



Full wwPDB EM Validation Report ⓘ

Jun 19, 2026 – 06:30 am BST

PDB ID : 9F1B / pdb_00009f1b
EMDB ID : EMD-50124
Title : Mammalian ternary complex of a translating 80S ribosome, NAC and NatA/E
Authors : Yudin, D.; Scaiola, A.; Ban, N.
Deposited on : 2024-04-18
Resolution : 3.01 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

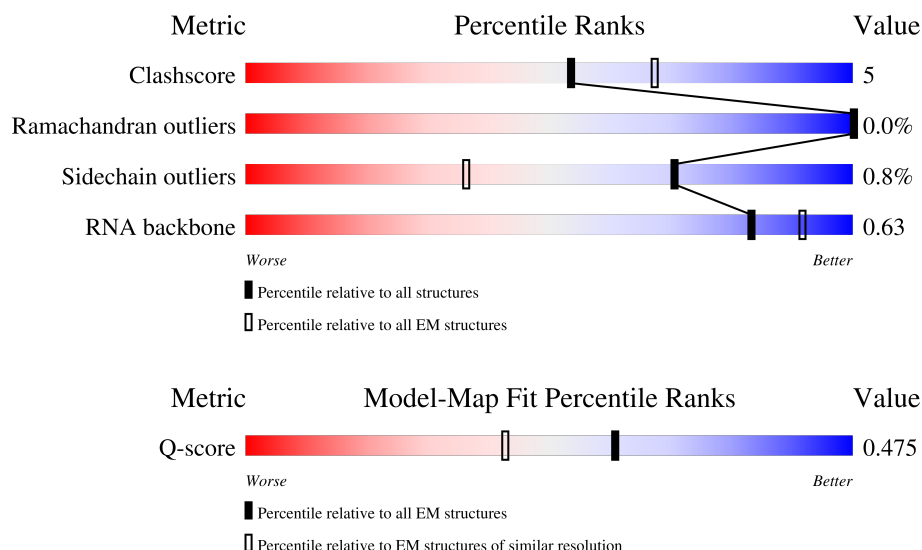
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.01 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	13882 (2.51 - 3.51)

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	BP	184	
2	Aq	135	
3	Bo	106	

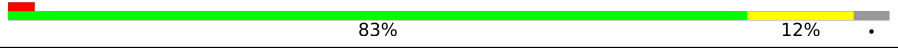
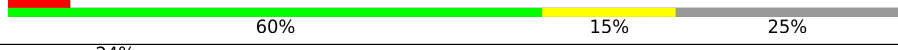
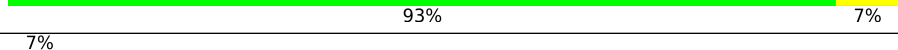
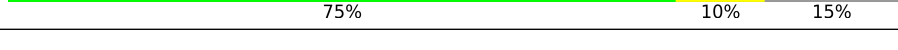
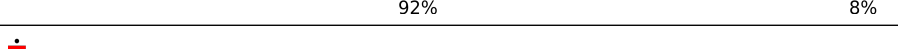
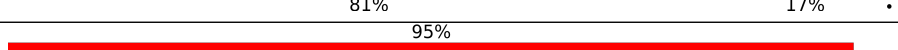
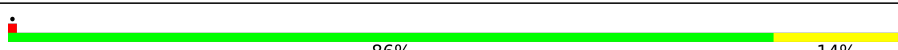
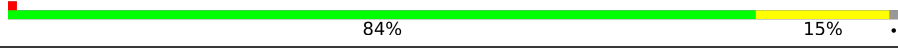
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Mol	Chain	Length	Quality of chain
4	AT	76	
5	Ar	151	
6	Cu	162	
7	BL	211	
8	BX	156	
9	Bp	92	
10	BQ	188	
11	As	145	
12	Br	136	
13	BR	196	
14	At	119	
15	Bs	318	
16	BG	266	
17	BU	128	
18	Av	130	
19	DB	915	
20	Ct	238	
21	BH	192	
22	BV	140	
23	Aw	143	
24	B5	4808	
25	BT	160	
26	BI	214	
27	BW	157	
28	Ax	130	

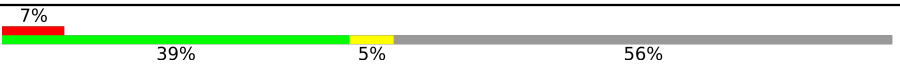
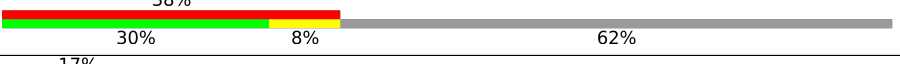
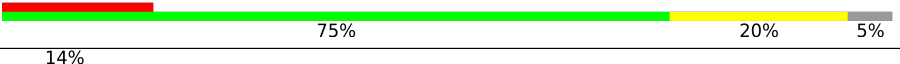
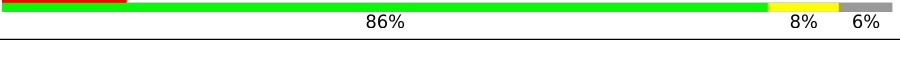
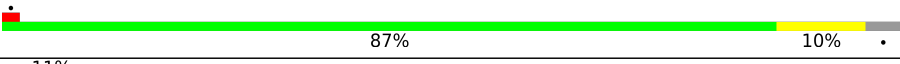
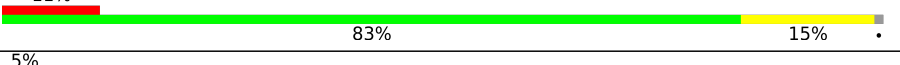
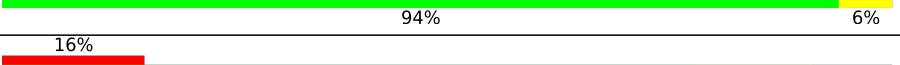
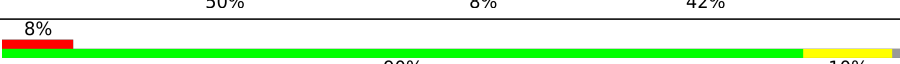
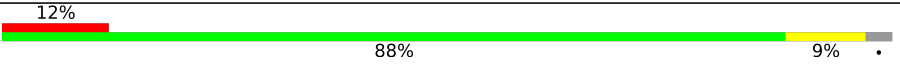
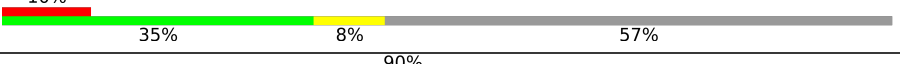
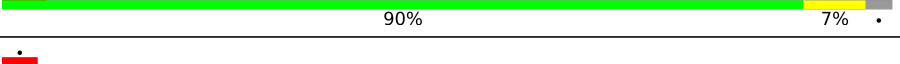
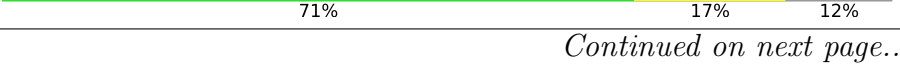
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Mol	Chain	Length	Quality of chain
29	B7	119	
30	Au	83	
31	BJ	178	
32	AZ	294	
33	Ay	124	
34	B8	158	
35	BK	29	
36	Aa	264	
37	Az	25	
38	BA	257	
39	Bt	165	
40	BM	218	
41	Ab	293	
42	BY	145	
43	BB	403	
44	BS	176	
45	Ac	281	
46	BZ	136	
47	BC	412	
48	BN	204	
49	Ad	263	
50	Ba	148	
51	B	297	
52	BO	203	
53	Ae	204	

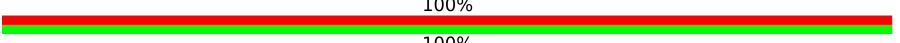
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Mol	Chain	Length	Quality of chain
54	Bb	245	
55	BE	291	
56	DA	403	
57	Af	249	
58	Bc	115	
59	BF	247	
60	DC	235	
61	Ag	432	
62	Bd	125	
63	A2	1870	
64	Ah	208	
65	Be	135	
66	AA	84	
67	Ai	194	
68	Bf	110	
69	AB	69	
70	Aj	165	
71	Bg	115	
72	AC	156	
73	Ak	158	
74	Bh	123	
75	AD	133	
76	Al	132	
77	Bi	105	
78	AE	115	

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Mol	Chain	Length	Quality of chain
79	Am	151	
80	Bj	97	
81	AF	317	
82	An	151	
83	Bk	70	
84	AG	56	
85	Ao	145	
86	Bl	51	
87	AH	3	
88	Ap	172	
89	Bm	128	

2 Entry composition

There are 97 unique types of molecules in this entry. The entry contains 234232 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 protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	BP	153	Total	C	N	O	S	0	0
			1242	777	241	215	9		

- Molecule 2 is a protein called 40S ribosomal protein eS17.

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

- Molecule 3 is a protein called Large ribosomal subunit protein eL42.

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

- 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 protein called Transcription factor BTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Cu	105	Total	C	N	O	S	0	0
			813	508	152	150	3		

- Molecule 7 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	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 8 is a protein called Ribosomal_L23eN domain-containing protein.

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

- Molecule 9 is a protein called 60S ribosomal protein L37a.

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

- Molecule 10 is a protein called Large ribosomal subunit protein eL18.

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

- Molecule 11 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	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 12 is a protein called Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	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 13 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	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 14 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 15 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 16 is a protein called 60S ribosomal protein L7a.

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

- Molecule 17 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	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 18 is a protein called Ribosomal protein S15a.

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

- Molecule 19 is a protein called N-alpha-acetyltransferase 15, NatA auxiliary subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 20 is a protein called Nascent polypeptide-associated complex subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	Ct	115	Total	C	N	O	S	
			895	561	163	167	4	0

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
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 21 is a protein called 60S ribosomal protein L9.

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

- Molecule 22 is a protein called Ribosomal protein L23.

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

- Molecule 23 is a protein called 40S ribosomal protein S23.

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

- Molecule 24 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	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 25 is a protein called 60S ribosomal protein L21.

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

- Molecule 26 is a protein called 60S ribosomal protein L10.

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

- Molecule 27 is a protein called Ribosomal protein L24.

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

- Molecule 28 is a protein called 40S ribosomal protein S24.

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

- Molecule 29 is a RNA chain called 5S rRNA.

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

- Molecule 30 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 31 is a protein called 60S ribosomal protein L11.

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

- Molecule 32 is a protein called Small ribosomal subunit protein uS2.

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

- Molecule 33 is a protein called 40S ribosomal protein S25.

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

- Molecule 34 is a RNA chain called 5.8S rRNA.

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

- Molecule 35 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	BK	29	Total	C	N	O	0	0
			145	87	29	29		

- Molecule 36 is a protein called 40S ribosomal protein S3a.

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

- Molecule 37 is a protein called 60S ribosomal protein L41.

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

- Molecule 38 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 39 is a protein called 60S ribosomal protein L12.

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

- Molecule 40 is a protein called 60S ribosomal protein L14.

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

- Molecule 41 is a protein called 40S ribosomal protein S2.

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

- Molecule 42 is a protein called Ribosomal protein L26.

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

- Molecule 43 is a protein called Ribosomal protein L3.

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

- Molecule 44 is a protein called Large ribosomal subunit protein eL20.

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

- Molecule 45 is a protein called 40S ribosomal protein S3.

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

- Molecule 46 is a protein called 60S ribosomal protein L27.

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

- Molecule 47 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 48 is a protein called Ribosomal protein L15.

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

- Molecule 49 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	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 50 is a protein called 60S ribosomal protein L27a.

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

- Molecule 51 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	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 52 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 53 is a protein called Ribosomal protein S5.

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

- Molecule 54 is a protein called 60S ribosomal protein L29.

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

- Molecule 55 is a protein called 60S ribosomal protein L6.

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

- Molecule 56 is a protein called Glutathione S-transferase class-mu 26 kDa isozyme,N-alpha-acetyltransferase 50.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	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
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 57 is a protein called 40S ribosomal protein S6.

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

- Molecule 58 is a protein called 60S ribosomal protein L30.

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

- Molecule 59 is a protein called Ribosomal Protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	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 60 is a protein called N-alpha-acetyltransferase 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	DC	165	Total	C	N	O	S	0	0
			1339	844	242	242	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 S7.

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

- Molecule 62 is a protein called 60S ribosomal protein L31.

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

- Molecule 63 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	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 64 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	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 65 is a protein called Ribosomal protein L32.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Be	22	ARG	CYS	variant	UNP G1U6S0
Be	75	ARG	HIS	variant	UNP G1U6S0

- Molecule 66 is a protein called 40S ribosomal protein S27.

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

- Molecule 67 is a protein called 40S ribosomal protein S9.

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

- Molecule 68 is a protein called 60S ribosomal protein L35a.

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

- Molecule 69 is a protein called 40S ribosomal protein S28.

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

- Molecule 70 is a protein called S10_pectin domain-containing protein.

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

- Molecule 71 is a protein called Large ribosomal subunit protein eL34.

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

- Molecule 72 is a protein called Ribosomal protein S27a.

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

- Molecule 73 is a protein called 40S ribosomal protein S11.

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

- Molecule 74 is a protein called 60S ribosomal protein L35.

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

- Molecule 75 is a protein called 40S ribosomal protein S30.

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

- Molecule 76 is a protein called 40S ribosomal protein S12.

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

- Molecule 77 is a protein called 60S ribosomal protein L36.

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

- Molecule 78 is a protein called Small ribosomal subunit protein eS26.

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

- Molecule 79 is a protein called 40S ribosomal protein S13.

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

- Molecule 80 is a protein called Ribosomal protein L37.

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

- Molecule 81 is a protein called Small ribosomal subunit protein RACK1.

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

- Molecule 82 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	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 83 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	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 84 is a protein called 40S ribosomal protein S29.

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

- Molecule 85 is a protein called 40S ribosomal protein uS19.

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

- Molecule 86 is a protein called 60S ribosomal protein L39-like.

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

- Molecule 87 is a RNA chain called mRNA.

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

- Molecule 88 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 89 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

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

- Molecule 90 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
90	BP	1	Total	Mg	0
			1	1	
90	AT	3	Total	Mg	0
			3	3	
90	BR	1	Total	Mg	0
			1	1	
90	Ct	1	Total	Mg	0
			1	1	
90	BV	1	Total	Mg	0
			1	1	
90	B5	282	Total	Mg	0
			282	282	
90	BI	1	Total	Mg	0
			1	1	
90	B7	9	Total	Mg	0
			9	9	
90	B8	9	Total	Mg	0
			9	9	
90	Ba	1	Total	Mg	0
			1	1	
90	Af	1	Total	Mg	0
			1	1	
90	A2	108	Total	Mg	0
			108	108	
90	Bj	1	Total	Mg	0
			1	1	
90	An	1	Total	Mg	0
			1	1	

- Molecule 91 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
91	Bo	1	Total	Zn	0
			1	1	
91	Bp	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
91	Bg	1	Total 1	Zn 1	0
91	AC	1	Total 1	Zn 1	0
91	AE	1	Total 1	Zn 1	0
91	Bj	1	Total 1	Zn 1	0
91	AG	1	Total 1	Zn 1	0
91	Bm	1	Total 1	Zn 1	0

- Molecule 92 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

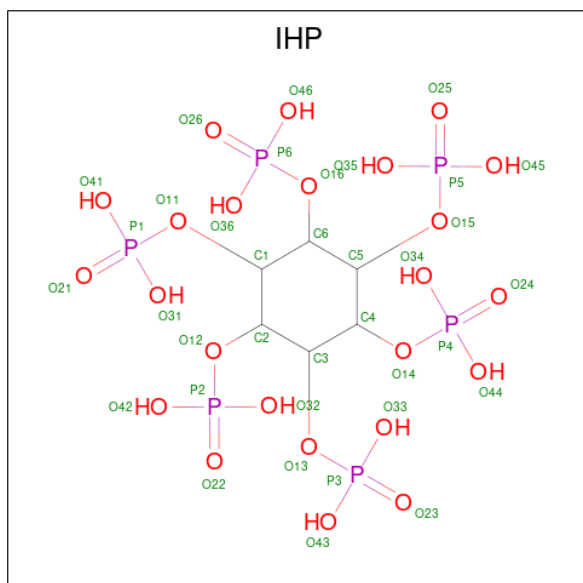
Mol	Chain	Residues	Atoms		AltConf
92	Bo	1	Total 1	X 1	0
92	AT	2	Total 2	X 2	0
92	Ar	1	Total 1	X 1	0
92	BL	1	Total 1	X 1	0
92	BQ	2	Total 2	X 2	0
92	BH	1	Total 1	X 1	0
92	B5	207	Total 207	X 207	0
92	BT	2	Total 2	X 2	0
92	BI	1	Total 1	X 1	0
92	B7	6	Total 6	X 6	0
92	B8	7	Total 7	X 7	0
92	BA	4	Total 4	X 4	0
92	BB	2	Total 2	X 2	0

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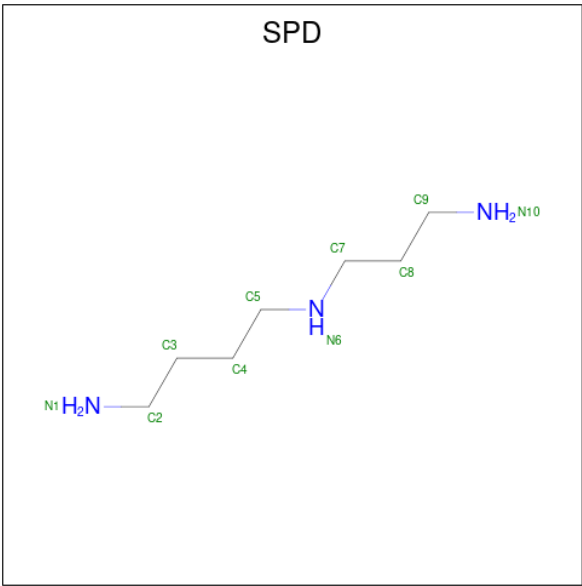
Mol	Chain	Residues	Atoms		AltConf
92	BN	1	Total	X	0
			1	1	
92	Ae	1	Total	X	0
			1	1	
92	Bb	2	Total	X	0
			2	2	
92	A2	57	Total	X	0
			57	57	
92	Be	3	Total	X	0
			3	3	
92	Bf	1	Total	X	0
			1	1	
92	Ak	1	Total	X	0
			1	1	
92	Bj	1	Total	X	0
			1	1	
92	An	1	Total	X	0
			1	1	
92	Bl	1	Total	X	0
			1	1	

- Molecule 93 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 94 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



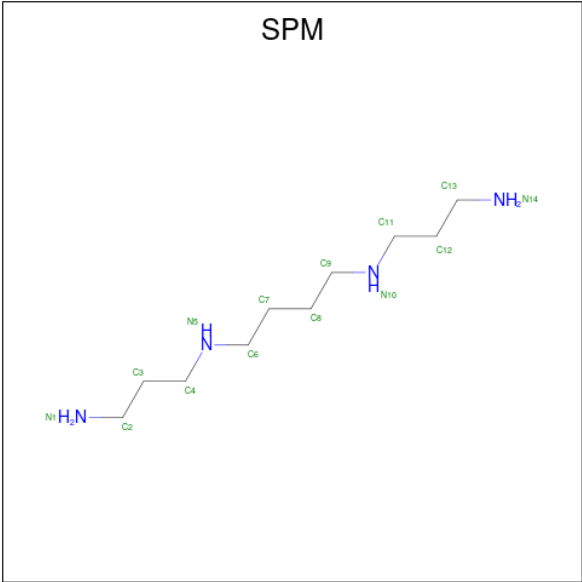
Mol	Chain	Residues	Atoms			AltConf
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N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

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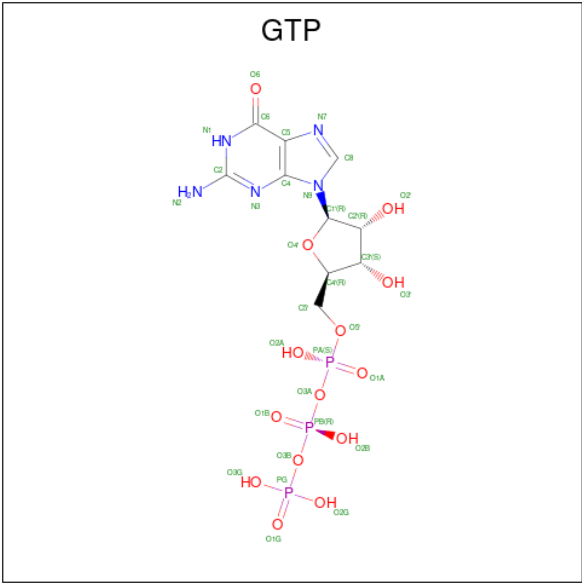
Mol	Chain	Residues	Atoms			AltConf
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	A2	1	Total	C	N	0
			10	7	3	
94	A2	1	Total	C	N	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	
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 GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

- Molecule 97 is water.

Mol	Chain	Residues	Atoms		AltConf
97	BP	3	Total 3	O 3	0
97	Bo	1	Total 1	O 1	0
97	AT	13	Total 13	O 13	0
97	Ar	1	Total 1	O 1	0
97	BL	2	Total 2	O 2	0
97	BX	1	Total 1	O 1	0
97	As	3	Total 3	O 3	0
97	BR	5	Total 5	O 5	0
97	At	1	Total 1	O 1	0
97	Ct	1	Total 1	O 1	0
97	BH	2	Total 2	O 2	0
97	BV	2	Total 2	O 2	0
97	Aw	5	Total 5	O 5	0
97	B5	1383	Total 1383	O 1383	0
97	BI	3	Total 3	O 3	0
97	B7	43	Total 43	O 43	0
97	BJ	1	Total 1	O 1	0
97	B8	50	Total 50	O 50	0
97	Aa	2	Total 2	O 2	0
97	BA	8	Total 8	O 8	0
97	BM	1	Total 1	O 1	0

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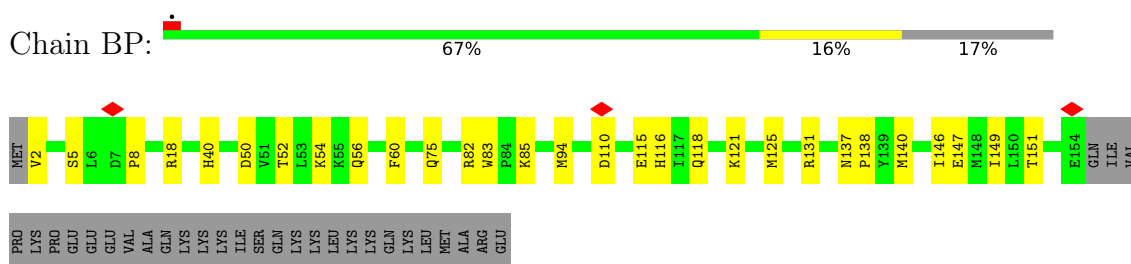
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Mol	Chain	Residues	Atoms		AltConf
97	BB	9	Total 9	O 9	0
97	BC	7	Total 7	O 7	0
97	BN	4	Total 4	O 4	0
97	Ba	8	Total 8	O 8	0
97	B	1	Total 1	O 1	0
97	BO	1	Total 1	O 1	0
97	Af	1	Total 1	O 1	0
97	BF	1	Total 1	O 1	0
97	Bd	1	Total 1	O 1	0
97	A2	526	Total 526	O 526	0
97	Be	5	Total 5	O 5	0
97	Bf	1	Total 1	O 1	0
97	Bg	2	Total 2	O 2	0
97	Ak	2	Total 2	O 2	0
97	AE	1	Total 1	O 1	0
97	Am	1	Total 1	O 1	0
97	Bj	3	Total 3	O 3	0
97	An	3	Total 3	O 3	0
97	Bl	1	Total 1	O 1	0
97	AH	5	Total 5	O 5	0
97	Ap	2	Total 2	O 2	0

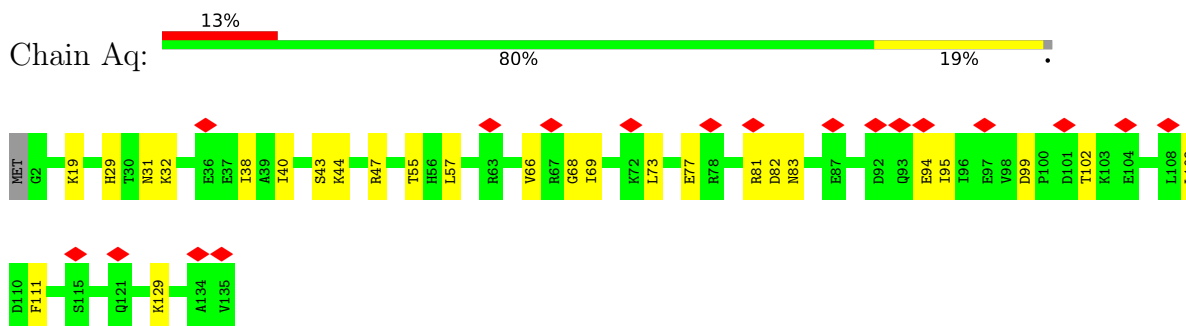
3 Residue-property plots [i](#)

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

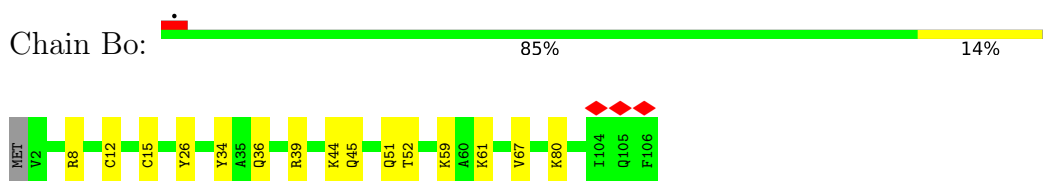
- Molecule 1: Large ribosomal subunit protein uL22



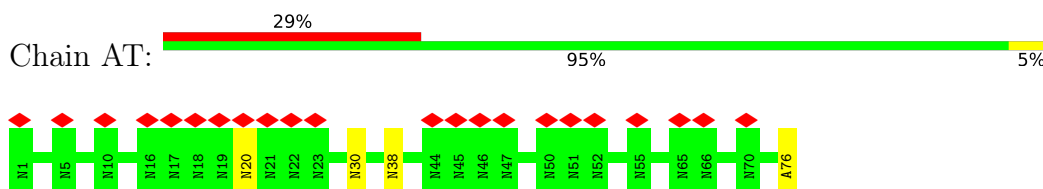
- Molecule 2: 40S ribosomal protein eS17



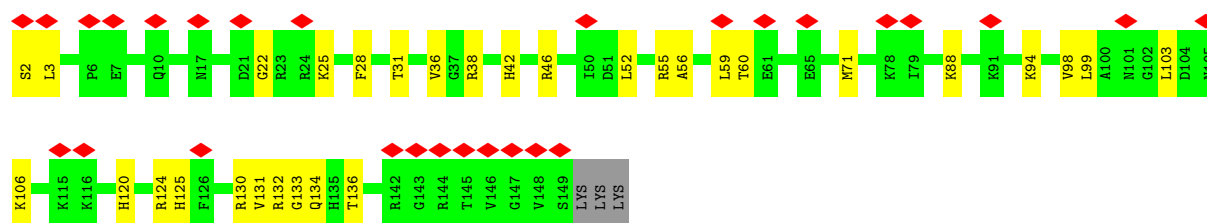
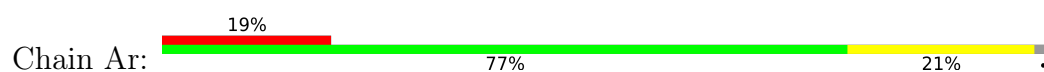
- Molecule 3: Large ribosomal subunit protein eL42



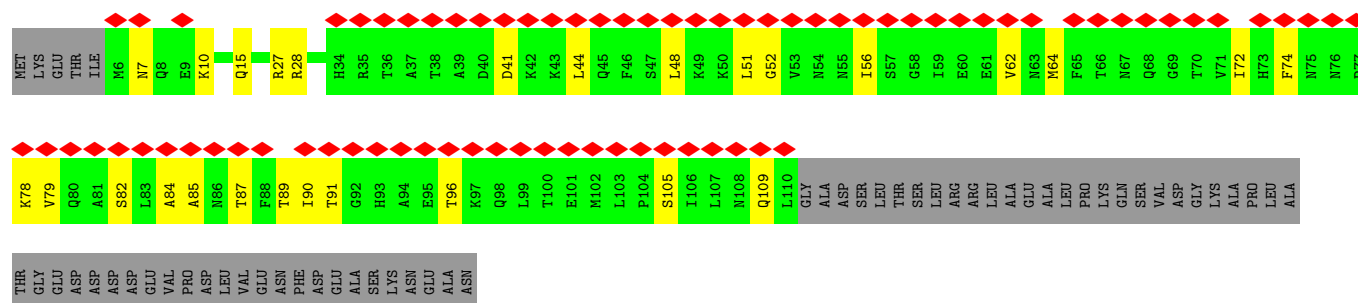
- Molecule 4: P-site tRNA



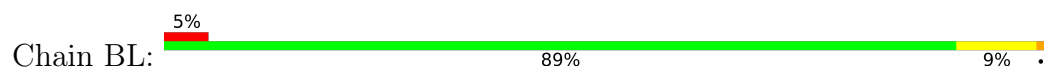
- Molecule 5: Small ribosomal subunit protein uS13



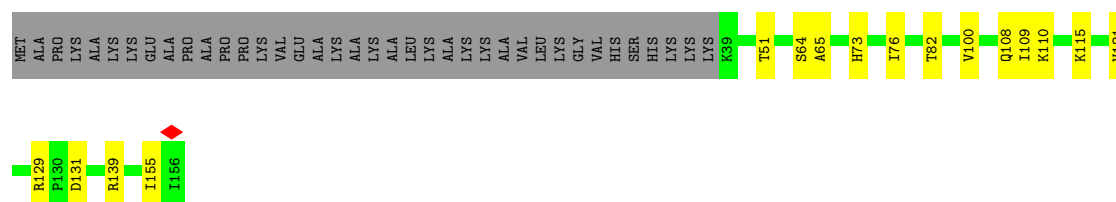
• Molecule 6: Transcription factor BTF3



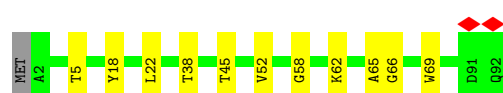
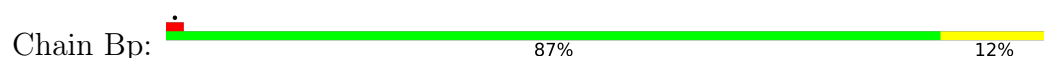
• Molecule 7: Large ribosomal subunit protein eL13



• Molecule 8: Ribosomal_L23eN domain-containing protein

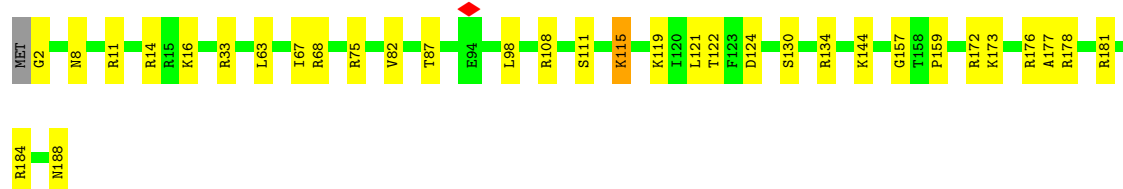


• Molecule 9: 60S ribosomal protein L37a



• Molecule 10: Large ribosomal subunit protein eL18

Chain BQ:  82% 17% ..



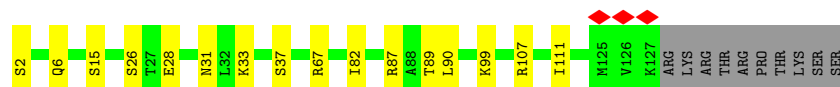
- Molecule 11: 40S ribosomal protein S19

Chain As:  12% 88% 10% .



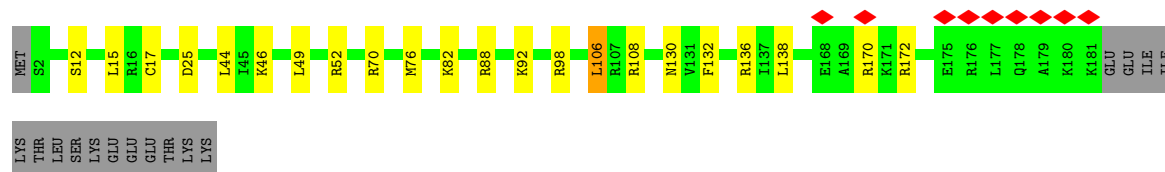
- Molecule 12: Large ribosomal subunit protein eL28

Chain Br:  81% 12% 7%



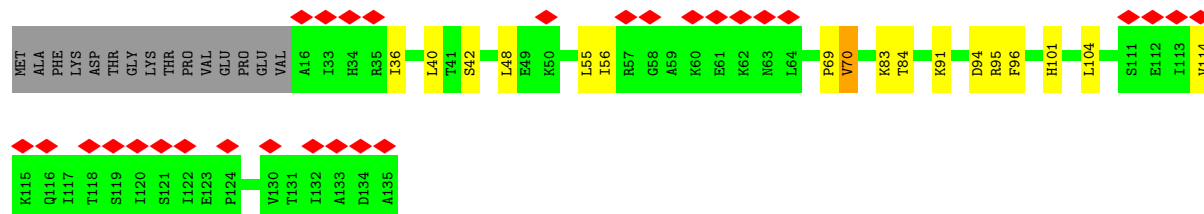
- Molecule 13: Ribosomal protein L19

Chain BR:  5% 81% 11% 8%

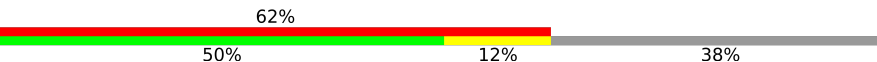


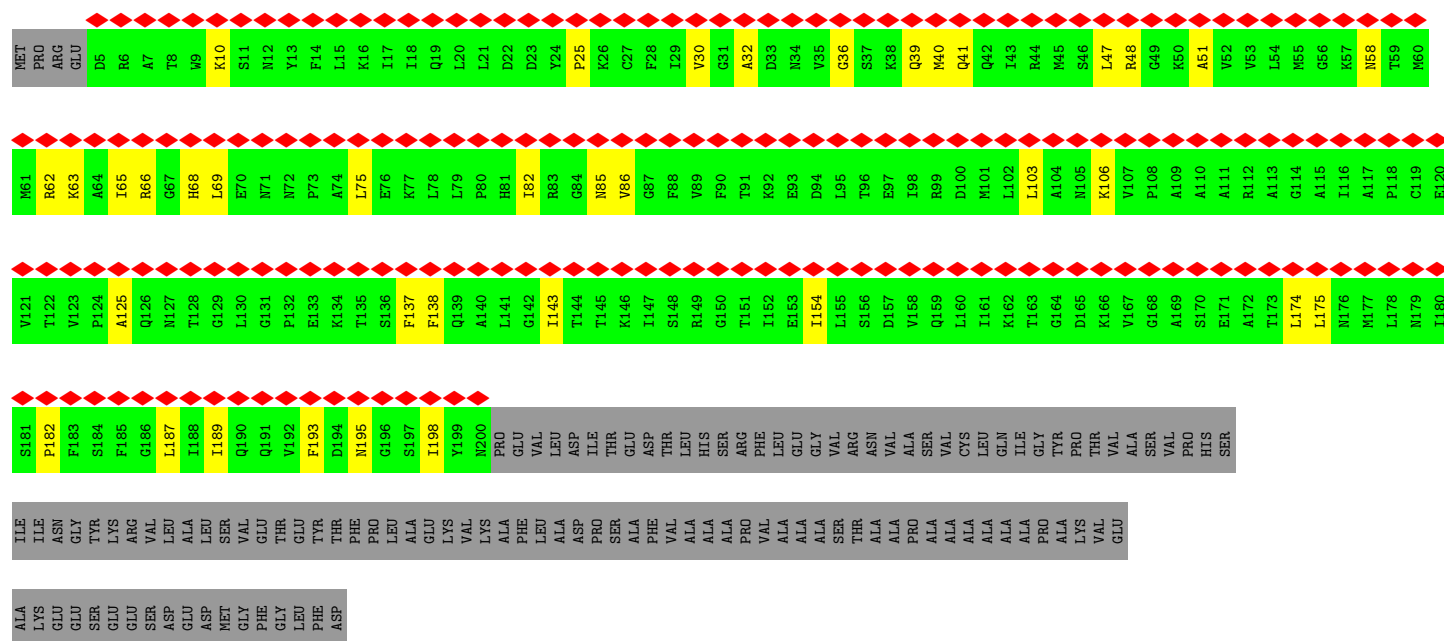
- Molecule 14: Small ribosomal subunit protein uS10

Chain At:  24% 73% 13% 13%

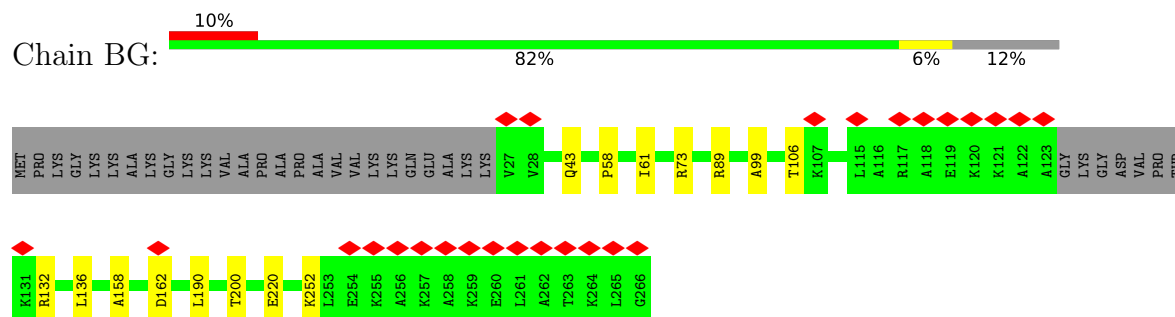


- Molecule 15: 60S acidic ribosomal protein P0

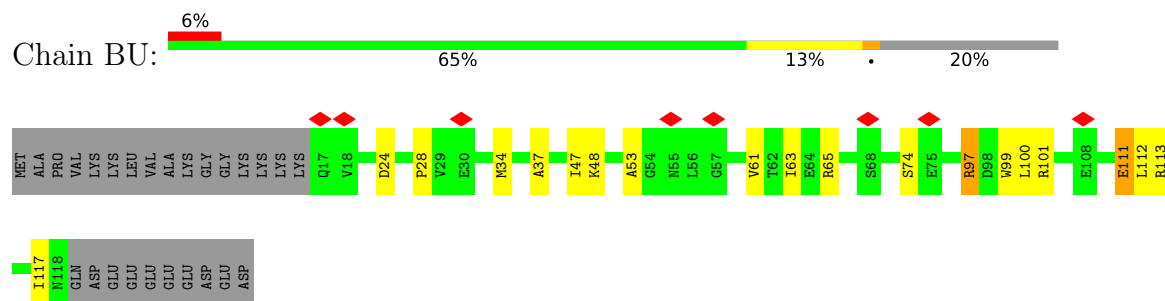
Chain Bs:  62% 50% 12% 38%



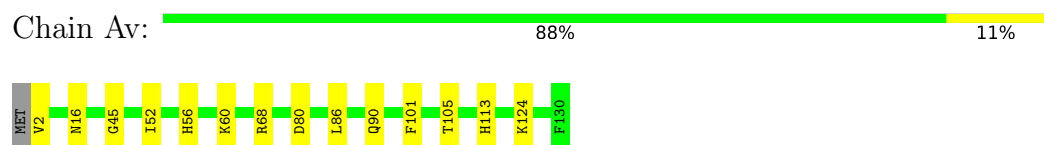
- Molecule 16: 60S ribosomal protein L7a



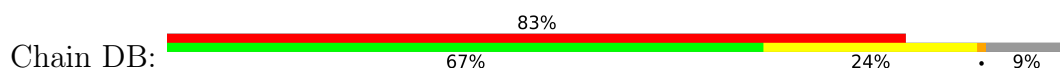
- Molecule 17: 60S ribosomal protein L22



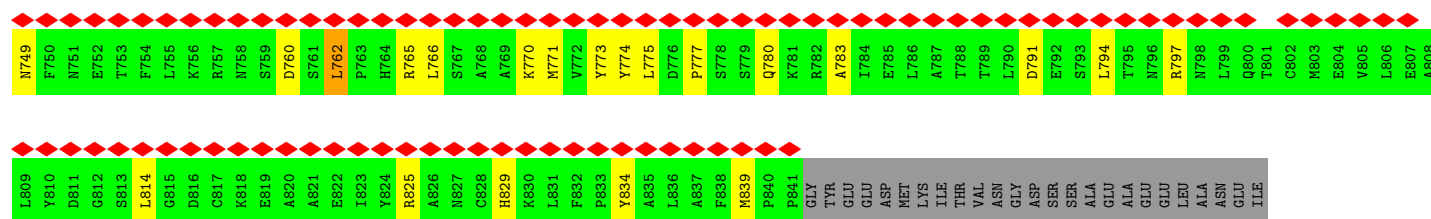
- Molecule 18: Ribosomal protein S15a



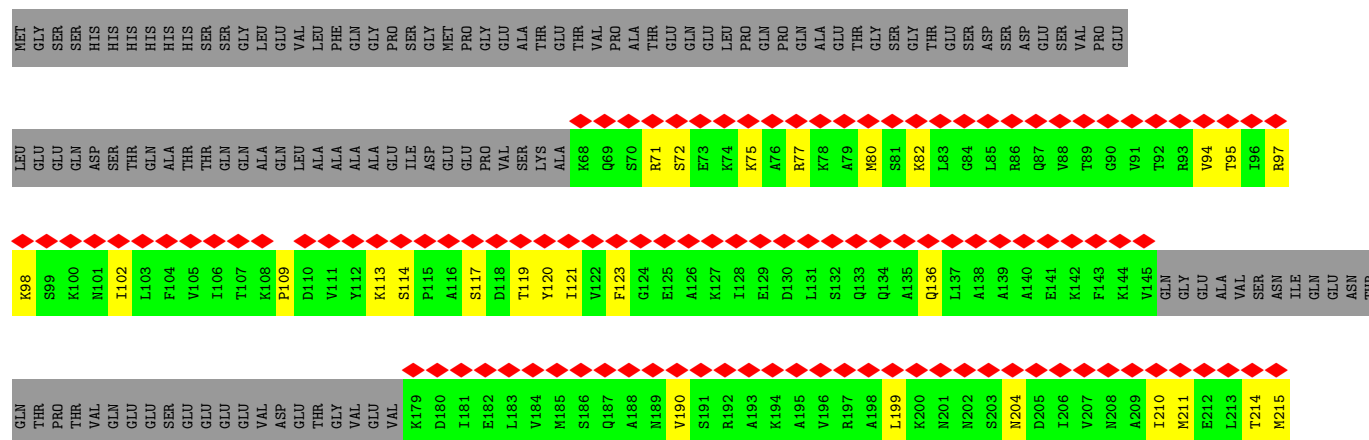
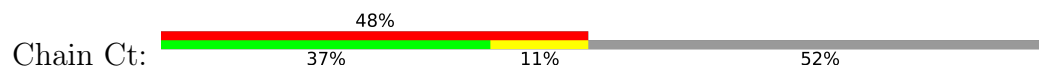
- Molecule 19: N-alpha-acetyltransferase 15, NatA auxiliary subunit



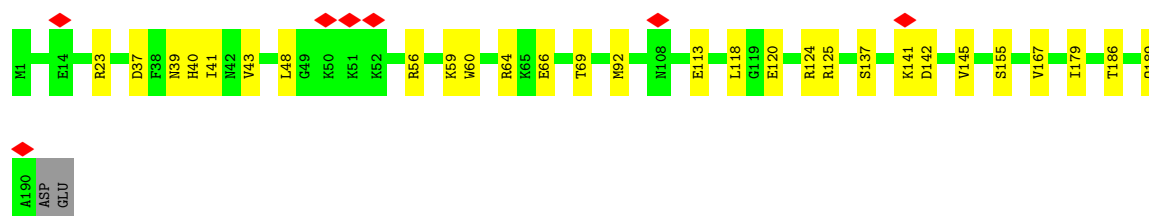
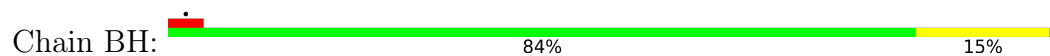
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A12	L13	F14	K15	R16	R19	C20	Y21	K24	Q25	Y26	R27	N28	K31	F32	C33	K34	L37	S38	N39	P40	K41	F42	E44	H45	G46	E47	T48	L49	A50	M51	K52	G53	L54	T55	L56	N57	C58	L59	G60	K61	K62	E63	E64	A65	Y66	E67	L68	V69	R70	R71	G72	L73	R74	N75						
D76	L77	K78	H80	V81	C82	H83	H84	Y86	G87	L88	L89	Q90	R91	S92	D93	K94	K95	Y96	D97	E98	A99	I100	C101	Y103	N105	A106	L107	K108	W109	D110	K111	D112	N113	L114	Q115	I116	L117	R118	D119	L120	S121	L122	L123	Q124	I125	Q126	M127	R128	D129	L130	Y133	R134	E135	T136						
R137	Y138	Q139	L140	L141	Q142	L143	R144	P145	A146	Q147	R148	A149	S150	W151	I152	G153	Y154	A155	I156	A157	Y158	H159	L160	L161	E162	D163	N164	E165	M166	A167	A168	K169	L170	L171	E172	E173	F174	R175	K176	T177	Q178	Q179	T180	S181	P182	D183	K184	V185	D186	Y187	E188	Y189	S190	E191	Q192	L193	L194	Y195	Q196	
N197	Q198	Y199	L200	R201	E202	A203	G204	L205	Y206	R207	E208	A209	L210	E211	H212	L213	C214	T215	Y216	E217	K218	Q219	L220	C221	D222	K223	L224	A225	V226	E227	E228	T229	K230	Q231	E232	L233	L234	L235	Q236	L237	C238	R239	L240	E241	D242	A243	A244	D245	V246	Y247	R248	G249	L250	Q251	E252	R253	L254	P255	E256	
N257	W258	A259	Y260	Y261	K262	G263	L264	E265	K266	A267	L268	K269	P270	A271	W272	H273	L274	E275	R276	L277	K278	T279	Y280	E281	E282	A283	W284	T285	K286	Y287	P288	R289	L290	L291	V292	P293	R294	R295	L296	P297	L298	N299	F300	L301	S302	G303	E304	K305	F306	K307	E308	C309	L310	D311	K312	F313	L314	R315	M316	
N317	F318	S319	K320	G321	C322	F323	P324	V325	F326	N327	T328	L329	R330	S331	H332	Y333	K334	D335	K336	E337	Y338	V339	A340	I341	L342	E343	E344	L345	V346	V347	G348	Y349	E350	T351	S352	L353	K354	S355	C356	R357	L358	F359	N360	P361	N362	D363	D364	G365	G366	E367	E368	P369	P370	T371	D372	L373	L374	W375	V376	
Q377	Y378	Y379	L380	A381	Q382	H383	Y384	D385	K386	I387	G388	Q389	S390	S391	Y392	A393	L394	E395	Y396	I397	N398	T399	A400	L401	E402	S403	T404	P405	T406	L407	L408	E409	L410	F411	L412	V413	K414	A415	K416	I417	Y418	K419	H420	A421	Q422	N423	I424	K425	E426	A427	A428	R429	W430	M431	D432	E433	A434	Q435	A436	
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R559	I560	A561	I562	E563	I564	Y565	L566	K567	L568	H569	D570	N571	P572	L573	T574	D575	E576	N577	K578	E579	H580	E581	A582	D583	T584	A585	N586	N587	S588	D589	K590	E591	R596	N597	K605	L608	E609	E610	E611	K612	K613	N614	A615	E616	K617	E618	K619	Q620	Q621	R622	N623	Q624	K625	K626	K627	K628				
D629	D630	D631	D632	E633	E634	L635	G636	G637	P638	K639	E640	E641	L642	L643	P644	E645	K646	L647	A648	K649	V650	E651	T652	P653	L654	E655	E656	A657	T658	D659	F660	L661	T662	P663	L664	K665	L666	L667	V668	K669	N670	K671	L672	N673	L674	T675	H676	L677	F677	E678	F679	E680	L681	F682	P683	R684	K685	E686	P687	K688
L689	L690	M691	L692	Q693	S694	V695	K696	R697	A698	F699	A700	I701	D702	S703	H705	P706	W707	L708	H709	E710	C711	M712	T713	R714	L715	F716	N717	T718	A719	V720	C721	T722	S723	K724	D725	L726	S727	D728	T729	W730	R731	T732	W733	L734	K735	Q736	F737	M738	N739	R740	L741	F742	G743	T745	N746	P747	K748			



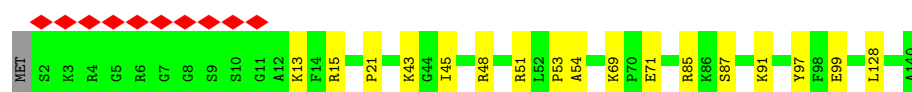
• Molecule 20: Nascent polypeptide-associated complex subunit alpha



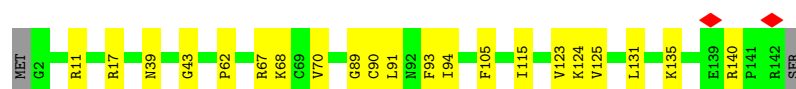
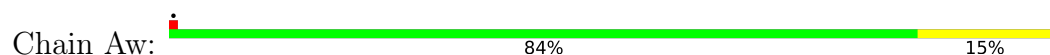
• Molecule 21: 60S ribosomal protein L9



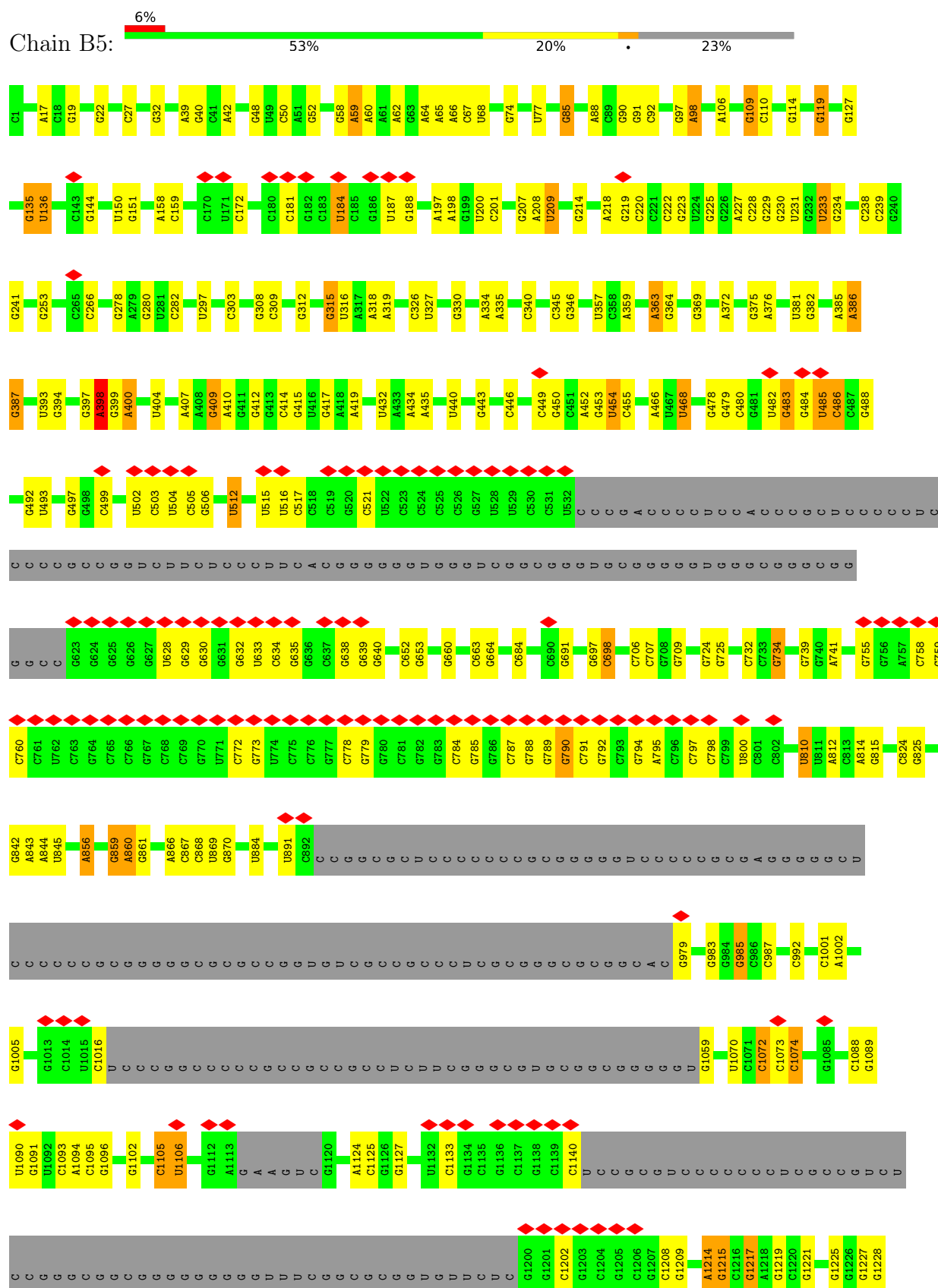
• Molecule 22: Ribosomal protein L23



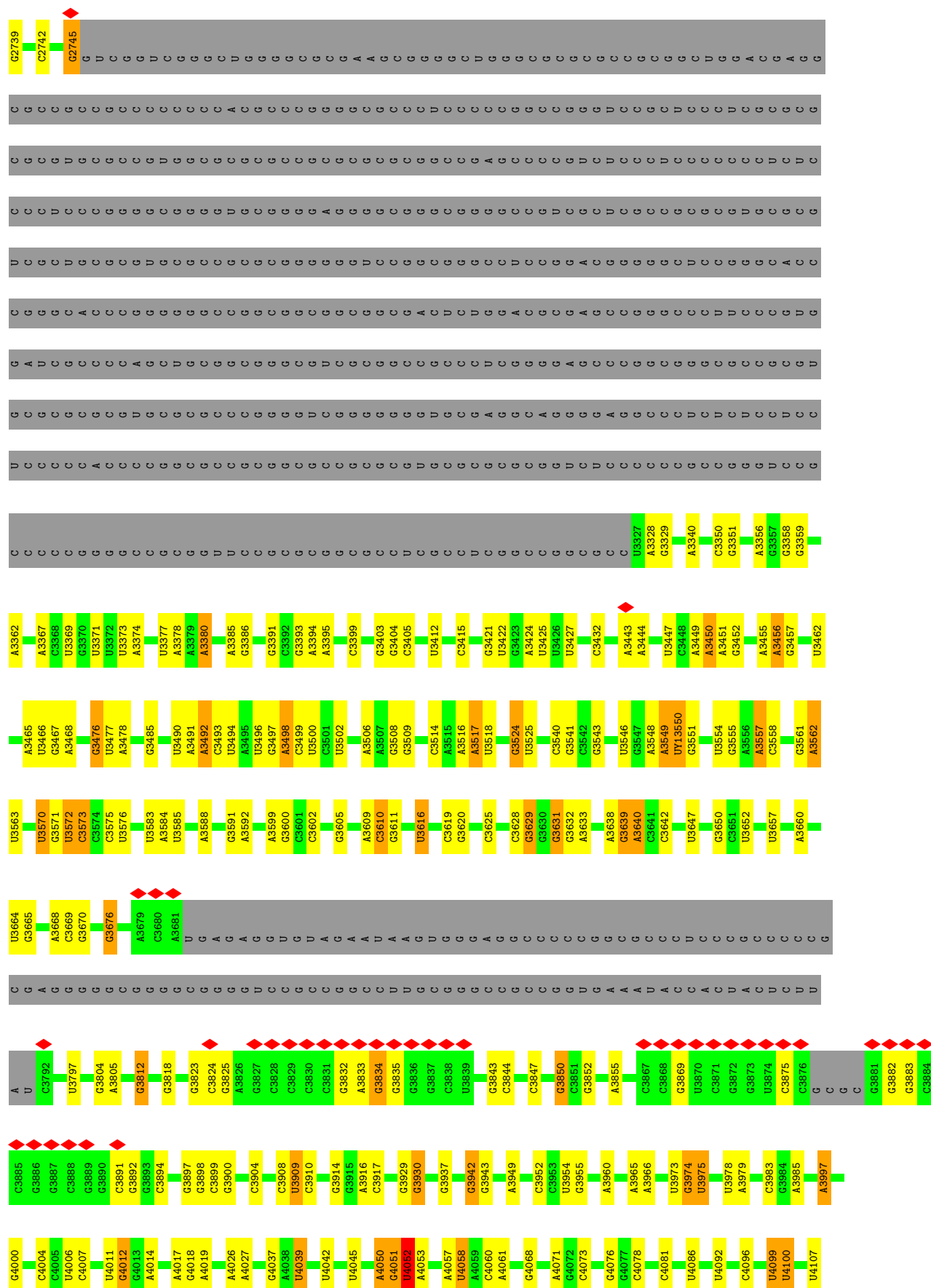
• Molecule 23: 40S ribosomal protein S23

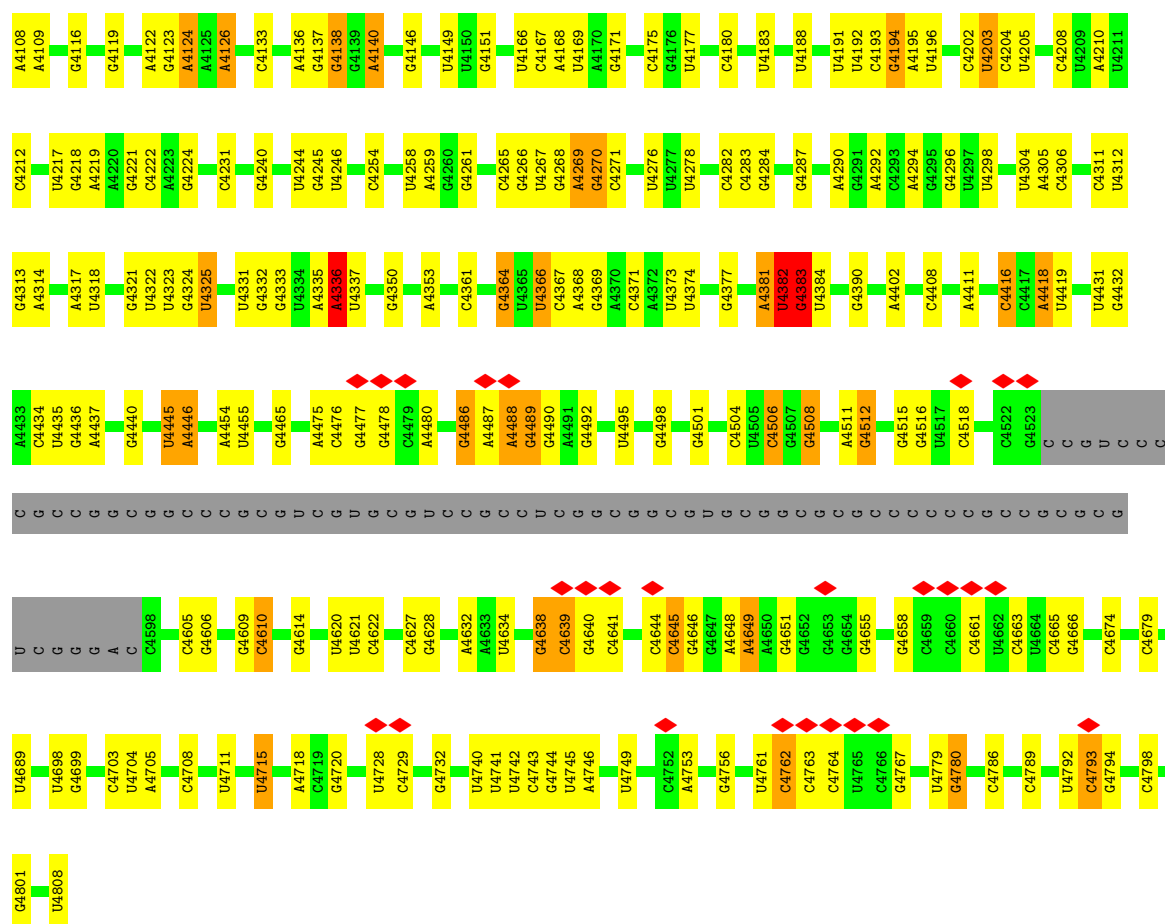


● Molecule 24: 28S rRNA



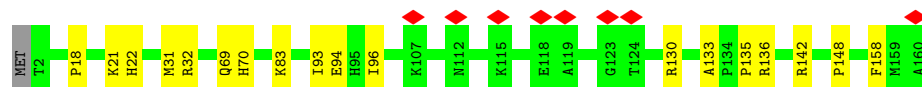






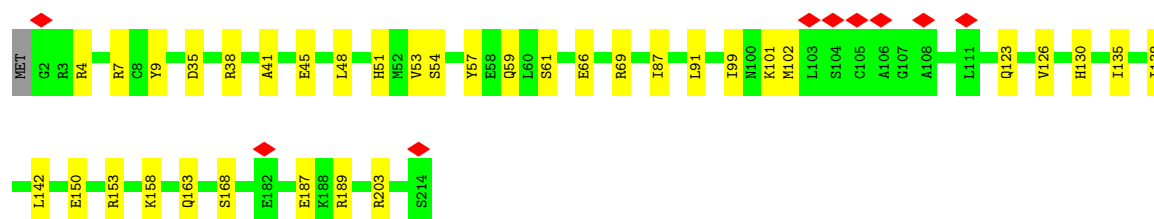
- Molecule 25: 60S ribosomal protein L21

Chain BT: 5% 88% 11%



- Molecule 26: 60S ribosomal protein L10

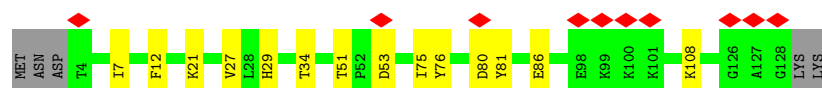
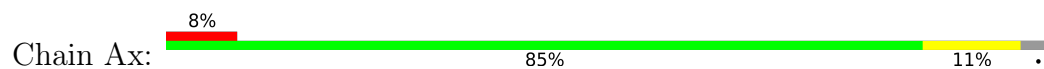
Chain BI: 83% 16%



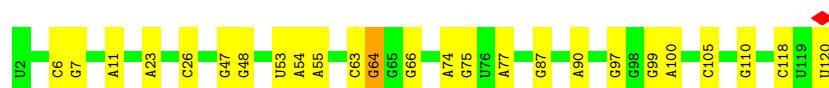
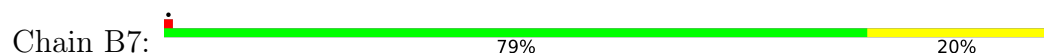
- Molecule 27: Ribosomal protein L24

Chain BW: 31% 67% 10% 23%

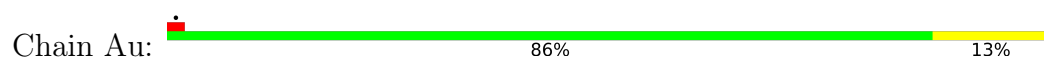
- Molecule 28: 40S ribosomal protein S24



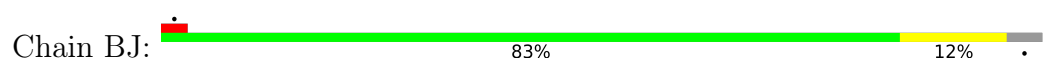
- Molecule 29: 5S rRNA



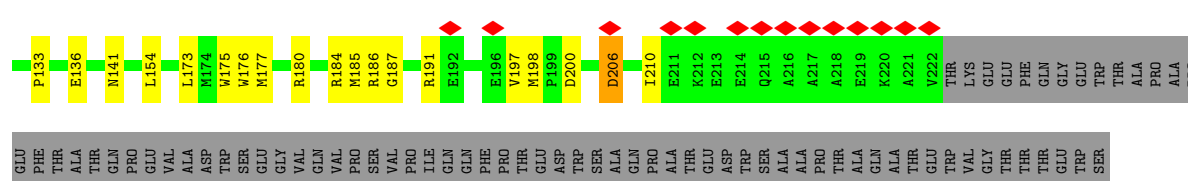
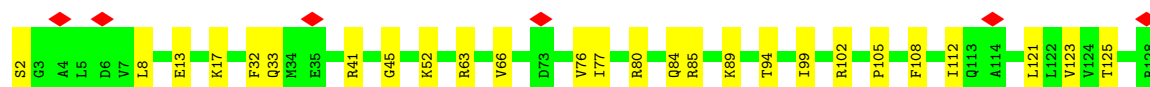
- Molecule 30: Small ribosomal subunit protein eS21



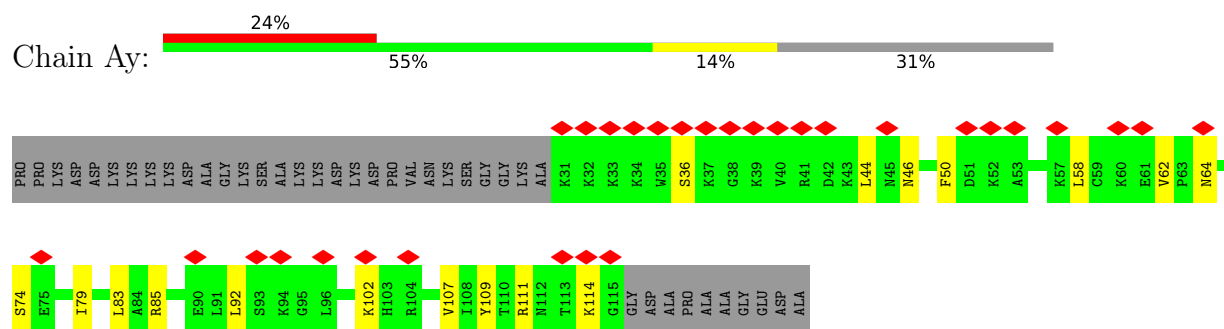
- Molecule 31: 60S ribosomal protein L11



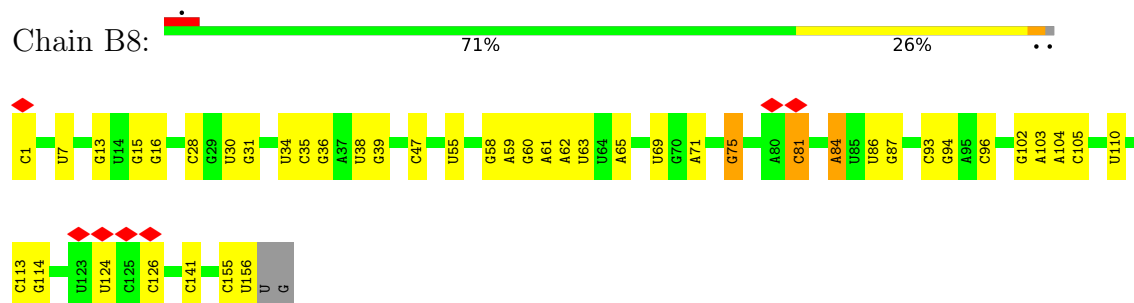
- Molecule 32: Small ribosomal subunit protein uS2



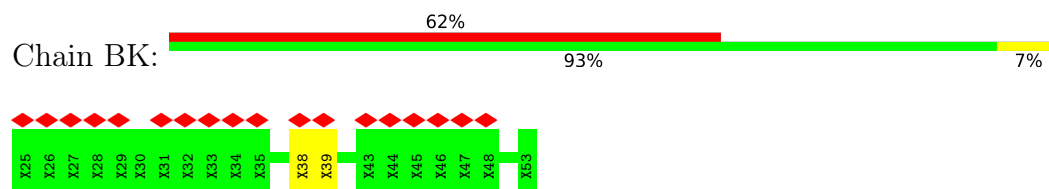
- Molecule 33: 40S ribosomal protein S25



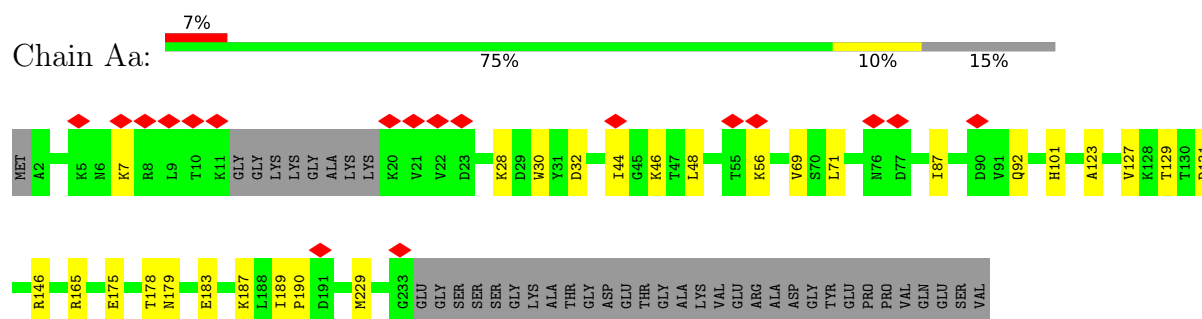
- Molecule 34: 5.8S rRNA



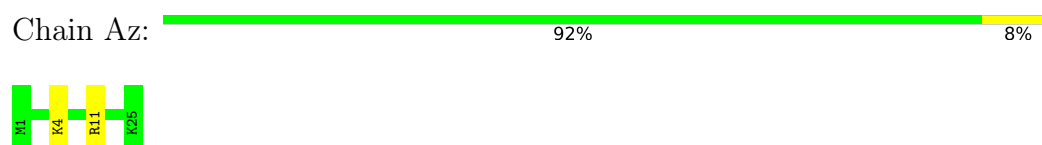
- Molecule 35: Nascent chain



- Molecule 36: 40S ribosomal protein S3a

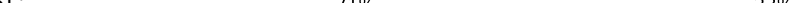


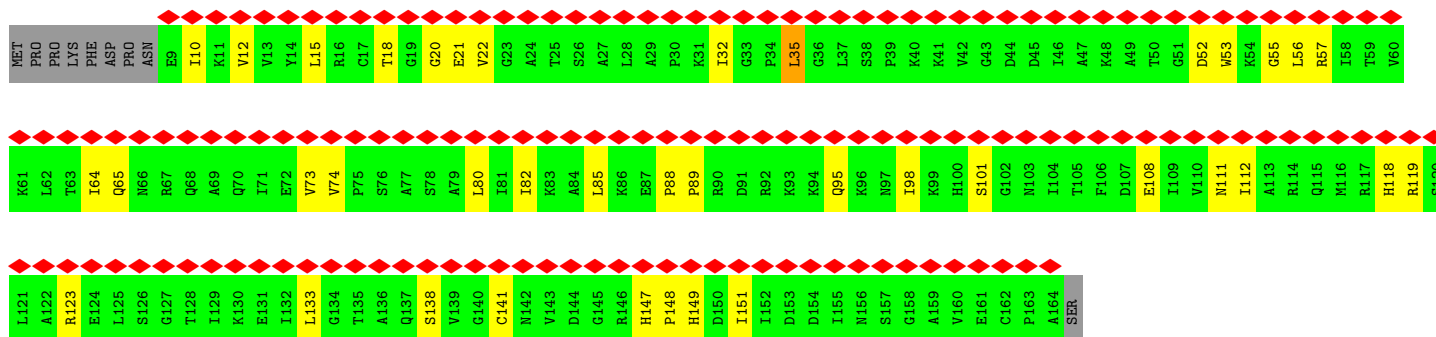
- Molecule 37: 60S ribosomal protein L41

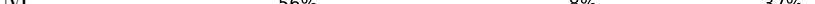


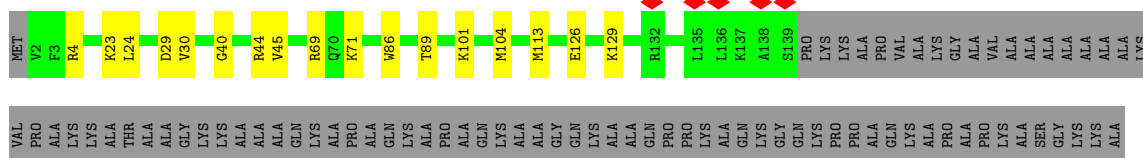
- Molecule 38: Large ribosomal subunit protein uL2

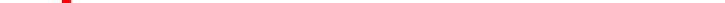
[illegible]

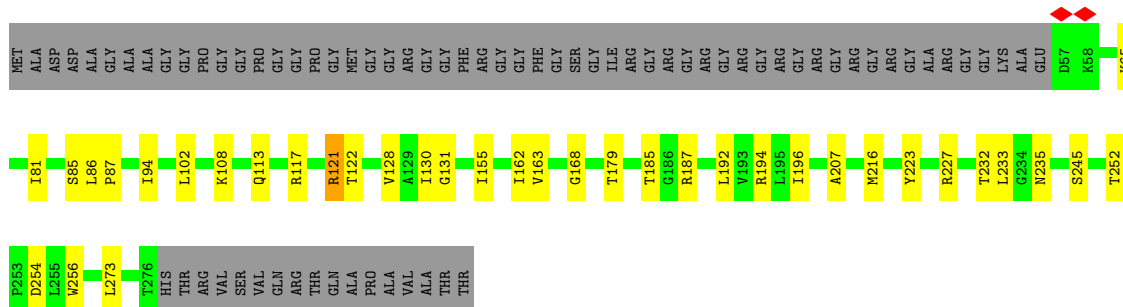
Chain Bt: 



Chain BM: 



Chain Ab: 

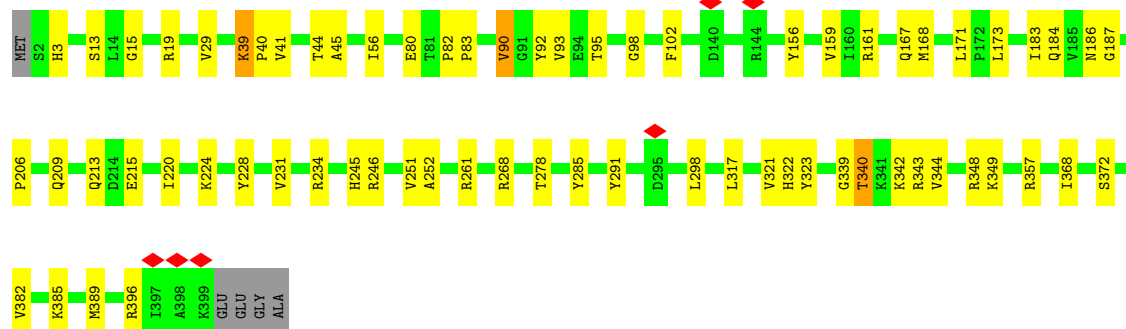


Chain BY: 



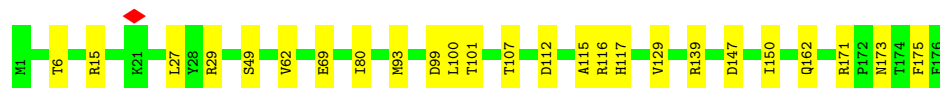
- Molecule 43: Ribosomal protein L3

Chain BB: 



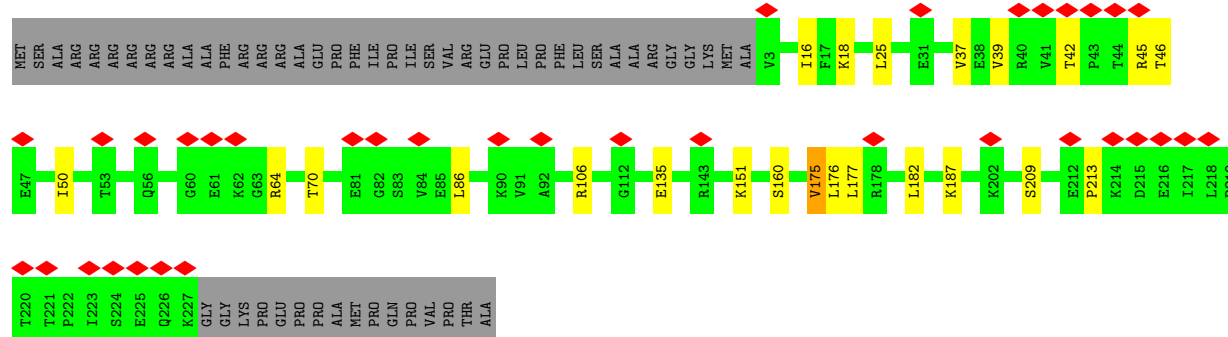
- Molecule 44: Large ribosomal subunit protein eL20

Chain BS: 



- Molecule 45: 40S ribosomal protein S3

Chain Ac: 

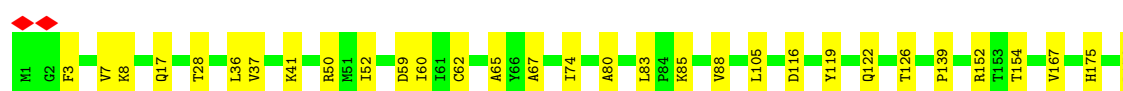
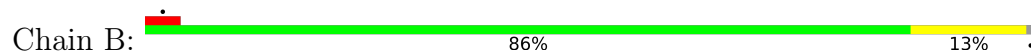
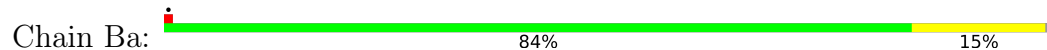
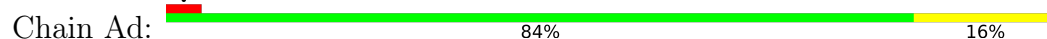
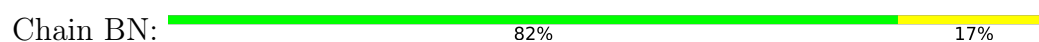


- Molecule 46: 60S ribosomal protein L27

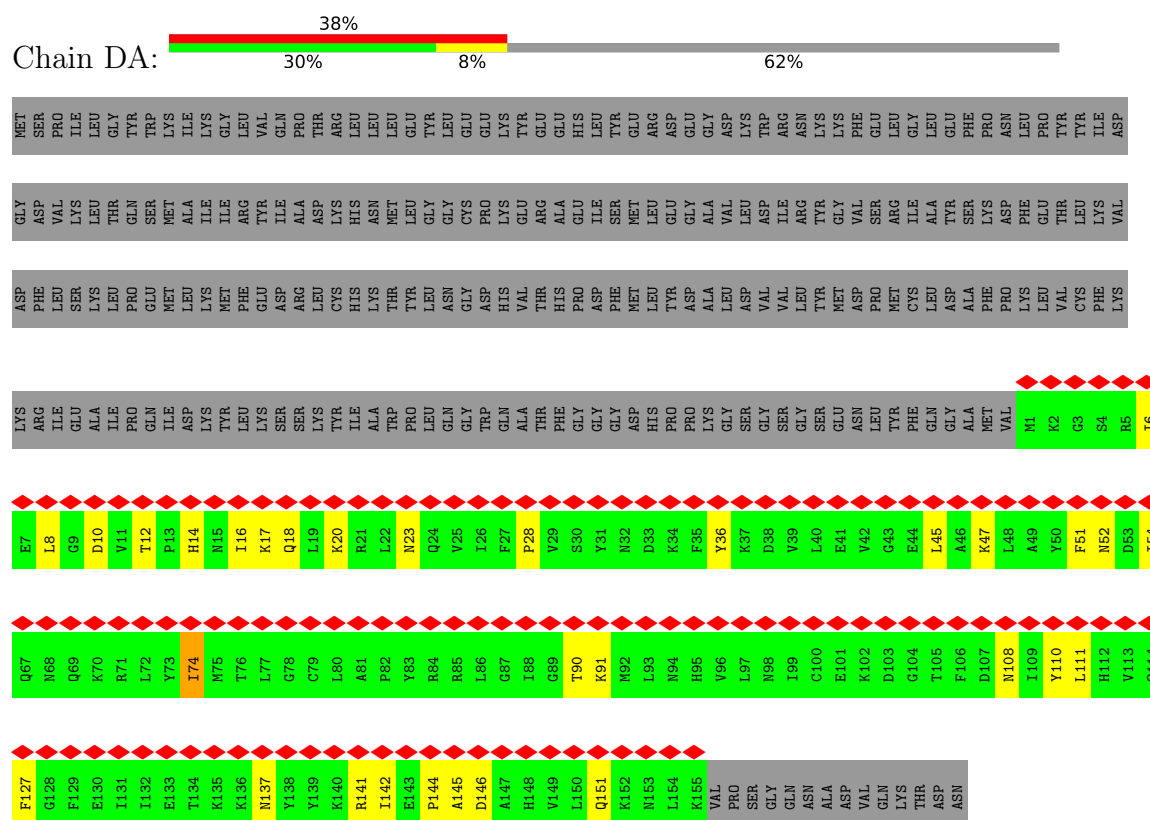
Chain BZ: 



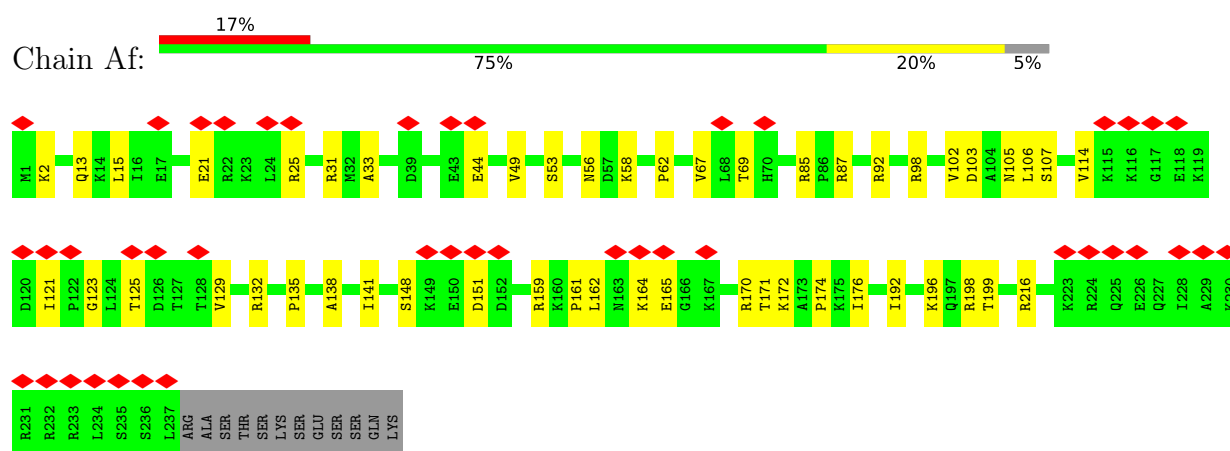
Chain BC: 77% 11% 12%



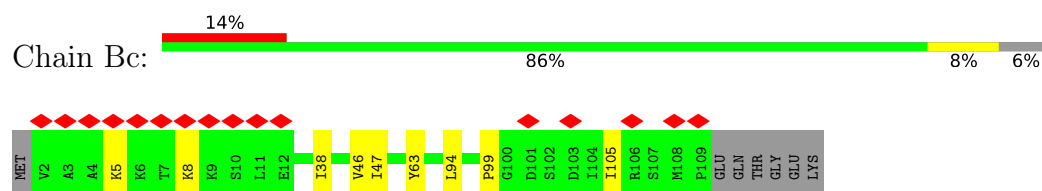
- Molecule 56: Glutathione S-transferase class-mu 26 kDa isozyme,N-alpha-acetyltransferase 50



- Molecule 57: 40S ribosomal protein S6



- Molecule 58: 60S ribosomal protein L30

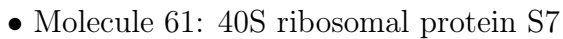


- Molecule 59: Ribosomal Protein uL30

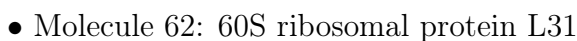
App Type	Percentage
Shopping app	78%
Social media app	14%
Productivity app	9%



Device Type	Percentage
Smartphone	66%
Tablet	53%
Feature phone	17%
Smartwatch	30%



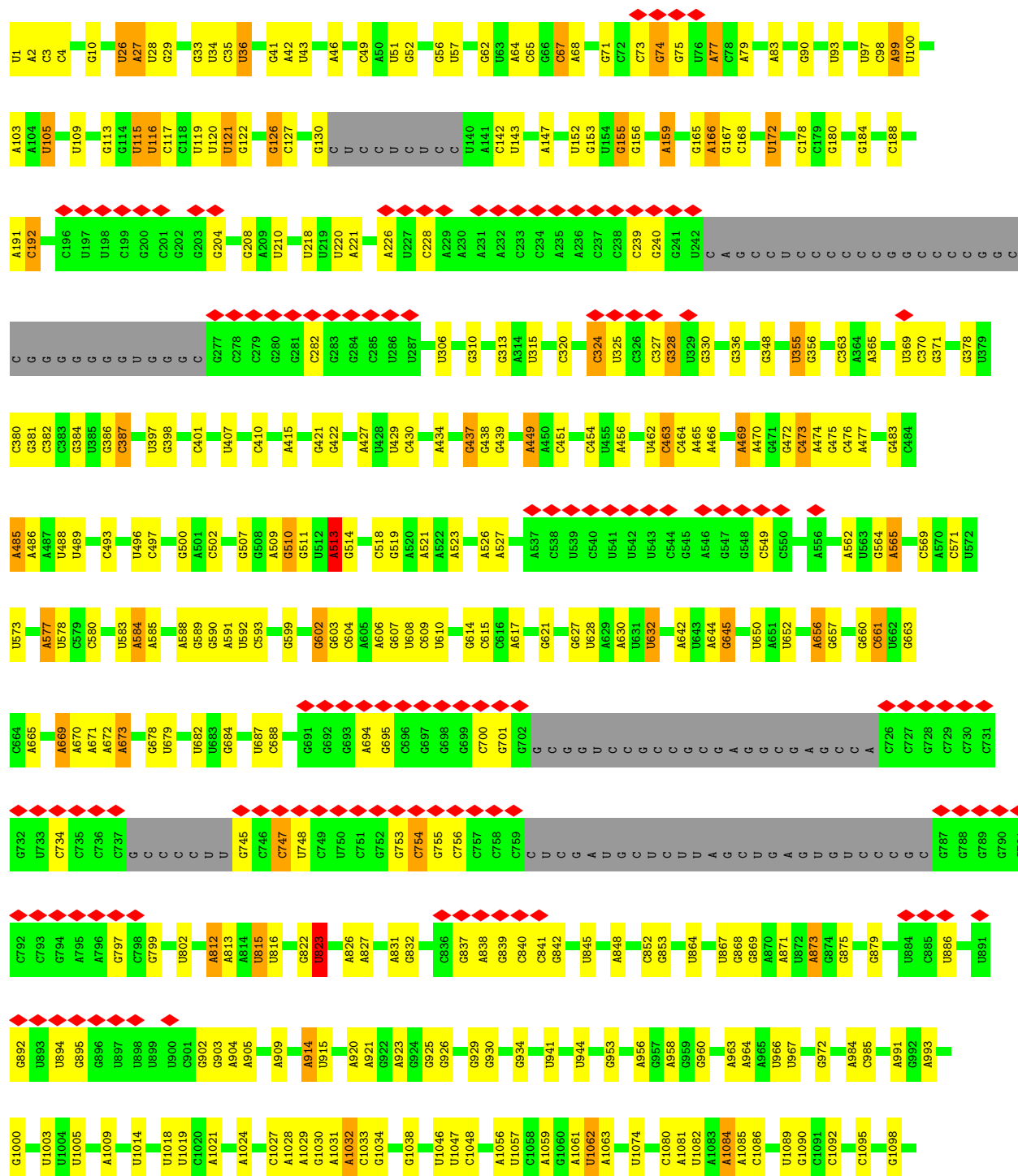
Response	Percentage
Very good	9%
Good	37%
Not good	7%
Very bad	56%

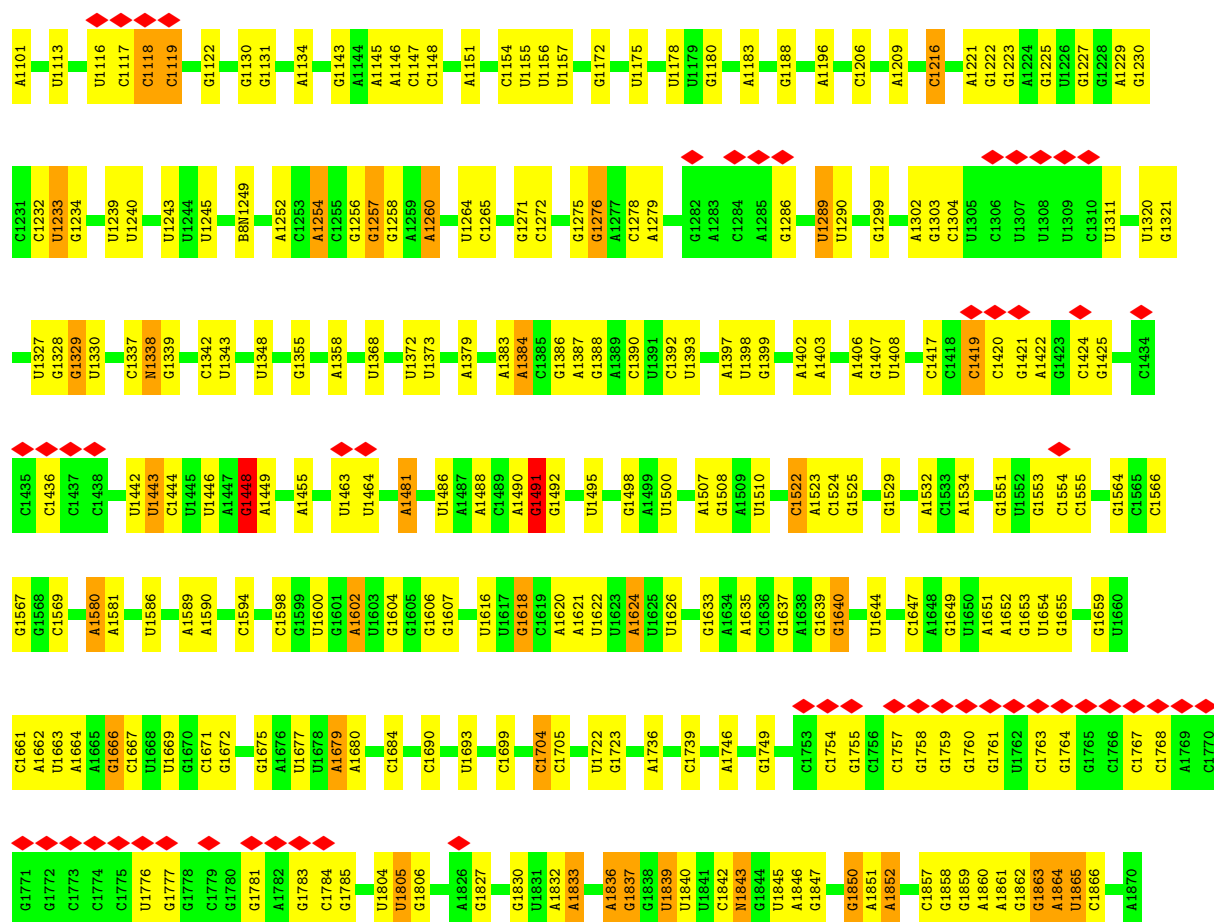


Frequency	Percentage
Very often	6%
Often	74%
Sometimes	11%
Never	14%

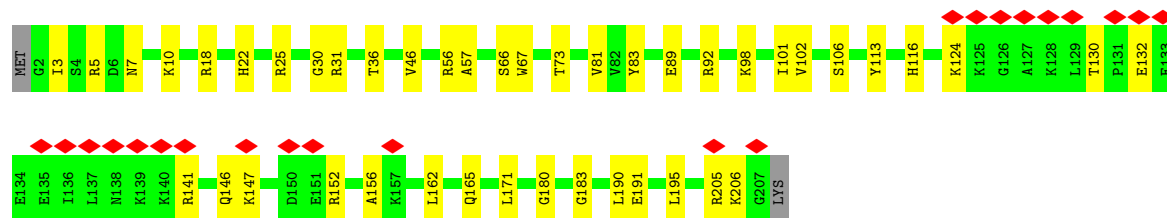
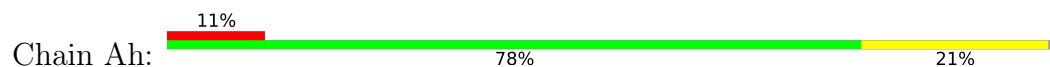


• Molecule 63: 18S rRNA

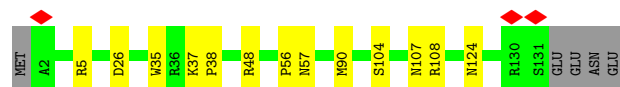
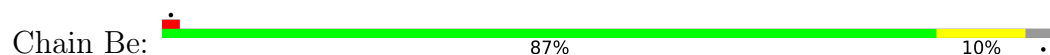




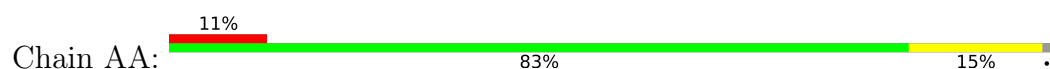
• Molecule 64: 40S ribosomal protein S8

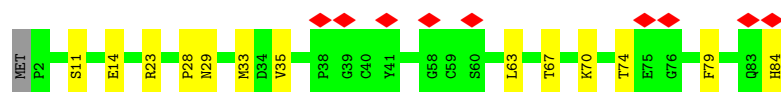


• Molecule 65: Ribosomal protein L32

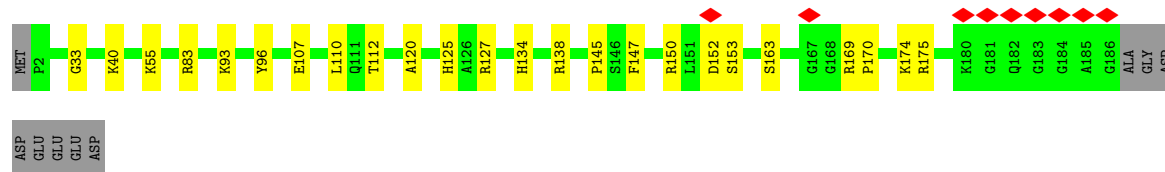
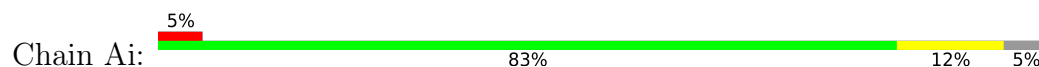


• Molecule 66: 40S ribosomal protein S27





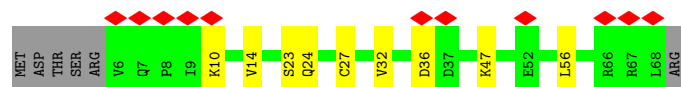
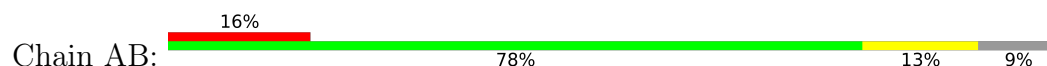
- Molecule 67: 40S ribosomal protein S9



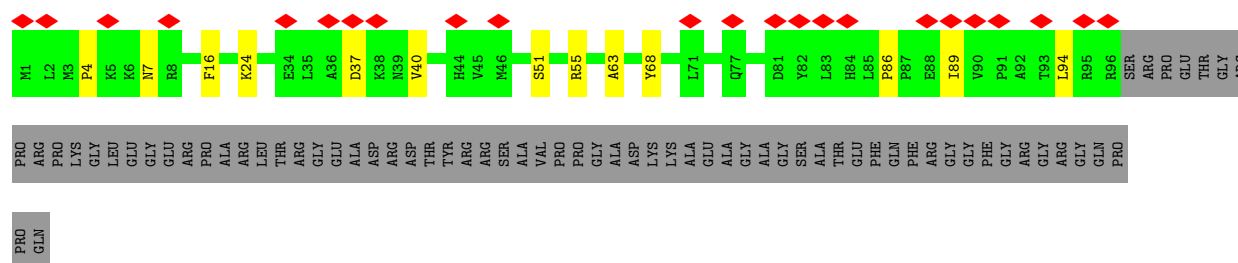
- Molecule 68: 60S ribosomal protein L35a



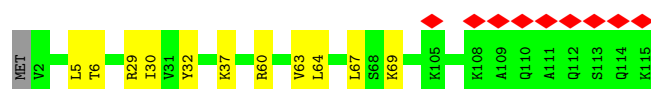
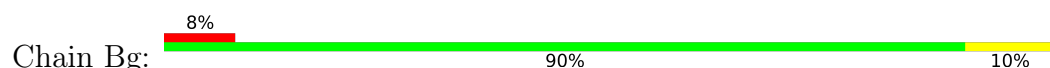
- Molecule 69: 40S ribosomal protein S28



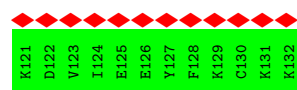
- Molecule 70: S10_ plectin domain-containing protein



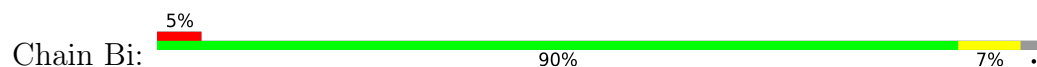
- Molecule 71: Large ribosomal subunit protein eL34



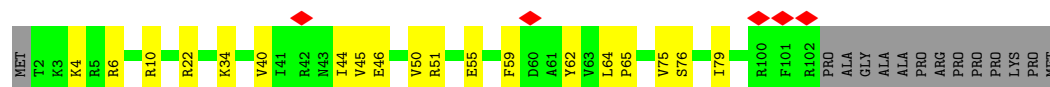
- Molecule 72: Ribosomal protein S27a



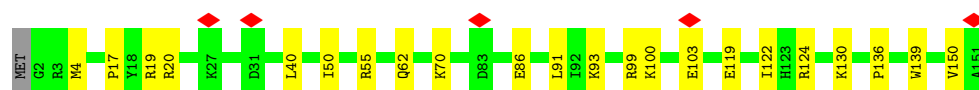
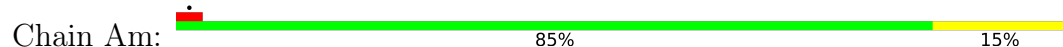
- Molecule 77: 60S ribosomal protein L36



- Molecule 78: Small ribosomal subunit protein eS26



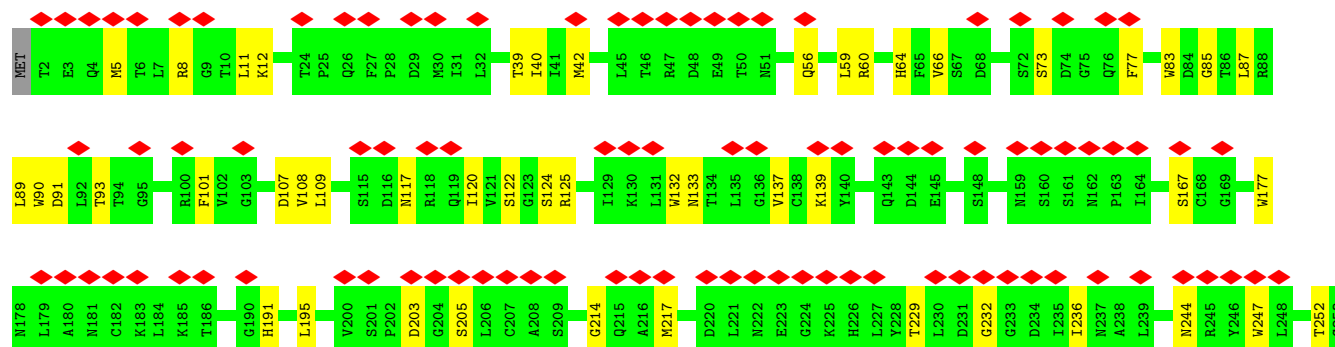
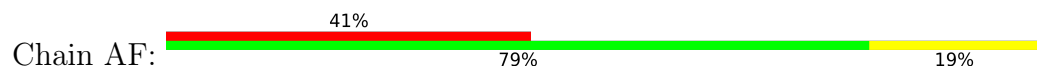
- Molecule 79: 40S ribosomal protein S13

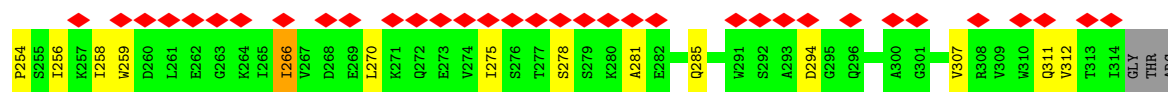


- Molecule 80: Ribosomal protein L37

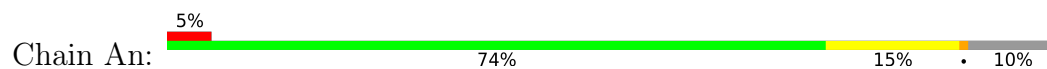


- Molecule 81: Small ribosomal subunit protein RACK1

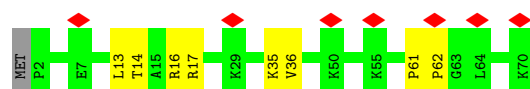




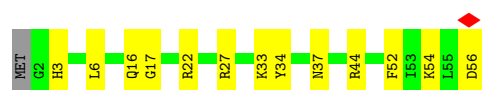
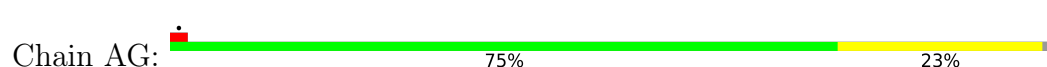
- Molecule 82: Small ribosomal subunit protein uS11



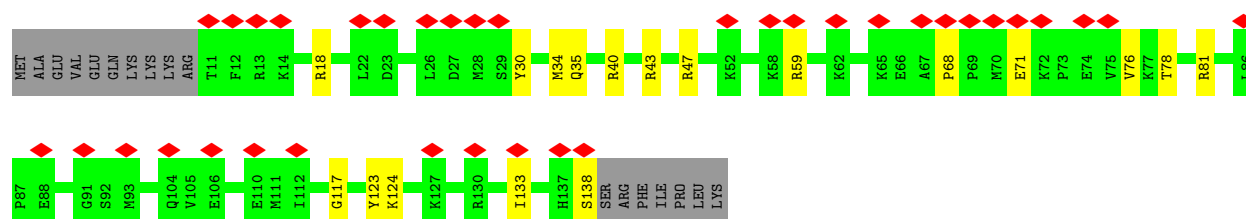
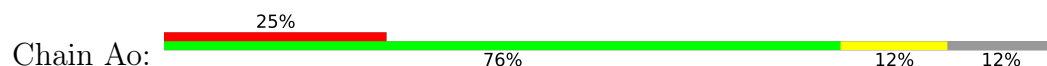
- Molecule 83: 60S ribosomal protein L38



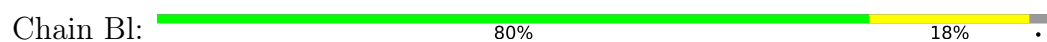
- Molecule 84: 40S ribosomal protein S29



- Molecule 85: 40S ribosomal protein uS19



- Molecule 86: 60S ribosomal protein L39-like

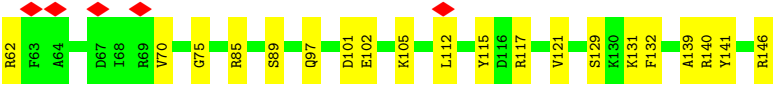
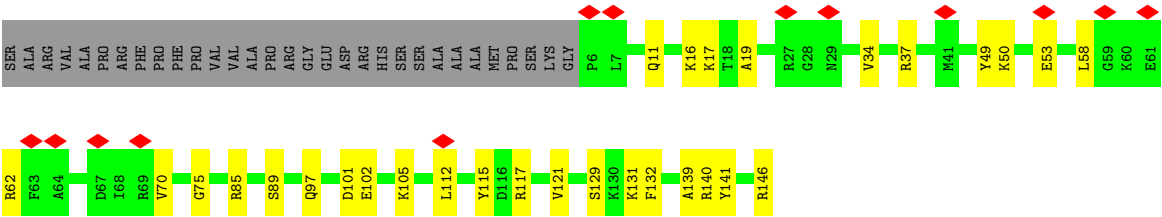


- Molecule 87: mRNA

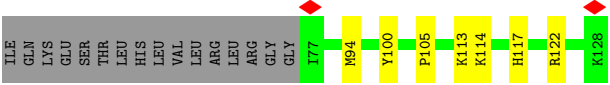
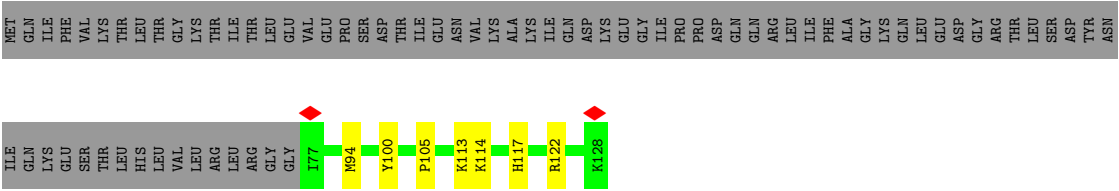
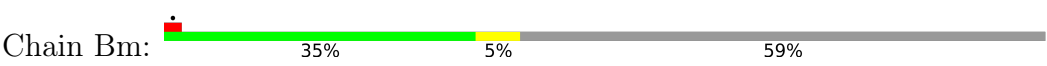




• Molecule 88: Small ribosomal subunit protein uS9



• Molecule 89: Ubiquitin-ribosomal protein eL40 fusion protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37182	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.360	Depositor
Minimum map value	-0.419	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.055	Depositor
Recommended contour level	0.275	Depositor
Map size (Å)	593.6, 593.6, 593.6	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	BP	0.07	0/1268	0.21	0/1700
2	Aq	0.07	0/1094	0.19	0/1469
3	Bo	0.13	0/866	0.25	0/1141
4	AT	0.07	0/68	0.15	0/103
5	Ar	0.06	0/1226	0.18	0/1643
6	Cu	0.16	0/821	0.35	0/1101
7	BL	0.07	0/1733	0.19	0/2316
8	BX	0.07	0/984	0.19	0/1323
9	Bp	0.08	0/718	0.21	0/953
10	BQ	0.07	0/1539	0.19	0/2054
11	As	0.06	0/1119	0.17	0/1498
12	Br	0.08	0/1020	0.22	0/1366
13	BR	0.06	0/1524	0.16	0/2013
14	At	0.14	0/832	0.22	0/1117
15	Bs	0.07	0/1530	0.19	0/2064
16	BG	0.07	0/1908	0.19	0/2566
17	BU	0.08	0/845	0.21	0/1134
18	Av	0.08	0/1051	0.18	0/1406
19	DB	0.11	0/7038	0.26	0/9468
20	Ct	0.22	0/900	0.35	0/1202
21	BH	0.07	0/1535	0.19	0/2063
22	BV	0.07	0/1048	0.19	0/1402
23	Aw	0.07	0/1107	0.20	0/1475
24	B5	0.11	2/86006 (0.0%)	0.13	0/134179
25	BT	0.07	0/1326	0.18	0/1770
26	BI	0.07	0/1756	0.20	0/2346
27	BW	0.06	0/1006	0.18	0/1334
28	Ax	0.06	0/1032	0.18	0/1371
29	B7	0.06	0/2835	0.10	0/4418
30	Au	0.07	0/636	0.18	0/852
31	BJ	0.07	0/1385	0.19	0/1852

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	AZ	0.08	0/1771	0.19	0/2406
33	Ay	0.07	0/691	0.18	0/922
34	B8	0.11	0/3635	0.15	0/5661
36	Aa	0.08	0/1841	0.20	0/2459
37	Az	0.06	0/240	0.13	0/305
38	BA	0.08	0/1965	0.22	0/2633
39	Bt	0.07	0/1193	0.21	0/1609
40	BM	0.07	0/1158	0.18	0/1547
41	Ab	0.07	0/1742	0.21	0/2354
42	BY	0.06	0/1132	0.19	0/1504
43	BB	0.08	0/3261	0.21	0/4364
44	BS	0.08	0/1497	0.20	0/2008
45	Ac	0.07	0/1779	0.19	0/2395
46	BZ	0.06	0/1130	0.17	0/1507
47	BC	0.07	0/2932	0.19	0/3939
48	BN	0.08	0/1746	0.19	0/2338
49	Ad	0.07	0/2118	0.20	0/2849
50	Ba	0.07	0/1179	0.20	0/1572
51	B	0.08	0/2444	0.20	0/3273
52	BO	0.08	0/1662	0.19	0/2222
53	Ae	0.07	0/1531	0.22	0/2059
54	Bb	0.06	0/884	0.18	0/1169
55	BE	0.08	0/1998	0.20	0/2673
56	DA	0.07	0/1284	0.21	0/1728
57	Af	0.06	0/1946	0.17	0/2590
58	Bc	0.07	0/847	0.18	0/1134
59	BF	0.07	0/1922	0.19	0/2563
60	DC	0.21	0/1368	0.37	0/1843
61	Ag	0.07	0/1552	0.19	0/2079
62	Bd	0.08	0/903	0.20	0/1216
63	A2	0.14	0/40342	0.13	0/62877
64	Ah	0.07	0/1715	0.19	0/2287
65	Be	0.07	0/1088	0.19	0/1451
66	AA	0.06	0/665	0.20	0/891
67	Ai	0.06	0/1550	0.18	0/2069
68	Bf	0.08	0/903	0.19	0/1208
69	AB	0.06	0/497	0.19	0/666
70	Aj	0.07	0/834	0.21	0/1125
71	Bg	0.07	0/916	0.19	0/1220
72	AC	0.06	0/622	0.18	0/822
73	Ak	0.07	0/1284	0.19	0/1717
74	Bh	0.06	0/1021	0.16	0/1348
75	AD	0.06	0/462	0.18	0/607

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	Al	0.07	0/968	0.20	0/1296
77	Bi	0.06	0/841	0.18	0/1112
78	AE	0.07	0/828	0.20	0/1109
79	Am	0.06	0/1232	0.18	0/1656
80	Bj	0.07	0/720	0.20	0/952
81	AF	0.08	0/2493	0.20	0/3394
82	An	0.07	0/1020	0.20	0/1366
83	Bk	0.07	0/575	0.17	0/761
84	AG	0.07	0/470	0.19	0/623
85	Ao	0.07	0/1069	0.19	0/1429
86	Bl	0.07	0/459	0.18	0/608
88	Ap	0.08	0/1142	0.25	0/1528
89	Bm	0.08	0/426	0.21	0/564
All	All	0.10	2/241249 (0.0%)	0.16	0/352306

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B5	4269	A2M	O3'-P	5.03	1.61	1.56
24	B5	3517	A2M	O3'-P	5.00	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BP	1242	0	1274	19	0
2	Aq	1080	0	1135	18	0
3	Bo	863	0	929	9	0
4	AT	939	0	617	3	0
5	Ar	1217	0	1279	20	0
6	Cu	813	0	856	23	0
7	BL	1702	0	1820	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	BX	967	0	1040	10	0
9	Bp	708	0	756	9	0
10	BQ	1515	0	1634	24	0
11	As	1113	0	1145	15	0
12	Br	1014	0	1083	12	0
13	BR	1508	0	1664	16	0
14	At	822	0	887	12	0
15	Bs	1507	0	1564	28	0
16	BG	1877	0	2023	11	0
17	BU	831	0	852	12	0
18	Av	1034	0	1080	12	0
19	DB	6900	0	6944	176	0
20	Ct	895	0	960	29	0
21	BH	1516	0	1597	17	0
22	BV	1034	0	1097	16	0
23	Aw	1099	0	1162	12	0
24	B5	79525	0	40251	628	0
25	BT	1298	0	1366	18	0
26	BI	1717	0	1764	21	0
27	BW	991	0	1048	12	0
28	Ax	1015	0	1086	9	0
29	B7	2538	0	1283	16	0
30	Au	640	0	633	9	0
31	BJ	1362	0	1399	15	0
32	AZ	1743	0	1748	28	0
33	Ay	683	0	761	11	0
34	B8	3319	0	1684	30	0
35	BK	145	0	32	1	0
36	Aa	1815	0	1908	20	0
37	Az	239	0	289	2	0
38	BA	1940	0	2028	33	0
39	Bt	1178	0	1235	24	0
40	BM	1137	0	1211	12	0
41	Ab	1706	0	1796	25	0
42	BY	1115	0	1205	12	0
43	BB	3206	0	3352	50	0
44	BS	1457	0	1492	16	0
45	Ac	1751	0	1846	15	0
46	BZ	1107	0	1182	13	0
47	BC	2886	0	3057	32	0
48	BN	1701	0	1749	29	0
49	Ad	2076	0	2177	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	Ba	1163	0	1202	19	0
51	B	2398	0	2428	30	0
52	BO	1630	0	1778	19	0
53	Ae	1509	0	1563	24	0
54	Bb	881	0	957	10	0
55	BE	1960	0	2153	29	0
56	DA	1260	0	1282	21	0
57	Af	1923	0	2089	41	0
58	Bc	836	0	888	6	0
59	BF	1886	0	2008	25	0
60	DC	1339	0	1315	31	0
61	Ag	1529	0	1627	19	0
62	Bd	888	0	930	10	0
63	A2	37833	0	19167	310	0
64	Ah	1686	0	1772	30	0
65	Be	1070	0	1164	10	0
66	AA	651	0	672	9	0
67	Ai	1525	0	1640	16	0
68	Bf	884	0	923	6	0
69	AB	495	0	523	5	0
70	Aj	810	0	836	8	0
71	Bg	906	0	998	7	0
72	AC	610	0	634	10	0
73	Ak	1262	0	1335	11	0
74	Bh	1013	0	1147	21	0
75	AD	457	0	502	11	0
76	Al	958	0	993	15	0
77	Bi	830	0	916	6	0
78	AE	814	0	863	12	0
79	Am	1208	0	1293	16	0
80	Bj	705	0	737	16	0
81	AF	2436	0	2393	36	0
82	An	1016	0	1038	17	0
83	Bk	569	0	637	5	0
84	AG	459	0	448	11	0
85	Ao	1048	0	1093	14	0
86	Bl	447	0	478	7	0
87	AH	36	0	25	0	0
88	Ap	1124	0	1193	23	0
89	Bm	432	0	470	6	0
90	A2	108	0	0	0	0
90	AT	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
90	Af	1	0	0	0	0
90	An	1	0	0	0	0
90	B5	282	0	0	0	0
90	B7	9	0	0	0	0
90	B8	9	0	0	0	0
90	BI	1	0	0	0	0
90	BP	1	0	0	0	0
90	BR	1	0	0	0	0
90	BV	1	0	0	0	0
90	Ba	1	0	0	0	0
90	Bj	1	0	0	0	0
90	Ct	1	0	0	0	0
91	AC	1	0	0	0	0
91	AE	1	0	0	0	0
91	AG	1	0	0	0	0
91	Bg	1	0	0	0	0
91	Bj	1	0	0	0	0
91	Bm	1	0	0	0	0
91	Bo	1	0	0	0	0
91	Bp	1	0	0	0	0
92	A2	57	0	0	1	0
92	AT	2	0	0	0	0
92	Ae	1	0	0	0	0
92	Ak	1	0	0	0	0
92	An	1	0	0	0	0
92	Ar	1	0	0	0	0
92	B5	207	0	0	4	0
92	B7	6	0	0	1	0
92	B8	7	0	0	0	0
92	BA	4	0	0	0	0
92	BB	2	0	0	0	0
92	BH	1	0	0	0	0
92	BI	1	0	0	0	0
92	BL	1	0	0	0	0
92	BN	1	0	0	0	0
92	BQ	2	0	0	0	0
92	BT	2	0	0	0	0
92	Bb	2	0	0	0	0
92	Be	3	0	0	0	0
92	Bf	1	0	0	0	0
92	Bj	1	0	0	0	0
92	Bl	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
92	Bo	1	0	0	0	0
93	DB	36	0	6	0	0
94	A2	80	0	152	9	0
94	B5	220	0	418	17	0
95	A2	14	0	26	3	0
95	B5	28	0	52	3	0
96	B7	32	0	11	0	0
97	A2	526	0	0	11	0
97	AE	1	0	0	0	0
97	AH	5	0	0	0	0
97	AT	13	0	0	0	0
97	Aa	2	0	0	0	0
97	Af	1	0	0	0	0
97	Ak	2	0	0	0	0
97	Am	1	0	0	0	0
97	An	3	0	0	0	0
97	Ap	2	0	0	0	0
97	Ar	1	0	0	0	0
97	As	3	0	0	0	0
97	At	1	0	0	1	0
97	Aw	5	0	0	0	0
97	B	1	0	0	0	0
97	B5	1383	0	0	36	0
97	B7	43	0	0	0	0
97	B8	50	0	0	0	0
97	BA	8	0	0	0	0
97	BB	9	0	0	0	0
97	BC	7	0	0	1	0
97	BF	1	0	0	0	0
97	BH	2	0	0	0	0
97	BI	3	0	0	0	0
97	BJ	1	0	0	0	0
97	BL	2	0	0	0	0
97	BM	1	0	0	0	0
97	BN	4	0	0	0	0
97	BO	1	0	0	0	0
97	BP	3	0	0	0	0
97	BR	5	0	0	0	0
97	BV	2	0	0	0	0
97	BX	1	0	0	0	0
97	Ba	8	0	0	1	0
97	Bd	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
97	Be	5	0	0	0	0
97	Bf	1	0	0	0	0
97	Bg	2	0	0	0	0
97	Bj	3	0	0	0	0
97	Bl	1	0	0	0	0
97	Bo	1	0	0	0	0
97	Ct	1	0	0	0	0
All	All	234232	0	175755	2016	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 (2016) 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)
92:B5:4968:UNX:UNK	97:B5:6243:HOH:O	1.45	0.96
34:B8:81:C:HO2'	74:Bh:2:ALA:N	1.66	0.93
18:Av:2:VAL:N	63:A2:1092:C:HO2'	1.66	0.92
82:An:34:PHE:HB3	82:An:41:PHE:HB2	1.66	0.77
49:Ad:125:LYS:H	49:Ad:142:HIS:HD2	1.34	0.76
24:B5:282:C:OP1	92:B5:5376:UNX:UNK	1.69	0.73
63:A2:1397:A:O2'	63:A2:1399:G:N7	2.21	0.73
63:A2:1491:OMG:HM22	63:A2:1492:G:H5'	1.71	0.73
24:B5:3540:OMC:HM22	24:B5:3541:G:H5'	1.70	0.73
15:Bs:63:LYS:HD3	24:B5:1899:A:H1'	1.71	0.72
19:DB:91:ARG:HH12	19:DB:119:ASP:HB3	1.54	0.72
19:DB:128:ARG:HH22	19:DB:545:GLU:HB2	1.54	0.72
19:DB:137:ARG:NH1	19:DB:153:GLY:O	2.23	0.72
10:BQ:119:LYS:HE3	10:BQ:121:LEU:HD21	1.70	0.72
15:Bs:36:GLY:HA2	24:B5:1908:G:H4'	1.72	0.72
24:B5:4292:A:N7	38:BA:215:ASN:ND2	2.37	0.71
32:AZ:94:THR:HG23	32:AZ:186:ARG:HH12	1.54	0.71
63:A2:1131:G:N2	63:A2:1131:G:OP2	2.23	0.71
24:B5:4018:G:N2	24:B5:4018:G:OP2	2.24	0.71
24:B5:4436:G:C8	97:B5:5694:HOH:O	2.42	0.71
6:Cu:27:ARG:HH12	17:BU:97:ARG:HB3	1.56	0.71
24:B5:2205:U:H2'	24:B5:2206:A2M:H8	1.73	0.71
24:B5:3909:U:H5'	24:B5:3910:C:H5''	1.73	0.71
24:B5:3373:U:OP2	24:B5:3378:A:N6	2.23	0.71
15:Bs:65:ILE:HG23	15:Bs:75:LEU:HB3	1.71	0.71
19:DB:626:LYS:HG3	24:B5:214:G:H21	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:AF:247:TRP:HB3	81:AF:258:ILE:HD11	1.73	0.71
56:DA:142:ILE:HG22	56:DA:144:PRO:HD2	1.72	0.71
56:DA:45:LEU:HB3	56:DA:61:CYS:HB2	1.73	0.71
24:B5:308:G:N2	24:B5:308:G:OP2	2.23	0.70
38:BA:6:ARG:HH12	38:BA:199:VAL:H	1.39	0.70
88:Ap:58:LEU:HB3	88:Ap:62:ARG:HD2	1.74	0.70
16:BG:58:PRO:HD2	16:BG:61:ILE:HD12	1.72	0.70
20:Ct:71:ARG:NH1	24:B5:394:G:OP2	2.25	0.70
24:B5:1237:G:OP2	24:B5:1237:G:N2	2.20	0.69
63:A2:926:G:H1	63:A2:1018:U:H3	1.40	0.69
24:B5:4361:C:H5''	43:BB:357:ARG:HE	1.57	0.69
51:B:83:LEU:HB3	51:B:88:VAL:HB	1.75	0.69
19:DB:100:ILE:HG23	19:DB:124:GLN:HE21	1.58	0.69
41:Ab:187:ARG:NH1	63:A2:1143:G:OP1	2.26	0.69
63:A2:1216:C:H42	63:A2:1221:A:H61	1.40	0.69
63:A2:228:C:H42	63:A2:902:G:H1'	1.58	0.68
63:A2:953:G:H21	82:An:52:THR:HG21	1.58	0.68
60:DC:10:ASP:HB3	60:DC:52:ILE:HD11	1.74	0.68
17:BU:101:ARG:NH2	24:B5:2545:C:OP1	2.24	0.68
24:B5:2143:A:N7	47:BC:143:ARG:NH1	2.42	0.68
25:BT:135:PRO:HB3	59:BF:85:GLU:HB2	1.76	0.68
64:Ah:101:ILE:HD12	64:Ah:190:LEU:HD11	1.75	0.68
10:BQ:144:LYS:HG2	24:B5:1415:C:H5''	1.75	0.68
19:DB:437:LEU:HB3	56:DA:18:GLN:HE21	1.59	0.67
22:BV:69:LYS:HG2	22:BV:71:GLU:HG2	1.76	0.67
33:Ay:46:ASN:ND2	63:A2:1600:U:OP2	2.26	0.67
8:BX:82:THR:HG22	8:BX:155:ILE:HG23	1.77	0.67
24:B5:3805:A:N1	24:B5:3917:C:N4	2.42	0.67
24:B5:2250:G:N2	86:Bl:51:LEU:OXT	2.28	0.67
63:A2:165:G:H2'	63:A2:166:A2M:H8	1.76	0.67
24:B5:3985:A:P	97:B5:5507:HOH:O	2.53	0.67
19:DB:354:LYS:HG3	19:DB:373:LEU:HD21	1.74	0.67
24:B5:755:G:H1	24:B5:800:U:H3	1.39	0.66
24:B5:4287:G:N2	24:B5:4290:A:OP2	2.28	0.66
66:AA:23:ARG:HH22	66:AA:29:ASN:HD21	1.42	0.66
19:DB:31:LYS:NZ	24:B5:207:G:OP2	2.27	0.66
36:Aa:28:LYS:HB3	36:Aa:48:LEU:HD11	1.75	0.66
14:At:94:ASP:OD2	84:AG:44:ARG:NH1	2.28	0.66
24:B5:788:G:H2'	24:B5:789:G:H8	1.58	0.66
24:B5:1550:G:P	97:B5:5517:HOH:O	2.53	0.66
24:B5:4271:C:OP1	43:BB:246:ARG:NH1	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
92:B5:4967:UNX:UNK	97:B5:6439:HOH:O	1.74	0.66
24:B5:1676:A:P	97:B5:5542:HOH:O	2.54	0.66
40:BM:40:GLY:HA3	40:BM:45:VAL:HB	1.76	0.66
29:B7:97:G:O6	92:B7:203:UNX:UNK	1.76	0.66
24:B5:4218:G:O2'	89:Bm:100:TYR:O	2.12	0.66
45:Ac:16:ILE:HG21	84:AG:22:ARG:HH11	1.60	0.66
55:BE:227:LYS:HE2	55:BE:241:GLU:H	1.61	0.66
24:B5:223:G:N3	47:BC:223:ASN:ND2	2.43	0.66
6:Cu:109:GLN:HB3	20:Ct:95:THR:HG21	1.78	0.66
24:B5:4411:A:P	97:B5:5687:HOH:O	2.54	0.66
63:A2:513:A2M:HM'2	63:A2:514:G:H5'	1.76	0.66
15:Bs:47:LEU:HB3	15:Bs:51:ALA:HB3	1.77	0.65
63:A2:1392:OMC:HM22	63:A2:1393:U:H5'	1.79	0.65
22:BV:15:ARG:NH2	24:B5:4416:C:O2'	2.29	0.65
24:B5:228:C:O2'	42:BY:14:ASN:ND2	2.28	0.65
63:A2:1034:G:N1	63:A2:1081:A:O2'	2.28	0.65
45:Ac:151:LYS:NZ	63:A2:1486:U:OP1	2.29	0.65
63:A2:166:A2M:HM'2	63:A2:167:G:H5'	1.78	0.65
85:Ao:59:ARG:HH11	85:Ao:76:VAL:HG13	1.61	0.65
43:BB:224:LYS:HG2	43:BB:340:THR:HG22	1.79	0.65
5:Ar:88:LYS:O	85:Ao:18:ARG:NH1	2.30	0.65
3:Bo:34:TYR:O	3:Bo:39:ARG:NH1	2.30	0.64
12:Br:107:ARG:NH2	24:B5:2106:A:OP1	2.30	0.64
59:BF:104:VAL:HG13	59:BF:135:VAL:HG12	1.80	0.64
19:DB:773:TYR:HE1	19:DB:780:GLN:HA	1.62	0.64
63:A2:43:U:P	97:A2:2177:HOH:O	2.56	0.64
24:B5:1810:A2M:HM'2	24:B5:1811:G:H5'	1.79	0.64
6:Cu:52:GLY:H	6:Cu:82:SER:HB2	1.62	0.64
24:B5:1848:G:C8	97:B5:5519:HOH:O	2.50	0.64
76:Al:89:VAL:HG11	76:Al:109:VAL:HG11	1.79	0.64
45:Ac:177:LEU:HD13	45:Ac:182:LEU:HD13	1.80	0.64
6:Cu:62:VAL:HG11	6:Cu:90:ILE:HD13	1.80	0.64
24:B5:2704:OMC:HM22	24:B5:2705:G:H5'	1.78	0.64
24:B5:1399:G:OP2	24:B5:1399:G:N2	2.29	0.63
24:B5:3555:G:N2	24:B5:3555:G:OP2	2.32	0.63
24:B5:4366:OMU:OP2	24:B5:4416:C:N4	2.31	0.63
63:A2:1555:C:O2	70:Aj:24:LYS:NZ	2.31	0.63
24:B5:369:G:N2	24:B5:372:A:OP2	2.30	0.63
54:Bb:56:LYS:O	54:Bb:60:ASN:ND2	2.30	0.63
63:A2:1386:G:P	97:A2:2106:HOH:O	2.55	0.63
49:Ad:11:ARG:HA	49:Ad:28:ALA:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:DC:162:LEU:HA	60:DC:165:LYS:HD2	1.81	0.63
62:Bd:64:ILE:HG23	62:Bd:68:LEU:HD23	1.80	0.63
63:A2:1286:G:H22	76:Al:57:ASP:HB2	1.62	0.63
81:AF:11:LEU:HB2	81:AF:307:VAL:HB	1.80	0.63
19:DB:407:LEU:HD21	56:DA:54:ILE:HB	1.80	0.63
24:B5:4194:G:H5''	24:B5:4195:A:H5''	1.80	0.63
48:BN:116:LEU:HD22	48:BN:135:ILE:HD11	1.80	0.63
63:A2:1080:C:O2'	63:A2:1183:A:N1	2.30	0.63
24:B5:432:U:H1'	94:B5:5263:SPD:HN6	1.64	0.63
24:B5:2207:OMG:N7	97:B5:5634:HOH:O	2.30	0.63
63:A2:642:A:OP1	67:Al:40:LYS:NZ	2.30	0.63
63:A2:905:A:O2'	73:Al:48:LYS:NZ	2.32	0.63
12:Br:87:ARG:NH1	55:BE:115:MET:O	2.31	0.63
24:B5:1937:A:N3	24:B5:1958:C:O2'	2.29	0.63
27:BW:91:MET:SD	27:BW:94:ARG:NH2	2.70	0.63
6:Cu:41:ASP:HA	6:Cu:44:LEU:HD12	1.81	0.62
17:BU:48:LYS:HG2	17:BU:53:ALA:HB2	1.81	0.62
22:BV:15:ARG:HB2	24:B5:4364:OMG:H5''	1.80	0.62
24:B5:734:G:OP2	40:BM:71:LYS:NZ	2.31	0.62
63:A2:97:U:OP1	92:A2:2073:UNX:UNK	1.81	0.62
38:BA:36:GLU:OE1	38:BA:163:ARG:NH1	2.30	0.62
24:B5:3541:G:OP2	24:B5:3541:G:N2	2.28	0.62
24:B5:1265:G:O6	97:B5:5514:HOH:O	2.13	0.62
24:B5:1624:A:N3	24:B5:1791:U:O2'	2.30	0.62
72:AC:126:CYS:HB3	72:AC:143:LYS:HD3	1.82	0.62
79:Am:136:PRO:HG2	79:Am:139:TRP:HB2	1.82	0.62
30:Au:38:GLU:HA	32:AZ:63:ARG:HH21	1.64	0.62
60:DC:18:ASN:ND2	60:DC:31:TYR:OH	2.33	0.62
63:A2:1089:U:OP1	95:A2:1994:SPM:N14	2.33	0.62
63:A2:1448:OMG:HM22	63:A2:1449:A:H5'	1.82	0.62
24:B5:1260:OMG:HM22	24:B5:1261:U:H5'	1.81	0.62
24:B5:1922:A:H1'	24:B5:1949:A:H4'	1.80	0.62
24:B5:2258:OMU:HM22	24:B5:2259:G:H5'	1.82	0.62
63:A2:1264:U:O2	84:AG:16:GLN:NE2	2.33	0.62
63:A2:1842:C:H2'	63:A2:1843:4AC:H6	1.82	0.62
24:B5:4779:U:OP2	43:BB:396:ARG:NH2	2.32	0.62
63:A2:191:A:H62	63:A2:208:G:H21	1.48	0.62
24:B5:741:A:N6	24:B5:810:U:O2	2.32	0.62
63:A2:577:A2M:HM'2	63:A2:578:U:H5'	1.82	0.62
19:DB:353:LEU:HB3	19:DB:373:LEU:HG	1.81	0.61
24:B5:1757:G:N2	24:B5:1757:G:OP2	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B5:1829:G:N2	24:B5:1829:G:OP2	2.31	0.61
53:Ae:56:TYR:HB3	53:Ae:63:LYS:HA	1.81	0.61
63:A2:165:G:N2	63:A2:165:G:OP2	2.32	0.61
63:A2:1529:G:O2'	63:A2:1667:C:OP1	2.17	0.61
19:DB:748:LYS:HG2	19:DB:775:LEU:HD13	1.82	0.61
25:BT:32:ARG:O	51:B:41:LYS:NZ	2.29	0.61
63:A2:747:C:O2	63:A2:797:G:N2	2.32	0.61
10:BQ:11:ARG:HB3	95:B5:5018:SPM:H22	1.82	0.61
11:As:101:ARG:NH2	63:A2:1567:G:N7	2.48	0.61
38:BA:27:ALA:O	38:BA:128:ARG:NH1	2.32	0.61
67:Ai:170:PRO:O	67:Ai:175:ARG:NH1	2.33	0.61
6:Cu:44:LEU:HD23	20:Ct:80:MET:HE2	1.83	0.61
15:Bs:48:ARG:HD3	39:Bt:123:ARG:HG2	1.80	0.61
19:DB:105:ASN:HD21	20:Ct:214:THR:HG21	1.64	0.61
24:B5:2444:A:N6	24:B5:2587:A:OP2	2.32	0.61
24:B5:4323:U:O4	92:B5:5315:UNX:UNK	1.79	0.61
63:A2:99:A2M:HM'2	63:A2:100:U:H5'	1.83	0.61
19:DB:608:ILE:HG22	19:DB:612:LYS:HE3	1.83	0.61
45:Ac:106:ARG:HG3	45:Ac:175:VAL:HB	1.82	0.61
24:B5:1423:C:OP1	50:Ba:132:ARG:NH2	2.34	0.61
24:B5:1694:C:O2	51:B:3:PHE:N	2.34	0.61
24:B5:1869:U:OP2	52:BO:49:ARG:NH1	2.31	0.61
12:Br:6:GLN:HE21	47:BC:133:LEU:HD13	1.65	0.61
24:B5:238:C:OP2	42:BY:45:ARG:NH2	2.34	0.61
63:A2:1624:A:OP2	94:A2:1950:SPD:N1	2.33	0.61
5:Ar:124:ARG:NH1	85:Ao:123:TYR:OH	2.34	0.61
6:Cu:72:ILE:HG12	6:Cu:96:THR:HG22	1.83	0.61
24:B5:2194:OMC:HM22	24:B5:2195:U:H5'	1.82	0.61
21:BH:23:ARG:HE	21:BH:39:ASN:HA	1.64	0.61
24:B5:1915:G:N3	39:Bt:138:SER:OG	2.33	0.61
53:Ae:60:ARG:HD2	63:A2:1680:A:H2'	1.83	0.61
63:A2:1018:U:OP1	79:Am:62:GLN:NE2	2.34	0.61
25:BT:133:ALA:HB3	59:BF:126:LYS:HB2	1.83	0.60
56:DA:10:ASP:OD1	56:DA:47:LYS:NZ	2.33	0.60
3:Bo:36:GLN:OE1	3:Bo:39:ARG:NH2	2.34	0.60
24:B5:4268:G:O2'	24:B5:4271:C:OP2	2.17	0.60
24:B5:375:G:OP2	80:Bj:52:LYS:NZ	2.34	0.60
53:Ae:125:SER:O	69:AB:47:LYS:NZ	2.34	0.60
63:A2:90:G:OP2	94:A2:1957:SPD:N10	2.33	0.60
63:A2:1839:U:P	97:A2:2115:HOH:O	2.59	0.60
66:AA:84:HIS:OXT	79:Am:19:ARG:NH1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:AF:5:MET:HG2	81:AF:312:VAL:HG22	1.83	0.60
24:B5:856:A:H1'	24:B5:2015:G:H5''	1.82	0.60
24:B5:1846:A:H4'	59:BF:222:LYS:HE3	1.84	0.60
24:B5:4304:U:OP2	43:BB:246:ARG:NH2	2.34	0.60
24:B5:4679:C:OP1	55:BE:159:ARG:NH1	2.34	0.60
33:Ay:85:ARG:NH2	63:A2:1598:C:OP2	2.33	0.60
49:Ad:45:ILE:HA	49:Ad:61:VAL:HG11	1.84	0.60
57:Af:13:GLN:NE2	63:A2:153:G:N3	2.50	0.60
73:Ak:135:SER:O	73:Ak:139:ARG:NH1	2.35	0.60
19:DB:188:GLU:HB3	19:DB:533:ILE:HD12	1.84	0.60
19:DB:441:ASP:O	19:DB:445:ASN:ND2	2.33	0.60
63:A2:75:G:O2'	63:A2:77:A:OP1	2.20	0.60
63:A2:121:OMU:HM22	63:A2:122:G:H5'	1.83	0.60
63:A2:852:C:H5''	63:A2:853:G:H5'	1.84	0.60
76:Al:11:VAL:HG13	76:Al:13:ASP:H	1.65	0.60
34:B8:141:C:OP1	48:BN:38:ARG:NH1	2.35	0.60
46:BZ:25:ILE:HA	46:BZ:43:VAL:HG12	1.84	0.60
78:AE:51:ARG:NH1	78:AE:55:GLU:OE2	2.35	0.60
88:Ap:53:GLU:OE1	88:Ap:85:ARG:NH2	2.34	0.60
11:As:12:GLN:HE22	63:A2:1594:C:H1'	1.67	0.60
24:B5:4282:OMC:HM22	24:B5:4283:C:H5'	1.84	0.60
94:B5:5263:SPD:H101	52:BO:91:LYS:HD3	1.66	0.60
56:DA:6:ILE:HG12	56:DA:51:PHE:HD1	1.67	0.60
19:DB:193:LEU:O	19:DB:197:ASN:ND2	2.35	0.60
22:BV:69:LYS:NZ	22:BV:71:GLU:OE2	2.35	0.60
24:B5:2161:G:N2	24:B5:2164:G:OP2	2.31	0.60
24:B5:1270:A2M:OP2	24:B5:4191:U:O2'	2.18	0.60
26:BI:87:ILE:HG12	26:BI:138:ILE:HG12	1.81	0.60
49:Ad:49:ARG:NH2	63:A2:497:C:OP1	2.31	0.60
78:AE:44:ILE:HD12	78:AE:65:PRO:HG2	1.84	0.60
79:Am:99:ARG:NH2	79:Am:119:GLU:OE2	2.34	0.60
14:At:101:HIS:ND1	63:A2:1448:OMG:OP1	2.35	0.59
17:BU:47:ILE:HD12	17:BU:63:ILE:HD11	1.84	0.59
24:B5:230:G:OP1	42:BY:15:ARG:NH1	2.35	0.59
24:B5:330:G:N7	94:B5:4912:SPD:N10	2.50	0.59
24:B5:4202:OMC:HM22	24:B5:4203:PSU:H5''	1.84	0.59
34:B8:81:C:O2'	74:Bh:2:ALA:N	2.33	0.59
3:Bo:26:TYR:HB3	3:Bo:67:VAL:HB	1.84	0.59
49:Ad:44:LEU:HD21	49:Ad:72:ILE:HD11	1.83	0.59
61:Ag:162:GLN:OE1	61:Ag:165:ASN:ND2	2.36	0.59
25:BT:136:ARG:NH1	59:BF:85:GLU:OE2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B5:1631:C:H41	24:B5:4124:A:H5''	1.68	0.59
24:B5:4666:G:N2	24:B5:4666:G:OP2	2.36	0.59
27:BW:80:ARG:NH2	57:Af:129:VAL:O	2.35	0.59
63:A2:1419:C:O2'	63:A2:1421:G:OP2	2.20	0.59
81:AF:133:ASN:HB3	81:AF:139:LYS:HE3	1.84	0.59
24:B5:4610:C:N4	44:BS:171:ARG:O	2.35	0.59
47:BC:327:LYS:NZ	59:BF:169:THR:O	2.36	0.59
5:Ar:22:GLY:HA2	5:Ar:56:ALA:HB3	1.83	0.59
24:B5:2486:G:N7	97:B5:5659:HOH:O	2.32	0.59
24:B5:3412:U:OP1	38:BA:54:ARG:NH2	2.31	0.59
57:Af:2:LYS:HB3	57:Af:15:LEU:HD11	1.84	0.59
63:A2:521:A:O2'	63:A2:826:A:N3	2.32	0.59
12:Br:99:LYS:NZ	24:B5:2103:C:O2	2.35	0.59
30:AU:39:VAL:HG11	32:AZ:8:LEU:HD11	1.85	0.59
59:BF:237:ASP:O	59:BF:240:ASN:ND2	2.35	0.59
63:A2:1342:C:N3	97:A2:2151:HOH:O	2.32	0.59
7:BL:5:ARG:NH2	24:B5:1789:A:OP2	2.33	0.59
16:BG:43:GLN:O	24:B5:3852:G:N2	2.35	0.59
19:DB:538:TYR:HE1	60:DC:36:LEU:HB3	1.67	0.59
24:B5:2364:G:H5'	24:B5:2483:G:H1'	1.84	0.59
26:BI:203:ARG:NH1	29:B7:105:C:OP2	2.36	0.59
63:A2:1651:A:H5''	88:Ap:139:ALA:HB2	1.83	0.59
63:A2:1663:U:O4	63:A2:1664:A:N6	2.35	0.59
11:As:60:THR:HG23	11:As:75:MET:HE2	1.85	0.59
19:DB:270:PRO:HG2	19:DB:276:ARG:HG2	1.83	0.59
45:Ac:42:THR:OG1	45:Ac:45:ARG:O	2.17	0.59
63:A2:1148:C:OP1	78:AE:6:ARG:NH1	2.35	0.59
81:AF:244:ASN:ND2	81:AF:294:ASP:O	2.36	0.59
2:Aq:57:LEU:HD13	2:Aq:69:ILE:HD11	1.83	0.59
24:B5:1809:C:H2'	24:B5:1810:A2M:H8	1.85	0.59
43:BB:213:GLN:NE2	43:BB:285:TYR:O	2.32	0.59
75:AD:109:ARG:O	75:AD:113:ASN:ND2	2.35	0.59
24:B5:1391:C:O2'	54:Bb:106:ARG:NH2	2.36	0.58
29:B7:6:C:O2'	51:B:50:ARG:NH2	2.36	0.58
30:AU:38:GLU:OE2	30:AU:51:LYS:NZ	2.35	0.58
4:AT:20:N:OP1	31:BJ:58:ARG:NH2	2.35	0.58
22:BV:13:LYS:HB3	22:BV:128:LEU:HD11	1.85	0.58
24:B5:2309:G:N7	97:B5:5661:HOH:O	2.32	0.58
33:Ay:111:ARG:HD2	33:Ay:114:LYS:HE3	1.85	0.58
61:Ag:114:GLN:NE2	63:A2:875:G:N3	2.49	0.58
24:B5:1539:G:N7	94:B5:4954:SPD:N10	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B5:1741:A:H5''	24:B5:1742:G:H5'	1.85	0.58
24:B5:4639:C:O2'	24:B5:4641:C:OP2	2.20	0.58
53:Ae:63:LYS:NZ	63:A2:1679:A2M:OP2	2.29	0.58
24:B5:1924:G:N2	24:B5:1924:G:OP1	2.36	0.58
47:BC:293:LEU:O	47:BC:299:GLN:NE2	2.35	0.58
63:A2:1402:A:N6	63:A2:1442:U:O2'	2.37	0.58
67:Ai:120:ALA:O	67:Ai:125:HIS:ND1	2.36	0.58
11:As:7:LYS:HB3	88:Ap:37:ARG:HG2	1.85	0.58
66:AA:11:SER:OG	66:AA:14:GLU:OE1	2.22	0.58
24:B5:1805:U:OP1	26:BI:4:ARG:NH1	2.35	0.58
27:BW:66:GLU:HG3	27:BW:68:GLN:HE22	1.69	0.58
53:Ae:47:LYS:NZ	88:Ap:115:TYR:O	2.37	0.58
63:A2:869:G:OP2	63:A2:869:G:N2	2.32	0.58
4:AT:38:N:O2'	63:A2:1059:A:OP1	2.21	0.58
15:Bs:32:ALA:O	15:Bs:85:ASN:ND2	2.37	0.58
24:B5:387:G:OP2	42:BY:89:LYS:NZ	2.34	0.58
24:B5:1834:G:O2'	24:B5:1846:A:N3	2.32	0.58
24:B5:2300:G:OP1	48:BN:65:ARG:NH2	2.35	0.58
51:B:37:VAL:HB	51:B:67:ALA:HB2	1.86	0.58
63:A2:430:C:O2'	63:A2:812:A:N1	2.35	0.58
69:AB:32:VAL:HG11	69:AB:56:LEU:HD12	1.85	0.58
5:Ar:136:THR:OG1	63:A2:1522:C:OP2	2.21	0.58
7:BL:59:VAL:HB	24:B5:74:G:H5''	1.85	0.58
24:B5:4151:G:OP2	26:BI:7:ARG:NH2	2.36	0.58
34:B8:47:C:H1'	34:B8:61:A:H2'	1.86	0.58
81:AF:120:ILE:HB	81:AF:132:TRP:HB2	1.84	0.58
19:DB:145:PRO:O	19:DB:151:TRP:NE1	2.35	0.58
24:B5:992:C:OP1	24:B5:1106:U:O2'	2.20	0.58
24:B5:4744:G:N2	24:B5:4780:G:O2'	2.37	0.58
27:BW:81:ALA:HB2	27:BW:87:LEU:HB2	1.85	0.58
63:A2:753:G:O2'	63:A2:754:C:O2	2.21	0.58
81:AF:87:LEU:HB2	81:AF:101:PHE:HB2	1.86	0.58
24:B5:3518:U:OP1	24:B5:4296:G:O2'	2.18	0.58
26:BI:38:ARG:HD2	26:BI:41:ALA:HB2	1.84	0.58
63:A2:463:OMC:HM22	63:A2:464:C:H5'	1.86	0.58
64:Ah:56:ARG:NH1	64:Ah:180:GLY:O	2.37	0.58
19:DB:517:GLU:OE2	19:DB:639:LYS:NZ	2.36	0.57
24:B5:3450:A2M:HM'2	24:B5:3451:A:H5'	1.86	0.57
27:BW:2:LYS:NZ	27:BW:4:GLU:OE2	2.37	0.57
32:AZ:198:MET:HG2	32:AZ:200:ASP:H	1.69	0.57
73:Ak:126:VAL:HG12	73:Ak:145:VAL:HG22	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:DB:156:ILE:HD11	19:DB:535:LEU:HD22	1.85	0.57
24:B5:3561:G:H2'	24:B5:3562:A2M:H8	1.85	0.57
38:BA:117:GLU:HG2	38:BA:124:GLY:H	1.69	0.57
57:Af:98:ARG:NH2	57:Af:103:ASP:OD1	2.37	0.57
63:A2:1864:A:OP2	78:AE:4:LYS:NZ	2.35	0.57
84:AG:3:HIS:HB3	84:AG:6:LEU:HB2	1.85	0.57
21:BH:64:ARG:NH1	24:B5:1888:U:OP1	2.37	0.57
49:Ad:100:ARG:HB2	49:Ad:114:ILE:HD13	1.86	0.57
57:Af:85:ARG:O	57:Af:87:ARG:NH1	2.37	0.57
60:DC:158:LEU:HA	60:DC:161:HIS:CD2	2.39	0.57
19:DB:277:LEU:HD21	19:DB:301:LEU:HD11	1.85	0.57
44:BS:147:ASP:HB3	44:BS:150:ILE:HB	1.86	0.57
63:A2:1355:G:N2	63:A2:1358:A:OP2	2.30	0.57
5:Ar:46:ARG:HG2	11:As:35:ASP:HB2	1.85	0.57
24:B5:327:U:O2'	77:Bi:30:ARG:NH1	2.36	0.57
43:BB:261:ARG:HB2	52:BO:64:THR:HG21	1.86	0.57
52:BO:54:TYR:OH	52:BO:73:PHE:O	2.22	0.57
63:A2:378:G:H5'	64:Ah:98:LYS:HB3	1.85	0.57
64:Ah:3:ILE:O	64:Ah:30:GLY:N	2.37	0.57
9:Bp:22:LEU:HB3	38:BA:180:LEU:HD21	1.87	0.57
18:Av:52:ILE:HB	61:Ag:144:ILE:HB	1.87	0.57
24:B5:1853:C:H4'	52:BO:89:PRO:HD3	1.87	0.57
24:B5:4073:C:OP1	25:BT:70:HIS:NE2	2.36	0.57
27:BW:70:LYS:NZ	57:Af:33:ALA:O	2.36	0.57
56:DA:8:LEU:HG	56:DA:91:LYS:HE3	1.87	0.57
60:DC:156:ASP:HA	60:DC:159:ARG:HD2	1.87	0.57
61:Ag:143:ARG:HB2	61:Ag:155:LYS:HB2	1.85	0.57
19:DB:80:HIS:CE1	19:DB:109:TRP:HB2	2.39	0.57
24:B5:2232:A:H4'	62:Bd:70:LYS:HG3	1.85	0.57
63:A2:437:OMG:HM22	63:A2:438:G:H5'	1.87	0.57
19:DB:770:LYS:HG2	19:DB:814:LEU:HD21	1.87	0.57
79:Am:4:MET:SD	79:Am:124:ARG:NH2	2.78	0.57
12:Br:28:GLU:OE2	12:Br:31:ASN:ND2	2.35	0.57
31:BJ:144:LYS:O	31:BJ:148:THR:OG1	2.18	0.57
32:AZ:33:GLN:HB3	32:AZ:154:LEU:HD12	1.86	0.57
63:A2:671:A:OP2	97:A2:2107:HOH:O	2.18	0.57
63:A2:1021:A:N7	79:Am:70:LYS:NZ	2.53	0.57
63:A2:1090:G:H4'	95:A2:1994:SPM:H111	1.86	0.57
81:AF:236:ILE:HG12	81:AF:252:THR:HG22	1.86	0.57
24:B5:3386:G:O2'	24:B5:3425:U:OP1	2.22	0.56
24:B5:3619:OMC:HM22	24:B5:3620:G:H5'	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:Ak:147:LYS:HD2	73:Ak:151:THR:HG21	1.87	0.56
2:Aq:19:LYS:HB3	45:Ac:213:PRO:HG3	1.87	0.56
24:B5:4140:A:OP1	97:B5:5514:HOH:O	2.17	0.56
41:Ab:207:ALA:HB2	63:A2:4:C:H4'	1.86	0.56
52:BO:81:TRP:HB2	52:BO:104:VAL:HG21	1.87	0.56
2:Aq:40:ILE:HB	45:Ac:209:SER:HB3	1.88	0.56
11:As:121:ARG:NH1	63:A2:1564:G:OP1	2.37	0.56
13:BR:46:LYS:NZ	24:B5:2548:G:O6	2.34	0.56
19:DB:128:ARG:NH2	19:DB:545:GLU:HB2	2.19	0.56
23:Aw:70:VAL:HG11	23:Aw:94:ILE:HG21	1.87	0.56
24:B5:1741:A:O2'	24:B5:1776:A:OP1	2.22	0.56
24:B5:3562:A2M:HM'2	24:B5:3563:U:H5'	1.87	0.56
37:Az:4:LYS:NZ	63:A2:1843:4AC:O7	2.39	0.56
81:AF:39:THR:HG22	81:AF:60:ARG:HG2	1.87	0.56
81:AF:77:PHE:HB3	81:AF:89:LEU:HD11	1.88	0.56
89:Bm:94:MET:HG2	89:Bm:105:PRO:HA	1.86	0.56
24:B5:707:C:O2	55:BE:133:LYS:NZ	2.38	0.56
24:B5:1546:U:OP2	24:B5:2699:C:O2'	2.21	0.56
24:B5:1641:C:OP1	54:Bb:19:ASN:ND2	2.36	0.56
24:B5:3639:G:P	97:B5:5520:HOH:O	2.63	0.56
52:BO:125:LYS:HG2	52:BO:129:LEU:HD12	1.86	0.56
6:Cu:48:LEU:HD23	6:Cu:51:LEU:HD12	1.87	0.56
63:A2:382:C:OP2	64:Ah:31:ARG:NH2	2.38	0.56
63:A2:1551:G:H3'	63:A2:1580:A:H61	1.71	0.56
71:Bg:5:LEU:HD21	71:Bg:30:ILE:HG22	1.88	0.56
19:DB:123:LEU:HD13	19:DB:126:GLN:HE22	1.71	0.56
19:DB:762:LEU:HD12	19:DB:797:ARG:HG2	1.87	0.56
24:B5:4383:OMG:HM22	24:B5:4384:U:H5'	1.87	0.56
32:AZ:17:LYS:HB3	32:AZ:173:LEU:HD11	1.88	0.56
39:Bt:147:HIS:HD2	39:Bt:149:HIS:HB2	1.70	0.56
12:Br:90:LEU:HD22	12:Br:111:ILE:HG23	1.86	0.56
24:B5:4336:A2M:HM'2	24:B5:4337:U:H5'	1.88	0.56
67:Ai:93:LYS:HB2	67:Ai:96:TYR:HD2	1.71	0.56
72:AC:114:ILE:HD12	76:Al:71:GLU:HG2	1.88	0.56
10:BQ:16:LYS:O	10:BQ:33:ARG:NH2	2.30	0.56
10:BQ:108:ARG:NH2	24:B5:1299:G:OP1	2.35	0.56
19:DB:371:THR:HG21	56:DA:52:ASN:HB2	1.88	0.56
19:DB:661:LEU:HB3	19:DB:665:LYS:HE3	1.87	0.56
24:B5:4366:OMU:HM22	24:B5:4367:C:H5'	1.86	0.56
24:B5:4632:A:OP1	52:BO:188:LYS:NZ	2.35	0.56
31:BJ:35:ARG:NH1	31:BJ:123:ILE:O	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:Af:49:VAL:HG23	57:Af:114:VAL:HB	1.88	0.56
57:Af:58:LYS:HA	57:Af:107:SER:HB2	1.88	0.56
63:A2:1014:U:OP1	63:A2:1130:G:O2'	2.23	0.56
63:A2:1180:G:N2	63:A2:1183:A:OP2	2.37	0.56
63:A2:1329:OMG:HM22	63:A2:1330:U:H5'	1.88	0.56
1:BP:52:THR:HG23	1:BP:85:LYS:HG3	1.88	0.56
1:BP:138:PRO:HB3	1:BP:140:MET:HE2	1.87	0.56
24:B5:1214:A:OP1	54:Bb:117:ARG:NH2	2.39	0.56
24:B5:3449:A:OP2	24:B5:3467:G:N2	2.34	0.56
24:B5:3942:OMG:HM22	24:B5:3943:G:H5'	1.88	0.56
24:B5:4004:C:OP2	31:BJ:54:ARG:NH1	2.39	0.56
13:BR:98:ARG:NH2	13:BR:132:PHE:O	2.30	0.56
17:BU:111:GLU:OE2	17:BU:113:ARG:NE	2.36	0.56
24:B5:1931:U:O2'	24:B5:1941:A:OP1	2.24	0.56
24:B5:4124:A:P	97:B5:5502:HOH:O	2.57	0.56
48:BN:115:VAL:O	48:BN:159:ARG:NH1	2.39	0.56
24:B5:136:U:O4	74:Bh:79:LYS:NZ	2.32	0.55
24:B5:2014:G:OP1	47:BC:312:ARG:NH2	2.38	0.55
47:BC:7:LEU:HB3	47:BC:21:ASN:HB3	1.88	0.55
48:BN:181:HIS:O	48:BN:195:ARG:NH2	2.37	0.55
57:Af:56:ASN:HD22	57:Af:62:PRO:HA	1.70	0.55
63:A2:1206:C:N4	97:A2:2187:HOH:O	2.38	0.55
63:A2:1675:G:N7	88:Ap:17:LYS:NZ	2.54	0.55
19:DB:254:ASN:HB2	19:DB:260:TYR:HE2	1.72	0.55
24:B5:3610:C:OP1	24:B5:4146:G:O2'	2.23	0.55
26:BI:54:SER:HB2	26:BI:135:ILE:HD11	1.87	0.55
32:AZ:102:ARG:HH12	32:AZ:105:PRO:HD3	1.69	0.55
38:BA:137:ILE:HD11	38:BA:149:LYS:HB2	1.87	0.55
51:B:152:ARG:HG3	51:B:154:THR:HG23	1.89	0.55
63:A2:1289:OMU:OP2	72:AC:97:LYS:NZ	2.39	0.55
63:A2:1508:G:N2	72:AC:87:THR:O	2.38	0.55
81:AF:214:GLY:HA2	81:AF:236:ILE:HG13	1.87	0.55
81:AF:217:MET:HG2	81:AF:229:THR:HG22	1.86	0.55
23:Aw:93:PHE:O	23:Aw:140:ARG:NH1	2.39	0.55
24:B5:3374:A:OP1	97:B5:5522:HOH:O	2.18	0.55
30:Au:83:PHE:O	32:AZ:52:LYS:NZ	2.39	0.55
63:A2:43:U:OP2	63:A2:486:A:N6	2.30	0.55
76:Al:75:ASN:N	76:Al:75:ASN:OD1	2.39	0.55
5:Ar:36:VAL:HG21	5:Ar:71:MET:HE3	1.89	0.55
24:B5:3625:C:O2'	24:B5:4718:A:N1	2.38	0.55
24:B5:4638:G:N2	24:B5:4661:C:O2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BI:101:LYS:NZ	26:BI:102:MET:O	2.39	0.55
31:BJ:17:ILE:HD12	31:BJ:80:GLU:HG2	1.88	0.55
63:A2:1704:OMC:HM22	63:A2:1705:C:H5'	1.89	0.55
24:B5:435:A:O2'	65:Be:26:ASP:OD2	2.25	0.55
25:BT:158:PHE:HZ	26:BI:53:VAL:HG11	1.71	0.55
30:Au:43:THR:OG1	30:Au:45:ARG:NH1	2.40	0.55
49:Ad:31:PRO:HG3	49:Ad:43:PRO:HG3	1.89	0.55
57:Af:159:ARG:HB3	57:Af:171:THR:HB	1.89	0.55
63:A2:220:U:H2'	63:A2:221:A:H8	1.72	0.55
72:AC:116:ARG:NH1	72:AC:120:GLU:OE2	2.40	0.55
16:BG:200:THR:OG1	24:B5:150:U:OP2	2.22	0.55
19:DB:100:ILE:HG12	19:DB:124:GLN:HG2	1.88	0.55
21:BH:92:MET:HE2	21:BH:179:ILE:HG22	1.87	0.55
23:Aw:91:LEU:HB3	75:AD:83:VAL:HG11	1.89	0.55
34:B8:102:G:OP1	80:Bj:20:ARG:NH1	2.38	0.55
50:Ba:89:ASN:OD1	50:Ba:92:LYS:NZ	2.39	0.55
76:Al:25:ALA:O	76:Al:30:GLY:N	2.37	0.55
84:AG:22:ARG:HH21	84:AG:37:ASN:HB2	1.70	0.55
19:DB:56:LEU:HD22	19:DB:61:LYS:HD2	1.88	0.55
19:DB:254:ASN:OD1	60:DC:93:GLN:NE2	2.40	0.55
24:B5:1980:A:N7	24:B5:4180:C:O2'	2.40	0.55
24:B5:2336:G:HO2'	34:B8:126:C:HO2'	1.55	0.55
24:B5:2623:C:N4	97:B5:5763:HOH:O	2.39	0.55
73:Ak:119:ASP:O	73:Ak:147:LYS:NZ	2.37	0.55
19:DB:124:GLN:HB3	19:DB:133:TYR:HE1	1.70	0.55
24:B5:835:G:OP1	40:BM:44:ARG:NH1	2.39	0.55
51:B:208:MET:HE3	51:B:233:PRO:HG3	1.87	0.55
24:B5:3557:A2M:HM'2	24:B5:3558:C:H5'	1.88	0.55
34:B8:60:G:O6	74:Bh:62:ASN:ND2	2.35	0.55
63:A2:1383:A:H2'	63:A2:1384:A2M:H8	1.89	0.55
64:Ah:67:TRP:NE1	64:Ah:191:GLU:OE2	2.38	0.55
3:Bo:44:LYS:HE2	3:Bo:52:THR:HB	1.88	0.55
24:B5:1334:G:N2	24:B5:1337:G:OP2	2.32	0.55
24:B5:2338:U:H2'	24:B5:2339:G:H8	1.72	0.55
24:B5:4099:PSU:H5'	24:B5:4100:U:H5'	1.87	0.55
47:BC:230:LEU:HD21	47:BC:236:ASN:H	1.72	0.55
63:A2:1443:OMU:HM22	63:A2:1444:C:H5'	1.89	0.55
63:A2:1618:G:N1	63:A2:1621:A:OP2	2.40	0.55
81:AF:232:GLY:HA3	81:AF:252:THR:HG21	1.88	0.55
24:B5:32:G:H21	24:B5:50:C:H5	1.55	0.54
24:B5:4745:U:H4'	24:B5:4746:A:H5'	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:Aa:44:ILE:HD12	36:Aa:69:VAL:HG21	1.88	0.54
63:A2:473:C:O2	63:A2:476:C:N4	2.40	0.54
63:A2:1084:A:N7	63:A2:1842:C:O2'	2.37	0.54
3:Bo:59:LYS:NZ	3:Bo:61:LYS:O	2.38	0.54
13:BR:15:LEU:HD13	13:BR:52:ARG:HB2	1.89	0.54
19:DB:326:PHE:CZ	19:DB:379:TYR:HA	2.42	0.54
24:B5:1284:OMC:OP1	50:Ba:6:ARG:NH2	2.40	0.54
24:B5:1315:A:N1	34:B8:28:C:O2'	2.38	0.54
24:B5:4368:A:H4'	43:BB:13:SER:HB2	1.88	0.54
58:Bc:8:LYS:NZ	63:A2:1009:A:OP2	2.36	0.54
63:A2:1289:OMU:HM22	63:A2:1290:U:H5'	1.89	0.54
81:AF:60:ARG:HE	88:Ap:97:GLN:HE22	1.56	0.54
49:Ad:87:MET:HE2	49:Ad:123:LEU:HB2	1.89	0.54
62:Bd:38:PHE:HB3	62:Bd:78:ARG:HG2	1.89	0.54
63:A2:1338:4AC:H2'	63:A2:1339:G:H8	1.73	0.54
19:DB:171:LEU:HB3	19:DB:196:GLN:HG2	1.90	0.54
24:B5:239:C:OP1	42:BY:46:SER:OG	2.26	0.54
26:BI:66:GLU:OE2	26:BI:69:ARG:NH2	2.41	0.54
31:BJ:136:ARG:NH2	31:BJ:161:GLU:OE1	2.40	0.54
36:Aa:179:ASN:ND2	36:Aa:183:GLU:OE1	2.41	0.54
57:Af:103:ASP:OD2	57:Af:105:ASN:ND2	2.34	0.54
63:A2:142:C:N4	63:A2:330:G:OP1	2.38	0.54
63:A2:1276:G:N2	63:A2:1507:A:OP2	2.36	0.54
63:A2:1839:U:P	97:A2:2103:HOH:O	2.64	0.54
88:Ap:132:PHE:O	88:Ap:140:ARG:NH2	2.37	0.54
12:Br:15:SER:HB2	24:B5:2142:G:H5'	1.89	0.54
19:DB:549:ARG:HB2	19:DB:667:LEU:HD12	1.88	0.54
24:B5:1678:G:N3	24:B5:1681:A:N6	2.55	0.54
24:B5:1955:C:H2'	24:B5:1956:A:H8	1.73	0.54
24:B5:4506:C:OP2	52:BO:171:LYS:NZ	2.38	0.54
85:Ao:81:ARG:NH2	85:Ao:117:GLY:O	2.40	0.54
6:Cu:84:ALA:O	20:Ct:72:SER:OG	2.23	0.54
24:B5:1738:G:N7	97:B5:5671:HOH:O	2.33	0.54
29:B7:6:C:H4'	51:B:52:ILE:HD13	1.90	0.54
61:Ag:44:ASN:OD1	61:Ag:68:GLN:NE2	2.33	0.54
63:A2:380:C:O2	64:Ah:5:ARG:NE	2.40	0.54
73:Ak:18:GLN:HG2	73:Ak:33:LEU:HD21	1.90	0.54
24:B5:381:U:H4'	24:B5:415:G:H5'	1.90	0.54
24:B5:859:G:O2'	24:B5:2106:A:N6	2.39	0.54
24:B5:3377:U:OP2	97:B5:5522:HOH:O	2.18	0.54
63:A2:1337:C:H41	63:A2:1338:4AC:HM73	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:Bf:43:LEU:O	68:Bf:109:ARG:NH1	2.32	0.54
19:DB:480:ASN:OD1	19:DB:488:GLN:NE2	2.35	0.54
21:BH:141:LYS:NZ	21:BH:142:ASP:OD2	2.41	0.54
23:Aw:68:LYS:HE2	75:AD:83:VAL:HG22	1.90	0.54
24:B5:1879:G:H22	24:B5:4180:C:H5'	1.73	0.54
63:A2:398:G:OP2	73:Ak:108:ASN:ND2	2.41	0.54
81:AF:167:SER:OG	81:AF:177:TRP:NE1	2.34	0.54
1:BP:121:LYS:O	34:B8:13:G:O2'	2.26	0.54
19:DB:326:PHE:HZ	19:DB:379:TYR:HA	1.72	0.54
19:DB:726:LEU:HB2	19:DB:731:ARG:CZ	2.37	0.54
24:B5:1125:C:H5	55:BE:62:SER:HB2	1.72	0.54
24:B5:1988:G:HO2'	24:B5:3616:PSU:HO2'	1.53	0.54
24:B5:2736:U:O3'	64:Ah:205:ARG:NH1	2.41	0.54
61:Ag:65:PRO:HD2	61:Ag:68:GLN:HE21	1.73	0.54
61:Ag:144:ILE:HG21	61:Ag:152:ARG:HH21	1.72	0.54
86:Bl:30:LYS:HB2	86:Bl:33:ASN:HB2	1.89	0.54
2:Aq:43:SER:OG	63:A2:1390:C:OP1	2.18	0.54
8:BX:73:HIS:CD2	8:BX:115:LYS:HD3	2.43	0.54
19:DB:124:GLN:O	19:DB:133:TYR:OH	2.16	0.54
31:BJ:15:LEU:HD12	31:BJ:165:TRP:HB2	1.89	0.54
53:Ae:83:ASN:HD22	63:A2:1652:A:H1'	1.73	0.54
64:Ah:162:LEU:HD11	64:Ah:191:GLU:HG2	1.90	0.54
82:An:98:ARG:HB3	82:An:132:VAL:HG23	1.90	0.54
19:DB:407:LEU:HB2	19:DB:410:LEU:HD12	1.90	0.53
19:DB:423:ASN:HB3	19:DB:426:GLU:HB2	1.89	0.53
24:B5:2249:G:N7	86:Bl:2:SER:N	2.56	0.53
51:B:65:ALA:HB2	51:B:74:ILE:HD13	1.90	0.53
11:As:129:ARG:NH1	63:A2:1417:C:OP1	2.40	0.53
24:B5:85:G:N2	24:B5:98:A:OP2	2.36	0.53
24:B5:483:G:O2'	24:B5:486:C:OP2	2.25	0.53
57:Af:135:PRO:HG2	57:Af:141:ILE:HD13	1.90	0.53
63:A2:64:A:H2	63:A2:83:A:H62	1.55	0.53
24:B5:4318:U:OP1	34:B8:1:C:N4	2.42	0.53
36:Aa:7:LYS:NZ	63:A2:966:U:OP1	2.35	0.53
53:Ae:130:ARG:HD2	63:A2:1684:C:H5'	1.91	0.53
57:Af:148:SER:N	57:Af:151:ASP:OD2	2.41	0.53
78:AE:59:PHE:HB2	78:AE:62:TYR:HB2	1.91	0.53
24:B5:1536:G:N7	97:B5:5685:HOH:O	2.34	0.53
24:B5:1610:C:O2	24:B5:4136:A:O2'	2.23	0.53
24:B5:2302:G:N2	24:B5:2305:C:OP2	2.41	0.53
12:Br:67:ARG:NH1	24:B5:480:C:OP1	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B5:2688:A:H61	24:B5:3575:C:H42	1.55	0.53
24:B5:3997:A:H5''	31:BJ:108:GLY:HA3	1.91	0.53
46:BZ:92:ASP:HB3	46:BZ:95:VAL:HG12	1.89	0.53
63:A2:510:OMG:HM22	63:A2:511:G:H5'	1.90	0.53
63:A2:523:A:H5''	67:AI:145:PRO:HD2	1.89	0.53
67:AI:138:ARG:NH1	67:AI:153:SER:OG	2.40	0.53
5:AR:38:ARG:O	5:AR:42:HIS:ND1	2.33	0.53
6:CU:56:ILE:HG21	20:CT:98:LYS:HE2	1.91	0.53
24:B5:3374:A:HO2'	80:BJ:2:THR:N	2.06	0.53
34:B8:96:C:H5''	74:Bh:66:LYS:HG2	1.90	0.53
40:BM:29:ASP:OD1	40:BM:30:VAL:N	2.42	0.53
56:DA:137:ASN:HA	56:DA:145:ALA:HB1	1.91	0.53
57:Af:162:LEU:HD11	57:Af:172:LYS:HG3	1.91	0.53
63:A2:387:C:H5'	64:Ah:7:ASN:HD22	1.73	0.53
24:B5:1934:G:O6	24:B5:1939:G:N2	2.41	0.53
24:B5:4140:A:N7	97:B5:5683:HOH:O	2.33	0.53
45:Ac:70:THR:HG22	45:Ac:86:LEU:HD13	1.90	0.53
63:A2:49:C:H2'	63:A2:473:C:H41	1.73	0.53
63:A2:1805:OMU:HM22	63:A2:1806:G:H5'	1.89	0.53
11:As:96:SER:OG	63:A2:1569:C:OP1	2.25	0.53
24:B5:4649:A:H4'	43:BB:95:THR:HG22	1.90	0.53
24:B5:4794:G:N2	62:Bd:118:GLN:OE1	2.40	0.53
36:Aa:189:ILE:HB	36:Aa:190:PRO:HD3	1.91	0.53
61:Ag:107:LYS:O	61:Ag:109:ARG:NH2	2.42	0.53
63:A2:204:G:OP2	64:Ah:147:LYS:NZ	2.36	0.53
3:Bo:8:ARG:NH2	24:B5:3978:U:O4	2.41	0.53
7:BL:115:GLN:OE1	24:B5:521:C:O2'	2.27	0.53
24:B5:1741:A:N3	25:BT:130:ARG:NH2	2.57	0.53
24:B5:2221:G:N2	24:B5:2224:A:OP2	2.42	0.53
24:B5:4269:A2M:H5''	24:B5:4270:G:H5'	1.91	0.53
24:B5:2420:C:OP1	46:BZ:111:ARG:NH1	2.42	0.53
24:B5:3629:G:OP2	97:B5:5523:HOH:O	2.19	0.53
57:Af:102:VAL:HG13	57:Af:106:LEU:HD12	1.91	0.53
59:BF:121:PHE:O	59:BF:204:ASN:ND2	2.42	0.53
63:A2:62:G:H1'	63:A2:172:OMU:HM23	1.91	0.53
71:Bg:64:LEU:HD23	71:Bg:67:LEU:HD12	1.91	0.53
1:BP:8:PRO:HG3	1:BP:149:ILE:HD13	1.91	0.52
19:DB:408:ILE:HD12	60:DC:79:ARG:HH22	1.74	0.52
21:BH:113:GLU:HG2	21:BH:125:ARG:HG2	1.90	0.52
24:B5:2658:A2M:HM'2	24:B5:2659:G:H5'	1.91	0.52
44:BS:99:ASP:OD1	44:BS:100:LEU:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:BC:110:ARG:O	47:BC:113:ARG:NH1	2.33	0.52
63:A2:1481:A:O2'	84:AG:56:ASP:OXT	2.24	0.52
64:Ah:165:GLN:HE22	64:Ah:195:LEU:HD11	1.74	0.52
73:Ak:120:VAL:HG22	73:Ak:145:VAL:HG11	1.89	0.52
84:AG:17:GLY:O	84:AG:27:ARG:NH1	2.42	0.52
63:A2:191:A:H3'	63:A2:192:C:H5''	1.92	0.52
19:DB:141:LEU:N	19:DB:154:TYR:OH	2.43	0.52
24:B5:3432:C:O2'	24:B5:3506:A:N3	2.37	0.52
24:B5:4068:G:N2	24:B5:4071:A:OP2	2.39	0.52
29:B7:23:A:N3	29:B7:118:C:O2'	2.36	0.52
38:BA:101:VAL:HG22	38:BA:165:VAL:HG22	1.91	0.52
48:BN:53:TYR:HB2	48:BN:133:ILE:HD13	1.91	0.52
63:A2:1338:4AC:H2'	63:A2:1339:G:C8	2.44	0.52
14:At:95:ARG:NH1	84:AG:56:ASP:OXT	2.41	0.52
16:BG:43:GLN:NE2	24:B5:3844:C:O2'	2.41	0.52
24:B5:1284:OMC:HM22	24:B5:1285:U:H5'	1.92	0.52
24:B5:1341:A:O2'	24:B5:1422:C:O2'	2.24	0.52
24:B5:2745:G:OP2	24:B5:3328:A:N6	2.39	0.52
34:B8:86:U:OP2	42:BY:113:LYS:NZ	2.41	0.52
48:BN:201:HIS:O	48:BN:204:ARG:NH1	2.38	0.52
2:Aq:77:GLU:OE2	2:Aq:81:ARG:NH2	2.43	0.52
10:BQ:157:GLY:O	10:BQ:188:ASN:ND2	2.42	0.52
19:DB:522:GLN:HA	19:DB:525:PHE:HD2	1.75	0.52
24:B5:364:G:O6	80:Bj:55:ARG:NH2	2.37	0.52
24:B5:1484:G:N7	97:B5:5688:HOH:O	2.34	0.52
24:B5:1503:G:OP1	94:B5:5082:SPD:N10	2.41	0.52
24:B5:2301:C:H5''	48:BN:67:ARG:HD2	1.90	0.52
67:Ai:110:LEU:HB2	67:Ai:147:PHE:HB3	1.91	0.52
24:B5:1093:C:H2'	24:B5:1094:A:H8	1.74	0.52
24:B5:1924:G:H1'	24:B5:1942:G:H2'	1.91	0.52
24:B5:2422:G:N2	24:B5:2425:A:OP2	2.35	0.52
43:BB:317:LEU:HB2	43:BB:372:SER:HB2	1.91	0.52
57:Af:170:ARG:NH1	63:A2:71:G:O6	2.41	0.52
63:A2:1620:A:OP2	85:Ao:47:ARG:NH2	2.40	0.52
10:BQ:63:LEU:N	10:BQ:87:THR:O	2.43	0.52
24:B5:2362:U:O2'	24:B5:2373:U:O2	2.26	0.52
24:B5:3421:G:O2'	24:B5:3550:UY1:OP2	2.26	0.52
24:B5:4480:A:H61	24:B5:4704:U:H3	1.56	0.52
29:B7:55:A:O2'	31:BJ:151:ILE:O	2.25	0.52
63:A2:1532:A:H4'	63:A2:1606:G:H4'	1.92	0.52
74:Bh:4:ILE:HD12	74:Bh:53:SER:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:BQ:67:ILE:HG12	10:BQ:98:LEU:HD11	1.92	0.52
24:B5:3930:G:H5'	38:BA:233:ARG:HB2	1.90	0.52
24:B5:4486:G:H2'	24:B5:4489:G:H5'	1.92	0.52
41:Ab:128:VAL:HG11	41:Ab:155:ILE:HG12	1.91	0.52
47:BC:14:LYS:HA	47:BC:173:LYS:HD3	1.91	0.52
60:DC:8:PRO:HA	60:DC:11:LEU:HG	1.92	0.52
63:A2:1222:G:O2'	63:A2:1677:U:O2	2.22	0.52
20:Ct:94:VAL:HG23	20:Ct:109:PRO:HG3	1.92	0.52
24:B5:788:G:H2'	24:B5:789:G:C8	2.43	0.52
58:Bc:5:LYS:NZ	63:A2:930:G:OP1	2.38	0.52
63:A2:1031:A:H2'	63:A2:1032:A2M:H8	1.91	0.52
1:BP:2:VAL:N	24:B5:409:G:OP2	2.43	0.51
24:B5:399:G:H2'	24:B5:400:A2M:H8	1.92	0.51
24:B5:2647:OMC:HM22	24:B5:2648:C:H5'	1.90	0.51
24:B5:3399:C:H4'	38:BA:8:GLN:HA	1.92	0.51
24:B5:3882:G:H2'	24:B5:3883:G:H8	1.75	0.51
57:Af:171:THR:OG1	63:A2:74:G:N2	2.42	0.51
61:Ag:134:VAL:O	61:Ag:137:SER:OG	2.27	0.51
8:BX:139:ARG:NH1	24:B5:2376:C:OP1	2.42	0.51
13:BR:136:ARG:NH1	24:B5:2739:G:OP1	2.44	0.51
24:B5:1611:U:OP2	50:Ba:26:ARG:NH2	2.30	0.51
24:B5:1823:C:N4	97:B5:5793:HOH:O	2.41	0.51
24:B5:1935:C:H42	24:B5:1939:G:H22	1.58	0.51
24:B5:2257:G:H2'	24:B5:2258:OMU:H6	1.92	0.51
41:Ab:187:ARG:HD2	41:Ab:192:LEU:HD12	1.92	0.51
43:BB:41:VAL:HA	43:BB:187:GLY:HA3	1.91	0.51
44:BS:15:ARG:HB3	44:BS:27:LEU:HD23	1.91	0.51
56:DA:90:THR:HG23	56:DA:127:PHE:HZ	1.73	0.51
9:Bp:5:THR:OG1	24:B5:1509:A:OP1	2.26	0.51
24:B5:2252:U:H4'	24:B5:2271:A:H4'	1.92	0.51
25:BT:93:ILE:HG21	51:B:41:LYS:HE2	1.93	0.51
43:BB:92:TYR:HB2	43:BB:159:VAL:HB	1.91	0.51
57:Af:31:ARG:NH1	63:A2:1746:A:O3'	2.43	0.51
63:A2:434:A:H5''	64:Ah:22:HIS:HB3	1.93	0.51
19:DB:326:PHE:O	19:DB:330:ARG:N	2.44	0.51
24:B5:1298:A:N6	24:B5:1458:A:O4'	2.43	0.51
38:BA:2:GLY:HA2	38:BA:207:VAL:HG23	1.92	0.51
39:Bt:10:ILE:HG12	39:Bt:65:GLN:HG2	1.93	0.51
51:B:223:PHE:HB3	51:B:226:TYR:HB2	1.91	0.51
1:BP:118:GLN:NE2	1:BP:147:GLU:OE2	2.43	0.51
15:Bs:30:VAL:HG21	15:Bs:187:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:DB:298:LEU:O	19:DB:338:LYS:NZ	2.41	0.51
24:B5:709:G:OP1	47:BC:321:ASN:ND2	2.43	0.51
28:Ax:7:ILE:HG22	28:Ax:27:VAL:HG22	1.93	0.51
41:Ab:81:ILE:HG23	41:Ab:86:LEU:HB2	1.93	0.51
63:A2:105:PSU:OP1	94:A2:1986:SPD:N10	2.44	0.51
63:A2:1085:A:OP1	63:A2:1859:G:O2'	2.27	0.51
81:AF:133:ASN:HD21	81:AF:137:VAL:HB	1.76	0.51
24:B5:2499:U:H5''	46:BZ:38:TYR:HB3	1.91	0.51
43:BB:95:THR:OG1	43:BB:98:GLY:O	2.21	0.51
55:BE:136:PHE:O	55:BE:141:ARG:NH2	2.44	0.51
63:A2:35:C:H2'	63:A2:36:PSU:H6	1.76	0.51
17:BU:28:PRO:HB2	17:BU:34:MET:HG2	1.93	0.51
24:B5:1335:A:H62	94:B5:5343:SPD:H102	1.59	0.51
24:B5:3404:G:OP2	24:B5:3404:G:N2	2.37	0.51
32:AZ:41:ARG:HE	32:AZ:45:GLY:HA2	1.76	0.51
62:Bd:19:GLU:OE1	62:Bd:92:ARG:NH1	2.44	0.51
63:A2:1260:A:H1'	63:A2:1265:C:H42	1.76	0.51
67:Ai:134:HIS:ND1	67:Ai:163:SER:OG	2.36	0.51
19:DB:673:GLU:HA	19:DB:676:LEU:HB2	1.93	0.51
24:B5:835:G:OP1	40:BM:23:LYS:NZ	2.40	0.51
24:B5:1449:U:H2'	24:B5:1450:G:H8	1.76	0.51
24:B5:1766:C:H1'	54:Bb:50:ASN:HD21	1.74	0.51
24:B5:4171:G:OP1	89:Bm:100:TYR:OH	2.27	0.51
24:B5:4445:U:H1'	24:B5:4446:A:H5''	1.93	0.51
26:BI:51:HIS:CD2	26:BI:168:SER:HB2	2.46	0.51
63:A2:1602:A:OP2	63:A2:1637:G:N2	2.43	0.51
66:AA:28:PRO:HG3	79:Am:17:PRO:HG3	1.93	0.51
13:BR:44:LEU:HD22	13:BR:49:LEU:HD12	1.92	0.51
13:BR:172:ARG:HH12	63:A2:909:A:H5''	1.74	0.51
21:BH:37:ASP:OD2	21:BH:39:ASN:ND2	2.44	0.51
24:B5:3391:G:OP1	38:BA:241:ARG:NH1	2.44	0.51
24:B5:3497:G:O2'	24:B5:3499:C:N4	2.44	0.51
24:B5:4416:C:O2'	24:B5:4418:A:OP2	2.26	0.51
41:Ab:192:LEU:HB3	41:Ab:227:ARG:HG2	1.93	0.51
55:BE:49:ASN:HD21	55:BE:57:GLY:HA3	1.75	0.51
55:BE:181:PRO:HD2	55:BE:184:LEU:HD12	1.93	0.51
66:AA:35:VAL:HG21	66:AA:63:LEU:HD13	1.93	0.51
19:DB:435:GLN:HE21	19:DB:448:CYS:HB2	1.76	0.51
19:DB:473:THR:OG1	19:DB:478:ASN:OD1	2.24	0.51
24:B5:2507:G:H4'	24:B5:2520:G:H4'	1.92	0.51
24:B5:4311:C:O2	43:BB:268:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B5:4764:C:O2'	24:B5:4767:G:N3	2.41	0.51
41:Ab:194:ARG:NH1	63:A2:1157:U:O4	2.44	0.51
44:BS:112:ASP:OD1	44:BS:116:ARG:NH1	2.40	0.51
56:DA:23:ASN:HD22	56:DA:36:TYR:HE1	1.58	0.51
60:DC:61:GLU:OE1	60:DC:69:HIS:NE2	2.37	0.51
19:DB:484:CYS:HA	60:DC:19:LEU:HD13	1.93	0.50
24:B5:2206:A2M:HM'2	24:B5:2207:OMG:H5'	1.92	0.50
61:Ag:160:LYS:HA	61:Ag:163:GLN:HB2	1.93	0.50
70:Aj:51:SER:OG	70:Aj:55:ARG:NH1	2.44	0.50
75:AD:91:LEU:HD23	75:AD:91:LEU:H	1.76	0.50
2:Aq:44:LYS:HG3	2:Aq:47:ARG:HH21	1.75	0.50
18:Av:45:GLY:O	18:Av:68:ARG:NH2	2.44	0.50
19:DB:125:ILE:HA	19:DB:133:TYR:CZ	2.45	0.50
24:B5:4051:G:O5'	25:BT:83:LYS:NZ	2.44	0.50
24:B5:4515:G:OP1	52:BO:168:TYR:OH	2.27	0.50
34:B8:75:OMG:OP2	42:BY:74:TYR:OH	2.25	0.50
49:Ad:112:HIS:NE2	49:Ad:237:SER:O	2.45	0.50
56:DA:115:ILE:HD13	56:DA:146:ASP:HB2	1.93	0.50
58:Bc:47:ILE:HD12	58:Bc:94:LEU:HD11	1.92	0.50
60:DC:12:MET:HA	60:DC:28:MET:HE1	1.92	0.50
63:A2:469:A2M:HM'2	63:A2:470:A:H5'	1.92	0.50
63:A2:963:A:N1	63:A2:1056:A:O2'	2.44	0.50
63:A2:1038:G:H4'	63:A2:1846:A:H4'	1.93	0.50
81:AF:256:ILE:HB	81:AF:270:LEU:HB2	1.93	0.50
14:At:94:ASP:OD1	84:AG:54:LYS:NZ	2.44	0.50
19:DB:213:LEU:O	19:DB:217:GLU:HG3	2.11	0.50
32:AZ:206:ASP:OD1	32:AZ:206:ASP:N	2.37	0.50
81:AF:8:ARG:NE	81:AF:311:GLN:OE1	2.42	0.50
24:B5:3468:A:OP2	97:B5:5524:HOH:O	2.20	0.50
24:B5:4741:U:OP2	43:BB:385:LYS:NZ	2.38	0.50
32:AZ:32:PHE:CD1	63:A2:1098:G:H4'	2.46	0.50
33:Ay:74:SER:OG	33:Ay:79:ILE:O	2.22	0.50
49:Ad:24:THR:HG22	63:A2:496:U:H4'	1.92	0.50
63:A2:1032:A2M:HM'2	63:A2:1033:C:H5'	1.93	0.50
63:A2:1604:G:P	97:A2:2244:HOH:O	2.69	0.50
63:A2:1618:G:H3'	85:Ao:47:ARG:HH22	1.77	0.50
19:DB:56:LEU:HB3	19:DB:61:LYS:HB2	1.94	0.50
49:Ad:124:CYS:HB3	49:Ad:141:THR:HB	1.93	0.50
51:B:122:GLN:NE2	51:B:126:THR:OG1	2.43	0.50
63:A2:1209:A:O2'	63:A2:1836:A:N7	2.38	0.50
81:AF:107:ASP:HB2	81:AF:125:ARG:HH11	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:BQ:178:ARG:N	50:Ba:51:GLY:HA2	2.26	0.50
19:DB:26:TYR:HB3	19:DB:55:THR:HG22	1.93	0.50
24:B5:419:A:N3	24:B5:1276:C:O2'	2.40	0.50
24:B5:1217:G:H4'	55:BE:77:ALA:HB2	1.93	0.50
36:Aa:32:ASP:OD1	36:Aa:46:LYS:NZ	2.44	0.50
39:Bt:18:THR:OG1	39:Bt:21:GLU:O	2.26	0.50
57:Af:174:PRO:HB3	63:A2:65:C:C6	2.47	0.50
63:A2:415:A:OP1	63:A2:815:PSU:O2'	2.26	0.50
67:Ai:33:GLY:HA3	75:AD:112:TYR:CG	2.47	0.50
85:Ao:40:ARG:HH21	85:Ao:43:ARG:HD3	1.77	0.50
2:Aq:31:ASN:ND2	2:Aq:55:THR:OG1	2.41	0.50
24:B5:2204:G:O2'	24:B5:3591:G:O6	2.24	0.50
24:B5:2691:G:O2'	24:B5:3570:U:O4	2.27	0.50
24:B5:3456:A2M:HM'2	24:B5:3457:G:H5'	1.92	0.50
26:BI:150:GLU:OE2	26:BI:153:ARG:NH2	2.37	0.50
36:Aa:179:ASN:HB3	36:Aa:183:GLU:HB2	1.94	0.50
64:Ah:10:LYS:O	64:Ah:18:ARG:NH1	2.45	0.50
5:Ar:98:VAL:HG11	5:Ar:106:LYS:HG3	1.92	0.50
11:As:101:ARG:NH1	63:A2:1566:C:OP2	2.45	0.50
24:B5:280:G:OP2	48:BN:44:ARG:NH2	2.42	0.50
24:B5:394:G:N2	24:B5:397:G:OP2	2.29	0.50
24:B5:860:A:N6	55:BE:129:LEU:O	2.42	0.50
24:B5:1095:C:H2'	24:B5:1096:G:H8	1.77	0.50
24:B5:1674:U:H5'	94:B5:5144:SPD:H41	1.94	0.50
24:B5:1779:G:OP2	59:BF:201:LYS:NZ	2.42	0.50
24:B5:4060:C:O2'	54:Bb:36:ASP:OD1	2.24	0.50
50:Ba:71:PRO:HG2	50:Ba:108:TYR:HA	1.94	0.50
63:A2:28:U:H2'	63:A2:29:G:H8	1.76	0.50
63:A2:1804:U:H2'	63:A2:1805:OMU:H6	1.93	0.50
7:BL:74:ARG:NH2	24:B5:109:G:OP2	2.44	0.50
11:As:91:HIS:HE2	63:A2:1666:G:P	2.35	0.50
12:Br:26:SER:OG	12:Br:28:GLU:OE1	2.15	0.50
19:DB:21:TYR:OH	19:DB:51:MET:O	2.22	0.50
19:DB:107:LEU:HB3	19:DB:111:LYS:HG2	1.93	0.50
19:DB:431:MET:HB3	19:DB:448:CYS:SG	2.51	0.50
24:B5:58:G:H4'	24:B5:59:A:H4'	1.93	0.50
24:B5:784:C:H2'	24:B5:785:G:H8	1.76	0.50
24:B5:1016:C:O2'	24:B5:1059:G:O4'	2.29	0.50
24:B5:1827:A:N6	24:B5:3605:G:O2'	2.44	0.50
24:B5:3491:A:HO2'	63:A2:1827:G:HO2'	1.60	0.50
26:BI:38:ARG:NH1	26:BI:45:GLU:OE1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:BE:189:LEU:HD21	55:BE:256:VAL:HG21	1.94	0.50
56:DA:28:PRO:O	56:DA:141:ARG:NH2	2.45	0.50
63:A2:355:OMU:HM22	63:A2:356:G:H5'	1.93	0.50
83:Bk:14:THR:HA	83:Bk:17:ARG:HD3	1.94	0.50
19:DB:20:CYS:O	19:DB:25:GLN:N	2.42	0.49
19:DB:134:ARG:HB3	19:DB:138:TYR:CZ	2.46	0.49
24:B5:184:U:H3	24:B5:253:G:H22	1.59	0.49
24:B5:3455:A:H2'	24:B5:3456:A2M:H8	1.93	0.49
32:AZ:177:MET:SD	32:AZ:180:ARG:NH2	2.85	0.49
57:Af:121:ILE:N	57:Af:125:THR:OG1	2.45	0.49
61:Ag:57:ARG:NH2	61:Ag:89:GLY:O	2.44	0.49
63:A2:694:A:H2'	63:A2:695:G:H8	1.76	0.49
67:Ai:107:GLU:HA	67:Ai:112:THR:HG21	1.94	0.49
6:Cu:15:GLN:HB2	17:BU:99:TRP:HE1	1.78	0.49
13:BR:12:SER:OG	13:BR:17:CYS:O	2.26	0.49
19:DB:69:VAL:HG21	19:DB:89:LEU:HD11	1.94	0.49
22:BV:13:LYS:HD2	22:BV:128:LEU:HD21	1.94	0.49
24:B5:454:U:H1'	65:Be:5:ARG:HE	1.77	0.49
24:B5:1564:U:O4	94:B5:4954:SPD:N6	2.45	0.49
24:B5:2550:U:C4	24:B5:2551:U:H1'	2.47	0.49
44:BS:173:ASN:ND2	44:BS:175:PHE:O	2.45	0.49
60:DC:128:PHE:HB3	60:DC:147:MET:HE2	1.95	0.49
63:A2:1299:G:H4'	85:Ao:78:THR:HA	1.94	0.49
72:AC:126:CYS:HB2	72:AC:130:VAL:HB	1.94	0.49
19:DB:145:PRO:HB2	20:Ct:136:GLN:HB3	1.94	0.49
19:DB:330:ARG:HA	19:DB:333:TYR:HD2	1.77	0.49
19:DB:745:THR:HB	19:DB:749:ASN:HD22	1.77	0.49
24:B5:2122:A:O2'	65:Be:48:ARG:NH2	2.45	0.49
24:B5:4495:U:H5''	68:Bf:54:LYS:HE3	1.93	0.49
81:AF:85:GLY:HA2	81:AF:108:VAL:HG23	1.94	0.49
24:B5:466:A:O2'	24:B5:468:U:OP2	2.31	0.49
24:B5:1458:A:H4'	24:B5:1459:G:H5'	1.93	0.49
41:Ab:185:THR:OG1	63:A2:1156:U:OP1	2.29	0.49
43:BB:39:LYS:HG2	43:BB:40:PRO:HD2	1.94	0.49
55:BE:246:THR:HG22	55:BE:248:GLN:H	1.76	0.49
88:Ap:16:LYS:HG3	88:Ap:17:LYS:H	1.77	0.49
1:BP:115:GLU:OE1	1:BP:151:THR:OG1	2.29	0.49
15:Bs:62:ARG:NH2	15:Bs:82:ILE:O	2.46	0.49
19:DB:541:LEU:HD12	60:DC:36:LEU:HD21	1.93	0.49
24:B5:2624:G:O2'	86:Bl:3:SER:O	2.30	0.49
25:BT:18:PRO:HG2	25:BT:21:LYS:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:Bt:32:ILE:HB	39:Bt:35:LEU:HD11	1.93	0.49
63:A2:920:A:O2'	94:A2:1971:SPD:N1	2.44	0.49
19:DB:544:LEU:HD21	60:DC:9:GLU:HB3	1.95	0.49
24:B5:1604:U:O2	94:B5:5165:SPD:N1	2.44	0.49
24:B5:2243:G:H21	71:Bg:6:THR:HG22	1.76	0.49
24:B5:4050:A:OP2	24:B5:4051:G:N2	2.45	0.49
34:B8:71:A:N1	34:B8:84:A:O2'	2.41	0.49
36:Aa:129:THR:OG1	36:Aa:131:ASP:OD1	2.27	0.49
55:BE:104:ASN:O	55:BE:108:ARG:NH2	2.41	0.49
59:BF:135:VAL:HG23	59:BF:139:ILE:HD13	1.94	0.49
63:A2:1227:G:N1	63:A2:1640:G7M:OP2	2.34	0.49
70:Aj:37:ASP:OD1	70:Aj:37:ASP:N	2.45	0.49
81:AF:259:TRP:HD1	81:AF:266:ILE:HA	1.78	0.49
1:BP:94:MET:HE1	1:BP:146:ILE:HB	1.95	0.49
12:Br:37:SER:OG	24:B5:2110:U:OP1	2.28	0.49
17:BU:101:ARG:NE	24:B5:2466:A:OP1	2.46	0.49
51:B:62:CYS:HB3	51:B:105:LEU:HD22	1.94	0.49
6:Cu:82:SER:HG	6:Cu:87:THR:HG1	1.50	0.49
19:DB:496:LYS:NZ	19:DB:560:ILE:O	2.45	0.49
19:DB:672:ILE:HG23	19:DB:698:ALA:HB1	1.94	0.49
32:AZ:176:TRP:HE1	32:AZ:197:VAL:HG23	1.76	0.49
56:DA:74:ILE:HG13	56:DA:111:LEU:HB3	1.95	0.49
60:DC:157:GLU:HA	60:DC:160:ARG:HD2	1.93	0.49
62:Bd:37:GLY:O	62:Bd:41:ARG:HG3	2.12	0.49
63:A2:1763:C:H2'	63:A2:1764:G:C8	2.48	0.49
19:DB:825:ARG:O	19:DB:829:HIS:ND1	2.46	0.49
24:B5:62:A:N3	24:B5:77:U:O2'	2.41	0.49
24:B5:4175:C:N3	26:BI:158:LYS:NZ	2.59	0.49
41:Ab:102:LEU:HD22	41:Ab:130:ILE:HG12	1.94	0.49
49:Ad:134:LYS:NZ	63:A2:127:C:O2	2.36	0.49
63:A2:116:OMU:HM22	63:A2:117:C:H5'	1.95	0.49
88:Ap:34:VAL:HG22	88:Ap:70:VAL:HB	1.94	0.49
2:Aq:29:HIS:HA	2:Aq:32:LYS:HE2	1.95	0.49
5:Ar:133:GLY:O	94:A2:1950:SPD:N1	2.43	0.49
7:BL:91:ALA:HB1	7:BL:96:ILE:HB	1.94	0.49
10:BQ:173:LYS:NZ	24:B5:88:A:N7	2.61	0.49
17:BU:100:LEU:HD13	17:BU:112:LEU:HD23	1.95	0.49
19:DB:436:ALA:HB1	56:DA:17:LYS:HG2	1.95	0.49
24:B5:2146:C:O2'	24:B5:2175:A:N1	2.40	0.49
43:BB:321:VAL:HG12	43:BB:322:HIS:HD1	1.78	0.49
47:BC:66:SER:HA	47:BC:77:PRO:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:Ba:84:GLU:OE2	50:Ba:87:ARG:NH2	2.45	0.49
63:A2:1758:G:H2'	63:A2:1759:G:H8	1.78	0.49
63:A2:1861:A:N7	78:AE:34:LYS:NZ	2.61	0.49
70:Aj:4:PRO:HB2	70:Aj:7:ASN:HD22	1.78	0.49
18:Av:2:VAL:N	63:A2:1092:C:O2'	2.39	0.48
19:DB:421:ALA:HB1	19:DB:834:TYR:HB2	1.95	0.48
30:Au:15:ARG:NH1	30:Au:33:GLN:OE1	2.46	0.48
34:B8:102:G:OP2	34:B8:104:A:O2'	2.27	0.48
41:Ab:232:THR:HG22	41:Ab:235:ASN:H	1.78	0.48
82:An:40:THR:HG21	82:An:74:ALA:HB2	1.94	0.48
13:BR:70:ARG:HD3	13:BR:76:MET:HE2	1.94	0.48
20:Ct:82:LYS:NZ	24:B5:2222:A:OP2	2.46	0.48
24:B5:3584:A:OP1	97:B5:5525:HOH:O	2.20	0.48
25:BT:148:PRO:HB2	44:BS:29:ARG:HB2	1.94	0.48
41:Ab:196:ILE:HB	41:Ab:223:TYR:HB2	1.96	0.48
63:A2:220:U:H2'	63:A2:221:A:C8	2.48	0.48
63:A2:477:A:N3	63:A2:489:U:O2'	2.38	0.48
23:Aw:131:LEU:HD11	23:Aw:135:LYS:HE3	1.93	0.48
24:B5:1907:G:H2'	24:B5:1908:G:C8	2.48	0.48
46:BZ:76:ASN:OD1	46:BZ:77:TYR:N	2.47	0.48
63:A2:1240:U:H5''	85:Ao:124:LYS:HD3	1.93	0.48
24:B5:1909:A:N6	24:B5:1955:C:OP2	2.47	0.48
24:B5:2652:G:O2'	24:B5:4390:G:OP1	2.26	0.48
30:Au:1:AME:HT23	30:Au:1:AME:HA	1.52	0.48
63:A2:1598:C:H4'	63:A2:1604:G:C6	2.49	0.48
74:Bh:80:PRO:HD2	74:Bh:83:LEU:HD12	1.95	0.48
20:Ct:71:ARG:O	20:Ct:75:LYS:HB2	2.12	0.48
20:Ct:77:ARG:HH21	20:Ct:123:PHE:HB3	1.78	0.48
24:B5:1548:A:H5''	24:B5:2682:U:H5''	1.96	0.48
24:B5:1984:G:O6	24:B5:3602:C:O2'	2.31	0.48
26:BI:187:GLU:HG3	26:BI:189:ARG:HG3	1.95	0.48
63:A2:941:U:H3	63:A2:1003:U:H3	1.59	0.48
63:A2:1865:U:H5'	78:AE:79:ILE:HD11	1.95	0.48
7:BL:12:PRO:HB2	7:BL:14:PHE:HD2	1.78	0.48
24:B5:4312:U:O2'	43:BB:234:ARG:NH1	2.36	0.48
24:B5:4323:U:H2'	24:B5:4324:G:C8	2.49	0.48
24:B5:4516:G:H5''	52:BO:176:ARG:HD3	1.95	0.48
48:BN:146:PRO:HB2	74:Bh:104:THR:HG23	1.95	0.48
63:A2:1229:A:O2'	63:A2:1635:A:N3	2.44	0.48
63:A2:1860:A:P	78:AE:10:ARG:HH12	2.37	0.48
85:Ao:138:SER:OG	88:Ap:146:ARG:O	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BL:176:PHE:HB2	77:Bi:3:LEU:HD23	1.96	0.48
14:At:91:LYS:NZ	97:At:201:HOH:O	2.46	0.48
24:B5:443:G:H5''	68:Bf:54:LYS:HB3	1.94	0.48
33:Ay:79:ILE:HB	33:Ay:83:LEU:HD23	1.95	0.48
41:Ab:121:ARG:O	41:Ab:121:ARG:NH1	2.47	0.48
58:Bc:38:ILE:HG21	58:Bc:63:TYR:HB3	1.96	0.48
63:A2:985:C:O2'	82:An:138:IAS:OD1	2.19	0.48
13:BR:170:ARG:HH22	63:A2:873:A:H5'	1.78	0.48
19:DB:400:ALA:O	19:DB:403:SER:OG	2.30	0.48
24:B5:1772:G:N2	24:B5:1774:G:O4'	2.47	0.48
47:BC:218:VAL:HA	47:BC:229:LEU:HG	1.95	0.48
56:DA:51:PHE:O	56:DA:54:ILE:HG12	2.14	0.48
76:Al:49:LEU:HB3	76:Al:111:VAL:HB	1.95	0.48
13:BR:98:ARG:NH2	13:BR:130:ASN:OD1	2.40	0.48
18:Av:56:HIS:HB3	79:Am:20:ARG:HH21	1.78	0.48
19:DB:418:TYR:O	19:DB:423:ASN:N	2.43	0.48
24:B5:1070:U:O2	51:B:286:SER:OG	2.29	0.48
24:B5:2539:A:H62	83:Bk:35:LYS:NZ	2.11	0.48
24:B5:3374:A:C4	80:Bj:3:LYS:HB3	2.48	0.48
24:B5:3812:G:O6	38:BA:72:ARG:NH2	2.46	0.48
24:B5:4037:G:H5'	24:B5:4039:PSU:C6	2.48	0.48
24:B5:4645:C:O2	24:B5:4655:G:N2	2.47	0.48
28:Ax:12:PHE:HZ	28:Ax:21:LYS:HD3	1.78	0.48
57:Af:15:LEU:HD22	63:A2:155:G:H4'	1.96	0.48
66:AA:67:THR:OG1	66:AA:70:LYS:O	2.32	0.48
74:Bh:13:LYS:NZ	74:Bh:16:GLU:OE2	2.46	0.48
1:BP:83:TRP:O	24:B5:3588:A:H5''	2.14	0.48
19:DB:469:THR:HB	19:DB:478:ASN:HD22	1.79	0.48
24:B5:135:G:N2	74:Bh:95:LEU:O	2.34	0.48
24:B5:4061:A:OP1	25:BT:69:GLN:NE2	2.47	0.48
24:B5:4512:G:O6	40:BM:4:ARG:NH2	2.42	0.48
24:B5:4762:C:H5'	64:Ah:124:LYS:HE2	1.95	0.48
26:BI:48:LEU:HB2	26:BI:142:LEU:HD23	1.94	0.48
49:Ad:49:ARG:NH1	63:A2:496:U:OP1	2.47	0.48
88:Ap:101:ASP:OD1	88:Ap:102:GLU:N	2.45	0.48
88:Ap:129:SER:O	88:Ap:131:LYS:NZ	2.42	0.48
5:Ar:124:ARG:HB2	5:Ar:131:VAL:HG12	1.96	0.47
13:BR:88:ARG:O	24:B5:2568:A:N6	2.47	0.47
15:Bs:39:GLN:HE22	15:Bs:106:LYS:HA	1.78	0.47
16:BG:132:ARG:NH1	24:B5:119:G:OP1	2.46	0.47
19:DB:265:GLU:OE2	19:DB:280:TYR:OH	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B5:303:C:OP2	48:BN:68:ARG:NH2	2.36	0.47
24:B5:1227:G:N1	24:B5:2015:G:OP1	2.42	0.47
24:B5:1921:G:N2	24:B5:1948:A:O2'	2.38	0.47
24:B5:4271:C:H5''	43:BB:245:HIC:HB2	1.96	0.47
28:Ax:108:LYS:NZ	63:A2:507:G:OP1	2.35	0.47
59:BF:153:ILE:HD12	59:BF:190:ILE:HG12	1.96	0.47
61:Ag:109:ARG:NH2	63:A2:745:G:N3	2.62	0.47
63:A2:823:PSU:HN3	63:A2:827:A:H62	1.61	0.47
68:Bf:4:ARG:NH1	68:Bf:6:TRP:O	2.43	0.47
3:Bo:45:GLN:HE22	3:Bo:51:GLN:HA	1.78	0.47
19:DB:672:ILE:HG22	19:DB:676:LEU:HG	1.95	0.47
19:DB:699:PHE:HE2	19:DB:741:LEU:HD13	1.78	0.47
23:Aw:11:ARG:NH2	73:Ak:104:LYS:O	2.40	0.47
24:B5:2620:G:H5''	24:B5:2621:G:H5'	1.96	0.47
53:Ae:49:LEU:HD12	88:Ap:50:LYS:HG2	1.95	0.47
63:A2:1607:G:N2	63:A2:1633:G:H1'	2.29	0.47
64:Ah:106:SER:HB3	64:Ah:171:LEU:HG	1.95	0.47
4:AT:30:N:OP1	63:A2:1525:G:O2'	2.30	0.47
5:Ar:3:LEU:HB3	33:Ay:50:PHE:HD2	1.79	0.47
15:Bs:48:ARG:HH11	39:Bt:123:ARG:HG2	1.80	0.47
16:BG:252:LYS:NZ	24:B5:3818:G:OP1	2.43	0.47
18:Av:16:ASN:ND2	63:A2:1095:C:O2	2.47	0.47
19:DB:495:TYR:HE2	19:DB:507:LYS:HE3	1.79	0.47
24:B5:40:G:N2	24:B5:4126:A:N7	2.62	0.47
24:B5:231:U:O2	42:BY:103:LYS:NZ	2.43	0.47
24:B5:3676:OMG:HN1	24:B5:3797:U:H3	1.60	0.47
24:B5:4440:G:OP1	24:B5:4440:G:N2	2.44	0.47
27:BW:102:LYS:HG2	27:BW:105:ARG:NH2	2.29	0.47
41:Ab:117:ARG:HH21	94:A2:1985:SPD:HN6	1.61	0.47
43:BB:90:VAL:HG13	43:BB:161:ARG:HB2	1.96	0.47
43:BB:291:TYR:HB3	43:BB:298:LEU:HD11	1.96	0.47
47:BC:221:PHE:HB3	47:BC:227:ILE:HG21	1.96	0.47
53:Ae:19:LEU:HD21	53:Ae:69:VAL:HG11	1.96	0.47
55:BE:97:LYS:HD2	55:BE:110:VAL:HG21	1.95	0.47
58:Bc:38:ILE:HD11	58:Bc:46:VAL:HG21	1.95	0.47
63:A2:599:G:O2'	63:A2:606:A:N1	2.45	0.47
63:A2:1172:G:O2'	63:A2:1188:G:O6	2.29	0.47
1:BP:5:SER:OG	1:BP:116:HIS:NE2	2.47	0.47
15:Bs:30:VAL:HG12	15:Bs:189:ILE:HA	1.97	0.47
19:DB:194:LEU:HB3	19:DB:536:ARG:CZ	2.45	0.47
24:B5:1639:A:OP1	50:Ba:47:LYS:NZ	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B5:1804:G:N2	24:B5:1807:A:OP2	2.38	0.47
24:B5:3668:A:OP1	94:B5:5244:SPD:N10	2.47	0.47
24:B5:4122:A:O2'	50:Ba:42:ARG:NH1	2.47	0.47
46:BZ:95:VAL:HG13	46:BZ:96:VAL:HG23	1.96	0.47
54:Bb:65:MET:HG2	54:Bb:68:ARG:HH22	1.79	0.47
57:Af:92:ARG:O	63:A2:454:C:O2'	2.24	0.47
6:Cu:82:SER:OG	6:Cu:87:THR:OG1	2.21	0.47
19:DB:198:GLN:HG3	19:DB:536:ARG:HH21	1.79	0.47
19:DB:326:PHE:CZ	19:DB:382:GLN:HB2	2.50	0.47
24:B5:3669:C:H1'	48:BN:125:SER:HB3	1.97	0.47
24:B5:4011:U:N3	51:B:17:GLN:O	2.48	0.47
39:Bt:53:TRP:HD1	39:Bt:56:LEU:HB2	1.79	0.47
55:BE:193:HIS:HB3	55:BE:196:PHE:HD2	1.78	0.47
56:DA:74:ILE:HD11	56:DA:111:LEU:HD22	1.97	0.47
64:Ah:130:THR:OG1	64:Ah:132:GLU:OE1	2.33	0.47
76:Al:79:VAL:HG11	76:Al:85:LEU:HB2	1.97	0.47
5:Ar:88:LYS:NZ	85:Ao:35:GLN:O	2.39	0.47
6:Cu:105:SER:O	20:Ct:97:ARG:NH2	2.27	0.47
19:DB:330:ARG:HA	19:DB:333:TYR:CD2	2.50	0.47
22:BV:87:SER:HB3	27:BW:19:ARG:HH21	1.80	0.47
24:B5:345:C:H2'	24:B5:346:G:C8	2.49	0.47
24:B5:1877:C:N3	97:B5:5696:HOH:O	2.35	0.47
24:B5:1922:A:H3'	24:B5:1926:C:H41	1.79	0.47
24:B5:2363:C:H2'	24:B5:2364:G:H8	1.79	0.47
24:B5:3422:U:O2'	24:B5:3549:A:N3	2.41	0.47
24:B5:3628:C:O2'	43:BB:268:ARG:NH2	2.47	0.47
32:AZ:184:ARG:HD3	32:AZ:191:ARG:HG2	1.96	0.47
46:BZ:87:VAL:HG12	46:BZ:89:ILE:HG13	1.96	0.47
63:A2:1143:G:N2	63:A2:1146:A:OP2	2.43	0.47
63:A2:1233:PSU:H2'	63:A2:1234:G:H8	1.80	0.47
9:Bp:69:TRP:NE1	38:BA:173:GLY:O	2.44	0.47
13:BR:92:LYS:NZ	24:B5:1528:G:OP1	2.48	0.47
15:Bs:103:LEU:HD12	15:Bs:106:LYS:HZ1	1.80	0.47
19:DB:661:LEU:HD23	19:DB:664:LEU:HD12	1.96	0.47
24:B5:1859:C:H3'	24:B5:1860:C:H5''	1.96	0.47
24:B5:3974:OMG:H5''	24:B5:3975:U:O4'	2.15	0.47
24:B5:4192:U:O2'	24:B5:4196:U:OP1	2.32	0.47
32:AZ:125:THR:HG22	32:AZ:175:TRP:HE1	1.79	0.47
41:Ab:113:GLN:OE1	63:A2:10:G:O2'	2.28	0.47
62:Bd:36:VAL:HG21	62:Bd:44:ARG:HD3	1.97	0.47
80:Bj:27:TYR:HA	80:Bj:34:CYS:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:DB:495:TYR:HB2	19:DB:504:ALA:HB2	1.96	0.47
19:DB:791:ASP:O	19:DB:797:ARG:NH1	2.47	0.47
23:Aw:67:ARG:HG3	23:Aw:115:ILE:HG12	1.97	0.47
24:B5:92:C:OP1	94:B5:4933:SPD:N10	2.47	0.47
24:B5:223:G:H4'	24:B5:225:G:N7	2.30	0.47
24:B5:1496:C:H5''	38:BA:21:LYS:HG2	1.97	0.47
24:B5:2007:C:OP1	68:Bf:15:LYS:NZ	2.48	0.47
24:B5:2365:G:OP2	71:Bg:29:ARG:NH2	2.46	0.47
25:BT:93:ILE:HA	25:BT:96:ILE:HG12	1.95	0.47
27:BW:102:LYS:HG2	27:BW:105:ARG:HH22	1.79	0.47
49:Ad:151:ASP:HB3	49:Ad:154:ILE:HG13	1.96	0.47
63:A2:960:G:OP1	82:An:104:ARG:NH1	2.48	0.47
1:BP:40:HIS:NE2	1:BP:110:ASP:O	2.40	0.47
6:Cu:89:THR:HG22	20:Ct:121:ILE:HG12	1.96	0.47
9:Bp:65:ALA:HB2	38:BA:48:ILE:HD13	1.96	0.47
19:DB:50:ALA:HA	19:DB:69:VAL:HG22	1.95	0.47
19:DB:134:ARG:NH2	19:DB:158:TYR:HA	2.29	0.47
19:DB:484:CYS:HB3	19:DB:487:PHE:HD2	1.79	0.47
24:B5:1225:G:H5'	47:BC:323:ARG:HB2	1.97	0.47
24:B5:2538:A:OP1	83:Bk:35:LYS:NZ	2.37	0.47
24:B5:4138:OMG:HM21	24:B5:4140:A:H2'	1.95	0.47
24:B5:4703:C:N4	24:B5:4704:U:O4	2.48	0.47
32:AZ:77:ILE:HD11	32:AZ:99:ILE:HD12	1.96	0.47
63:A2:614:G:N2	63:A2:627:G:OP1	2.47	0.47
63:A2:1018:U:H5'	79:Am:55:ARG:HE	1.79	0.47
15:Bs:137:PHE:HB3	15:Bs:174:LEU:HD11	1.97	0.47
19:DB:107:LEU:O	19:DB:111:LYS:HG3	2.15	0.47
33:Ay:36:SER:HB3	63:A2:1639:G:H4'	1.96	0.47
49:Ad:87:MET:HE1	49:Ad:236:ILE:HG21	1.97	0.47
52:BO:130:LYS:HB2	52:BO:133:ARG:HG2	1.96	0.47
63:A2:485:A2M:O5'	63:A2:485:A2M:H8	2.15	0.47
13:BR:106:LEU:HD13	13:BR:138:LEU:HD21	1.97	0.46
19:DB:765:ARG:CZ	19:DB:794:LEU:HD21	2.45	0.46
24:B5:684:C:OP2	55:BE:114:LYS:NZ	2.42	0.46
24:B5:1568:A:H5'	38:BA:183:GLY:HA2	1.97	0.46
24:B5:1596:G:N3	24:B5:3650:G:O2'	2.44	0.46
24:B5:2232:A:H5'	62:Bd:70:LYS:HE2	1.98	0.46
24:B5:2639:G:N3	97:B5:5716:HOH:O	2.36	0.46
24:B5:3843:G:H4'	24:B5:3844:C:H5'	1.96	0.46
24:B5:3952:C:O2'	24:B5:4081:C:O2'	2.31	0.46
31:BJ:81:GLU:OE2	31:BJ:85:LYS:NZ	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:BC:60:HIS:HA	47:BC:92:PHE:HE1	1.80	0.46
57:Af:164:LYS:HG2	57:Af:165:GLU:H	1.80	0.46
63:A2:98:C:OP2	63:A2:427:A:O2'	2.25	0.46
63:A2:630:A:O2'	63:A2:632:U:OP1	2.32	0.46
63:A2:679:U:OP2	63:A2:1027:C:N4	2.37	0.46
79:Am:130:LYS:NZ	79:Am:139:TRP:O	2.35	0.46
10:BQ:177:ALA:O	10:BQ:184:ARG:HB2	2.15	0.46
19:DB:146:ALA:HA	20:Ct:136:GLN:HE22	1.80	0.46
24:B5:1572:G:H1'	24:B5:2356:A:N6	2.30	0.46
24:B5:3983:C:OP1	24:B5:4073:C:O2'	2.32	0.46
29:B7:87:G:N2	29:B7:90:A:OP2	2.45	0.46
43:BB:220:ILE:HG12	43:BB:278:THR:HG23	1.97	0.46
19:DB:146:ALA:HA	20:Ct:136:GLN:NE2	2.31	0.46
24:B5:1412:G:N7	97:B5:5718:HOH:O	2.36	0.46
24:B5:2486:G:H1	24:B5:2534:U:H3	1.62	0.46
34:B8:38:U:O2'	74:Bh:86:LYS:NZ	2.41	0.46
47:BC:201:ARG:NH2	97:BC:503:HOH:O	2.49	0.46
63:A2:903:G:H2'	63:A2:904:A:H8	1.80	0.46
67:Ai:170:PRO:HB3	67:Ai:174:LYS:HE3	1.96	0.46
82:An:16:SER:OG	82:An:17:LEU:N	2.48	0.46
89:Bm:113:LYS:HG2	89:Bm:117:HIS:HE1	1.81	0.46
19:DB:195:TYR:HE2	19:DB:533:ILE:HG22	1.80	0.46
19:DB:525:PHE:O	19:DB:529:CYS:N	2.44	0.46
24:B5:3642:C:O2'	24:B5:3942:OMG:N2	2.38	0.46
31:BJ:90:ARG:NH2	31:BJ:108:GLY:O	2.49	0.46
32:AZ:77:ILE:HG21	32:AZ:133:PRO:HG3	1.97	0.46
50:Ba:14:HIS:ND1	97:Ba:401:HOH:O	2.36	0.46
63:A2:562:A:O2'	67:Ai:134:HIS:NE2	2.35	0.46
63:A2:602:OMG:HM22	63:A2:603:G:H5'	1.97	0.46
63:A2:1652:A:H2'	63:A2:1653:G:H8	1.80	0.46
65:Be:37:LYS:HD2	65:Be:38:PRO:HD2	1.95	0.46
13:BR:108:ARG:NH2	24:B5:2742:C:OP1	2.36	0.46
16:BG:162:ASP:O	24:B5:150:U:N3	2.42	0.46
19:DB:171:LEU:O	19:DB:196:GLN:NE2	2.48	0.46
19:DB:714:ARG:HG3	19:DB:771:MET:HE1	1.96	0.46
22:BV:21:PRO:HA	22:BV:54:ALA:HA	1.96	0.46
24:B5:85:G:O2'	24:B5:97:G:O6	2.24	0.46
24:B5:1005:G:OP1	25:BT:142:ARG:NH1	2.43	0.46
24:B5:1601:A:O2'	80:Bj:49:TRP:O	2.26	0.46
27:BW:84:GLY:HA2	57:Af:161:PRO:HD3	1.97	0.46
29:B7:47:G:H21	51:B:222:GLN:HE22	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Au:25:GLY:O	41:Ab:85:SER:OG	2.33	0.46
36:Aa:48:LEU:O	82:An:51:GLU:HG3	2.15	0.46
55:BE:134:LYS:O	55:BE:139:HIS:NE2	2.48	0.46
63:A2:371:G:O2'	64:Ah:10:LYS:NZ	2.49	0.46
14:At:36:ILE:HG12	14:At:114:VAL:HG21	1.96	0.46
19:DB:191:GLU:HB3	19:DB:195:TYR:OH	2.16	0.46
24:B5:106:A:O2'	24:B5:335:A:N3	2.42	0.46
24:B5:663:C:H2'	24:B5:664:G:H8	1.81	0.46
51:B:7:VAL:HG23	51:B:8:LYS:HG3	1.96	0.46
53:Ae:124:ASP:OD1	53:Ae:125:SER:N	2.44	0.46
63:A2:929:G:H1	63:A2:1014:U:H3	1.64	0.46
18:Av:101:PHE:HA	18:Av:113:HIS:CE1	2.51	0.46
19:DB:58:CYS:HA	19:DB:635:ILE:HG23	1.98	0.46
19:DB:435:GLN:NE2	19:DB:445:ASN:HA	2.30	0.46
34:B8:84:A:O4'	74:Bh:3:LYS:NZ	2.49	0.46
39:Bt:20:GLY:H	39:Bt:55:GLY:N	2.14	0.46
46:BZ:41:ALA:HB2	46:BZ:77:TYR:HE1	1.81	0.46
60:DC:122:TYR:HB3	60:DC:128:PHE:HB2	1.97	0.46
81:AF:87:LEU:HD21	81:AF:108:VAL:HG11	1.97	0.46
82:An:45:THR:HG22	82:An:52:THR:HG22	1.98	0.46
21:BH:118:LEU:HD11	21:BH:167:VAL:HG22	1.98	0.46
24:B5:512:U:OP2	50:Ba:85:GLN:NE2	2.42	0.46
24:B5:1463:A:OP1	47:BC:110:ARG:NH1	2.39	0.46
24:B5:3452:G:H22	24:B5:3465:A:H2	1.64	0.46
28:Ax:34:THR:O	63:A2:571:C:O2'	2.30	0.46
30:Au:45:ARG:HE	32:AZ:187:GLY:HA2	1.80	0.46
47:BC:329:ASN:ND2	59:BF:187:GLU:OE2	2.49	0.46
57:Af:92:ARG:NH1	63:A2:1739:C:OP1	2.40	0.46
57:Af:192:ILE:HG22	57:Af:196:LYS:HE2	1.97	0.46
6:Cu:28:ARG:NH2	13:BR:25:ASP:OD2	2.41	0.46
24:B5:1687:U:O2'	26:BI:35:ASP:OD1	2.34	0.46
24:B5:1897:A:O2'	24:B5:1964:A:N1	2.47	0.46
24:B5:4627:C:H2'	24:B5:4628:G:H8	1.81	0.46
28:Ax:21:LYS:HB2	28:Ax:75:ILE:HB	1.98	0.46
47:BC:316:LYS:HB2	47:BC:324:ILE:HG13	1.98	0.46
55:BE:156:LEU:HD11	55:BE:198:ILE:HG13	1.98	0.46
64:Ah:57:ALA:HB2	64:Ah:183:GLY:HA2	1.98	0.46
1:BP:131:ARG:HG3	1:BP:137:ASN:ND2	2.31	0.46
10:BQ:178:ARG:H	50:Ba:51:GLY:HA2	1.80	0.46
33:Ay:102:LYS:HD2	33:Ay:107:VAL:HG12	1.97	0.46
43:BB:168:MET:HE1	43:BB:173:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:A2:925:G:H5'	79:Am:4:MET:HE3	1.97	0.46
73:Ak:24:LEU:HD23	73:Ak:24:LEU:H	1.80	0.46
10:BQ:122:THR:OG1	10:BQ:124:ASP:OD1	2.17	0.45
19:DB:21:TYR:CZ	19:DB:55:THR:HG23	2.51	0.45
24:B5:1672:G:N3	24:B5:3960:A:H2'	2.31	0.45
24:B5:1838:G:O2'	65:Be:57:ASN:OD1	2.28	0.45
24:B5:2146:C:OP1	65:Be:107:ASN:ND2	2.44	0.45
24:B5:4086:U:O2	94:B5:4933:SPD:N10	2.49	0.45
25:BT:22:HIS:O	51:B:17:GLN:NE2	2.46	0.45
25:BT:94:GLU:OE1	25:BT:94:GLU:N	2.46	0.45
34:B8:65:A:O2'	74:Bh:10:ARG:NH2	2.48	0.45
56:DA:16:ILE:HG13	56:DA:20:LYS:HE3	1.98	0.45
64:Ah:89:GLU:OE1	64:Ah:92:ARG:NH2	2.49	0.45
71:Bg:60:ARG:HB2	71:Bg:63:VAL:HG23	1.97	0.45
19:DB:158:TYR:HB3	19:DB:167:ALA:HB2	1.98	0.45
22:BV:48:ARG:HD2	24:B5:4367:C:OP1	2.17	0.45
22:BV:85:ARG:NH1	22:BV:99:GLU:O	2.44	0.45
24:B5:632:G:H5''	24:B5:633:U:H5'	1.98	0.45
24:B5:772:C:H2'	24:B5:773:G:H8	1.81	0.45
24:B5:2678:A:O2'	43:BB:228:TYR:O	2.34	0.45
24:B5:3524:OMG:HM22	24:B5:3525:U:H5'	1.98	0.45
26:BI:99:ILE:HG22	26:BI:123:GLN:HB2	1.99	0.45
41:Ab:131:GLY:HA3	41:Ab:216:MET:HB3	1.97	0.45
47:BC:60:HIS:NE2	47:BC:100:ARG:HD3	2.31	0.45
63:A2:1062:U:H1'	94:A2:1964:SPD:H41	1.98	0.45
1:BP:50:ASP:OD2	1:BP:56:GLN:NE2	2.49	0.45
24:B5:3548:A:OP1	24:B5:3550:UY1:N1	2.50	0.45
24:B5:4283:C:H2'	24:B5:4284:G:C8	2.52	0.45
24:B5:4333:G:N2	43:BB:15:GLY:O	2.36	0.45
43:BB:19:ARG:HB2	43:BB:234:ARG:NH2	2.31	0.45
49:Ad:12:VAL:O	63:A2:813:A:O2'	2.31	0.45
63:A2:98:C:H2'	63:A2:427:A:H4'	1.98	0.45
63:A2:1311:U:H5''	72:AC:130:VAL:HG13	1.97	0.45
63:A2:1767:C:H4'	63:A2:1768:C:H5	1.81	0.45
7:BL:163:LYS:NZ	24:B5:512:U:O5'	2.48	0.45
10:BQ:87:THR:HG21	24:B5:1458:A:H62	1.82	0.45
19:DB:424:ILE:HG22	19:DB:455:ALA:HB2	1.99	0.45
21:BH:60:TRP:O	24:B5:4511:A:N6	2.37	0.45
24:B5:22:G:OP1	80:Bj:44:LYS:N	2.38	0.45
24:B5:66:A:O2'	24:B5:326:C:O2	2.28	0.45
24:B5:197:A:N3	24:B5:222:C:O2'	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B5:308:G:O6	48:BN:12:ARG:NH1	2.49	0.45
24:B5:385:A:H4'	24:B5:386:A:H5'	1.97	0.45
24:B5:1943:U:H2'	24:B5:1944:G:C8	2.51	0.45
24:B5:2318:G:H4'	24:B5:2319:G:H8	1.81	0.45
24:B5:3432:C:H2'	24:B5:3478:A:H61	1.82	0.45
45:Ac:64:ARG:HD2	70:Aj:94:LEU:HD21	1.99	0.45
46:BZ:12:LEU:HB2	46:BZ:81:MET:HB3	1.98	0.45
46:BZ:36:ARG:NH1	46:BZ:38:TYR:OH	2.42	0.45
55:BE:164:ARG:O	55:BE:185:ASN:ND2	2.48	0.45
63:A2:159:A2M:H8	63:A2:159:A2M:O5'	2.17	0.45
63:A2:1233:PSU:H2'	63:A2:1234:G:C8	2.52	0.45
15:Bs:10:LYS:HD2	15:Bs:63:LYS:NZ	2.32	0.45
15:Bs:82:ILE:HG23	15:Bs:86:VAL:HG21	1.99	0.45
19:DB:541:LEU:HD23	19:DB:544:LEU:HD12	1.97	0.45
47:BC:25:PRO:HB2	47:BC:27:VAL:HG12	1.98	0.45
53:Ae:74:ASN:HA	53:Ae:77:MET:HE2	1.98	0.45
59:BF:226:PHE:N	59:BF:232:ALA:O	2.49	0.45
1:BP:75:GLN:NE2	24:B5:4708:C:O2'	2.50	0.45
19:DB:773:TYR:CE1	19:DB:780:GLN:HA	2.48	0.45
20:Ct:98:LYS:HB2	20:Ct:102:ILE:HB	1.98	0.45
24:B5:151:G:OP2	48:BN:4:TYR:OH	2.23	0.45
24:B5:410:A:O2'	24:B5:414:C:O2'	2.31	0.45
24:B5:1493:U:H2'	24:B5:1494:G:H8	1.81	0.45
24:B5:3450:A2M:H8	24:B5:3450:A2M:O5'	2.17	0.45
24:B5:4323:U:H2'	24:B5:4324:G:H8	1.82	0.45
29:B7:74:A:N1	29:B7:100:A:H5''	2.31	0.45
31:BJ:40:LEU:HD12	31:BJ:70:VAL:HG22	1.99	0.45
38:BA:30:ARG:HG3	38:BA:76:PHE:HZ	1.82	0.45
46:BZ:48:ARG:HB3	46:BZ:69:LYS:HB3	1.98	0.45
81:AF:64:HIS:HB3	81:AF:83:TRP:HB2	1.98	0.45
82:An:46:ASP:N	82:An:46:ASP:OD1	2.48	0.45
15:Bs:193:PHE:HD1	15:Bs:198:ILE:HD11	1.82	0.45
19:DB:201:ARG:NH2	19:DB:229:THR:HB	2.31	0.45
19:DB:375:TRP:O	19:DB:379:TYR:HD1	2.00	0.45
24:B5:2322:G:H2'	24:B5:2323:G:H8	1.82	0.45
24:B5:3834:G:H1'	24:B5:3835:G:C8	2.52	0.45
36:Aa:30:TRP:CE2	36:Aa:48:LEU:HD13	2.52	0.45
60:DC:160:ARG:O	60:DC:164:LEU:HG	2.17	0.45
78:AE:22:ARG:NH2	82:An:145:GLY:O	2.49	0.45
15:Bs:25:PRO:HB2	15:Bs:195:ASN:HD21	1.82	0.45
24:B5:1811:G:O2'	24:B5:3965:A:N3	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B5:1915:G:N2	39:Bt:138:SER:O	2.46	0.45
24:B5:2247:A:H1'	80:Bj:12:ARG:HH11	1.82	0.45
24:B5:2635:C:O2'	80:Bj:8:PHE:O	2.32	0.45
24:B5:4620:U:C4	40:BM:113:MET:HG3	2.52	0.45
94:B5:5405:SPD:N6	48:BN:70:GLY:O	2.45	0.45
26:BI:61:SER:HA	26:BI:126:VAL:HG12	1.99	0.45
36:Aa:71:LEU:HD11	36:Aa:189:ILE:HG23	1.98	0.45
39:Bt:95:GLN:HG3	39:Bt:98:ILE:HG12	1.97	0.45
45:Ac:176:LEU:HD13	63:A2:1500:U:H4'	1.99	0.45
61:Ag:116:ARG:NH2	63:A2:688:C:O3'	2.50	0.45
63:A2:42:A:O2'	63:A2:98:C:OP1	2.32	0.45
63:A2:397:U:OP2	73:Ak:79:LYS:NZ	2.45	0.45
65:Be:104:SER:O	65:Be:108:ARG:HG3	2.16	0.45
81:AF:91:ASP:OD2	81:AF:93:THR:OG1	2.34	0.45
88:Ap:89:SER:HB3	88:Ap:112:LEU:HD13	1.99	0.45
2:Aq:109:LEU:HD13	32:AZ:52:LYS:HB2	1.98	0.45
5:Ar:125:HIS:CD2	5:Ar:131:VAL:HG11	2.52	0.45
19:DB:134:ARG:HH21	19:DB:158:TYR:HA	1.81	0.45
19:DB:192:LEU:HG	19:DB:533:ILE:HG21	1.99	0.45
19:DB:226:VAL:HG12	19:DB:230:LYS:HE2	1.99	0.45
19:DB:569:HIS:CE1	19:DB:654:LEU:HG	2.52	0.45
19:DB:771:MET:HA	19:DB:774:TYR:HD2	1.82	0.45
21:BH:41:ILE:HG22	21:BH:43:VAL:HG13	1.97	0.45
21:BH:59:LYS:HE2	21:BH:66:GLU:HB3	1.98	0.45
24:B5:407:A:N3	97:B5:5709:HOH:O	2.35	0.45
24:B5:4331:U:H2'	24:B5:4332:G:C8	2.52	0.45
40:BM:86:TRP:O	40:BM:89:THR:OG1	2.32	0.45
52:BO:61:ARG:HA	52:BO:70:PRO:HD2	1.98	0.45
63:A2:589:G:OP2	63:A2:589:G:N2	2.39	0.45
67:AI:83:ARG:HH21	67:AI:150:ARG:NH1	2.14	0.45
2:Aq:129:LYS:NZ	63:A2:1101:A:OP1	2.41	0.45
24:B5:1270:A2M:HM'2	24:B5:1271:C:H5'	1.99	0.45
39:Bt:80:LEU:HD13	39:Bt:112:ILE:HG23	1.99	0.45
48:BN:143:ARG:NH1	74:Bh:95:LEU:HD23	2.32	0.45
52:BO:10:ASP:OD2	52:BO:37:ARG:NH2	2.37	0.45
63:A2:1659:G:OP2	63:A2:1661:C:N4	2.50	0.45
81:AF:59:LEU:HD23	81:AF:90:TRP:CE3	2.52	0.45
88:Ap:131:LYS:HB2	88:Ap:140:ARG:HH12	1.81	0.45
2:Aq:83:ASN:OD1	32:AZ:89:LYS:NZ	2.49	0.44
19:DB:80:HIS:CE1	19:DB:110:ASP:HB2	2.52	0.44
24:B5:407:A:O2'	24:B5:410:A:OP1	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B5:1072:C:H1'	24:B5:1074:C:C2	2.51	0.44
24:B5:2250:G:O6	86:Bl:2:SER:N	2.50	0.44
24:B5:3476:OMG:HM22	24:B5:3477:U:H5'	1.99	0.44
24:B5:4052:OMU:HM22	24:B5:4053:A:H5'	1.98	0.44
24:B5:4057:A:H2'	24:B5:4058:PSU:H6	1.82	0.44
39:Bt:147:HIS:CD2	39:Bt:149:HIS:HB2	2.50	0.44
47:BC:76:ILE:HD12	47:BC:77:PRO:HD2	1.99	0.44
47:BC:278:ASN:OD1	47:BC:279:LEU:N	2.49	0.44
63:A2:99:A2M:H8	63:A2:99:A2M:O5'	2.16	0.44
63:A2:1524:C:H2'	63:A2:1525:G:H8	1.82	0.44
63:A2:1763:C:H2'	63:A2:1764:G:H8	1.81	0.44
63:A2:1776:U:H2'	63:A2:1777:G:H8	1.82	0.44
63:A2:1863:G:N2	78:AE:76:SER:OG	2.47	0.44
72:AC:133:ALA:N	72:AC:140:TYR:O	2.31	0.44
76:Al:31:LEU:HD11	76:Al:109:VAL:HB	2.00	0.44
83:Bk:13:LEU:HD23	83:Bk:16:ARG:HH21	1.81	0.44
1:BP:125:MET:HE1	24:B5:2261:A:H5''	2.00	0.44
21:BH:120:GLU:OE1	21:BH:124:ARG:NH2	2.45	0.44
24:B5:842:G:H3'	59:BF:147:LYS:HD2	1.98	0.44
26:Bl:91:LEU:HD12	26:Bl:135:ILE:HG23	1.99	0.44
43:BB:161:ARG:HG2	43:BB:184:GLN:HA	1.99	0.44
55:BE:45:HIS:ND1	55:BE:46:CYS:O	2.50	0.44
63:A2:657:G:H5'	63:A2:663:G:N2	2.32	0.44
63:A2:1758:G:H1	63:A2:1776:U:H3	1.65	0.44
16:BG:73:ARG:HH12	24:B5:3908:C:H5	1.65	0.44
24:B5:48:G:OP1	48:BN:192:TRP:NE1	2.39	0.44
24:B5:345:C:H2'	24:B5:346:G:H8	1.83	0.44
24:B5:484:G:H3'	24:B5:485:U:H2'	1.98	0.44
24:B5:1726:A:O5'	94:B5:5144:SPD:N1	2.51	0.44
24:B5:1736:G:OP1	59:BF:103:LYS:NZ	2.49	0.44
24:B5:2612:U:C2	71:Bg:69:LYS:HB2	2.52	0.44
24:B5:4508:G:OP2	52:BO:37:ARG:NH1	2.44	0.44
32:AZ:76:VAL:HG12	32:AZ:123:VAL:HB	1.99	0.44
43:BB:56:ILE:HG22	43:BB:368:ILE:HA	1.99	0.44
43:BB:231:VAL:HG21	43:BB:251:VAL:HG23	1.99	0.44
51:B:119:TYR:OH	51:B:139:PRO:O	2.33	0.44
57:Af:121:ILE:HG22	57:Af:123:GLY:H	1.82	0.44
63:A2:120:U:H2'	63:A2:121:OMU:H6	1.99	0.44
63:A2:518:OMC:HM22	63:A2:519:G:H5'	1.99	0.44
63:A2:1833:6MZ:H8	63:A2:1833:6MZ:O5'	2.18	0.44
64:Ah:81:VAL:HG22	64:Ah:102:VAL:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ar:132:ARG:HB2	5:Ar:134:GLN:HE22	1.82	0.44
6:Cu:62:VAL:HB	6:Cu:74:PHE:HB2	1.99	0.44
19:DB:79:SER:OG	19:DB:82:CYS:SG	2.55	0.44
23:Aw:123:VAL:HG12	23:Aw:124:LYS:HG3	1.99	0.44
24:B5:3340:A:N7	97:B5:5727:HOH:O	2.36	0.44
36:Aa:56:LYS:NZ	63:A2:953:G:OP1	2.50	0.44
42:BY:30:MET:HB3	42:BY:101:PRO:HG2	2.00	0.44
45:Ac:160:SER:OG	63:A2:1387:A:OP2	2.26	0.44
63:A2:1649:G:C5	88:Ap:17:LYS:HE2	2.52	0.44
77:Bi:73:ILE:O	77:Bi:77:VAL:HG22	2.18	0.44
86:Bl:23:ILE:HG23	86:Bl:38:ASN:HB2	1.98	0.44
15:Bs:10:LYS:HD2	15:Bs:63:LYS:HZ1	1.83	0.44
15:Bs:125:ALA:HA	15:Bs:154:ILE:HB	1.98	0.44
20:Ct:210:ILE:O	20:Ct:214:THR:HG23	2.17	0.44
24:B5:2131:G:O2'	24:B5:2133:C:O5'	2.36	0.44
24:B5:2363:C:H2'	24:B5:2364:G:C8	2.53	0.44
24:B5:3477:U:HO2'	38:BA:243:THR:H	1.60	0.44
35:BK:38:UNK:O	35:BK:39:UNK:C	2.66	0.44
63:A2:26:U:H2'	63:A2:27:A2M:H8	1.99	0.44
63:A2:1222:G:H2'	63:A2:1223:G:C8	2.53	0.44
81:AF:254:PRO:HA	81:AF:285:GLN:HA	1.98	0.44
82:An:136:PRO:HB2	82:An:139:SER:HB2	1.98	0.44
7:BL:81:LEU:HD12	7:BL:86:ILE:HB	2.00	0.44
18:Av:86:LEU:HG	18:Av:90:GLN:HE21	1.82	0.44
21:BH:41:ILE:HD13	21:BH:69:THR:HB	2.00	0.44
24:B5:67:C:OP2	24:B5:312:G:N2	2.50	0.44
24:B5:772:C:H2'	24:B5:773:G:C8	2.52	0.44
24:B5:1001:C:H2'	24:B5:1002:A:H8	1.82	0.44
24:B5:2293:G:OP1	38:BA:17:ARG:NH1	2.50	0.44
24:B5:4261:G:H5''	43:BB:3:HIS:CE1	2.53	0.44
43:BB:44:THR:HG21	43:BB:186:ASN:ND2	2.32	0.44
48:BN:42:PRO:HG3	48:BN:61:ILE:HG13	1.99	0.44
56:DA:108:ASN:ND2	56:DA:151:GLN:HE21	2.15	0.44
57:Af:67:VAL:HG12	57:Af:69:THR:HG22	2.00	0.44
59:BF:136:GLU:HG3	59:BF:233:GLY:HA2	2.00	0.44
61:Ag:7:LYS:NZ	61:Ag:40:LEU:O	2.51	0.44
61:Ag:100:ILE:HG12	61:Ag:125:VAL:HG21	1.99	0.44
63:A2:1256:G:OP1	63:A2:1257:G:O2'	2.29	0.44
6:Cu:91:THR:HG22	20:Ct:119:THR:HG22	2.00	0.44
24:B5:1276:C:H2'	24:B5:1277:A:C8	2.52	0.44
24:B5:1391:C:H4'	24:B5:1393:C:H5'	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B5:1919:U:O4	39:Bt:57:ARG:NH2	2.48	0.44
33:Ay:92:LEU:HD22	33:Ay:109:TYR:HE1	1.82	0.44
34:B8:36:G:C5	74:Bh:89:ARG:HD3	2.52	0.44
59:BF:181:TYR:CZ	59:BF:202:GLU:HG2	2.52	0.44
67:Ai:127:ARG:HD3	75:AD:105:ARG:HD3	2.00	0.44
14:At:42:SER:HB3	14:At:48:LEU:HB2	1.99	0.44
18:Av:68:ARG:HD2	41:Ab:256:TRP:CG	2.53	0.44
19:DB:151:TRP:HZ2	20:Ct:136:GLN:HG2	1.83	0.44
24:B5:2400:G:H1	24:B5:2413:U:H3	1.65	0.44
24:B5:2621:G:N2	34:B8:113:C:OP2	2.50	0.44
61:Ag:43:LEU:HB3	61:Ag:72:PHE:CE1	2.51	0.44
63:A2:984:A:OP1	63:A2:1074:U:O2'	2.29	0.44
63:A2:1118:C:O2'	63:A2:1119:C:O4'	2.36	0.44
63:A2:1320:U:H2'	63:A2:1321:G:C8	2.53	0.44
63:A2:1760:G:H2'	63:A2:1761:G:H8	1.83	0.44
12:Br:33:LYS:HA	65:Be:90:MET:HG3	1.99	0.44
15:Bs:68:HIS:HB3	15:Bs:75:LEU:HD22	1.99	0.44
19:DB:441:ASP:HB3	19:DB:443:PHE:HD1	1.83	0.44
19:DB:482:MET:HE2	60:DC:25:ASN:HB2	2.00	0.44
20:Ct:211:MET:O	20:Ct:214:THR:OG1	2.35	0.44
24:B5:1620:C:O2'	95:B5:5018:SPM:N1	2.51	0.44
24:B5:1621:C:O2'	24:B5:1643:G:OP1	2.31	0.44
24:B5:1946:G:H21	24:B5:1951:A:H62	1.64	0.44
24:B5:2216:C:H5'	62:Bd:46:LEU:HD22	2.00	0.44
24:B5:2654:G:N2	24:B5:2657:C:OP2	2.44	0.44
24:B5:2687:A:O2'	24:B5:4377:G:H4'	2.17	0.44
26:BI:9:TYR:O	26:BI:59:GLN:NE2	2.51	0.44
34:B8:93:C:OP1	80:Bj:76:HIS:NE2	2.40	0.44
63:A2:57:U:O2'	63:A2:500:G:N3	2.51	0.44
63:A2:1690:C:OP1	94:A2:1985:SPD:N1	2.51	0.44
70:Aj:63:ALA:HB3	70:Aj:68:TYR:HE2	1.82	0.44
78:AE:45:VAL:HB	78:AE:64:LEU:HD13	2.00	0.44
81:AF:87:LEU:HD11	81:AF:122:SER:HB3	2.00	0.44
19:DB:408:ILE:HD13	19:DB:444:ILE:HD11	1.99	0.43
19:DB:417:ILE:O	19:DB:421:ALA:N	2.48	0.43
24:B5:385:A:H1'	24:B5:387:G:H5''	1.98	0.43
24:B5:1567:G:OP1	97:B5:5530:HOH:O	2.21	0.43
24:B5:2256:U:H2'	24:B5:2257:G:C8	2.53	0.43
38:BA:83:HIS:CE1	38:BA:86:GLN:HB2	2.53	0.43
39:Bt:101:SER:HA	39:Bt:141:CYS:HA	2.00	0.43
49:Ad:55:ALA:HB1	49:Ad:60:GLU:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Ad:104:ASP:OD1	49:Ad:108:ARG:N	2.36	0.43
57:Af:176:ILE:HG22	63:A2:77:A:N3	2.32	0.43
63:A2:381:G:N1	63:A2:384:G:OP2	2.42	0.43
63:A2:1388:G:P	97:A2:2130:HOH:O	2.75	0.43
66:AA:23:ARG:HH22	66:AA:29:ASN:ND2	2.13	0.43
6:Cu:85:ALA:HB2	20:Ct:72:SER:HB2	1.99	0.43
18:Av:80:ASP:OD1	18:Av:124:LYS:NZ	2.49	0.43
21:BH:48:LEU:HD11	21:BH:56:ARG:HH11	1.83	0.43
24:B5:417:G:H1'	34:B8:16:G:N2	2.32	0.43
24:B5:1924:G:H21	24:B5:1924:G:P	2.41	0.43
25:BT:93:ILE:H	25:BT:93:ILE:HG13	1.67	0.43
43:BB:82:PRO:HG3	43:BB:171:LEU:HD21	2.00	0.43
53:Ae:131:ALA:HB2	53:Ae:135:ARG:HH21	1.83	0.43
63:A2:1408:U:O2'	88:Ap:11:GLN:NE2	2.46	0.43
76:Al:37:GLU:HA	76:Al:40:LYS:HD2	2.00	0.43
80:Bj:22:CYS:SG	80:Bj:24:SER:OG	2.75	0.43
1:BP:18:ARG:HA	1:BP:147:GLU:HA	2.00	0.43
2:Aq:109:LEU:HG	2:Aq:111:PHE:HD2	1.82	0.43
10:BQ:14:ARG:NH2	24:B5:2022:C:OP2	2.50	0.43
15:Bs:175:LEU:HD13	15:Bs:182:PRO:HG2	1.98	0.43
16:BG:99:ALA:HB1	16:BG:136:LEU:HD11	2.01	0.43
19:DB:301:LEU:HD23	19:DB:301:LEU:HA	1.84	0.43
19:DB:695:VAL:HG11	19:DB:712:MET:SD	2.57	0.43
23:Aw:90:CYS:HA	23:Aw:93:PHE:HD2	1.84	0.43
24:B5:492:G:H4'	47:BC:3:CYS:HB3	2.00	0.43
24:B5:1249:C:OP1	34:B8:7:U:O2'	2.36	0.43
24:B5:2183:C:H4'	47:BC:42:THR:HG23	2.01	0.43
24:B5:3380:A:H1'	24:B5:3517:A2M:N6	2.34	0.43
48:BN:9:GLU:HB2	77:Bi:44:ILE:HG13	2.00	0.43
55:BE:182:LEU:HD12	55:BE:186:ARG:HA	1.98	0.43
60:DC:158:LEU:HA	60:DC:161:HIS:HD2	1.80	0.43
63:A2:1754:C:O2	63:A2:1781:G:N2	2.51	0.43
63:A2:1857:C:H2'	63:A2:1858:G:C8	2.53	0.43
79:Am:93:LYS:HA	79:Am:150:VAL:HG21	2.00	0.43
86:Bl:20:ASN:ND2	86:Bl:42:ARG:O	2.51	0.43
8:BX:51:THR:O	24:B5:2318:G:N2	2.34	0.43
20:Ct:71:ARG:HD3	20:Ct:71:ARG:HA	1.82	0.43
24:B5:697:G:N2	24:B5:698:C:O2	2.51	0.43
24:B5:1271:C:H2'	24:B5:1272:G:C8	2.52	0.43
24:B5:4140:A:N6	97:B5:5679:HOH:O	2.33	0.43
24:B5:4331:U:H2'	24:B5:4332:G:H8	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:AZ:108:PHE:HB2	32:AZ:136:GLU:HG2	2.00	0.43
40:BM:101:LYS:HA	40:BM:104:MET:HG3	2.01	0.43
41:Ab:65:LYS:HE3	41:Ab:273:LEU:HD13	2.00	0.43
53:Ae:71:ARG:NH2	53:Ae:148:ASN:OD1	2.52	0.43
55:BE:103:LYS:HE2	55:BE:103:LYS:HB2	1.84	0.43
2:Aq:82:ASP:O	32:AZ:85:ARG:NH2	2.41	0.43
6:Cu:64:MET:HB2	6:Cu:72:ILE:HB	2.01	0.43
10:BQ:8:ASN:O	95:B5:5018:SPM:N5	2.52	0.43
19:DB:137:ARG:HH11	19:DB:157:ALA:HB2	1.83	0.43
22:BV:48:ARG:NH1	24:B5:4367:C:OP1	2.50	0.43
24:B5:2649:A:O2'	94:B5:5082:SPD:N1	2.52	0.43
24:B5:4004:C:H5'	31:BJ:68:ILE:HD11	2.00	0.43
24:B5:4026:A:N6	51:B:28:THR:O	2.45	0.43
24:B5:4488:A:H2'	24:B5:4689:U:H3	1.84	0.43
36:Aa:30:TRP:CE2	82:An:19:PRO:HD3	2.52	0.43
45:Ac:18:LYS:HE2	45:Ac:39:VAL:HB	2.01	0.43
60:DC:18:ASN:HD21	60:DC:26:PHE:H	1.67	0.43
63:A2:678:G:H21	63:A2:1029:A:H62	1.64	0.43
63:A2:1837:G:OP1	63:A2:1840:U:H4'	2.19	0.43
65:Be:35:TRP:CZ2	65:Be:56:PRO:HD2	2.53	0.43
76:Al:49:LEU:HD11	76:Al:77:ILE:HD13	1.99	0.43
7:BL:116:ARG:NH2	7:BL:155:MET:O	2.44	0.43
19:DB:191:GLU:HB3	19:DB:195:TYR:CZ	2.53	0.43
19:DB:280:TYR:O	19:DB:284:TRP:HD1	2.02	0.43
19:DB:625:LYS:O	19:DB:629:ASP:HB2	2.19	0.43
24:B5:2362:U:H1'	24:B5:2363:C:C6	2.54	0.43
24:B5:2549:G:C6	24:B5:2551:U:H5''	2.54	0.43
24:B5:2658:A2M:P	24:B5:2658:A2M:H8	2.59	0.43
24:B5:3631:OMG:HM22	24:B5:3632:G:H5'	2.01	0.43
24:B5:3894:C:OP1	46:BZ:59:LYS:NZ	2.34	0.43
24:B5:4324:G:H2'	24:B5:4325:PSU:H6	1.84	0.43
24:B5:4335:A:N1	24:B5:4367:C:O2'	2.51	0.43
39:Bt:82:ILE:HA	39:Bt:85:LEU:HD12	2.00	0.43
43:BB:93:VAL:HG23	43:BB:102:PHE:HB2	2.00	0.43
47:BC:65:GLU:HB3	47:BC:80:ARG:HD3	2.00	0.43
53:Ae:30:ILE:HG23	53:Ae:117:ILE:HD11	2.00	0.43
56:DA:12:THR:HG22	56:DA:14:HIS:H	1.83	0.43
70:Aj:16:PHE:HE2	70:Aj:89:ILE:HG22	1.83	0.43
9:Bp:58:GLY:O	24:B5:2495:G:N1	2.40	0.43
19:DB:258:TRP:CZ3	19:DB:296:LEU:HG	2.54	0.43
24:B5:3403:G:OP1	48:BN:72:LYS:NZ	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B5:3640:A:N7	24:B5:4195:A:N6	2.67	0.43
24:B5:4314:A:O2'	24:B5:4720:G:N7	2.52	0.43
28:Ax:80:ASP:OD1	28:Ax:81:TYR:N	2.52	0.43
32:AZ:66:VAL:HG21	32:AZ:185:MET:HB2	1.99	0.43
43:BB:19:ARG:HB2	43:BB:234:ARG:HH21	1.83	0.43
55:BE:172:SER:OG	55:BE:217:ASP:OD2	2.31	0.43
59:BF:53:ALA:HB2	59:BF:187:GLU:HG3	2.01	0.43
63:A2:35:C:H5''	63:A2:580:C:H5''	2.01	0.43
63:A2:894:U:H2'	63:A2:895:G:H8	1.84	0.43
63:A2:1278:C:H2'	63:A2:1279:A:H8	1.83	0.43
75:AD:113:ASN:HA	75:AD:117:VAL:HB	2.01	0.43
88:Ap:49:TYR:O	88:Ap:53:GLU:HG3	2.19	0.43
11:As:104:LEU:HD13	11:As:121:ARG:HD3	2.01	0.43
14:At:40:LEU:HD11	14:At:55:LEU:HD12	2.01	0.43
17:BU:61:VAL:HG22	17:BU:74:SER:HB2	2.00	0.43
19:DB:713:ILE:HB	19:DB:771:MET:HE2	2.00	0.43
20:Ct:71:ARG:HH12	24:B5:393:U:H3'	1.84	0.43
20:Ct:113:LYS:HE2	20:Ct:120:TYR:CE2	2.54	0.43
24:B5:1215:G:H5''	54:Bb:110:ALA:HB1	2.00	0.43
38:BA:3:ARG:HG2	38:BA:207:VAL:HG22	2.00	0.43
41:Ab:94:ILE:HG21	41:Ab:162:ILE:HD12	2.00	0.43
41:Ab:168:GLY:N	41:Ab:179:THR:O	2.38	0.43
51:B:59:ASP:OD1	51:B:60:ILE:N	2.52	0.43
53:Ae:58:ALA:HB3	53:Ae:62:ARG:HH21	1.84	0.43
64:Ah:36:THR:OG1	64:Ah:57:ALA:O	2.29	0.43
72:AC:118:ARG:NH1	72:AC:134:SER:OG	2.52	0.43
88:Ap:117:ARG:HE	88:Ap:121:VAL:HG21	1.84	0.43
8:BX:100:VAL:HG21	8:BX:109:ILE:HD11	2.00	0.43
16:BG:89:ARG:NH2	34:B8:155:C:OP1	2.52	0.43
18:Av:68:ARG:HD2	41:Ab:256:TRP:CD2	2.54	0.43
23:Aw:17:ARG:NH2	63:A2:660:G:H21	2.17	0.43
24:B5:68:U:OP1	48:BN:178:HIS:ND1	2.38	0.43
24:B5:4715:U:H1'	43:BB:343:ARG:HH12	1.84	0.43
36:Aa:146:ARG:HH22	63:A2:1113:U:H1'	1.84	0.43
38:BA:30:ARG:HG2	38:BA:74:GLU:HG3	2.00	0.43
39:Bt:52:ASP:OD1	39:Bt:52:ASP:N	2.41	0.43
49:Ad:86:PHE:CD2	49:Ad:87:MET:HG2	2.54	0.43
53:Ae:63:LYS:HD2	53:Ae:71:ARG:HH12	1.83	0.43
79:Am:100:LYS:O	79:Am:103:GLU:HG2	2.19	0.43
5:Ar:28:PHE:O	5:Ar:31:THR:OG1	2.27	0.43
19:DB:21:TYR:CE2	19:DB:55:THR:HG23	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:DB:301:LEU:HB3	19:DB:306:PHE:CE1	2.54	0.43
24:B5:2358:G:OP1	71:Bg:37:LYS:NZ	2.34	0.43
24:B5:3351:G:H22	24:B5:3356:A:H1'	1.83	0.43
51:B:60:ILE:HB	51:B:80:ALA:HB2	1.99	0.43
57:Af:132:ARG:HD2	63:A2:152:U:H1'	2.00	0.43
63:A2:1590:A:N3	63:A2:1654:U:O2'	2.48	0.43
67:Ai:152:ASP:OD1	67:Ai:152:ASP:N	2.50	0.43
69:AB:10:LYS:NZ	69:AB:36:ASP:OD2	2.46	0.43
88:Ap:19:ALA:HB2	88:Ap:75:GLY:HA3	2.01	0.43
2:Aq:81:ARG:HD3	32:AZ:210:ILE:HG21	2.00	0.42
3:Bo:80:LYS:O	24:B5:4092:U:O2'	2.28	0.42
6:Cu:79:VAL:HG22	6:Cu:90:ILE:HG23	2.00	0.42
19:DB:371:THR:O	19:DB:375:TRP:N	2.46	0.42
19:DB:419:LYS:HD2	19:DB:451:TYR:CE2	2.53	0.42
19:DB:569:HIS:HB2	19:DB:684:ARG:HH11	1.84	0.42
24:B5:1208:C:H2'	24:B5:1209:G:H8	1.84	0.42
24:B5:3650:G:OP1	94:B5:4975:SPD:H82	2.19	0.42
24:B5:4741:U:H2'	24:B5:4742:U:C6	2.53	0.42
29:B7:48:G:OP1	51:B:226:TYR:OH	2.31	0.42
34:B8:15:G:C6	34:B8:16:G:N1	2.87	0.42
63:A2:239:C:H2'	63:A2:240:G:C8	2.54	0.42
63:A2:1147:C:O2'	63:A2:1151:A:N1	2.48	0.42
80:Bj:2:THR:O	80:Bj:7:SER:OG	2.23	0.42
24:B5:639:G:H2'	24:B5:640:G:H8	1.84	0.42
24:B5:1095:C:H2'	24:B5:1096:G:C8	2.54	0.42
24:B5:1341:A:N1	24:B5:1453:G:O2'	2.46	0.42
24:B5:1701:C:H2'	24:B5:1702:C:C6	2.55	0.42
29:B7:63:C:H5'	29:B7:64:G:H5''	2.00	0.42
43:BB:206:PRO:HG2	43:BB:209:GLN:HG3	2.00	0.42
43:BB:322:HIS:O	43:BB:342:LYS:NZ	2.34	0.42
44:BS:69:GLU:HG2	44:BS:101:THR:HG22	2.00	0.42
52:BO:18:ARG:CZ	52:BO:128:ARG:HH21	2.32	0.42
53:Ae:40:ALA:HB1	53:Ae:45:TYR:CG	2.55	0.42
55:BE:216:THR:OG1	55:BE:217:ASP:N	2.52	0.42
59:BF:170:ASP:OD1	59:BF:171:ASN:N	2.52	0.42
63:A2:324:C:H42	63:A2:328:G:N2	2.17	0.42
81:AF:107:ASP:C	81:AF:124:SER:HG	2.23	0.42
18:Av:60:LYS:NZ	66:AA:23:ARG:O	2.53	0.42
19:DB:120:LEU:O	19:DB:124:GLN:N	2.48	0.42
19:DB:448:CYS:O	19:DB:452:MET:HG2	2.20	0.42
19:DB:773:TYR:CZ	19:DB:783:ALA:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Ct:114:SER:OG	20:Ct:117:SER:O	2.36	0.42
24:B5:1549:C:O2'	24:B5:1552:G:H1'	2.19	0.42
24:B5:4381:A:OP1	24:B5:4382:PSU:O2'	2.32	0.42
29:B7:26:C:O2'	31:BJ:147:ARG:NH1	2.53	0.42
34:B8:141:C:H5''	48:BN:60:VAL:HG11	2.00	0.42
40:BM:126:GLU:HA	40:BM:129:LYS:HE2	2.01	0.42
44:BS:6:THR:HA	44:BS:107:THR:HG21	2.02	0.42
45:Ac:25:LEU:HD12	45:Ac:37:VAL:HG11	2.02	0.42
55:BE:273:TYR:O	55:BE:276:SER:OG	2.36	0.42
57:Af:172:LYS:NZ	63:A2:67:C:OP2	2.44	0.42
60:DC:18:ASN:HD21	60:DC:25:ASN:HA	1.85	0.42
61:Ag:20:GLU:HG2	61:Ag:48:ALA:HB3	2.01	0.42
63:A2:381:G:OP1	64:Ah:56:ARG:NH2	2.52	0.42
63:A2:462:U:H2'	63:A2:463:OMC:H6	1.84	0.42
63:A2:678:G:N1	63:A2:1028:A:OP2	2.33	0.42
81:AF:73:SER:OG	81:AF:117:ASN:OD1	2.25	0.42
12:Br:82:ILE:HG22	12:Br:89:THR:HG22	2.01	0.42
24:B5:209:U:H5'	42:BY:59:ARG:HD2	2.01	0.42
24:B5:1999:G:N2	44:BS:115:ALA:HB2	2.34	0.42
24:B5:3517:A2M:HM'1	24:B5:4283:C:H1'	2.00	0.42
49:Ad:153:LEU:HD13	57:Af:216:ARG:HD2	2.02	0.42
50:Ba:14:HIS:O	50:Ba:16:SER:N	2.52	0.42
65:Be:124:ASN:OD1	65:Be:124:ASN:N	2.52	0.42
66:AA:33:MET:HB2	66:AA:79:PHE:HB2	2.01	0.42
10:BQ:75:ARG:NH2	24:B5:1412:G:O2'	2.52	0.42
11:As:65:TYR:HE1	11:As:128:GLN:HG3	1.85	0.42
24:B5:1105:C:C5	54:Bb:92:LYS:HD2	2.54	0.42
24:B5:1793:G:N2	24:B5:4140:A:O4'	2.53	0.42
36:Aa:30:TRP:CG	82:An:19:PRO:HB3	2.55	0.42
63:A2:502:C:OP1	94:A2:1978:SPD:N6	2.52	0.42
72:AC:102:VAL:HG21	76:Al:35:ILE:HG21	2.00	0.42
81:AF:203:ASP:OD1	81:AF:205:SER:OG	2.33	0.42
15:Bs:58:ASN:O	15:Bs:62:ARG:HG3	2.19	0.42
19:DB:121:SER:O	19:DB:125:ILE:HG13	2.20	0.42
19:DB:184:LYS:HG2	19:DB:189:TYR:CZ	2.54	0.42
19:DB:446:SER:O	19:DB:450:LYS:HG3	2.20	0.42
19:DB:708:LEU:HD23	19:DB:708:LEU:HA	1.87	0.42
20:Ct:199:LEU:HB3	20:Ct:204:ASN:HA	2.02	0.42
24:B5:19:G:P	74:Bh:93:ARG:HE	2.42	0.42
24:B5:652:C:H2'	24:B5:653:G:H8	1.84	0.42
24:B5:787:C:H2'	24:B5:788:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B5:2396:A:OP2	24:B5:2417:G:O2'	2.35	0.42
24:B5:3850:G:O2'	46:BZ:136:PHE:OXT	2.37	0.42
24:B5:4715:U:O2	43:BB:343:ARG:NH1	2.52	0.42
39:Bt:133:LEU:HG	39:Bt:148:PRO:HB3	2.02	0.42
40:BM:24:LEU:HD11	40:BM:86:TRP:CG	2.54	0.42
43:BB:339:GLY:HA3	43:BB:343:ARG:HG2	2.00	0.42
57:Af:2:LYS:NZ	63:A2:156:G:OP1	2.53	0.42
61:Ag:66:VAL:HG11	63:A2:914:A:N3	2.34	0.42
63:A2:1754:C:H2'	63:A2:1755:G:H8	1.85	0.42
70:Aj:86:PRO:HG2	70:Aj:89:ILE:HG13	2.01	0.42
10:BQ:172:ARG:HA	10:BQ:176:ARG:HD2	2.00	0.42
19:DB:418:TYR:HB3	19:DB:423:ASN:HB2	2.00	0.42
24:B5:27:C:O2'	24:B5:60:A:N3	2.45	0.42
24:B5:318:A:H2'	24:B5:319:A:C8	2.55	0.42
24:B5:1284:OMC:HM21	47:BC:106:LYS:HB2	2.02	0.42
24:B5:2431:C:OP1	24:B5:2611:C:O2'	2.33	0.42
24:B5:3882:G:H2'	24:B5:3883:G:C8	2.54	0.42
36:Aa:175:GLU:O	36:Aa:187:LYS:NZ	2.48	0.42
37:Az:11:ARG:NH2	63:A2:1845:U:OP1	2.40	0.42
53:Ae:14:THR:HB	53:Ae:15:PRO:HD3	2.01	0.42
60:DC:159:ARG:O	60:DC:163:GLU:HG3	2.20	0.42
63:A2:1048:C:H5''	82:An:143:LYS:HB2	2.00	0.42
63:A2:1229:A:H2'	63:A2:1230:G:C8	2.55	0.42
8:BX:65:ALA:HB2	74:Bh:69:LEU:HD11	2.01	0.42
10:BQ:111:SER:O	10:BQ:115:LYS:HB2	2.20	0.42
10:BQ:181:ARG:HH22	24:B5:1335:A:P	2.43	0.42
14:At:96:PHE:HB3	84:AG:52:PHE:HB3	2.02	0.42
19:DB:431:MET:HE3	19:DB:448:CYS:SG	2.60	0.42
23:Aw:89:GLY:HA2	75:AD:83:VAL:HG12	2.02	0.42
24:B5:1271:C:H5''	24:B5:4195:A:OP1	2.20	0.42
24:B5:4780:G:N1	43:BB:389:MET:O	2.38	0.42
63:A2:449:A:H5''	64:Ah:25:ARG:HA	2.02	0.42
63:A2:564:G:O2'	63:A2:565:A:H8	2.03	0.42
63:A2:583:U:H2'	63:A2:584:A:H5''	2.02	0.42
10:BQ:130:SER:OG	10:BQ:134:ARG:N	2.52	0.42
13:BR:82:LYS:O	24:B5:2706:G:O2'	2.28	0.42
23:Aw:39:ASN:HD22	23:Aw:43:GLY:H	1.68	0.42
24:B5:172:C:O2	74:Bh:112:ARG:NH1	2.53	0.42
24:B5:1769:G:H2'	24:B5:1770:G:H8	1.84	0.42
24:B5:2235:C:OP2	97:B5:5526:HOH:O	2.20	0.42
24:B5:3897:G:H2'	24:B5:3898:G:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B5:4012:G:N3	24:B5:4012:G:H2'	2.34	0.42
36:Aa:87:ILE:HG22	36:Aa:101:HIS:HB2	2.01	0.42
43:BB:215:GLU:OE2	43:BB:349:LYS:NZ	2.53	0.42
60:DC:13:ASN:HB2	60:DC:52:ILE:HD12	2.02	0.42
63:A2:115:U:O2'	63:A2:382:C:O2	2.26	0.42
69:AB:23:SER:OG	69:AB:24:GLN:OE1	2.27	0.42
15:Bs:66:ARG:HA	15:Bs:69:LEU:HG	2.00	0.42
19:DB:506:LYS:HD2	19:DB:644:PRO:HD3	2.01	0.42
19:DB:538:TYR:CD1	60:DC:36:LEU:HD22	2.55	0.42
19:DB:581:GLU:O	19:DB:584:THR:OG1	2.34	0.42
19:DB:766:LEU:O	19:DB:770:LYS:HG3	2.20	0.42
19:DB:777:PRO:O	19:DB:780:GLN:HG3	2.20	0.42
20:Ct:72:SER:HA	20:Ct:75:LYS:HB2	2.02	0.42
22:BV:45:ILE:HG21	22:BV:53:PRO:HB3	2.02	0.42
24:B5:114:G:N2	24:B5:158:A:H61	2.17	0.42
24:B5:891:U:H3	24:B5:979:G:H1	1.68	0.42
24:B5:1317:A:H2	47:BC:234:LYS:HD2	1.85	0.42
24:B5:1688:A:H2'	24:B5:1689:G:C8	2.55	0.42
24:B5:2602:G:H1'	24:B5:2607:A:H2	1.84	0.42
24:B5:3954:U:H2'	24:B5:3955:G:H8	1.85	0.42
24:B5:4408:C:O2'	24:B5:4743:C:OP1	2.34	0.42
25:BT:31:MET:HE2	51:B:67:ALA:HB1	2.01	0.42
33:Ay:64:ASN:HD22	33:Ay:114:LYS:HE2	1.85	0.42
45:Ac:50:ILE:HD11	45:Ac:86:LEU:HD23	2.02	0.42
45:Ac:135:GLU:HB3	45:Ac:187:LYS:HB2	2.02	0.42
51:B:85:LYS:NZ	51:B:254:GLU:OE2	2.37	0.42
57:Af:172:LYS:HD3	63:A2:65:C:H4'	2.02	0.42
63:A2:1232:C:O2'	63:A2:1254:A:N6	2.52	0.42
77:Bi:26:HIS:O	77:Bi:29:ARG:HG3	2.20	0.42
5:Ar:46:ARG:HH12	5:Ar:52:LEU:HD11	1.84	0.41
9:Bp:18:TYR:HB3	38:BA:180:LEU:HD22	2.01	0.41
9:Bp:62:LYS:HE3	9:Bp:62:LYS:HB2	1.91	0.41
9:Bp:66:GLY:HA2	38:BA:80:GLU:HG3	2.02	0.41
16:BG:158:ALA:HB2	16:BG:190:LEU:HD12	2.02	0.41
19:DB:347:VAL:HG22	19:DB:380:LEU:HD11	2.00	0.41
24:B5:184:U:H3	24:B5:253:G:H1	1.68	0.41
24:B5:985:G:OP2	55:BE:67:ARG:NH1	2.53	0.41
24:B5:1225:G:OP1	47:BC:316:LYS:NZ	2.43	0.41
24:B5:1695:U:H2'	24:B5:1696:U:C6	2.55	0.41
24:B5:1718:PSU:H2'	24:B5:1719:A:C8	2.55	0.41
24:B5:2712:U:O2'	24:B5:2724:A:N7	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B5:3395:A:N6	24:B5:3914:G:O2'	2.53	0.41
24:B5:3415:C:OP1	38:BA:132:ASN:ND2	2.47	0.41
24:B5:4648:A:OP2	43:BB:156:TYR:OH	2.32	0.41
29:B7:55:A:H4'	31:BJ:155:HIS:HB2	2.00	0.41
36:Aa:92:GLN:NE2	36:Aa:229:MET:SD	2.83	0.41
48:BN:138:PHE:HA	48:BN:143:ARG:HE	1.85	0.41
49:Ad:18:TRP:C	49:Ad:51:ARG:HH22	2.28	0.41
55:BE:59:TYR:HB3	55:BE:63:ALA:HB3	2.02	0.41
58:Bc:99:PRO:HG3	58:Bc:105:ILE:HG13	2.02	0.41
74:Bh:6:ALA:O	74:Bh:10:ARG:HG3	2.20	0.41
75:AD:122:THR:HG21	75:AD:126:LYS:HG2	2.02	0.41
81:AF:40:ILE:HD11	81:AF:66:VAL:HG11	2.02	0.41
3:Bo:12:CYS:HB3	3:Bo:15:CYS:HB2	2.01	0.41
19:DB:19:ARG:NH2	24:B5:404:U:OP1	2.54	0.41
19:DB:47:GLU:HG2	19:DB:81:VAL:HB	2.02	0.41
24:B5:1981:A:O4'	24:B5:4208:C:O2'	2.38	0.41
24:B5:4108:A:H2'	24:B5:4109:A:H8	1.84	0.41
24:B5:4231:C:O2'	89:Bm:114:LYS:NZ	2.50	0.41
24:B5:4270:G:C2	43:BB:252:ALA:HB1	2.55	0.41
24:B5:4381:A:H3'	24:B5:4382:PSU:H4'	2.01	0.41
24:B5:4698:U:H2'	24:B5:4699:G:C8	2.56	0.41
38:BA:117:GLU:HG2	38:BA:124:GLY:N	2.35	0.41
43:BB:80:GLU:OE1	43:BB:323:TYR:OH	2.31	0.41
49:Ad:71:LYS:HG2	49:Ad:76:VAL:HG22	2.01	0.41
53:Ae:35:LEU:HD22	53:Ae:117:ILE:HG12	2.01	0.41
57:Af:138:ALA:HA	57:Af:176:ILE:HD11	2.02	0.41
64:Ah:83:TYR:HB3	64:Ah:101:ILE:HB	2.03	0.41
81:AF:42:MET:O	81:AF:56:GLN:N	2.51	0.41
88:Ap:97:GLN:HB2	88:Ap:105:LYS:HG3	2.02	0.41
19:DB:69:VAL:HG12	19:DB:86:TYR:CZ	2.56	0.41
19:DB:101:LYS:HD3	20:Ct:214:THR:OG1	2.21	0.41
19:DB:296:LEU:N	19:DB:297:PRO:HD2	2.35	0.41
19:DB:301:LEU:HB3	19:DB:306:PHE:CZ	2.55	0.41
24:B5:315:G:C8	50:Ba:62:HIS:HB2	2.54	0.41
24:B5:1632:PSU:H4'	24:B5:1635:G:N1	2.35	0.41
24:B5:2450:C:H2'	24:B5:2451:G:C8	2.56	0.41
27:BW:73:ARG:NH1	63:A2:1781:G:OP2	2.53	0.41
28:Ax:29:HIS:ND1	28:Ax:29:HIS:O	2.51	0.41
28:Ax:51:THR:OG1	28:Ax:53:ASP:OD1	2.31	0.41
38:BA:245:ARG:NH1	38:BA:247:ARG:HH21	2.18	0.41
39:Bt:35:LEU:H	39:Bt:35:LEU:HG	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:Ab:108:LYS:HB2	41:Ab:233:LEU:HD13	2.02	0.41
49:Ad:229:GLY:HA3	49:Ad:234:PRO:HA	2.03	0.41
53:Ae:43:GLU:H	53:Ae:43:GLU:CD	2.27	0.41
55:BE:98:PRO:HA	55:BE:107:THR:HA	2.01	0.41
59:BF:219:MET:HB3	59:BF:231:ASP:OD2	2.20	0.41
63:A2:421:G:O2'	63:A2:661:C:N3	2.52	0.41
63:A2:585:A:OP1	67:Ai:169:ARG:NH2	2.46	0.41
63:A2:614:G:N1	63:A2:630:A:OP2	2.40	0.41
63:A2:700:C:H2'	63:A2:701:G:C8	2.55	0.41
79:Am:40:LEU:HD12	79:Am:50:ILE:HG23	2.02	0.41
7:BL:87:HIS:HB3	7:BL:90:VAL:HG23	2.02	0.41
19:DB:496:LYS:HE2	19:DB:504:ALA:HB1	2.01	0.41
24:B5:382:G:H4'	24:B5:407:A:N1	2.35	0.41
24:B5:432:U:O2'	94:B5:5263:SPD:H92	2.21	0.41
24:B5:706:C:OP1	55:BE:142:LYS:NZ	2.41	0.41
24:B5:1088:C:H2'	24:B5:1089:G:H8	1.85	0.41
24:B5:1576:A:OP2	80:Bj:30:GLN:NE2	2.54	0.41
24:B5:1922:A:H4'	24:B5:1923:A:C8	2.55	0.41
24:B5:3478:A:H5''	38:BA:244:GLY:HA3	2.01	0.41
24:B5:3664:U:H2'	24:B5:3665:G:C8	2.55	0.41
24:B5:4204:C:H2'	24:B5:4205:U:C6	2.55	0.41
24:B5:4663:C:O2	24:B5:4665:C:N4	2.51	0.41
48:BN:94:PHE:CE2	48:BN:96:ARG:HB2	2.56	0.41
60:DC:72:ILE:HG13	60:DC:91:MET:HE1	2.03	0.41
60:DC:158:LEU:O	60:DC:162:LEU:HG	2.20	0.41
63:A2:617:A:H1'	75:AD:86:VAL:HG23	2.01	0.41
63:A2:1030:G:N7	97:A2:2182:HOH:O	2.37	0.41
63:A2:1671:C:H2'	63:A2:1672:G:C8	2.56	0.41
2:Aq:99:ASP:OD1	2:Aq:102:THR:N	2.49	0.41
14:At:56:ILE:HD11	14:At:69:PRO:HD3	2.01	0.41
19:DB:509:HIS:HD2	19:DB:647:LEU:HD13	1.85	0.41
24:B5:17:A:OP1	74:Bh:84:ARG:NH2	2.43	0.41
24:B5:440:U:O2'	68:Bf:91:ASN:O	2.29	0.41
24:B5:3572:U:H2'	24:B5:3573:OMC:O4'	2.20	0.41
24:B5:4219:A:O2'	89:Bm:122:ARG:NH2	2.53	0.41
24:B5:4350:G:N2	24:B5:4353:A:OP2	2.54	0.41
24:B5:4792:U:H3'	24:B5:4793:C:C6	2.55	0.41
39:Bt:108:GLU:HA	39:Bt:111:ASN:HD21	1.86	0.41
43:BB:83:PRO:O	43:BB:167:GLN:NE2	2.54	0.41
44:BS:162:GLN:HE22	52:BO:128:ARG:HH11	1.66	0.41
47:BC:150:LEU:HD12	47:BC:151:PRO:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Ad:137:PRO:HG2	49:Ad:150:PRO:HD2	2.03	0.41
57:Af:21:GLU:OE1	57:Af:25:ARG:NH2	2.52	0.41
57:Af:196:LYS:NZ	63:A2:126:G:O6	2.33	0.41
57:Af:199:THR:HG21	63:A2:126:G:H2'	2.02	0.41
63:A2:28:U:H2'	63:A2:29:G:C8	2.53	0.41
63:A2:1669:U:OP2	88:Ap:141:TYR:OH	2.25	0.41
64:Ah:206:LYS:HE3	64:Ah:206:LYS:HB3	1.90	0.41
5:Ar:25:LYS:HD2	5:Ar:55:ARG:HD3	2.02	0.41
19:DB:105:ASN:ND2	20:Ct:214:THR:HG21	2.33	0.41
22:BV:43:LYS:HD3	24:B5:4254:C:H5''	2.01	0.41
24:B5:1283:U:OP1	50:Ba:8:THR:OG1	2.27	0.41
24:B5:1394:U:O2'	59:BF:33:ARG:NE	2.33	0.41
24:B5:1423:C:H5''	50:Ba:132:ARG:CZ	2.51	0.41
24:B5:2034:A:N6	24:B5:2035:G:O6	2.54	0.41
24:B5:2250:G:N2	24:B5:2250:G:OP2	2.49	0.41
24:B5:2450:C:H2'	24:B5:2451:G:H8	1.85	0.41
24:B5:3600:G:H22	24:B5:3632:G:H1'	1.85	0.41
24:B5:4732:G:N2	24:B5:4798:C:O2	2.54	0.41
29:B7:11:A:N1	29:B7:66:G:O2'	2.48	0.41
34:B8:58:G:N7	80:Bj:63:ARG:NH2	2.61	0.41
38:BA:140:ASN:ND2	38:BA:143:THR:OG1	2.53	0.41
39:Bt:88:PRO:HA	39:Bt:89:PRO:HD3	1.99	0.41
39:Bt:118:HIS:CD2	39:Bt:119:ARG:HG2	2.56	0.41
47:BC:11:TYR:CZ	47:BC:148:PRO:HB2	2.55	0.41
49:Ad:62:LYS:HE3	49:Ad:62:LYS:HB3	1.90	0.41
64:Ah:116:HIS:O	64:Ah:152:ARG:NH2	2.53	0.41
6:Cu:7:ASN:H	6:Cu:10:LYS:HD2	1.84	0.41
17:BU:24:ASP:HB3	17:BU:111:GLU:HB2	2.02	0.41
19:DB:155:ALA:O	19:DB:159:HIS:N	2.52	0.41
19:DB:444:ILE:HG22	19:DB:448:CYS:SG	2.61	0.41
19:DB:760:ASP:HA	19:DB:794:LEU:HD23	2.03	0.41
21:BH:137:SER:HB2	21:BH:145:VAL:HG23	2.01	0.41
24:B5:2360:A:N3	24:B5:2382:C:O2'	2.52	0.41
24:B5:3498:A:O2'	63:A2:1850:G:N3	2.43	0.41
24:B5:4605:C:H2'	24:B5:4606:G:C8	2.56	0.41
28:Ax:76:TYR:OH	28:Ax:86:GLU:OE1	2.31	0.41
39:Bt:35:LEU:HD13	39:Bt:64:ILE:HG21	2.03	0.41
39:Bt:133:LEU:HD11	39:Bt:151:ILE:HG13	2.03	0.41
41:Ab:163:VAL:HG21	41:Ab:245:SER:HB3	2.03	0.41
49:Ad:240:ARG:NH2	63:A2:845:U:OP1	2.52	0.41
52:BO:181:ALA:O	52:BO:185:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:DA:64:ASP:OD2	56:DA:110:TYR:OH	2.33	0.41
61:Ag:37:LYS:O	61:Ag:41:ARG:HG3	2.20	0.41
63:A2:527:A:H5'	75:AD:105:ARG:HH21	1.85	0.41
63:A2:1757:C:H2'	63:A2:1758:G:C8	2.56	0.41
63:A2:1758:G:H2'	63:A2:1759:G:C8	2.54	0.41
76:Al:72:HIS:CD2	76:Al:74:ILE:HD11	2.56	0.41
8:BX:110:LYS:HG3	8:BX:121:VAL:HB	2.03	0.41
14:At:70:VAL:HG13	14:At:104:LEU:HB2	2.03	0.41
14:At:83:LYS:HB3	63:A2:1338:4AC:H5''	2.02	0.41
15:Bs:138:PHE:HB3	15:Bs:143:ILE:HB	2.02	0.41
17:BU:37:ALA:HB2	17:BU:65:ARG:NH1	2.36	0.41
24:B5:363:A:N1	24:B5:376:A:H5''	2.36	0.41
24:B5:629:G:H2'	24:B5:630:G:C8	2.56	0.41
24:B5:2239:A:N7	24:B5:2657:C:H2'	2.36	0.41
24:B5:2418:U:H5''	24:B5:2419:G:H5'	2.02	0.41
24:B5:2601:G:O2'	24:B5:2608:A:N3	2.38	0.41
26:BI:57:TYR:HD1	26:BI:130:HIS:HA	1.85	0.41
32:AZ:13:GLU:HG2	32:AZ:17:LYS:HE2	2.02	0.41
43:BB:29:VAL:HG13	43:BB:348:ARG:HD3	2.02	0.41
52:BO:189:ILE:HA	52:BO:192:PHE:HD2	1.86	0.41
60:DC:41:LEU:HB3	60:DC:58:ALA:HB3	2.02	0.41
63:A2:673:A:H5'	95:A2:1994:SPM:H92	2.03	0.41
63:A2:1649:G:O2'	63:A2:1675:G:O6	2.37	0.41
81:AF:73:SER:H	81:AF:117:ASN:HD21	1.68	0.41
82:An:151:LEU:H	82:An:151:LEU:HD23	1.85	0.41
83:Bk:61:PRO:HA	83:Bk:62:PRO:HD3	1.91	0.41
2:Aq:66:VAL:HG12	2:Aq:68:GLY:H	1.85	0.41
5:Ar:124:ARG:NE	5:Ar:130:ARG:O	2.39	0.41
6:Cu:78:LYS:HB2	6:Cu:91:THR:HG1	1.86	0.41
7:BL:34:ARG:NH2	34:B8:30:U:OP1	2.54	0.41
10:BQ:68:ARG:HE	24:B5:1375:A:H5'	1.86	0.41
10:BQ:159:PRO:HD2	24:B5:4052:OMU:OP2	2.21	0.41
11:As:84:ARG:NH2	63:A2:1606:G:OP1	2.54	0.41
11:As:91:HIS:NE2	63:A2:1666:G:OP1	2.40	0.41
15:Bs:41:GLN:HE22	24:B5:1934:G:H21	1.67	0.41
19:DB:6:LEU:O	19:DB:11:ASN:ND2	2.53	0.41
19:DB:57:ASN:ND2	19:DB:89:LEU:HD22	2.35	0.41
19:DB:134:ARG:NH2	19:DB:161:LEU:HB2	2.36	0.41
19:DB:280:TYR:CE1	19:DB:296:LEU:HD13	2.56	0.41
19:DB:372:THR:O	19:DB:376:VAL:HG23	2.21	0.41
19:DB:412:LEU:HD21	19:DB:444:ILE:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:DB:626:LYS:HE2	24:B5:214:G:H1'	2.01	0.41
22:BV:51:ARG:NH1	24:B5:4366:OMU:OP1	2.52	0.41
24:B5:90:G:OP2	24:B5:92:C:N4	2.53	0.41
24:B5:198:A:OP2	42:BY:126:ARG:NH2	2.54	0.41
24:B5:227:A:N6	24:B5:241:G:O2'	2.52	0.41
24:B5:1420:G:OP1	54:Bb:44:ARG:NH1	2.54	0.41
24:B5:1868:A:C8	24:B5:1871:A:H1'	2.56	0.41
24:B5:1891:G:OP1	44:BS:139:ARG:NE	2.45	0.41
24:B5:3497:G:H21	24:B5:3498:A:N6	2.19	0.41
24:B5:3660:A:OP1	48:BN:90:ASN:ND2	2.45	0.41
24:B5:4194:G:C8	97:B5:5594:HOH:O	2.70	0.41
29:B7:77:A:H62	29:B7:99:G:H21	1.69	0.41
32:AZ:80:ARG:O	32:AZ:84:GLN:HG3	2.21	0.41
32:AZ:141:ASN:ND2	41:Ab:87:PRO:HD3	2.36	0.41
33:Ay:58:LEU:HD12	33:Ay:62:VAL:HG21	2.03	0.41
34:B8:124:U:O4	34:B8:126:C:N4	2.54	0.41
41:Ab:252:THR:OG1	41:Ab:254:ASP:OD1	2.33	0.41
51:B:263:LYS:HA	51:B:263:LYS:HD2	1.89	0.41
53:Ae:125:SER:HB3	53:Ae:136:ARG:HB3	2.03	0.41
57:Af:53:SER:HB2	63:A2:165:G:H4'	2.03	0.41
63:A2:51:U:H2'	63:A2:52:G:C8	2.56	0.41
63:A2:604:C:N4	63:A2:621:G:O6	2.54	0.41
63:A2:1846:A:H2'	63:A2:1847:G:C8	2.56	0.41
79:Am:91:LEU:HB3	79:Am:122:ILE:HG12	2.02	0.41
84:AG:33:LYS:HE2	84:AG:34:TYR:CZ	2.56	0.41
1:BP:54:LYS:HA	1:BP:83:TRP:CD1	2.56	0.41
1:BP:131:ARG:HH22	24:B5:3592:A:H2	1.69	0.41
2:Aq:94:GLU:HG2	2:Aq:95:ILE:HG13	2.03	0.41
9:Bp:38:THR:HA	9:Bp:45:THR:HA	2.03	0.41
24:B5:52:G:H4'	24:B5:1484:G:H4'	2.02	0.41
24:B5:327:U:HO2'	77:Bi:30:ARG:HH11	1.63	0.41
24:B5:375:G:N7	80:Bj:56:ARG:NH2	2.62	0.41
24:B5:478:G:H2'	24:B5:479:G:H8	1.86	0.41
24:B5:724:G:OP2	59:BF:75:ARG:NE	2.53	0.41
24:B5:778:C:H2'	24:B5:779:G:C8	2.55	0.41
24:B5:1503:G:O2'	24:B5:2655:A:N3	2.44	0.41
24:B5:1699:G:H2'	24:B5:1700:G:H8	1.85	0.41
24:B5:3393:G:N7	38:BA:152:SER:OG	2.46	0.41
34:B8:30:U:H2'	34:B8:31:G:C8	2.56	0.41
36:Aa:30:TRP:CD2	36:Aa:48:LEU:HD13	2.56	0.41
38:BA:80:GLU:HB2	38:BA:170:ALA:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:Ba:26:ARG:HD3	50:Ba:26:ARG:HA	1.84	0.41
60:DC:1:MET:HE3	60:DC:81:HIS:HD2	1.85	0.41
63:A2:172:OMU:H6	63:A2:315:U:H1'	2.03	0.41
63:A2:456:A:O2'	63:A2:1736:A:N3	2.46	0.41
63:A2:656:A:H4'	63:A2:657:G:H3'	2.02	0.41
63:A2:1271:G:O2'	63:A2:1302:A:N7	2.52	0.41
64:Ah:113:TYR:OH	64:Ah:156:ALA:O	2.38	0.41
76:Al:11:VAL:HG21	76:Al:16:THR:HG21	2.02	0.41
7:BL:60:ARG:O	24:B5:74:G:H5'	2.22	0.40
8:BX:64:SER:HB2	74:Bh:69:LEU:HD13	2.03	0.40
8:BX:76:ILE:HD13	8:BX:108:GLN:HB3	2.03	0.40
8:BX:129:ARG:NH2	8:BX:131:ASP:OD2	2.54	0.40
15:Bs:40:MET:HE1	15:Bs:187:LEU:HD11	2.02	0.40
19:DB:148:ARG:NH2	19:DB:189:TYR:OH	2.54	0.40
21:BH:40:HIS:ND1	21:BH:41:ILE:HG13	2.35	0.40
24:B5:278:G:H5''	48:BN:8:GLN:NE2	2.35	0.40
24:B5:357:U:O2	24:B5:359:A:N6	2.54	0.40
24:B5:434:A:H2'	24:B5:435:A:O4'	2.21	0.40
24:B5:1696:U:H2'	24:B5:1697:G:C8	2.56	0.40
24:B5:2568:A:N1	97:B5:5728:HOH:O	2.36	0.40
24:B5:4265:C:OP1	24:B5:4266:G:H5''	2.21	0.40
24:B5:4269:A2M:HM'3	24:B5:4305:A:N7	2.36	0.40
44:BS:62:VAL:HA	59:BF:82:VAL:HG22	2.03	0.40
44:BS:80:ILE:HG12	44:BS:129:VAL:HG22	2.04	0.40
44:BS:93:MET:HE1	44:BS:117:HIS:CE1	2.55	0.40
48:BN:178:HIS:HA	48:BN:181:HIS:NE2	2.36	0.40
49:Ad:100:ARG:HH12	49:Ad:122:LYS:HA	1.86	0.40
50:Ba:36:GLY:HA3	50:Ba:40:HIS:CE1	2.56	0.40
57:Af:198:ARG:NH2	63:A2:126:G:OP2	2.45	0.40
63:A2:958:A:OP1	82:An:57:THR:OG1	2.36	0.40
85:Ao:68:PRO:HD2	85:Ao:71:GLU:HB2	2.03	0.40
5:Ar:120:HIS:CE1	5:Ar:124:ARG:HD2	2.56	0.40
19:DB:324:PRO:HB3	60:DC:80:SER:O	2.21	0.40
22:BV:91:LYS:HD3	22:BV:91:LYS:HA	1.93	0.40
24:B5:62:A:OP1	48:BN:172:ARG:NH1	2.54	0.40
24:B5:208:A:C2	24:B5:233:U:H5''	2.56	0.40
24:B5:229:G:H5''	42:BY:11:ARG:HG3	2.02	0.40
24:B5:1381:G:N2	24:B5:1413:C:OP2	2.49	0.40
24:B5:2012:C:H5''	59:BF:211:LYS:HB3	2.02	0.40
24:B5:4071:A:H1'	51:B:36:LEU:HD23	2.03	0.40
24:B5:4431:U:H2'	24:B5:4432:G:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B5:4605:C:H2'	24:B5:4606:G:H8	1.86	0.40
57:Af:162:LEU:HB3	63:A2:67:C:C5	2.56	0.40
63:A2:1616:U:O4	85:Ao:40:ARG:NH2	2.55	0.40
64:Ah:66:SER:HA	64:Ah:73:THR:HA	2.03	0.40
78:AE:46:GLU:O	78:AE:50:VAL:HG23	2.21	0.40
10:BQ:2:GLY:N	24:B5:2011:C:OP1	2.55	0.40
19:DB:87:GLY:HA3	19:DB:103:TYR:CE2	2.56	0.40
22:BV:97:TYR:OH	27:BW:37:GLU:OE2	2.33	0.40
24:B5:223:G:H4'	24:B5:225:G:C8	2.56	0.40
24:B5:789:G:H2'	24:B5:790:G:H5'	2.03	0.40
24:B5:1316:A:OP1	48:BN:202:ARG:NH2	2.33	0.40
24:B5:1600:C:H2'	24:B5:1601:A:C8	2.56	0.40
24:B5:3899:C:H2'	24:B5:3900:G:C8	2.57	0.40
24:B5:4371:C:OP1	43:BB:224:LYS:HG3	2.22	0.40
29:B7:75:G:H5''	44:BS:49:SER:O	2.21	0.40
53:Ae:51:HIS:HA	53:Ae:86:LYS:HE2	2.03	0.40
53:Ae:126:THR:HG21	69:AB:27:CYS:SG	2.61	0.40
63:A2:665:A:O2'	63:A2:671:A:N1	2.40	0.40
64:Ah:141:ARG:HB2	64:Ah:146:GLN:HG2	2.04	0.40
76:Al:33:ARG:HG3	76:Al:109:VAL:HG12	2.04	0.40
2:Aq:38:ILE:H	2:Aq:38:ILE:HG13	1.79	0.40
19:DB:154:TYR:HD1	19:DB:154:TYR:N	2.20	0.40
19:DB:442:ARG:CZ	60:DC:23:PRO:HA	2.51	0.40
19:DB:555:PHE:HB3	19:DB:559:ARG:NE	2.36	0.40
24:B5:1449:U:H2'	24:B5:1450:G:C8	2.55	0.40
24:B5:2432:C:H2'	24:B5:2433:G:O4'	2.22	0.40
24:B5:2687:A:N6	24:B5:3571:G:O2'	2.54	0.40
24:B5:4006:U:H2'	24:B5:4007:C:C6	2.57	0.40
40:BM:69:ARG:HH12	40:BM:71:LYS:HE3	1.86	0.40
51:B:116:ASP:OD1	51:B:116:ASP:N	2.52	0.40
51:B:167:VAL:HG11	51:B:175:HIS:CE1	2.56	0.40
53:Ae:73:THR:O	53:Ae:89:THR:HG21	2.22	0.40
59:BF:240:ASN:O	59:BF:244:ARG:HG2	2.21	0.40
63:A2:588:A:H5'	63:A2:593:C:H41	1.86	0.40
63:A2:1019:U:O2'	79:Am:86:GLU:OE2	2.39	0.40
1:BP:60:PHE:CE1	1:BP:82:ARG:HB2	2.57	0.40
5:Ar:36:VAL:HG23	5:Ar:99:LEU:HD22	2.03	0.40
7:BL:7:GLY:O	50:Ba:49:HIS:NE2	2.47	0.40
7:BL:128:PRO:HG3	7:BL:138:ASP:HB3	2.04	0.40
7:BL:162:LYS:NZ	24:B5:638:G:OP2	2.46	0.40
11:As:71:GLY:O	11:As:75:MET:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Bs:63:LYS:NZ	24:B5:1899:A:N3	2.68	0.40
15:Bs:85:ASN:OD1	15:Bs:85:ASN:N	2.46	0.40
19:DB:120:LEU:HD22	19:DB:124:GLN:NE2	2.37	0.40
19:DB:447:LYS:O	19:DB:451:TYR:HD1	2.05	0.40
19:DB:672:ILE:HD12	19:DB:705:HIS:CD2	2.57	0.40
21:BH:155:SER:OG	24:B5:4434:C:O2'	2.36	0.40
21:BH:186:THR:O	21:BH:189:GLN:NE2	2.53	0.40
24:B5:398:A2M:O5'	24:B5:398:A2M:H8	2.21	0.40
24:B5:856:A:N6	24:B5:1227:G:H1'	2.36	0.40
24:B5:1093:C:H2'	24:B5:1094:A:C8	2.56	0.40
24:B5:1673:G:N2	24:B5:1674:U:O4	2.39	0.40
24:B5:4222:C:O2'	24:B5:4224:G:OP2	2.35	0.40
36:Aa:123:ALA:HB2	36:Aa:165:ARG:HG3	2.02	0.40
43:BB:45:ALA:HB3	43:BB:183:ILE:HG23	2.03	0.40
43:BB:317:LEU:HD22	43:BB:382:VAL:HG13	2.04	0.40
51:B:179:ARG:HA	51:B:179:ARG:HD3	1.91	0.40
62:Bd:92:ARG:HA	62:Bd:102:LEU:HD23	2.03	0.40
63:A2:1328:G:OP1	97:A2:2108:HOH:O	2.22	0.40
81:AF:109:LEU:HD21	81:AF:125:ARG:CZ	2.52	0.40
81:AF:191:HIS:CE1	81:AF:195:LEU:HD11	2.57	0.40
81:AF:278:SER:HB2	81:AF:281:ALA:HB3	2.04	0.40
85:Ao:30:TYR:O	85:Ao:34:MET:HG3	2.22	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	
1	BP	151/184 (82%)	149 (99%)	2 (1%)	0	100	100
2	Aq	132/135 (98%)	132 (100%)	0	0	100	100
3	Bo	102/106 (96%)	100 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Ar	146/151 (97%)	143 (98%)	3 (2%)	0	100	100
6	Cu	103/162 (64%)	95 (92%)	8 (8%)	0	100	100
7	BL	208/211 (99%)	204 (98%)	4 (2%)	0	100	100
8	BX	116/156 (74%)	115 (99%)	1 (1%)	0	100	100
9	Bp	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
10	BQ	185/188 (98%)	182 (98%)	3 (2%)	0	100	100
11	As	140/145 (97%)	140 (100%)	0	0	100	100
12	Br	124/136 (91%)	122 (98%)	2 (2%)	0	100	100
13	BR	178/196 (91%)	178 (100%)	0	0	100	100
14	At	102/119 (86%)	98 (96%)	4 (4%)	0	100	100
15	Bs	194/318 (61%)	189 (97%)	5 (3%)	0	100	100
16	BG	229/266 (86%)	228 (100%)	1 (0%)	0	100	100
17	BU	100/128 (78%)	97 (97%)	3 (3%)	0	100	100
18	Av	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
19	DB	835/915 (91%)	822 (98%)	13 (2%)	0	100	100
20	Ct	111/238 (47%)	110 (99%)	1 (1%)	0	100	100
21	BH	188/192 (98%)	188 (100%)	0	0	100	100
22	BV	137/140 (98%)	135 (98%)	2 (2%)	0	100	100
23	Aw	138/143 (96%)	136 (99%)	2 (1%)	0	100	100
25	BT	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
26	BI	211/214 (99%)	206 (98%)	5 (2%)	0	100	100
27	BW	119/157 (76%)	118 (99%)	1 (1%)	0	100	100
28	Ax	123/130 (95%)	122 (99%)	1 (1%)	0	100	100
30	Au	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
31	BJ	168/178 (94%)	167 (99%)	1 (1%)	0	100	100
32	AZ	219/294 (74%)	214 (98%)	5 (2%)	0	100	100
33	Ay	83/124 (67%)	81 (98%)	2 (2%)	0	100	100
36	Aa	220/264 (83%)	217 (99%)	3 (1%)	0	100	100
37	Az	23/25 (92%)	23 (100%)	0	0	100	100
38	BA	250/257 (97%)	240 (96%)	10 (4%)	0	100	100
39	Bt	154/165 (93%)	153 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	BM	136/218 (62%)	134 (98%)	2 (2%)	0	100	100
41	Ab	218/293 (74%)	218 (100%)	0	0	100	100
42	BY	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
43	BB	395/403 (98%)	392 (99%)	3 (1%)	0	100	100
44	BS	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
45	Ac	223/281 (79%)	221 (99%)	2 (1%)	0	100	100
46	BZ	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
47	BC	360/412 (87%)	357 (99%)	3 (1%)	0	100	100
48	BN	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
49	Ad	260/263 (99%)	256 (98%)	4 (2%)	0	100	100
50	Ba	144/148 (97%)	137 (95%)	6 (4%)	1 (1%)	18	51
51	B	293/297 (99%)	289 (99%)	4 (1%)	0	100	100
52	BO	197/203 (97%)	197 (100%)	0	0	100	100
53	Ae	189/204 (93%)	185 (98%)	4 (2%)	0	100	100
54	Bb	103/245 (42%)	97 (94%)	6 (6%)	0	100	100
55	BE	239/291 (82%)	235 (98%)	4 (2%)	0	100	100
56	DA	153/403 (38%)	152 (99%)	1 (1%)	0	100	100
57	Af	235/249 (94%)	234 (100%)	1 (0%)	0	100	100
58	Bc	106/115 (92%)	106 (100%)	0	0	100	100
59	BF	224/247 (91%)	218 (97%)	5 (2%)	1 (0%)	30	63
60	DC	163/235 (69%)	162 (99%)	1 (1%)	0	100	100
61	Ag	188/432 (44%)	185 (98%)	3 (2%)	0	100	100
62	Bd	105/125 (84%)	105 (100%)	0	0	100	100
64	Ah	204/208 (98%)	200 (98%)	4 (2%)	0	100	100
65	Be	128/135 (95%)	127 (99%)	1 (1%)	0	100	100
66	AA	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
67	Ai	183/194 (94%)	179 (98%)	4 (2%)	0	100	100
68	Bf	108/110 (98%)	108 (100%)	0	0	100	100
69	AB	61/69 (88%)	61 (100%)	0	0	100	100
70	Aj	94/165 (57%)	91 (97%)	3 (3%)	0	100	100
71	Bg	112/115 (97%)	111 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
72	AC	72/156 (46%)	71 (99%)	1 (1%)	0	100	100
73	Ak	152/158 (96%)	148 (97%)	4 (3%)	0	100	100
74	Bh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
75	AD	55/133 (41%)	54 (98%)	1 (2%)	0	100	100
76	Al	122/132 (92%)	118 (97%)	4 (3%)	0	100	100
77	Bi	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
78	AE	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
79	Am	148/151 (98%)	147 (99%)	1 (1%)	0	100	100
80	Bj	84/97 (87%)	84 (100%)	0	0	100	100
81	AF	311/317 (98%)	305 (98%)	6 (2%)	0	100	100
82	An	132/151 (87%)	128 (97%)	4 (3%)	0	100	100
83	Bk	67/70 (96%)	67 (100%)	0	0	100	100
84	AG	53/56 (95%)	53 (100%)	0	0	100	100
85	Ao	126/145 (87%)	123 (98%)	3 (2%)	0	100	100
86	Bl	48/51 (94%)	48 (100%)	0	0	100	100
88	Ap	139/172 (81%)	133 (96%)	6 (4%)	0	100	100
89	Bm	49/128 (38%)	49 (100%)	0	0	100	100
All	All	13062/15567 (84%)	12867 (98%)	193 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
50	Ba	15	VAL
59	BF	196	VAL

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	
1	BP	134/163 (82%)	134 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Aq	120/121 (99%)	119 (99%)	1 (1%)	73	85
3	Bo	92/93 (99%)	92 (100%)	0	100	100
5	Ar	127/130 (98%)	123 (97%)	4 (3%)	35	67
6	Cu	89/136 (65%)	89 (100%)	0	100	100
7	BL	175/176 (99%)	173 (99%)	2 (1%)	65	82
8	BX	106/134 (79%)	106 (100%)	0	100	100
9	Bp	74/75 (99%)	73 (99%)	1 (1%)	59	79
10	BQ	164/165 (99%)	162 (99%)	2 (1%)	63	81
11	As	112/114 (98%)	112 (100%)	0	100	100
12	Br	109/119 (92%)	109 (100%)	0	100	100
13	BR	159/175 (91%)	158 (99%)	1 (1%)	78	87
14	At	94/107 (88%)	92 (98%)	2 (2%)	47	74
15	Bs	164/258 (64%)	164 (100%)	0	100	100
16	BG	199/223 (89%)	197 (99%)	2 (1%)	68	83
17	BU	91/113 (80%)	88 (97%)	3 (3%)	33	65
18	Av	112/113 (99%)	111 (99%)	1 (1%)	70	84
19	DB	746/806 (93%)	729 (98%)	17 (2%)	44	72
20	Ct	99/202 (49%)	97 (98%)	2 (2%)	48	75
21	BH	169/171 (99%)	169 (100%)	0	100	100
22	BV	106/107 (99%)	106 (100%)	0	100	100
23	Aw	112/114 (98%)	110 (98%)	2 (2%)	51	76
25	BT	139/140 (99%)	139 (100%)	0	100	100
26	BI	180/181 (99%)	179 (99%)	1 (1%)	78	87
27	BW	100/126 (79%)	99 (99%)	1 (1%)	68	83
28	Ax	107/112 (96%)	107 (100%)	0	100	100
30	Au	67/67 (100%)	65 (97%)	2 (3%)	36	68
31	BJ	143/149 (96%)	143 (100%)	0	100	100
32	AZ	182/242 (75%)	179 (98%)	3 (2%)	55	78
33	Ay	75/102 (74%)	74 (99%)	1 (1%)	61	80
36	Aa	203/231 (88%)	201 (99%)	2 (1%)	68	83
37	Az	24/24 (100%)	24 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	BA	194/198 (98%)	193 (100%)	1 (0%)	81	88
39	Bt	128/137 (93%)	122 (95%)	6 (5%)	23	56
40	BM	117/161 (73%)	117 (100%)	0	100	100
41	Ab	185/223 (83%)	183 (99%)	2 (1%)	65	82
42	BY	124/135 (92%)	124 (100%)	0	100	100
43	BB	344/347 (99%)	340 (99%)	4 (1%)	63	81
44	BS	154/154 (100%)	154 (100%)	0	100	100
45	Ac	189/232 (82%)	187 (99%)	2 (1%)	65	82
46	BZ	117/118 (99%)	117 (100%)	0	100	100
47	BC	302/336 (90%)	302 (100%)	0	100	100
48	BN	171/172 (99%)	171 (100%)	0	100	100
49	Ad	224/225 (100%)	224 (100%)	0	100	100
50	Ba	118/119 (99%)	118 (100%)	0	100	100
51	B	247/250 (99%)	247 (100%)	0	100	100
52	BO	171/173 (99%)	169 (99%)	2 (1%)	63	81
53	Ae	161/170 (95%)	161 (100%)	0	100	100
54	Bb	87/183 (48%)	87 (100%)	0	100	100
55	BE	216/251 (86%)	215 (100%)	1 (0%)	81	88
56	DA	137/355 (39%)	136 (99%)	1 (1%)	76	85
57	Af	207/218 (95%)	206 (100%)	1 (0%)	81	88
58	Bc	92/98 (94%)	92 (100%)	0	100	100
59	BF	197/215 (92%)	197 (100%)	0	100	100
60	DC	141/202 (70%)	140 (99%)	1 (1%)	76	85
61	Ag	170/360 (47%)	169 (99%)	1 (1%)	78	87
62	Bd	98/110 (89%)	98 (100%)	0	100	100
64	Ah	178/180 (99%)	177 (99%)	1 (1%)	78	87
65	Be	116/121 (96%)	116 (100%)	0	100	100
66	AA	75/76 (99%)	74 (99%)	1 (1%)	61	80
67	Ai	161/168 (96%)	160 (99%)	1 (1%)	78	87
68	Bf	89/89 (100%)	89 (100%)	0	100	100
69	AB	56/62 (90%)	55 (98%)	1 (2%)	51	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
70	Aj	87/136 (64%)	86 (99%)	1 (1%)	65	82
71	Bg	98/99 (99%)	97 (99%)	1 (1%)	68	83
72	AC	67/140 (48%)	67 (100%)	0	100	100
73	Ak	139/142 (98%)	139 (100%)	0	100	100
74	Bh	109/110 (99%)	109 (100%)	0	100	100
75	AD	47/106 (44%)	47 (100%)	0	100	100
76	Al	104/108 (96%)	101 (97%)	3 (3%)	37	68
77	Bi	86/89 (97%)	86 (100%)	0	100	100
78	AE	88/98 (90%)	86 (98%)	2 (2%)	44	72
79	Am	130/131 (99%)	130 (100%)	0	100	100
80	Bj	73/80 (91%)	73 (100%)	0	100	100
81	AF	272/275 (99%)	269 (99%)	3 (1%)	65	82
82	An	105/118 (89%)	102 (97%)	3 (3%)	37	68
83	Bk	64/65 (98%)	63 (98%)	1 (2%)	55	78
84	AG	48/49 (98%)	48 (100%)	0	100	100
85	Ao	114/130 (88%)	113 (99%)	1 (1%)	70	84
86	Bl	47/48 (98%)	47 (100%)	0	100	100
88	Ap	117/140 (84%)	117 (100%)	0	100	100
89	Bm	47/115 (41%)	47 (100%)	0	100	100
All	All	11381/13206 (86%)	11290 (99%)	91 (1%)	70	85

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Aq	73	LEU
5	Ar	59	LEU
5	Ar	60	THR
5	Ar	94	LYS
5	Ar	103	LEU
7	BL	81	LEU
7	BL	115	GLN
9	Bp	52	VAL
10	BQ	82	VAL
10	BQ	115	LYS
13	BR	106	LEU

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Mol	Chain	Res	Type
14	At	70	VAL
14	At	84	THR
16	BG	106	THR
16	BG	220	GLU
17	BU	97	ARG
17	BU	111	GLU
17	BU	117	ILE
18	Av	105	THR
19	DB	55	THR
19	DB	126	GLN
19	DB	210	LEU
19	DB	296	LEU
19	DB	306	PHE
19	DB	373	LEU
19	DB	374	LEU
19	DB	397	ILE
19	DB	401	ILE
19	DB	444	ILE
19	DB	534	THR
19	DB	547	VAL
19	DB	560	ILE
19	DB	662	THR
19	DB	683	PHE
19	DB	762	LEU
19	DB	839	MET
20	Ct	190	VAL
20	Ct	215	MET
23	Aw	105	PHE
23	Aw	125	VAL
26	BI	163	GLN
27	BW	68	GLN
30	Au	42	VAL
30	Au	61	ARG
32	AZ	112	ILE
32	AZ	121	LEU
32	AZ	206	ASP
33	Ay	44	LEU
36	Aa	127	VAL
36	Aa	178	THR
38	BA	32	VAL
39	Bt	12	VAL
39	Bt	15	LEU

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Mol	Chain	Res	Type
39	Bt	22	VAL
39	Bt	35	LEU
39	Bt	73	VAL
39	Bt	74	VAL
41	Ab	121	ARG
41	Ab	122	THR
43	BB	39	LYS
43	BB	90	VAL
43	BB	340	THR
43	BB	344	VAL
45	Ac	46	THR
45	Ac	175	VAL
52	BO	126	VAL
52	BO	174	LEU
55	BE	289	LEU
56	DA	74	ILE
57	Af	44	GLU
60	DC	153	GLN
61	Ag	53	VAL
64	Ah	46	VAL
66	AA	74	THR
67	Ai	55	LYS
69	AB	14	VAL
70	Aj	40	VAL
71	Bg	32	TYR
76	Al	75	ASN
76	Al	94	ILE
76	Al	104	VAL
78	AE	40	VAL
78	AE	75	VAL
81	AF	12	LYS
81	AF	266	ILE
81	AF	275	ILE
82	An	21	VAL
82	An	100	THR
82	An	113	GLN
83	Bk	36	VAL
85	Ao	133	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (146) such sidechains are listed below:

Mol	Chain	Res	Type
1	BP	75	GLN
1	BP	120	ASN
1	BP	137	ASN
2	Aq	56	HIS
2	Aq	121	GLN
6	Cu	76	ASN
8	BX	107	HIS
8	BX	111	GLN
10	BQ	125	GLN
11	As	12	GLN
12	Br	4	HIS
12	Br	6	GLN
12	Br	30	ASN
13	BR	39	GLN
13	BR	40	GLN
13	BR	143	HIS
15	Bs	34	ASN
15	Bs	41	GLN
15	Bs	179	ASN
15	Bs	195	ASN
16	BG	43	GLN
16	BG	64	GLN
16	BG	81	ASN
16	BG	236	HIS
17	BU	17	GLN
18	Av	90	GLN
18	Av	91	ASN
19	DB	23	HIS
19	DB	25	GLN
19	DB	124	GLN
19	DB	327	ASN
19	DB	435	GLN
19	DB	456	ASN
19	DB	509	HIS
19	DB	551	HIS
19	DB	569	HIS
19	DB	705	HIS
19	DB	749	ASN
19	DB	764	HIS
20	Ct	134	GLN
21	BH	39	ASN
21	BH	42	ASN
21	BH	98	HIS

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Mol	Chain	Res	Type
23	Aw	92	ASN
26	BI	59	GLN
26	BI	73	ASN
26	BI	163	GLN
27	BW	68	GLN
27	BW	120	GLN
28	Ax	15	ASN
28	Ax	19	GLN
28	Ax	85	ASN
30	Au	2	GLN
31	BJ	97	ASN
32	AZ	113	GLN
33	Ay	64	ASN
33	Ay	112	ASN
36	Aa	76	ASN
36	Aa	124	HIS
38	BA	50	HIS
38	BA	140	ASN
38	BA	205	ASN
39	Bt	118	HIS
40	BM	33	GLN
40	BM	34	ASN
40	BM	48	GLN
40	BM	125	ASN
41	Ab	115	GLN
42	BY	14	ASN
42	BY	61	HIS
43	BB	184	GLN
43	BB	289	GLN
43	BB	354	GLN
44	BS	173	ASN
45	Ac	4	GLN
46	BZ	78	ASN
47	BC	21	ASN
47	BC	48	ASN
47	BC	50	GLN
47	BC	61	GLN
47	BC	89	GLN
47	BC	212	ASN
47	BC	276	ASN
47	BC	310	HIS
47	BC	329	ASN

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Mol	Chain	Res	Type
49	Ad	142	HIS
50	Ba	34	ASN
50	Ba	60	HIS
51	B	122	GLN
51	B	275	GLN
52	BO	63	ASN
52	BO	180	GLN
53	Ae	65	GLN
53	Ae	82	ASN
53	Ae	83	ASN
53	Ae	118	ASN
54	Bb	50	ASN
55	BE	131	HIS
56	DA	18	GLN
56	DA	24	GLN
56	DA	52	ASN
56	DA	69	GLN
56	DA	95	HIS
58	Bc	33	GLN
58	Bc	40	GLN
59	BF	55	HIS
59	BF	57	HIS
59	BF	115	GLN
59	BF	118	ASN
60	DC	24	GLN
60	DC	25	ASN
60	DC	93	GLN
60	DC	101	ASN
60	DC	161	HIS
61	Ag	91	HIS
64	Ah	7	ASN
64	Ah	167	GLN
65	Be	34	ASN
66	AA	9	HIS
66	AA	29	ASN
66	AA	51	GLN
70	Aj	7	ASN
70	Aj	50	GLN
70	Aj	77	GLN
71	Bg	114	GLN
73	Ak	19	ASN
73	Ak	108	ASN

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Mol	Chain	Res	Type
74	Bh	98	HIS
75	AD	89	GLN
76	Al	28	HIS
77	Bi	15	HIS
77	Bi	26	HIS
78	AE	72	HIS
79	Am	36	GLN
80	Bj	30	GLN
80	Bj	57	ASN
80	Bj	66	HIS
81	AF	147	HIS
81	AF	159	ASN
81	AF	196	ASN
83	Bk	58	GLN
84	AG	37	ASN
86	Bl	25	GLN
88	Ap	97	GLN
88	Ap	114	GLN
89	Bm	117	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	B5	3694/4808 (76%)	434 (11%)	2 (0%)
29	B7	118/119 (99%)	6 (5%)	0
34	B8	155/158 (98%)	15 (9%)	0
4	AT	2/76 (2%)	1 (50%)	0
63	A2	1765/1870 (94%)	208 (11%)	1 (0%)
87	AH	0/3	-	-
All	All	5734/7034 (81%)	664 (11%)	3 (0%)

All (664) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	AT	76	A
24	B5	39	A
24	B5	42	A
24	B5	59	A
24	B5	64	A
24	B5	65	A
24	B5	85	G

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Mol	Chain	Res	Type
24	B5	91	G
24	B5	98	A
24	B5	109	G
24	B5	110	C
24	B5	119	G
24	B5	127	G
24	B5	135	G
24	B5	136	U
24	B5	144	G
24	B5	159	C
24	B5	181	C
24	B5	184	U
24	B5	187	U
24	B5	188	G
24	B5	200	U
24	B5	201	C
24	B5	209	U
24	B5	218	A
24	B5	219	G
24	B5	220	C
24	B5	233	U
24	B5	234	G
24	B5	266	C
24	B5	297	U
24	B5	309	C
24	B5	315	G
24	B5	316	U
24	B5	334	A
24	B5	340	C
24	B5	363	A
24	B5	386	A
24	B5	387	G
24	B5	398	A2M
24	B5	409	G
24	B5	412	G
24	B5	446	C
24	B5	449	C
24	B5	450	G
24	B5	452	A
24	B5	453	G
24	B5	454	U
24	B5	455	C

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Mol	Chain	Res	Type
24	B5	468	U
24	B5	482	U
24	B5	483	G
24	B5	485	U
24	B5	486	C
24	B5	488	G
24	B5	493	U
24	B5	497	G
24	B5	499	C
24	B5	502	U
24	B5	503	C
24	B5	504	U
24	B5	505	C
24	B5	506	G
24	B5	512	U
24	B5	515	U
24	B5	516	U
24	B5	517	C
24	B5	628	U
24	B5	634	C
24	B5	635	G
24	B5	660	G
24	B5	691	G
24	B5	698	C
24	B5	725	G
24	B5	732	C
24	B5	734	G
24	B5	739	G
24	B5	758	C
24	B5	759	G
24	B5	760	C
24	B5	790	G
24	B5	791	C
24	B5	792	G
24	B5	794	G
24	B5	795	A
24	B5	797	C
24	B5	798	C
24	B5	810	U
24	B5	812	A
24	B5	814	A
24	B5	815	G

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Mol	Chain	Res	Type
24	B5	824	C
24	B5	825	G
24	B5	831	A
24	B5	832	G
24	B5	833	C
24	B5	834	A
24	B5	835	G
24	B5	843	A
24	B5	844	A
24	B5	845	U
24	B5	856	A
24	B5	859	G
24	B5	860	A
24	B5	861	G
24	B5	866	A
24	B5	867	C
24	B5	868	C
24	B5	869	U
24	B5	870	G
24	B5	884	U
24	B5	983	G
24	B5	985	G
24	B5	987	C
24	B5	1072	C
24	B5	1073	C
24	B5	1074	C
24	B5	1090	U
24	B5	1091	G
24	B5	1102	G
24	B5	1105	C
24	B5	1106	U
24	B5	1124	A
24	B5	1127	G
24	B5	1133	C
24	B5	1140	C
24	B5	1202	C
24	B5	1214	A
24	B5	1215	G
24	B5	1217	G
24	B5	1219	G
24	B5	1221	G
24	B5	1228	G

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Mol	Chain	Res	Type
24	B5	1231	G
24	B5	1238	A
24	B5	1240	G
24	B5	1246	U
24	B5	1247	A
24	B5	1270	A2M
24	B5	1298	A
24	B5	1299	G
24	B5	1303	G
24	B5	1309	C
24	B5	1310	G
24	B5	1323	C
24	B5	1331	A
24	B5	1341	A
24	B5	1351	G
24	B5	1362	C
24	B5	1375	A
24	B5	1391	C
24	B5	1393	C
24	B5	1401	C
24	B5	1452	A
24	B5	1453	G
24	B5	1457	G
24	B5	1469	U
24	B5	1489	A2M
24	B5	1502	A
24	B5	1521	C
24	B5	1533	U
24	B5	1546	U
24	B5	1551	U
24	B5	1579	G
24	B5	1580	OMG
24	B5	1586	A
24	B5	1588	G
24	B5	1589	A
24	B5	1593	A
24	B5	1609	G
24	B5	1616	C
24	B5	1631	C
24	B5	1632	PSU
24	B5	1653	C
24	B5	1657	C

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Mol	Chain	Res	Type
24	B5	1658	C
24	B5	1673	G
24	B5	1704	A
24	B5	1705	A
24	B5	1726	A
24	B5	1743	A
24	B5	1774	G
24	B5	1775	G
24	B5	1776	A
24	B5	1781	G
24	B5	1794	G
24	B5	1808	G
24	B5	1836	A
24	B5	1857	U
24	B5	1859	C
24	B5	1860	C
24	B5	1861	G
24	B5	1870	C
24	B5	1871	A
24	B5	1879	G
24	B5	1898	U
24	B5	1899	A
24	B5	1900	G
24	B5	1913	U
24	B5	1914	G
24	B5	1922	A
24	B5	1923	A
24	B5	1924	G
24	B5	1925	U
24	B5	1926	C
24	B5	1936	U
24	B5	1940	G
24	B5	1942	G
24	B5	1943	U
24	B5	1963	G
24	B5	1965	A
24	B5	1985	G
24	B5	1987	U
24	B5	1994	G
24	B5	1995	G
24	B5	2008	A
24	B5	2023	U

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Mol	Chain	Res	Type
24	B5	2032	G
24	B5	2034	A
24	B5	2037	G
24	B5	2041	G
24	B5	2044	A
24	B5	2045	G
24	B5	2046	A
24	B5	2132	C
24	B5	2143	A
24	B5	2144	G
24	B5	2156	A
24	B5	2159	G
24	B5	2174	G
24	B5	2191	G
24	B5	2194	OMC
24	B5	2203	A
24	B5	2207	OMG
24	B5	2238	A
24	B5	2241	U
24	B5	2253	C
24	B5	2264	G
24	B5	2268	U
24	B5	2332	C
24	B5	2333	U
24	B5	2334	C
24	B5	2349	G
24	B5	2356	A
24	B5	2372	A
24	B5	2380	A
24	B5	2387	G
24	B5	2388	U
24	B5	2390	G
24	B5	2409	G
24	B5	2429	G
24	B5	2430	A
24	B5	2432	C
24	B5	2444	A
24	B5	2470	C
24	B5	2496	C
24	B5	2503	A
24	B5	2512	C
24	B5	2530	U

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Mol	Chain	Res	Type
24	B5	2537	G
24	B5	2538	A
24	B5	2539	A
24	B5	2546	G
24	B5	2551	U
24	B5	2552	C
24	B5	2553	C
24	B5	2554	G
24	B5	2586	A
24	B5	2606	U
24	B5	2612	U
24	B5	2630	A2M
24	B5	2631	U
24	B5	2633	U
24	B5	2641	A
24	B5	2657	C
24	B5	2669	U
24	B5	2670	G
24	B5	2672	U
24	B5	2698	G
24	B5	2745	G
24	B5	3329	G
24	B5	3350	C
24	B5	3358	G
24	B5	3362	A
24	B5	3367	A
24	B5	3380	A
24	B5	3385	A
24	B5	3394	A
24	B5	3405	C
24	B5	3424	A
24	B5	3443	A
24	B5	3444	A
24	B5	3485	G
24	B5	3492	A2M
24	B5	3493	C
24	B5	3498	A
24	B5	3508	G
24	B5	3509	G
24	B5	3516	A
24	B5	3543	G
24	B5	3546	U

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Mol	Chain	Res	Type
24	B5	3549	A
24	B5	3551	G
24	B5	3570	U
24	B5	3572	U
24	B5	3609	A
24	B5	3610	C
24	B5	3611	G
24	B5	3629	G
24	B5	3633	A
24	B5	3638	A
24	B5	3639	G
24	B5	3640	A
24	B5	3647	U
24	B5	3670	G
24	B5	3804	G
24	B5	3812	G
24	B5	3823	G
24	B5	3824	C
24	B5	3825	G
24	B5	3832	G
24	B5	3833	A
24	B5	3834	G
24	B5	3847	C
24	B5	3850	G
24	B5	3855	A
24	B5	3869	G
24	B5	3875	C
24	B5	3891	C
24	B5	3892	G
24	B5	3904	C
24	B5	3909	U
24	B5	3916	A
24	B5	3929	G
24	B5	3930	G
24	B5	3937	G
24	B5	3949	A
24	B5	3975	U
24	B5	3979	A
24	B5	3997	A
24	B5	4000	G
24	B5	4012	G
24	B5	4014	A

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Mol	Chain	Res	Type
24	B5	4017	A
24	B5	4019	A
24	B5	4027	A
24	B5	4050	A
24	B5	4051	G
24	B5	4052	OMU
24	B5	4076	G
24	B5	4078	C
24	B5	4096	C
24	B5	4100	U
24	B5	4119	G
24	B5	4123	G
24	B5	4124	A
24	B5	4126	A
24	B5	4133	C
24	B5	4137	G
24	B5	4140	A
24	B5	4167	C
24	B5	4168	A
24	B5	4183	U
24	B5	4194	G
24	B5	4210	A
24	B5	4212	C
24	B5	4221	G
24	B5	4258	U
24	B5	4259	A
24	B5	4270	G
24	B5	4294	A
24	B5	4306	C
24	B5	4313	G
24	B5	4321	G
24	B5	4336	A2M
24	B5	4373	U
24	B5	4381	A
24	B5	4382	PSU
24	B5	4383	OMG
24	B5	4402	A
24	B5	4416	C
24	B5	4418	A
24	B5	4437	A
24	B5	4446	A
24	B5	4454	A

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Mol	Chain	Res	Type
24	B5	4455	U
24	B5	4465	G
24	B5	4475	A
24	B5	4476	C
24	B5	4477	G
24	B5	4478	G
24	B5	4486	G
24	B5	4487	A
24	B5	4488	A
24	B5	4489	G
24	B5	4490	G
24	B5	4492	G
24	B5	4498	G
24	B5	4501	G
24	B5	4504	C
24	B5	4506	C
24	B5	4508	G
24	B5	4512	G
24	B5	4518	C
24	B5	4609	G
24	B5	4610	C
24	B5	4614	G
24	B5	4621	U
24	B5	4622	C
24	B5	4634	U
24	B5	4638	G
24	B5	4639	C
24	B5	4640	G
24	B5	4644	C
24	B5	4645	C
24	B5	4646	G
24	B5	4649	A
24	B5	4651	G
24	B5	4658	G
24	B5	4674	C
24	B5	4705	A
24	B5	4715	U
24	B5	4728	U
24	B5	4729	C
24	B5	4753	A
24	B5	4756	G
24	B5	4761	U

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Mol	Chain	Res	Type
24	B5	4762	C
24	B5	4763	C
24	B5	4780	G
24	B5	4786	C
24	B5	4789	C
24	B5	4793	C
24	B5	4801	G
24	B5	4808	U
29	B7	7	G
29	B7	53	U
29	B7	54	A
29	B7	64	G
29	B7	110	G
29	B7	120	U
34	B8	34	U
34	B8	35	C
34	B8	39	G
34	B8	59	A
34	B8	62	A
34	B8	63	U
34	B8	81	C
34	B8	84	A
34	B8	87	G
34	B8	94	G
34	B8	103	A
34	B8	105	C
34	B8	110	U
34	B8	114	G
34	B8	156	U
63	A2	2	A
63	A2	3	C
63	A2	26	U
63	A2	33	G
63	A2	41	G
63	A2	46	A
63	A2	56	G
63	A2	67	C
63	A2	68	A
63	A2	73	C
63	A2	74	G
63	A2	77	A
63	A2	79	A

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Mol	Chain	Res	Type
63	A2	103	A
63	A2	113	G
63	A2	115	U
63	A2	126	G
63	A2	130	G
63	A2	143	U
63	A2	147	A
63	A2	155	G
63	A2	168	C
63	A2	178	C
63	A2	180	G
63	A2	184	G
63	A2	188	C
63	A2	192	C
63	A2	226	A
63	A2	282	C
63	A2	306	U
63	A2	310	G
63	A2	313	G
63	A2	320	C
63	A2	324	C
63	A2	325	U
63	A2	327	C
63	A2	328	G
63	A2	336	G
63	A2	348	G
63	A2	363	C
63	A2	365	A
63	A2	369	U
63	A2	370	C
63	A2	386	G
63	A2	387	C
63	A2	401	C
63	A2	410	C
63	A2	422	G
63	A2	439	G
63	A2	449	A
63	A2	451	C
63	A2	465	A
63	A2	466	A
63	A2	472	G
63	A2	473	C

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Mol	Chain	Res	Type
63	A2	474	A
63	A2	475	G
63	A2	483	G
63	A2	488	U
63	A2	493	C
63	A2	509	A
63	A2	513	A2M
63	A2	526	A
63	A2	549	C
63	A2	565	A
63	A2	569	C
63	A2	584	A
63	A2	590	G
63	A2	592	U
63	A2	607	G
63	A2	608	U
63	A2	609	C
63	A2	615	C
63	A2	632	U
63	A2	644	A
63	A2	645	OMG
63	A2	656	A
63	A2	661	C
63	A2	669	A2M
63	A2	670	A
63	A2	672	A
63	A2	673	A
63	A2	734	C
63	A2	747	C
63	A2	748	U
63	A2	754	C
63	A2	755	G
63	A2	756	C
63	A2	799	G
63	A2	812	A
63	A2	822	G
63	A2	823	PSU
63	A2	831	A
63	A2	832	G
63	A2	837	G
63	A2	838	A
63	A2	839	G

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Mol	Chain	Res	Type
63	A2	840	C
63	A2	841	C
63	A2	842	G
63	A2	848	A
63	A2	871	A
63	A2	873	A
63	A2	879	G
63	A2	886	U
63	A2	892	G
63	A2	914	A
63	A2	915	U
63	A2	921	A
63	A2	923	A
63	A2	934	G
63	A2	944	U
63	A2	956	A
63	A2	964	A
63	A2	972	G
63	A2	991	A
63	A2	993	A
63	A2	1000	G
63	A2	1024	A
63	A2	1061	A
63	A2	1062	U
63	A2	1063	A
63	A2	1084	A
63	A2	1086	C
63	A2	1116	U
63	A2	1117	C
63	A2	1118	C
63	A2	1119	C
63	A2	1122	G
63	A2	1134	A
63	A2	1145	A
63	A2	1154	C
63	A2	1155	U
63	A2	1196	A
63	A2	1216	C
63	A2	1225	G
63	A2	1243	U
63	A2	1252	A
63	A2	1254	A

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Mol	Chain	Res	Type
63	A2	1257	G
63	A2	1258	G
63	A2	1260	A
63	A2	1272	C
63	A2	1275	G
63	A2	1276	G
63	A2	1303	G
63	A2	1304	C
63	A2	1343	U
63	A2	1372	U
63	A2	1373	U
63	A2	1379	A
63	A2	1398	U
63	A2	1403	A
63	A2	1406	A
63	A2	1407	G
63	A2	1419	C
63	A2	1420	C
63	A2	1422	A
63	A2	1424	C
63	A2	1425	G
63	A2	1436	C
63	A2	1448	OMG
63	A2	1455	A
63	A2	1463	U
63	A2	1464	U
63	A2	1481	A
63	A2	1488	A
63	A2	1490	A
63	A2	1491	OMG
63	A2	1495	U
63	A2	1498	G
63	A2	1510	U
63	A2	1522	C
63	A2	1523	A
63	A2	1534	A
63	A2	1553	G
63	A2	1554	C
63	A2	1580	A
63	A2	1581	A
63	A2	1586	U
63	A2	1589	A

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Mol	Chain	Res	Type
63	A2	1602	A
63	A2	1618	G
63	A2	1622	U
63	A2	1624	A
63	A2	1647	C
63	A2	1655	G
63	A2	1662	A
63	A2	1666	G
63	A2	1699	C
63	A2	1722	U
63	A2	1723	G
63	A2	1749	G
63	A2	1783	G
63	A2	1784	C
63	A2	1785	G
63	A2	1830	G
63	A2	1832	A
63	A2	1836	A
63	A2	1837	G
63	A2	1839	U
63	A2	1850	G
63	A2	1852	MA6
63	A2	1862	G
63	A2	1863	G
63	A2	1864	A
63	A2	1865	U
63	A2	1866	C

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	B5	1588	G
24	B5	4445	U
63	A2	1	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
63	PSU	A2	1239	63	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
89	M3L	Bm	98	89	10,11,12	0.83	0	9,14,16	0.53	0
63	OMU	A2	429	63	19,22,23	1.20	2 (10%)	26,31,34	1.69	4 (15%)
47	AYA	BC	2	47	6,7,8	0.71	0	5,8,10	0.36	0
63	PSU	A2	36	63	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
24	PSU	B5	1718	24	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
24	PSU	B5	4298	24	18,21,22	1.33	2 (11%)	22,30,33	1.90	3 (13%)
24	A2M	B5	3557	24	22,25,26	1.46	4 (18%)	31,36,39	2.13	10 (32%)
24	PSU	B5	4169	24	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
24	OMG	B5	1477	24	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
63	PSU	A2	109	63	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
63	PSU	A2	1057	63	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
24	PSU	B5	1491	24	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
24	PSU	B5	4267	90,24	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
63	PSU	A2	967	63	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
24	OMG	B5	4240	24	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
24	PSU	B5	3462	24	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
63	PSU	A2	573	63	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
63	A2M	A2	577	63	22,25,26	1.47	4 (18%)	31,36,39	2.11	10 (32%)
63	OMG	A2	645	63	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
63	PSU	A2	1046	63	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
63	PSU	A2	1175	63	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
24	A2M	B5	400	24	22,25,26	1.47	4 (18%)	31,36,39	2.09	10 (32%)
24	PSU	B5	3585	90,24	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
63	PSU	A2	610	63	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
38	V5N	BA	216	38	9,11,12	2.09	2 (22%)	9,14,16	1.72	2 (22%)
63	OMG	A2	1448	63	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
24	A2M	B5	4269	90,24	22,25,26	1.46	4 (18%)	31,36,39	2.13	10 (32%)
30	AME	Au	1	30	9,10,11	0.48	0	9,11,13	0.86	1 (11%)
24	OMG	B5	1260	24	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
24	UY1	B5	3550	24	19,22,23	1.39	3 (15%)	22,31,34	1.89	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
63	4AC	A2	1843	63	21,24,25	1.11	2 (9%)	29,34,37	1.27	3 (10%)
63	PSU	A2	1693	63	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
63	OMU	A2	1443	90,63	19,22,23	1.24	3 (15%)	26,31,34	1.69	5 (19%)
24	OMG	B5	3524	24	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
63	PSU	A2	867	63	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
24	6MZ	B5	3966	24	22,25,26	1.44	4 (18%)	30,36,39	2.18	9 (30%)
34	OMG	B8	75	34	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
24	OMC	B5	2647	24	19,22,23	0.81	0	26,31,34	0.82	0
63	OMG	A2	868	63	23,26,27	1.18	3 (13%)	33,38,41	1.92	6 (18%)
24	PSU	B5	3554	24	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
24	OMC	B5	2208	90,24	19,22,23	0.81	0	26,31,34	0.83	0
24	PSU	B5	4374	24	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
63	PSU	A2	119	63	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
63	PSU	A2	1626	63	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
63	OMC	A2	174	90,63	19,22,23	0.81	0	26,31,34	0.82	0
63	PSU	A2	650	63	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
63	PSU	A2	1082	63	18,21,22	1.36	2 (11%)	22,30,33	1.84	3 (13%)
63	PSU	A2	407	63	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
24	OMC	B5	4202	24	19,22,23	0.81	0	26,31,34	0.77	0
24	OMC	B5	2704	24	19,22,23	0.81	0	26,31,34	0.83	0
24	PSU	B5	4749	24	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
43	HIC	BB	245	43	10,11,12	0.61	0	8,14,16	0.39	0
63	A2M	A2	1679	63	22,25,26	1.45	4 (18%)	31,36,39	2.24	10 (32%)
63	MA6	A2	1851	63	23,26,27	2.28	5 (21%)	34,38,41	3.71	13 (38%)
24	PSU	B5	4099	24	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
63	6MZ	A2	1833	90,63	22,25,26	1.45	4 (18%)	30,36,39	2.16	9 (30%)
63	A2M	A2	669	90,63	22,25,26	1.45	4 (18%)	31,36,39	2.12	10 (32%)
24	OMG	B5	2207	24	23,26,27	1.18	3 (13%)	33,38,41	1.93	6 (18%)
24	PSU	B5	4435	24	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
63	PSU	A2	34	63	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
24	UR3	B5	4276	24	19,22,23	0.99	0	26,32,35	1.41	1 (3%)
63	A2M	A2	513	63	22,25,26	1.48	4 (18%)	31,36,39	2.13	10 (32%)
24	PSU	B5	2351	24	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
24	OMG	B5	4369	24	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
24	A2M	B5	2206	90,24	22,25,26	1.47	4 (18%)	31,36,39	2.11	9 (29%)
24	OMG	B5	4138	24	23,26,27	1.19	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
24	PSU	B5	3427	24	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
24	PSU	B5	4177	24	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
24	A2M	B5	2658	90,24	22,25,26	1.46	4 (18%)	31,36,39	2.10	9 (29%)
24	OMG	B5	3676	24	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
24	A2M	B5	2244	90,24	22,25,26	1.47	4 (18%)	31,36,39	2.14	10 (32%)
63	PSU	A2	218	63	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
24	PSU	B5	3500	24	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
63	A2M	A2	99	90,63	22,25,26	1.47	4 (18%)	31,36,39	2.13	9 (29%)
63	PSU	A2	1233	63	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
24	PSU	B5	4042	24	18,21,22	1.33	2 (11%)	22,30,33	1.90	3 (13%)
24	A2M	B5	3450	24	22,25,26	1.47	4 (18%)	31,36,39	2.11	9 (29%)
24	A2M	B5	4317	24	22,25,26	1.47	4 (18%)	31,36,39	2.14	9 (29%)
63	PSU	A2	93	63	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
24	OMU	B5	4244	24	19,22,23	1.21	2 (10%)	26,31,34	1.70	5 (19%)
63	OMU	A2	355	63	19,22,23	1.23	2 (10%)	26,31,34	1.71	4 (15%)
24	PSU	B5	3466	24	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
24	PSU	B5	1799	24	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
24	PSU	B5	3494	24	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
24	PSU	B5	4149	24	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
24	PSU	B5	4217	24	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
63	OMU	A2	1805	63	19,22,23	1.22	3 (15%)	26,31,34	1.69	4 (15%)
63	B8N	A2	1249	63	24,29,30	1.31	3 (12%)	29,42,45	1.30	3 (10%)
63	4AC	A2	1338	63	21,24,25	1.07	2 (9%)	29,34,37	1.21	3 (10%)
63	PSU	A2	802	63	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
63	OMU	A2	121	63	19,22,23	1.21	3 (15%)	26,31,34	1.66	4 (15%)
24	OMG	B5	4245	24	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
24	A2M	B5	3517	24	22,25,26	1.44	4 (18%)	31,36,39	2.22	11 (35%)
24	PSU	B5	3652	90,24	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
63	PSU	A2	105	63	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
63	PSU	A2	682	63	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
63	OMC	A2	463	63	19,22,23	0.81	0	26,31,34	0.86	1 (3%)
24	OMG	B5	2267	24	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
24	OMC	B5	3573	24	19,22,23	0.81	0	26,31,34	0.91	1 (3%)
24	OMC	B5	3601	24	19,22,23	0.81	0	26,31,34	0.80	0
50	V5N	Ba	39	50	9,11,12	2.09	2 (22%)	9,14,16	1.71	2 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	PSU	B5	4058	24	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
63	A2M	A2	591	63	22,25,26	1.49	4 (18%)	31,36,39	2.20	7 (22%)
63	A2M	A2	1032	63	22,25,26	1.46	4 (18%)	31,36,39	2.11	10 (32%)
24	A2M	B5	1270	24	22,25,26	1.46	4 (18%)	31,36,39	2.10	10 (32%)
24	OMC	B5	3433	24	19,22,23	0.79	0	26,31,34	0.75	0
24	PSU	B5	3583	24	18,21,22	1.36	2 (11%)	22,30,33	1.84	3 (13%)
24	OMC	B5	4282	90,24	19,22,23	0.82	0	26,31,34	0.85	0
24	A2M	B5	1479	24	22,25,26	1.46	4 (18%)	31,36,39	2.11	8 (25%)
63	PSU	A2	1047	63	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
24	OMG	B5	4116	24	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
63	A2M	A2	485	63	22,25,26	1.47	4 (18%)	31,36,39	2.09	9 (29%)
24	PSU	B5	2475	24	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
24	PSU	B5	4278	24	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
24	PSU	B5	4382	24	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
24	A2M	B5	1489	90,24	22,25,26	1.46	4 (18%)	31,36,39	2.09	9 (29%)
24	OMG	B5	3359	24	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
63	PSU	A2	864	63	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
24	PSU	B5	4166	24	18,21,22	1.37	2 (11%)	22,30,33	1.81	3 (13%)
63	OMG	A2	684	63	23,26,27	1.19	3 (13%)	33,38,41	1.92	6 (18%)
24	PSU	B5	1720	24	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
24	PSU	B5	1638	24	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
63	PSU	A2	210	63	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
24	OMC	B5	3540	24	19,22,23	0.82	0	26,31,34	0.81	0
24	PSU	B5	3447	24	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
24	A2M	B5	4336	24	22,25,26	1.45	4 (18%)	31,36,39	2.15	10 (32%)
63	OMG	A2	510	90,63	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
63	PSU	A2	1368	63	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
63	OMG	A2	437	63	23,26,27	1.19	3 (13%)	33,38,41	1.95	6 (18%)
63	A2M	A2	469	63	22,25,26	1.47	4 (18%)	31,36,39	2.12	9 (29%)
24	PSU	B5	4107	24	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
34	PSU	B8	55	34	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
63	PSU	A2	816	63	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
63	PSU	A2	1348	63	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
24	PSU	B5	3496	24	18,21,22	1.33	2 (11%)	22,30,33	1.86	3 (13%)
24	OMG	B5	3974	24	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
63	OMC	A2	518	63	19,22,23	0.82	0	26,31,34	0.81	0
24	A2M	B5	2630	90,24	22,25,26	1.45	4 (18%)	31,36,39	2.15	9 (29%)
24	1MA	B5	1266	90,24	21,25,26	1.38	4 (19%)	31,37,40	1.71	5 (16%)
63	MA6	A2	1852	63	23,26,27	2.25	5 (21%)	34,38,41	3.68	13 (38%)
24	OMU	B5	3657	24	19,22,23	1.23	2 (10%)	26,31,34	1.71	4 (15%)
24	PSU	B5	3576	24	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
24	PSU	B5	4740	24	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
24	PSU	B5	1537	24	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
24	OMC	B5	2265	90,24	19,22,23	0.82	0	26,31,34	0.90	1 (3%)
63	OMU	A2	172	63	19,22,23	1.20	2 (10%)	26,31,34	1.68	5 (19%)
63	OMU	A2	116	63	19,22,23	1.18	2 (10%)	26,31,34	1.69	5 (19%)
63	A2M	A2	1384	63	22,25,26	1.47	4 (18%)	31,36,39	2.11	10 (32%)
24	OMC	B5	1820	90,24	19,22,23	0.80	0	26,31,34	0.79	0
82	IAS	An	138	82	6,7,8	0.97	0	6,8,10	1.38	1 (16%)
63	PSU	A2	1178	63	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
63	PSU	A2	1005	63	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
23	HY3	Aw	62	23	6,8,9	2.06	1 (16%)	5,10,12	1.12	1 (20%)
24	PSU	B5	3502	24	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
63	A2M	A2	27	90,63	22,25,26	1.47	4 (18%)	31,36,39	2.13	9 (29%)
24	PSU	B5	4039	24	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
24	5MC	B5	4193	24	18,22,23	0.99	2 (11%)	26,32,35	1.17	2 (7%)
3	MLZ	Bo	53	3	8,9,10	0.40	0	4,9,11	0.15	0
63	OMG	A2	1329	63	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
63	PSU	A2	687	63	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
24	OMC	B5	1284	24	19,22,23	0.81	0	26,31,34	0.79	0
11	NMM	As	67	11	9,11,12	0.60	0	6,12,14	0.43	0
24	PSU	B5	1801	24	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
63	PSU	A2	1245	63	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
63	OMC	A2	1392	63	19,22,23	0.82	0	26,31,34	0.83	0
24	PSU	B5	4045	24	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
24	OMU	B5	4052	24	19,22,23	1.22	3 (15%)	26,31,34	1.69	4 (15%)
24	PSU	B5	1632	24	18,21,22	1.36	2 (11%)	22,30,33	1.87	4 (18%)
24	PSU	B5	1721	24	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
24	PSU	B5	4203	24	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
63	PSU	A2	1446	63	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
24	OMG	B5	4383	24	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SAC	Ar	2	5	7,8,9	0.54	0	8,9,11	0.90	1 (12%)
24	OMU	B5	2680	24	19,22,23	1.21	2 (10%)	26,31,34	1.72	4 (15%)
63	OMU	A2	1289	63	19,22,23	1.23	3 (15%)	26,31,34	1.68	5 (19%)
12	SAC	Br	2	12	7,8,9	0.52	0	8,9,11	0.83	1 (12%)
24	PSU	B5	4419	24	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
63	OMC	A2	1704	63	19,22,23	0.82	0	26,31,34	0.85	1 (3%)
63	G7M	A2	1640	63	23,26,27	3.14	9 (39%)	35,39,42	3.33	13 (37%)
63	OMG	A2	602	63	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
54	MLZ	Bb	5	54	8,9,10	0.49	0	4,9,11	0.18	0
24	5MC	B5	3514	90,24	18,22,23	0.95	2 (11%)	26,32,35	1.14	3 (11%)
24	OMC	B5	2194	90,24	19,22,23	0.82	0	26,31,34	0.90	1 (3%)
63	A2M	A2	159	63	22,25,26	1.47	4 (18%)	31,36,39	2.15	10 (32%)
63	PSU	A2	823	63	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
24	PSU	B5	1731	24	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
24	OMU	B5	2258	24	19,22,23	1.22	3 (15%)	26,31,34	1.67	4 (15%)
24	OMG	B5	3631	24	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
63	OMU	A2	1327	90,63	19,22,23	1.18	2 (10%)	26,31,34	1.71	5 (19%)
24	PSU	B5	1683	24	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
24	PSU	B5	3490	24	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
24	PSU	B5	4325	24	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
24	A2M	B5	3456	24	22,25,26	1.47	4 (18%)	31,36,39	2.14	10 (32%)
34	PSU	B8	69	34	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
24	OMG	B5	3942	4,24	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
24	PSU	B5	4188	24	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
24	A2M	B5	398	24	22,25,26	1.47	4 (18%)	31,36,39	2.16	10 (32%)
24	PSU	B5	4322	24	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
24	A2M	B5	3492	24,63	22,25,26	1.47	4 (18%)	31,36,39	2.17	10 (32%)
24	OMU	B5	4366	24	19,22,23	1.22	2 (10%)	26,31,34	1.71	4 (15%)
24	OMU	B5	3973	24	19,22,23	1.22	3 (15%)	26,31,34	1.70	4 (15%)
24	OMG	B5	1580	24	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
24	PSU	B5	3369	24	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
24	PSU	B5	3371	24	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
63	OMU	A2	628	63	19,22,23	1.17	2 (10%)	26,31,34	1.69	5 (19%)
24	OMG	B5	3476	24	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
24	OMG	B5	2719	24	23,26,27	1.20	3 (13%)	33,38,41	1.97	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	PSU	B5	4246	24	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
63	PSU	A2	815	63	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
24	OMC	B5	2667	24	19,22,23	0.81	0	26,31,34	0.80	0
24	OMG	B5	4364	24	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
24	A2M	B5	3599	24	22,25,26	1.46	4 (18%)	31,36,39	2.13	9 (29%)
63	OMG	A2	1491	90,63	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
63	PSU	A2	652	63	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
24	PSU	B5	3616	24	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
63	PSU	A2	1644	90,63	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
24	OMC	B5	3619	24	19,22,23	0.81	0	26,31,34	0.84	0
24	A2M	B5	1810	90,24	22,25,26	1.47	4 (18%)	31,36,39	2.18	10 (32%)
24	A2M	B5	3562	24	22,25,26	1.47	4 (18%)	31,36,39	2.15	10 (32%)
32	SAC	AZ	2	32	7,8,9	0.53	0	8,9,11	0.86	1 (12%)
24	PSU	B5	4711	24	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
63	A2M	A2	166	63	22,25,26	1.46	4 (18%)	31,36,39	2.17	10 (32%)

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
63	PSU	A2	1239	63	-	0/7/25/26	0/2/2/2
89	M3L	Bm	98	89	-	0/9/10/12	-
63	OMU	A2	429	63	-	6/9/27/28	0/2/2/2
47	AYA	BC	2	47	-	3/4/6/8	-
63	PSU	A2	36	63	-	0/7/25/26	0/2/2/2
24	PSU	B5	1718	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	4298	24	-	0/7/25/26	0/2/2/2
24	A2M	B5	3557	24	-	1/9/27/28	0/3/3/3
24	PSU	B5	4169	24	-	0/7/25/26	0/2/2/2
24	OMG	B5	1477	24	-	0/9/27/28	0/3/3/3
63	PSU	A2	109	63	-	0/7/25/26	0/2/2/2
63	PSU	A2	1057	63	-	0/7/25/26	0/2/2/2
24	PSU	B5	1491	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	4267	90,24	-	0/7/25/26	0/2/2/2
63	PSU	A2	967	63	-	0/7/25/26	0/2/2/2
24	OMG	B5	4240	24	-	0/9/27/28	0/3/3/3
24	PSU	B5	3462	24	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	PSU	A2	573	63	-	0/7/25/26	0/2/2/2
63	A2M	A2	577	63	-	2/9/27/28	0/3/3/3
63	OMG	A2	645	63	-	3/9/27/28	0/3/3/3
63	PSU	A2	1046	63	-	0/7/25/26	0/2/2/2
63	PSU	A2	1175	63	-	0/7/25/26	0/2/2/2
24	A2M	B5	400	24	-	0/9/27/28	0/3/3/3
24	PSU	B5	3585	90,24	-	0/7/25/26	0/2/2/2
63	PSU	A2	610	63	-	0/7/25/26	0/2/2/2
38	V5N	BA	216	38	-	3/9/10/12	0/1/1/1
63	OMG	A2	1448	63	-	3/9/27/28	0/3/3/3
24	A2M	B5	4269	90,24	-	0/9/27/28	0/3/3/3
30	AME	Au	1	30	-	2/9/10/12	-
24	OMG	B5	1260	24	-	1/9/27/28	0/3/3/3
24	UY1	B5	3550	24	-	1/9/27/28	0/2/2/2
63	4AC	A2	1843	63	-	4/11/29/30	0/2/2/2
63	PSU	A2	1693	63	-	0/7/25/26	0/2/2/2
63	OMU	A2	1443	90,63	-	0/9/27/28	0/2/2/2
24	OMG	B5	3524	24	-	0/9/27/28	0/3/3/3
63	PSU	A2	867	63	-	0/7/25/26	0/2/2/2
24	6MZ	B5	3966	24	-	0/9/27/28	0/3/3/3
34	OMG	B8	75	34	-	0/9/27/28	0/3/3/3
24	OMC	B5	2647	24	-	0/9/27/28	0/2/2/2
63	OMG	A2	868	63	-	2/9/27/28	0/3/3/3
24	PSU	B5	3554	24	-	0/7/25/26	0/2/2/2
24	OMC	B5	2208	90,24	-	0/9/27/28	0/2/2/2
24	PSU	B5	4374	24	-	0/7/25/26	0/2/2/2
63	PSU	A2	119	63	-	0/7/25/26	0/2/2/2
63	PSU	A2	1626	63	-	0/7/25/26	0/2/2/2
63	OMC	A2	174	90,63	-	0/9/27/28	0/2/2/2
63	PSU	A2	650	63	-	0/7/25/26	0/2/2/2
63	PSU	A2	1082	63	-	0/7/25/26	0/2/2/2
63	PSU	A2	407	63	-	0/7/25/26	0/2/2/2
24	OMC	B5	4202	24	-	0/9/27/28	0/2/2/2
24	OMC	B5	2704	24	-	1/9/27/28	0/2/2/2
24	PSU	B5	4749	24	-	0/7/25/26	0/2/2/2
43	HIC	BB	245	43	-	2/5/6/8	0/1/1/1
63	A2M	A2	1679	63	-	0/9/27/28	0/3/3/3
63	MA6	A2	1851	63	-	0/11/29/30	0/3/3/3
24	PSU	B5	4099	24	-	0/7/25/26	0/2/2/2
63	6MZ	A2	1833	90,63	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	A2M	A2	669	90,63	-	3/9/27/28	0/3/3/3
24	OMG	B5	2207	24	-	3/9/27/28	0/3/3/3
24	PSU	B5	4435	24	-	0/7/25/26	0/2/2/2
63	PSU	A2	34	63	-	0/7/25/26	0/2/2/2
24	UR3	B5	4276	24	-	0/7/25/26	0/2/2/2
63	A2M	A2	513	63	-	2/9/27/28	0/3/3/3
24	PSU	B5	2351	24	-	0/7/25/26	0/2/2/2
24	OMG	B5	4369	24	-	0/9/27/28	0/3/3/3
24	A2M	B5	2206	90,24	-	0/9/27/28	0/3/3/3
24	OMG	B5	4138	24	-	1/9/27/28	0/3/3/3
24	PSU	B5	3427	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	4177	24	-	0/7/25/26	0/2/2/2
24	A2M	B5	2658	90,24	-	0/9/27/28	0/3/3/3
24	OMG	B5	3676	24	-	2/9/27/28	0/3/3/3
24	A2M	B5	2244	90,24	-	0/9/27/28	0/3/3/3
63	PSU	A2	218	63	-	0/7/25/26	0/2/2/2
24	PSU	B5	3500	24	-	0/7/25/26	0/2/2/2
63	A2M	A2	99	90,63	-	2/9/27/28	0/3/3/3
63	PSU	A2	1233	63	-	0/7/25/26	0/2/2/2
24	PSU	B5	4042	24	-	0/7/25/26	0/2/2/2
24	A2M	B5	3450	24	-	0/9/27/28	0/3/3/3
24	A2M	B5	4317	24	-	0/9/27/28	0/3/3/3
63	PSU	A2	93	63	-	0/7/25/26	0/2/2/2
24	OMU	B5	4244	24	-	0/9/27/28	0/2/2/2
63	OMU	A2	355	63	-	1/9/27/28	0/2/2/2
24	PSU	B5	3466	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	1799	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	3494	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	4149	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	4217	24	-	0/7/25/26	0/2/2/2
63	OMU	A2	1805	63	-	0/9/27/28	0/2/2/2
63	B8N	A2	1249	63	-	4/16/34/35	0/2/2/2
63	4AC	A2	1338	63	-	3/11/29/30	0/2/2/2
63	PSU	A2	802	63	-	0/7/25/26	0/2/2/2
63	OMU	A2	121	63	-	0/9/27/28	0/2/2/2
24	OMG	B5	4245	24	-	0/9/27/28	0/3/3/3
24	A2M	B5	3517	24	-	2/9/27/28	0/3/3/3
24	PSU	B5	3652	90,24	-	0/7/25/26	0/2/2/2
63	PSU	A2	105	63	-	0/7/25/26	0/2/2/2
63	PSU	A2	682	63	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	OMC	A2	463	63	-	0/9/27/28	0/2/2/2
24	OMG	B5	2267	24	-	0/9/27/28	0/3/3/3
24	OMC	B5	3573	24	-	0/9/27/28	0/2/2/2
24	OMC	B5	3601	24	-	0/9/27/28	0/2/2/2
50	V5N	Ba	39	50	-	1/9/10/12	0/1/1/1
24	PSU	B5	4058	24	-	0/7/25/26	0/2/2/2
63	A2M	A2	591	63	-	4/9/27/28	0/3/3/3
63	A2M	A2	1032	63	-	0/9/27/28	0/3/3/3
24	A2M	B5	1270	24	-	0/9/27/28	0/3/3/3
24	OMC	B5	3433	24	-	4/9/27/28	0/2/2/2
24	PSU	B5	3583	24	-	0/7/25/26	0/2/2/2
24	OMC	B5	4282	90,24	-	1/9/27/28	0/2/2/2
24	A2M	B5	1479	24	-	0/9/27/28	0/3/3/3
63	PSU	A2	1047	63	-	0/7/25/26	0/2/2/2
24	OMG	B5	4116	24	-	0/9/27/28	0/3/3/3
63	A2M	A2	485	63	-	0/9/27/28	0/3/3/3
24	PSU	B5	2475	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	4278	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	4382	24	-	4/7/25/26	0/2/2/2
24	A2M	B5	1489	90,24	-	2/9/27/28	0/3/3/3
24	OMG	B5	3359	24	-	0/9/27/28	0/3/3/3
63	PSU	A2	864	63	-	0/7/25/26	0/2/2/2
24	PSU	B5	4166	24	-	2/7/25/26	0/2/2/2
63	OMG	A2	684	63	-	1/9/27/28	0/3/3/3
24	PSU	B5	1720	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	1638	24	-	0/7/25/26	0/2/2/2
63	PSU	A2	210	63	-	0/7/25/26	0/2/2/2
24	OMC	B5	3540	24	-	0/9/27/28	0/2/2/2
24	PSU	B5	3447	24	-	0/7/25/26	0/2/2/2
24	A2M	B5	4336	24	-	1/9/27/28	0/3/3/3
63	OMG	A2	510	90,63	-	2/9/27/28	0/3/3/3
63	PSU	A2	1368	63	-	0/7/25/26	0/2/2/2
63	OMG	A2	437	63	-	0/9/27/28	0/3/3/3
63	A2M	A2	469	63	-	0/9/27/28	0/3/3/3
24	PSU	B5	4107	24	-	0/7/25/26	0/2/2/2
34	PSU	B8	55	34	-	0/7/25/26	0/2/2/2
63	PSU	A2	816	63	-	0/7/25/26	0/2/2/2
63	PSU	A2	1348	63	-	0/7/25/26	0/2/2/2
24	PSU	B5	3496	24	-	0/7/25/26	0/2/2/2
24	OMG	B5	3974	24	-	0/9/27/28	0/3/3/3
63	OMC	A2	518	63	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	A2M	B5	2630	90,24	-	2/9/27/28	0/3/3/3
24	1MA	B5	1266	90,24	-	0/7/25/26	0/3/3/3
63	MA6	A2	1852	63	-	2/11/29/30	0/3/3/3
24	OMU	B5	3657	24	-	0/9/27/28	0/2/2/2
24	PSU	B5	3576	24	-	1/7/25/26	0/2/2/2
24	PSU	B5	4740	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	1537	24	-	0/7/25/26	0/2/2/2
24	OMC	B5	2265	90,24	-	1/9/27/28	0/2/2/2
63	OMU	A2	172	63	-	0/9/27/28	0/2/2/2
63	OMU	A2	116	63	-	0/9/27/28	0/2/2/2
63	A2M	A2	1384	63	-	0/9/27/28	0/3/3/3
24	OMC	B5	1820	90,24	-	1/9/27/28	0/2/2/2
82	IAS	An	138	82	-	2/7/7/8	-
63	PSU	A2	1178	63	-	0/7/25/26	0/2/2/2
63	PSU	A2	1005	63	-	0/7/25/26	0/2/2/2
23	HY3	Aw	62	23	-	1/1/12/14	0/1/1/1
24	PSU	B5	3502	24	-	0/7/25/26	0/2/2/2
63	A2M	A2	27	90,63	-	1/9/27/28	0/3/3/3
24	PSU	B5	4039	24	-	0/7/25/26	0/2/2/2
24	5MC	B5	4193	24	-	4/7/25/26	0/2/2/2
3	MLZ	Bo	53	3	-	1/7/8/10	-
63	OMG	A2	1329	63	-	0/9/27/28	0/3/3/3
63	PSU	A2	687	63	-	0/7/25/26	0/2/2/2
24	OMC	B5	1284	24	-	1/9/27/28	0/2/2/2
11	NMM	As	67	11	-	0/9/11/13	-
24	PSU	B5	1801	24	-	0/7/25/26	0/2/2/2
63	PSU	A2	1245	63	-	0/7/25/26	0/2/2/2
63	OMC	A2	1392	63	-	0/9/27/28	0/2/2/2
24	PSU	B5	4045	24	-	0/7/25/26	0/2/2/2
24	OMU	B5	4052	24	-	0/9/27/28	0/2/2/2
24	PSU	B5	1632	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	1721	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	4203	24	-	0/7/25/26	0/2/2/2
63	PSU	A2	1446	63	-	0/7/25/26	0/2/2/2
24	OMG	B5	4383	24	-	1/9/27/28	0/3/3/3
5	SAC	Ar	2	5	-	0/7/8/10	-
24	OMU	B5	2680	24	-	1/9/27/28	0/2/2/2
63	OMU	A2	1289	63	-	0/9/27/28	0/2/2/2
12	SAC	Br	2	12	-	0/7/8/10	-
24	PSU	B5	4419	24	-	0/7/25/26	0/2/2/2
63	OMC	A2	1704	63	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	G7M	A2	1640	63	-	2/7/25/26	0/3/3/3
63	OMG	A2	602	63	-	0/9/27/28	0/3/3/3
54	MLZ	Bb	5	54	-	2/7/8/10	-
24	5MC	B5	3514	90,24	-	0/7/25/26	0/2/2/2
24	OMC	B5	2194	90,24	-	2/9/27/28	0/2/2/2
63	A2M	A2	159	63	-	0/9/27/28	0/3/3/3
63	PSU	A2	823	63	-	0/7/25/26	0/2/2/2
24	PSU	B5	1731	24	-	0/7/25/26	0/2/2/2
24	OMU	B5	2258	24	-	0/9/27/28	0/2/2/2
24	OMG	B5	3631	24	-	1/9/27/28	0/3/3/3
63	OMU	A2	1327	90,63	-	0/9/27/28	0/2/2/2
24	PSU	B5	1683	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	3490	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	4325	24	-	0/7/25/26	0/2/2/2
24	A2M	B5	3456	24	-	0/9/27/28	0/3/3/3
34	PSU	B8	69	34	-	0/7/25/26	0/2/2/2
24	OMG	B5	3942	4,24	-	0/9/27/28	0/3/3/3
24	PSU	B5	4188	24	-	0/7/25/26	0/2/2/2
24	A2M	B5	398	24	-	4/9/27/28	0/3/3/3
24	PSU	B5	4322	24	-	0/7/25/26	0/2/2/2
24	A2M	B5	3492	24,63	-	2/9/27/28	0/3/3/3
24	OMU	B5	4366	24	-	0/9/27/28	0/2/2/2
24	OMU	B5	3973	24	-	0/9/27/28	0/2/2/2
24	OMG	B5	1580	24	-	0/9/27/28	0/3/3/3
24	PSU	B5	3369	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	3371	24	-	0/7/25/26	0/2/2/2
63	OMU	A2	628	63	-	4/9/27/28	0/2/2/2
24	OMG	B5	3476	24	-	1/9/27/28	0/3/3/3
24	OMG	B5	2719	24	-	0/9/27/28	0/3/3/3
24	PSU	B5	4246	24	-	1/7/25/26	0/2/2/2
63	PSU	A2	815	63	-	0/7/25/26	0/2/2/2
24	OMC	B5	2667	24	-	1/9/27/28	0/2/2/2
24	OMG	B5	4364	24	-	0/9/27/28	0/3/3/3
24	A2M	B5	3599	24	-	0/9/27/28	0/3/3/3
63	OMG	A2	1491	90,63	-	0/9/27/28	0/3/3/3
63	PSU	A2	652	63	-	0/7/25/26	0/2/2/2
24	PSU	B5	3616	24	-	0/7/25/26	0/2/2/2
63	PSU	A2	1644	90,63	-	0/7/25/26	0/2/2/2
24	OMC	B5	3619	24	-	3/9/27/28	0/2/2/2
24	A2M	B5	1810	90,24	-	1/9/27/28	0/3/3/3
24	A2M	B5	3562	24	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	SAC	AZ	2	32	-	2/7/8/10	-
24	PSU	B5	4711	24	-	0/7/25/26	0/2/2/2
63	A2M	A2	166	63	-	0/9/27/28	0/3/3/3

All (505) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	A2	1640	G7M	C4-N9	7.86	1.58	1.38
63	A2	1640	G7M	O6-C6	7.68	1.38	1.23
63	A2	1851	MA6	C5-N7	6.88	1.52	1.39
63	A2	1852	MA6	C5-N7	6.78	1.51	1.39
63	A2	1640	G7M	C5-C4	6.21	1.54	1.38
63	A2	1851	MA6	C8-N9	-5.44	1.27	1.37
63	A2	1852	MA6	C8-N9	-5.37	1.27	1.37
50	Ba	39	V5N	CG-ND1	-4.92	1.33	1.37
38	BA	216	V5N	CG-ND1	-4.90	1.33	1.37
23	Aw	62	HY3	C3-CA	-4.68	1.50	1.55
63	A2	591	A2M	C5-C4	4.66	1.47	1.39
24	B5	3492	A2M	C5-C4	4.56	1.47	1.39
63	A2	99	A2M	C5-C4	4.54	1.47	1.39
63	A2	469	A2M	C5-C4	4.54	1.47	1.39
63	A2	1833	6MZ	C5-C4	4.53	1.47	1.39
24	B5	400	A2M	C5-C4	4.53	1.47	1.39
63	A2	513	A2M	C5-C4	4.53	1.47	1.39
24	B5	4317	A2M	C5-C4	4.53	1.47	1.39
63	A2	159	A2M	C5-C4	4.52	1.47	1.39
24	B5	1479	A2M	C5-C4	4.52	1.47	1.39
63	A2	1384	A2M	C5-C4	4.52	1.47	1.39
24	B5	398	A2M	C5-C4	4.51	1.47	1.39
24	B5	2244	A2M	C5-C4	4.51	1.47	1.39
63	A2	166	A2M	C5-C4	4.51	1.47	1.39
24	B5	2206	A2M	C5-C4	4.50	1.47	1.39
63	A2	485	A2M	C5-C4	4.50	1.47	1.39
63	A2	577	A2M	C5-C4	4.50	1.47	1.39
24	B5	3456	A2M	C5-C4	4.50	1.47	1.39
24	B5	3562	A2M	C5-C4	4.49	1.47	1.39
24	B5	3599	A2M	C5-C4	4.49	1.47	1.39
63	A2	669	A2M	C5-C4	4.49	1.47	1.39
24	B5	2630	A2M	C5-C4	4.48	1.47	1.39
63	A2	27	A2M	C5-C4	4.48	1.47	1.39
24	B5	3450	A2M	C5-C4	4.48	1.47	1.39
24	B5	1810	A2M	C5-C4	4.48	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B5	3966	6MZ	C5-C4	4.47	1.47	1.39
63	A2	1640	G7M	C2-N2	4.47	1.44	1.34
24	B5	2658	A2M	C5-C4	4.46	1.47	1.39
24	B5	3557	A2M	C5-C4	4.46	1.47	1.39
24	B5	1270	A2M	C5-C4	4.45	1.47	1.39
24	B5	4336	A2M	C5-C4	4.44	1.47	1.39
63	A2	1032	A2M	C5-C4	4.43	1.47	1.39
24	B5	4269	A2M	C5-C4	4.43	1.47	1.39
24	B5	1489	A2M	C5-C4	4.42	1.47	1.39
63	A2	1679	A2M	C5-C4	4.41	1.47	1.39
24	B5	3517	A2M	C5-C4	4.37	1.47	1.39
63	A2	1640	G7M	C2-N1	3.87	1.47	1.37
24	B5	3550	UY1	C6-C5	3.73	1.39	1.35
63	A2	1851	MA6	C4-N9	-3.69	1.29	1.37
63	A2	1852	MA6	C4-N9	-3.60	1.29	1.37
63	A2	1640	G7M	C2-N3	3.31	1.41	1.33
63	A2	1851	MA6	C5-C4	3.30	1.45	1.39
63	A2	1852	MA6	C5-C4	3.30	1.45	1.39
24	B5	1632	PSU	C6-C5	3.25	1.39	1.35
24	B5	4166	PSU	C6-C5	3.25	1.39	1.35
24	B5	1266	1MA	C6-N6	3.23	1.35	1.28
24	B5	3583	PSU	C6-C5	3.21	1.39	1.35
63	A2	1348	PSU	C6-C5	3.21	1.39	1.35
63	A2	573	PSU	C6-C5	3.20	1.39	1.35
24	B5	3494	PSU	C6-C5	3.20	1.39	1.35
24	B5	4058	PSU	C6-C5	3.20	1.39	1.35
24	B5	4749	PSU	C6-C5	3.20	1.39	1.35
63	A2	967	PSU	C6-C5	3.19	1.39	1.35
24	B5	4740	PSU	C6-C5	3.19	1.39	1.35
24	B5	4711	PSU	C6-C5	3.19	1.39	1.35
24	B5	4203	PSU	C6-C5	3.18	1.39	1.35
63	A2	109	PSU	C6-C5	3.18	1.39	1.35
63	A2	867	PSU	C6-C5	3.18	1.39	1.35
34	B8	69	PSU	C6-C5	3.18	1.39	1.35
24	B5	3447	PSU	C6-C5	3.17	1.39	1.35
63	A2	1239	PSU	C6-C5	3.17	1.39	1.35
63	A2	823	PSU	C6-C5	3.17	1.39	1.35
63	A2	210	PSU	C6-C5	3.17	1.39	1.35
63	A2	816	PSU	C6-C5	3.17	1.39	1.35
24	B5	4188	PSU	C6-C5	3.17	1.39	1.35
24	B5	2475	PSU	C6-C5	3.16	1.39	1.35
24	B5	3576	PSU	C6-C5	3.16	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	A2	1245	PSU	C6-C5	3.16	1.39	1.35
63	A2	1082	PSU	C6-C5	3.16	1.39	1.35
63	A2	119	PSU	C6-C5	3.16	1.39	1.35
24	B5	3371	PSU	C6-C5	3.16	1.39	1.35
63	A2	1047	PSU	C6-C5	3.16	1.39	1.35
24	B5	4217	PSU	C6-C5	3.15	1.39	1.35
63	A2	1233	PSU	C6-C5	3.15	1.39	1.35
24	B5	1638	PSU	C6-C5	3.15	1.39	1.35
24	B5	4267	PSU	C6-C5	3.15	1.39	1.35
63	A2	1249	B8N	C6-C5	3.15	1.39	1.34
24	B5	1683	PSU	C6-C5	3.14	1.39	1.35
24	B5	1799	PSU	C6-C5	3.14	1.39	1.35
24	B5	4435	PSU	C6-C5	3.14	1.39	1.35
24	B5	1718	PSU	C6-C5	3.14	1.39	1.35
24	B5	1491	PSU	C6-C5	3.14	1.39	1.35
63	A2	1693	PSU	C6-C5	3.13	1.39	1.35
24	B5	4099	PSU	C6-C5	3.13	1.39	1.35
24	B5	3500	PSU	C6-C5	3.13	1.39	1.35
24	B5	4169	PSU	C6-C5	3.13	1.39	1.35
63	A2	1046	PSU	C6-C5	3.13	1.39	1.35
24	B5	3427	PSU	C6-C5	3.12	1.39	1.35
63	A2	1626	PSU	C6-C5	3.12	1.39	1.35
24	B5	4322	PSU	C6-C5	3.12	1.39	1.35
63	A2	815	PSU	C6-C5	3.12	1.39	1.35
24	B5	4045	PSU	C6-C5	3.12	1.39	1.35
24	B5	4278	PSU	C6-C5	3.12	1.39	1.35
24	B5	1266	1MA	C5-C4	3.12	1.47	1.38
63	A2	1005	PSU	C6-C5	3.12	1.39	1.35
63	A2	1644	PSU	C6-C5	3.12	1.39	1.35
24	B5	3652	PSU	C6-C5	3.12	1.39	1.35
63	A2	864	PSU	C6-C5	3.12	1.39	1.35
24	B5	2719	OMG	C5-C4	3.12	1.47	1.38
24	B5	4042	PSU	C6-C5	3.12	1.39	1.35
24	B5	3466	PSU	C6-C5	3.11	1.38	1.35
63	A2	650	PSU	C6-C5	3.11	1.38	1.35
24	B5	3462	PSU	C6-C5	3.11	1.38	1.35
63	A2	105	PSU	C6-C5	3.11	1.38	1.35
24	B5	4177	PSU	C6-C5	3.11	1.38	1.35
24	B5	1721	PSU	C6-C5	3.11	1.38	1.35
24	B5	2351	PSU	C6-C5	3.11	1.38	1.35
63	A2	687	PSU	C6-C5	3.11	1.38	1.35
63	A2	1057	PSU	C6-C5	3.11	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	A2	1175	PSU	C6-C5	3.11	1.38	1.35
63	A2	218	PSU	C6-C5	3.10	1.38	1.35
63	A2	510	OMG	C5-C4	3.10	1.47	1.38
24	B5	4325	PSU	C6-C5	3.10	1.38	1.35
63	A2	1446	PSU	C6-C5	3.10	1.38	1.35
63	A2	610	PSU	C6-C5	3.10	1.38	1.35
63	A2	93	PSU	C6-C5	3.10	1.38	1.35
63	A2	1329	OMG	C5-C4	3.10	1.47	1.38
24	B5	4245	OMG	C5-C4	3.10	1.47	1.38
63	A2	36	PSU	C6-C5	3.10	1.38	1.35
24	B5	1720	PSU	C6-C5	3.10	1.38	1.35
63	A2	802	PSU	C6-C5	3.10	1.38	1.35
24	B5	3554	PSU	C6-C5	3.10	1.38	1.35
63	A2	1178	PSU	C6-C5	3.10	1.38	1.35
24	B5	1537	PSU	C6-C5	3.10	1.38	1.35
24	B5	3490	PSU	C6-C5	3.10	1.38	1.35
34	B8	75	OMG	C5-C4	3.10	1.47	1.38
24	B5	1731	PSU	C6-C5	3.09	1.38	1.35
24	B5	1580	OMG	C5-C4	3.09	1.47	1.38
24	B5	3942	OMG	C5-C4	3.09	1.47	1.38
24	B5	3496	PSU	C6-C5	3.09	1.38	1.35
24	B5	4107	PSU	C6-C5	3.09	1.38	1.35
24	B5	4374	PSU	C6-C5	3.09	1.38	1.35
63	A2	1491	OMG	C5-C4	3.09	1.47	1.38
63	A2	1249	B8N	C4-N3	-3.09	1.34	1.40
24	B5	3524	OMG	C5-C4	3.09	1.47	1.38
63	A2	652	PSU	C6-C5	3.09	1.38	1.35
24	B5	4246	PSU	C6-C5	3.09	1.38	1.35
63	A2	602	OMG	C5-C4	3.09	1.47	1.38
63	A2	34	PSU	C6-C5	3.08	1.38	1.35
63	A2	1448	OMG	C5-C4	3.08	1.47	1.38
63	A2	407	PSU	C6-C5	3.08	1.38	1.35
24	B5	4138	OMG	C5-C4	3.08	1.47	1.38
24	B5	4240	OMG	C5-C4	3.08	1.47	1.38
24	B5	4419	PSU	C6-C5	3.07	1.38	1.35
63	A2	1368	PSU	C6-C5	3.07	1.38	1.35
24	B5	4382	PSU	C6-C5	3.07	1.38	1.35
24	B5	4149	PSU	C6-C5	3.07	1.38	1.35
24	B5	3359	OMG	C5-C4	3.07	1.47	1.38
24	B5	3369	PSU	C6-C5	3.07	1.38	1.35
24	B5	2267	OMG	C5-C4	3.07	1.47	1.38
24	B5	3476	OMG	C5-C4	3.07	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B5	1477	OMG	C5-C4	3.07	1.47	1.38
24	B5	4364	OMG	C5-C4	3.06	1.47	1.38
63	A2	645	OMG	C5-C4	3.06	1.47	1.38
63	A2	437	OMG	C5-C4	3.06	1.47	1.38
24	B5	4039	PSU	C6-C5	3.06	1.38	1.35
34	B8	55	PSU	C6-C5	3.06	1.38	1.35
24	B5	4383	OMG	C5-C4	3.06	1.47	1.38
24	B5	3502	PSU	C6-C5	3.06	1.38	1.35
24	B5	1801	PSU	C6-C5	3.05	1.38	1.35
24	B5	4298	PSU	C6-C5	3.05	1.38	1.35
24	B5	3676	OMG	C5-C4	3.04	1.47	1.38
24	B5	3974	OMG	C5-C4	3.04	1.47	1.38
24	B5	4116	OMG	C5-C4	3.04	1.47	1.38
24	B5	3616	PSU	C6-C5	3.04	1.38	1.35
63	A2	1852	MA6	C6-N6	3.04	1.45	1.36
24	B5	4369	OMG	C5-C4	3.04	1.47	1.38
24	B5	3585	PSU	C6-C5	3.04	1.38	1.35
24	B5	3631	OMG	C5-C4	3.04	1.47	1.38
63	A2	684	OMG	C5-C4	3.03	1.47	1.38
63	A2	868	OMG	C5-C4	3.03	1.47	1.38
63	A2	682	PSU	C6-C5	3.03	1.38	1.35
63	A2	1851	MA6	C6-N6	3.02	1.45	1.36
24	B5	1260	OMG	C5-C4	3.01	1.47	1.38
24	B5	2207	OMG	C5-C4	2.99	1.47	1.38
63	A2	1843	4AC	C4-N4	-2.99	1.35	1.39
38	BA	216	V5N	CD2-NE2	-2.85	1.33	1.37
50	Ba	39	V5N	CD2-NE2	-2.84	1.33	1.37
24	B5	4193	5MC	C6-C5	2.84	1.39	1.34
63	A2	1338	4AC	C4-N4	-2.82	1.35	1.39
24	B5	3514	5MC	C6-C5	2.76	1.39	1.34
63	A2	591	A2M	C5-C6	2.75	1.48	1.41
63	A2	652	PSU	C4-N3	-2.73	1.33	1.38
24	B5	3369	PSU	C4-N3	-2.73	1.33	1.38
24	B5	4042	PSU	C4-N3	-2.72	1.33	1.38
24	B5	4317	A2M	C5-C6	2.71	1.48	1.41
63	A2	1679	A2M	C5-C6	2.71	1.48	1.41
24	B5	3550	UY1	C2-N1	2.71	1.40	1.36
24	B5	3652	PSU	C4-N3	-2.71	1.33	1.38
24	B5	3616	PSU	C4-N3	-2.71	1.33	1.38
24	B5	4149	PSU	C4-N3	-2.71	1.33	1.38
63	A2	513	A2M	C5-C6	2.71	1.48	1.41
63	A2	469	A2M	C5-C6	2.70	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	A2	166	A2M	C5-C6	2.70	1.48	1.41
24	B5	4711	PSU	C4-N3	-2.70	1.33	1.38
24	B5	398	A2M	C5-C6	2.70	1.48	1.41
24	B5	4107	PSU	C4-N3	-2.70	1.33	1.38
63	A2	577	A2M	C5-C6	2.70	1.48	1.41
24	B5	3500	PSU	C4-N3	-2.69	1.33	1.38
34	B8	69	PSU	C4-N3	-2.69	1.33	1.38
24	B5	4169	PSU	C4-N3	-2.69	1.33	1.38
24	B5	3450	A2M	C5-C6	2.69	1.48	1.41
63	A2	682	PSU	C4-N3	-2.69	1.33	1.38
24	B5	1721	PSU	C4-N3	-2.69	1.33	1.38
24	B5	2206	A2M	C5-C6	2.69	1.48	1.41
24	B5	3562	A2M	C5-C6	2.68	1.48	1.41
24	B5	4267	PSU	C4-N3	-2.68	1.33	1.38
24	B5	4740	PSU	C4-N3	-2.68	1.33	1.38
34	B8	55	PSU	C4-N3	-2.68	1.33	1.38
24	B5	1489	A2M	C5-C6	2.68	1.48	1.41
24	B5	1720	PSU	C4-N3	-2.68	1.33	1.38
24	B5	2658	A2M	C5-C6	2.68	1.48	1.41
63	A2	1005	PSU	C4-N3	-2.68	1.33	1.38
24	B5	4039	PSU	C4-N3	-2.68	1.33	1.38
63	A2	867	PSU	C4-N3	-2.68	1.33	1.38
63	A2	1384	A2M	C5-C6	2.68	1.48	1.41
63	A2	93	PSU	C4-N3	-2.68	1.33	1.38
63	A2	159	A2M	C5-C6	2.68	1.48	1.41
24	B5	4336	A2M	C5-C6	2.68	1.48	1.41
63	A2	485	A2M	C5-C6	2.68	1.48	1.41
63	A2	1233	PSU	C4-N3	-2.68	1.33	1.38
63	A2	1032	A2M	C5-C6	2.68	1.48	1.41
63	A2	105	PSU	C4-N3	-2.68	1.33	1.38
24	B5	4246	PSU	C4-N3	-2.68	1.33	1.38
24	B5	4269	A2M	C5-C6	2.67	1.48	1.41
24	B5	3371	PSU	C4-N3	-2.67	1.33	1.38
24	B5	4435	PSU	C4-N3	-2.67	1.33	1.38
63	A2	1245	PSU	C4-N3	-2.67	1.33	1.38
24	B5	4374	PSU	C4-N3	-2.67	1.33	1.38
24	B5	3492	A2M	C5-C6	2.67	1.48	1.41
24	B5	1801	PSU	C4-N3	-2.67	1.33	1.38
24	B5	3427	PSU	C4-N3	-2.67	1.33	1.38
24	B5	2244	A2M	C5-C6	2.67	1.48	1.41
24	B5	3557	A2M	C5-C6	2.67	1.48	1.41
63	A2	34	PSU	C4-N3	-2.67	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B5	3554	PSU	C4-N3	-2.67	1.33	1.38
24	B5	1270	A2M	C5-C6	2.67	1.48	1.41
63	A2	407	PSU	C4-N3	-2.67	1.33	1.38
24	B5	3583	PSU	C4-N3	-2.67	1.33	1.38
24	B5	4203	PSU	C4-N3	-2.67	1.33	1.38
63	A2	27	A2M	C5-C6	2.67	1.48	1.41
24	B5	4382	PSU	C4-N3	-2.67	1.33	1.38
24	B5	1731	PSU	C4-N3	-2.66	1.33	1.38
63	A2	1239	PSU	C4-N3	-2.66	1.33	1.38
24	B5	3462	PSU	C4-N3	-2.66	1.33	1.38
63	A2	1626	PSU	C4-N3	-2.66	1.33	1.38
24	B5	3599	A2M	C5-C6	2.66	1.48	1.41
24	B5	1718	PSU	C4-N3	-2.66	1.33	1.38
63	A2	573	PSU	C4-N3	-2.66	1.33	1.38
24	B5	4045	PSU	C4-N3	-2.66	1.33	1.38
24	B5	1810	A2M	C5-C6	2.66	1.48	1.41
63	A2	669	A2M	C5-C6	2.66	1.48	1.41
63	A2	650	PSU	C4-N3	-2.66	1.33	1.38
63	A2	1693	PSU	C4-N3	-2.66	1.33	1.38
24	B5	3490	PSU	C4-N3	-2.65	1.33	1.38
24	B5	1683	PSU	C4-N3	-2.65	1.33	1.38
24	B5	4419	PSU	C4-N3	-2.65	1.33	1.38
63	A2	109	PSU	C4-N3	-2.65	1.33	1.38
24	B5	3456	A2M	C5-C6	2.65	1.48	1.41
24	B5	1491	PSU	C4-N3	-2.65	1.33	1.38
24	B5	1638	PSU	C4-N3	-2.65	1.33	1.38
24	B5	3576	PSU	C4-N3	-2.65	1.33	1.38
24	B5	4177	PSU	C4-N3	-2.65	1.33	1.38
63	A2	1082	PSU	C4-N3	-2.65	1.33	1.38
24	B5	2475	PSU	C4-N3	-2.65	1.33	1.38
24	B5	4278	PSU	C4-N3	-2.65	1.33	1.38
63	A2	119	PSU	C4-N3	-2.65	1.33	1.38
63	A2	1644	PSU	C4-N3	-2.65	1.33	1.38
63	A2	1348	PSU	C4-N3	-2.65	1.33	1.38
24	B5	400	A2M	C5-C6	2.65	1.48	1.41
63	A2	610	PSU	C4-N3	-2.65	1.33	1.38
24	B5	4188	PSU	C4-N3	-2.65	1.33	1.38
24	B5	4298	PSU	C4-N3	-2.64	1.33	1.38
24	B5	3585	PSU	C4-N3	-2.64	1.33	1.38
24	B5	1537	PSU	C4-N3	-2.64	1.33	1.38
24	B5	4749	PSU	C4-N3	-2.64	1.33	1.38
24	B5	1479	A2M	C5-C6	2.64	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B5	4322	PSU	C4-N3	-2.64	1.33	1.38
24	B5	4217	PSU	C4-N3	-2.64	1.33	1.38
63	A2	1046	PSU	C4-N3	-2.64	1.33	1.38
63	A2	1178	PSU	C4-N3	-2.64	1.33	1.38
24	B5	2630	A2M	C5-C6	2.64	1.48	1.41
63	A2	815	PSU	C4-N3	-2.64	1.33	1.38
24	B5	3502	PSU	C4-N3	-2.63	1.33	1.38
63	A2	1446	PSU	C4-N3	-2.63	1.33	1.38
63	A2	36	PSU	C4-N3	-2.63	1.34	1.38
24	B5	2351	PSU	C4-N3	-2.63	1.34	1.38
63	A2	1368	PSU	C4-N3	-2.63	1.34	1.38
63	A2	99	A2M	C5-C6	2.63	1.48	1.41
63	A2	1047	PSU	C4-N3	-2.63	1.34	1.38
63	A2	1175	PSU	C4-N3	-2.63	1.34	1.38
24	B5	4325	PSU	C4-N3	-2.63	1.34	1.38
24	B5	1799	PSU	C4-N3	-2.63	1.34	1.38
63	A2	1057	PSU	C4-N3	-2.63	1.34	1.38
63	A2	687	PSU	C4-N3	-2.62	1.34	1.38
63	A2	816	PSU	C4-N3	-2.62	1.34	1.38
24	B5	4058	PSU	C4-N3	-2.62	1.34	1.38
63	A2	218	PSU	C4-N3	-2.62	1.34	1.38
63	A2	802	PSU	C4-N3	-2.62	1.34	1.38
63	A2	864	PSU	C4-N3	-2.62	1.34	1.38
24	B5	3447	PSU	C4-N3	-2.61	1.34	1.38
24	B5	3517	A2M	C5-C6	2.61	1.48	1.41
24	B5	4099	PSU	C4-N3	-2.61	1.34	1.38
63	A2	967	PSU	C4-N3	-2.61	1.34	1.38
24	B5	1632	PSU	C4-N3	-2.60	1.34	1.38
24	B5	3496	PSU	C4-N3	-2.60	1.34	1.38
24	B5	3466	PSU	C4-N3	-2.60	1.34	1.38
24	B5	3494	PSU	C4-N3	-2.59	1.34	1.38
63	A2	823	PSU	C4-N3	-2.59	1.34	1.38
63	A2	210	PSU	C4-N3	-2.58	1.34	1.38
24	B5	3657	OMU	C4-N3	-2.58	1.33	1.38
24	B5	4244	OMU	C4-N3	-2.56	1.34	1.38
24	B5	4366	OMU	C4-N3	-2.56	1.34	1.38
63	A2	355	OMU	C4-N3	-2.54	1.34	1.38
24	B5	3966	6MZ	C5-C6	2.53	1.48	1.41
24	B5	2258	OMU	C4-N3	-2.53	1.34	1.38
63	A2	1249	B8N	C2-N3	-2.53	1.34	1.38
63	A2	1289	OMU	C4-N3	-2.52	1.34	1.38
24	B5	2719	OMG	C6-N1	-2.51	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B5	4052	OMU	C4-N3	-2.51	1.34	1.38
63	A2	429	OMU	C4-N3	-2.50	1.34	1.38
24	B5	3942	OMG	C6-N1	-2.50	1.34	1.38
63	A2	1833	6MZ	C5-C6	2.50	1.48	1.41
24	B5	4138	OMG	C6-N1	-2.50	1.34	1.38
24	B5	1580	OMG	C6-N1	-2.50	1.34	1.38
24	B5	2680	OMU	C4-N3	-2.50	1.34	1.38
24	B5	4166	PSU	C4-N3	-2.50	1.34	1.38
24	B5	1489	A2M	C8-N7	2.50	1.36	1.31
24	B5	3973	OMU	C4-N3	-2.49	1.34	1.38
24	B5	3476	OMG	C6-N1	-2.48	1.34	1.38
24	B5	3524	OMG	C6-N1	-2.48	1.34	1.38
24	B5	4369	OMG	C6-N1	-2.48	1.34	1.38
63	A2	1443	OMU	C4-N3	-2.48	1.34	1.38
24	B5	3359	OMG	C6-N1	-2.48	1.34	1.38
24	B5	4116	OMG	C6-N1	-2.48	1.34	1.38
24	B5	2267	OMG	C6-N1	-2.47	1.34	1.38
24	B5	1260	OMG	C6-N1	-2.47	1.34	1.38
63	A2	172	OMU	C4-N3	-2.47	1.34	1.38
63	A2	645	OMG	C6-N1	-2.47	1.34	1.38
24	B5	1477	OMG	C6-N1	-2.47	1.34	1.38
63	A2	121	OMU	C4-N3	-2.47	1.34	1.38
63	A2	1491	OMG	C6-N1	-2.46	1.34	1.38
24	B5	4240	OMG	C6-N1	-2.46	1.34	1.38
34	B8	75	OMG	C6-N1	-2.46	1.34	1.38
63	A2	510	OMG	C6-N1	-2.46	1.34	1.38
63	A2	513	A2M	C8-N7	2.45	1.36	1.31
24	B5	3974	OMG	C6-N1	-2.45	1.34	1.38
24	B5	4245	OMG	C6-N1	-2.45	1.34	1.38
63	A2	1805	OMU	C4-N3	-2.44	1.34	1.38
63	A2	684	OMG	C6-N1	-2.44	1.34	1.38
63	A2	602	OMG	C6-N1	-2.44	1.34	1.38
63	A2	116	OMU	C4-N3	-2.44	1.34	1.38
63	A2	1329	OMG	C6-N1	-2.43	1.34	1.38
24	B5	2207	OMG	C6-N1	-2.43	1.34	1.38
24	B5	3631	OMG	C6-N1	-2.43	1.34	1.38
24	B5	3450	A2M	C8-N7	2.43	1.36	1.31
24	B5	4364	OMG	C6-N1	-2.43	1.34	1.38
24	B5	4317	A2M	C8-N7	2.43	1.36	1.31
63	A2	469	A2M	C8-N7	2.42	1.36	1.31
63	A2	1327	OMU	C4-N3	-2.42	1.34	1.38
63	A2	159	A2M	C8-N7	2.42	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B5	3456	A2M	C8-N7	2.42	1.36	1.31
63	A2	577	A2M	C8-N7	2.42	1.36	1.31
24	B5	4383	OMG	C6-N1	-2.42	1.34	1.38
63	A2	99	A2M	C8-N7	2.42	1.36	1.31
63	A2	437	OMG	C6-N1	-2.41	1.34	1.38
63	A2	1679	A2M	C8-N7	2.41	1.36	1.31
24	B5	1810	A2M	C8-N7	2.41	1.36	1.31
24	B5	2658	A2M	C8-N7	2.41	1.36	1.31
24	B5	3676	OMG	C6-N1	-2.41	1.34	1.38
63	A2	1032	A2M	C8-N7	2.41	1.36	1.31
24	B5	4336	A2M	C8-N7	2.41	1.36	1.31
63	A2	628	OMU	C4-N3	-2.41	1.34	1.38
24	B5	1479	A2M	C8-N7	2.41	1.36	1.31
24	B5	1270	A2M	C8-N7	2.40	1.36	1.31
63	A2	1448	OMG	C6-N1	-2.40	1.34	1.38
63	A2	669	A2M	C8-N7	2.40	1.36	1.31
24	B5	398	A2M	C8-N7	2.40	1.36	1.31
24	B5	4269	A2M	C8-N7	2.39	1.36	1.31
63	A2	166	A2M	C8-N7	2.39	1.36	1.31
63	A2	485	A2M	C8-N7	2.39	1.36	1.31
24	B5	400	A2M	C8-N7	2.38	1.36	1.31
24	B5	3599	A2M	C8-N7	2.38	1.36	1.31
24	B5	3492	A2M	C8-N7	2.38	1.36	1.31
24	B5	2206	A2M	C8-N7	2.37	1.36	1.31
63	A2	1384	A2M	C8-N7	2.37	1.36	1.31
63	A2	868	OMG	C6-N1	-2.37	1.34	1.38
63	A2	1640	G7M	C5-N7	2.37	1.41	1.39
24	B5	3557	A2M	C8-N7	2.37	1.36	1.31
24	B5	3517	A2M	C8-N7	2.37	1.36	1.31
24	B5	3562	A2M	C8-N7	2.37	1.36	1.31
63	A2	27	A2M	C8-N7	2.36	1.36	1.31
24	B5	2244	A2M	C8-N7	2.36	1.36	1.31
63	A2	591	A2M	C8-N7	2.36	1.36	1.31
24	B5	2630	A2M	C8-N7	2.31	1.36	1.31
24	B5	3966	6MZ	C8-N7	2.31	1.36	1.31
63	A2	591	A2M	C5-N7	-2.28	1.34	1.39
63	A2	1833	6MZ	C5-N7	-2.28	1.34	1.39
63	A2	1833	6MZ	C8-N7	2.26	1.35	1.31
24	B5	1266	1MA	C2-N3	2.26	1.34	1.30
24	B5	3514	5MC	C6-N1	-2.24	1.34	1.38
24	B5	3550	UY1	C6-N1	-2.23	1.32	1.36
24	B5	3517	A2M	C5-N7	-2.22	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B5	2206	A2M	C5-N7	-2.21	1.34	1.39
24	B5	4193	5MC	C6-N1	-2.21	1.34	1.38
24	B5	2244	A2M	C5-N7	-2.21	1.34	1.39
63	A2	355	OMU	C2-N3	-2.21	1.34	1.38
24	B5	1479	A2M	C5-N7	-2.21	1.34	1.39
24	B5	3657	OMU	C2-N3	-2.21	1.34	1.38
24	B5	3966	6MZ	C5-N7	-2.20	1.34	1.39
24	B5	2719	OMG	C5-N7	-2.20	1.34	1.39
63	A2	1443	OMU	C2-N1	2.20	1.42	1.38
63	A2	1032	A2M	C5-N7	-2.20	1.34	1.39
24	B5	4366	OMU	C2-N3	-2.20	1.34	1.38
63	A2	485	A2M	C5-N7	-2.20	1.34	1.39
24	B5	3524	OMG	C5-N7	-2.19	1.34	1.39
63	A2	1843	4AC	C7-N4	-2.19	1.33	1.37
63	A2	99	A2M	C5-N7	-2.19	1.34	1.39
63	A2	27	A2M	C5-N7	-2.19	1.34	1.39
24	B5	2658	A2M	C5-N7	-2.19	1.34	1.39
24	B5	3599	A2M	C5-N7	-2.19	1.34	1.39
24	B5	3492	A2M	C5-N7	-2.19	1.34	1.39
63	A2	1289	OMU	C2-N1	2.19	1.42	1.38
24	B5	4240	OMG	C5-N7	-2.18	1.34	1.39
63	A2	1384	A2M	C5-N7	-2.18	1.34	1.39
24	B5	3562	A2M	C5-N7	-2.18	1.34	1.39
24	B5	1580	OMG	C5-N7	-2.18	1.34	1.39
24	B5	400	A2M	C5-N7	-2.18	1.34	1.39
63	A2	1640	G7M	C4-N3	2.18	1.39	1.34
63	A2	513	A2M	C5-N7	-2.17	1.34	1.39
63	A2	510	OMG	C5-N7	-2.17	1.34	1.39
24	B5	3450	A2M	C5-N7	-2.17	1.34	1.39
24	B5	3942	OMG	C5-N7	-2.17	1.34	1.39
63	A2	159	A2M	C5-N7	-2.17	1.34	1.39
63	A2	1491	OMG	C5-N7	-2.16	1.34	1.39
24	B5	2630	A2M	C5-N7	-2.16	1.34	1.39
24	B5	3973	OMU	C2-N3	-2.16	1.34	1.38
24	B5	1270	A2M	C5-N7	-2.16	1.34	1.39
34	B8	75	OMG	C5-N7	-2.16	1.34	1.39
24	B5	1477	OMG	C5-N7	-2.16	1.34	1.39
24	B5	2680	OMU	C2-N3	-2.16	1.34	1.38
24	B5	4269	A2M	C5-N7	-2.16	1.34	1.39
24	B5	4245	OMG	C5-N7	-2.16	1.34	1.39
63	A2	429	OMU	C2-N3	-2.15	1.34	1.38
63	A2	1327	OMU	C2-N3	-2.15	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B5	3557	A2M	C5-N7	-2.15	1.35	1.39
24	B5	4052	OMU	C2-N3	-2.15	1.34	1.38
24	B5	398	A2M	C5-N7	-2.15	1.35	1.39
24	B5	4317	A2M	C5-N7	-2.15	1.35	1.39
24	B5	3359	OMG	C5-N7	-2.15	1.34	1.39
24	B5	3476	OMG	C5-N7	-2.15	1.34	1.39
63	A2	577	A2M	C5-N7	-2.14	1.35	1.39
63	A2	121	OMU	C2-N3	-2.14	1.34	1.38
24	B5	3974	OMG	C5-N7	-2.14	1.34	1.39
24	B5	1810	A2M	C5-N7	-2.14	1.35	1.39
24	B5	2267	OMG	C5-N7	-2.14	1.34	1.39
24	B5	4244	OMU	C2-N3	-2.14	1.34	1.38
63	A2	172	OMU	C2-N3	-2.14	1.34	1.38
24	B5	3456	A2M	C5-N7	-2.14	1.35	1.39
63	A2	1329	OMG	C5-N7	-2.13	1.35	1.39
63	A2	469	A2M	C5-N7	-2.13	1.35	1.39
63	A2	628	OMU	C2-N3	-2.13	1.34	1.38
63	A2	1443	OMU	C2-N3	-2.13	1.34	1.38
63	A2	645	OMG	C5-N7	-2.13	1.35	1.39
24	B5	4138	OMG	C5-N7	-2.13	1.35	1.39
24	B5	1489	A2M	C5-N7	-2.13	1.35	1.39
24	B5	4369	OMG	C5-N7	-2.12	1.35	1.39
24	B5	1260	OMG	C5-N7	-2.12	1.35	1.39
24	B5	3676	OMG	C5-N7	-2.12	1.35	1.39
24	B5	4364	OMG	C5-N7	-2.12	1.35	1.39
63	A2	669	A2M	C5-N7	-2.12	1.35	1.39
63	A2	1679	A2M	C5-N7	-2.12	1.35	1.39
24	B5	1266	1MA	C5-N7	-2.11	1.35	1.39
24	B5	4116	OMG	C5-N7	-2.11	1.35	1.39
24	B5	2258	OMU	C2-N3	-2.11	1.34	1.38
63	A2	166	A2M	C5-N7	-2.11	1.35	1.39
24	B5	2207	OMG	C5-N7	-2.11	1.35	1.39
63	A2	602	OMG	C5-N7	-2.10	1.35	1.39
63	A2	437	OMG	C5-N7	-2.10	1.35	1.39
63	A2	1805	OMU	C2-N3	-2.10	1.34	1.38
63	A2	1289	OMU	C2-N3	-2.09	1.34	1.38
24	B5	4383	OMG	C5-N7	-2.09	1.35	1.39
63	A2	116	OMU	C2-N3	-2.09	1.34	1.38
63	A2	1640	G7M	C6-N1	2.09	1.42	1.38
24	B5	4336	A2M	C5-N7	-2.09	1.35	1.39
63	A2	1448	OMG	C5-N7	-2.09	1.35	1.39
63	A2	1805	OMU	C2-N1	2.09	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	A2	684	OMG	C5-N7	-2.08	1.35	1.39
24	B5	2258	OMU	C2-N1	2.08	1.41	1.38
24	B5	4052	OMU	C2-N1	2.07	1.41	1.38
24	B5	3631	OMG	C5-N7	-2.07	1.35	1.39
24	B5	3973	OMU	C2-N1	2.06	1.41	1.38
63	A2	868	OMG	C5-N7	-2.05	1.35	1.39
63	A2	121	OMU	C5-C4	-2.05	1.39	1.43
63	A2	1338	4AC	C7-N4	-2.01	1.33	1.37

All (956) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	A2	1851	MA6	C4-N9-C8	14.73	121.69	105.73
63	A2	1852	MA6	C4-N9-C8	14.45	121.39	105.73
63	A2	1640	G7M	C8-N7-C5	11.45	122.10	107.78
63	A2	591	A2M	C5-C4-N3	-6.94	117.69	126.75
63	A2	1852	MA6	N3-C4-N9	6.89	138.43	127.08
63	A2	1851	MA6	N3-C4-N9	6.62	137.99	127.08
63	A2	1640	G7M	N9-C4-N3	6.61	139.21	125.94
63	A2	1833	6MZ	C5-C4-N3	-6.43	118.36	126.75
63	A2	1640	G7M	C6-C5-N7	6.43	140.03	132.25
24	B5	2719	OMG	C5-C4-N3	-6.38	118.11	128.46
24	B5	1479	A2M	C5-C4-N3	-6.30	118.53	126.75
63	A2	513	A2M	C5-C4-N3	-6.30	118.53	126.75
24	B5	2658	A2M	C5-C4-N3	-6.30	118.53	126.75
63	A2	166	A2M	C5-C4-N3	-6.26	118.58	126.75
24	B5	2206	A2M	C5-C4-N3	-6.25	118.59	126.75
24	B5	4317	A2M	C5-C4-N3	-6.24	118.61	126.75
63	A2	159	A2M	C5-C4-N3	-6.24	118.61	126.75
63	A2	485	A2M	C5-C4-N3	-6.23	118.62	126.75
24	B5	3966	6MZ	C5-C4-N3	-6.23	118.62	126.75
63	A2	99	A2M	C5-C4-N3	-6.20	118.66	126.75
24	B5	4336	A2M	C5-C4-N3	-6.20	118.66	126.75
24	B5	3450	A2M	C5-C4-N3	-6.18	118.69	126.75
63	A2	27	A2M	C5-C4-N3	-6.18	118.69	126.75
24	B5	3599	A2M	C5-C4-N3	-6.17	118.70	126.75
24	B5	400	A2M	C5-C4-N3	-6.17	118.70	126.75
24	B5	2630	A2M	C5-C4-N3	-6.17	118.70	126.75
24	B5	3562	A2M	C5-C4-N3	-6.17	118.70	126.75
24	B5	1580	OMG	C5-C4-N3	-6.16	118.47	128.46
24	B5	2244	A2M	C5-C4-N3	-6.16	118.71	126.75
24	B5	3524	OMG	C5-C4-N3	-6.16	118.47	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B5	3942	OMG	C5-C4-N3	-6.16	118.47	128.46
63	A2	469	A2M	C5-C4-N3	-6.16	118.72	126.75
63	A2	669	A2M	C5-C4-N3	-6.15	118.72	126.75
24	B5	398	A2M	C5-C4-N3	-6.15	118.73	126.75
63	A2	1640	G7M	CN7-N7-C5	-6.14	119.14	126.77
34	B8	75	OMG	C5-C4-N3	-6.13	118.51	128.46
24	B5	4138	OMG	C5-C4-N3	-6.13	118.52	128.46
63	A2	1491	OMG	C5-C4-N3	-6.12	118.53	128.46
24	B5	1270	A2M	C5-C4-N3	-6.12	118.77	126.75
24	B5	3517	A2M	C5-C4-N3	-6.12	118.77	126.75
63	A2	1384	A2M	C5-C4-N3	-6.11	118.77	126.75
24	B5	3494	PSU	N1-C2-N3	6.11	122.06	115.13
24	B5	4269	A2M	C5-C4-N3	-6.11	118.78	126.75
24	B5	1477	OMG	C5-C4-N3	-6.10	118.56	128.46
24	B5	4245	OMG	C5-C4-N3	-6.10	118.57	128.46
24	B5	1489	A2M	C5-C4-N3	-6.10	118.80	126.75
63	A2	510	OMG	C5-C4-N3	-6.09	118.58	128.46
24	B5	4149	PSU	N1-C2-N3	6.09	122.03	115.13
24	B5	4240	OMG	C5-C4-N3	-6.09	118.58	128.46
24	B5	3476	OMG	C5-C4-N3	-6.09	118.59	128.46
24	B5	3492	A2M	C5-C4-N3	-6.08	118.81	126.75
24	B5	3557	A2M	C5-C4-N3	-6.07	118.83	126.75
24	B5	3616	PSU	N1-C2-N3	6.07	122.01	115.13
63	A2	577	A2M	C5-C4-N3	-6.07	118.83	126.75
63	A2	1679	A2M	C5-C4-N3	-6.07	118.84	126.75
34	B8	69	PSU	N1-C2-N3	6.06	122.00	115.13
24	B5	3369	PSU	N1-C2-N3	6.06	122.00	115.13
63	A2	602	OMG	C5-C4-N3	-6.06	118.64	128.46
24	B5	2267	OMG	C5-C4-N3	-6.06	118.64	128.46
24	B5	4246	PSU	N1-C2-N3	6.05	121.99	115.13
63	A2	437	OMG	C5-C4-N3	-6.05	118.64	128.46
24	B5	3456	A2M	C5-C4-N3	-6.05	118.86	126.75
63	A2	1448	OMG	C5-C4-N3	-6.05	118.65	128.46
24	B5	4364	OMG	C5-C4-N3	-6.05	118.65	128.46
24	B5	1810	A2M	C5-C4-N3	-6.05	118.86	126.75
24	B5	1799	PSU	N1-C2-N3	6.04	121.98	115.13
63	A2	1047	PSU	N1-C2-N3	6.04	121.98	115.13
34	B8	55	PSU	N1-C2-N3	6.04	121.98	115.13
63	A2	645	OMG	C5-C4-N3	-6.04	118.66	128.46
63	A2	1644	PSU	N1-C2-N3	6.04	121.97	115.13
24	B5	4116	OMG	C5-C4-N3	-6.04	118.67	128.46
24	B5	4369	OMG	C5-C4-N3	-6.04	118.67	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	A2	1329	OMG	C5-C4-N3	-6.04	118.67	128.46
24	B5	3359	OMG	C5-C4-N3	-6.03	118.67	128.46
24	B5	4374	PSU	N1-C2-N3	6.03	121.96	115.13
24	B5	4711	PSU	N1-C2-N3	6.03	121.96	115.13
63	A2	1239	PSU	N1-C2-N3	6.02	121.95	115.13
63	A2	1032	A2M	C5-C4-N3	-6.02	118.90	126.75
63	A2	610	PSU	N1-C2-N3	6.02	121.95	115.13
63	A2	109	PSU	N1-C2-N3	6.02	121.95	115.13
63	A2	105	PSU	N1-C2-N3	6.02	121.94	115.13
24	B5	1491	PSU	N1-C2-N3	6.01	121.94	115.13
24	B5	1638	PSU	N1-C2-N3	6.01	121.94	115.13
24	B5	4382	PSU	N1-C2-N3	6.01	121.94	115.13
63	A2	682	PSU	N1-C2-N3	6.01	121.94	115.13
63	A2	823	PSU	N1-C2-N3	6.01	121.94	115.13
63	A2	1446	PSU	N1-C2-N3	6.01	121.94	115.13
24	B5	4217	PSU	N1-C2-N3	6.00	121.93	115.13
24	B5	4188	PSU	N1-C2-N3	6.00	121.93	115.13
63	A2	1851	MA6	N9-C8-N7	-6.00	105.71	113.91
63	A2	34	PSU	N1-C2-N3	6.00	121.92	115.13
24	B5	4298	PSU	N1-C2-N3	6.00	121.92	115.13
24	B5	1537	PSU	N1-C2-N3	5.99	121.92	115.13
24	B5	3490	PSU	N1-C2-N3	5.99	121.92	115.13
63	A2	1175	PSU	N1-C2-N3	5.99	121.92	115.13
24	B5	3652	PSU	N1-C2-N3	5.99	121.92	115.13
24	B5	3447	PSU	N1-C2-N3	5.99	121.92	115.13
63	A2	816	PSU	N1-C2-N3	5.99	121.92	115.13
63	A2	1368	PSU	N1-C2-N3	5.99	121.92	115.13
24	B5	3427	PSU	N1-C2-N3	5.99	121.92	115.13
24	B5	3466	PSU	N1-C2-N3	5.99	121.91	115.13
63	A2	1233	PSU	N1-C2-N3	5.99	121.91	115.13
24	B5	4099	PSU	N1-C2-N3	5.98	121.91	115.13
24	B5	1720	PSU	N1-C2-N3	5.98	121.91	115.13
24	B5	4749	PSU	N1-C2-N3	5.98	121.91	115.13
63	A2	1245	PSU	N1-C2-N3	5.98	121.91	115.13
63	A2	815	PSU	N1-C2-N3	5.98	121.91	115.13
24	B5	4435	PSU	N1-C2-N3	5.98	121.90	115.13
63	A2	1178	PSU	N1-C2-N3	5.98	121.90	115.13
63	A2	687	PSU	N1-C2-N3	5.98	121.90	115.13
63	A2	1693	PSU	N1-C2-N3	5.98	121.90	115.13
63	A2	1851	MA6	C4-C5-N7	-5.97	103.34	110.62
24	B5	4419	PSU	N1-C2-N3	5.97	121.90	115.13
24	B5	4042	PSU	N1-C2-N3	5.97	121.90	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	A2	650	PSU	N1-C2-N3	5.97	121.89	115.13
24	B5	4267	PSU	N1-C2-N3	5.97	121.89	115.13
63	A2	652	PSU	N1-C2-N3	5.97	121.89	115.13
24	B5	3576	PSU	N1-C2-N3	5.97	121.89	115.13
24	B5	4169	PSU	N1-C2-N3	5.97	121.89	115.13
24	B5	4058	PSU	N1-C2-N3	5.97	121.89	115.13
24	B5	3462	PSU	N1-C2-N3	5.96	121.89	115.13
24	B5	2475	PSU	N1-C2-N3	5.96	121.89	115.13
24	B5	4278	PSU	N1-C2-N3	5.96	121.89	115.13
63	A2	1348	PSU	N1-C2-N3	5.96	121.89	115.13
24	B5	2351	PSU	N1-C2-N3	5.96	121.88	115.13
63	A2	36	PSU	N1-C2-N3	5.96	121.88	115.13
63	A2	864	PSU	N1-C2-N3	5.96	121.88	115.13
24	B5	4383	OMG	C5-C4-N3	-5.96	118.80	128.46
63	A2	967	PSU	N1-C2-N3	5.96	121.88	115.13
63	A2	407	PSU	N1-C2-N3	5.95	121.88	115.13
24	B5	3500	PSU	N1-C2-N3	5.95	121.88	115.13
24	B5	3554	PSU	N1-C2-N3	5.95	121.88	115.13
24	B5	4322	PSU	N1-C2-N3	5.95	121.88	115.13
24	B5	4045	PSU	N1-C2-N3	5.95	121.87	115.13
24	B5	3631	OMG	C5-C4-N3	-5.95	118.81	128.46
24	B5	3974	OMG	C5-C4-N3	-5.95	118.81	128.46
63	A2	802	PSU	N1-C2-N3	5.95	121.87	115.13
24	B5	3371	PSU	N1-C2-N3	5.95	121.87	115.13
63	A2	218	PSU	N1-C2-N3	5.95	121.87	115.13
24	B5	1260	OMG	C5-C4-N3	-5.95	118.81	128.46
63	A2	573	PSU	N1-C2-N3	5.94	121.86	115.13
24	B5	4177	PSU	N1-C2-N3	5.94	121.86	115.13
24	B5	1721	PSU	N1-C2-N3	5.94	121.86	115.13
24	B5	4740	PSU	N1-C2-N3	5.94	121.86	115.13
24	B5	1731	PSU	N1-C2-N3	5.94	121.86	115.13
24	B5	1801	PSU	N1-C2-N3	5.94	121.86	115.13
63	A2	867	PSU	N1-C2-N3	5.94	121.86	115.13
63	A2	1057	PSU	N1-C2-N3	5.93	121.85	115.13
63	A2	93	PSU	N1-C2-N3	5.93	121.85	115.13
24	B5	1718	PSU	N1-C2-N3	5.93	121.85	115.13
24	B5	1683	PSU	N1-C2-N3	5.93	121.85	115.13
24	B5	4325	PSU	N1-C2-N3	5.93	121.85	115.13
24	B5	3676	OMG	C5-C4-N3	-5.93	118.84	128.46
24	B5	1632	PSU	N1-C2-N3	5.93	121.84	115.13
63	A2	1046	PSU	N1-C2-N3	5.93	121.84	115.13
24	B5	4039	PSU	N1-C2-N3	5.92	121.84	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B5	3585	PSU	N1-C2-N3	5.92	121.84	115.13
63	A2	1626	PSU	N1-C2-N3	5.92	121.84	115.13
63	A2	119	PSU	N1-C2-N3	5.92	121.84	115.13
63	A2	210	PSU	N1-C2-N3	5.92	121.84	115.13
63	A2	1005	PSU	N1-C2-N3	5.92	121.83	115.13
24	B5	3502	PSU	N1-C2-N3	5.91	121.83	115.13
63	A2	684	OMG	C5-C4-N3	-5.91	118.88	128.46
24	B5	4203	PSU	N1-C2-N3	5.90	121.82	115.13
63	A2	1852	MA6	C5-C4-N3	-5.88	119.07	126.75
24	B5	3496	PSU	N1-C2-N3	5.88	121.79	115.13
24	B5	3583	PSU	N1-C2-N3	5.87	121.78	115.13
24	B5	4107	PSU	N1-C2-N3	5.86	121.77	115.13
63	A2	1082	PSU	N1-C2-N3	5.85	121.76	115.13
24	B5	2207	OMG	C5-C4-N3	-5.84	118.99	128.46
63	A2	868	OMG	C5-C4-N3	-5.80	119.06	128.46
63	A2	1852	MA6	C4-C5-N7	-5.77	103.59	110.62
63	A2	1852	MA6	N9-C8-N7	-5.77	106.02	113.91
24	B5	4276	UR3	C4-N3-C2	-5.77	119.13	124.56
24	B5	4166	PSU	N1-C2-N3	5.75	121.64	115.13
63	A2	1851	MA6	C5-C4-N3	-5.62	119.42	126.75
24	B5	1266	1MA	C5-C4-N3	-5.47	119.09	127.26
63	A2	591	A2M	N3-C4-N9	5.47	136.09	127.08
24	B5	3550	UY1	C4-N3-C2	-5.22	118.83	126.34
63	A2	1833	6MZ	N3-C4-N9	5.15	135.57	127.08
24	B5	2719	OMG	C2-N3-C4	5.05	121.30	112.30
24	B5	4369	OMG	C2-N3-C4	4.92	121.07	112.30
63	A2	437	OMG	C2-N3-C4	4.92	121.06	112.30
63	A2	645	OMG	C2-N3-C4	4.91	121.05	112.30
63	A2	602	OMG	C2-N3-C4	4.91	121.05	112.30
34	B8	75	OMG	C2-N3-C4	4.91	121.04	112.30
24	B5	3524	OMG	C2-N3-C4	4.90	121.04	112.30
24	B5	1477	OMG	C2-N3-C4	4.90	121.03	112.30
24	B5	4138	OMG	C2-N3-C4	4.89	121.01	112.30
24	B5	4245	OMG	C2-N3-C4	4.89	121.01	112.30
24	B5	3476	OMG	C2-N3-C4	4.89	121.01	112.30
24	B5	1479	A2M	N3-C4-N9	4.88	135.13	127.08
24	B5	3942	OMG	C2-N3-C4	4.87	120.98	112.30
63	A2	1491	OMG	C2-N3-C4	4.87	120.98	112.30
24	B5	1580	OMG	C2-N3-C4	4.87	120.98	112.30
63	A2	1448	OMG	C2-N3-C4	4.87	120.98	112.30
24	B5	4364	OMG	C2-N3-C4	4.87	120.98	112.30
24	B5	4116	OMG	C2-N3-C4	4.87	120.97	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B5	3359	OMG	C2-N3-C4	4.87	120.97	112.30
24	B5	4240	OMG	C2-N3-C4	4.86	120.96	112.30
24	B5	3676	OMG	C2-N3-C4	4.86	120.96	112.30
63	A2	1329	OMG	C2-N3-C4	4.86	120.96	112.30
24	B5	2267	OMG	C2-N3-C4	4.85	120.95	112.30
24	B5	4317	A2M	N3-C4-N9	4.85	135.08	127.08
24	B5	3966	6MZ	N3-C4-N9	4.85	135.08	127.08
24	B5	3974	OMG	C2-N3-C4	4.85	120.94	112.30
63	A2	99	A2M	N3-C4-N9	4.85	135.07	127.08
63	A2	684	OMG	C2-N3-C4	4.85	120.94	112.30
63	A2	513	A2M	N3-C4-N9	4.85	135.07	127.08
24	B5	1260	OMG	C2-N3-C4	4.85	120.93	112.30
63	A2	510	OMG	C2-N3-C4	4.84	120.93	112.30
63	A2	1640	G7M	C2-N3-C4	4.84	120.93	112.30
24	B5	2207	OMG	C2-N3-C4	4.84	120.93	112.30
63	A2	159	A2M	N3-C4-N9	4.84	135.06	127.08
63	A2	166	A2M	N3-C4-N9	4.84	135.05	127.08
24	B5	2630	A2M	N3-C4-N9	4.84	135.05	127.08
24	B5	3631	OMG	C2-N3-C4	4.83	120.91	112.30
24	B5	2658	A2M	N3-C4-N9	4.83	135.04	127.08
24	B5	3599	A2M	N3-C4-N9	4.82	135.03	127.08
24	B5	4383	OMG	C2-N3-C4	4.82	120.89	112.30
63	A2	27	A2M	N3-C4-N9	4.82	135.03	127.08
63	A2	485	A2M	N3-C4-N9	4.82	135.03	127.08
24	B5	3517	A2M	N3-C4-N9	4.82	135.02	127.08
24	B5	2244	A2M	N3-C4-N9	4.81	135.01	127.08
24	B5	3562	A2M	N3-C4-N9	4.81	135.01	127.08
63	A2	868	OMG	C2-N3-C4	4.81	120.87	112.30
24	B5	3492	A2M	N3-C4-N9	4.80	135.00	127.08
24	B5	398	A2M	N3-C4-N9	4.80	134.99	127.08
24	B5	4336	A2M	N3-C4-N9	4.80	134.99	127.08
63	A2	469	A2M	N3-C4-N9	4.80	134.99	127.08
63	A2	669	A2M	N3-C4-N9	4.78	134.96	127.08
63	A2	1384	A2M	N3-C4-N9	4.78	134.96	127.08
24	B5	400	A2M	N3-C4-N9	4.78	134.95	127.08
24	B5	2719	OMG	N9-C4-N3	4.77	135.53	125.94
24	B5	2206	A2M	N3-C4-N9	4.77	134.94	127.08
24	B5	1270	A2M	N3-C4-N9	4.76	134.93	127.08
24	B5	1266	1MA	C2-N3-C4	4.75	121.74	112.41
24	B5	3450	A2M	N3-C4-N9	4.74	134.90	127.08
63	A2	1679	A2M	N3-C4-N9	4.74	134.90	127.08
24	B5	3557	A2M	N3-C4-N9	4.73	134.88	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B5	3456	A2M	N3-C4-N9	4.73	134.87	127.08
24	B5	4269	A2M	N3-C4-N9	4.72	134.86	127.08
24	B5	1810	A2M	N3-C4-N9	4.71	134.85	127.08
63	A2	577	A2M	N3-C4-N9	4.71	134.84	127.08
63	A2	1032	A2M	N3-C4-N9	4.69	134.82	127.08
63	A2	1843	4AC	N4-C4-N3	4.68	121.71	113.85
24	B5	1580	OMG	N9-C4-N3	4.65	135.28	125.94
24	B5	1489	A2M	N3-C4-N9	4.63	134.72	127.08
63	A2	1491	OMG	N9-C4-N3	4.60	135.18	125.94
24	B5	3524	OMG	N9-C4-N3	4.60	135.18	125.94
24	B5	3942	OMG	N9-C4-N3	4.59	135.15	125.94
24	B5	4240	OMG	N9-C4-N3	4.57	135.11	125.94
34	B8	75	OMG	N9-C4-N3	4.56	135.10	125.94
24	B5	1477	OMG	N9-C4-N3	4.55	135.08	125.94
24	B5	4138	OMG	N9-C4-N3	4.55	135.08	125.94
24	B5	4245	OMG	N9-C4-N3	4.55	135.08	125.94
63	A2	510	OMG	N9-C4-N3	4.55	135.07	125.94
24	B5	2267	OMG	N9-C4-N3	4.53	135.03	125.94
63	A2	1327	OMU	C4-N3-C2	-4.52	120.62	126.58
63	A2	628	OMU	C4-N3-C2	-4.51	120.63	126.58
24	B5	3476	OMG	N9-C4-N3	4.51	135.00	125.94
24	B5	4116	OMG	N9-C4-N3	4.50	134.98	125.94
24	B5	3359	OMG	N9-C4-N3	4.50	134.97	125.94
63	A2	437	OMG	N9-C4-N3	4.49	134.95	125.94
24	B5	2680	OMU	C4-N3-C2	-4.48	120.67	126.58
63	A2	1640	G7M	C5-C4-N3	-4.47	119.57	128.15
63	A2	1338	4AC	N4-C4-N3	4.47	121.35	113.85
24	B5	3657	OMU	C4-N3-C2	-4.47	120.69	126.58
24	B5	4364	OMG	N9-C4-N3	4.47	134.91	125.94
63	A2	1329	OMG	N9-C4-N3	4.46	134.90	125.94
24	B5	4369	OMG	N9-C4-N3	4.46	134.90	125.94
63	A2	645	OMG	N9-C4-N3	4.46	134.89	125.94
63	A2	602	OMG	N9-C4-N3	4.45	134.88	125.94
24	B5	4244	OMU	C4-N3-C2	-4.45	120.71	126.58
63	A2	355	OMU	C4-N3-C2	-4.45	120.72	126.58
24	B5	3973	OMU	C4-N3-C2	-4.44	120.72	126.58
63	A2	1448	OMG	N9-C4-N3	4.44	134.86	125.94
63	A2	429	OMU	C4-N3-C2	-4.42	120.76	126.58
24	B5	3974	OMG	N9-C4-N3	4.41	134.79	125.94
24	B5	4383	OMG	N9-C4-N3	4.41	134.79	125.94
63	A2	172	OMU	C4-N3-C2	-4.41	120.77	126.58
24	B5	3676	OMG	N9-C4-N3	4.40	134.77	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B5	1260	OMG	N9-C4-N3	4.39	134.76	125.94
63	A2	116	OMU	C4-N3-C2	-4.39	120.79	126.58
24	B5	4366	OMU	C4-N3-C2	-4.39	120.80	126.58
24	B5	3631	OMG	N9-C4-N3	4.38	134.74	125.94
63	A2	684	OMG	N9-C4-N3	4.35	134.67	125.94
24	B5	2258	OMU	C4-N3-C2	-4.32	120.89	126.58
24	B5	4052	OMU	C4-N3-C2	-4.31	120.89	126.58
63	A2	1805	OMU	C4-N3-C2	-4.31	120.89	126.58
24	B5	2207	OMG	N9-C4-N3	4.31	134.60	125.94
63	A2	121	OMU	C4-N3-C2	-4.29	120.92	126.58
63	A2	1851	MA6	N1-C2-N3	-4.28	121.91	128.60
63	A2	1443	OMU	C4-N3-C2	-4.26	120.95	126.58
63	A2	1289	OMU	C4-N3-C2	-4.24	120.99	126.58
24	B5	3550	UY1	N1-C2-N3	4.24	119.93	115.13
63	A2	1679	A2M	C2'-C1'-N9	-4.21	106.44	113.53
63	A2	868	OMG	N9-C4-N3	4.21	134.38	125.94
63	A2	1851	MA6	C2-N1-C6	4.19	121.66	111.75
24	B5	1810	A2M	C2'-C1'-N9	-4.16	106.53	113.53
63	A2	591	A2M	C2-N3-C4	4.15	121.56	111.75
63	A2	1327	OMU	N3-C2-N1	4.15	120.40	114.89
63	A2	1852	MA6	N1-C2-N3	-4.15	122.12	128.60
63	A2	429	OMU	N3-C2-N1	4.14	120.39	114.89
24	B5	4366	OMU	N3-C2-N1	4.14	120.38	114.89
24	B5	2680	OMU	N3-C2-N1	4.13	120.37	114.89
24	B5	3973	OMU	N3-C2-N1	4.12	120.36	114.89
63	A2	355	OMU	N3-C2-N1	4.11	120.35	114.89
24	B5	4244	OMU	N3-C2-N1	4.10	120.34	114.89
24	B5	3657	OMU	N3-C2-N1	4.10	120.34	114.89
63	A2	628	OMU	N3-C2-N1	4.07	120.30	114.89
63	A2	116	OMU	N3-C2-N1	4.07	120.29	114.89
24	B5	2258	OMU	N3-C2-N1	4.04	120.25	114.89
63	A2	1805	OMU	N3-C2-N1	4.04	120.25	114.89
63	A2	172	OMU	N3-C2-N1	4.03	120.23	114.89
24	B5	4052	OMU	N3-C2-N1	4.02	120.23	114.89
63	A2	1852	MA6	C2-N1-C6	4.02	121.25	111.75
24	B5	4188	PSU	C4-N3-C2	-3.99	120.59	126.34
63	A2	1443	OMU	N3-C2-N1	3.99	120.19	114.89
24	B5	4149	PSU	C4-N3-C2	-3.97	120.61	126.34
63	A2	1289	OMU	N3-C2-N1	3.97	120.16	114.89
34	B8	69	PSU	C4-N3-C2	-3.96	120.63	126.34
24	B5	3616	PSU	C4-N3-C2	-3.96	120.63	126.34
24	B5	4267	PSU	C4-N3-C2	-3.95	120.64	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B5	4042	PSU	C4-N3-C2	-3.95	120.65	126.34
63	A2	1644	PSU	C4-N3-C2	-3.95	120.65	126.34
63	A2	1233	PSU	C4-N3-C2	-3.95	120.65	126.34
63	A2	121	OMU	N3-C2-N1	3.94	120.12	114.89
63	A2	1047	PSU	C4-N3-C2	-3.94	120.66	126.34
24	B5	4298	PSU	C4-N3-C2	-3.94	120.66	126.34
24	B5	3369	PSU	C4-N3-C2	-3.94	120.67	126.34
63	A2	1175	PSU	C4-N3-C2	-3.94	120.67	126.34
34	B8	55	PSU	C4-N3-C2	-3.94	120.67	126.34
63	A2	1640	G7M	CN7-N7-C8	-3.94	118.77	124.84
24	B5	1491	PSU	C4-N3-C2	-3.93	120.67	126.34
24	B5	3490	PSU	C4-N3-C2	-3.93	120.67	126.34
63	A2	610	PSU	C4-N3-C2	-3.93	120.67	126.34
24	B5	4336	A2M	C2-N3-C4	3.93	121.03	111.75
24	B5	4374	PSU	C4-N3-C2	-3.93	120.68	126.34
24	B5	4711	PSU	C4-N3-C2	-3.93	120.68	126.34
24	B5	4246	PSU	C4-N3-C2	-3.92	120.69	126.34
63	A2	166	A2M	C2-N3-C4	3.92	121.00	111.75
24	B5	1801	PSU	C4-N3-C2	-3.91	120.70	126.34
24	B5	4099	PSU	C4-N3-C2	-3.91	120.70	126.34
63	A2	652	PSU	C4-N3-C2	-3.91	120.70	126.34
24	B5	1799	PSU	C4-N3-C2	-3.91	120.70	126.34
63	A2	650	PSU	C4-N3-C2	-3.91	120.70	126.34
63	A2	1245	PSU	C4-N3-C2	-3.91	120.71	126.34
24	B5	4419	PSU	C4-N3-C2	-3.91	120.71	126.34
63	A2	218	PSU	C4-N3-C2	-3.91	120.71	126.34
63	A2	1178	PSU	C4-N3-C2	-3.90	120.71	126.34
24	B5	3462	PSU	C4-N3-C2	-3.90	120.72	126.34
24	B5	1731	PSU	C4-N3-C2	-3.90	120.72	126.34
24	B5	4325	PSU	C4-N3-C2	-3.90	120.72	126.34
63	A2	1679	A2M	C2-N3-C4	3.90	120.96	111.75
63	A2	1693	PSU	C4-N3-C2	-3.90	120.72	126.34
24	B5	2351	PSU	C4-N3-C2	-3.90	120.73	126.34
24	B5	3466	PSU	C4-N3-C2	-3.89	120.73	126.34
63	A2	1368	PSU	C4-N3-C2	-3.89	120.73	126.34
24	B5	1638	PSU	C4-N3-C2	-3.89	120.73	126.34
24	B5	4217	PSU	C4-N3-C2	-3.89	120.73	126.34
24	B5	3576	PSU	C4-N3-C2	-3.89	120.73	126.34
63	A2	867	PSU	C4-N3-C2	-3.89	120.73	126.34
63	A2	513	A2M	C2-N3-C4	3.89	120.94	111.75
63	A2	34	PSU	C4-N3-C2	-3.89	120.74	126.34
24	B5	1721	PSU	C4-N3-C2	-3.89	120.74	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B5	4058	PSU	C4-N3-C2	-3.89	120.74	126.34
24	B5	3427	PSU	C4-N3-C2	-3.88	120.74	126.34
24	B5	4317	A2M	C2-N3-C4	3.88	120.93	111.75
24	B5	2206	A2M	C2-N3-C4	3.88	120.92	111.75
24	B5	1718	PSU	C4-N3-C2	-3.88	120.74	126.34
24	B5	4177	PSU	C4-N3-C2	-3.88	120.74	126.34
24	B5	2658	A2M	C2-N3-C4	3.88	120.92	111.75
63	A2	816	PSU	C4-N3-C2	-3.88	120.75	126.34
24	B5	3447	PSU	C4-N3-C2	-3.88	120.75	126.34
63	A2	815	PSU	C4-N3-C2	-3.88	120.75	126.34
24	B5	1479	A2M	C2-N3-C4	3.88	120.91	111.75
63	A2	407	PSU	C4-N3-C2	-3.88	120.75	126.34
63	A2	682	PSU	C4-N3-C2	-3.88	120.75	126.34
63	A2	1348	PSU	C4-N3-C2	-3.88	120.75	126.34
24	B5	1489	A2M	C2-N3-C4	3.88	120.91	111.75
24	B5	4749	PSU	C4-N3-C2	-3.87	120.76	126.34
63	A2	1046	PSU	C4-N3-C2	-3.87	120.76	126.34
24	B5	3599	A2M	C2-N3-C4	3.87	120.90	111.75
63	A2	109	PSU	C4-N3-C2	-3.87	120.76	126.34
24	B5	2475	PSU	C4-N3-C2	-3.87	120.77	126.34
24	B5	3502	PSU	C4-N3-C2	-3.87	120.77	126.34
63	A2	1446	PSU	C4-N3-C2	-3.87	120.77	126.34
63	A2	1833	6MZ	C2-N3-C4	3.87	120.89	111.75
63	A2	1239	PSU	C4-N3-C2	-3.87	120.77	126.34
63	A2	93	PSU	C4-N3-C2	-3.86	120.77	126.34
24	B5	1683	PSU	C4-N3-C2	-3.86	120.77	126.34
24	B5	2244	A2M	C2-N3-C4	3.86	120.88	111.75
63	A2	99	A2M	C2-N3-C4	3.86	120.88	111.75
24	B5	398	A2M	C2-N3-C4	3.86	120.88	111.75
24	B5	3562	A2M	C2-N3-C4	3.86	120.87	111.75
24	B5	4435	PSU	C4-N3-C2	-3.86	120.78	126.34
24	B5	3496	PSU	C4-N3-C2	-3.86	120.78	126.34
63	A2	802	PSU	C4-N3-C2	-3.86	120.78	126.34
24	B5	3517	A2M	C2-N3-C4	3.86	120.87	111.75
63	A2	469	A2M	C2-N3-C4	3.86	120.87	111.75
63	A2	105	PSU	C4-N3-C2	-3.86	120.78	126.34
63	A2	159	A2M	C2-N3-C4	3.86	120.86	111.75
63	A2	864	PSU	C4-N3-C2	-3.86	120.78	126.34
24	B5	4045	PSU	C4-N3-C2	-3.85	120.79	126.34
24	B5	4039	PSU	C4-N3-C2	-3.85	120.79	126.34
63	A2	687	PSU	C4-N3-C2	-3.85	120.79	126.34
24	B5	3500	PSU	C4-N3-C2	-3.85	120.79	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B5	3652	PSU	C4-N3-C2	-3.85	120.79	126.34
24	B5	1270	A2M	C2-N3-C4	3.85	120.84	111.75
63	A2	27	A2M	C2-N3-C4	3.84	120.83	111.75
24	B5	3456	A2M	C2-N3-C4	3.84	120.82	111.75
24	B5	3450	A2M	C2-N3-C4	3.84	120.82	111.75
63	A2	36	PSU	C4-N3-C2	-3.84	120.81	126.34
63	A2	1005	PSU	C4-N3-C2	-3.84	120.81	126.34
63	A2	823	PSU	C4-N3-C2	-3.84	120.81	126.34
24	B5	3494	PSU	C4-N3-C2	-3.84	120.81	126.34
24	B5	4740	PSU	C4-N3-C2	-3.84	120.81	126.34
63	A2	485	A2M	C2-N3-C4	3.84	120.81	111.75
24	B5	4269	A2M	C2-N3-C4	3.83	120.81	111.75
63	A2	573	PSU	C4-N3-C2	-3.83	120.82	126.34
63	A2	669	A2M	C2-N3-C4	3.83	120.80	111.75
24	B5	3966	6MZ	C2-N3-C4	3.83	120.80	111.75
63	A2	1057	PSU	C4-N3-C2	-3.83	120.82	126.34
24	B5	1810	A2M	C2-N3-C4	3.83	120.79	111.75
24	B5	3585	PSU	C4-N3-C2	-3.83	120.83	126.34
24	B5	4193	5MC	C5-C6-N1	-3.82	119.41	123.34
63	A2	1032	A2M	C2-N3-C4	3.82	120.78	111.75
24	B5	3554	PSU	C4-N3-C2	-3.82	120.83	126.34
63	A2	119	PSU	C4-N3-C2	-3.82	120.83	126.34
63	A2	1384	A2M	C2-N3-C4	3.82	120.78	111.75
24	B5	3557	A2M	C2-N3-C4	3.82	120.77	111.75
24	B5	3492	A2M	C2-N3-C4	3.82	120.77	111.75
24	B5	1720	PSU	C4-N3-C2	-3.82	120.84	126.34
63	A2	577	A2M	C2-N3-C4	3.81	120.76	111.75
24	B5	4203	PSU	C4-N3-C2	-3.81	120.85	126.34
24	B5	4107	PSU	C4-N3-C2	-3.81	120.85	126.34
24	B5	400	A2M	C2-N3-C4	3.81	120.75	111.75
24	B5	3583	PSU	C4-N3-C2	-3.81	120.86	126.34
63	A2	967	PSU	C4-N3-C2	-3.80	120.86	126.34
24	B5	2630	A2M	C2-N3-C4	3.80	120.73	111.75
24	B5	4169	PSU	C4-N3-C2	-3.80	120.86	126.34
24	B5	1537	PSU	C4-N3-C2	-3.80	120.87	126.34
63	A2	1626	PSU	C4-N3-C2	-3.79	120.87	126.34
24	B5	4382	PSU	C4-N3-C2	-3.79	120.87	126.34
63	A2	1640	G7M	C5-C6-N1	3.79	119.70	111.79
24	B5	4322	PSU	C4-N3-C2	-3.78	120.89	126.34
24	B5	3371	PSU	C4-N3-C2	-3.78	120.89	126.34
24	B5	4278	PSU	C4-N3-C2	-3.77	120.90	126.34
63	A2	1082	PSU	C4-N3-C2	-3.74	120.94	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	A2	210	PSU	C4-N3-C2	-3.73	120.97	126.34
24	B5	1632	PSU	C4-N3-C2	-3.72	120.98	126.34
63	A2	1640	G7M	N9-C8-N7	-3.71	103.03	112.21
63	A2	1640	G7M	C4-C5-N7	-3.64	101.71	107.67
24	B5	4244	OMU	C5-C4-N3	3.61	120.24	114.84
63	A2	1851	MA6	C6-C5-N7	3.60	139.32	133.28
63	A2	628	OMU	C5-C4-N3	3.58	120.20	114.84
24	B5	398	A2M	C2'-C1'-N9	-3.58	107.50	113.53
24	B5	2680	OMU	C5-C4-N3	3.58	120.20	114.84
24	B5	3557	A2M	C2'-C1'-N9	-3.57	107.53	113.53
24	B5	3973	OMU	C5-C4-N3	3.56	120.16	114.84
24	B5	3562	A2M	C2'-C1'-N9	-3.56	107.54	113.53
63	A2	355	OMU	C5-C4-N3	3.56	120.16	114.84
24	B5	3494	PSU	O2-C2-N1	-3.55	118.88	122.79
24	B5	3657	OMU	C5-C4-N3	3.55	120.16	114.84
63	A2	116	OMU	C5-C4-N3	3.55	120.15	114.84
63	A2	429	OMU	C5-C4-N3	3.53	120.12	114.84
63	A2	1327	OMU	C5-C4-N3	3.53	120.12	114.84
24	B5	2258	OMU	C5-C4-N3	3.53	120.12	114.84
63	A2	1443	OMU	C5-C4-N3	3.52	120.11	114.84
24	B5	3456	A2M	C2'-C1'-N9	-3.52	107.60	113.53
24	B5	4435	PSU	O2-C2-N1	-3.51	118.92	122.79
63	A2	1289	OMU	C5-C4-N3	3.51	120.10	114.84
24	B5	4052	OMU	C5-C4-N3	3.51	120.09	114.84
63	A2	172	OMU	C5-C4-N3	3.51	120.09	114.84
63	A2	121	OMU	C5-C4-N3	3.51	120.09	114.84
24	B5	4366	OMU	C5-C4-N3	3.51	120.09	114.84
63	A2	1805	OMU	C5-C4-N3	3.51	120.08	114.84
24	B5	4382	PSU	O2-C2-N1	-3.50	118.94	122.79
63	A2	1852	MA6	C1'-N9-C8	-3.50	119.24	127.14
24	B5	4166	PSU	C4-N3-C2	-3.49	121.31	126.34
34	B8	55	PSU	O2-C2-N1	-3.49	118.94	122.79
63	A2	1852	MA6	C2-N3-C4	3.48	119.98	111.75
24	B5	4246	PSU	O2-C2-N1	-3.47	118.97	122.79
63	A2	1047	PSU	O2-C2-N1	-3.47	118.97	122.79
63	A2	166	A2M	C2'-C1'-N9	-3.47	107.70	113.53
63	A2	802	PSU	O2-C2-N1	-3.46	118.98	122.79
63	A2	1368	PSU	O2-C2-N1	-3.46	118.98	122.79
24	B5	1799	PSU	O2-C2-N1	-3.46	118.98	122.79
24	B5	3462	PSU	O2-C2-N1	-3.46	118.99	122.79
63	A2	36	PSU	O2-C2-N1	-3.46	118.99	122.79
63	A2	967	PSU	O2-C2-N1	-3.45	118.99	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	A2	1851	MA6	C2-N3-C4	3.45	119.91	111.75
63	A2	868	OMG	C6-C5-N7	3.45	136.66	130.25
50	Ba	39	V5N	CD2-CG-ND1	3.45	110.23	105.71
24	B5	1720	PSU	O2-C2-N1	-3.45	119.00	122.79
24	B5	4058	PSU	O2-C2-N1	-3.44	119.00	122.79
24	B5	4298	PSU	O2-C2-N1	-3.44	119.00	122.79
63	A2	1693	PSU	O2-C2-N1	-3.44	119.00	122.79
63	A2	109	PSU	O2-C2-N1	-3.44	119.00	122.79
24	B5	1638	PSU	O2-C2-N1	-3.44	119.00	122.79
24	B5	1491	PSU	O2-C2-N1	-3.43	119.01	122.79
63	A2	1446	PSU	O2-C2-N1	-3.43	119.01	122.79
24	B5	1683	PSU	O2-C2-N1	-3.43	119.01	122.79
63	A2	99	A2M	C2'-C1'-N9	-3.43	107.75	113.53
63	A2	34	PSU	O2-C2-N1	-3.43	119.02	122.79
24	B5	1632	PSU	O2-C2-N1	-3.42	119.02	122.79
63	A2	1057	PSU	O2-C2-N1	-3.42	119.02	122.79
24	B5	4374	PSU	O2-C2-N1	-3.42	119.02	122.79
24	B5	4278	PSU	O2-C2-N1	-3.42	119.02	122.79
63	A2	1175	PSU	O2-C2-N1	-3.42	119.02	122.79
24	B5	2244	A2M	C2'-C1'-N9	-3.42	107.77	113.53
24	B5	3514	5MC	C5-C6-N1	-3.42	119.82	123.34
24	B5	1718	PSU	O2-C2-N1	-3.41	119.03	122.79
24	B5	4322	PSU	O2-C2-N1	-3.41	119.03	122.79
63	A2	687	PSU	O2-C2-N1	-3.41	119.03	122.79
24	B5	3554	PSU	O2-C2-N1	-3.41	119.03	122.79
24	B5	4188	PSU	O2-C2-N1	-3.41	119.03	122.79
63	A2	1348	PSU	O2-C2-N1	-3.41	119.04	122.79
63	A2	1626	PSU	O2-C2-N1	-3.41	119.04	122.79
24	B5	3427	PSU	O2-C2-N1	-3.41	119.04	122.79
63	A2	1178	PSU	O2-C2-N1	-3.41	119.04	122.79
63	A2	210	PSU	O2-C2-N1	-3.41	119.04	122.79
24	B5	3502	PSU	O2-C2-N1	-3.40	119.05	122.79
63	A2	1245	PSU	O2-C2-N1	-3.40	119.05	122.79
24	B5	3500	PSU	O2-C2-N1	-3.40	119.05	122.79
24	B5	4149	PSU	O2-C2-N1	-3.40	119.05	122.79
24	B5	4419	PSU	O2-C2-N1	-3.40	119.05	122.79
63	A2	650	PSU	O2-C2-N1	-3.39	119.05	122.79
24	B5	1489	A2M	C4-C5-N7	-3.39	106.49	110.62
63	A2	407	PSU	O2-C2-N1	-3.39	119.06	122.79
24	B5	2207	OMG	C6-C5-N7	3.39	136.56	130.25
24	B5	3616	PSU	O2-C2-N1	-3.39	119.06	122.79
63	A2	823	PSU	O2-C2-N1	-3.39	119.06	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	A2	1005	PSU	O2-C2-N1	-3.39	119.06	122.79
24	B5	3466	PSU	O2-C2-N1	-3.39	119.06	122.79
24	B5	3585	PSU	O2-C2-N1	-3.39	119.06	122.79
24	B5	4749	PSU	O2-C2-N1	-3.39	119.06	122.79
63	A2	864	PSU	O2-C2-N1	-3.38	119.07	122.79
24	B5	4166	PSU	O2-C2-N1	-3.38	119.07	122.79
63	A2	1239	PSU	O2-C2-N1	-3.38	119.07	122.79
24	B5	4267	PSU	O2-C2-N1	-3.38	119.07	122.79
24	B5	1537	PSU	O2-C2-N1	-3.38	119.07	122.79
63	A2	513	A2M	C4-C5-N7	-3.38	106.50	110.62
63	A2	652	PSU	O2-C2-N1	-3.38	119.07	122.79
63	A2	1644	PSU	O2-C2-N1	-3.38	119.07	122.79
24	B5	3447	PSU	O2-C2-N1	-3.38	119.07	122.79
24	B5	4177	PSU	O2-C2-N1	-3.38	119.07	122.79
63	A2	1046	PSU	O2-C2-N1	-3.38	119.07	122.79
63	A2	105	PSU	O2-C2-N1	-3.37	119.08	122.79
24	B5	3369	PSU	O2-C2-N1	-3.37	119.08	122.79
24	B5	4711	PSU	O2-C2-N1	-3.37	119.08	122.79
24	B5	4045	PSU	O2-C2-N1	-3.36	119.09	122.79
24	B5	4203	PSU	O2-C2-N1	-3.36	119.09	122.79
24	B5	1731	PSU	O2-C2-N1	-3.36	119.09	122.79
24	B5	3496	PSU	O2-C2-N1	-3.36	119.09	122.79
63	A2	218	PSU	O2-C2-N1	-3.36	119.09	122.79
63	A2	610	PSU	O2-C2-N1	-3.36	119.09	122.79
24	B5	2206	A2M	C4-C5-N7	-3.36	106.53	110.62
24	B5	3652	PSU	O2-C2-N1	-3.36	119.09	122.79
63	A2	573	PSU	O2-C2-N1	-3.36	119.09	122.79
38	BA	216	V5N	CD2-CG-ND1	3.36	110.12	105.71
24	B5	3576	PSU	O2-C2-N1	-3.36	119.10	122.79
24	B5	4099	PSU	O2-C2-N1	-3.36	119.10	122.79
24	B5	4169	PSU	O2-C2-N1	-3.36	119.10	122.79
24	B5	1801	PSU	O2-C2-N1	-3.35	119.10	122.79
63	A2	93	PSU	O2-C2-N1	-3.35	119.10	122.79
63	A2	119	PSU	O2-C2-N1	-3.35	119.10	122.79
34	B8	69	PSU	O2-C2-N1	-3.35	119.10	122.79
24	B5	2475	PSU	O2-C2-N1	-3.35	119.10	122.79
63	A2	577	A2M	C2'-C1'-N9	-3.35	107.89	113.53
24	B5	2351	PSU	O2-C2-N1	-3.35	119.10	122.79
24	B5	3490	PSU	O2-C2-N1	-3.35	119.11	122.79
63	A2	1233	PSU	O2-C2-N1	-3.35	119.11	122.79
24	B5	4336	A2M	C4-C5-N7	-3.34	106.55	110.62
63	A2	1851	MA6	C1'-N9-C8	-3.34	119.59	127.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	A2	682	PSU	O2-C2-N1	-3.34	119.11	122.79
63	A2	867	PSU	O2-C2-N1	-3.34	119.12	122.79
63	A2	816	PSU	O2-C2-N1	-3.34	119.12	122.79
63	A2	166	A2M	C4-C5-N7	-3.34	106.56	110.62
63	A2	159	A2M	C4-C5-N7	-3.33	106.56	110.62
63	A2	684	OMG	C6-C5-N7	3.33	136.44	130.25
24	B5	4042	PSU	O2-C2-N1	-3.33	119.12	122.79
24	B5	4740	PSU	O2-C2-N1	-3.33	119.13	122.79
63	A2	1852	MA6	C6-C5-N7	3.33	138.87	133.28
24	B5	3450	A2M	C4-C5-N7	-3.32	106.57	110.62
24	B5	4383	OMG	C6-C5-N7	3.32	136.43	130.25
24	B5	4039	PSU	O2-C2-N1	-3.32	119.13	122.79
24	B5	400	A2M	C4-C5-N7	-3.32	106.57	110.62
63	A2	1679	A2M	C4-C5-N7	-3.32	106.57	110.62
63	A2	577	A2M	C4-C5-N7	-3.32	106.58	110.62
24	B5	3583	PSU	O2-C2-N1	-3.32	119.14	122.79
24	B5	1266	1MA	N9-C4-N3	3.32	134.67	126.94
24	B5	1260	OMG	C6-C5-N7	3.31	136.41	130.25
63	A2	815	PSU	O2-C2-N1	-3.31	119.14	122.79
24	B5	3371	PSU	O2-C2-N1	-3.31	119.15	122.79
24	B5	1810	A2M	C4-C5-N7	-3.31	106.59	110.62
24	B5	4269	A2M	C4-C5-N7	-3.31	106.59	110.62
63	A2	1851	MA6	C4-N9-C1'	-3.31	118.72	126.59
24	B5	2658	A2M	C4-C5-N7	-3.30	106.60	110.62
63	A2	27	A2M	C4-C5-N7	-3.30	106.60	110.62
24	B5	1721	PSU	O2-C2-N1	-3.30	119.16	122.79
24	B5	4217	PSU	O2-C2-N1	-3.30	119.16	122.79
24	B5	3456	A2M	C4-C5-N7	-3.29	106.61	110.62
24	B5	2244	A2M	C4-C5-N7	-3.29	106.61	110.62
24	B5	4325	PSU	O2-C2-N1	-3.29	119.17	122.79
24	B5	3562	A2M	C4-C5-N7	-3.29	106.61	110.62
24	B5	398	A2M	C4-C5-N7	-3.29	106.61	110.62
24	B5	4317	A2M	C4-C5-N7	-3.29	106.61	110.62
63	A2	669	A2M	C4-C5-N7	-3.29	106.61	110.62
63	A2	645	OMG	C6-C5-N7	3.29	136.36	130.25
24	B5	4107	PSU	O2-C2-N1	-3.28	119.17	122.79
24	B5	3631	OMG	C6-C5-N7	3.28	136.35	130.25
63	A2	602	OMG	C6-C5-N7	3.28	136.35	130.25
63	A2	1640	G7M	O6-C6-C5	-3.28	120.66	128.06
63	A2	469	A2M	C4-C5-N7	-3.28	106.63	110.62
24	B5	4369	OMG	C6-C5-N7	3.27	136.34	130.25
24	B5	3974	OMG	C6-C5-N7	3.27	136.34	130.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B5	1479	A2M	C4-C5-N7	-3.27	106.63	110.62
63	A2	1384	A2M	C4-C5-N7	-3.27	106.64	110.62
24	B5	3557	A2M	C4-C5-N7	-3.26	106.64	110.62
24	B5	3676	OMG	C6-C5-N7	3.26	136.31	130.25
63	A2	1679	A2M	N3-C2-N1	-3.26	123.50	128.60
63	A2	99	A2M	C4-C5-N7	-3.26	106.65	110.62
63	A2	485	A2M	C4-C5-N7	-3.25	106.66	110.62
63	A2	1032	A2M	C4-C5-N7	-3.25	106.66	110.62
63	A2	1032	A2M	C2'-C1'-N9	-3.25	108.06	113.53
24	B5	3966	6MZ	C6-C5-N7	3.25	135.91	132.39
63	A2	1249	B8N	C4-N3-C2	-3.24	121.36	125.46
24	B5	1270	A2M	C4-C5-N7	-3.24	106.67	110.62
24	B5	3966	6MZ	C9-N6-C6	-3.24	120.08	122.87
63	A2	1448	OMG	C6-C5-N7	3.24	136.28	130.25
63	A2	1329	OMG	C6-C5-N7	3.24	136.27	130.25
24	B5	3599	A2M	C4-C5-N7	-3.24	106.68	110.62
63	A2	437	OMG	C6-C5-N7	3.24	136.26	130.25
24	B5	3476	OMG	C6-C5-N7	3.23	136.26	130.25
63	A2	1082	PSU	O2-C2-N1	-3.22	119.24	122.79
24	B5	3966	6MZ	C4-C5-N7	-3.22	106.70	110.62
24	B5	4336	A2M	C2'-C1'-N9	-3.22	108.12	113.53
24	B5	4364	OMG	C6-C5-N7	3.21	136.22	130.25
24	B5	3359	OMG	C6-C5-N7	3.21	136.22	130.25
24	B5	4336	A2M	N3-C2-N1	-3.21	123.58	128.60
63	A2	1032	A2M	N3-C2-N1	-3.20	123.59	128.60
24	B5	4116	OMG	C6-C5-N7	3.20	136.19	130.25
24	B5	3456	A2M	N3-C2-N1	-3.19	123.61	128.60
24	B5	4138	OMG	C6-C5-N7	3.19	136.18	130.25
24	B5	3517	A2M	C4-C5-N7	-3.19	106.73	110.62
24	B5	1489	A2M	N3-C2-N1	-3.19	123.61	128.60
24	B5	2630	A2M	C4-C5-N7	-3.19	106.73	110.62
63	A2	166	A2M	N3-C2-N1	-3.19	123.61	128.60
63	A2	469	A2M	C2'-C1'-N9	-3.19	108.16	113.53
24	B5	4245	OMG	C6-C5-N7	3.19	136.18	130.25
24	B5	3450	A2M	C2'-C1'-N9	-3.19	108.17	113.53
24	B5	3492	A2M	C4-C5-N7	-3.18	106.75	110.62
24	B5	4269	A2M	C2'-C1'-N9	-3.17	108.19	113.53
24	B5	1477	OMG	C6-C5-N7	3.17	136.15	130.25
24	B5	398	A2M	N3-C2-N1	-3.17	123.65	128.60
24	B5	1810	A2M	N3-C2-N1	-3.17	123.65	128.60
24	B5	3517	A2M	N3-C2-N1	-3.17	123.65	128.60
24	B5	3599	A2M	N3-C2-N1	-3.17	123.65	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B5	3492	A2M	N3-C2-N1	-3.16	123.66	128.60
63	A2	510	OMG	C6-C5-N7	3.16	136.12	130.25
24	B5	4269	A2M	N3-C2-N1	-3.15	123.67	128.60
24	B5	2244	A2M	N3-C2-N1	-3.15	123.67	128.60
24	B5	2267	OMG	C6-C5-N7	3.15	136.11	130.25
63	A2	591	A2M	C4-C5-N7	-3.15	106.78	110.62
24	B5	3562	A2M	N3-C2-N1	-3.14	123.69	128.60
24	B5	2206	A2M	N3-C2-N1	-3.14	123.69	128.60
24	B5	2630	A2M	C2'-C1'-N9	-3.14	108.24	113.53
63	A2	591	A2M	N3-C2-N1	-3.14	123.69	128.60
34	B8	75	OMG	C6-C5-N7	3.14	136.08	130.25
63	A2	469	A2M	N3-C2-N1	-3.13	123.70	128.60
63	A2	99	A2M	N3-C2-N1	-3.13	123.70	128.60
24	B5	3942	OMG	C6-C5-N7	3.13	136.07	130.25
24	B5	3557	A2M	N3-C2-N1	-3.13	123.71	128.60
63	A2	27	A2M	N3-C2-N1	-3.13	123.71	128.60
63	A2	1384	A2M	N3-C2-N1	-3.12	123.73	128.60
24	B5	1270	A2M	N3-C2-N1	-3.11	123.73	128.60
24	B5	4317	A2M	N3-C2-N1	-3.11	123.73	128.60
63	A2	513	A2M	N3-C2-N1	-3.11	123.74	128.60
24	B5	4240	OMG	C6-C5-N7	3.10	136.02	130.25
63	A2	577	A2M	N3-C2-N1	-3.10	123.75	128.60
24	B5	1479	A2M	N3-C2-N1	-3.10	123.76	128.60
24	B5	3524	OMG	C6-C5-N7	3.09	136.00	130.25
63	A2	159	A2M	N3-C2-N1	-3.09	123.77	128.60
63	A2	159	A2M	C2'-C1'-N9	-3.08	108.34	113.53
63	A2	669	A2M	N3-C2-N1	-3.08	123.78	128.60
24	B5	400	A2M	N3-C2-N1	-3.08	123.78	128.60
63	A2	27	A2M	C2'-C1'-N9	-3.08	108.34	113.53
24	B5	3450	A2M	N3-C2-N1	-3.08	123.79	128.60
24	B5	2658	A2M	N3-C2-N1	-3.08	123.79	128.60
63	A2	1491	OMG	C6-C5-N7	3.07	135.96	130.25
24	B5	3966	6MZ	N1-C2-N3	-3.07	123.80	128.60
63	A2	485	A2M	N3-C2-N1	-3.07	123.81	128.60
24	B5	2630	A2M	N3-C2-N1	-3.06	123.81	128.60
63	A2	116	OMU	O4-C4-C5	-3.06	119.78	125.16
24	B5	4244	OMU	O4-C4-C5	-3.05	119.79	125.16
63	A2	1833	6MZ	C4-C5-N7	-3.04	106.91	110.62
63	A2	1852	MA6	C4-N9-C1'	-3.03	119.37	126.59
24	B5	1580	OMG	C6-C5-N7	3.02	135.87	130.25
63	A2	1833	6MZ	N1-C2-N3	-3.02	123.88	128.60
24	B5	2206	A2M	C2'-C1'-N9	-3.01	108.46	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B5	2719	OMG	C6-C5-N7	3.01	135.85	130.25
63	A2	1805	OMU	O4-C4-C5	-3.00	119.88	125.16
63	A2	1289	OMU	O4-C4-C5	-3.00	119.89	125.16
63	A2	1640	G7M	C2-N1-C6	-3.00	119.64	125.10
63	A2	1249	B8N	N3-C2-N1	2.99	120.97	116.76
24	B5	3599	A2M	C2'-C1'-N9	-2.98	108.51	113.53
63	A2	1443	OMU	O4-C4-C5	-2.98	119.92	125.16
24	B5	4317	A2M	C2'-C1'-N9	-2.98	108.51	113.53
24	B5	2680	OMU	O4-C4-C5	-2.97	119.93	125.16
24	B5	4366	OMU	O4-C4-C5	-2.97	119.94	125.16
63	A2	429	OMU	O4-C4-C5	-2.96	119.95	125.16
24	B5	2258	OMU	O4-C4-C5	-2.96	119.95	125.16
24	B5	3657	OMU	O4-C4-C5	-2.96	119.96	125.16
24	B5	3517	A2M	O4'-C1'-N9	2.96	113.88	108.06
63	A2	628	OMU	O4-C4-C5	-2.95	119.96	125.16
63	A2	172	OMU	O4-C4-C5	-2.95	119.97	125.16
63	A2	355	OMU	O4-C4-C5	-2.95	119.97	125.16
63	A2	121	OMU	O4-C4-C5	-2.94	119.98	125.16
24	B5	4052	OMU	O4-C4-C5	-2.94	119.99	125.16
63	A2	1327	OMU	O4-C4-C5	-2.94	119.99	125.16
24	B5	3973	OMU	O4-C4-C5	-2.94	119.99	125.16
24	B5	3517	A2M	C2'-C1'-N9	-2.92	108.62	113.53
24	B5	3492	A2M	C2'-C1'-N9	-2.91	108.63	113.53
63	A2	513	A2M	C2'-C1'-N9	-2.88	108.68	113.53
63	A2	1384	A2M	C2'-C1'-N9	-2.85	108.74	113.53
63	A2	513	A2M	C5-N7-C8	2.83	107.53	103.51
24	B5	4336	A2M	C5-N7-C8	2.83	107.53	103.51
63	A2	1679	A2M	C5-N7-C8	2.83	107.52	103.51
63	A2	1852	MA6	C5-C4-N9	-2.82	102.50	105.78
63	A2	166	A2M	C5-N7-C8	2.80	107.49	103.51
63	A2	1833	6MZ	C6-C5-N7	2.80	135.42	132.39
24	B5	2244	A2M	C5-N7-C8	2.79	107.47	103.51
63	A2	159	A2M	C5-N7-C8	2.78	107.47	103.51
24	B5	1489	A2M	C5-N7-C8	2.78	107.46	103.51
63	A2	1032	A2M	C5-N7-C8	2.78	107.45	103.51
24	B5	2206	A2M	C5-N7-C8	2.78	107.45	103.51
63	A2	577	A2M	C5-N7-C8	2.78	107.45	103.51
24	B5	3562	A2M	C5-N7-C8	2.78	107.45	103.51
63	A2	1679	A2M	C4-N9-C8	2.77	108.73	105.73
63	A2	27	A2M	C5-N7-C8	2.77	107.45	103.51
24	B5	4269	A2M	C5-N7-C8	2.76	107.43	103.51
24	B5	400	A2M	C5-N7-C8	2.76	107.43	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	A2	1384	A2M	C5-N7-C8	2.76	107.43	103.51
24	B5	3456	A2M	C5-N7-C8	2.76	107.43	103.51
24	B5	3517	A2M	C5-N7-C8	2.76	107.42	103.51
24	B5	398	A2M	C5-N7-C8	2.75	107.42	103.51
82	An	138	IAS	OD1-CG-CB	-2.75	117.42	125.43
63	A2	1851	MA6	C5-C4-N9	-2.74	102.59	105.78
63	A2	669	A2M	C5-N7-C8	2.74	107.41	103.51
24	B5	2658	A2M	C5-N7-C8	2.74	107.40	103.51
24	B5	1810	A2M	C5-N7-C8	2.74	107.39	103.51
63	A2	469	A2M	C5-N7-C8	2.73	107.39	103.51
24	B5	3450	A2M	C5-N7-C8	2.73	107.39	103.51
24	B5	3557	A2M	C5-N7-C8	2.73	107.38	103.51
24	B5	4317	A2M	C5-N7-C8	2.72	107.37	103.51
24	B5	1479	A2M	C5-N7-C8	2.72	107.37	103.51
63	A2	485	A2M	C5-N7-C8	2.71	107.36	103.51
24	B5	3599	A2M	C5-N7-C8	2.71	107.36	103.51
63	A2	99	A2M	C5-N7-C8	2.71	107.36	103.51
24	B5	1270	A2M	C5-N7-C8	2.71	107.36	103.51
24	B5	3492	A2M	C5-N7-C8	2.71	107.36	103.51
24	B5	3517	A2M	C4-N9-C8	2.70	108.65	105.73
63	A2	591	A2M	C5-N7-C8	2.70	107.34	103.51
24	B5	3966	6MZ	C5-N7-C8	2.70	107.34	103.51
63	A2	868	OMG	C4-C5-N7	-2.69	106.47	110.72
24	B5	1810	A2M	C4-N9-C8	2.68	108.64	105.73
24	B5	4383	OMG	C4-C5-N7	-2.68	106.48	110.72
24	B5	3456	A2M	C4-N9-C8	2.68	108.63	105.73
63	A2	602	OMG	C4-C5-N7	-2.67	106.49	110.72
24	B5	2207	OMG	C4-C5-N7	-2.67	106.50	110.72
63	A2	645	OMG	C4-C5-N7	-2.67	106.50	110.72
24	B5	1260	OMG	C4-C5-N7	-2.66	106.50	110.72
24	B5	4369	OMG	C4-C5-N7	-2.66	106.51	110.72
63	A2	1448	OMG	C4-C5-N7	-2.66	106.51	110.72
24	B5	2630	A2M	C5-N7-C8	2.66	107.28	103.51
63	A2	1329	OMG	C4-C5-N7	-2.65	106.53	110.72
63	A2	684	OMG	C4-C5-N7	-2.64	106.53	110.72
24	B5	3476	OMG	C4-C5-N7	-2.64	106.54	110.72
63	A2	1032	A2M	C4-N9-C8	2.64	108.59	105.73
24	B5	3631	OMG	C4-C5-N7	-2.63	106.55	110.72
24	B5	4138	OMG	C4-C5-N7	-2.63	106.55	110.72
63	A2	437	OMG	C4-C5-N7	-2.63	106.55	110.72
24	B5	4364	OMG	C4-C5-N7	-2.63	106.57	110.72
24	B5	3974	OMG	C4-C5-N7	-2.62	106.58	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B5	3359	OMG	C4-C5-N7	-2.62	106.58	110.72
24	B5	4336	A2M	C4-N9-C8	2.61	108.56	105.73
24	B5	3514	5MC	C5-C4-N3	-2.61	118.86	121.67
24	B5	4245	OMG	C4-C5-N7	-2.61	106.59	110.72
24	B5	3942	OMG	C4-C5-N7	-2.61	106.59	110.72
63	A2	577	A2M	C4-N9-C8	2.61	108.55	105.73
24	B5	3557	A2M	C4-N9-C8	2.60	108.55	105.73
24	B5	4116	OMG	C4-C5-N7	-2.60	106.60	110.72
24	B5	3562	A2M	C4-N9-C8	2.60	108.55	105.73
63	A2	510	OMG	C4-C5-N7	-2.60	106.61	110.72
24	B5	1477	OMG	C4-C5-N7	-2.60	106.61	110.72
24	B5	1266	1MA	C4-C5-N7	-2.60	106.61	110.72
63	A2	1833	6MZ	C5-N7-C8	2.60	107.20	103.51
24	B5	1270	A2M	C4-N9-C8	2.59	108.54	105.73
34	B8	75	OMG	C4-C5-N7	-2.59	106.62	110.72
24	B5	398	A2M	C4-N9-C8	2.59	108.54	105.73
63	A2	1384	A2M	C4-N9-C8	2.59	108.53	105.73
24	B5	3676	OMG	C4-C5-N7	-2.59	106.63	110.72
24	B5	4269	A2M	C4-N9-C8	2.59	108.53	105.73
24	B5	3492	A2M	C4-N9-C8	2.58	108.53	105.73
24	B5	2244	A2M	C4-N9-C8	2.58	108.52	105.73
63	A2	159	A2M	C4-N9-C8	2.58	108.52	105.73
24	B5	2719	OMG	C4-C5-N7	-2.58	106.64	110.72
63	A2	1833	6MZ	C9-N6-C6	-2.58	120.65	122.87
63	A2	669	A2M	C4-N9-C8	2.57	108.51	105.73
24	B5	2267	OMG	C4-C5-N7	-2.56	106.66	110.72
24	B5	3524	OMG	C4-C5-N7	-2.56	106.67	110.72
63	A2	469	A2M	C4-N9-C8	2.56	108.50	105.73
63	A2	27	A2M	C4-N9-C8	2.56	108.50	105.73
63	A2	1843	4AC	C5-C4-N4	-2.55	118.48	122.92
24	B5	4240	OMG	C4-C5-N7	-2.55	106.68	110.72
24	B5	1270	A2M	C2'-C1'-N9	-2.55	109.24	113.53
24	B5	3599	A2M	C4-N9-C8	2.55	108.49	105.73
24	B5	4317	A2M	C4-N9-C8	2.54	108.48	105.73
24	B5	400	A2M	C4-N9-C8	2.54	108.48	105.73
63	A2	1491	OMG	C4-C5-N7	-2.53	106.72	110.72
63	A2	513	A2M	C4-N9-C8	2.53	108.47	105.73
63	A2	99	A2M	C4-N9-C8	2.52	108.46	105.73
24	B5	1580	OMG	C4-C5-N7	-2.52	106.73	110.72
24	B5	1489	A2M	C4-N9-C8	2.52	108.46	105.73
24	B5	3550	UY1	CM2-O2'-C2'	-2.52	107.91	114.52
38	BA	216	V5N	O-C-CA	-2.52	118.18	124.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B5	2658	A2M	C2'-C1'-N9	-2.52	109.29	113.53
24	B5	400	A2M	C2'-C1'-N9	-2.51	109.31	113.53
63	A2	166	A2M	C4-N9-C8	2.48	108.41	105.73
63	A2	1338	4AC	C6-C5-C4	2.47	119.99	116.96
24	B5	3450	A2M	C4-N9-C8	2.47	108.41	105.73
24	B5	2630	A2M	C4-N9-C8	2.47	108.41	105.73
24	B5	4193	5MC	C5-C4-N3	-2.47	119.01	121.67
30	Au	1	AME	O-C-CA	-2.46	118.33	124.78
63	A2	1833	6MZ	C4-N9-C8	2.45	108.38	105.73
24	B5	3966	6MZ	C4-N9-C8	2.44	108.37	105.73
24	B5	3550	UY1	C6-C5-C4	2.44	119.90	118.20
24	B5	1479	A2M	C4-N9-C8	2.42	108.36	105.73
63	A2	485	A2M	C4-N9-C8	2.42	108.35	105.73
5	Ar	2	SAC	O-C-CA	-2.42	118.45	124.78
63	A2	1443	OMU	C1'-N1-C2	2.40	121.91	117.57
24	B5	2658	A2M	C4-N9-C8	2.38	108.31	105.73
32	AZ	2	SAC	O-C-CA	-2.34	118.64	124.78
24	B5	1489	A2M	C6-C5-N7	2.34	136.38	132.02
24	B5	2206	A2M	C4-N9-C8	2.33	108.26	105.73
24	B5	3550	UY1	O2-C2-N1	-2.33	120.23	122.79
50	Ba	39	V5N	O-C-CA	-2.32	118.69	124.78
24	B5	2265	OMC	O2-C2-N3	-2.31	118.57	122.33
63	A2	1679	A2M	C6-C5-N7	2.31	136.33	132.02
63	A2	1843	4AC	C6-C5-C4	2.30	119.78	116.96
24	B5	3573	OMC	O2-C2-N3	-2.30	118.59	122.33
63	A2	1289	OMU	C1'-N1-C2	2.30	121.73	117.57
24	B5	3456	A2M	C6-C5-N7	2.28	136.28	132.02
24	B5	4336	A2M	C6-C5-N7	2.28	136.26	132.02
24	B5	1810	A2M	C6-C5-N7	2.27	136.25	132.02
63	A2	628	OMU	O2-C2-N1	-2.27	119.77	122.79
63	A2	1338	4AC	C5-C4-N4	-2.26	119.00	122.92
63	A2	577	A2M	C6-C5-N7	2.24	136.20	132.02
12	Br	2	SAC	O-C-CA	-2.23	118.92	124.78
63	A2	1032	A2M	C6-C5-N7	2.23	136.18	132.02
63	A2	1851	MA6	C5-N7-C8	2.23	106.67	103.51
24	B5	398	A2M	C6-C5-N7	2.22	136.16	132.02
24	B5	3557	A2M	C6-C5-N7	2.22	136.16	132.02
63	A2	513	A2M	C6-C5-N7	2.22	136.16	132.02
24	B5	4269	A2M	C6-C5-N7	2.22	136.16	132.02
24	B5	2207	OMG	O6-C6-C5	-2.22	120.71	126.60
23	Aw	62	HY3	O-C-CA	-2.22	118.64	124.83
63	A2	166	A2M	C6-C5-N7	2.21	136.15	132.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B5	3562	A2M	C6-C5-N7	2.21	136.14	132.02
24	B5	2244	A2M	C6-C5-N7	2.21	136.14	132.02
24	B5	1270	A2M	C6-C5-N7	2.21	136.14	132.02
24	B5	2206	A2M	C6-C5-N7	2.21	136.13	132.02
63	A2	485	A2M	C2'-C1'-N9	-2.20	109.82	113.53
24	B5	400	A2M	C6-C5-N7	2.20	136.13	132.02
63	A2	1679	A2M	N9-C8-N7	-2.20	110.90	113.91
24	B5	3517	A2M	C6-C5-N7	2.20	136.11	132.02
63	A2	469	A2M	C6-C5-N7	2.19	136.11	132.02
24	B5	2194	OMC	O2-C2-N3	-2.19	118.77	122.33
63	A2	1384	A2M	C6-C5-N7	2.19	136.10	132.02
24	B5	3450	A2M	C6-C5-N7	2.19	136.09	132.02
63	A2	159	A2M	C6-C5-N7	2.18	136.09	132.02
63	A2	27	A2M	C6-C5-N7	2.18	136.08	132.02
63	A2	1327	OMU	O2-C2-N1	-2.18	119.89	122.79
63	A2	669	A2M	C6-C5-N7	2.18	136.08	132.02
24	B5	3599	A2M	C6-C5-N7	2.18	136.07	132.02
24	B5	1580	OMG	O6-C6-C5	-2.17	120.85	126.60
63	A2	1491	OMG	O6-C6-C5	-2.17	120.85	126.60
24	B5	4317	A2M	C6-C5-N7	2.16	136.05	132.02
63	A2	99	A2M	C6-C5-N7	2.16	136.04	132.02
63	A2	1249	B8N	C5-C4-N3	2.16	120.17	116.17
63	A2	669	A2M	C2'-C1'-N9	-2.15	109.91	113.53
24	B5	4245	OMG	O6-C6-C5	-2.15	120.90	126.60
24	B5	2267	OMG	O6-C6-C5	-2.15	120.91	126.60
24	B5	3517	A2M	N9-C8-N7	-2.14	110.98	113.91
24	B5	3492	A2M	C6-C5-N7	2.14	136.01	132.02
63	A2	591	A2M	C4-N9-C8	2.14	108.05	105.73
24	B5	2658	A2M	C6-C5-N7	2.14	136.00	132.02
24	B5	3942	OMG	O6-C6-C5	-2.14	120.93	126.60
63	A2	1640	G7M	C5-C4-N9	-2.13	101.22	105.89
24	B5	3974	OMG	O6-C6-C5	-2.13	120.94	126.60
24	B5	4244	OMU	O2-C2-N1	-2.13	119.95	122.79
24	B5	1266	1MA	C6-C5-N7	2.13	136.06	132.20
63	A2	1032	A2M	N9-C8-N7	-2.12	111.01	113.91
24	B5	3359	OMG	O6-C6-C5	-2.12	120.97	126.60
24	B5	1479	A2M	C6-C5-N7	2.12	135.97	132.02
24	B5	4116	OMG	O6-C6-C5	-2.12	120.99	126.60
24	B5	1477	OMG	O6-C6-C5	-2.11	120.99	126.60
24	B5	4336	A2M	N9-C8-N7	-2.11	111.02	113.91
24	B5	4364	OMG	O6-C6-C5	-2.11	121.00	126.60
24	B5	4240	OMG	O6-C6-C5	-2.11	121.01	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	A2	1852	MA6	C5-N7-C8	2.11	106.50	103.51
63	A2	485	A2M	C6-C5-N7	2.11	135.94	132.02
34	B8	75	OMG	O6-C6-C5	-2.10	121.02	126.60
24	B5	3676	OMG	O6-C6-C5	-2.10	121.02	126.60
24	B5	3631	OMG	O6-C6-C5	-2.10	121.02	126.60
24	B5	4383	OMG	O6-C6-C5	-2.10	121.02	126.60
24	B5	3476	OMG	O6-C6-C5	-2.10	121.03	126.60
63	A2	645	OMG	O6-C6-C5	-2.10	121.03	126.60
24	B5	1260	OMG	O6-C6-C5	-2.10	121.04	126.60
24	B5	2719	OMG	O6-C6-C5	-2.09	121.05	126.60
24	B5	3524	OMG	O6-C6-C5	-2.09	121.05	126.60
63	A2	1448	OMG	O6-C6-C5	-2.09	121.06	126.60
24	B5	3456	A2M	N9-C8-N7	-2.09	111.06	113.91
24	B5	4138	OMG	O6-C6-C5	-2.09	121.06	126.60
63	A2	510	OMG	O6-C6-C5	-2.08	121.07	126.60
63	A2	602	OMG	O6-C6-C5	-2.08	121.07	126.60
63	A2	463	OMC	O2-C2-N3	-2.08	118.95	122.33
63	A2	1329	OMG	O6-C6-C5	-2.08	121.09	126.60
63	A2	684	OMG	O6-C6-C5	-2.08	121.09	126.60
24	B5	4369	OMG	O6-C6-C5	-2.08	121.09	126.60
63	A2	437	OMG	O6-C6-C5	-2.07	121.10	126.60
24	B5	1632	PSU	O4'-C1'-C2'	2.07	108.06	105.14
63	A2	577	A2M	N9-C8-N7	-2.07	111.09	113.91
24	B5	2630	A2M	C6-C5-N7	2.06	135.87	132.02
24	B5	1810	A2M	N9-C8-N7	-2.06	111.09	113.91
24	B5	4269	A2M	N9-C8-N7	-2.06	111.09	113.91
24	B5	3562	A2M	N9-C8-N7	-2.06	111.10	113.91
63	A2	513	A2M	N9-C8-N7	-2.05	111.10	113.91
24	B5	1489	A2M	N9-C8-N7	-2.05	111.11	113.91
24	B5	3514	5MC	O2-C2-N3	-2.05	119.00	122.33
24	B5	2244	A2M	N9-C8-N7	-2.04	111.12	113.91
63	A2	159	A2M	N9-C8-N7	-2.04	111.12	113.91
24	B5	3557	A2M	N9-C8-N7	-2.04	111.12	113.91
63	A2	1384	A2M	N9-C8-N7	-2.04	111.13	113.91
24	B5	1270	A2M	N9-C8-N7	-2.04	111.13	113.91
63	A2	669	A2M	N9-C8-N7	-2.02	111.15	113.91
63	A2	1704	OMC	O2-C2-N3	-2.02	119.05	122.33
24	B5	398	A2M	N9-C8-N7	-2.02	111.16	113.91
63	A2	172	OMU	O2-C2-N1	-2.02	120.11	122.79
63	A2	116	OMU	O2-C2-N1	-2.01	120.11	122.79
63	A2	868	OMG	O6-C6-C5	-2.01	121.26	126.60
63	A2	166	A2M	N9-C8-N7	-2.01	111.17	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B5	3492	A2M	N9-C8-N7	-2.00	111.17	113.91
24	B5	400	A2M	N9-C8-N7	-2.00	111.17	113.91

There are no chirality outliers.

All (125) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Bo	53	MLZ	O-C-CA-CB
24	B5	3433	OMC	C2'-C1'-N1-C2
24	B5	3433	OMC	C2'-C1'-N1-C6
24	B5	3517	A2M	O4'-C4'-C5'-O5'
24	B5	4166	PSU	C2'-C1'-C5-C4
24	B5	4166	PSU	C2'-C1'-C5-C6
24	B5	4193	5MC	C2'-C1'-N1-C6
24	B5	4336	A2M	C4'-C5'-O5'-P
24	B5	4382	PSU	O4'-C1'-C5-C4
24	B5	4382	PSU	O4'-C1'-C5-C6
24	B5	4382	PSU	C3'-C4'-C5'-O5'
38	BA	216	V5N	O-C-CA-CB
63	A2	429	OMU	C2'-C1'-N1-C2
63	A2	429	OMU	C2'-C1'-N1-C6
63	A2	513	A2M	O4'-C4'-C5'-O5'
63	A2	645	OMG	O4'-C4'-C5'-O5'
63	A2	1448	OMG	C3'-C4'-C5'-O5'
63	A2	1249	B8N	N34-C33-C34-O35
63	A2	1338	4AC	O7-C7-N4-C4
63	A2	1338	4AC	CM7-C7-N4-C4
63	A2	1843	4AC	N3-C4-N4-C7
63	A2	1843	4AC	C5-C4-N4-C7
63	A2	1843	4AC	O7-C7-N4-C4
63	A2	1843	4AC	CM7-C7-N4-C4
47	BC	2	AYA	OT-CT-N-CA
47	BC	2	AYA	CM-CT-N-CA
24	B5	398	A2M	O4'-C4'-C5'-O5'
24	B5	398	A2M	C3'-C4'-C5'-O5'
24	B5	1489	A2M	O4'-C4'-C5'-O5'
24	B5	2207	OMG	O4'-C4'-C5'-O5'
63	A2	513	A2M	C3'-C4'-C5'-O5'
63	A2	645	OMG	C3'-C4'-C5'-O5'
63	A2	669	A2M	O4'-C4'-C5'-O5'
63	A2	669	A2M	C3'-C4'-C5'-O5'
30	Au	1	AME	CT2-CT1-N-CA

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Mol	Chain	Res	Type	Atoms
30	Au	1	AME	OT-CT1-N-CA
63	A2	1249	B8N	N34-C33-C34-O36
24	B5	2207	OMG	C3'-C4'-C5'-O5'
24	B5	3517	A2M	C3'-C4'-C5'-O5'
24	B5	4382	PSU	O4'-C4'-C5'-O5'
63	A2	99	A2M	O4'-C4'-C5'-O5'
63	A2	628	OMU	C2'-C1'-N1-C6
24	B5	4193	5MC	C2'-C1'-N1-C2
24	B5	1489	A2M	C3'-C4'-C5'-O5'
63	A2	577	A2M	C3'-C4'-C5'-O5'
63	A2	1448	OMG	O4'-C4'-C5'-O5'
63	A2	1852	MA6	C5-C6-N6-C9
43	BB	245	HIC	CA-CB-CG-ND1
63	A2	628	OMU	C2'-C1'-N1-C2
63	A2	1640	G7M	O4'-C4'-C5'-O5'
63	A2	628	OMU	O4'-C1'-N1-C6
63	A2	99	A2M	C3'-C4'-C5'-O5'
63	A2	577	A2M	O4'-C4'-C5'-O5'
63	A2	429	OMU	O4'-C4'-C5'-O5'
63	A2	429	OMU	O4'-C1'-N1-C6
63	A2	1249	B8N	C32-C33-C34-O36
47	BC	2	AYA	C-CA-N-CT
24	B5	3576	PSU	C4'-C5'-O5'-P
63	A2	645	OMG	C4'-C5'-O5'-P
63	A2	1852	MA6	C4'-C5'-O5'-P
24	B5	3550	UY1	C4'-C5'-O5'-P
63	A2	1640	G7M	C3'-C4'-C5'-O5'
63	A2	591	A2M	C2'-C1'-N9-C4
24	B5	2630	A2M	C2'-C1'-N9-C8
32	AZ	2	SAC	C-CA-N-C1A
32	AZ	2	SAC	CB-CA-N-C1A
63	A2	429	OMU	O4'-C1'-N1-C2
24	B5	1260	OMG	C3'-C2'-O2'-CM2
24	B5	1284	OMC	C3'-C2'-O2'-CM2
24	B5	1810	A2M	C3'-C2'-O2'-CM'
24	B5	2680	OMU	C3'-C2'-O2'-CM2
24	B5	3631	OMG	C3'-C2'-O2'-CM2
63	A2	1448	OMG	C3'-C2'-O2'-CM2
63	A2	1338	4AC	N3-C4-N4-C7
82	An	138	IAS	C-CA-CB-CG
54	Bb	5	MLZ	N-CA-CB-CG
63	A2	591	A2M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
63	A2	1249	B8N	C32-C33-C34-O35
24	B5	4193	5MC	O4'-C1'-N1-C2
24	B5	4246	PSU	C4'-C5'-O5'-P
63	A2	628	OMU	O4'-C1'-N1-C2
24	B5	4193	5MC	O4'-C1'-N1-C6
63	A2	591	A2M	C2'-C1'-N9-C8
24	B5	3433	OMC	O4'-C1'-N1-C6
38	BA	216	V5N	O2-CB-CG-CD2
50	Ba	39	V5N	O2-CB-CG-CD2
24	B5	398	A2M	C3'-C2'-O2'-CM'
24	B5	3557	A2M	C3'-C2'-O2'-CM'
24	B5	4282	OMC	C3'-C2'-O2'-CM2
24	B5	4383	OMG	C3'-C2'-O2'-CM2
63	A2	355	OMU	C3'-C2'-O2'-CM2
24	B5	3619	OMC	C4'-C5'-O5'-P
63	A2	429	OMU	C3'-C4'-C5'-O5'
43	BB	245	HIC	CA-CB-CG-CD2
24	B5	2207	OMG	C3'-C2'-O2'-CM2
24	B5	2265	OMC	C3'-C2'-O2'-CM2
24	B5	2667	OMC	C3'-C2'-O2'-CM2
24	B5	2704	OMC	C3'-C2'-O2'-CM2
24	B5	3619	OMC	C3'-C2'-O2'-CM2
24	B5	4138	OMG	C3'-C2'-O2'-CM2
63	A2	868	OMG	C3'-C2'-O2'-CM2
63	A2	591	A2M	O4'-C1'-N9-C8
63	A2	684	OMG	O4'-C4'-C5'-O5'
54	Bb	5	MLZ	C-CA-CB-CG
24	B5	398	A2M	C1'-C2'-O2'-CM'
24	B5	3619	OMC	C1'-C2'-O2'-CM2
24	B5	3676	OMG	C1'-C2'-O2'-CM2
63	A2	510	OMG	C1'-C2'-O2'-CM2
63	A2	868	OMG	C1'-C2'-O2'-CM2
24	B5	1820	OMC	C3'-C2'-O2'-CM2
24	B5	3676	OMG	C3'-C2'-O2'-CM2
24	B5	2630	A2M	O4'-C1'-N9-C8
24	B5	2194	OMC	O4'-C4'-C5'-O5'
23	Aw	62	HY3	O-C-CA-C3
24	B5	3433	OMC	O4'-C1'-N1-C2
24	B5	3492	A2M	O4'-C4'-C5'-O5'
82	An	138	IAS	N-CA-CB-CG
63	A2	669	A2M	C2'-C1'-N9-C8
24	B5	3476	OMG	C3'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
63	A2	27	A2M	C3'-C2'-O2'-CM'
63	A2	510	OMG	C3'-C2'-O2'-CM2
63	A2	1704	OMC	C3'-C2'-O2'-CM2
38	BA	216	V5N	CA-CB-CG-ND1
24	B5	3492	A2M	C2'-C1'-N9-C8
24	B5	2194	OMC	C2'-C1'-N1-C2

There are no ring outliers.

87 monomers are involved in 118 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	A2	36	PSU	1	0
24	B5	1718	PSU	1	0
24	B5	3557	A2M	1	0
63	A2	577	A2M	1	0
24	B5	400	A2M	1	0
63	A2	1448	OMG	2	0
24	B5	4269	A2M	2	0
30	Au	1	AME	1	0
24	B5	1260	OMG	1	0
24	B5	3550	UY1	2	0
63	A2	1843	4AC	2	0
63	A2	1443	OMU	1	0
24	B5	3524	OMG	1	0
34	B8	75	OMG	1	0
24	B5	2647	OMC	1	0
24	B5	4202	OMC	1	0
24	B5	2704	OMC	1	0
43	BB	245	HIC	1	0
63	A2	1679	A2M	1	0
24	B5	4099	PSU	1	0
63	A2	1833	6MZ	1	0
24	B5	2207	OMG	2	0
63	A2	513	A2M	1	0
24	B5	2206	A2M	2	0
24	B5	4138	OMG	1	0
24	B5	2658	A2M	2	0
24	B5	3676	OMG	1	0
63	A2	99	A2M	2	0
63	A2	1233	PSU	2	0
24	B5	3450	A2M	2	0
63	A2	355	OMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	A2	1805	OMU	2	0
63	A2	1338	4AC	4	0
63	A2	121	OMU	2	0
24	B5	3517	A2M	2	0
63	A2	105	PSU	1	0
63	A2	463	OMC	2	0
24	B5	3573	OMC	1	0
24	B5	4058	PSU	1	0
63	A2	1032	A2M	2	0
24	B5	1270	A2M	2	0
24	B5	4282	OMC	1	0
63	A2	485	A2M	1	0
24	B5	4382	PSU	2	0
24	B5	3540	OMC	1	0
24	B5	4336	A2M	1	0
63	A2	510	OMG	1	0
63	A2	437	OMG	1	0
63	A2	469	A2M	1	0
24	B5	3974	OMG	1	0
63	A2	518	OMC	1	0
63	A2	172	OMU	2	0
63	A2	116	OMU	1	0
63	A2	1384	A2M	1	0
82	An	138	IAS	1	0
63	A2	27	A2M	1	0
24	B5	4039	PSU	1	0
63	A2	1329	OMG	1	0
24	B5	1284	OMC	3	0
63	A2	1392	OMC	1	0
24	B5	4052	OMU	2	0
24	B5	1632	PSU	1	0
24	B5	4203	PSU	1	0
24	B5	4383	OMG	1	0
63	A2	1289	OMU	2	0
63	A2	1704	OMC	1	0
63	A2	1640	G7M	1	0
63	A2	602	OMG	1	0
24	B5	2194	OMC	1	0
63	A2	159	A2M	1	0
63	A2	823	PSU	1	0
24	B5	2258	OMU	2	0
24	B5	3631	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B5	4325	PSU	1	0
24	B5	3456	A2M	2	0
24	B5	3942	OMG	2	0
24	B5	398	A2M	1	0
24	B5	4366	OMU	3	0
24	B5	3476	OMG	1	0
63	A2	815	PSU	1	0
24	B5	4364	OMG	1	0
63	A2	1491	OMG	1	0
24	B5	3616	PSU	1	0
24	B5	3619	OMC	1	0
24	B5	1810	A2M	2	0
24	B5	3562	A2M	2	0
63	A2	166	A2M	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 769 ligands modelled in this entry, 428 are monoatomic and 306 are unknown - 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	A2	1978	-	9,9,9	0.15	0	8,8,8	0.20	0
94	SPD	A2	1971	-	9,9,9	0.15	0	8,8,8	0.19	0
94	SPD	A2	1950	-	9,9,9	0.15	0	8,8,8	0.19	0
94	SPD	B5	5041	-	9,9,9	0.14	0	8,8,8	0.20	0
94	SPD	A2	1985	-	9,9,9	0.16	0	8,8,8	0.17	0
94	SPD	B5	5082	-	9,9,9	0.15	0	8,8,8	0.17	0
94	SPD	B5	5343	-	9,9,9	0.15	0	8,8,8	0.17	0
95	SPM	B5	5018	-	13,13,13	0.15	0	12,12,12	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
94	SPD	A2	1957	-	9,9,9	0.15	0	8,8,8	0.19	0
95	SPM	A2	1994	-	13,13,13	0.15	0	12,12,12	0.16	0
96	GTP	B7	216	29	30,34,34	0.50	0	46,54,54	0.55	0
94	SPD	A2	1964	-	9,9,9	0.15	0	8,8,8	0.17	0
94	SPD	B5	4933	-	9,9,9	0.15	0	8,8,8	0.17	0
94	SPD	B5	5244	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	B5	5205	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	A2	1943	-	9,9,9	0.15	0	8,8,8	0.17	0
94	SPD	B5	5322	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	B5	4975	-	9,9,9	0.16	0	8,8,8	0.19	0
95	SPM	B5	5061	-	13,13,13	0.15	0	12,12,12	0.14	0
94	SPD	B5	4945	-	9,9,9	0.16	0	8,8,8	0.19	0
94	SPD	B5	5144	-	9,9,9	0.15	0	8,8,8	0.22	0
94	SPD	B5	4997	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	B5	5103	-	9,9,9	0.15	0	8,8,8	0.17	0
94	SPD	A2	1986	-	9,9,9	0.16	0	8,8,8	0.18	0
94	SPD	B5	4912	-	9,9,9	0.16	0	8,8,8	0.17	0
94	SPD	B5	5165	-	9,9,9	0.16	0	8,8,8	0.19	0
94	SPD	B5	5405	-	9,9,9	0.16	0	8,8,8	0.18	0
94	SPD	B5	5363	-	9,9,9	0.16	0	8,8,8	0.19	0
94	SPD	B5	5123	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	B5	4954	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	B5	5385	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	B5	5263	-	9,9,9	0.16	0	8,8,8	0.15	0
94	SPD	B5	5302	-	9,9,9	0.15	0	8,8,8	0.15	0
93	IHP	DB	901	-	36,36,36	1.55	6 (16%)	54,60,60	1.09	3 (5%)
94	SPD	B5	5224	-	9,9,9	0.16	0	8,8,8	0.18	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	A2	1978	-	-	1/7/7/7	-
94	SPD	A2	1971	-	-	0/7/7/7	-
94	SPD	A2	1950	-	-	0/7/7/7	-
94	SPD	B5	5041	-	-	0/7/7/7	-
94	SPD	A2	1985	-	-	1/7/7/7	-
94	SPD	B5	5082	-	-	0/7/7/7	-
94	SPD	B5	5343	-	-	1/7/7/7	-
95	SPM	B5	5018	-	-	1/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
94	SPD	A2	1957	-	-	0/7/7/7	-
95	SPM	A2	1994	-	-	2/11/11/11	-
96	GTP	B7	216	29	-	0/22/38/38	0/3/3/3
94	SPD	A2	1964	-	-	0/7/7/7	-
94	SPD	B5	4933	-	-	0/7/7/7	-
94	SPD	B5	5244	-	-	0/7/7/7	-
94	SPD	B5	5205	-	-	0/7/7/7	-
94	SPD	A2	1943	-	-	0/7/7/7	-
94	SPD	B5	5322	-	-	1/7/7/7	-
94	SPD	B5	4975	-	-	2/7/7/7	-
95	SPM	B5	5061	-	-	0/11/11/11	-
94	SPD	B5	4945	-	-	0/7/7/7	-
94	SPD	B5	5144	-	-	0/7/7/7	-
94	SPD	B5	4997	-	-	0/7/7/7	-
94	SPD	B5	5103	-	-	0/7/7/7	-
94	SPD	A2	1986	-	-	0/7/7/7	-
94	SPD	B5	4912	-	-	0/7/7/7	-
94	SPD	B5	5165	-	-	1/7/7/7	-
94	SPD	B5	5405	-	-	1/7/7/7	-
94	SPD	B5	5363	-	-	0/7/7/7	-
94	SPD	B5	5123	-	-	0/7/7/7	-
94	SPD	B5	4954	-	-	0/7/7/7	-
94	SPD	B5	5385	-	-	1/7/7/7	-
94	SPD	B5	5263	-	-	1/7/7/7	-
94	SPD	B5	5302	-	-	1/7/7/7	-
93	IHP	DB	901	-	-	8/30/54/54	0/1/1/1
94	SPD	B5	5224	-	-	1/7/7/7	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
93	DB	901	IHP	P2-O12	3.53	1.66	1.59
93	DB	901	IHP	P5-O15	3.43	1.65	1.59
93	DB	901	IHP	P1-O11	3.25	1.65	1.59
93	DB	901	IHP	P6-O16	3.24	1.65	1.59
93	DB	901	IHP	P4-O14	3.18	1.65	1.59
93	DB	901	IHP	P3-O13	3.12	1.65	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
93	DB	901	IHP	C6-C5-C4	4.26	119.74	110.41
93	DB	901	IHP	C5-C4-C3	3.49	118.05	110.41
93	DB	901	IHP	C5-C6-C1	3.40	117.86	110.41

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
93	DB	901	IHP	C1-C2-O12-P2
93	DB	901	IHP	C4-C5-O15-P5
93	DB	901	IHP	C4-O14-P4-O24
95	A2	1994	SPM	C8-C9-N10-C11
93	DB	901	IHP	C2-O12-P2-O32
93	DB	901	IHP	C2-O12-P2-O42
95	A2	1994	SPM	C12-C11-N10-C9
94	B5	5263	SPD	C2-C3-C4-C5
93	DB	901	IHP	C1-O11-P1-O21
94	B5	5224	SPD	C2-C3-C4-C5
94	B5	5322	SPD	C2-C3-C4-C5
94	B5	5405	SPD	C2-C3-C4-C5
94	A2	1978	SPD	C2-C3-C4-C5
93	DB	901	IHP	C5-O15-P5-O45
93	DB	901	IHP	C6-O16-P6-O36
94	B5	5343	SPD	C2-C3-C4-C5
94	A2	1985	SPD	C2-C3-C4-C5
94	B5	5385	SPD	C2-C3-C4-C5
94	B5	4975	SPD	C4-C5-N6-C7
95	B5	5018	SPM	C8-C9-N10-C11
94	B5	5302	SPD	C2-C3-C4-C5
94	B5	4975	SPD	C2-C3-C4-C5
94	B5	5165	SPD	C2-C3-C4-C5

There are no ring outliers.

20 monomers are involved in 32 short contacts:

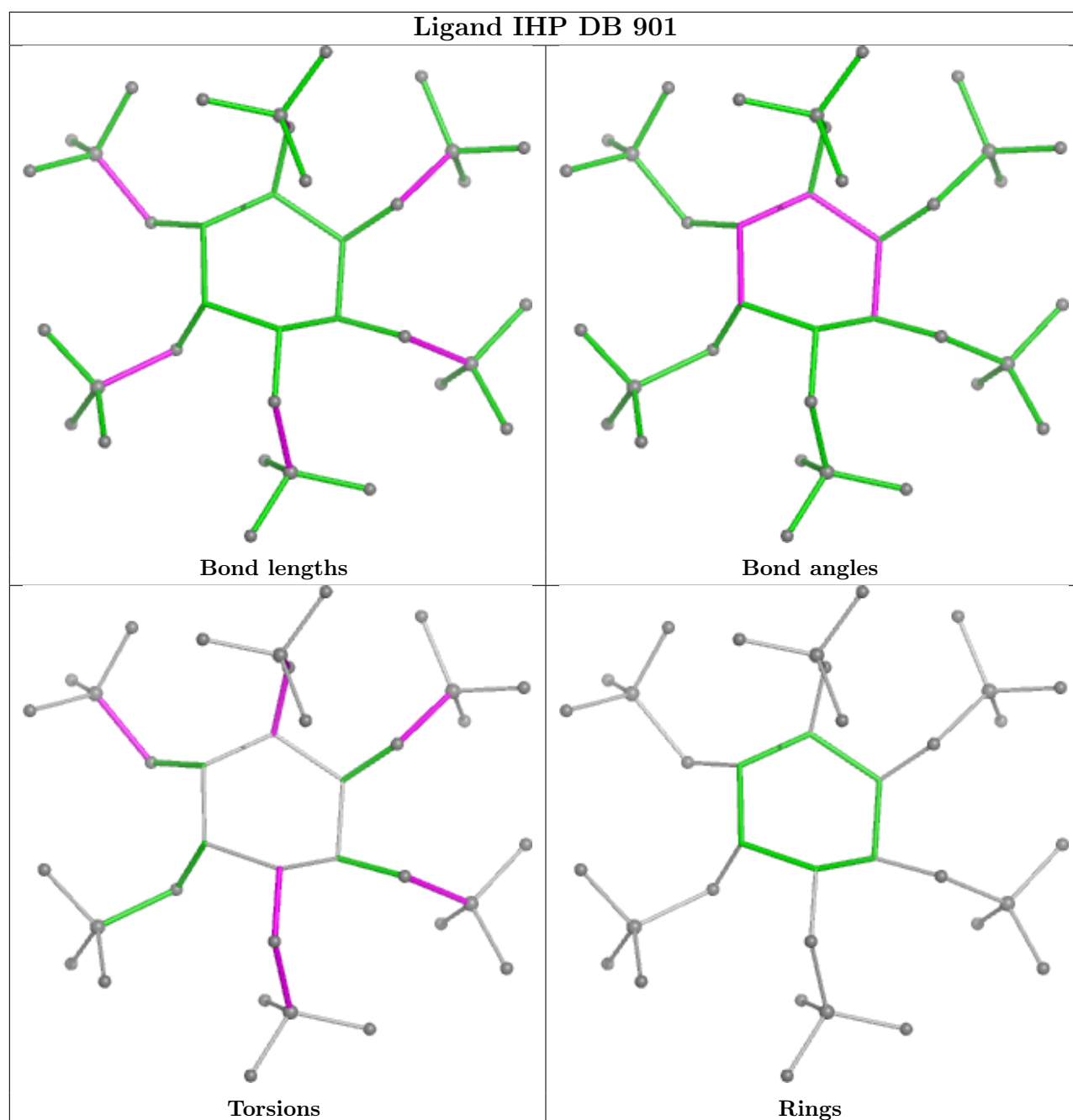
Mol	Chain	Res	Type	Clashes	Symm-Clashes
94	A2	1978	SPD	1	0
94	A2	1971	SPD	1	0
94	A2	1950	SPD	2	0
94	A2	1985	SPD	2	0
94	B5	5082	SPD	2	0
94	B5	5343	SPD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
95	B5	5018	SPM	3	0
94	A2	1957	SPD	1	0
95	A2	1994	SPM	3	0
94	A2	1964	SPD	1	0
94	B5	4933	SPD	2	0
94	B5	5244	SPD	1	0
94	B5	4975	SPD	1	0
94	B5	5144	SPD	2	0
94	A2	1986	SPD	1	0
94	B5	4912	SPD	1	0
94	B5	5165	SPD	1	0
94	B5	5405	SPD	1	0
94	B5	4954	SPD	2	0
94	B5	5263	SPD	3	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.

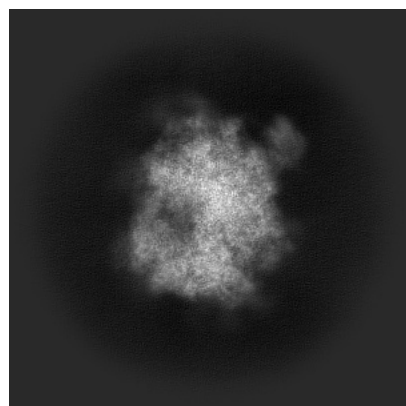
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50124. These allow visual inspection of the internal detail of the map and identification of artifacts.

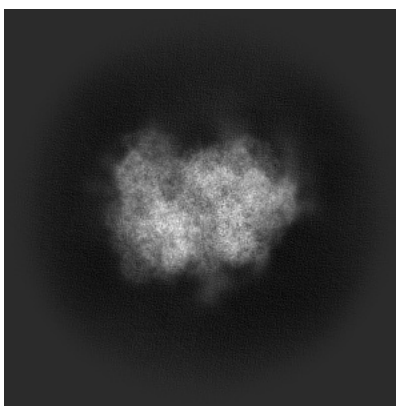
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

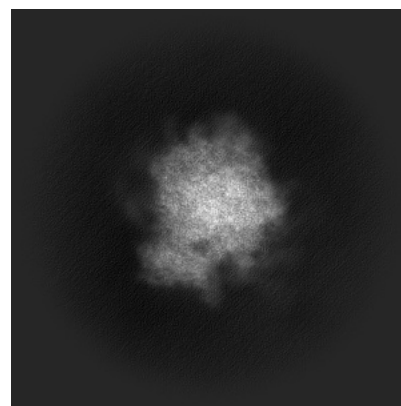
6.1.1 Primary map



X

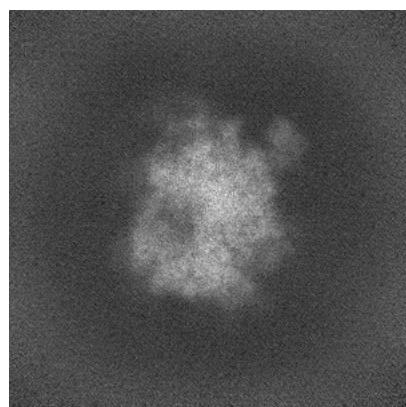


Y

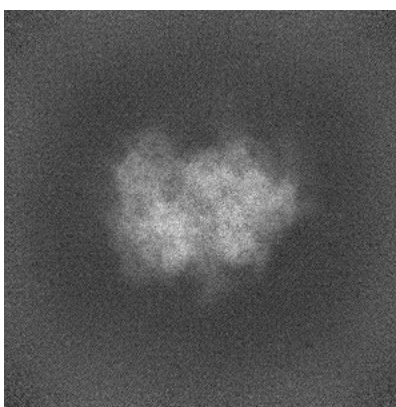


Z

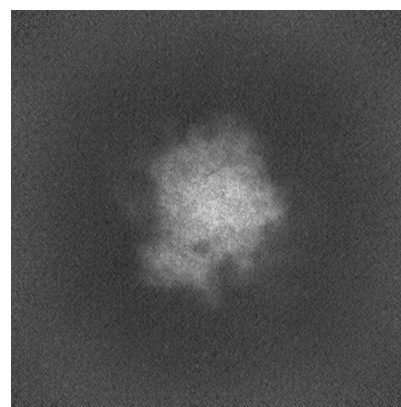
6.1.2 Raw map



X



Y

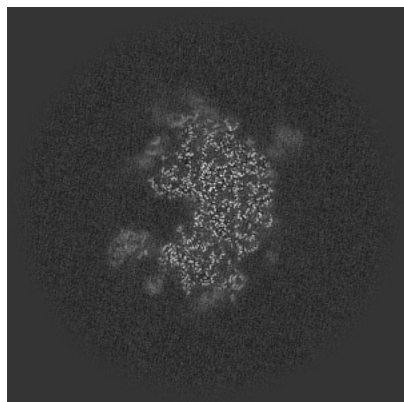


Z

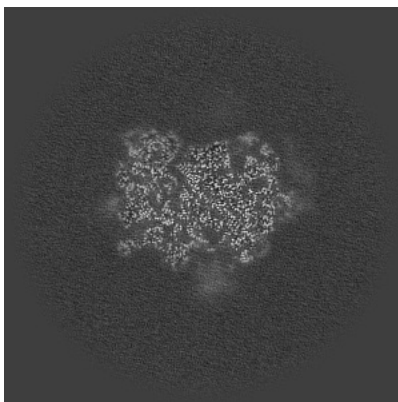
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

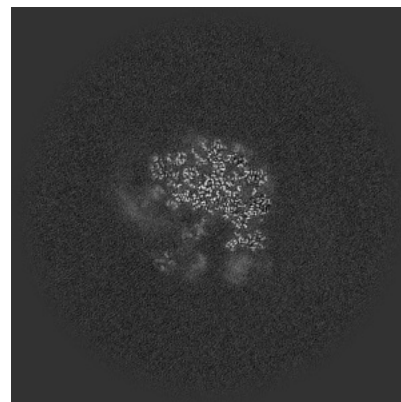
6.2.1 Primary map



X Index: 280

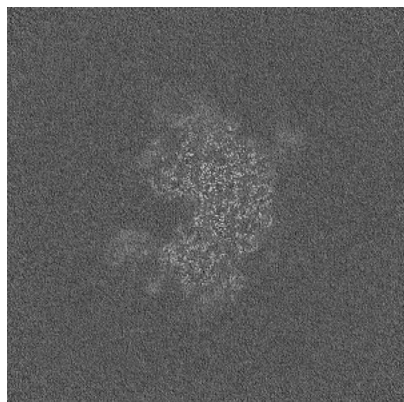


Y Index: 280

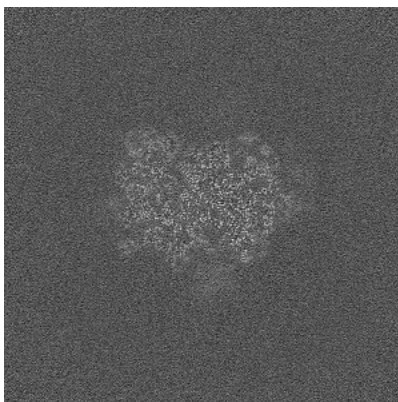


Z Index: 280

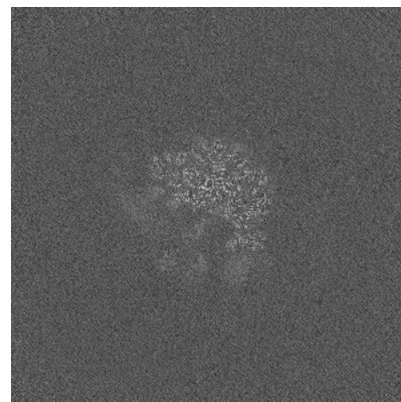
6.2.2 Raw map



X Index: 280



Y Index: 280

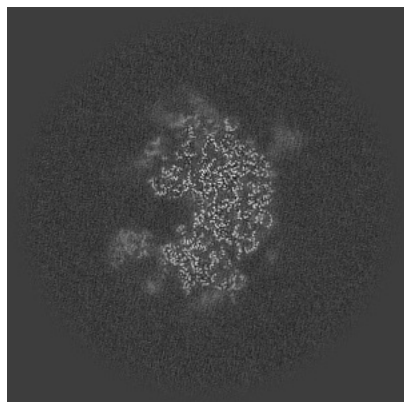


Z Index: 280

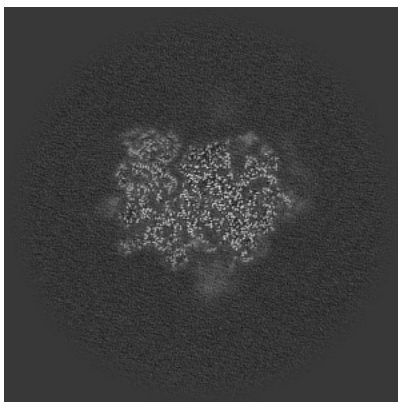
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

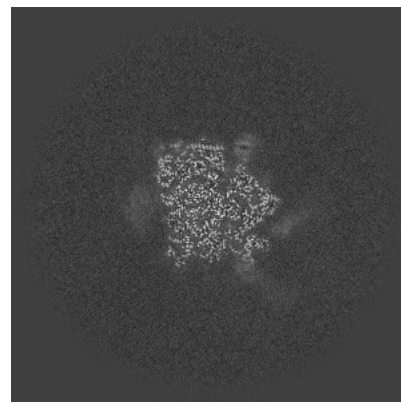
6.3.1 Primary map



X Index: 279

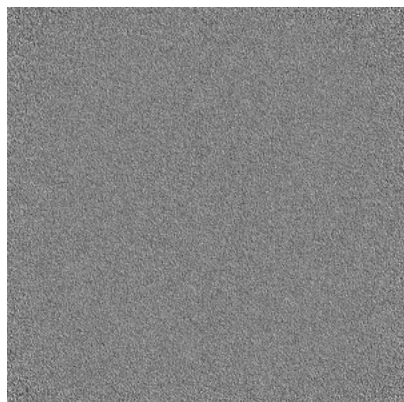


Y Index: 281

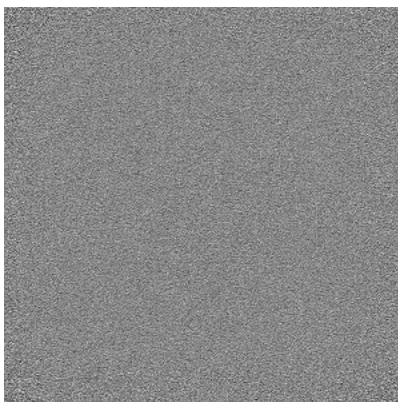


Z Index: 309

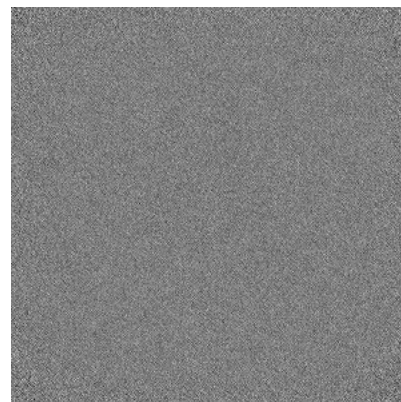
6.3.2 Raw map



X Index: 0



Y Index: 0

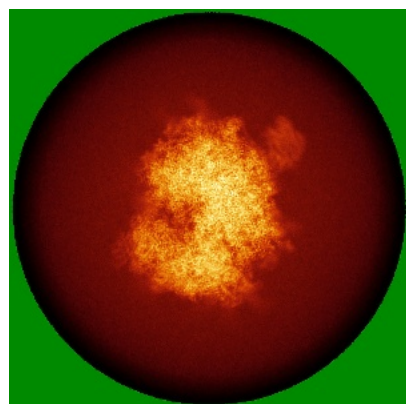


Z Index: 0

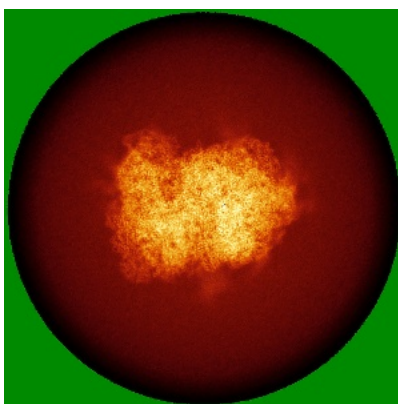
The images above show the largest variance slices of the map in three orthogonal directions.

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

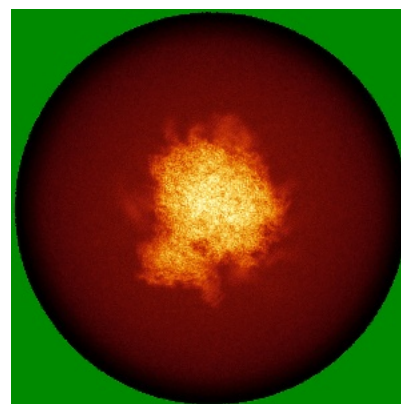
6.4.1 Primary map



X

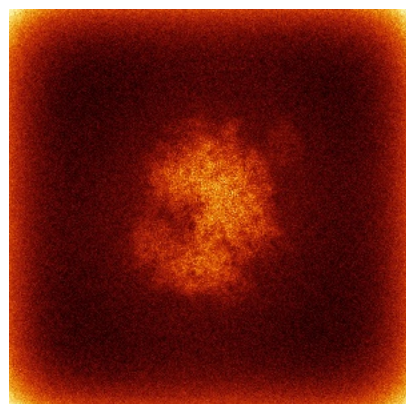


Y

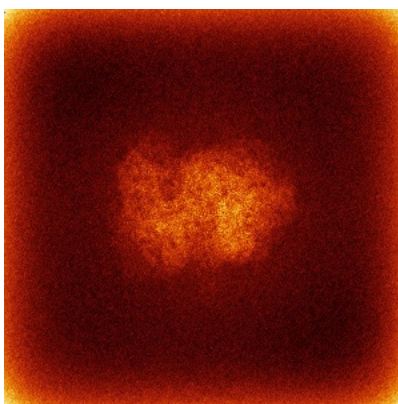


Z

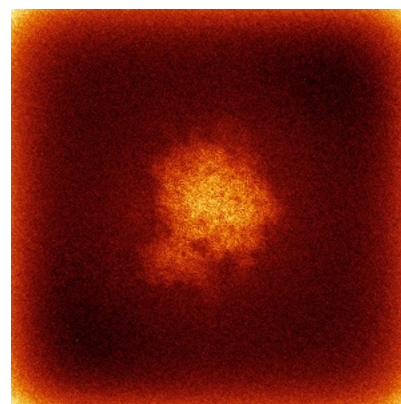
6.4.2 Raw map



X



Y

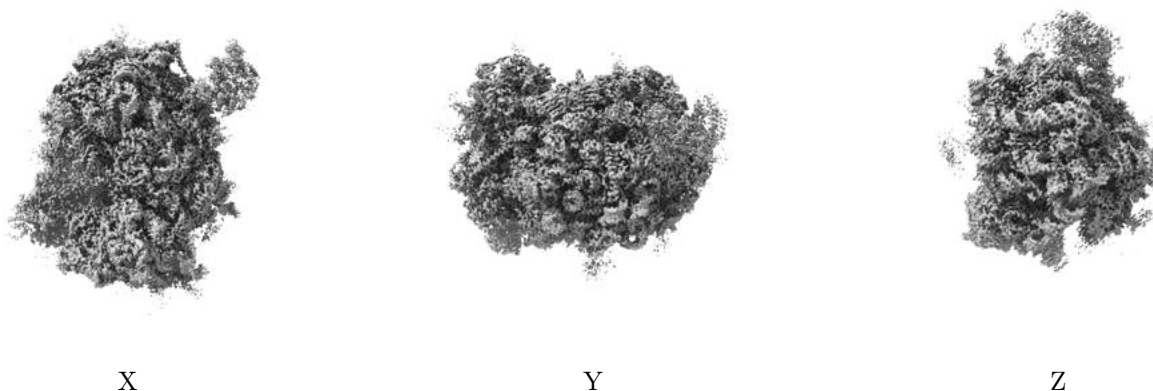


Z

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.

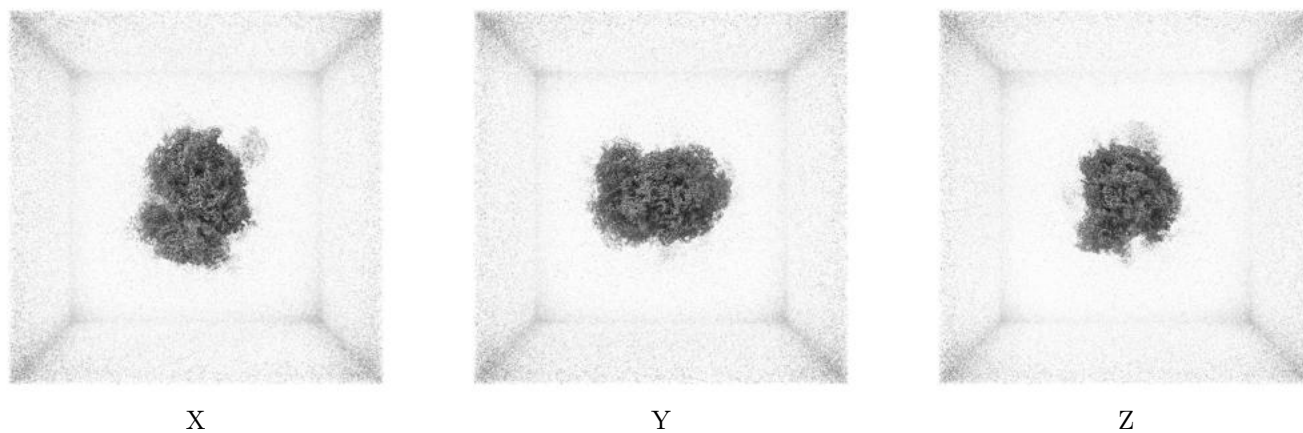
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.275. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

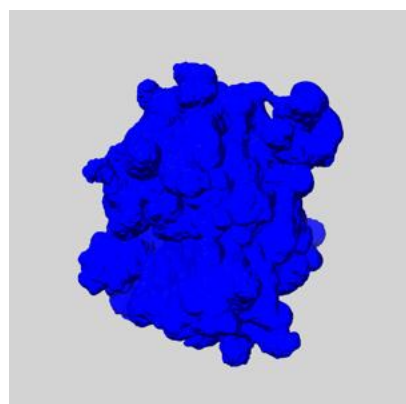
6.6 Mask visualisation [i](#)

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

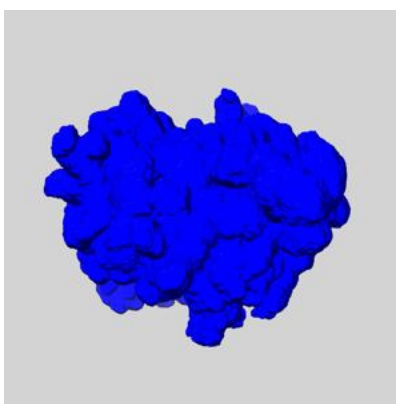
A mask typically either:

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

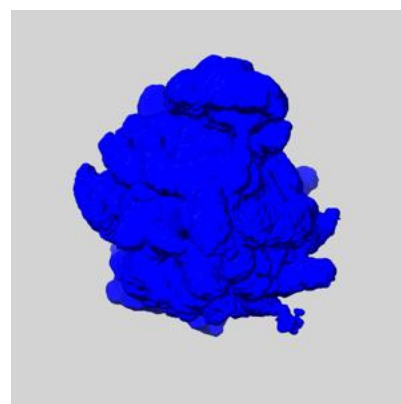
6.6.1 emd_50124_msk_1.map [i](#)



X

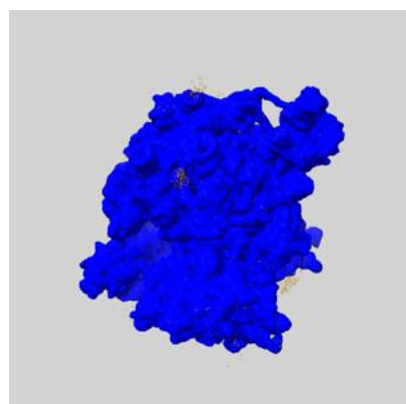


Y

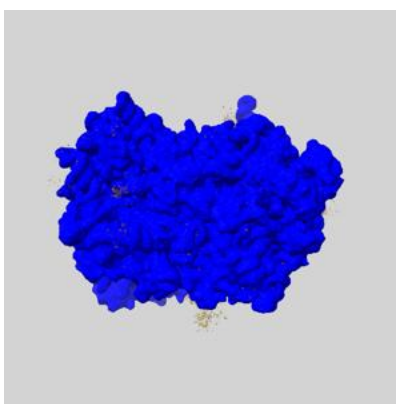


Z

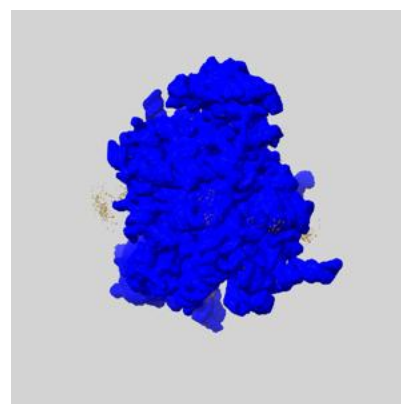
6.6.2 emd_50124_msk_2.map [i](#)



X



Y

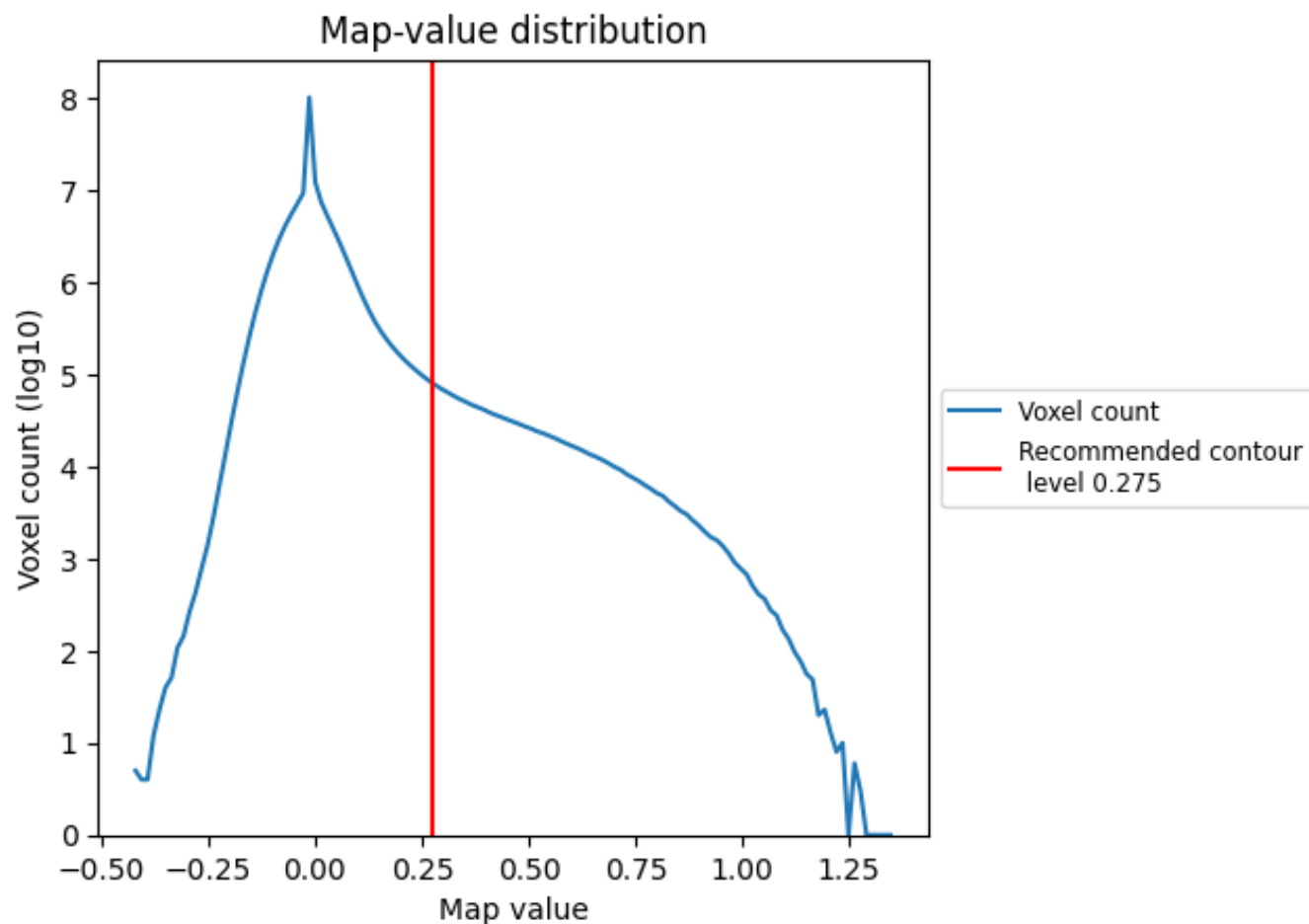


Z

7 Map analysis [i](#)

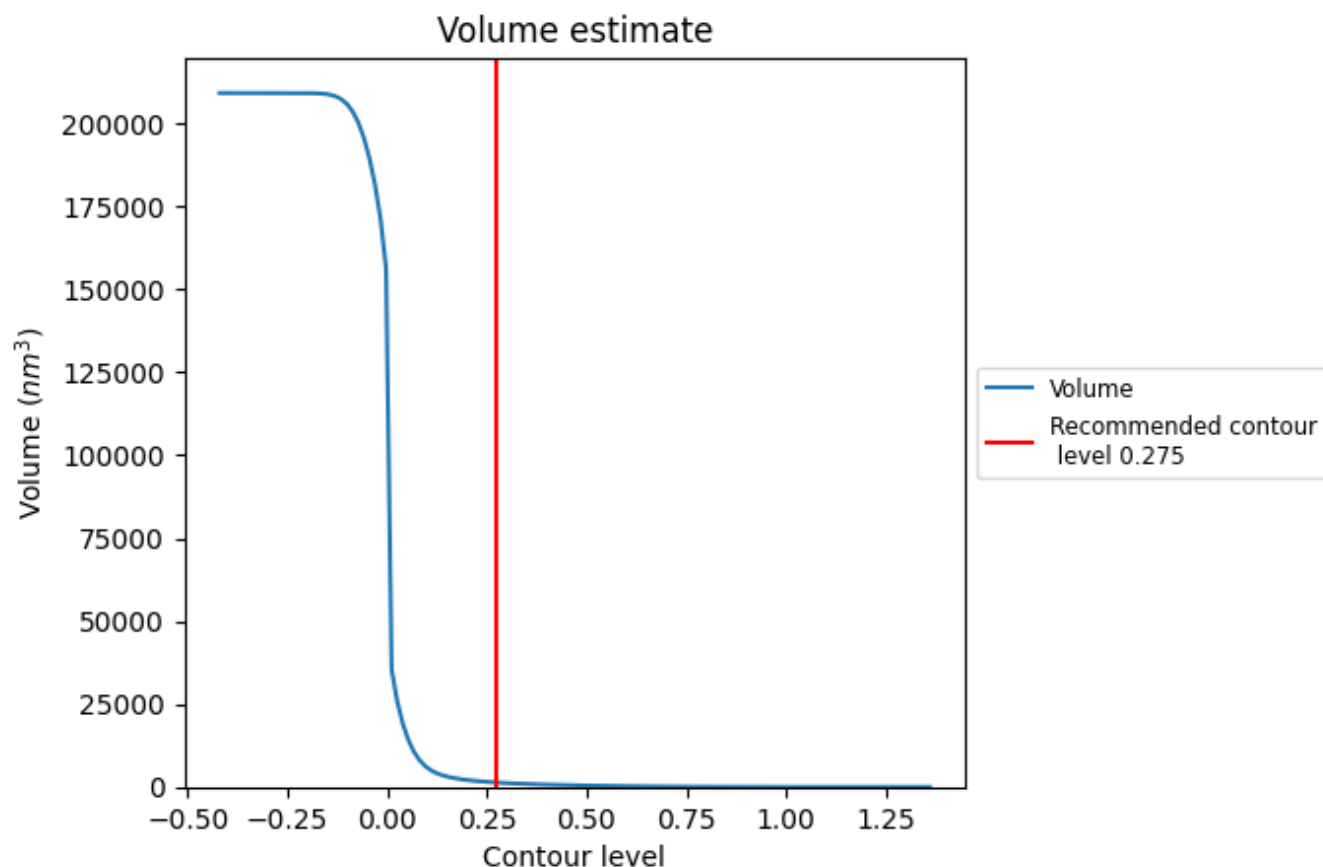
This section contains the results of statistical analysis of the map.

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.

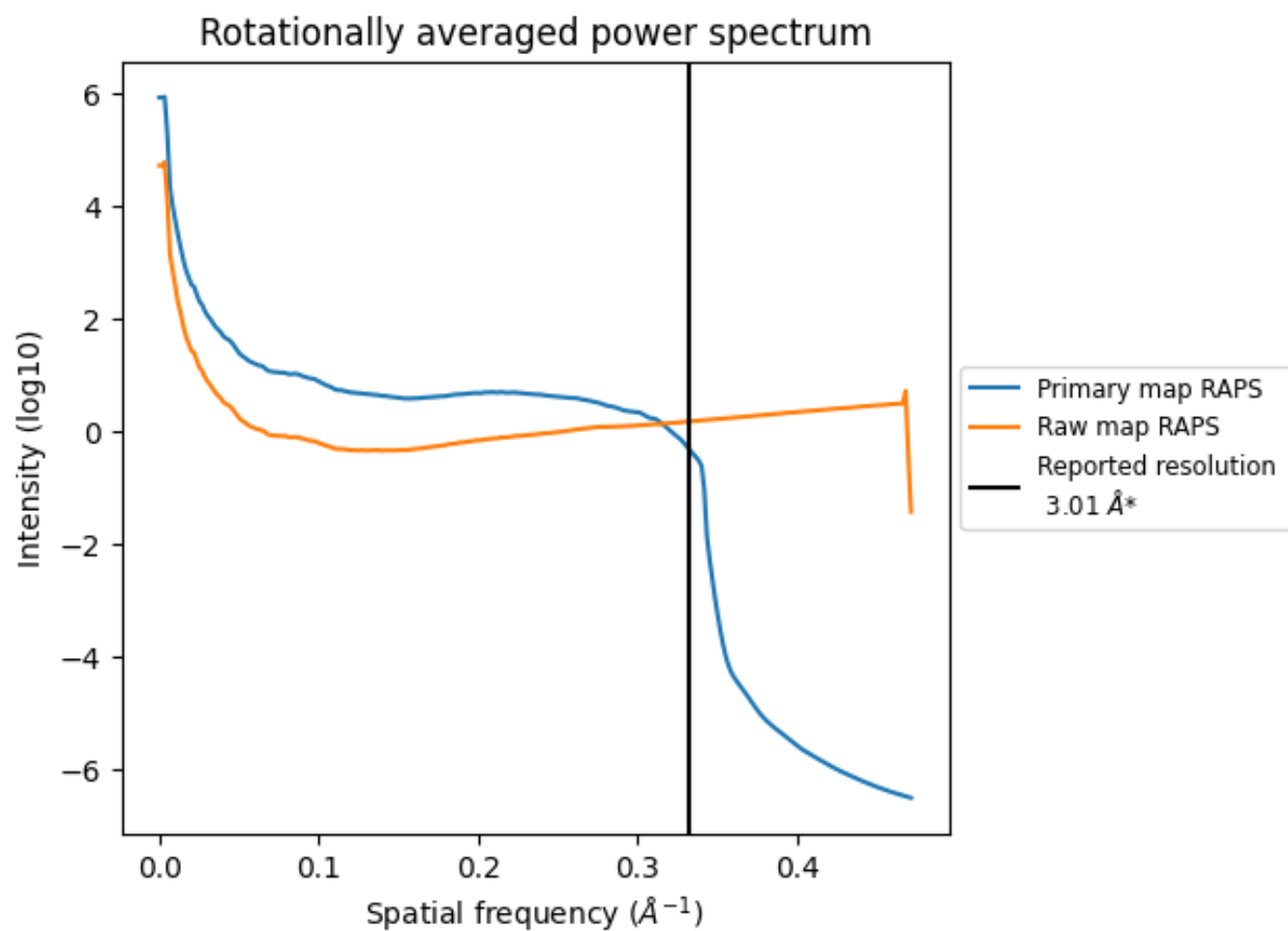
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1330 nm³; this corresponds to an approximate mass of 1201 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 ⓘ

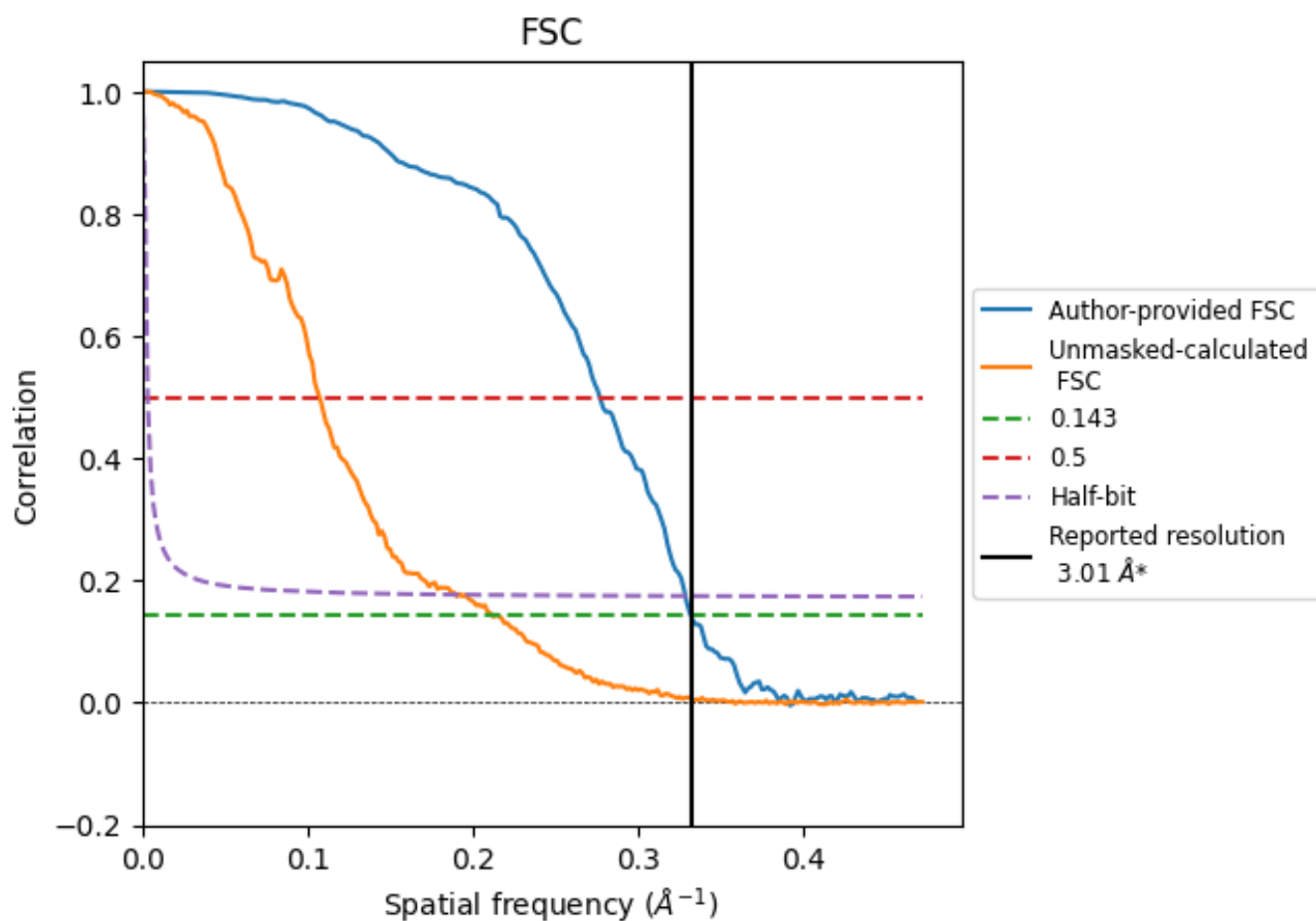


*Reported resolution corresponds to spatial frequency of 0.332 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.332 Å⁻¹

8.2 Resolution estimates [i](#)

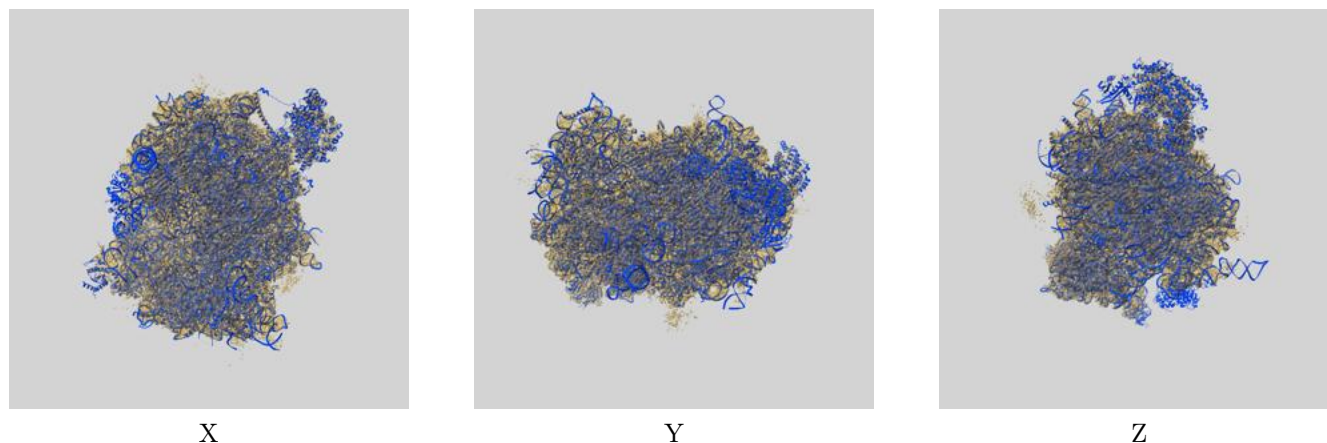
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.01	-	-
Author-provided FSC curve	3.01	3.61	3.04
Unmasked-calculated*	4.73	9.33	5.27

*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 4.73 differs from the reported value 3.01 by more than 10 %

9 Map-model fit [i](#)

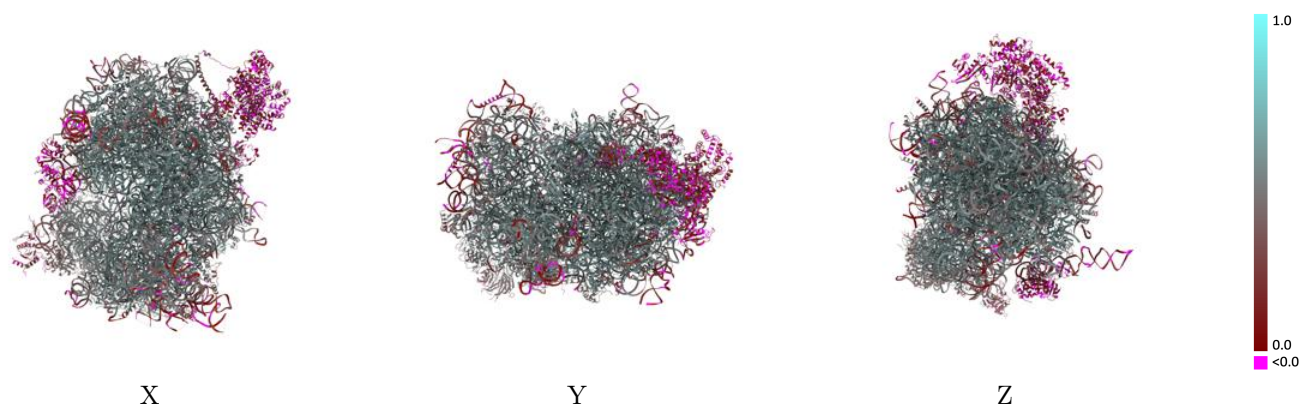
This section contains information regarding the fit between EMDB map EMD-50124 and PDB model 9F1B. Per-residue inclusion information can be found in [section 3](#) on [page 32](#).

9.1 Map-model overlay [i](#)



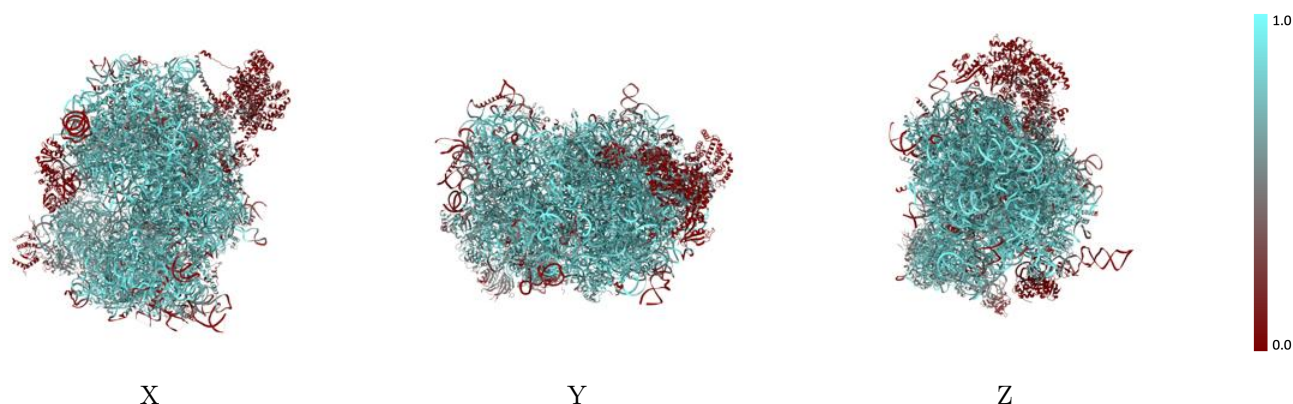
The images above show the 3D surface view of the map at the recommended contour level 0.275 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



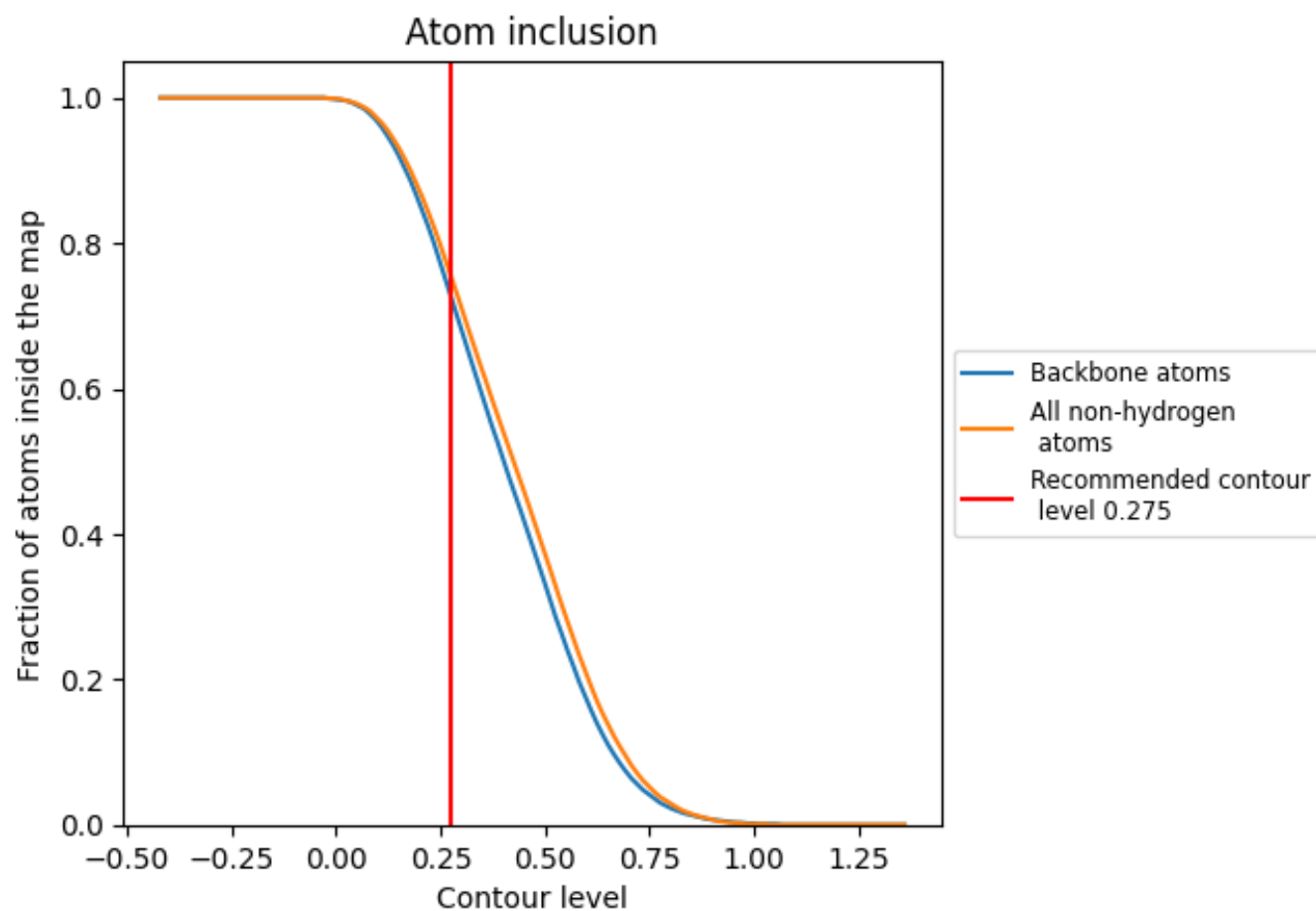
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.275).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 76% 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 (0.275) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7550	 0.4750
A2	 0.8340	 0.4770
AA	 0.6760	 0.4940
AB	 0.6040	 0.4780
AC	 0.1580	 0.2200
AD	 0.5770	 0.4370
AE	 0.7980	 0.5180
AF	 0.4480	 0.3760
AG	 0.8120	 0.4960
AH	 0.1110	 0.3930
AT	 0.5350	 0.4300
AZ	 0.7000	 0.5000
Aa	 0.6880	 0.5030
Ab	 0.7800	 0.5250
Ac	 0.6100	 0.4320
Ad	 0.7770	 0.5190
Ae	 0.6640	 0.4740
Af	 0.6150	 0.4160
Ag	 0.5810	 0.4320
Ah	 0.7380	 0.5060
Ai	 0.7500	 0.4960
Aj	 0.5520	 0.3920
Ak	 0.7490	 0.5000
Al	 0.0760	 0.1840
Am	 0.7700	 0.5270
An	 0.7710	 0.5310
Ao	 0.5590	 0.4140
Ap	 0.7010	 0.4760
Aq	 0.6430	 0.4560
Ar	 0.6120	 0.4400
As	 0.6700	 0.4420
At	 0.6020	 0.4150
Au	 0.7330	 0.5060
Av	 0.8070	 0.5460
Aw	 0.8050	 0.5450



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Chain	Atom inclusion	Q-score
Ax	 0.7070	 0.4830
Ay	 0.5010	 0.3960
Az	 0.7390	 0.5400
B	 0.7510	 0.5210
B5	 0.8560	 0.5010
B7	 0.9420	 0.5520
B8	 0.9030	 0.5280
BA	 0.8510	 0.5690
BB	 0.8300	 0.5580
BC	 0.8460	 0.5570
BE	 0.7190	 0.4990
BF	 0.8490	 0.5600
BG	 0.7080	 0.4880
BH	 0.7620	 0.5330
BI	 0.7880	 0.5470
BJ	 0.6930	 0.5030
BK	 0.3310	 0.3920
BL	 0.7930	 0.5170
BM	 0.7900	 0.5200
BN	 0.9040	 0.5760
BO	 0.8470	 0.5610
BP	 0.8530	 0.5640
BQ	 0.8600	 0.5680
BR	 0.7950	 0.5200
BS	 0.8660	 0.5670
BT	 0.7900	 0.5340
BU	 0.6780	 0.4800
BV	 0.7760	 0.5450
BW	 0.5410	 0.3730
BX	 0.8060	 0.5380
BY	 0.7740	 0.5400
BZ	 0.7880	 0.5270
Ba	 0.8760	 0.5730
Bb	 0.6860	 0.4710
Bc	 0.6760	 0.4860
Bd	 0.8030	 0.5370
Be	 0.8540	 0.5620
Bf	 0.8500	 0.5750
Bg	 0.7930	 0.5360
Bh	 0.7850	 0.5290
Bi	 0.7700	 0.5150
Bj	 0.9140	 0.5780

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Chain	Atom inclusion	Q-score
Bk	 0.6550	 0.4820
Bl	 0.8760	 0.5530
Bm	 0.8190	 0.5500
Bo	 0.7960	 0.5480
Bp	 0.7920	 0.5460
Br	 0.8380	 0.5520
Bs	 0.0050	 0.0570
Bt	 0.0020	 0.0470
Ct	 0.1020	 0.1340
Cu	 0.2310	 0.2170
DA	 0.0050	 0.0410
DB	 0.1280	 0.1010
DC	 0.1200	 0.0860