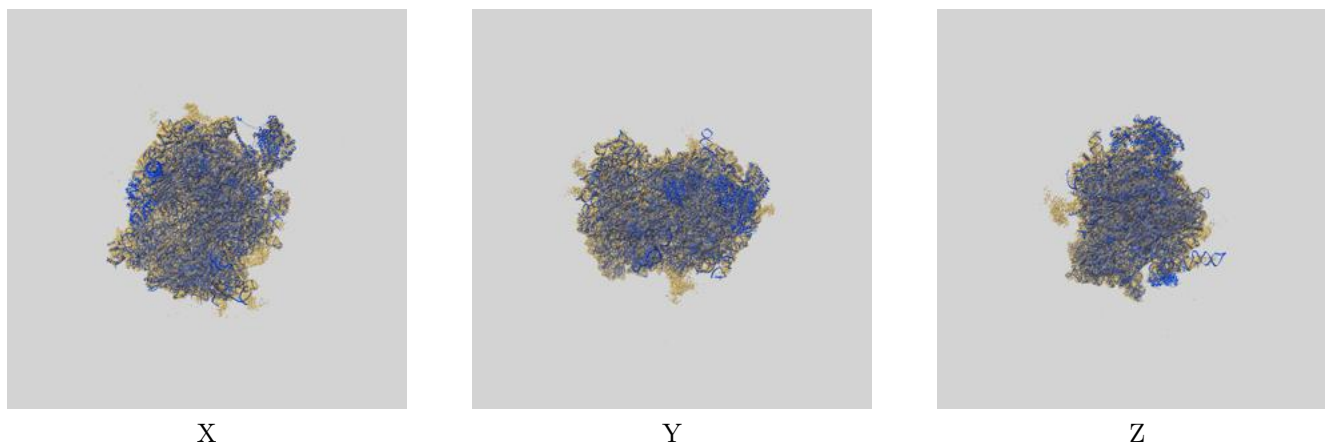
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.78	-	-
Author-provided FSC curve	3.79	4.25	3.81
Unmasked-calculated*	5.64	9.95	6.44

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.64 differs from the reported value 3.78 by more than 10 %

9 Map-model fit [i](#)

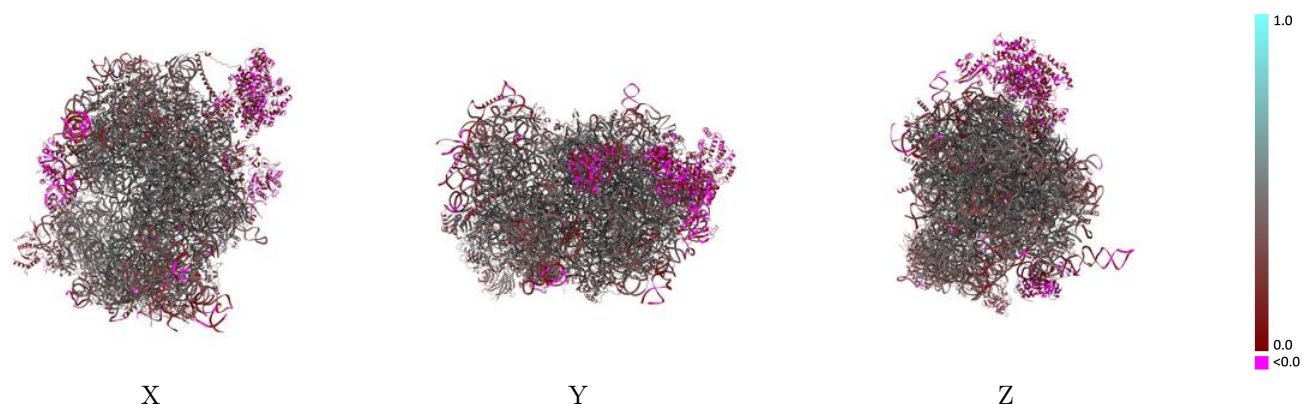
This section contains information regarding the fit between EMDB map EMD-50125 and PDB model 9F1C. Per-residue inclusion information can be found in section [3](#) on page [33](#).

9.1 Map-model overlay [i](#)



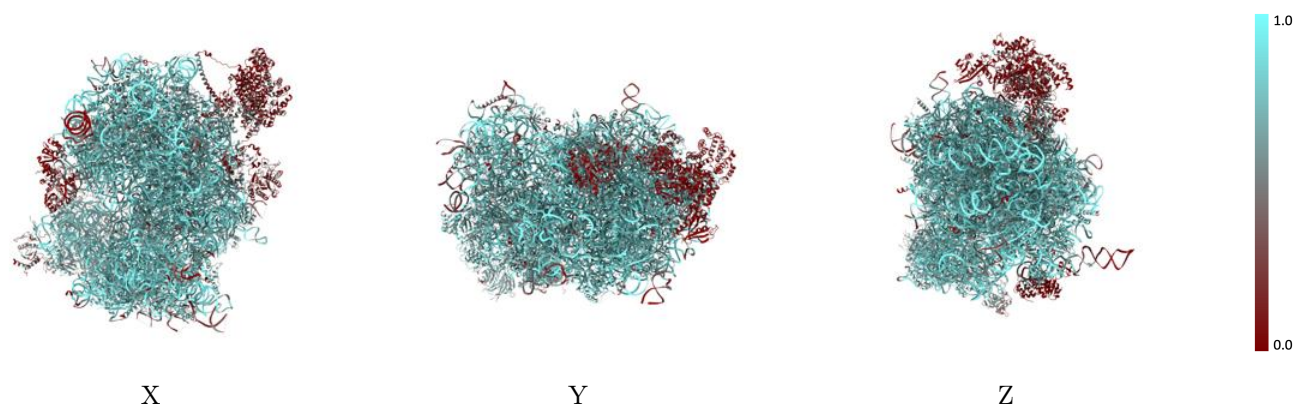
The images above show the 3D surface view of the map at the recommended contour level 0.175 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



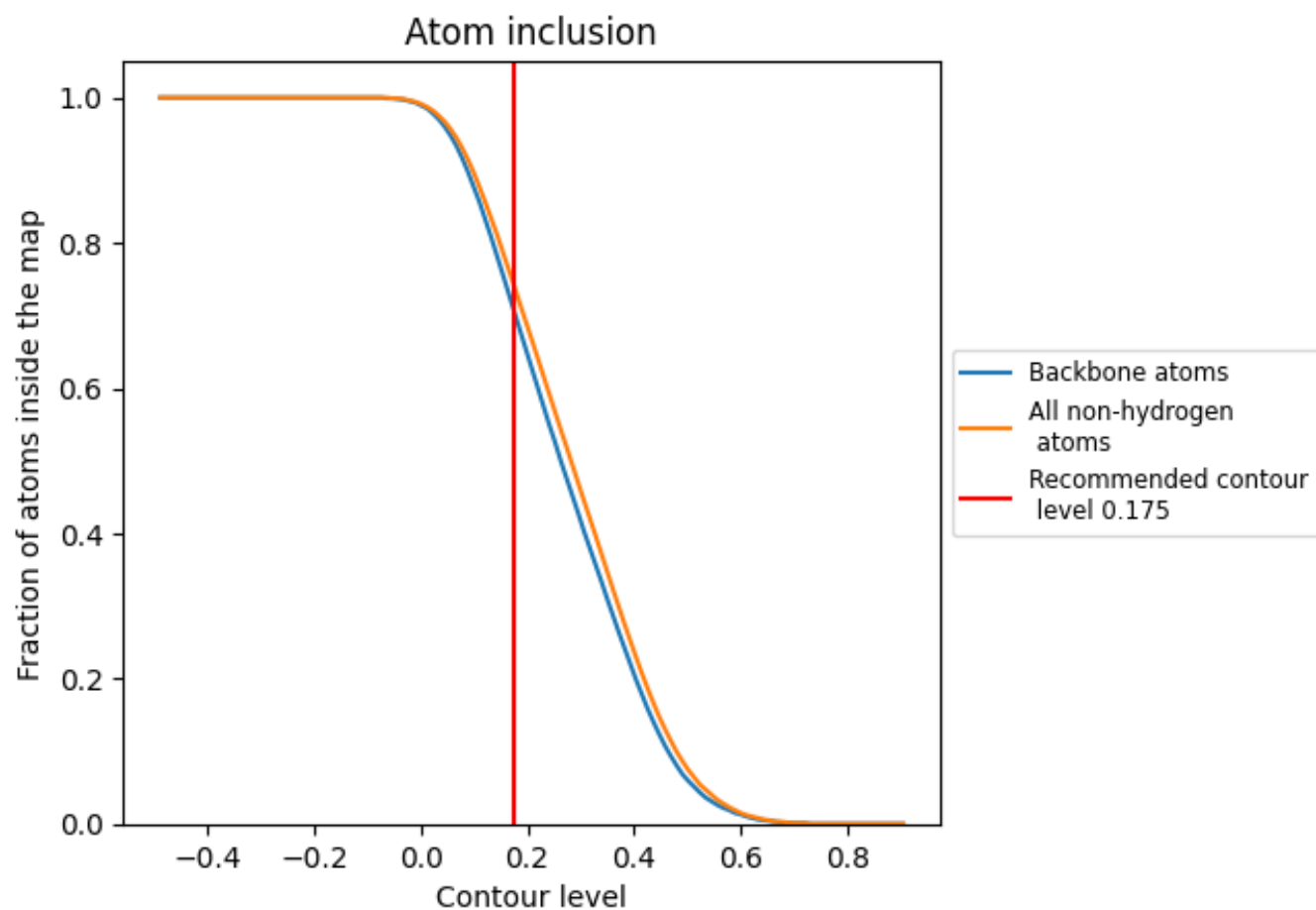
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.175) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7410	 0.3710
A2	 0.8600	 0.3810
AA	 0.6760	 0.4110
AB	 0.6600	 0.3880
AC	 0.3940	 0.1490
AD	 0.5930	 0.3680
AE	 0.7560	 0.4390
AF	 0.6470	 0.3060
AG	 0.7510	 0.4020
AH	 0.0280	 0.3250
AT	 0.6350	 0.3910
AZ	 0.7240	 0.4020
Aa	 0.6740	 0.3990
Ab	 0.7340	 0.4300
Ac	 0.6500	 0.3710
Ad	 0.7290	 0.4210
Ae	 0.6520	 0.3620
Af	 0.6510	 0.3130
Ag	 0.6710	 0.3600
Ah	 0.7170	 0.4040
Ai	 0.7510	 0.4030
Aj	 0.6900	 0.3310
Ak	 0.6670	 0.4120
Al	 0.3330	 0.1440
Am	 0.7160	 0.4190
An	 0.7180	 0.4140
Ao	 0.6340	 0.3030
Ap	 0.6990	 0.3720
Aq	 0.6880	 0.3610
Ar	 0.6410	 0.3170
As	 0.6820	 0.3330
At	 0.6270	 0.3340
Au	 0.7240	 0.4110
Av	 0.6950	 0.4460
Aw	 0.7440	 0.4470



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Chain	Atom inclusion	Q-score
Ax	 0.7400	 0.3790
Ay	 0.5380	 0.2820
Az	 0.6060	 0.4180
B	 0.7560	 0.3920
B5	 0.8520	 0.3890
B7	 0.9210	 0.4170
B8	 0.8800	 0.4080
BA	 0.7300	 0.4580
BB	 0.7510	 0.4410
BC	 0.7560	 0.4440
BE	 0.6790	 0.3760
BF	 0.7450	 0.4340
BG	 0.7050	 0.3870
BH	 0.7190	 0.4120
BI	 0.7360	 0.4420
BJ	 0.7080	 0.3880
BK	 0.2060	 0.4310
BL	 0.7220	 0.4110
BM	 0.7450	 0.4020
BN	 0.7720	 0.4610
BO	 0.7430	 0.4370
BP	 0.7280	 0.4460
BQ	 0.7530	 0.4590
BR	 0.7160	 0.3890
BS	 0.7550	 0.4500
BT	 0.7140	 0.4400
BU	 0.7220	 0.4260
BV	 0.7000	 0.4500
BW	 0.5760	 0.3170
BX	 0.7130	 0.4280
BY	 0.7160	 0.4270
BZ	 0.7470	 0.3990
Ba	 0.7950	 0.4520
Bb	 0.6600	 0.3700
Bc	 0.6290	 0.3620
Bd	 0.7350	 0.4430
Be	 0.7580	 0.4550
Bf	 0.7740	 0.4620
Bg	 0.7120	 0.4330
Bh	 0.7340	 0.4130
Bi	 0.7240	 0.4000
Bj	 0.8250	 0.4710

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Chain	Atom inclusion	Q-score
Bk	 0.6340	 0.3640
Bl	 0.7260	 0.4500
Bm	 0.7280	 0.4220
Bo	 0.7080	 0.4360
Bp	 0.7130	 0.4270
Br	 0.7430	 0.4560
Bs	 0.0440	 0.0350
Bt	 0.0450	 0.0550
Ct	 0.1950	 0.1080
Cu	 0.3250	 0.2200
DA	 0.0350	 0.0460
DB	 0.1690	 0.0860
DC	 0.1490	 0.0510
EA	 0.1620	 0.0470