



Full wwPDB EM Validation Report ⓘ

Jun 1, 2026 – 05:37 pm BST

PDB ID : 28LN / pdb_000028ln
EMDB ID : EMD-56598
Title : XBP1u-stalled RPL4 RNC in complex with NAC
Authors : Santos, J.; Guennigmann, M.; Gora, R.J.; Iljina, M.; Predin, M.; Kotan, I.E.;
De, P.; Choudhary, D.; Jang, J.; Tippmann, F.; Hins, C.; Ban, N.; Tans, S.J.;
Shan, S.; Kramer, G.; Bukau, B.
Deposited on : 2026-02-05
Resolution : 2.70 Å (reported)
Based on initial models : 6r7q, 7qwr, 8qoi

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:

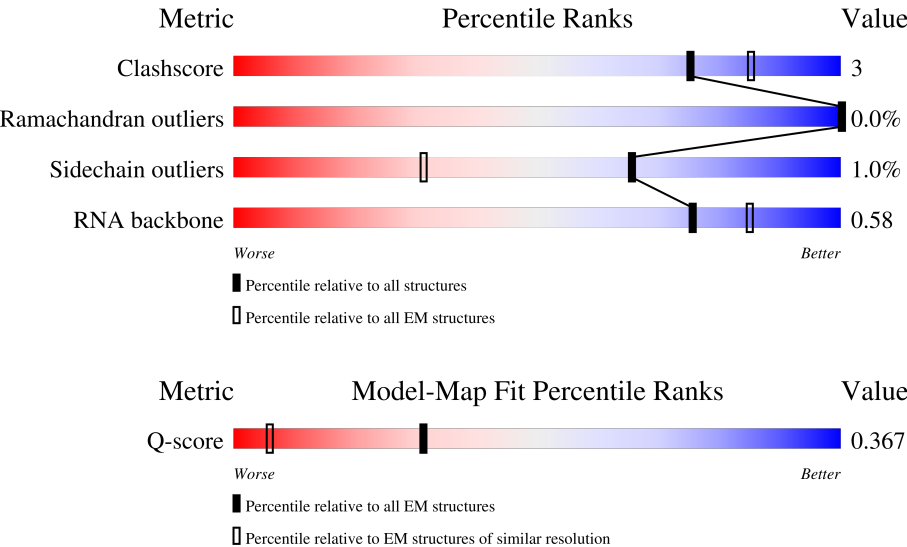
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal 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 2.70 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	10327 (2.20 - 3.20)

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	B1	184	
2	B2	76	
3	B4	6	

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Mol	Chain	Length	Quality of chain
4	B5	5069	
5	B7	120	
6	B8	157	
7	BA	257	
8	BB	403	
9	BC	427	
10	BD	297	
11	BE	288	
12	BF	248	
13	BG	266	
14	BH	192	
15	BI	214	
16	BJ	178	
17	BL	211	
18	BM	215	
19	BN	204	
20	BO	203	
21	BP	184	
22	BQ	188	
23	BR	196	
24	BS	176	
25	BT	160	
26	BU	128	
27	BV	140	
28	BW	157	

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Mol	Chain	Length	Quality of chain
29	BX	156	
30	BY	145	
31	BZ	136	
32	Ba	148	
33	Bb	159	
34	Bc	115	
35	Bd	125	
36	Be	135	
37	Bf	110	
38	Bg	117	
39	Bh	123	
40	Bi	105	
41	Bj	97	
42	Bk	70	
43	Bl	51	
44	Bm	128	
45	Bo	106	
46	Bp	92	
47	Br	137	
48	Bs	317	
49	Bt	165	
50	Bu	215	
51	Bv	206	
52	A2	1869	
53	AA	295	

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Mol	Chain	Length	Quality of chain
54	AB	264	
55	AC	293	
56	AD	243	
57	AE	263	
58	AF	204	
59	AG	249	
60	AH	194	
61	AI	208	
62	AJ	194	
63	AK	165	
64	AL	158	
65	AM	132	
66	AN	151	
67	AO	151	
68	AP	145	
69	AQ	146	
70	AR	135	
71	AS	152	
72	AT	145	
73	AU	119	
74	AV	84	
75	AW	130	
76	AX	143	
77	AY	133	
78	AZ	125	

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Mol	Chain	Length	Quality of chain
79	Aa	115	
80	Ab	84	
81	Ac	69	
82	Ad	56	
83	Ae	133	
84	Af	156	
85	Ag	317	
86	Ah	25	

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 220645 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 uL4,X-box-binding protein 1, luminal form,X-box-binding protein 1, luminal form,X-box-binding protein 1, luminal form.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B1	34	Total	C	N	O	S	0	0
			283	187	48	45	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	178	CYS	PRO	conflict	UNP P17861
B1	179	ALA	SER	conflict	UNP P17861

- Molecule 2 is a RNA chain called tRNA-Met-CAT.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B2	76	Total	C	N	O	P	0	0
			1638	736	288	538	76		

- Molecule 3 is a RNA chain called mRNA fragment (6-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B4	6	Total	C	N	O	P	0	0
			127	57	21	43	6		

- Molecule 4 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B5	3638	Total	C	N	O	P	0	0
			78039	34791	14254	25356	3638		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B7	120	Total	C	N	O	P	0	0
			2570	1141	456	851	122		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B8	156	Total	C	N	O	P	0	0
			3320	1482	585	1097	156		

- Molecule 7 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BA	248	Total	C	N	O	S	0	0
			1899	1189	389	315	6		

- Molecule 8 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BB	402	Total	C	N	O	S	0	0
			3239	2061	608	556	14		

- Molecule 9 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BC	367	Total	C	N	O	S	0	0
			2919	1835	582	488	14		

- Molecule 10 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	BD	293	Total	C	N	O	S	0	0
			2386	1510	435	427	14		

- Molecule 11 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BE	221	Total	C	N	O	S	0	0
			1773	1142	335	292	4		

- Molecule 12 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BF	225	Total	C	N	O	S	1	0
			1878	1207	361	301	9		

- Molecule 13 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BG	240	Total	C	N	O	S	0	0
			1927	1229	370	324	4		

- Molecule 14 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BH	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 15 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BI	205	Total	C	N	O	S	0	0
			1660	1054	319	274	13		

- Molecule 16 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BJ	171	Total	C	N	O	S	0	0
			1371	867	256	242	6		

- Molecule 17 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BL	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 18 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	BM	136	Total	C	N	O	S	0	0
			1120	719	215	179	7		

- Molecule 19 is a protein called 60S ribosomal protein L15.

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

- Molecule 20 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BO	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 21 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BP	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 22 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BQ	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 23 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BR	187	Total	C	N	O	S	0	0
			1566	971	336	250	9		

- Molecule 24 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BS	176	Total	C	N	O	S	0	0
			1461	930	284	236	11		

- 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 L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BU	104	Total	C	N	O	S	0	0
			851	544	150	155	2		

- Molecule 27 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BV	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 28 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BW	122	Total	C	N	O	S	0	0
			997	622	203	168	4		

- Molecule 29 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BX	126	Total	C	N	O	S	0	0
			1031	658	196	176	1		

- Molecule 30 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BY	132	Total	C	N	O	S	0	0
			1102	692	223	184	3		

- Molecule 31 is a protein called 60S ribosomal protein L27.

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

- Molecule 32 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ba	147	Total	C	N	O	S	0	0
			1163	736	237	187	3		

- Molecule 33 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Bb	99	Total	C	N	O	S	0	0
			809	503	177	125	4		

- Molecule 34 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Bc	106	Total	C	N	O	S	0	0
			824	523	146	148	7		

- Molecule 35 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Bd	107	Total	C	N	O	S	0	0
			883	558	171	152	2		

- Molecule 36 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Be	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 37 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Bf	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 38 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Bg	109	Total	C	N	O	S	0	0
			868	544	179	139	6		

- Molecule 39 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Bh	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 40 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Bi	99	Total	C	N	O	S	0	0
			813	509	173	126	5		

- Molecule 41 is a protein called Large ribosomal subunit protein eL37.

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

- Molecule 42 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Bk	68	Total	C	N	O	S	0	0
			559	360	101	97	1		

- Molecule 43 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Bl	50	Total	C	N	O	S	1	0
			451	286	100	64	1		

- Molecule 44 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Bm	51	Total	C	N	O	S	0	0
			419	260	88	65	6		

- Molecule 45 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Bo	102	Total	C	N	O	S	1	0
			843	528	174	135	6		

- Molecule 46 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Bp	88	Total	C	N	O	S	0	0
			681	430	131	113	7		

- Molecule 47 is a protein called Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Br	124	Total	C	N	O	S	0	0
			990	614	205	167	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Br	2	ACE	-	acetylation	UNP P46779

- Molecule 48 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Bs	196	Total	C	N	O	S	0	0
			1506	958	263	276	9		

- Molecule 49 is a protein called Large ribosomal subunit protein uL11.

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

- Molecule 50 is a protein called Nascent polypeptide-associated complex subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Bu	66	Total	C	N	O	S	0	0
			522	330	95	96	1		

- Molecule 51 is a protein called Transcription factor BTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Bv	109	Total	C	N	O	S	0	0
			846	528	157	157	4		

- Molecule 52 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	A2	1779	Total	C	N	O	P	0	0
			38027	16999	6818	12431	1779		

- Molecule 53 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AA	217	Total	C	N	O	S	0	0
			1708	1085	299	316	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	2	ACE	-	acetylation	UNP P08865

- Molecule 54 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AB	223	Total	C	N	O	S	0	0
			1806	1146	326	320	14		

- Molecule 55 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AC	218	Total	C	N	O	S	0	0
			1690	1094	289	297	10		

- Molecule 56 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AD	225	Total	C	N	O	S	0	0
			1752	1117	315	313	7		

- Molecule 57 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 58 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AF	192	Total	C	N	O	S	0	0
			1517	948	287	275	7		

- Molecule 59 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AG	240	Total	C	N	O	S	0	0
			1945	1212	393	333	7		

- Molecule 60 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AH	188	Total	C	N	O	S	0	0
			1515	966	279	269	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AI	203	Total	C	N	O	S	0	0
			1670	1048	329	288	5		

- Molecule 62 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AJ	180	Total	C	N	O	S	0	0
			1499	955	300	242	2		

- Molecule 63 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AK	97	Total	C	N	O	S	0	0
			816	533	144	133	6		

- Molecule 64 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AL	151	Total	C	N	O	S	0	0
			1229	782	230	211	6		

- Molecule 65 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AM	123	Total	C	N	O	S	0	0
			953	598	169	177	9		

- Molecule 66 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	AN	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 67 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	AO	135	Total	C	N	O	S	0	0
			1010	618	198	188	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AO	138	IAS	ASP	modified residue	UNP P62263

- Molecule 68 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	AP	127	Total	C	N	O	S	0	0
			1044	663	197	177	7		

- Molecule 69 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	AQ	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 70 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	AR	134	Total	C	N	O	S	0	0
			1082	680	201	197	4		

- Molecule 71 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	AS	146	Total	C	N	O	S	0	0
			1200	753	242	204	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AS	2	ACE	-	acetylation	UNP P62269

- Molecule 72 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	AT	144	Total	C	N	O	S	0	0
			1123	704	217	199	3		

- Molecule 73 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	AU	101	Total	C	N	O	S	0	0
			803	504	153	142	4		

- Molecule 74 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	AV	84	Total	C	N	O	S	0	0
			639	395	117	122	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AV	0	ACE	-	acetylation	UNP P63220

- Molecule 75 is a protein called 40S ribosomal protein S15a.

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

- Molecule 76 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	AX	141	Total	C	N	O	S	1	0
			1105	698	220	184	3		

- Molecule 77 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	AY	124	Total	C	N	O	S	0	0
			1014	641	198	170	5		

- Molecule 78 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	AZ	72	Total	C	N	O	S	0	0
			574	368	104	101	1		

- Molecule 79 is a protein called 40S ribosomal protein S26.

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

- Molecule 80 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Ab	83	Total	C	N	O	S	0	0
			650	408	121	114	7		

- Molecule 81 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Ac	65	Total	C	N	O	S	0	0
			512	311	103	96	2		

- Molecule 82 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Ad	55	Total	C	N	O	S	0	0
			458	286	94	73	5		

- Molecule 83 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Ae	57	Total	C	N	O	S	0	0
			451	279	99	72	1		

- Molecule 84 is a protein called Ubiquitin.

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

- Molecule 85 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Ag	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

- Molecule 86 is a protein called 60S ribosomal protein L41.

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

- Molecule 87 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
87	B5	285	Total 285	Mg 285	0
87	B7	4	Total 4	Mg 4	0
87	B8	6	Total 6	Mg 6	0
87	BA	3	Total 3	Mg 3	0
87	BB	1	Total 1	Mg 1	0
87	BN	1	Total 1	Mg 1	0
87	BV	1	Total 1	Mg 1	0
87	Ba	1	Total 1	Mg 1	0
87	Be	1	Total 1	Mg 1	0
87	Bf	2	Total 2	Mg 2	0
87	Bg	1	Total 1	Mg 1	0
87	Bj	1	Total 1	Mg 1	0
87	A2	123	Total 123	Mg 123	0
87	AI	1	Total 1	Mg 1	0
87	AX	1	Total 1	Mg 1	0

- Molecule 88 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
88	Bg	1	Total 1	Zn 1	0
88	Bj	1	Total 1	Zn 1	0
88	Bm	1	Total 1	Zn 1	0
88	Bo	1	Total 1	Zn 1	0
88	Bp	1	Total 1	Zn 1	0

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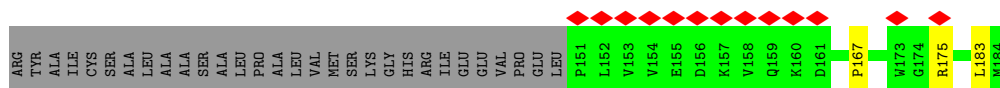
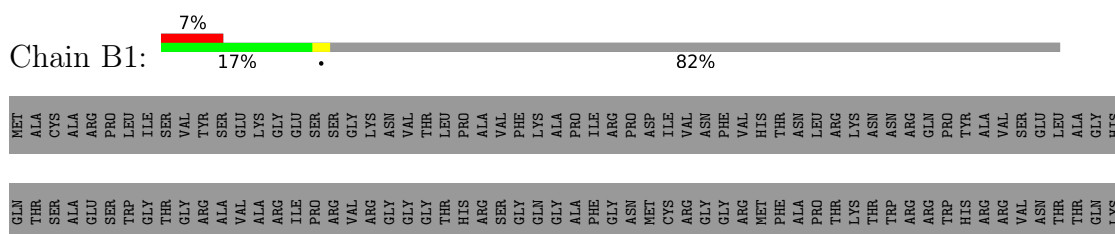
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Mol	Chain	Residues	Atoms		AltConf
88	Aa	1	Total 1	Zn 1	0
88	Ad	1	Total 1	Zn 1	0
88	Af	1	Total 1	Zn 1	0

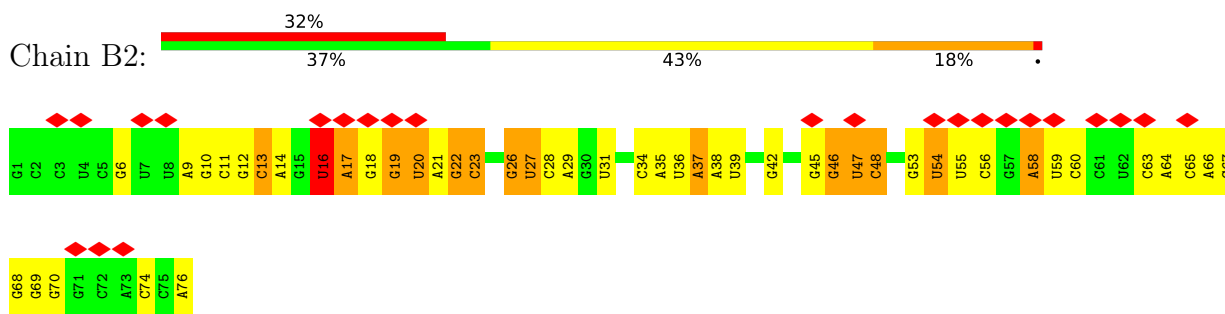
3 Residue-property plots

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

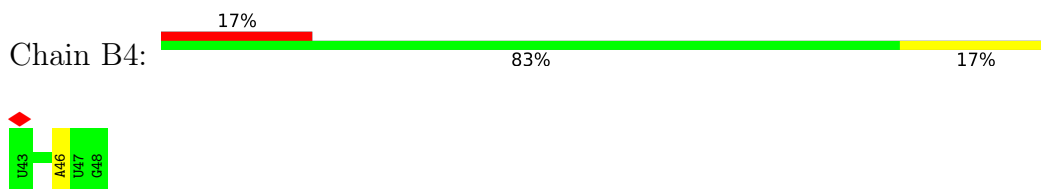
- Molecule 1: Large ribosomal subunit protein uL4,X-box-binding protein 1, luminal form,X-box-binding protein 1, luminal form,X-box-binding protein 1, luminal form



- Molecule 2: tRNA-Met-CAT



- Molecule 3: mRNA fragment (6-MER)



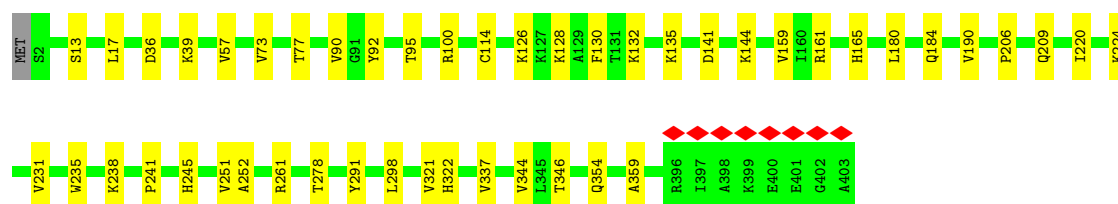
- Molecule 4: 28S rRNA



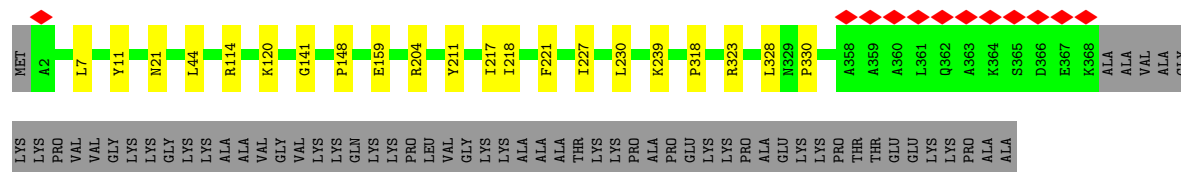
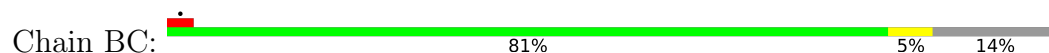


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A1396	G1503	U1690	A1779	C1920	G2002	G	A2373	G2517	G2685	G2826	U
A1397	U1513	G1690	U1780	G1921	U2003	C	A2394	U2518	U2686	U2827	G
G1398	A1514	G1696	C1784	C1930	G2004	G	U2397	G2519	G2687	G2828	G
C1401	A1517	C1697	A1785	A1931	U2005	C	U2400	G2543	G2693	U2836	G
G1402	G1521	A1698	A1786	C1934	G2006	C	A2409	U2544	A2694	G2837	A
G1403	A1522	G1699	A1787	G1939	U2007	G	U2413	G2553	A2695	U2838	G
C1406	A1523	A1700	U1791	A1941	A2008	U	G2414	G2554	A2696	G2839	C
G1407	A1533	G1702	A1792	A1944	A2009	C	U2415	C2559	G2702	A2843	C
C1408	C1534	C1703	A1793	G1945	C2010	C	G2420	G2560	G2703	A2844	C
U1409	U1535	G1704	A1801	G1946	A2011	C	A2421	G2561	G2704	G2854	G
C1410	A1536	C1705	A1802	U1945	A2012	G	G2422	G2562	U2705	C2855	C
G1411	U1537	C1706	A1803	U1953	C2013	C	U2423	G2563	U2706	A2856	C
G1414	G1538	C1707	A1804	G1954	U2014	C	U2424	A2664	G2707	G2857	C
G1415	C1539	C1708	C1811	G1955	C2015	C	G2433	G2565	C2708	C2858	C
G1418	A1546	A1711	C1819	U1958	A2016	C	U2436	G2566	G2709	C2859	C
A1419	G1549	C1712	A1820	A1959	C2017	G	G2460	G2567	G2710	G2875	C
C1438	G1560	G1713	U1821	G1960	U2018	A	G2461	G2568	G2711	G2876	A
A1442	G1573	A1718	C1827	C1965	C2021	C	G2462	U2569	G2715	G2889	C
A1451	U1576	C1719	G1828	A1966	C2022	C	G2468	C2570	G2716	G2897	G
G1452	U1577	G1720	U1832	G1967	G2023	C	C2469	A2571	G2723	A2724	C
G1456	U1581	G1740	U1833	G1968	A2024	C	G2470	G2572	G2725	G2726	C
C1457	C1589	A1741	G1834	A1969	A2025	C	G2473	G2573	U2740	U2898	C
A1458	U1590	A1742	G1835	C1970	A2032	C	G2474	G2574	G2741	G2900	C
C1459	U1595	U1743	A1836	G1971	G2033	C	U2477	G2575	A2742	G2901	G
G1474	G1475	A1748	G1841	G1972	G2038	C	U2483	C2582	G2753	G	U
C1476	C1477	G1749	G1854	G1973	G2045	A	U2484	G2585	G2758	G	C
G1478	G1481	A1750	C1858	G1974	A2046	G	G2485	A2586	G2759	G	C
G1482	G1483	G1756	U1859	G1975	U2047	G	C2488	C2587	U2760	U2837	C
C1484	A1630	C1757	U1860	C1976	U2054	C	U2489	C2588	G2761	G2888	C
G1485	A1631	G1760	U1861	C1977	G2055	C	U2494	A2600	G2762	A2600	C
G1486	G1632	C1761	G1868	A1978	G2058	C	G2495	C2612	U2763	G2763	C
G1487	A1633	C1762	C1869	U1979	A2068	C	U2496	C2626	U2766	U2766	C
G1488	G1640	G1763	A1870	G1980	C2072	C	G2497	U2631	G2769	G2770	C
G1491	G1653	A1764	C1874	A1981	G2075	C	U2498	U2632	G2776	G2777	C
U1493	C1660	A1765	G1884	A1982	C2082	C	U2499	G2639	A2786	A2786	C
G1494	C1675	A1766	U1885	A1983	C2083	C	G2500	A2646	U2767	U2767	C
A1496	U1676	G1767	U1886	G1984	G2084	C	G2501	G2651	U2769	U2769	C
G1497	G1679	C1770	C1913	U1887	G2088	C	G2502	G2657	C2803	C2803	C
C1500	G1501	C1771	C1914	G1988	U2089	C	C2503	G2661	C2804	C2804	C
		U1772	G1915	A1989	G2091	C	U2507	G2668	C2813	C2813	C
		C1773	A1916	A1990	G2092	C	A2512	G2674	A2814	A2814	C
			U1917	U1991	A2093	C					
			G1918	C1992	A2094	C					
				C1993	U2095	C					
				G1994	U2096	C					
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				A1998		C					
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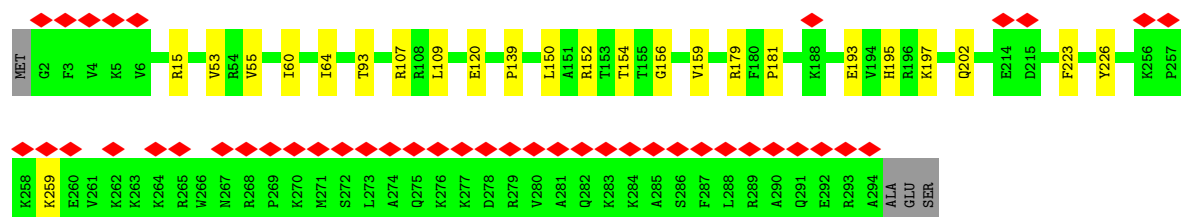
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U4422	U4311	G4168	U3914	C3811	U3712	G	C
A4423	U4325	A4169	U3919	A3812	G3713	C	U
U4430	G4328	C4170	U3924	U3813	U3714	C	U
U4436	G4329	G4182	G3932	A3816	A3717	U3594	U
U4437	G4330	G4183	G3937	U413817	A3718	A3595	U
U4438	C4331	G4190	G3938	G3818	G3719	G3596	U
U4441	A4335	G4195	C3936	U3821	A3724	A3597	U
U4442	C4336	G4203	G3943	A3824	G3724	A3598	U
C4443	G4337	A4204	A3944	C3825	U3729	C3601	U
C4446	A4338	C4205	A3945	A3828	G3730	G3602	U
C4447	A4347	G4213	G3946	A3829	A3731	A3603	U
A4448	C4348	U4219	C3947	U3830	G3732	U3606	U
U4451	U4352	G4225	U3949	G3837	G3734	G3607	U
C4455	U4353	U4226	A4096	A3838	G3743	G3608	U
U4456	G4356	G4227	A4097	U3839	U3744	A3609	U
A4463	U4360	U4228	G3950	C3840	A3745	A3610	U
U4464	A4361	G4232	A3951	C3842	U3746	C3617	U
C4465	A4362	U4248	G3952	U3843	A3747	G3618	U
U4470	G4369	G4249	A3953	U3847	C3751	A3623	U
G4474	C4370	A4250	G3954	A3848	G3752	G3624	U
C4482	U4371	G4251	U	U3850	G3753	G3625	U
A4483	G4372	A4252	G	A3851	U3757	G3626	U
C4374	U4373	G4253	U	U3852	A3758	A3634	U
A4375	C4374	A4254	G	A3855	A3759	C3635	U
C4376	A4375	G4255	A	C3856	C3760	U3636	U
A4488	G4376	A4256	C	A3866	U3761	G3637	U
U4492	A4377	G4265	U	U	A3762	U3638	U
G4493	U4378	G4266	A	A3876	U3763	U3640	U
U4497	A4386	A4267	G	C3877	G3764	A3645	U
C4498	C4387	G4270	C	G3878	A3765	A3652	U
U4499	A4388	A4280	U	U3883	U3767	A3661	U
U4511	C4389	G4290	C	C3886	G3768	A3662	U
A4512	G4391	U4291	G	G3887	U3769	G3663	U
C4518	A4392	A4292	G	U3891	G3770	C3672	U
U4520	G4393	G4293	C	G3896	U3771	G3673	U
G4521	U4397	U4294	C	G3897	G3776	A3691	U
A4522	C4398	G4296	C	G3898	C3781	U3694	U
C4524	U4402	A4297	G	G3899	A3782	G3695	U
U4529	U4403	U4298	U	A3900	A3784	U3696	U
U4530	G4404	U4299	C	A3904	G3791	G3697	U
U4531	U4418	A4303	A	A3905	U3792	G3698	U
C4535	U4419	G4304	A	A3906	C3807	C3699	U
	C4420	U4305	U	G3907	G3808	G3709	U
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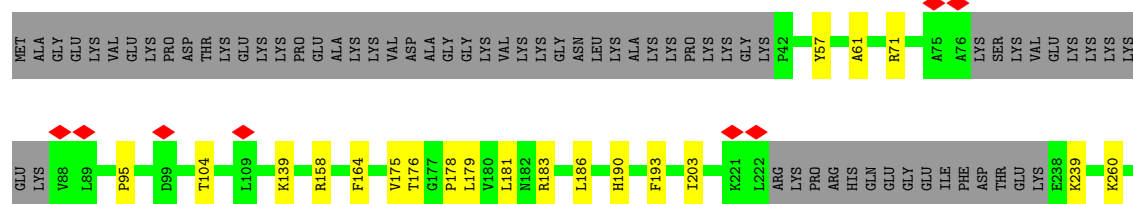
• Molecule 9: 60S ribosomal protein L4



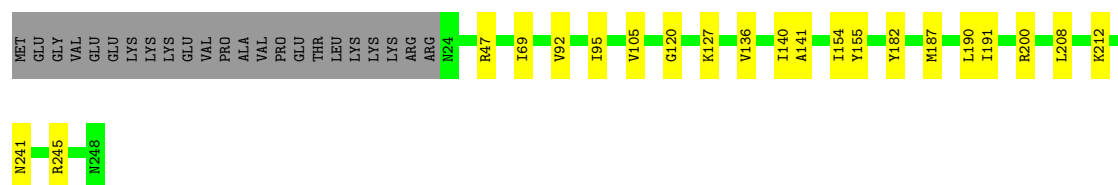
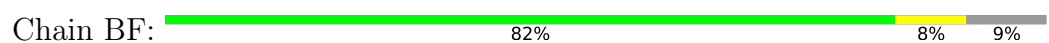
• Molecule 10: 60S ribosomal protein L5



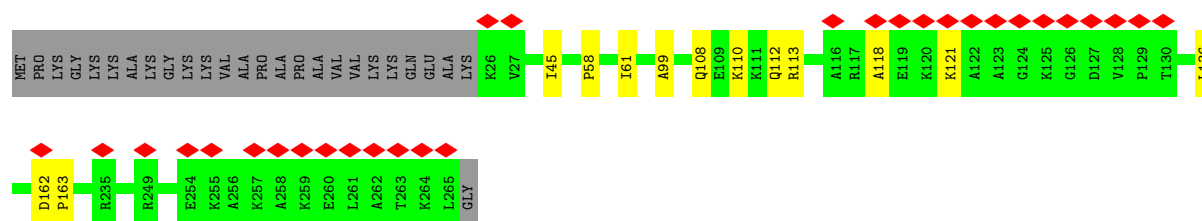
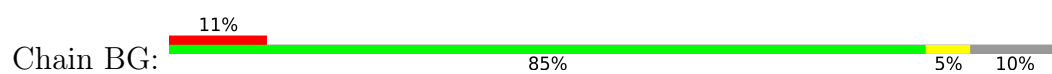
• Molecule 11: Large ribosomal subunit protein eL6



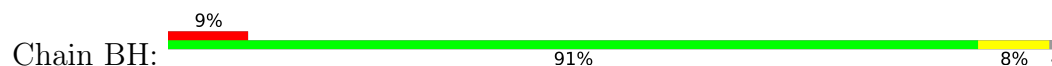
• Molecule 12: Large ribosomal subunit protein uL30



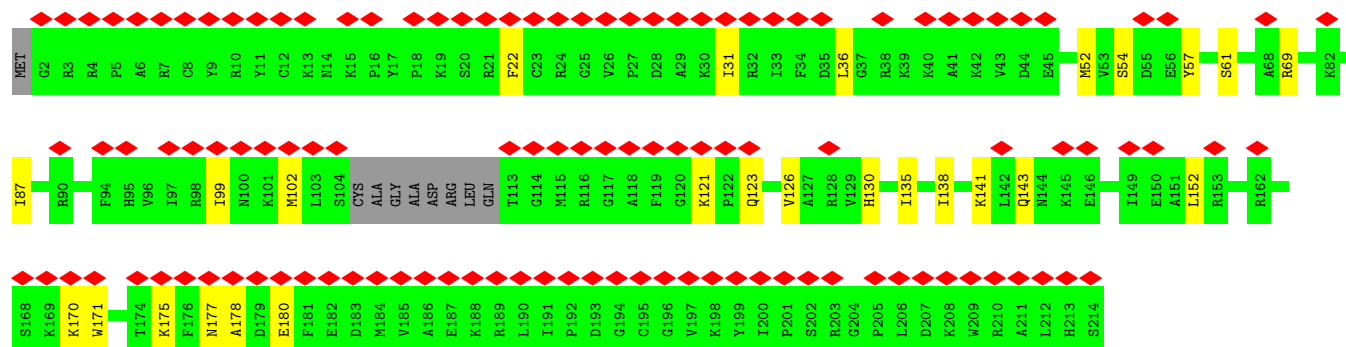
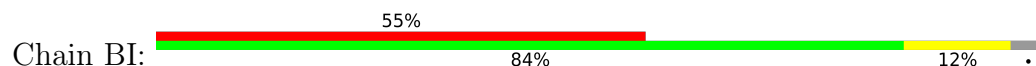
• Molecule 13: 60S ribosomal protein L7a



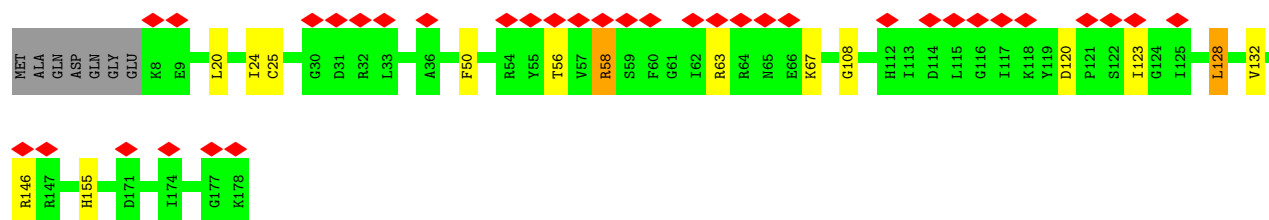
• Molecule 14: 60S ribosomal protein L9



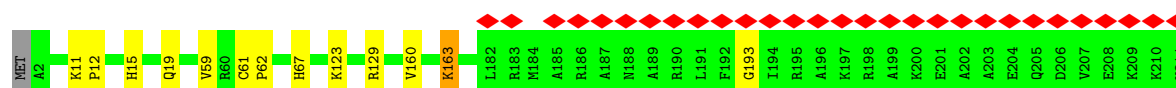
• Molecule 15: 60S ribosomal protein L10



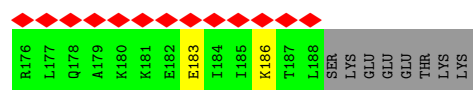
• Molecule 16: 60S ribosomal protein L11



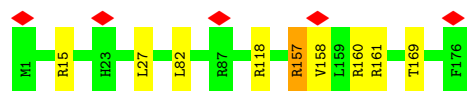
• Molecule 17: 60S ribosomal protein L13



- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| MET | S2 | M3 | L4 | L15 | K21 | T29 | K45 | R52 | V55 | A61 | R62 | G63 | M65 | T67 | L68 | A69 | R70 | R71 | K72 | G73 | R74 | H75 | M76 | K82 | L101 | L106 | K135 | D157 | Q158 | A159 | E160 | A161 | R162 | R163 | S164 | K165 | T166 | K167 | E168 | A169 | R170 | K171 | R172 | R173 | E174 |
|-----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|



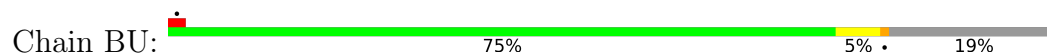
- Molecule 24: 60S ribosomal protein L18a



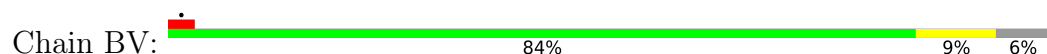
- Molecule 25: 60S ribosomal protein L21



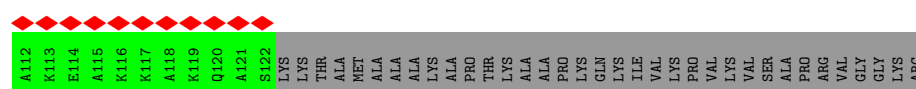
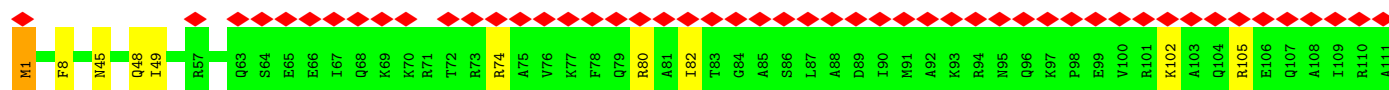
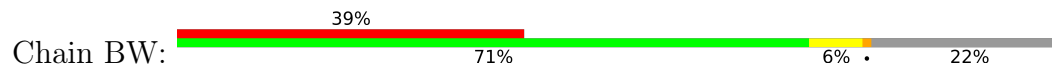
- Molecule 26: 60S ribosomal protein L22



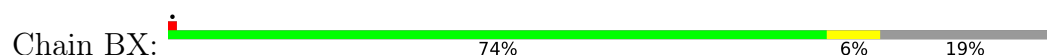
- Molecule 27: 60S ribosomal protein L23

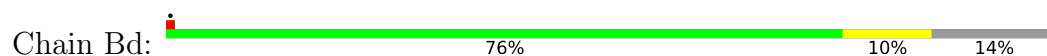


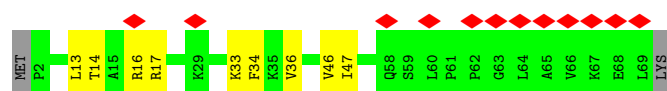
- Molecule 28: 60S ribosomal protein L24



- Molecule 29: 60S ribosomal protein L23a



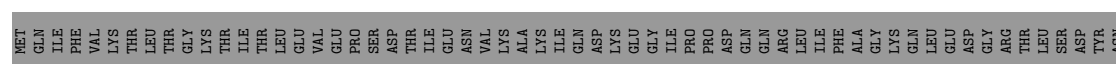


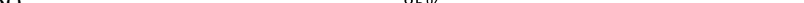


- Chain Bl: 88% 10%



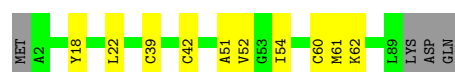
- Chain Bm: 



- Chain Bo:  34% 85% 11%

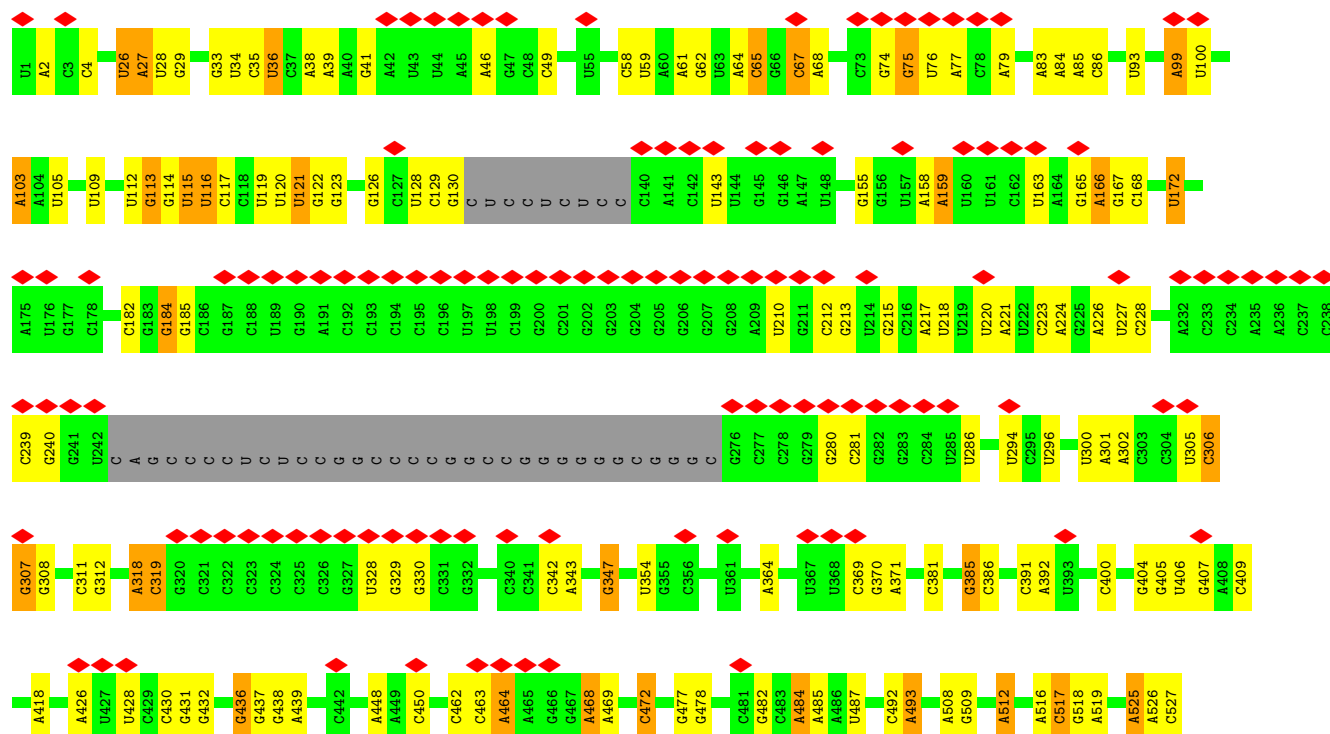


- Chain Bp: 85% 11% 4%

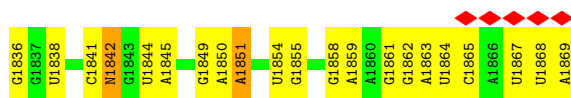


- Chain Br: 87% 9%

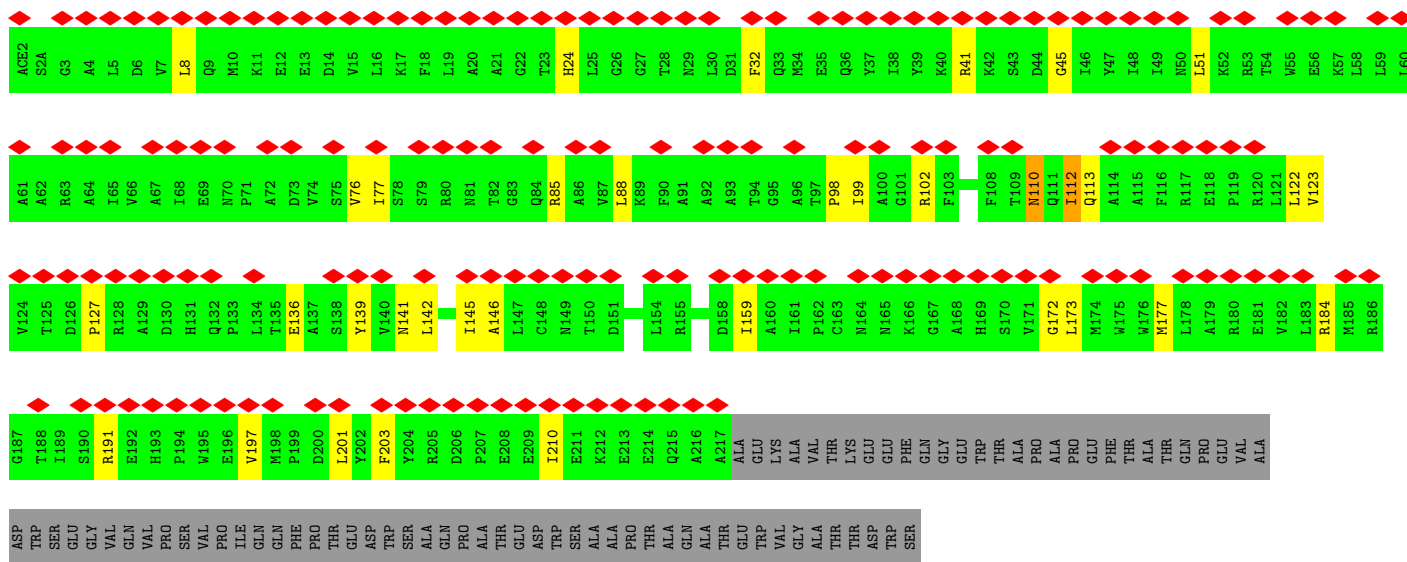




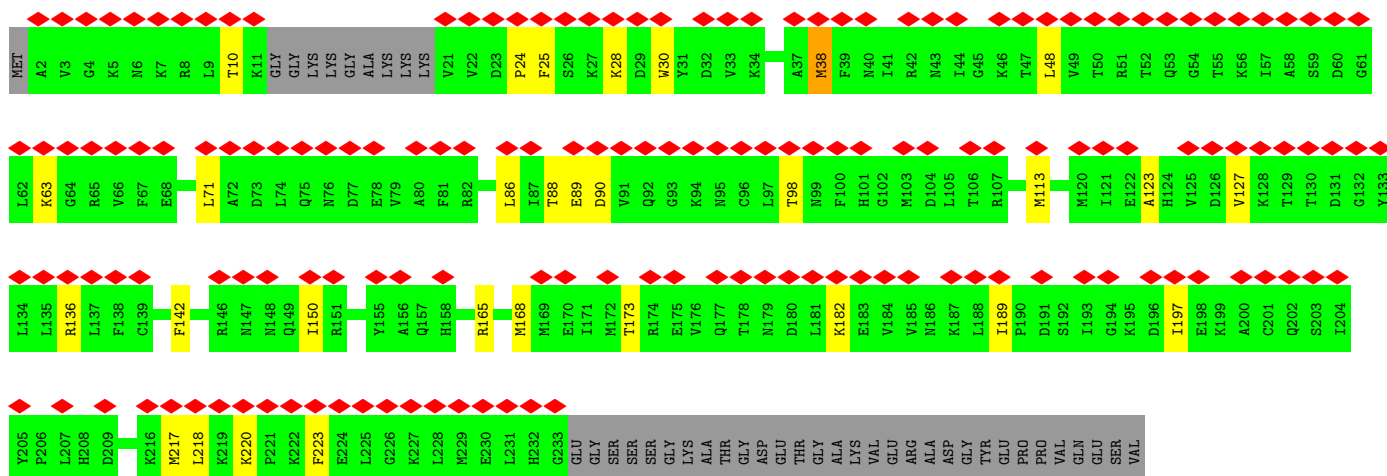
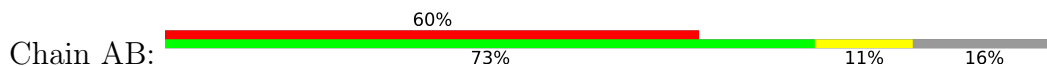




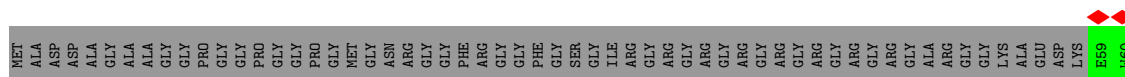
• Molecule 53: Small ribosomal subunit protein uS2

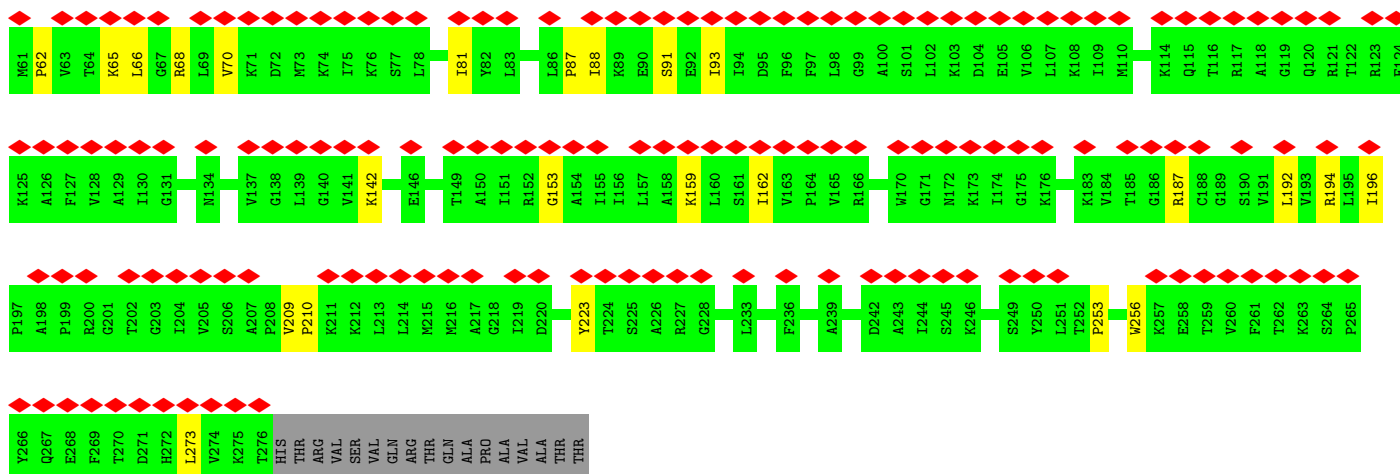


• Molecule 54: 40S ribosomal protein S3a

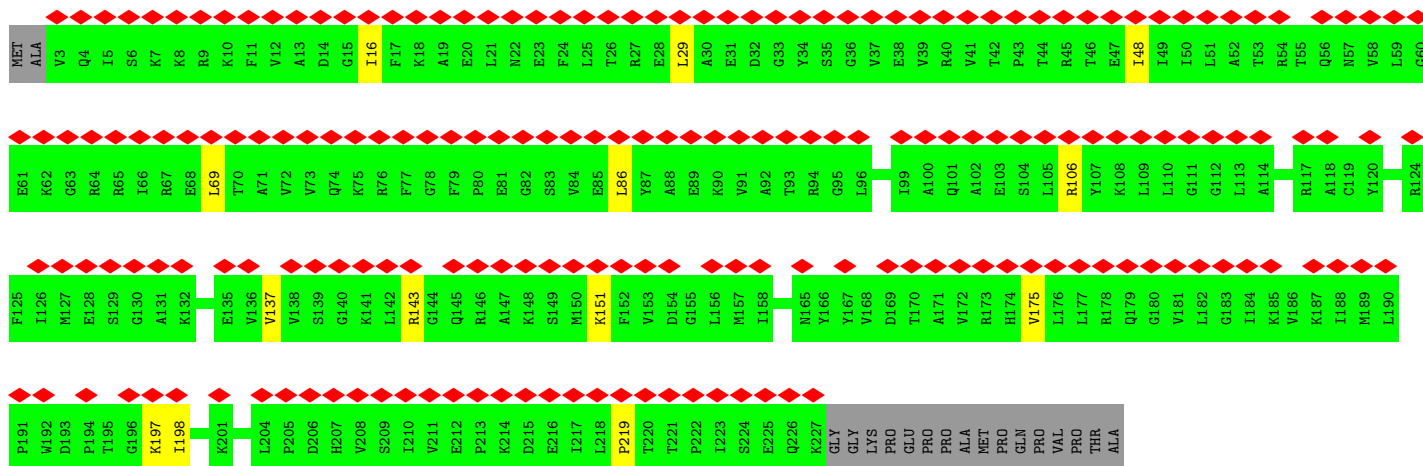
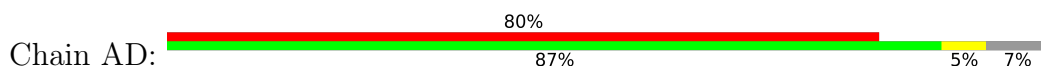


• Molecule 55: 40S ribosomal protein S2

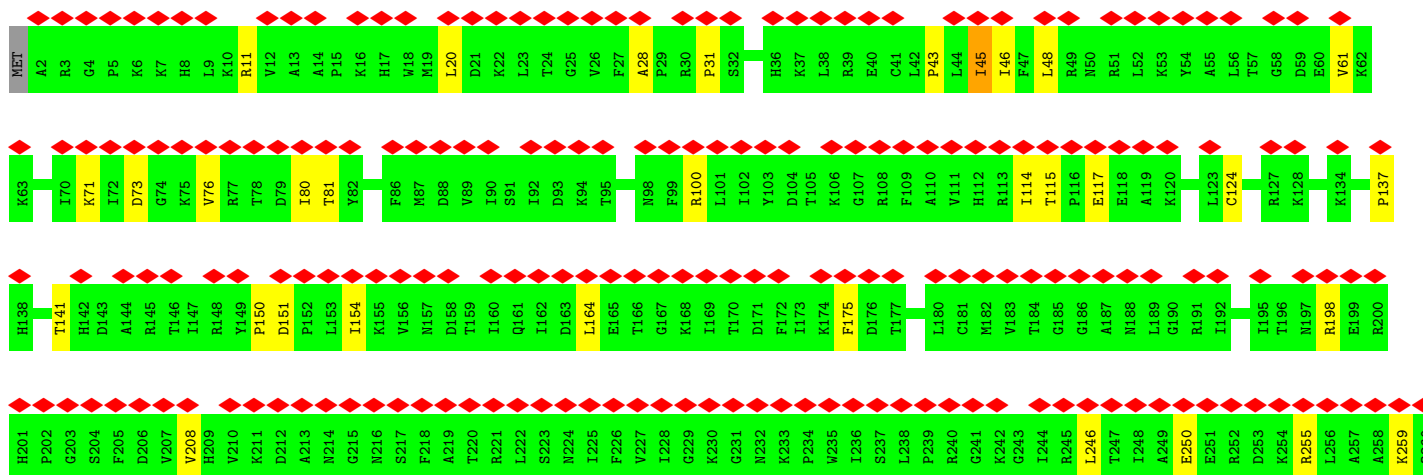
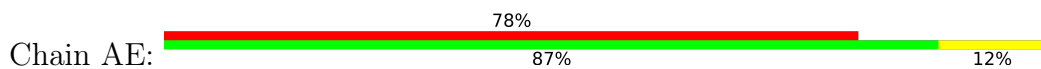




• Molecule 56: 40S ribosomal protein S3



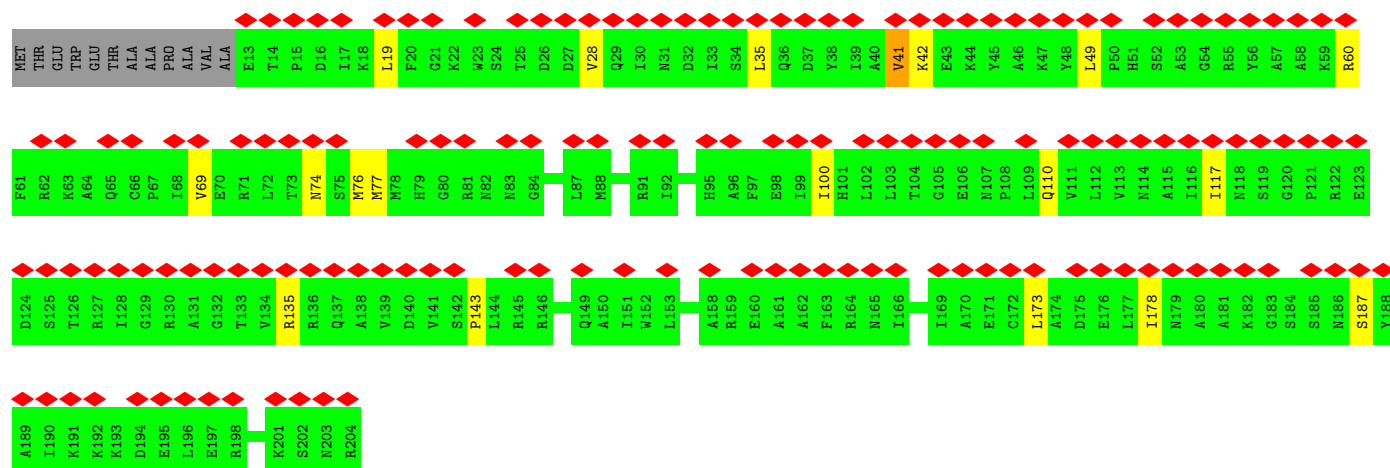
• Molecule 57: Small ribosomal subunit protein eS4, X isoform





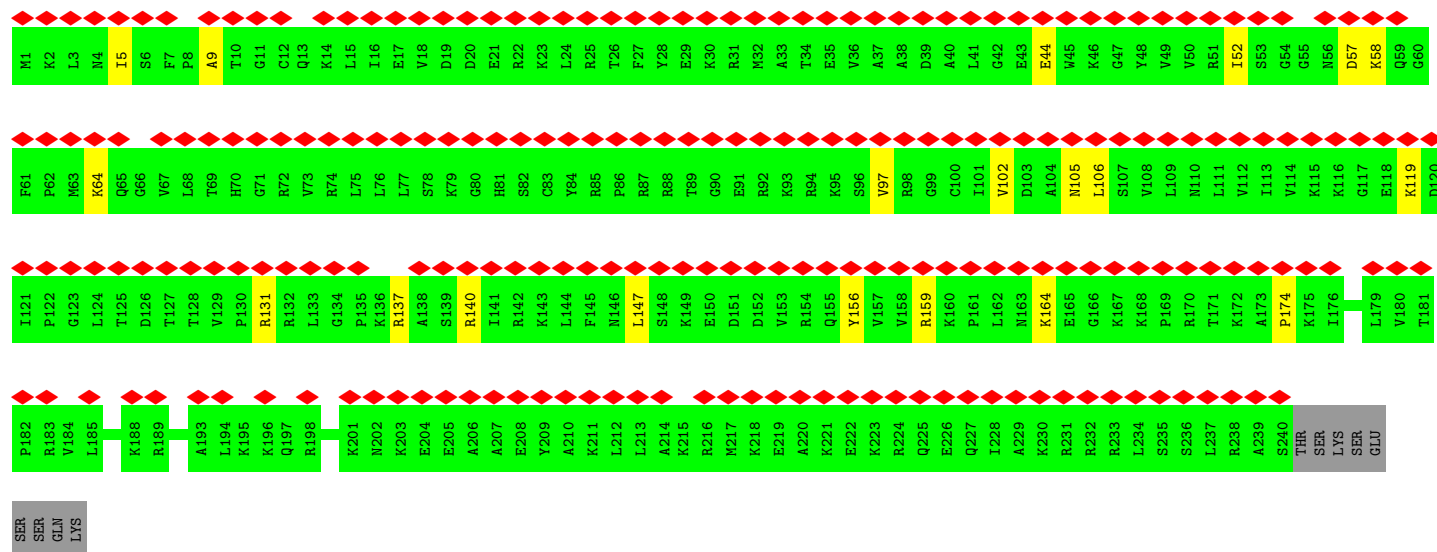
• Molecule 58: 40S ribosomal protein S5

Chain AF:



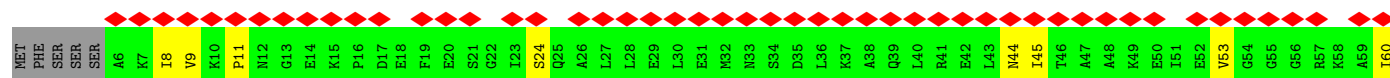
• Molecule 59: 40S ribosomal protein S6

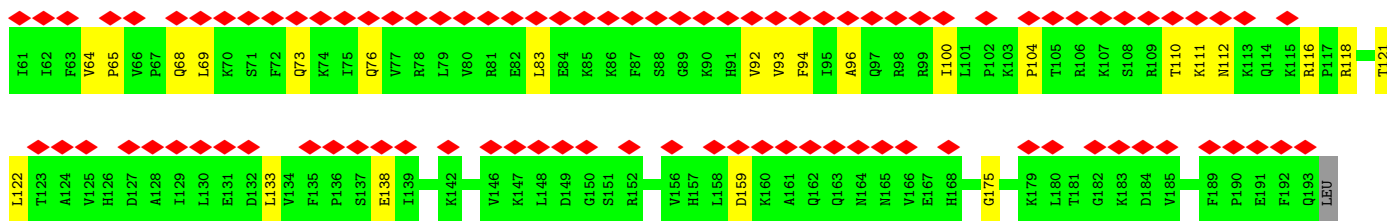
Chain AG:



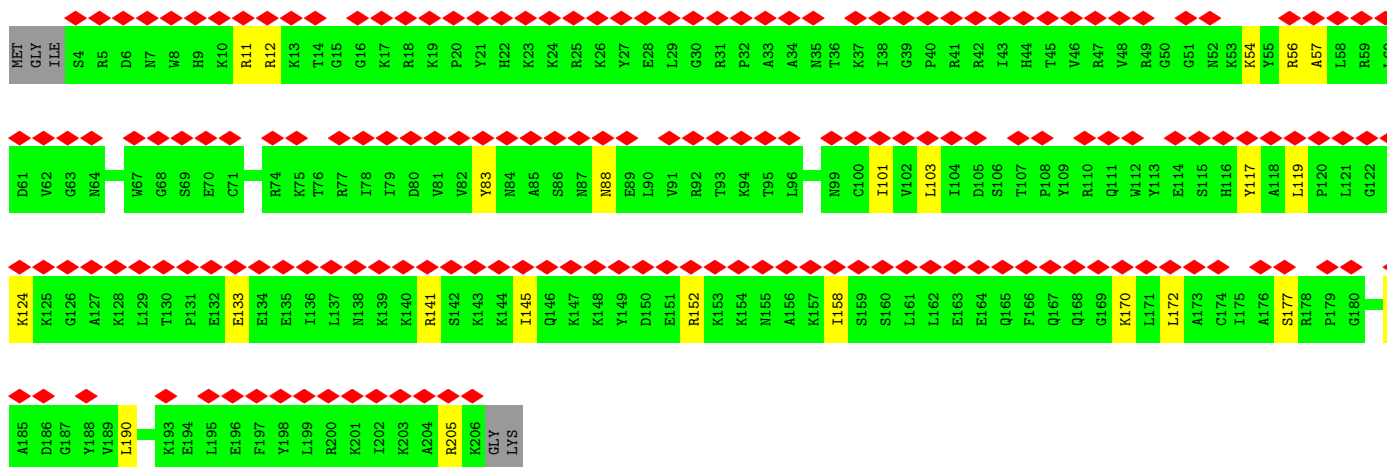
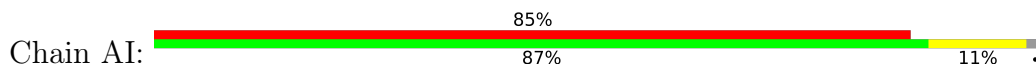
• Molecule 60: 40S ribosomal protein S7

Chain AH:

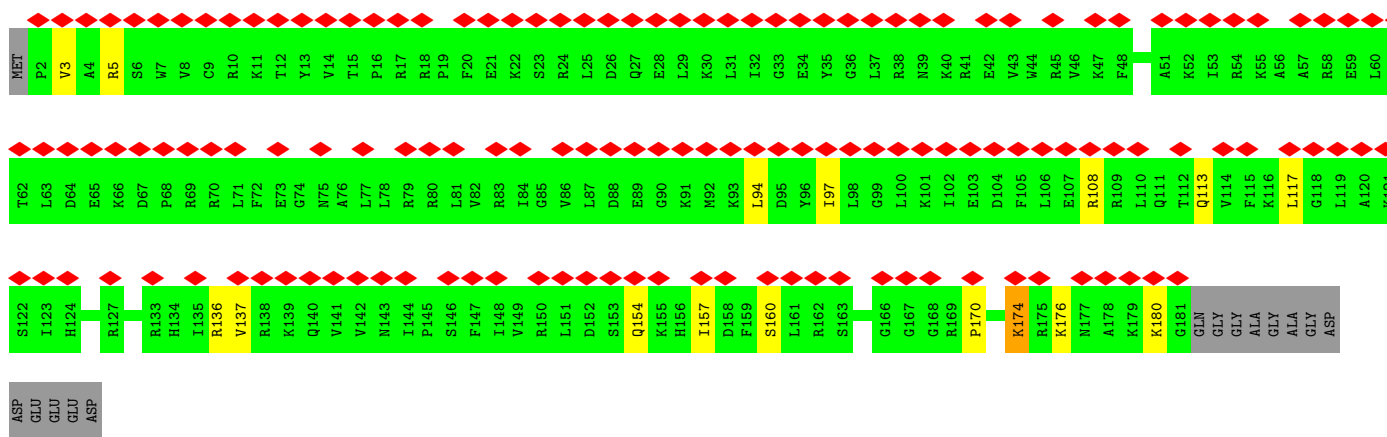
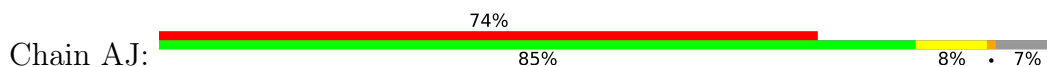




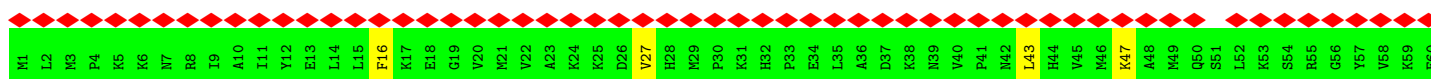
• Molecule 61: 40S ribosomal protein S8

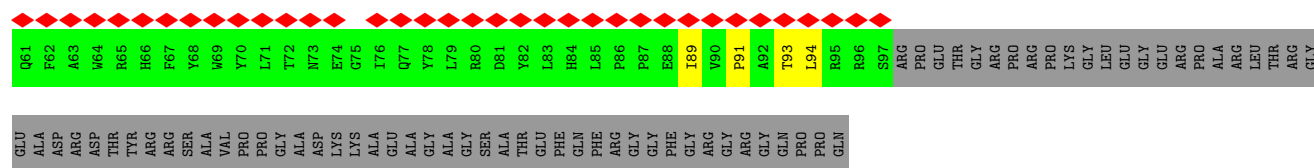


• Molecule 62: 40S ribosomal protein S9

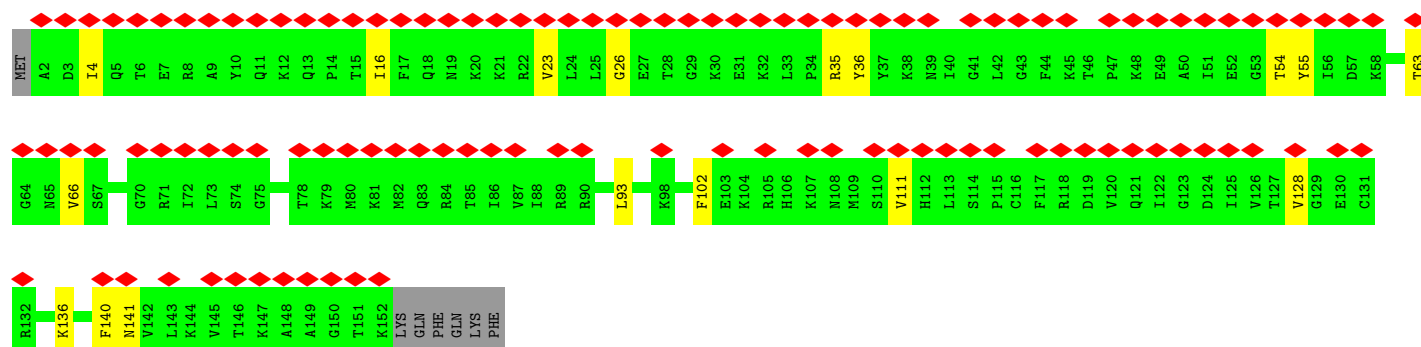
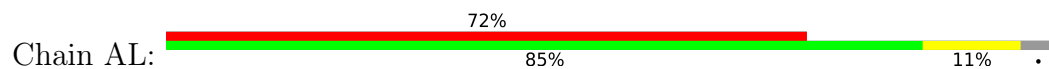


• Molecule 63: 40S ribosomal protein S10

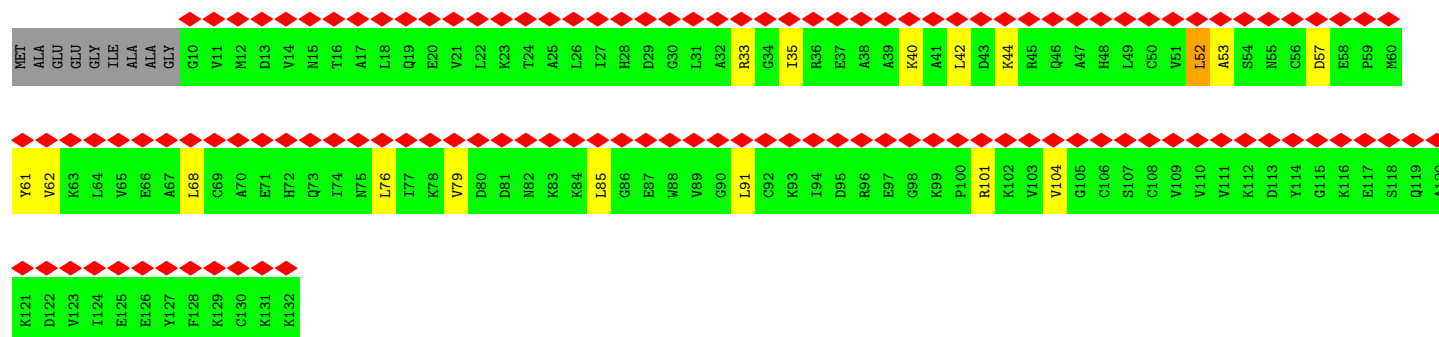
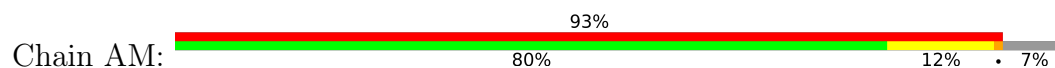




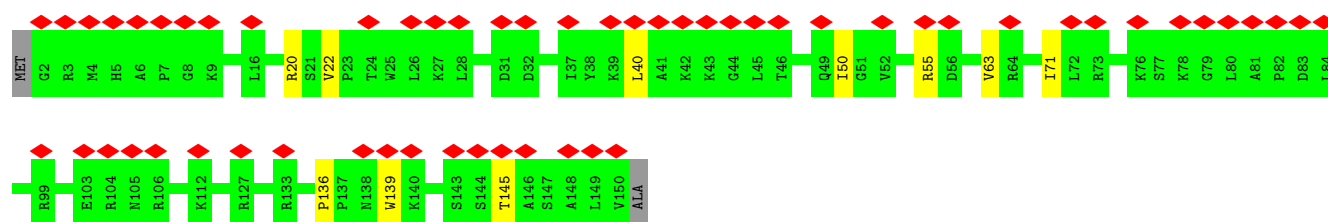
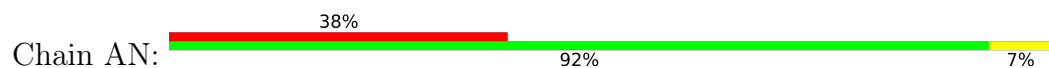
- Molecule 64: Small ribosomal subunit protein uS17



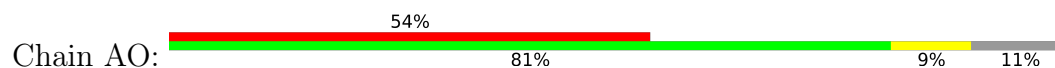
- Molecule 65: 40S ribosomal protein S12

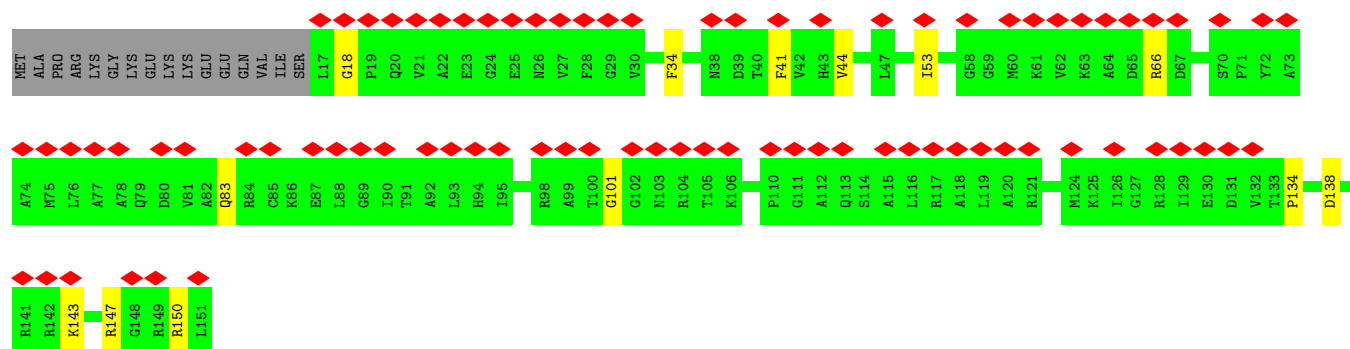


- Molecule 66: 40S ribosomal protein S13

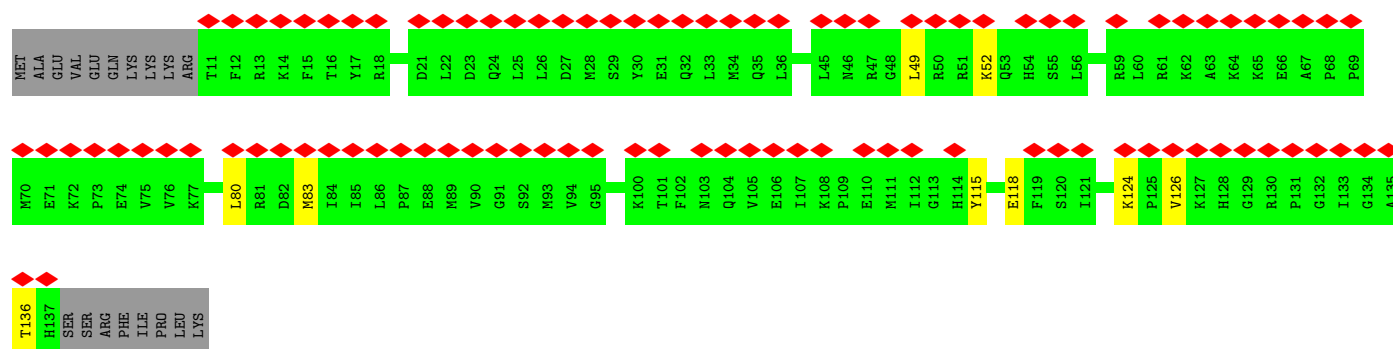
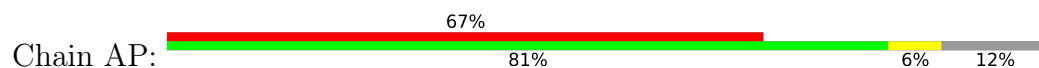


- Molecule 67: 40S ribosomal protein S14

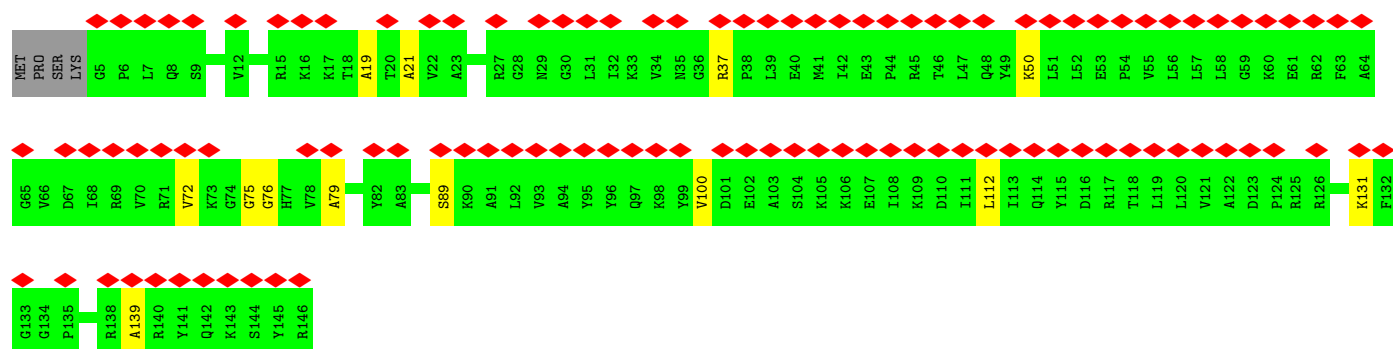
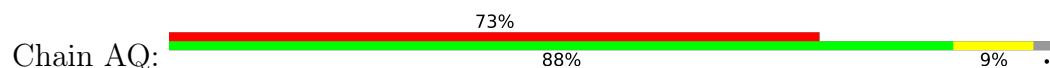




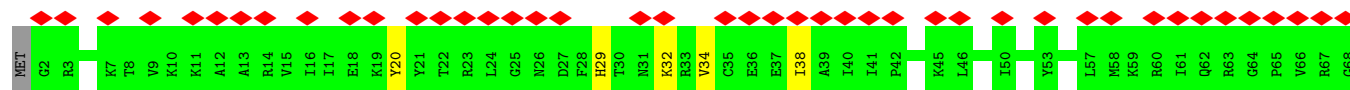
• Molecule 68: 40S ribosomal protein S15

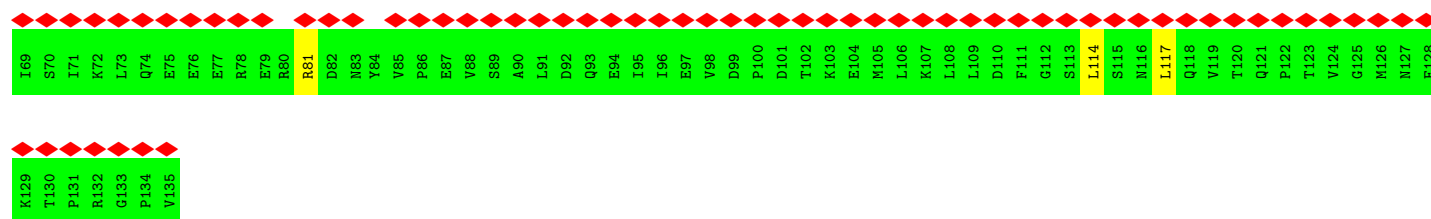


• Molecule 69: 40S ribosomal protein S16

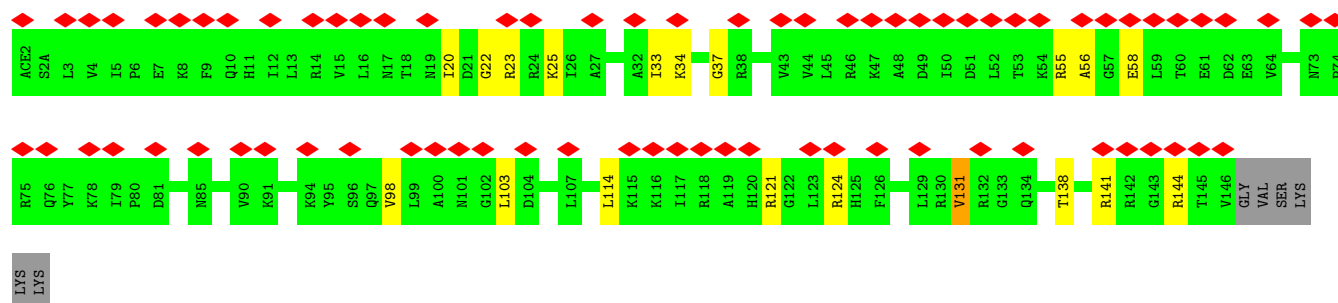
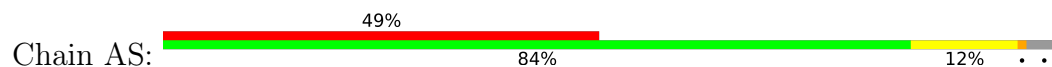


• Molecule 70: 40S ribosomal protein S17

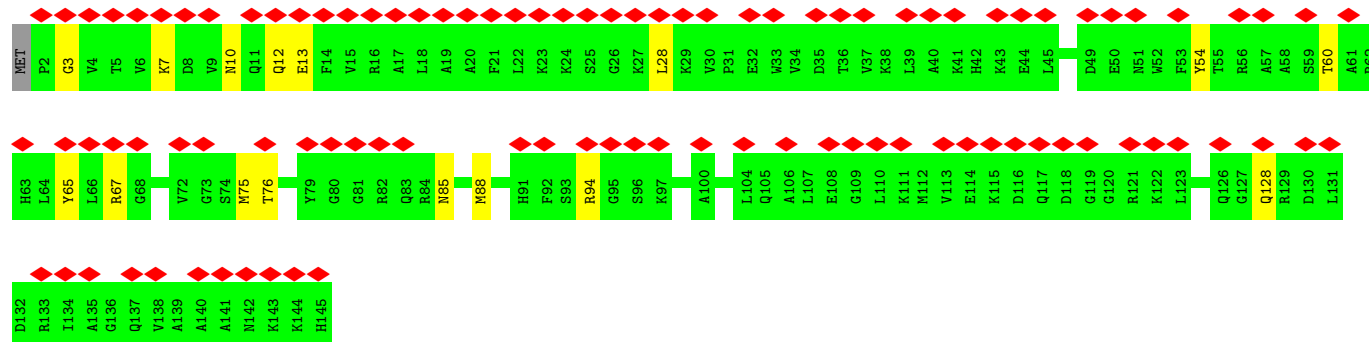
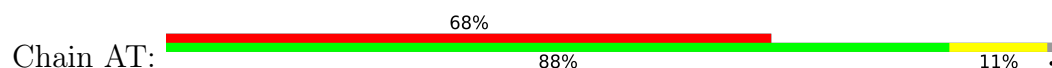




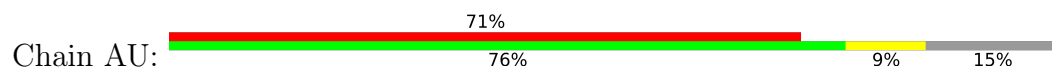
• Molecule 71: Small ribosomal subunit protein uS13



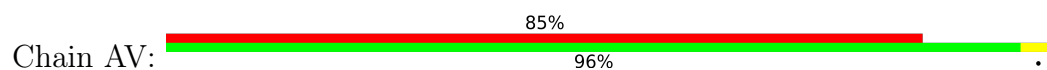
• Molecule 72: Small ribosomal subunit protein eS19

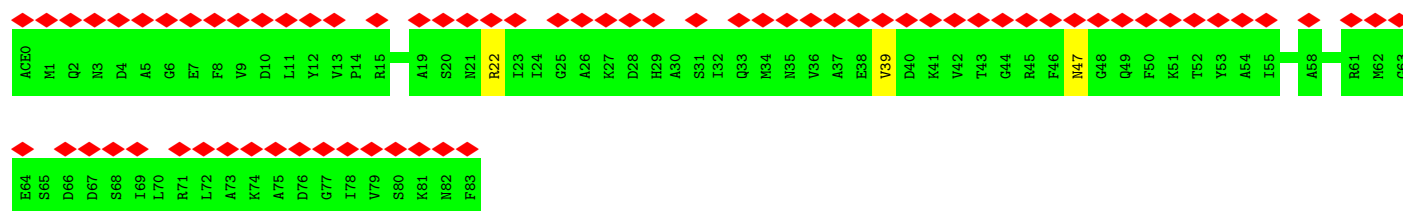


• Molecule 73: 40S ribosomal protein S20



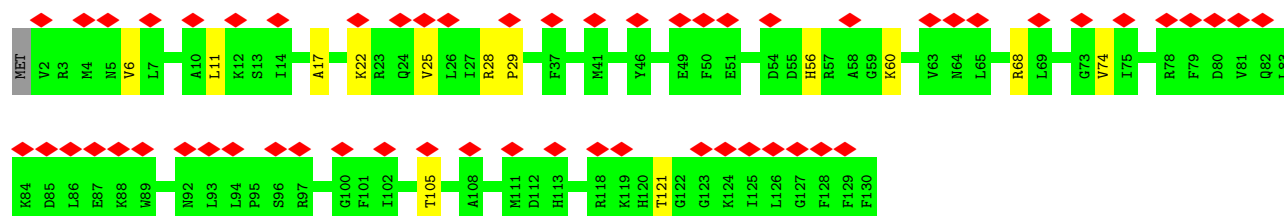
• Molecule 74: Small ribosomal subunit protein eS21





• Molecule 75: 40S ribosomal protein S15a

Chain AW: 44% 89% 10%



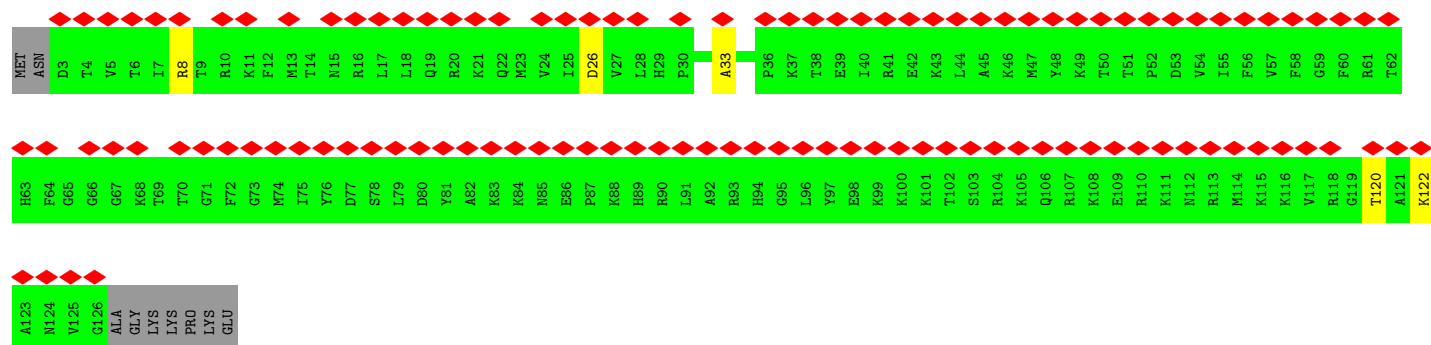
• Molecule 76: Small ribosomal subunit protein uS12

Chain AX: 87% 90% 9%

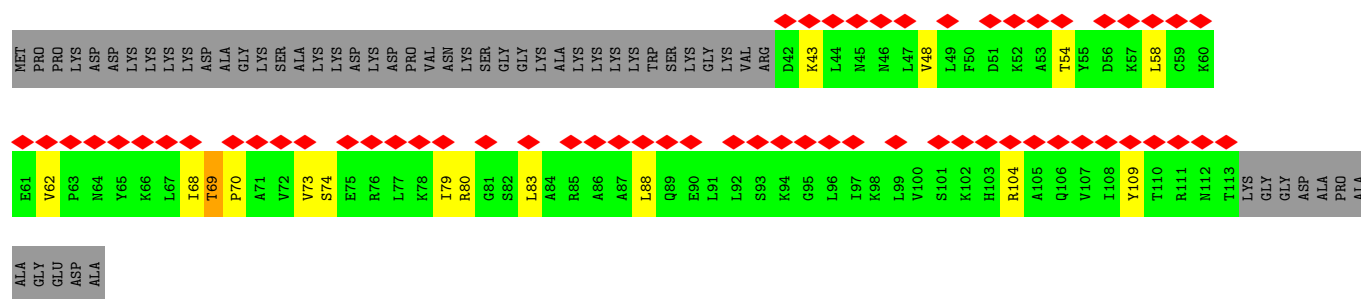


• Molecule 77: 40S ribosomal protein S24

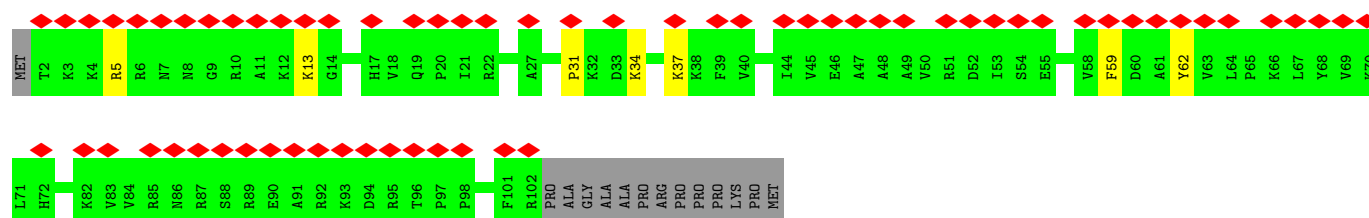
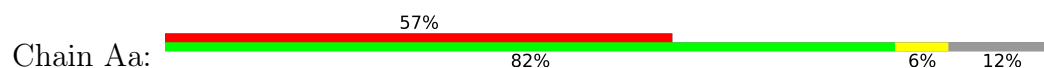
Chain AY: 84% 89% 7%



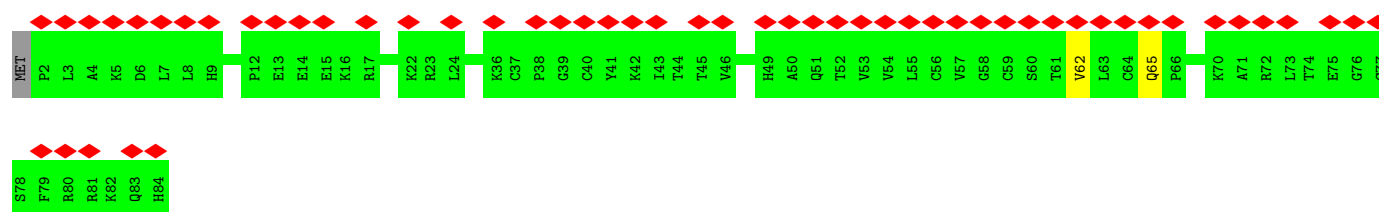
• Molecule 78: Small ribosomal subunit protein eS25



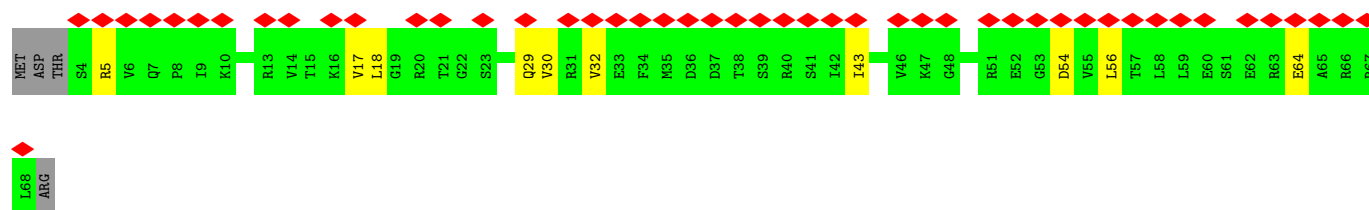
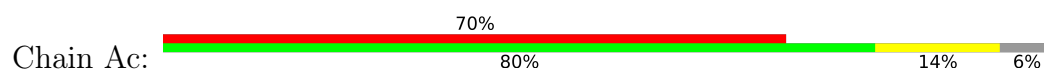
- Molecule 79: 40S ribosomal protein S26



- Molecule 80: 40S ribosomal protein S27

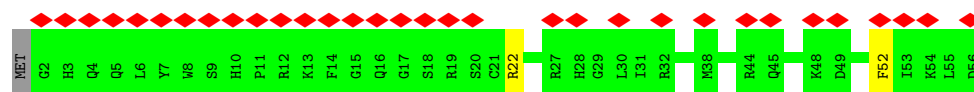


- Molecule 81: 40S ribosomal protein S28

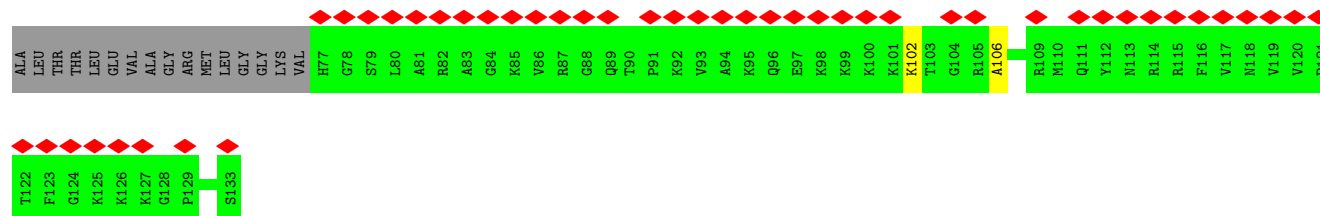
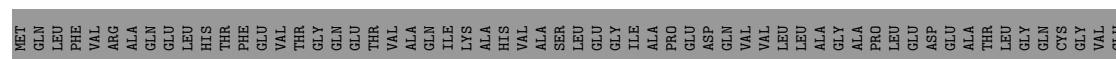
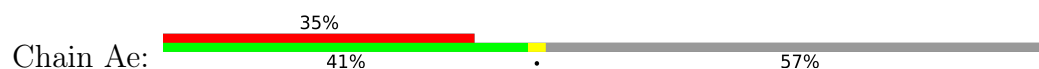


- Molecule 82: 40S ribosomal protein S29

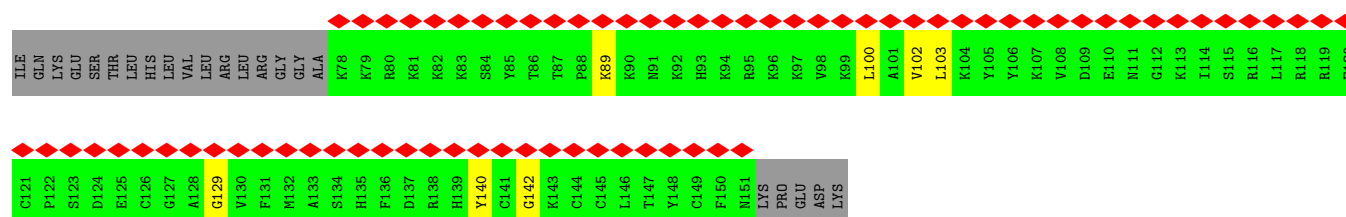
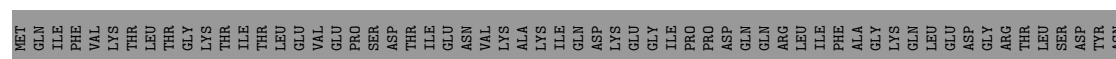




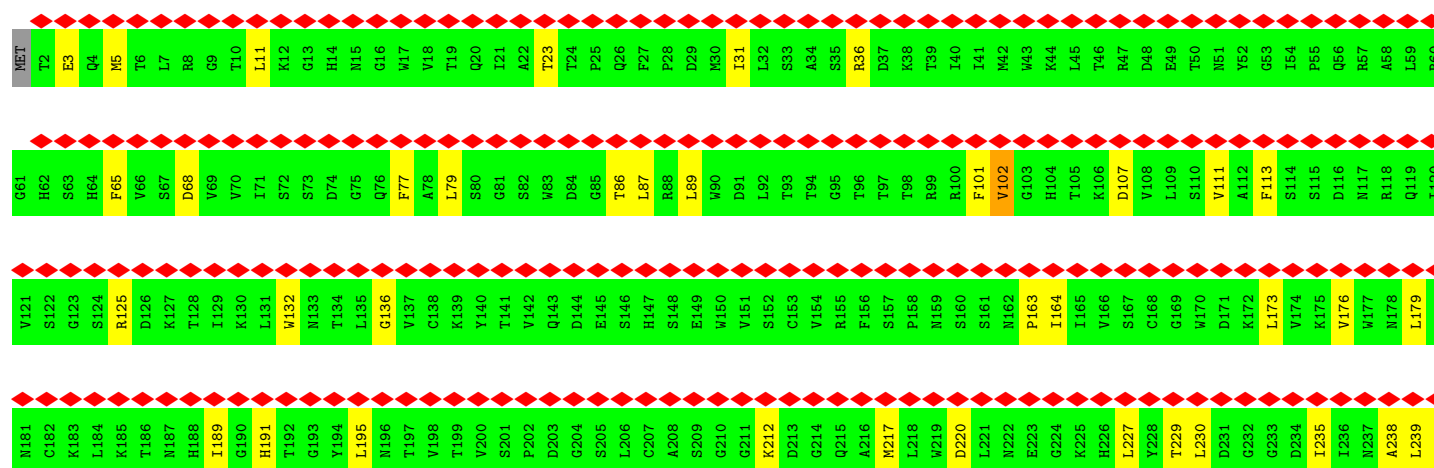
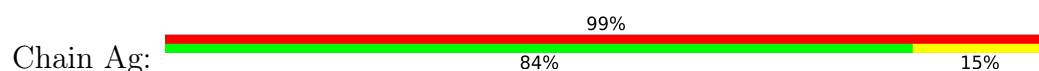
- Molecule 83: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein

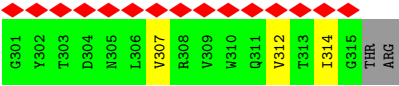
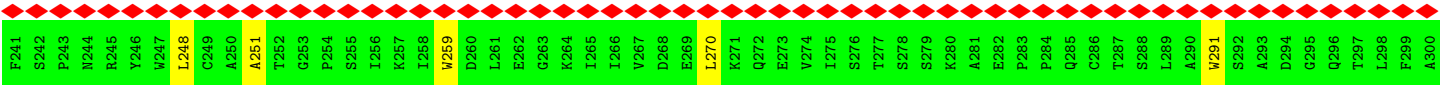


- Molecule 84: Ubiquitin

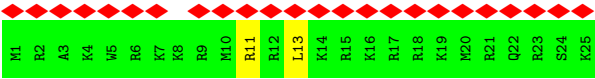
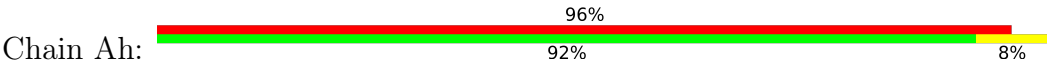


- Molecule 85: Receptor of activated protein C kinase 1





● Molecule 86: 60S ribosomal protein L41



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	104588	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.263	Depositor
Minimum map value	-0.461	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.149	Depositor
Map size (Å)	586.32, 586.32, 586.32	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.047, 1.047, 1.047	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, T6A, 5MC, IAS, ACE, MG, UR3, 5MU, A2M, OMC, B8N, HY3, NMM, UY1, MLZ, V5N, MA6, 4AC, G7M, PSU, GTP, 1MA, HIC, M2G, ZN, H2U, 6MZ, 2MG, 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	B1	0.10	0/295	0.25	0/403
2	B2	0.25	1/1434 (0.1%)	0.29	0/2232
3	B4	0.09	0/141	0.25	0/217
4	B5	0.14	0/84341	0.19	0/131575
5	B7	0.08	0/2835	0.16	0/4418
6	B8	0.14	0/3613	0.16	0/5627
7	BA	0.12	0/1924	0.24	0/2578
8	BB	0.11	0/3294	0.24	0/4406
9	BC	0.12	0/2973	0.23	0/3992
10	BD	0.08	0/2432	0.20	0/3256
11	BE	0.09	0/1807	0.22	0/2425
12	BF	0.11	0/1916	0.22	0/2553
13	BG	0.10	0/1960	0.23	0/2639
14	BH	0.07	0/1537	0.19	0/2066
15	BI	0.07	0/1698	0.20	0/2266
16	BJ	0.07	0/1394	0.19	0/1863
17	BL	0.11	0/1732	0.24	0/2315
18	BM	0.21	0/1142	0.30	0/1527
19	BN	0.12	0/1746	0.23	0/2338
20	BO	0.11	0/1682	0.23	0/2250
21	BP	0.10	0/1268	0.23	0/1701
22	BQ	0.11	0/1537	0.25	0/2052
23	BR	0.09	0/1582	0.18	0/2091
24	BS	0.09	0/1501	0.20	0/2013
25	BT	0.09	0/1326	0.19	0/1770
26	BU	0.08	0/865	0.22	0/1160
27	BV	0.11	0/993	0.24	0/1332
28	BW	0.08	0/1012	0.20	0/1342
29	BX	0.10	0/1050	0.21	0/1409
30	BY	0.10	0/1119	0.21	0/1488
31	BZ	0.09	0/1130	0.20	0/1507

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Ba	0.10	0/1179	0.24	0/1573
33	Bb	0.07	0/811	0.19	0/1070
34	Bc	0.09	0/835	0.22	0/1118
35	Bd	0.10	0/898	0.22	0/1210
36	Be	0.12	0/1071	0.22	0/1429
37	Bf	0.13	0/895	0.23	0/1198
38	Bg	0.10	0/878	0.22	0/1170
39	Bh	0.08	0/1023	0.18	0/1351
40	Bi	0.07	0/824	0.20	0/1090
41	Bj	0.11	0/720	0.26	0/952
42	Bk	0.06	0/565	0.17	0/750
43	Bl	0.10	0/465	0.19	0/614
44	Bm	0.06	0/425	0.20	0/564
45	Bo	0.08	0/848	0.21	0/1116
46	Bp	0.10	0/691	0.22	0/919
47	Br	0.12	0/1003	0.23	0/1346
48	Bs	0.07	0/1529	0.20	0/2063
49	Bt	0.08	0/1193	0.22	0/1609
50	Bu	0.07	0/527	0.22	0/703
51	Bv	0.10	0/854	0.29	0/1144
52	A2	0.14	4/40445 (0.0%)	0.16	0/63039
53	AA	0.08	0/1743	0.21	0/2369
54	AB	0.08	0/1832	0.21	0/2448
55	AC	0.08	0/1726	0.22	0/2332
56	AD	0.07	0/1780	0.20	0/2397
57	AE	0.08	0/2118	0.22	0/2849
58	AF	0.08	0/1539	0.24	0/2071
59	AG	0.07	0/1968	0.20	0/2619
60	AH	0.08	0/1538	0.22	0/2060
61	AI	0.08	0/1699	0.21	0/2266
62	AJ	0.06	0/1524	0.19	0/2035
63	AK	0.07	0/840	0.21	0/1133
64	AL	0.07	0/1250	0.20	0/1673
65	AM	0.09	0/963	0.27	0/1291
66	AN	0.07	0/1226	0.19	0/1649
67	AO	0.08	0/1014	0.21	0/1358
68	AP	0.07	0/1065	0.19	0/1424
69	AQ	0.08	0/1146	0.22	0/1534
70	AR	0.07	0/1097	0.20	0/1474
71	AS	0.09	0/1216	0.25	0/1630
72	AT	0.07	0/1130	0.20	0/1513
73	AU	0.07	0/813	0.21	0/1092
74	AV	0.08	0/644	0.19	0/862

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	AW	0.07	0/1051	0.20	0/1406
76	AX	0.08	0/1116	0.23	0/1486
77	AY	0.07	0/1031	0.20	0/1370
78	AZ	0.10	0/580	0.29	0/780
79	Aa	0.08	0/828	0.23	0/1109
80	Ab	0.07	0/664	0.21	0/891
81	Ac	0.06	0/514	0.17	0/688
82	Ad	0.07	0/469	0.20	0/623
83	Ae	0.07	0/457	0.20	0/602
84	Af	0.08	0/622	0.26	0/822
85	Ag	0.07	0/2497	0.23	0/3399
86	Ah	0.06	0/240	0.15	0/305
All	All	0.12	5/230898 (0.0%)	0.20	0/338399

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B2	37	T6A	O3'-P	5.11	1.61	1.56
52	A2	799	OMU	O3'-P	5.06	1.61	1.56
52	A2	512	A2M	O3'-P	5.04	1.61	1.56
52	A2	172	OMU	O3'-P	5.01	1.61	1.56
52	A2	484	A2M	O3'-P	5.01	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	B1	283	0	281	3	0
2	B2	1638	0	850	21	0
3	B4	127	0	64	0	0
4	B5	78039	0	39528	403	0
5	B7	2570	0	1295	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B8	3320	0	1686	12	0
7	BA	1899	0	1986	15	0
8	BB	3239	0	3376	29	0
9	BC	2919	0	3092	14	0
10	BD	2386	0	2421	14	0
11	BE	1773	0	1928	11	0
12	BF	1878	0	2009	14	0
13	BG	1927	0	2080	7	0
14	BH	1518	0	1601	8	0
15	BI	1660	0	1710	13	0
16	BJ	1371	0	1412	11	0
17	BL	1701	0	1818	11	0
18	BM	1120	0	1187	6	0
19	BN	1701	0	1749	14	0
20	BO	1650	0	1794	9	0
21	BP	1242	0	1267	9	0
22	BQ	1513	0	1628	8	0
23	BR	1566	0	1729	13	0
24	BS	1461	0	1502	5	0
25	BT	1298	0	1366	8	0
26	BU	851	0	877	4	0
27	BV	979	0	1039	10	0
28	BW	997	0	1053	8	0
29	BX	1031	0	1110	5	0
30	BY	1102	0	1189	7	0
31	BZ	1107	0	1182	7	0
32	Ba	1163	0	1206	9	0
33	Bb	809	0	875	4	0
34	Bc	824	0	874	8	0
35	Bd	883	0	923	8	0
36	Be	1053	0	1147	8	0
37	Bf	876	0	912	4	0
38	Bg	868	0	959	4	0
39	Bh	1015	0	1148	9	0
40	Bi	813	0	894	9	0
41	Bj	705	0	737	4	0
42	Bk	559	0	624	4	0
43	Bl	451	0	490	2	0
44	Bm	419	0	452	2	0
45	Bo	843	0	914	6	0
46	Bp	681	0	731	6	0
47	Br	990	0	1054	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	Bs	1506	0	1562	22	0
49	Bt	1178	0	1235	10	0
50	Bu	522	0	565	7	0
51	Bv	846	0	891	13	0
52	A2	38027	0	19276	230	0
53	AA	1708	0	1710	22	0
54	AB	1806	0	1895	19	0
55	AC	1690	0	1777	14	0
56	AD	1752	0	1848	7	0
57	AE	2076	0	2177	17	0
58	AF	1517	0	1569	11	0
59	AG	1945	0	2112	12	0
60	AH	1515	0	1611	19	0
61	AI	1670	0	1755	13	0
62	AJ	1499	0	1618	9	0
63	AK	816	0	841	3	0
64	AL	1229	0	1302	10	0
65	AM	953	0	990	11	0
66	AN	1202	0	1289	4	0
67	AO	1010	0	1033	9	0
68	AP	1044	0	1089	6	0
69	AQ	1128	0	1195	9	0
70	AR	1082	0	1137	5	0
71	AS	1200	0	1262	10	0
72	AT	1123	0	1152	11	0
73	AU	803	0	873	6	0
74	AV	639	0	638	1	0
75	AW	1034	0	1080	6	0
76	AX	1105	0	1175	6	0
77	AY	1014	0	1082	4	0
78	AZ	574	0	627	11	0
79	Aa	814	0	863	5	0
80	Ab	650	0	672	1	0
81	Ac	512	0	541	6	0
82	Ad	458	0	448	2	0
83	Ae	451	0	494	1	0
84	Af	610	0	634	8	0
85	Ag	2440	0	2396	26	0
86	Ah	239	0	289	2	0
87	A2	123	0	0	0	0
87	AI	1	0	0	0	0
87	AX	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	B5	285	0	0	0	0
87	B7	4	0	0	0	0
87	B8	6	0	0	0	0
87	BA	3	0	0	0	0
87	BB	1	0	0	0	0
87	BN	1	0	0	0	0
87	BV	1	0	0	0	0
87	Ba	1	0	0	0	0
87	Be	1	0	0	0	0
87	Bf	2	0	0	0	0
87	Bg	1	0	0	0	0
87	Bj	1	0	0	0	0
88	Aa	1	0	0	0	0
88	Ad	1	0	0	0	0
88	Af	1	0	0	0	0
88	Bg	1	0	0	0	0
88	Bj	1	0	0	0	0
88	Bm	1	0	0	0	0
88	Bo	1	0	0	0	0
88	Bp	1	0	0	0	0
All	All	220645	0	164452	1202	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 3.

All (1202) 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)
18:BM:128:LYS:O	18:BM:132:LYS:HG3	1.44	1.18
5:B7:72:U:H3	5:B7:103:A:H61	1.15	0.94
4:B5:1858:C:H42	4:B5:1874:C:H42	1.32	0.77
16:BJ:56:THR:HG22	16:BJ:58:ARG:HH12	1.50	0.77
52:A2:84:A:H5''	77:AY:122:LYS:HD2	1.66	0.76
4:B5:733:A:H62	4:B5:929:G:H21	1.34	0.74
4:B5:2574:U:H5''	4:B5:2575:G:H5'	1.68	0.73
4:B5:2646:A:H62	4:B5:2685:G:H21	1.33	0.73
4:B5:4870:C:H5'	4:B5:4871:G:H4'	1.72	0.72
4:B5:3757:U:H3	4:B5:3765:A:H61	1.39	0.70
51:Bv:105:GLU:HB2	51:Bv:117:HIS:HE1	1.57	0.69
8:BB:291:TYR:HB3	8:BB:298:LEU:HD11	1.74	0.69
50:Bu:95:THR:HG21	51:Bv:153:GLN:HB3	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B5:1474:G:H22	4:B5:1488:G:H1	1.40	0.69
4:B5:3807:OMC:HM22	4:B5:3808:G:H5'	1.75	0.69
4:B5:1358:G:H5'	9:BC:114:ARG:HD2	1.75	0.69
4:B5:4570:A2M:HM'2	4:B5:4571:U:H5'	1.75	0.69
62:AJ:108:ARG:HA	62:AJ:113:GLN:HE21	1.58	0.68
13:BG:58:PRO:HD2	13:BG:61:ILE:HD12	1.74	0.68
4:B5:1212:G:H4'	4:B5:1213:C:H2'	1.75	0.68
53:AA:184:ARG:HD2	53:AA:191:ARG:HG2	1.76	0.68
4:B5:1760:G:H1	4:B5:1770:U:H3	1.42	0.68
52:A2:38:A:H5''	62:AJ:5:ARG:HB3	1.76	0.67
52:A2:1743:G:H21	52:A2:1791:A:H62	1.42	0.67
4:B5:388:A:H62	4:B5:412:G:H22	1.42	0.67
60:AH:69:LEU:HD22	60:AH:96:ALA:HB2	1.77	0.66
85:Ag:87:LEU:HB2	85:Ag:101:PHE:HB2	1.77	0.66
16:BJ:56:THR:HG23	16:BJ:63:ARG:HA	1.78	0.66
4:B5:1869:C:H2'	4:B5:1870:A2M:H8	1.78	0.66
52:A2:1137:U:H3	52:A2:1148:A:H62	1.42	0.66
60:AH:93:VAL:HG11	60:AH:133:LEU:HD12	1.78	0.66
67:AO:83:GLN:HB2	81:Ac:5:ARG:HH21	1.59	0.66
4:B5:2361:U:H2'	4:B5:2362:A2M:H8	1.78	0.65
52:A2:165:G:H2'	52:A2:166:A2M:H8	1.79	0.65
57:AE:11:ARG:HA	57:AE:28:ALA:HB2	1.79	0.65
18:BM:128:LYS:O	18:BM:132:LYS:CG	2.35	0.64
50:Bu:98:LYS:HB3	50:Bu:102:ILE:HB	1.77	0.64
2:B2:36:U:H2'	2:B2:37:T6A:C8	2.32	0.64
48:Bs:65:ILE:HG23	48:Bs:75:LEU:HB3	1.78	0.64
26:BU:39:PHE:HZ	26:BU:87:THR:HG22	1.63	0.64
52:A2:217:A:H2	52:A2:306:C:H42	1.46	0.64
4:B5:2612:C:H42	4:B5:2723:G:H1	1.46	0.64
4:B5:2860:OMC:HM22	4:B5:2861:G:H5'	1.80	0.64
62:AJ:170:PRO:HB3	62:AJ:174:LYS:HE3	1.80	0.63
12:BF:105:VAL:HG13	12:BF:136:VAL:HG12	1.80	0.63
33:Bb:8:THR:HG22	33:Bb:10:HIS:H	1.63	0.63
54:AB:28:LYS:HB3	54:AB:48:LEU:HD11	1.80	0.63
52:A2:1490:OMG:HM22	52:A2:1491:G:H5'	1.81	0.63
4:B5:1459:C:H5''	22:BQ:144:LYS:HG2	1.80	0.63
4:B5:4522:A2M:H5''	4:B5:4523:G:H5'	1.81	0.63
52:A2:1030:A:H2'	52:A2:1031:A2M:H8	1.80	0.63
60:AH:83:LEU:HD23	60:AH:92:VAL:HG11	1.80	0.63
27:BV:35:LYS:HB2	27:BV:67:LYS:HG3	1.80	0.62
52:A2:166:A2M:HM'2	52:A2:167:G:H5'	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:A2:1650:A:H5''	69:AQ:139:ALA:HB2	1.80	0.62
52:A2:1758:G:H2'	52:A2:1759:G:H8	1.64	0.62
52:A2:1831:A:H2'	52:A2:1832:6MZ:H8	1.81	0.62
53:AA:110:ASN:HD21	53:AA:112:ILE:HG12	1.65	0.62
23:BR:173:ARG:HH22	52:A2:911:C:H41	1.47	0.62
57:AE:31:PRO:HG3	57:AE:43:PRO:HG3	1.82	0.62
85:Ag:68:ASP:HB3	85:Ag:111:VAL:HG22	1.80	0.62
52:A2:560:A:H5'	62:AJ:174:LYS:HG3	1.81	0.62
4:B5:1984:G:H1'	4:B5:2002:G:H2'	1.81	0.62
10:BD:223:PHE:HB3	10:BD:226:TYR:HB2	1.81	0.62
67:AO:101:GLY:HA3	67:AO:134:PRO:HG2	1.82	0.62
21:BP:57:CYS:HB2	21:BP:72:GLN:HB2	1.81	0.62
8:BB:165:HIS:HB3	8:BB:180:LEU:HD23	1.82	0.61
20:BO:130:LYS:HB2	20:BO:133:ARG:HG2	1.81	0.61
52:A2:1350:U:H3	52:A2:1379:A:H61	1.49	0.61
52:A2:1703:OMC:HM22	52:A2:1704:C:H5'	1.81	0.61
67:AO:34:PHE:HB3	67:AO:41:PHE:HB2	1.82	0.61
4:B5:696:C:H5'	4:B5:697:G:H5'	1.83	0.61
48:Bs:13:TYR:HA	48:Bs:16:LYS:HE2	1.82	0.61
78:AZ:58:LEU:HD12	78:AZ:62:VAL:HG21	1.82	0.61
78:AZ:73:VAL:HG21	78:AZ:88:LEU:HD21	1.84	0.60
52:A2:1656:G:H1	52:A2:1668:U:H3	1.46	0.60
9:BC:159:GLU:HA	9:BC:217:ILE:HB	1.83	0.60
85:Ag:173:LEU:HD22	85:Ag:189:ILE:HG12	1.84	0.60
52:A2:868:G:H22	60:AH:118:ARG:HH21	1.50	0.60
15:BI:99:ILE:HD11	15:BI:102:MET:HG3	1.81	0.60
4:B5:173:C:H5''	17:BL:129:ARG:HH12	1.65	0.60
51:Bv:126:SER:HB3	51:Bv:131:THR:HB	1.84	0.60
4:B5:74:G:H5''	17:BL:59:VAL:HB	1.83	0.60
56:AD:197:LYS:HG2	56:AD:198:ILE:HG23	1.83	0.59
4:B5:5023:C:H4'	61:AI:124:LYS:HE2	1.83	0.59
14:BH:48:LEU:HD11	14:BH:56:ARG:HH11	1.66	0.59
52:A2:74:G:H5''	52:A2:75:G:H5'	1.83	0.59
29:BX:89:LYS:HD3	29:BX:93:ASN:HD22	1.67	0.59
4:B5:4204:A:H61	4:B5:4226:OMU:HN3	1.51	0.59
4:B5:3717:A2M:HM'2	4:B5:3718:A:H5'	1.84	0.59
61:AI:101:ILE:HD12	61:AI:190:LEU:HD11	1.85	0.59
9:BC:221:PHE:HB3	9:BC:227:ILE:HG21	1.83	0.59
65:AM:44:LYS:HE2	84:Af:129:GLY:H	1.68	0.59
4:B5:2814:A2M:H5'	4:B5:2814:A2M:H8	1.84	0.59
15:BI:54:SER:HB2	15:BI:135:ILE:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:A2:1391:OMC:HM22	52:A2:1392:U:H5'	1.84	0.59
4:B5:3696:U:H5''	4:B5:3697:G:H5'	1.83	0.58
4:B5:3738:C:H2'	4:B5:3739:G:H8	1.69	0.58
52:A2:858:A:H2'	52:A2:859:G:H8	1.68	0.58
55:AC:70:VAL:HG21	55:AC:93:ILE:HG23	1.85	0.58
4:B5:1315:OMG:HM22	4:B5:1316:U:H5'	1.85	0.58
48:Bs:40:MET:HE1	48:Bs:187:LEU:HD11	1.85	0.58
52:A2:525:A:H2'	52:A2:526:A:H8	1.68	0.58
4:B5:2015:C:H2'	4:B5:2016:A:H8	1.67	0.58
61:AI:172:LEU:HB3	61:AI:190:LEU:HD12	1.85	0.58
73:AU:20:ILE:HG12	73:AU:116:ILE:HG12	1.86	0.58
56:AD:106:ARG:HG3	56:AD:175:VAL:HG22	1.85	0.58
4:B5:2473:G:H1	4:B5:2502:G:H5'	1.69	0.58
4:B5:1418:G:H21	4:B5:1419:A:H62	1.52	0.58
4:B5:2553:U:H1'	4:B5:2573:G:H22	1.69	0.57
27:BV:13:LYS:HB2	27:BV:128:LEU:HD21	1.86	0.57
51:Bv:99:ASN:HA	51:Bv:124:GLN:HA	1.85	0.57
69:AQ:89:SER:HB3	69:AQ:112:LEU:HD13	1.86	0.57
52:A2:536:A:H2	52:A2:548:C:H41	1.51	0.57
4:B5:4254:A:H2'	4:B5:4255:A:H8	1.70	0.57
19:BN:138:PHE:HA	19:BN:143:ARG:HE	1.69	0.57
4:B5:1972:G:H1	4:B5:1992:C:H42	1.51	0.57
4:B5:3753:G:H1	4:B5:3769:PSU:HN3	1.52	0.57
57:AE:255:ARG:HG2	57:AE:259:LYS:HE3	1.86	0.57
4:B5:739:G:H2'	4:B5:740:G:H8	1.69	0.57
41:Bj:2:THR:HG22	41:Bj:4:GLY:H	1.70	0.57
39:Bh:73:TYR:HB3	39:Bh:79:LYS:HG2	1.87	0.57
4:B5:1749:G:H2'	4:B5:1750:A:H8	1.70	0.57
27:BV:92:ASP:HB2	28:BW:1:MET:HE2	1.87	0.57
52:A2:62:G:H1'	52:A2:172:OMU:HM23	1.87	0.57
5:B7:2:U:H3	5:B7:117:G:H1	1.53	0.57
5:B7:72:U:H3	5:B7:103:A:N6	1.95	0.57
4:B5:912:U:H1'	4:B5:913:U:H5	1.70	0.56
4:B5:3950:G:H22	4:B5:4060:G:H1	1.53	0.56
7:BA:101:VAL:HG22	7:BA:165:VAL:HG22	1.85	0.56
26:BU:22:THR:HG23	26:BU:109:SER:HB3	1.87	0.56
2:B2:34:OMC:HM22	2:B2:35:A:H5'	1.87	0.56
4:B5:1870:A2M:HM'2	4:B5:1871:G:H5'	1.87	0.56
4:B5:1968:G:H4'	48:Bs:36:GLY:HA2	1.85	0.56
4:B5:4248:G:H2'	4:B5:4249:G:H8	1.70	0.56
11:BE:95:PRO:HA	11:BE:104:THR:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BV:13:LYS:HD3	27:BV:128:LEU:HD11	1.86	0.56
47:Br:2:ACE:H1	47:Br:5:LEU:HD23	1.86	0.56
52:A2:844:U:H2'	52:A2:845:G:H8	1.68	0.56
4:B5:3936:C:H1'	19:BN:125:SER:HB3	1.88	0.56
5:B7:63:C:H5'	5:B7:64:G:H5''	1.87	0.56
21:BP:122:ALA:HB3	21:BP:143:PRO:HB2	1.87	0.56
35:Bd:32:ARG:HD3	35:Bd:48:GLU:HB3	1.87	0.56
60:AH:100:ILE:HD13	60:AH:122:LEU:HD12	1.87	0.56
72:AT:60:THR:HG23	72:AT:75:MET:HE2	1.86	0.56
78:AZ:68:ILE:HB	78:AZ:109:TYR:HB2	1.86	0.56
4:B5:280:G:H5''	19:BN:14:LYS:HE2	1.87	0.56
13:BG:99:ALA:HB1	13:BG:136:LEU:HD11	1.86	0.56
52:A2:1060:A:H4'	52:A2:1061:U:H5'	1.87	0.56
4:B5:2350:OMC:HM22	4:B5:2351:U:H5'	1.87	0.56
4:B5:3824:A2M:HM'2	4:B5:3825:C:H5'	1.88	0.56
48:Bs:175:LEU:HD13	48:Bs:182:PRO:HG2	1.86	0.56
52:A2:436:OMG:HM22	52:A2:437:G:H5'	1.87	0.56
64:AL:111:VAL:HG12	64:AL:140:PHE:HB2	1.88	0.56
42:Bk:33:LYS:HG2	42:Bk:46:VAL:HG22	1.88	0.56
52:A2:1063:C:H4'	67:AO:150:ARG:HH12	1.70	0.56
55:AC:196:ILE:HB	55:AC:223:TYR:HB2	1.88	0.56
4:B5:2844:A:H61	4:B5:3842:C:H42	1.54	0.56
4:B5:4455:OMC:HM22	4:B5:4456:PSU:H5''	1.87	0.56
65:AM:53:ALA:HB2	65:AM:85:LEU:HD13	1.88	0.56
85:Ag:11:LEU:HB2	85:Ag:307:VAL:HB	1.88	0.56
4:B5:2468:C:H5	4:B5:2470:G:H22	1.53	0.56
52:A2:484:A2M:O5'	52:A2:484:A2M:H8	2.06	0.56
60:AH:9:VAL:HG23	60:AH:24:SER:HB3	1.88	0.56
65:AM:33:ARG:HD2	65:AM:91:LEU:HD21	1.86	0.56
71:AS:124:ARG:HB2	71:AS:131:VAL:HG13	1.86	0.56
83:Ae:102:LYS:HD3	83:Ae:106:ALA:HB1	1.88	0.56
52:A2:371:A:H5''	61:AI:11:ARG:HB2	1.88	0.55
70:AR:29:HIS:HA	70:AR:32:LYS:HE2	1.87	0.55
4:B5:2703:C:H2'	4:B5:2704:G:C8	2.41	0.55
69:AQ:37:ARG:HG2	72:AT:7:LYS:HB3	1.87	0.55
78:AZ:79:ILE:HG23	78:AZ:83:LEU:HD23	1.88	0.55
23:BR:68:LEU:HA	23:BR:71:ARG:HD2	1.87	0.55
31:BZ:29:ILE:HG22	31:BZ:32:GLY:H	1.71	0.55
69:AQ:19:ALA:HB2	69:AQ:75:GLY:HA3	1.87	0.55
52:A2:1543:U:H5''	69:AQ:37:ARG:HH12	1.70	0.55
64:AL:66:VAL:HG11	64:AL:141:ASN:HD22	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:Ag:79:LEU:HD11	85:Ag:87:LEU:HD23	1.88	0.55
4:B5:1995:C:H42	4:B5:1999:G:H22	1.53	0.55
52:A2:381:C:H5''	61:Al:54:LYS:HE3	1.89	0.55
19:BN:53:TYR:HB2	19:BN:133:ILE:HD13	1.87	0.55
20:BO:61:ARG:HA	20:BO:70:PRO:HD2	1.87	0.55
64:AL:4:ILE:HD11	64:AL:54:THR:HG23	1.87	0.55
78:AZ:69:THR:HG22	78:AZ:70:PRO:HD2	1.89	0.55
4:B5:4251:C:H42	16:BJ:25:CYS:HB3	1.71	0.55
4:B5:5005:U:H4'	4:B5:5006:A:H5'	1.88	0.55
11:BE:203:ILE:HA	11:BE:260:LYS:HZ2	1.71	0.55
51:Bv:92:LEU:HD23	51:Bv:95:LEU:HD12	1.89	0.55
52:A2:582:U:H2'	52:A2:583:A:H8	1.71	0.55
52:A2:1841:C:H2'	52:A2:1842:4AC:H6	1.88	0.55
52:A2:1593:C:H1'	72:AT:12:GLN:HE22	1.71	0.54
8:BB:132:LYS:HA	8:BB:135:LYS:HE2	1.89	0.54
14:BH:103:VAL:HG21	14:BH:144:LEU:HD11	1.90	0.54
4:B5:173:C:H3'	17:BL:129:ARG:HH22	1.72	0.54
4:B5:1801:A:H5''	4:B5:1802:G:H5'	1.89	0.54
4:B5:4362:A:H5''	45:Bo:36:GLN:HG2	1.89	0.54
52:A2:116:OMU:HN3	52:A2:347:G:H1	1.55	0.54
16:BJ:120:ASP:HB3	16:BJ:123:ILE:HG12	1.89	0.54
57:AE:45:ILE:HA	57:AE:61:VAL:HG11	1.89	0.54
4:B5:1476:C:H41	4:B5:1488:G:H22	1.55	0.54
14:BH:94:SER:HB2	14:BH:142:ASP:HB3	1.90	0.54
52:A2:468:A2M:HM'2	52:A2:469:A:H5'	1.89	0.54
34:Bc:38:ILE:HG21	34:Bc:63:TYR:HB3	1.88	0.54
48:Bs:122:THR:HG22	48:Bs:159:GLN:HG2	1.90	0.54
52:A2:1864:U:H3'	79:Aa:5:ARG:HH21	1.71	0.54
62:AJ:94:LEU:HD12	62:AJ:97:ILE:HD12	1.90	0.54
81:Ac:17:VAL:HA	81:Ac:30:VAL:HG12	1.88	0.54
1:B1:167:PRO:HB3	21:BP:135:ARG:HG2	1.90	0.54
4:B5:2484:U:H2'	4:B5:2485:G:C8	2.42	0.54
28:BW:45:ASN:HD22	28:BW:48:GLN:HG3	1.72	0.54
48:Bs:48:ARG:HD3	49:Bt:123:ARG:HG2	1.88	0.54
52:A2:307:G:H21	52:A2:311:C:H42	1.56	0.54
52:A2:1099:G:H22	52:A2:1133:A:H2	1.55	0.54
4:B5:163:A:H61	4:B5:272:U:H3	1.55	0.54
4:B5:4391:OMG:HM21	4:B5:4393:A:H2'	1.89	0.54
14:BH:113:GLU:HG2	14:BH:125:ARG:HG2	1.90	0.54
52:A2:576:A2M:HM'2	52:A2:577:U:H5'	1.88	0.54
52:A2:1172:U:H2'	52:A2:1173:A:H8	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B5:2646:A:H62	4:B5:2685:G:N2	2.05	0.54
63:AK:91:PRO:HG2	63:AK:94:LEU:HD23	1.89	0.54
4:B5:2875:OMG:HM22	4:B5:2876:G:H5'	1.90	0.54
28:BW:74:ARG:HH12	52:A2:1781:A:H62	1.55	0.54
52:A2:618:C:H41	76:AX:67:ARG:HH21	1.55	0.54
52:A2:1630:A:H5''	71:AS:37:GLY:H	1.72	0.54
58:AF:143:PRO:HG2	81:Ac:54:ASP:HB3	1.90	0.54
52:A2:1133:A:H5'	79:Aa:13:LYS:HB3	1.90	0.53
59:AG:64:LYS:HB2	59:AG:97:VAL:HG11	1.90	0.53
4:B5:1502:A:H4'	4:B5:1503:G:H5'	1.90	0.53
4:B5:1819:C:H5'	10:BD:139:PRO:HB3	1.90	0.53
4:B5:2473:G:N1	4:B5:2502:G:H5'	2.23	0.53
7:BA:137:ILE:HD11	7:BA:149:LYS:HB2	1.90	0.53
4:B5:4935:G:C5	11:BE:183:ARG:HD3	2.44	0.53
8:BB:57:VAL:HG22	8:BB:73:VAL:HG22	1.90	0.53
19:BN:116:LEU:HD22	19:BN:135:ILE:HD11	1.91	0.53
52:A2:385:G:H3'	64:AL:136:LYS:HB2	1.89	0.53
52:A2:1239:U:H5''	68:AP:124:LYS:HD3	1.91	0.53
4:B5:4652:C:H5''	35:Bd:79:ASN:HD22	1.72	0.53
4:B5:4698:U:H1'	4:B5:4699:A:H5''	1.90	0.53
58:AF:49:LEU:HD12	69:AQ:50:LYS:HG2	1.90	0.53
71:AS:138:THR:HA	71:AS:141:ARG:HH21	1.73	0.53
52:A2:28:U:H2'	52:A2:29:G:H8	1.74	0.53
52:A2:1803:U:H2'	52:A2:1804:OMU:H6	1.90	0.53
85:Ag:5:MET:HB2	85:Ag:270:LEU:HD21	1.89	0.53
4:B5:3886:OMC:HM22	4:B5:3887:G:H5'	1.91	0.53
45:Bo:26:TYR:HB3	45:Bo:67:VAL:HB	1.90	0.53
73:AU:56:MET:HB2	73:AU:86:LYS:HB3	1.90	0.53
4:B5:463:A:H2'	4:B5:464:G:H8	1.73	0.53
35:Bd:64:ILE:HG23	35:Bd:68:LEU:HD23	1.91	0.53
39:Bh:80:PRO:HD2	39:Bh:83:LEU:HD12	1.91	0.53
30:BY:55:VAL:HG12	30:BY:106:ILE:HA	1.91	0.53
4:B5:2094:A:H1'	4:B5:2095:G:C2	2.44	0.53
65:AM:52:LEU:HB2	65:AM:76:LEU:HD11	1.90	0.53
11:BE:190:HIS:HB3	11:BE:193:PHE:HD2	1.73	0.52
15:BI:36:LEU:HD11	15:BI:69:ARG:HH11	1.73	0.52
4:B5:2482:G:H1	4:B5:2494:U:H3	1.58	0.52
43:BI:9:ILE:HD12	43:BI:51:LEU:HD21	1.89	0.52
4:B5:1410:C:H2'	4:B5:1411:G:H8	1.75	0.52
4:B5:3943:OMG:HM22	4:B5:3944:A:H5'	1.92	0.52
11:BE:164:PHE:HA	11:BE:175:VAL:HG12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BH:92:MET:HE2	14:BH:179:ILE:HG22	1.90	0.52
52:A2:1433:C:H3'	52:A2:1437:C:H41	1.74	0.52
55:AC:159:LYS:HA	55:AC:162:ILE:HG13	1.92	0.52
7:BA:3:ARG:HG2	7:BA:207:VAL:HG22	1.91	0.52
52:A2:1584:G:H4'	72:AT:67:NMM:HAA1	1.91	0.52
54:AB:123:ALA:HB2	54:AB:165:ARG:HG3	1.91	0.52
4:B5:168:C:H2'	4:B5:169:G:H8	1.74	0.52
38:Bg:48:VAL:HG23	46:Bp:61:MET:HB2	1.90	0.52
60:AH:45:ILE:HG22	60:AH:64:VAL:HG12	1.90	0.52
1:B1:183:LEU:HD13	4:B5:4451:U:H1'	1.91	0.52
4:B5:927:C:H2'	4:B5:928:A:C8	2.43	0.52
52:A2:1124:C:H5''	54:AB:150:ILE:HG12	1.92	0.52
52:A2:1597:C:H5'	71:AS:25:LYS:HD2	1.92	0.52
53:AA:110:ASN:ND2	53:AA:112:ILE:HG12	2.24	0.52
4:B5:267:G:H2'	4:B5:268:G:H8	1.75	0.52
68:AP:52:LYS:HG2	68:AP:80:LEU:HD11	1.92	0.52
78:AZ:54:THR:HG21	78:AZ:79:ILE:HD11	1.91	0.52
31:BZ:25:ILE:HA	31:BZ:43:VAL:HG12	1.92	0.52
53:AA:76:VAL:HG12	53:AA:123:VAL:HB	1.92	0.52
15:BI:171:TRP:HB2	15:BI:178:ALA:HA	1.91	0.52
31:BZ:12:LEU:HB2	31:BZ:81:MET:HB3	1.92	0.52
50:Bu:119:THR:HG21	51:Bv:88:LEU:HD21	1.91	0.52
53:AA:8:LEU:HD11	74:AV:39:VAL:HG21	1.92	0.52
60:AH:110:THR:HG22	60:AH:112:ASN:H	1.75	0.52
13:BG:110:LYS:HA	13:BG:113:ARG:HG2	1.92	0.51
52:A2:26:U:H2'	52:A2:27:A2M:H8	1.92	0.51
2:B2:19:G:H1	2:B2:56:C:H42	1.58	0.51
4:B5:158:A:H4'	4:B5:159:C:H2'	1.92	0.51
4:B5:1616:G:H1'	4:B5:2512:A:N6	2.25	0.51
12:BF:127:LYS:HB2	25:BT:133:ALA:HB3	1.91	0.51
48:Bs:30:VAL:HG21	48:Bs:187:LEU:HD13	1.92	0.51
52:A2:116:OMU:HM22	52:A2:117:C:H5'	1.93	0.51
85:Ag:163:PRO:HB2	85:Ag:179:LEU:HB3	1.90	0.51
4:B5:134:G:H4'	4:B5:135:G:OP1	2.09	0.51
4:B5:454:U:H3	4:B5:701:G:H22	1.59	0.51
4:B5:4729:C:H2'	4:B5:4731:G:N7	2.26	0.51
8:BB:220:ILE:HB	8:BB:346:THR:HB	1.92	0.51
9:BC:328:LEU:HB3	12:BF:187:MET:HG3	1.93	0.51
56:AD:219:PRO:HB3	85:Ag:189:ILE:HG22	1.91	0.51
64:AL:23:VAL:HG23	64:AL:26:GLY:H	1.76	0.51
58:AF:41:VAL:HG13	58:AF:42:LYS:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BA:117:GLU:HG2	7:BA:124:GLY:H	1.76	0.51
85:Ag:240:CYS:HG	85:Ag:291:TRP:CD1	2.27	0.51
52:A2:798:G:H5'	60:AH:111:LYS:HG3	1.91	0.51
54:AB:63:LYS:HE3	54:AB:90:ASP:HA	1.92	0.51
62:AJ:137:VAL:HG22	62:AJ:157:ILE:HG12	1.93	0.51
4:B5:411:G:H4'	4:B5:412:G:H5''	1.93	0.51
4:B5:4589:A2M:HM'2	4:B5:4590:U:H5'	1.92	0.51
8:BB:92:TYR:HB2	8:BB:159:VAL:HB	1.93	0.51
52:A2:77:A:H5''	59:AG:159:ARG:HH12	1.74	0.51
52:A2:1780:G:H2'	52:A2:1781:A:C8	2.45	0.51
49:Bt:10:ILE:HG12	49:Bt:65:GLN:HG2	1.93	0.51
52:A2:1480:A:H5'	69:AQ:131:LYS:HD3	1.93	0.51
10:BD:150:LEU:HD12	16:BJ:146:ARG:HG3	1.93	0.51
14:BH:111:LEU:HD11	14:BH:125:ARG:HB3	1.92	0.51
22:BQ:18:PRO:HG3	22:BQ:29:VAL:HG21	1.93	0.51
49:Bt:147:HIS:HD2	49:Bt:149:HIS:HB2	1.76	0.51
4:B5:1418:G:N2	4:B5:1419:A:H62	2.09	0.51
10:BD:107:ARG:HH12	10:BD:120:GLU:HA	1.76	0.51
15:BI:141:LYS:HD2	15:BI:143:GLN:HE22	1.76	0.51
52:A2:1112:U:H2'	52:A2:1113:A:C8	2.45	0.51
70:AR:114:LEU:HB2	70:AR:117:LEU:HG	1.92	0.51
71:AS:22:GLY:HA2	71:AS:56:ALA:HB3	1.93	0.51
32:Ba:119:LYS:HA	32:Ba:140:VAL:HG13	1.91	0.50
52:A2:49:C:H2'	52:A2:472:C:H41	1.75	0.50
75:AW:28:ARG:HB3	75:AW:60:LYS:HG2	1.93	0.50
4:B5:137:G:H2'	4:B5:138:G:H8	1.76	0.50
4:B5:3719:G:H22	4:B5:3732:A:H2	1.59	0.50
49:Bt:28:LEU:HD13	49:Bt:42:VAL:HG23	1.94	0.50
54:AB:38:MET:HE2	54:AB:182:LYS:HA	1.93	0.50
4:B5:137:G:H2'	4:B5:138:G:C8	2.46	0.50
4:B5:1793:A:H5''	4:B5:4213:A:H61	1.75	0.50
4:B5:658:C:H2'	4:B5:659:G:C8	2.47	0.50
4:B5:3877:C:H5	4:B5:4399:G:H4'	1.76	0.50
23:BR:183:GLU:HA	23:BR:186:LYS:HE2	1.92	0.50
71:AS:20:ILE:HD11	71:AS:33:ILE:HG13	1.93	0.50
4:B5:1749:G:H2'	4:B5:1750:A:C8	2.46	0.50
4:B5:1920:C:H5''	24:BS:161:ARG:HH12	1.76	0.50
4:B5:4535:OMC:HM22	4:B5:4536:C:H5'	1.93	0.50
55:AC:187:ARG:HD3	55:AC:192:LEU:HD12	1.93	0.50
85:Ag:5:MET:HG2	85:Ag:312:VAL:HG22	1.93	0.50
4:B5:1500:C:H1'	22:BQ:68:ARG:HD3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BB:141:ASP:HA	8:BB:144:LYS:HE2	1.93	0.50
40:Bi:26:HIS:CE1	40:Bi:29:ARG:HH11	2.30	0.50
52:A2:1275:G:H1'	52:A2:1321:G:H22	1.77	0.50
60:AH:8:ILE:HG22	60:AH:44:ASN:HA	1.94	0.50
4:B5:955:A:H1'	4:B5:2075:G:H5''	1.93	0.50
4:B5:1700:A:H2'	4:B5:1702:C:H41	1.77	0.50
4:B5:4767:G:H2'	4:B5:4768:G:C8	2.46	0.50
13:BG:162:ASP:HB3	13:BG:163:PRO:HD3	1.94	0.50
52:A2:1415:C:H2'	52:A2:1416:C:C6	2.47	0.50
4:B5:2740:U:H2'	7:BA:50:HIS:HD2	1.77	0.50
4:B5:3856:G:H5''	21:BP:86:LYS:HB2	1.92	0.50
4:B5:4621:A:H4'	8:BB:13:SER:HB2	1.92	0.50
52:A2:1478:U:H2'	52:A2:1479:G:C8	2.46	0.50
57:AE:20:LEU:HD21	57:AE:46:ILE:HD13	1.94	0.50
4:B5:203:U:H3	4:B5:212:A:H61	1.60	0.50
4:B5:4536:C:H2'	4:B5:4537:G:C8	2.47	0.50
4:B5:4617:OMG:H5''	27:BV:15:ARG:HB2	1.94	0.50
57:AE:48:LEU:HD12	57:AE:61:VAL:HG13	1.94	0.50
34:Bc:21:VAL:HG11	34:Bc:96:ILE:HD12	1.93	0.49
52:A2:1010:G:H2'	52:A2:1011:A:H8	1.77	0.49
58:AF:35:LEU:HD12	58:AF:117:ILE:HG12	1.94	0.49
61:AI:57:ALA:HB2	61:AI:183:GLY:HA2	1.93	0.49
4:B5:734:G:H1	4:B5:928:A:H61	1.60	0.49
4:B5:2889:C:H42	4:B5:3610:A:H61	1.60	0.49
4:B5:4749:G:H2'	4:B5:4750:G:C8	2.47	0.49
4:B5:4774:C:H2'	4:B5:4775:G:C8	2.47	0.49
57:AE:246:LEU:HB3	57:AE:250:GLU:HG3	1.94	0.49
4:B5:743:G:H2'	4:B5:744:G:H8	1.78	0.49
4:B5:2776:G:H5''	4:B5:2777:G:H5'	1.94	0.49
7:BA:180:LEU:HD22	46:Bp:18:TYR:HB3	1.94	0.49
10:BD:55:VAL:HG13	10:BD:60:ILE:HG12	1.94	0.49
48:Bs:106:LYS:HD3	48:Bs:184:SER:HB2	1.93	0.49
52:A2:159:A2M:H2	52:A2:468:A2M:H1'	1.94	0.49
4:B5:1953:U:H2'	4:B5:1954:G:C8	2.47	0.49
7:BA:2:GLY:HA2	7:BA:207:VAL:HG23	1.93	0.49
30:BY:31:SER:HA	30:BY:48:PRO:HA	1.94	0.49
52:A2:1867:U:H4'	52:A2:1868:U:H5'	1.93	0.49
67:AO:44:VAL:HG12	67:AO:53:ILE:HB	1.93	0.49
4:B5:3759:A:N6	4:B5:3764:G:H21	2.11	0.49
4:B5:3855:A:H5''	21:BP:83:TRP:O	2.13	0.49
49:Bt:133:LEU:HD11	49:Bt:151:ILE:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:AD:137:VAL:HG22	56:AD:151:LYS:HG3	1.95	0.49
76:AX:101:LEU:HD22	76:AX:124:LYS:HE2	1.94	0.49
4:B5:665:C:H2'	4:B5:669:C:C6	2.48	0.49
4:B5:4097:A:H61	4:B5:4110:U:H3	1.61	0.49
15:BI:99:ILE:HG22	15:BI:123:GLN:HB2	1.95	0.49
23:BR:4:LEU:HD11	23:BR:29:THR:HG23	1.94	0.49
25:BT:75:VAL:HG22	25:BT:88:ARG:HG2	1.94	0.49
34:Bc:47:ILE:HD12	34:Bc:94:LEU:HD11	1.94	0.49
52:A2:159:A2M:O5'	52:A2:159:A2M:H8	2.13	0.49
60:AH:76:GLN:HE22	60:AH:94:PHE:HB2	1.78	0.49
85:Ag:191:HIS:CG	85:Ag:195:LEU:HD21	2.48	0.49
1:B1:175:ARG:HH21	4:B5:3907:A:H1'	1.77	0.49
4:B5:4124:C:H5'	13:BG:45:ILE:HD12	1.95	0.49
4:B5:4296:G:H2'	4:B5:4297:A:H8	1.78	0.49
53:AA:145:ILE:HG12	53:AA:159:ILE:HB	1.94	0.49
4:B5:4893:A:H5''	4:B5:4894:C:H2'	1.94	0.49
52:A2:220:U:H5'	61:AI:177:SER:HB3	1.95	0.49
52:A2:1844:U:H3	52:A2:1855:G:H1	1.60	0.49
64:AL:16:ILE:HD11	64:AL:36:TYR:HB2	1.94	0.49
84:Af:140:TYR:CZ	84:Af:142:GLY:HA2	2.48	0.49
4:B5:142:G:H2'	4:B5:144:G:C8	2.48	0.49
4:B5:4482:C:H2'	4:B5:4483:A:H8	1.78	0.49
10:BD:181:PRO:HD2	10:BD:195:HIS:CD2	2.48	0.49
16:BJ:50:PHE:HB3	16:BJ:67:LYS:HB3	1.94	0.49
52:A2:1455:A:H2'	52:A2:1456:G:H8	1.78	0.49
59:AG:58:LYS:HE3	59:AG:105:ASN:HA	1.94	0.49
4:B5:741:C:H2'	4:B5:742:G:C8	2.47	0.49
4:B5:4254:A:H2'	4:B5:4255:A:C8	2.47	0.49
28:BW:80:ARG:HG2	59:AG:9:ALA:HA	1.95	0.49
52:A2:1710:C:H42	52:A2:1823:A:H61	1.60	0.49
54:AB:89:GLU:HB3	54:AB:223:PHE:HE1	1.78	0.49
81:Ac:18:LEU:HD12	81:Ac:29:GLN:HG2	1.94	0.49
85:Ag:238:ALA:H	85:Ag:251:ALA:HB3	1.78	0.49
85:Ag:239:LEU:HD22	85:Ag:248:LEU:HD11	1.94	0.49
4:B5:267:G:H2'	4:B5:268:G:C8	2.48	0.48
4:B5:1493:U:H2'	4:B5:1494:G:H8	1.78	0.48
4:B5:1811:C:H5''	33:Bb:56:LYS:HE3	1.94	0.48
4:B5:2554:G:H1	4:B5:2571:C:H42	1.61	0.48
65:AM:61:TYR:HD2	84:Af:100:LEU:HD11	1.78	0.48
4:B5:142:G:H2'	4:B5:144:G:H8	1.77	0.48
4:B5:3618:G:H22	4:B5:3623:A:H1'	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B5:4652:C:H2'	4:B5:4653:C:C6	2.47	0.48
7:BA:6:ARG:HH12	7:BA:199:VAL:H	1.61	0.48
42:Bk:14:THR:HA	42:Bk:17:ARG:HD3	1.95	0.48
4:B5:3745:A:H5''	7:BA:244:GLY:HA3	1.95	0.48
4:B5:4141:C:H4'	4:B5:4142:G:H5'	1.94	0.48
4:B5:4760:G:H2'	4:B5:4761:A:H8	1.78	0.48
4:B5:4858:C:H2'	4:B5:4859:G:C8	2.49	0.48
4:B5:4888:G:H2'	4:B5:4889:G:C8	2.48	0.48
9:BC:318:PRO:HG2	12:BF:155:TYR:HB3	1.95	0.48
52:A2:853:C:H2'	52:A2:854:A:C8	2.47	0.48
52:A2:1824:A:H2'	52:A2:1825:A:O4'	2.13	0.48
72:AT:10:ASN:HD22	72:AT:13:GLU:HG3	1.79	0.48
4:B5:486:C:H2'	4:B5:487:G:C8	2.48	0.48
4:B5:927:C:H2'	4:B5:928:A:H8	1.78	0.48
4:B5:1589:C:H4'	4:B5:2856:A:H5'	1.94	0.48
52:A2:1337:4AC:H2'	52:A2:1338:G:C8	2.48	0.48
52:A2:1536:G:H2'	52:A2:1537:A:C8	2.48	0.48
4:B5:1280:G:H5'	9:BC:323:ARG:HB2	1.95	0.48
6:B8:114:G:H1	6:B8:136:U:H3	1.60	0.48
7:BA:180:LEU:HD21	46:Bp:22:LEU:HB3	1.96	0.48
40:Bi:70:LEU:HD22	40:Bi:87:ARG:HH21	1.78	0.48
44:Bm:110:CYS:HB3	44:Bm:117:HIS:HA	1.94	0.48
52:A2:1854:U:P	67:AO:147:ARG:HH22	2.37	0.48
2:B2:29:A:H5''	68:AP:136:THR:HG21	1.95	0.48
48:Bs:10:LYS:HG3	48:Bs:60:MET:HE1	1.95	0.48
52:A2:1208:A:H2'	52:A2:1209:A:C8	2.49	0.48
52:A2:1593:C:H2'	52:A2:1594:A:H8	1.79	0.48
54:AB:24:PRO:O	54:AB:28:LYS:HG2	2.13	0.48
72:AT:85:ASN:HB2	72:AT:88:MET:HB2	1.96	0.48
2:B2:53:G:H3'	2:B2:54:5MU:H73	1.94	0.48
4:B5:2054:G:C2	20:BO:130:LYS:HE3	2.49	0.48
10:BD:156:GLY:HA2	10:BD:181:PRO:HG3	1.96	0.48
68:AP:49:LEU:HD13	68:AP:83:MET:HE1	1.96	0.48
4:B5:3829:A2M:HM'2	4:B5:3830:U:H5'	1.95	0.48
10:BD:193:GLU:HG3	10:BD:197:LYS:HE3	1.96	0.48
15:BI:170:LYS:HD3	15:BI:175:LYS:HA	1.96	0.48
20:BO:118:MET:HG2	24:BS:169:THR:HG22	1.94	0.48
52:A2:1113:A:H61	52:A2:1119:A:H61	1.62	0.48
66:AN:40:LEU:HD12	66:AN:50:ILE:HG23	1.96	0.48
69:AQ:21:ALA:HB2	69:AQ:72:VAL:HG13	1.95	0.48
26:BU:117:ILE:HA	51:Bv:75:LYS:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:A2:1808:U:H2'	52:A2:1809:A:C8	2.49	0.48
4:B5:1612:A:H5'	7:BA:183:GLY:HA2	1.96	0.48
4:B5:1748:A:H2'	4:B5:1749:G:C8	2.49	0.48
52:A2:1337:4AC:H2'	52:A2:1338:G:H8	1.78	0.48
4:B5:4901:C:H2'	4:B5:4902:G:C8	2.48	0.47
23:BR:21:LYS:HE3	23:BR:55:VAL:HA	1.96	0.47
35:Bd:53:ALA:HA	35:Bd:88:LEU:HD21	1.95	0.47
52:A2:462:OMC:HM22	52:A2:463:C:H5'	1.95	0.47
52:A2:525:A:H2'	52:A2:526:A:C8	2.48	0.47
62:AJ:136:ARG:HG2	62:AJ:160:SER:HA	1.96	0.47
71:AS:34:LYS:HB3	71:AS:103:LEU:HD23	1.95	0.47
4:B5:1240:C:H2'	4:B5:1241:G:C8	2.50	0.47
4:B5:3828:G:H2'	4:B5:3829:A2M:H8	1.95	0.47
8:BB:220:ILE:HG12	8:BB:278:THR:HG23	1.96	0.47
11:BE:178:PRO:HD2	11:BE:181:LEU:HD12	1.96	0.47
32:Ba:72:THR:HG22	32:Ba:110:LYS:HB3	1.96	0.47
52:A2:300:U:H2'	52:A2:301:A:H8	1.80	0.47
52:A2:864:A:H2'	52:A2:865:A:C8	2.49	0.47
52:A2:874:G:H2'	52:A2:875:A:C8	2.49	0.47
2:B2:13:C:H2'	2:B2:14:A:H8	1.78	0.47
4:B5:229:G:H5''	30:BY:11:ARG:HG3	1.95	0.47
4:B5:1482:C:H41	4:B5:1483:G:H21	1.61	0.47
4:B5:2715:C:H2'	4:B5:2716:G:C8	2.49	0.47
4:B5:5056:C:H2'	4:B5:5057:A:C8	2.49	0.47
44:Bm:94:MET:HG2	44:Bm:105:PRO:HA	1.96	0.47
52:A2:1208:A:H2'	52:A2:1209:A:H8	1.78	0.47
55:AC:142:LYS:HG2	55:AC:153:GLY:HA3	1.96	0.47
52:A2:1284:A:N6	52:A2:1313:A:H2'	2.30	0.47
52:A2:1285:G:H22	65:AM:57:ASP:HB3	1.79	0.47
52:A2:1324:G:H1	52:A2:1504:U:H3	1.63	0.47
4:B5:2709:C:H41	23:BR:46:LYS:NZ	2.13	0.47
4:B5:4888:G:H2'	4:B5:4889:G:H8	1.80	0.47
51:Bv:147:LEU:HA	51:Bv:150:ILE:HG22	1.96	0.47
52:A2:792:C:H2'	52:A2:793:G:C8	2.49	0.47
56:AD:29:LEU:HD21	56:AD:69:LEU:HD11	1.97	0.47
2:B2:9:A:H62	2:B2:23:C:H5	1.63	0.47
4:B5:3723:A2M:HM'2	4:B5:3724:G:H5'	1.96	0.47
4:B5:3791:OMG:HM22	4:B5:3792:U:H5'	1.97	0.47
19:BN:84:PRO:HA	19:BN:87:HIS:CG	2.50	0.47
52:A2:1029:G:H2'	52:A2:1030:A:H8	1.79	0.47
60:AH:60:ILE:HB	60:AH:92:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:Ag:220:ASP:HB2	85:Ag:227:LEU:HD21	1.96	0.47
2:B2:34:OMC:H5'	52:A2:1248:B8N:C4	2.45	0.47
2:B2:65:C:H2'	2:B2:66:A:H8	1.80	0.47
4:B5:1451:A:H2'	4:B5:1452:G:O4'	2.15	0.47
4:B5:2033:G:H4'	24:BS:118:ARG:HG2	1.97	0.47
5:B7:55:A:H4'	16:BJ:155:HIS:HB2	1.95	0.47
52:A2:65:C:C5	59:AG:174:PRO:HB3	2.49	0.47
72:AT:65:TYR:HE1	72:AT:128:GLN:HG3	1.79	0.47
4:B5:658:C:H2'	4:B5:659:G:H8	1.78	0.47
60:AH:53:VAL:HG11	60:AH:175:GLY:HA3	1.97	0.47
61:AI:103:LEU:HD22	61:AI:170:LYS:HB3	1.97	0.47
81:Ac:32:VAL:HG11	81:Ac:56:LEU:HD12	1.97	0.47
4:B5:4205:C:H42	4:B5:4225:G:H1	1.62	0.47
27:BV:106:VAL:HG12	27:BV:112:MET:HA	1.97	0.47
52:A2:122:G:H2'	52:A2:123:G:H8	1.80	0.47
52:A2:1098:C:H2'	52:A2:1099:G:C8	2.50	0.47
52:A2:1679:A:H2'	58:AF:60:ARG:HD2	1.97	0.47
52:A2:1858:G:H2'	52:A2:1859:A:H8	1.80	0.47
4:B5:114:G:N2	4:B5:158:A:H61	2.13	0.47
4:B5:4299:U:H4'	25:BT:89:ILE:HG22	1.97	0.47
4:B5:4760:G:H2'	4:B5:4761:A:C8	2.49	0.47
11:BE:179:LEU:HD12	11:BE:183:ARG:HA	1.97	0.47
24:BS:15:ARG:HB3	24:BS:27:LEU:HD23	1.97	0.47
51:Bv:142:GLN:HB2	51:Bv:145:GLU:HG3	1.97	0.47
4:B5:935:C:C4	18:BM:19:PRO:HB3	2.50	0.46
4:B5:1295:G:H2'	4:B5:1296:U:O4'	2.14	0.46
4:B5:2093:G:H1'	4:B5:2094:A:C8	2.50	0.46
4:B5:2564:A:H3'	4:B5:2565:G:H8	1.80	0.46
4:B5:2803:OMC:HM22	4:B5:2804:C:H5'	1.96	0.46
4:B5:4418:U:H5	4:B5:4474:G:H21	1.63	0.46
9:BC:141:GLY:HA3	9:BC:204:ARG:HH12	1.80	0.46
12:BF:154:ILE:HD12	12:BF:191:ILE:HG12	1.97	0.46
19:BN:9:GLU:HB2	40:Bi:44:ILE:HG13	1.97	0.46
52:A2:1109:C:H2'	52:A2:1110:G:C8	2.49	0.46
65:AM:79:VAL:HG11	65:AM:85:LEU:HB2	1.96	0.46
4:B5:3606:U:H2'	4:B5:3607:A:C8	2.49	0.46
5:B7:59:G:H2'	5:B7:60:G:H8	1.80	0.46
15:BI:177:ASN:HB2	15:BI:180:GLU:HG2	1.97	0.46
21:BP:16:LYS:HG2	21:BP:149:ILE:HG12	1.97	0.46
52:A2:28:U:H2'	52:A2:29:G:C8	2.50	0.46
55:AC:88:ILE:HG23	55:AC:93:ILE:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:AE:137:PRO:HG2	57:AE:150:PRO:HD2	1.97	0.46
60:AH:65:PRO:HG2	60:AH:68:GLN:HB2	1.97	0.46
75:AW:17:ALA:HB1	75:AW:22:LYS:HB2	1.98	0.46
10:BD:152:ARG:HG3	10:BD:154:THR:HG23	1.97	0.46
30:BY:2:LYS:HE3	30:BY:2:LYS:HB3	1.73	0.46
52:A2:391:C:H2'	52:A2:392:A:H8	1.80	0.46
52:A2:1593:C:H2'	52:A2:1594:A:C8	2.50	0.46
52:A2:1717:C:H2'	52:A2:1718:G:C8	2.50	0.46
52:A2:1740:C:H42	52:A2:1794:C:H42	1.62	0.46
53:AA:77:ILE:HG12	53:AA:99:ILE:HB	1.96	0.46
76:AX:67:ARG:HG3	76:AX:115:ILE:HG12	1.97	0.46
12:BF:190:LEU:HD21	12:BF:208:LEU:HD21	1.98	0.46
48:Bs:68:HIS:HB3	48:Bs:75:LEU:HD22	1.96	0.46
57:AE:175:PHE:HE2	57:AE:198:ARG:HD2	1.80	0.46
4:B5:1178:U:H4'	4:B5:1180:C:H41	1.80	0.46
4:B5:4619:OMU:HM22	4:B5:4620:C:H5'	1.98	0.46
7:BA:30:ARG:HG2	7:BA:74:GLU:HG3	1.97	0.46
28:BW:82:ILE:HG23	59:AG:131:ARG:HB2	1.97	0.46
46:Bp:39:CYS:HB3	46:Bp:42:CYS:SG	2.55	0.46
52:A2:1125:C:H2'	52:A2:1126:G:H8	1.81	0.46
60:AH:9:VAL:HG12	60:AH:11:PRO:HD3	1.98	0.46
84:Af:100:LEU:HD13	84:Af:103:LEU:HD11	1.98	0.46
4:B5:1083:C:H42	4:B5:1212:G:H1	1.64	0.46
4:B5:2094:A:H4'	4:B5:2095:G:H5'	1.97	0.46
4:B5:3601:C:H2'	4:B5:3602:G:C8	2.51	0.46
4:B5:3950:G:H1	4:B5:4060:G:H1	1.63	0.46
4:B5:4991:G:H2'	4:B5:4992:G:C8	2.51	0.46
8:BB:321:VAL:HG12	8:BB:322:HIS:HD1	1.80	0.46
52:A2:120:U:H2'	52:A2:121:OMU:H6	1.98	0.46
53:AA:24:HIS:HB3	53:AA:51:LEU:HD21	1.97	0.46
55:AC:256:TRP:CD2	75:AW:68:ARG:HD3	2.50	0.46
59:AG:57:ASP:HA	59:AG:106:LEU:HA	1.96	0.46
4:B5:168:C:H2'	4:B5:169:G:C8	2.50	0.46
4:B5:4523:G:C2	8:BB:252:ALA:HB1	2.50	0.46
4:B5:4913:C:H2'	4:B5:4914:G:C8	2.51	0.46
25:BT:44:GLY:HA2	25:BT:95:HIS:HB3	1.97	0.46
58:AF:76:MET:HE3	58:AF:173:LEU:HD22	1.98	0.46
65:AM:42:LEU:HD13	65:AM:68:LEU:HB3	1.98	0.46
73:AU:80:PHE:HB3	82:Ad:52:PHE:HB3	1.98	0.46
4:B5:480:C:H2'	4:B5:481:G:C8	2.51	0.46
4:B5:2520:G:H5'	4:B5:2639:G:H1'	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B5:5024:C:H41	4:B5:5027:G:H21	1.63	0.46
36:Be:108:ARG:HE	36:Be:128:ARG:HD2	1.80	0.46
45:Bo:74:GLU:HB3	45:Bo:77:CYS:HB3	1.98	0.46
49:Bt:46:ILE:HD11	49:Bt:62:LEU:HD21	1.98	0.46
51:Bv:106:VAL:HG11	51:Bv:134:ILE:HD13	1.98	0.46
52:A2:300:U:H2'	52:A2:301:A:C8	2.50	0.46
52:A2:844:U:H2'	52:A2:845:G:C8	2.50	0.46
65:AM:40:LYS:HG3	84:Af:129:GLY:HA3	1.96	0.46
4:B5:32:G:H21	4:B5:50:C:H5	1.64	0.46
4:B5:245:C:H4'	4:B5:246:G:OP1	2.15	0.46
4:B5:4254:A:C8	4:B5:4255:A:H2'	2.51	0.46
27:BV:107:ASN:HD21	27:BV:111:GLU:HB3	1.80	0.46
31:BZ:64:LYS:HA	31:BZ:67:LYS:HE3	1.98	0.46
52:A2:103:A:H5'	61:AI:12:ARG:HH12	1.81	0.46
52:A2:879:C:H2'	52:A2:880:G:H8	1.81	0.46
52:A2:1097:G:H4'	53:AA:32:PHE:CG	2.51	0.46
52:A2:1315:U:H2'	52:A2:1316:C:C6	2.51	0.46
4:B5:254:G:H2'	4:B5:255:C:H4'	1.98	0.46
4:B5:663:G:H2'	4:B5:664:G:C8	2.51	0.46
4:B5:1331:C:H2'	4:B5:1332:A:C8	2.51	0.46
4:B5:1698:A:H3'	4:B5:1699:G:H21	1.81	0.46
4:B5:1913:C:H4'	20:BO:89:PRO:HD3	1.97	0.46
4:B5:1982:A:H4'	4:B5:1983:A:C8	2.51	0.46
4:B5:1993:C:H2'	4:B5:1994:G:H8	1.81	0.46
4:B5:4868:U:H4'	4:B5:4870:C:H4'	1.97	0.46
12:BF:182:TYR:HB3	12:BF:200:ARG:HG3	1.98	0.46
16:BJ:24:ILE:HG12	16:BJ:128:LEU:HB3	1.98	0.46
52:A2:1228:A:H2'	52:A2:1229:G:C8	2.51	0.46
52:A2:1412:C:H2'	52:A2:1413:G:C8	2.51	0.46
58:AF:19:LEU:HD21	58:AF:69:VAL:HG11	1.98	0.46
85:Ag:86:THR:HG22	85:Ag:102:VAL:HG13	1.98	0.46
4:B5:275:C:H2'	4:B5:276:C:C6	2.50	0.45
4:B5:742:G:H2'	4:B5:743:G:C8	2.52	0.45
4:B5:743:G:H2'	4:B5:744:G:C8	2.51	0.45
4:B5:1092:C:H2'	4:B5:1093:G:H8	1.81	0.45
4:B5:1203:C:H2'	4:B5:1204:G:H8	1.80	0.45
8:BB:161:ARG:HG2	8:BB:184:GLN:HA	1.97	0.45
18:BM:13:ALA:HB1	18:BM:55:MET:HB3	1.98	0.45
29:BX:81:LEU:HG	29:BX:83:THR:HG23	1.98	0.45
32:Ba:75:LEU:HD13	32:Ba:117:LEU:HD12	1.98	0.45
48:Bs:102:LEU:HD11	48:Bs:187:LEU:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:AI:141:ARG:HD3	61:AI:145:ILE:HG22	1.98	0.45
78:AZ:48:VAL:HG12	78:AZ:80:ARG:HD2	1.97	0.45
4:B5:502:C:H5'	4:B5:504:G:H5''	1.97	0.45
4:B5:4620:C:OP1	27:BV:48:ARG:HD2	2.16	0.45
8:BB:238:LYS:HE3	27:BV:50:ASN:HD22	1.79	0.45
11:BE:176:THR:HB	11:BE:186:LEU:HD23	1.97	0.45
13:BG:118:ALA:HA	13:BG:121:LYS:HG2	1.98	0.45
48:Bs:39:GLN:HE21	48:Bs:186:GLY:HA2	1.80	0.45
52:A2:678:U:H2'	52:A2:679:A:C8	2.51	0.45
52:A2:799:OMU:HM22	52:A2:800:U:H5'	1.97	0.45
4:B5:137:G:H4'	39:Bh:98:HIS:CG	2.52	0.45
49:Bt:82:ILE:HA	49:Bt:85:LEU:HD12	1.98	0.45
52:A2:1047:C:H5''	67:AO:143:LYS:HB2	1.99	0.45
62:AJ:176:LYS:HG2	62:AJ:180:LYS:HE3	1.98	0.45
6:B8:77:A:H2'	6:B8:78:G:O4'	2.16	0.45
8:BB:36:ASP:HB3	8:BB:39:LYS:HE2	1.99	0.45
36:Be:35:TRP:CZ2	36:Be:56:PRO:HD2	2.51	0.45
37:Bf:50:VAL:HG22	37:Bf:69:VAL:HG22	1.98	0.45
38:Bg:60:ARG:HB2	38:Bg:63:VAL:HG23	1.98	0.45
52:A2:115:U:H2'	52:A2:116:OMU:H6	1.98	0.45
52:A2:1612:G:H2'	52:A2:1613:G:H8	1.82	0.45
57:AE:115:THR:HG22	57:AE:117:GLU:H	1.82	0.45
59:AG:137:ARG:HB3	59:AG:140:ARG:HB2	1.99	0.45
4:B5:1244:C:H2'	4:B5:1245:G:H8	1.81	0.45
4:B5:1777:C:H2'	4:B5:1778:PSU:H6	1.82	0.45
4:B5:1827:C:H2'	4:B5:1828:G:C8	2.52	0.45
4:B5:2899:U:H3	4:B5:3598:A:H61	1.64	0.45
7:BA:118:GLU:HG3	7:BA:156:LYS:HE2	1.99	0.45
52:A2:1758:G:H2'	52:A2:1759:G:C8	2.49	0.45
53:AA:173:LEU:HD11	53:AA:177:MET:HE2	1.99	0.45
64:AL:111:VAL:HG11	64:AL:128:VAL:HG11	1.99	0.45
4:B5:390:C:H42	4:B5:401:G:H1	1.63	0.45
4:B5:1365:G:H5''	9:BC:218:ILE:HD12	1.99	0.45
4:B5:4913:C:H2'	4:B5:4914:G:H8	1.81	0.45
54:AB:88:THR:HA	54:AB:98:THR:HG22	1.99	0.45
66:AN:63:VAL:HG21	66:AN:71:ILE:HD11	1.99	0.45
4:B5:1501:G:H1	22:BQ:89:ASP:HA	1.82	0.45
4:B5:1705:A:O5'	4:B5:1705:A:H8	2.00	0.45
4:B5:1793:A:H5''	4:B5:4213:A:N6	2.31	0.45
4:B5:2896:G:H5''	23:BR:101:ILE:HD13	1.99	0.45
4:B5:3603:A:P	23:BR:71:ARG:HH12	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BF:95:ILE:HD13	12:BF:141:ALA:HB2	1.97	0.45
52:A2:874:G:H2'	52:A2:875:A:H8	1.81	0.45
52:A2:1114:U:H3	52:A2:1119:A:H62	1.63	0.45
59:AG:44:GLU:HA	59:AG:119:LYS:HD2	1.99	0.45
4:B5:417:G:H1'	6:B8:16:G:N2	2.32	0.45
4:B5:1967:G:H2'	4:B5:1968:G:C8	2.52	0.45
4:B5:1414:G:H2'	4:B5:1415:G:C8	2.52	0.45
4:B5:2500:C:H2'	4:B5:2501:G:C8	2.52	0.45
4:B5:2715:C:H2'	4:B5:2716:G:H8	1.82	0.45
28:BW:102:LYS:HD2	28:BW:105:ARG:HD2	1.99	0.45
31:BZ:50:PRO:HD3	31:BZ:68:ILE:HG12	1.99	0.45
52:A2:907:G:H2'	52:A2:908:A:C8	2.52	0.45
52:A2:1380:C:H1'	53:AA:113:GLN:HE22	1.81	0.45
52:A2:1678:A2M:H1'	52:A2:1678:A2M:HM'2	1.71	0.45
4:B5:1756:U:H2'	4:B5:1757:G:H8	1.82	0.45
8:BB:354:GLN:HB3	8:BB:359:ALA:HB1	1.98	0.45
36:Be:28:TYR:HB3	36:Be:30:LYS:HG2	1.99	0.45
48:Bs:191:GLN:HG3	48:Bs:200:ASN:HA	1.99	0.45
52:A2:1711:U:H2'	52:A2:1712:A:C8	2.52	0.45
59:AG:52:ILE:HD13	59:AG:102:VAL:HG21	1.98	0.45
4:B5:381:U:H4'	4:B5:415:G:H5'	2.00	0.44
4:B5:1485:C:H2'	4:B5:1486:G:C8	2.52	0.44
4:B5:3944:A:H2'	4:B5:3945:G:C8	2.52	0.44
49:Bt:32:ILE:HB	49:Bt:35:LEU:HD11	2.00	0.44
52:A2:906:U:H2'	52:A2:907:G:H8	1.81	0.44
52:A2:1447:OMG:HM22	52:A2:1448:A:H5'	1.98	0.44
54:AB:30:TRP:CE2	54:AB:48:LEU:HD13	2.52	0.44
66:AN:136:PRO:HG2	66:AN:139:TRP:HB2	1.97	0.44
4:B5:37:U:H4'	32:Ba:32:ARG:HD2	2.00	0.44
4:B5:1325:A2M:HM'2	4:B5:1326:C:O4'	2.17	0.44
4:B5:2632:U:H5''	23:BR:61:ALA:HB2	1.99	0.44
4:B5:3606:U:H2'	4:B5:3607:A:H8	1.81	0.44
4:B5:4248:G:H2'	4:B5:4249:G:C8	2.52	0.44
4:B5:4766:C:H2'	4:B5:4767:G:C8	2.52	0.44
5:B7:36:C:H2'	5:B7:37:G:C8	2.53	0.44
6:B8:141:C:H5''	19:BN:60:VAL:HG11	1.99	0.44
52:A2:1815:A:H2'	52:A2:1816:G:H8	1.82	0.44
4:B5:174:C:H2'	4:B5:175:C:C6	2.53	0.44
4:B5:477:C:H2'	4:B5:478:G:H8	1.83	0.44
4:B5:4391:OMG:N3	4:B5:4446:5MC:HM52	2.33	0.44
9:BC:44:LEU:HD11	9:BC:120:LYS:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:BM:53:LYS:HG2	24:BS:157:ARG:HD3	1.99	0.44
34:Bc:38:ILE:HD11	34:Bc:46:VAL:HG21	1.99	0.44
36:Be:82:VAL:HG13	36:Be:114:ARG:HG2	1.99	0.44
54:AB:71:LEU:HD11	54:AB:189:ILE:HG23	1.99	0.44
64:AL:93:LEU:HB3	64:AL:102:PHE:HB3	1.99	0.44
4:B5:654:C:H2'	4:B5:655:C:C6	2.53	0.44
4:B5:1485:C:H2'	4:B5:1486:G:H8	1.83	0.44
4:B5:3602:G:H2'	4:B5:3603:A:C8	2.52	0.44
4:B5:3712:U:H2'	4:B5:3713:G:C8	2.52	0.44
4:B5:3717:A2M:O5'	4:B5:3717:A2M:H8	2.17	0.44
39:Bh:89:ARG:O	39:Bh:93:ARG:HG2	2.18	0.44
52:A2:1272:OMC:HM22	52:A2:1273:C:H5'	1.99	0.44
52:A2:1815:A:H2'	52:A2:1816:G:C8	2.53	0.44
55:AC:209:VAL:HB	55:AC:210:PRO:HD3	1.98	0.44
76:AX:94:ILE:HD11	76:AX:130:LEU:HD11	1.99	0.44
4:B5:1377:C:H42	17:BL:160:VAL:HG22	1.82	0.44
4:B5:1491:G:H4'	33:Bb:41:ARG:HE	1.82	0.44
4:B5:4310:A:H2'	4:B5:4311:PSU:H6	1.82	0.44
4:B5:4866:G:H2'	4:B5:4867:G:H8	1.83	0.44
9:BC:7:LEU:HB3	9:BC:21:ASN:HB3	1.99	0.44
23:BR:15:LEU:HD13	23:BR:52:ARG:HB2	1.99	0.44
46:Bp:62:LYS:HE2	46:Bp:62:LYS:HB2	1.86	0.44
52:A2:678:U:H2'	52:A2:679:A:H8	1.81	0.44
52:A2:1521:C:H5'	68:AP:126:VAL:HB	2.00	0.44
52:A2:1594:A:N7	78:AZ:104:ARG:HD3	2.33	0.44
57:AE:100:ARG:HB2	57:AE:114:ILE:HD13	1.99	0.44
73:AU:17:ILE:HD13	73:AU:94:PRO:HD3	1.98	0.44
4:B5:1708:C:N4	4:B5:1709:A:H62	2.15	0.44
4:B5:5062:G:H2'	4:B5:5063:G:H8	1.82	0.44
8:BB:261:ARG:HB2	20:BO:64:THR:HG21	1.98	0.44
58:AF:74:ASN:HA	58:AF:77:MET:HE2	2.00	0.44
4:B5:1401:C:H2'	4:B5:1402:G:C8	2.53	0.44
4:B5:4295:PSU:H2'	4:B5:4296:G:C8	2.53	0.44
46:Bp:51:ALA:HB3	46:Bp:54:ILE:HD12	2.00	0.44
4:B5:699:C:H2'	4:B5:700:G:C8	2.52	0.44
4:B5:2516:A:H5'	38:Bg:62:LYS:HE3	1.99	0.44
50:Bu:97:ARG:HB2	51:Bv:105:GLU:HG2	2.00	0.44
52:A2:750:C:H2'	52:A2:751:G:C8	2.53	0.44
57:AE:71:LYS:HG2	57:AE:76:VAL:HG22	1.99	0.44
76:AX:46:HIS:CD2	76:AX:103:ALA:HB2	2.53	0.44
2:B2:63:C:H2'	2:B2:64:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B5:178:C:H2'	4:B5:179:G:H8	1.83	0.44
4:B5:1477:C:H2'	4:B5:1478:G:C8	2.53	0.44
10:BD:179:ARG:HA	10:BD:179:ARG:HD3	1.82	0.44
15:BI:87:ILE:HG12	15:BI:138:ILE:HG12	1.98	0.44
19:BN:15:GLN:HB3	40:Bi:52:PRO:HD2	1.99	0.44
22:BQ:65:ARG:O	22:BQ:69:LYS:HG2	2.18	0.44
48:Bs:20:LEU:HD22	48:Bs:52:VAL:HG11	2.00	0.44
52:A2:112:U:H5''	52:A2:113:G:H2'	1.99	0.44
52:A2:518:G:H2'	52:A2:519:A:C8	2.53	0.44
52:A2:1775:U:H2'	52:A2:1776:G:C8	2.53	0.44
55:AC:62:PRO:HG2	55:AC:68:ARG:HG2	2.00	0.44
60:AH:69:LEU:O	60:AH:73:GLN:HG2	2.17	0.44
77:AY:8:ARG:HB2	77:AY:26:ASP:HB2	2.00	0.44
4:B5:487:G:H2'	4:B5:488:G:C8	2.53	0.43
4:B5:4348:C:H4'	4:B5:4348:C:OP2	2.18	0.43
7:BA:66:PRO:HG2	7:BA:67:TYR:CE2	2.53	0.43
10:BD:197:LYS:HB3	10:BD:202:GLN:HB2	2.00	0.43
21:BP:50:ASP:HB3	21:BP:55:LYS:HB2	2.00	0.43
36:Be:23:HIS:HA	36:Be:53:ILE:HD12	2.00	0.43
45:Bo:23:VAL:HG13	45:Bo:68:LEU:HB3	2.00	0.43
48:Bs:5:ASP:HB2	48:Bs:8:THR:HG22	1.98	0.43
52:A2:223:C:H2'	52:A2:224:A:C8	2.53	0.43
52:A2:558:G:H2'	52:A2:559:G:C8	2.53	0.43
52:A2:980:A:H2'	52:A2:981:A:C8	2.53	0.43
54:AB:25:PHE:HE2	67:AO:18:GLY:HA2	1.84	0.43
60:AH:138:GLU:H	60:AH:159:ASP:HB2	1.82	0.43
4:B5:1827:C:H2'	4:B5:1828:G:H8	1.83	0.43
4:B5:4356:G:O3'	17:BL:193:GLY:HA3	2.17	0.43
4:B5:4914:G:H2'	4:B5:4915:G:H8	1.84	0.43
20:BO:12:ARG:HE	20:BO:37:ARG:NH2	2.15	0.43
21:BP:94:MET:HE1	21:BP:146:ILE:HB	1.99	0.43
52:A2:239:C:H2'	52:A2:240:G:C8	2.53	0.43
52:A2:677:G:H21	52:A2:1028:A:H62	1.67	0.43
52:A2:1587:G:C6	72:AT:67:NMM:HD2	2.54	0.43
2:B2:11:C:H2'	2:B2:12:G:C8	2.53	0.43
4:B5:1193:G:H2'	4:B5:1194:G:C8	2.53	0.43
4:B5:2092:A:H4'	4:B5:2093:G:O5'	2.19	0.43
4:B5:4296:G:H2'	4:B5:4297:A:C8	2.54	0.43
16:BJ:20:LEU:HD13	16:BJ:132:VAL:HG22	2.00	0.43
52:A2:1478:U:H2'	52:A2:1479:G:H8	1.83	0.43
52:A2:1560:U:H2'	52:A2:1561:A:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:AA:41:ARG:HE	53:AA:45:GLY:HA2	1.83	0.43
4:B5:1540:C:H5''	7:BA:21:LYS:HG2	1.99	0.43
4:B5:2769:C:H2'	4:B5:2770:G:H8	1.83	0.43
4:B5:2899:U:H2'	4:B5:2900:G:C8	2.53	0.43
5:B7:69:U:H2'	5:B7:70:G:C8	2.53	0.43
9:BC:230:LEU:HD11	9:BC:239:LYS:HB2	1.99	0.43
28:BW:8:PHE:HZ	28:BW:49:ILE:HG13	1.82	0.43
51:Bv:65:GLY:HA3	51:Bv:69:THR:HG21	2.01	0.43
52:A2:431:G:H2'	52:A2:432:G:H8	1.84	0.43
52:A2:536:A:H61	52:A2:547:G:H1	1.66	0.43
52:A2:908:A:H2'	52:A2:909:G:C8	2.53	0.43
52:A2:1536:G:H2'	52:A2:1537:A:H8	1.84	0.43
54:AB:217:MET:HE2	54:AB:220:LYS:HZ3	1.83	0.43
64:AL:4:ILE:HD12	64:AL:55:TYR:HA	2.00	0.43
66:AN:20:ARG:HH21	75:AW:56:HIS:HB3	1.83	0.43
76:AX:124:LYS:HA	76:AX:129:SER:HA	1.98	0.43
79:Aa:59:PHE:HB2	79:Aa:62:TYR:HB2	2.00	0.43
6:B8:96:C:H5''	39:Bh:66:LYS:HG2	2.00	0.43
31:BZ:67:LYS:HE2	31:BZ:67:LYS:HB3	1.81	0.43
61:AI:117:TYR:CD1	61:AI:152:ARG:HB3	2.54	0.43
2:B2:69:G:H2'	2:B2:70:G:C8	2.53	0.43
4:B5:1457:C:H5''	22:BQ:69:LYS:HE2	2.00	0.43
4:B5:3709:G:H1'	4:B5:3711:A:H62	1.82	0.43
4:B5:4253:G:H2'	4:B5:4254:A:C8	2.54	0.43
17:BL:123:LYS:HB2	39:Bh:122:LYS:HB2	2.00	0.43
37:Bf:63:LYS:HA	37:Bf:63:LYS:HD3	1.86	0.43
45:Bo:6:LYS:HE2	45:Bo:94:GLY:HA3	1.99	0.43
52:A2:535:G:H2'	52:A2:536:A:C8	2.54	0.43
53:AA:172:GLY:HA3	53:AA:203:PHE:HD1	1.83	0.43
53:AA:210:ILE:HG21	70:AR:81:ARG:HD3	2.00	0.43
4:B5:398:A2M:O5'	4:B5:398:A2M:H8	2.17	0.43
4:B5:1513:U:H2'	4:B5:1514:A:C8	2.53	0.43
4:B5:1537:U:H2'	4:B5:1538:G:H8	1.84	0.43
4:B5:2769:C:H2'	4:B5:2770:G:C8	2.54	0.43
4:B5:4487:A:H4'	4:B5:4488:G:C8	2.53	0.43
8:BB:231:VAL:HG21	8:BB:251:VAL:HG23	2.00	0.43
35:Bd:41:ARG:HG3	35:Bd:78:ARG:HA	2.00	0.43
52:A2:281:C:H41	52:A2:891:G:H1'	1.84	0.43
52:A2:1101:U:H2'	52:A2:1102:G:C8	2.54	0.43
52:A2:1412:C:H2'	52:A2:1413:G:H8	1.83	0.43
52:A2:1753:C:H2'	52:A2:1754:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:AE:151:ASP:HB3	57:AE:154:ILE:HG13	2.01	0.43
63:AK:27:VAL:HB	63:AK:43:LEU:HD13	2.00	0.43
2:B2:9:A:N3	2:B2:45:G:H2'	2.34	0.43
2:B2:67:C:H2'	2:B2:68:G:C8	2.53	0.43
4:B5:1729:U:H4'	25:BT:100:LYS:HB2	2.00	0.43
4:B5:2032:A:H2'	4:B5:2033:G:C8	2.54	0.43
4:B5:4168:G:H4'	4:B5:4170:C:C2	2.54	0.43
4:B5:4577:G:H2'	4:B5:4578:PSU:H6	1.84	0.43
4:B5:4726:A:H5'	8:BB:130:PHE:H	1.84	0.43
4:B5:5062:G:H2'	4:B5:5063:G:C8	2.54	0.43
52:A2:184:G:H2'	52:A2:185:G:C8	2.54	0.43
70:AR:34:VAL:HG12	70:AR:38:ILE:HD13	2.00	0.43
4:B5:85:G:C5	17:BL:11:LYS:HE2	2.54	0.43
4:B5:1778:PSU:H2'	4:B5:1779:A:C8	2.54	0.43
4:B5:2276:C:H5''	22:BQ:3:VAL:HG11	2.00	0.43
4:B5:2460:G:H2'	4:B5:2461:C:C6	2.54	0.43
4:B5:3731:A:H2'	4:B5:3732:A:H8	1.84	0.43
4:B5:4524:C:H5''	8:BB:245:HIC:HB2	2.00	0.43
20:BO:81:TRP:HB2	20:BO:104:VAL:HG21	2.00	0.43
52:A2:518:G:H2'	52:A2:519:A:H8	1.84	0.43
55:AC:66:LEU:HD21	55:AC:81:ILE:HD13	2.01	0.43
57:AE:124:CYS:HB3	57:AE:141:THR:HB	2.00	0.43
58:AF:28:VAL:HG13	58:AF:110:GLN:HA	2.00	0.43
2:B2:16:H2U:H2'	2:B2:16:H2U:H61	1.51	0.43
4:B5:315:G:C8	32:Ba:62:HIS:HB2	2.54	0.43
4:B5:2490:C:H2'	4:B5:2491:C:C6	2.54	0.43
4:B5:2519:C:H2'	4:B5:2520:G:C8	2.54	0.43
4:B5:3662:A:H4'	4:B5:3663:G:O5'	2.19	0.43
4:B5:3699:C:H2'	4:B5:3745:A:H61	1.84	0.43
6:B8:19:C:H2'	6:B8:20:A:C8	2.54	0.43
8:BB:77:THR:HG21	8:BB:337:VAL:HG22	2.00	0.43
32:Ba:125:LYS:HG2	32:Ba:145:VAL:HB	2.00	0.43
36:Be:8:VAL:HG23	36:Be:10:PRO:HD3	2.00	0.43
52:A2:582:U:H1'	77:AY:33:ALA:HB2	2.01	0.43
52:A2:1242:U:H4'	52:A2:1243:U:H5''	2.01	0.43
52:A2:1520:G:H5''	52:A2:1521:C:OP2	2.18	0.43
52:A2:1655:C:H2'	52:A2:1656:G:C8	2.54	0.43
52:A2:1786:U:H2'	52:A2:1787:G:C8	2.54	0.43
55:AC:65:LYS:HD3	55:AC:273:LEU:HD13	2.01	0.43
64:AL:35:ARG:HH21	64:AL:63:THR:HG21	1.84	0.43
4:B5:178:C:H2'	4:B5:179:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B5:2570:C:H2'	4:B5:2571:C:H6	1.84	0.42
9:BC:211:TYR:OH	9:BC:218:ILE:HD11	2.19	0.42
9:BC:330:PRO:HG3	12:BF:47:ARG:NH2	2.33	0.42
15:BI:57:TYR:HD1	15:BI:130:HIS:HA	1.84	0.42
52:A2:1377:U:H3'	53:AA:102:ARG:HH12	1.84	0.42
52:A2:1424:G:N2	72:AT:3:GLY:HA3	2.34	0.42
54:AB:136:ARG:HB2	54:AB:218:LEU:HD11	2.00	0.42
2:B2:26:M2G:HM23	2:B2:27:PSU:H1'	2.00	0.42
4:B5:137:G:H4'	39:Bh:98:HIS:CD2	2.54	0.42
4:B5:247:G:O2'	30:BY:128:VAL:HG11	2.19	0.42
4:B5:2567:C:H2'	4:B5:2568:G:C8	2.54	0.42
4:B5:3662:A:H1'	4:B5:3663:G:OP2	2.19	0.42
4:B5:3950:G:H22	4:B5:4060:G:H22	1.67	0.42
4:B5:4137:C:H2'	4:B5:4138:G:C8	2.53	0.42
4:B5:4397:C:H2'	4:B5:4398:U:C6	2.55	0.42
34:Bc:31:TYR:HD1	34:Bc:60:ILE:HD11	1.84	0.42
52:A2:122:G:H2'	52:A2:123:G:C8	2.55	0.42
52:A2:220:U:H2'	52:A2:221:A:C8	2.54	0.42
85:Ag:217:MET:HG2	85:Ag:229:THR:HG23	2.02	0.42
2:B2:22:G:O2'	2:B2:23:C:H5''	2.19	0.42
4:B5:257:C:H2'	4:B5:258:G:C8	2.53	0.42
4:B5:734:G:H2'	4:B5:735:G:H8	1.83	0.42
4:B5:1088:G:H2'	4:B5:1089:G:H8	1.84	0.42
4:B5:2896:G:H2'	4:B5:2897:G:H8	1.84	0.42
4:B5:4335:A:H5''	4:B5:4336:C:H5'	2.00	0.42
4:B5:4388:C:H2'	4:B5:4389:A:C8	2.55	0.42
4:B5:4569:G:H2'	4:B5:4570:A2M:H8	2.02	0.42
4:B5:4722:A:H4'	8:BB:100:ARG:HD2	2.01	0.42
4:B5:4965:A:H5'	8:BB:128:LYS:HG3	2.01	0.42
10:BD:64:ILE:HG13	10:BD:109:LEU:HD22	2.00	0.42
11:BE:57:TYR:HB3	11:BE:61:ALA:HB3	2.01	0.42
13:BG:108:GLN:O	13:BG:112:GLN:HG2	2.20	0.42
19:BN:73:ARG:HB2	19:BN:92:LEU:HD12	2.01	0.42
52:A2:477:G:H2'	52:A2:478:G:H8	1.84	0.42
52:A2:1610:G:H2'	52:A2:1611:G:H8	1.84	0.42
4:B5:477:C:H2'	4:B5:478:G:C8	2.55	0.42
4:B5:670:G:H2'	4:B5:671:G:C8	2.55	0.42
4:B5:3913:U:H3	4:B5:4377:A:H2	1.66	0.42
4:B5:3931:U:H2'	4:B5:3932:G:C8	2.54	0.42
4:B5:5001:U:H2'	4:B5:5002:U:C6	2.54	0.42
40:Bi:26:HIS:CE1	40:Bi:29:ARG:HD3	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:A2:1420:G:H2'	52:A2:1421:A:O4'	2.19	0.42
4:B5:161:G:H2'	4:B5:162:A:C8	2.54	0.42
4:B5:712:C:H5''	11:BE:139:LYS:HE3	2.01	0.42
4:B5:1698:A:H2'	4:B5:1699:G:O4'	2.19	0.42
4:B5:2409:C:H42	4:B5:2433:G:H1	1.67	0.42
4:B5:2759:G:H21	4:B5:2761:G:H22	1.68	0.42
4:B5:3945:G:H2'	4:B5:3946:A:H8	1.85	0.42
4:B5:4144:C:H2'	4:B5:4145:G:C8	2.54	0.42
4:B5:4944:G:C2	11:BE:158:ARG:HD2	2.55	0.42
6:B8:121:G:H2'	6:B8:122:G:C8	2.54	0.42
16:BJ:67:LYS:HE3	16:BJ:67:LYS:HB2	1.84	0.42
32:Ba:147:VAL:HA	40:Bi:6:PRO:HG2	2.00	0.42
36:Be:58:ILE:HD12	36:Be:58:ILE:HA	1.94	0.42
49:Bt:118:HIS:HD1	49:Bt:119:ARG:HG2	1.84	0.42
52:A2:35:C:H2'	52:A2:36:PSU:H6	1.84	0.42
55:AC:194:ARG:HD3	55:AC:196:ILE:HD11	2.01	0.42
71:AS:23:ARG:HA	78:AZ:48:VAL:HG21	2.02	0.42
2:B2:58:1MA:H1'	2:B2:60:C:H5	1.85	0.42
4:B5:456:C:H42	4:B5:700:G:H1	1.66	0.42
4:B5:739:G:H2'	4:B5:740:G:C8	2.52	0.42
4:B5:1742:A:H1'	10:BD:15:ARG:HD2	2.01	0.42
4:B5:2484:U:H3	4:B5:2492:G:H1	1.67	0.42
4:B5:3945:G:H2'	4:B5:3946:A:C8	2.54	0.42
14:BH:29:GLY:HA3	14:BH:84:VAL:HB	2.01	0.42
19:BN:178:HIS:HA	19:BN:181:HIS:NE2	2.35	0.42
42:Bk:13:LEU:HD23	42:Bk:16:ARG:HH21	1.83	0.42
52:A2:38:A:H2'	52:A2:39:A:C8	2.54	0.42
52:A2:1120:U:H2'	52:A2:1121:G:C8	2.55	0.42
52:A2:1280:G:H5''	65:AM:101:ARG:HH12	1.84	0.42
52:A2:1600:G:H4'	78:AZ:43:LYS:HE3	2.02	0.42
73:AU:54:VAL:HB	73:AU:88:LEU:HB2	2.02	0.42
85:Ag:212:LYS:HA	85:Ag:235:ILE:HG23	2.02	0.42
4:B5:1451:A:O2'	4:B5:1708:C:H4'	2.20	0.42
4:B5:1741:A:H2'	4:B5:1742:A:C8	2.54	0.42
4:B5:2032:A:H2'	4:B5:2033:G:H8	1.85	0.42
4:B5:2373:A:H5'	35:Bd:64:ILE:O	2.19	0.42
4:B5:2564:A:H3'	4:B5:2565:G:C8	2.53	0.42
4:B5:3607:A:H2'	4:B5:3608:G:C8	2.55	0.42
52:A2:527:C:H2'	52:A2:528:A:H8	1.85	0.42
52:A2:601:OMG:HM22	52:A2:602:G:H5'	2.02	0.42
58:AF:135:ARG:HD2	67:AO:66:ARG:NH2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:AH:116:ARG:HH12	60:AH:121:THR:HA	1.85	0.42
65:AM:35:ILE:HG23	84:Af:102:VAL:HG21	2.01	0.42
84:Af:100:LEU:HD22	84:Af:103:LEU:HG	2.02	0.42
20:BO:143:HIS:HA	20:BO:147:TRP:HB3	2.02	0.42
21:BP:94:MET:HE3	21:BP:94:MET:HB2	1.89	0.42
29:BX:64:SER:HB2	39:Bh:69:LEU:HD13	2.02	0.42
29:BX:87:MET:HE1	29:BX:156:ILE:HG12	2.02	0.42
41:Bj:27:TYR:HA	41:Bj:34:CYS:HA	2.01	0.42
52:A2:1753:C:H2'	52:A2:1754:G:H8	1.84	0.42
54:AB:86:LEU:HB3	54:AB:98:THR:HB	2.02	0.42
60:AH:104:PRO:HD3	60:AH:116:ARG:HE	1.84	0.42
61:AI:83:TYR:HB3	61:AI:101:ILE:HB	2.01	0.42
70:AR:20:TYR:CD1	70:AR:38:ILE:HD12	2.54	0.42
81:Ac:43:ILE:H	81:Ac:64:GLU:HG3	1.85	0.42
85:Ag:164:ILE:HG23	85:Ag:176:VAL:HG13	2.00	0.42
2:B2:28:C:H2'	2:B2:29:A:H8	1.83	0.42
4:B5:1065:G:H2'	4:B5:1066:G:H8	1.85	0.42
4:B5:1288:C:H2'	4:B5:1289:G:H8	1.83	0.42
4:B5:1343:C:H2'	4:B5:1344:A:C8	2.55	0.42
4:B5:2570:C:H2'	4:B5:2571:C:C6	2.55	0.42
4:B5:4738:C:H2'	4:B5:4739:G:C8	2.55	0.42
8:BB:206:PRO:HG2	8:BB:209:GLN:HG3	2.02	0.42
14:BH:41:ILE:HG22	14:BH:43:VAL:HG13	2.02	0.42
35:Bd:68:LEU:HA	35:Bd:108:TYR:HB2	2.02	0.42
36:Be:91:CYS:HB3	36:Be:95:TYR:HD2	1.84	0.42
47:Br:84:LYS:HB3	47:Br:84:LYS:HE2	1.85	0.42
48:Bs:13:TYR:CZ	48:Bs:17:ILE:HD11	2.55	0.42
48:Bs:58:ASN:O	48:Bs:62:ARG:HG3	2.19	0.42
52:A2:99:A2M:HM'2	52:A2:100:U:H5'	2.02	0.42
52:A2:951:C:H2'	52:A2:952:G:C8	2.55	0.42
52:A2:1574:C:H2'	52:A2:1575:G:C8	2.55	0.42
53:AA:127:PRO:HG3	53:AA:146:ALA:HB1	2.02	0.42
54:AB:89:GLU:HB3	54:AB:223:PHE:CE1	2.55	0.42
85:Ag:3:GLU:HG3	85:Ag:314:ILE:HA	2.02	0.42
52:A2:342:C:H2'	52:A2:343:A:H8	1.84	0.42
52:A2:906:U:H2'	52:A2:907:G:C8	2.54	0.42
52:A2:1037:G:H4'	52:A2:1845:A:H4'	2.02	0.42
52:A2:1320:G:H2'	52:A2:1321:G:O4'	2.19	0.42
59:AG:147:LEU:HD11	59:AG:156:TYR:HB2	2.01	0.42
71:AS:55:ARG:HB2	71:AS:58:GLU:HG3	2.01	0.42
2:B2:16:H2U:O3'	2:B2:17:A:H3'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B5:141:C:H2'	4:B5:142:G:C8	2.55	0.41
4:B5:231:U:H4'	30:BY:100:HIS:CD2	2.55	0.41
4:B5:499:G:H2'	4:B5:499:G:N3	2.34	0.41
4:B5:925:G:H2'	4:B5:926:G:C8	2.55	0.41
4:B5:1193:G:H2'	4:B5:1194:G:H8	1.83	0.41
4:B5:1784:C:H2'	4:B5:1785:A:C8	2.56	0.41
4:B5:4250:A:H5''	16:BJ:108:GLY:HA3	2.02	0.41
4:B5:4455:OMC:HM21	8:BB:241:PRO:HD3	2.02	0.41
34:Bc:28:VAL:HG21	34:Bc:37:MET:HG3	2.02	0.41
52:A2:212:C:H2'	52:A2:213:G:C8	2.55	0.41
52:A2:582:U:H2'	52:A2:583:A:C8	2.54	0.41
52:A2:794:A:H2'	52:A2:795:A:C8	2.55	0.41
52:A2:908:A:H2'	52:A2:909:G:H8	1.84	0.41
52:A2:1787:G:H2'	52:A2:1788:A:H8	1.85	0.41
53:AA:122:LEU:HB2	53:AA:142:LEU:HD21	2.02	0.41
57:AE:198:ARG:HG3	57:AE:208:VAL:HG22	2.03	0.41
85:Ag:23:THR:HG22	85:Ag:31:ILE:HG22	2.02	0.41
85:Ag:77:PHE:HB3	85:Ag:89:LEU:HD11	2.01	0.41
4:B5:1741:A:H2'	4:B5:1742:A:H8	1.85	0.41
4:B5:1787:A:H2'	15:BI:22:PHE:CZ	2.54	0.41
4:B5:4140:G:H1'	4:B5:4142:G:N2	2.35	0.41
4:B5:4965:A:H5''	8:BB:126:LYS:HD2	2.01	0.41
12:BF:136:VAL:HG23	12:BF:140:ILE:HD13	2.02	0.41
15:BI:52:MET:HE3	15:BI:152:LEU:HD22	2.01	0.41
38:Bg:56:VAL:HG13	38:Bg:72:LYS:HA	2.02	0.41
41:Bj:67:LEU:HD23	41:Bj:67:LEU:HA	1.87	0.41
52:A2:158:A:H1'	52:A2:464:A:C5	2.55	0.41
52:A2:438:G:H2'	52:A2:439:A:C8	2.54	0.41
54:AB:127:VAL:HG21	54:AB:173:THR:HA	2.02	0.41
71:AS:114:LEU:HD13	71:AS:121:ARG:HG2	2.02	0.41
4:B5:182:G:H1'	4:B5:183:C:C6	2.55	0.41
4:B5:1379:G:H4'	4:B5:1380:U:H6	1.85	0.41
4:B5:1517:A:H61	17:BL:19:GLN:HE22	1.69	0.41
4:B5:2364:OMC:HM21	4:B5:2827:U:H2'	2.01	0.41
4:B5:4106:G:H2'	4:B5:4107:G:H8	1.86	0.41
4:B5:4294:U:H2'	4:B5:4295:PSU:H6	1.85	0.41
4:B5:4909:A:H4'	8:BB:95:THR:HG22	2.02	0.41
39:Bh:31:LEU:HB3	39:Bh:47:ILE:HG12	2.02	0.41
48:Bs:57:LYS:HB3	48:Bs:60:MET:HB2	2.01	0.41
52:A2:692:G:H2'	52:A2:693:A:O4'	2.20	0.41
52:A2:755:C:H2'	52:A2:756:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:A2:1128:C:H2'	52:A2:1129:G:C8	2.55	0.41
53:AA:85:ARG:HD3	53:AA:203:PHE:O	2.20	0.41
4:B5:1201:C:H2'	4:B5:1202:G:C8	2.55	0.41
4:B5:1402:G:H2'	4:B5:1403:G:C8	2.55	0.41
4:B5:1559:A:H2'	4:B5:1560:G:C8	2.55	0.41
4:B5:1632:G:H5'	4:B5:1633:A:OP1	2.20	0.41
4:B5:2436:C:H5'	29:BX:127:LEU:HB3	2.02	0.41
4:B5:2473:G:H1	4:B5:2501:G:H2'	1.84	0.41
4:B5:3640:U:H5	4:B5:3645:A:N7	2.19	0.41
4:B5:3847:U:H2'	4:B5:3848:A:C8	2.55	0.41
4:B5:4914:G:H2'	4:B5:4915:G:C8	2.56	0.41
5:B7:74:A:N1	5:B7:100:A:H5''	2.36	0.41
8:BB:17:LEU:HD21	8:BB:235:TRP:HH2	1.85	0.41
9:BC:11:TYR:CZ	9:BC:148:PRO:HB2	2.56	0.41
22:BQ:8:ASN:ND2	22:BQ:9:LYS:HG3	2.35	0.41
31:BZ:73:LYS:HE2	31:BZ:73:LYS:HB3	1.96	0.41
35:Bd:29:ILE:O	35:Bd:33:ILE:HG12	2.21	0.41
48:Bs:21:LEU:HD13	48:Bs:75:LEU:HD21	2.01	0.41
48:Bs:102:LEU:HD21	48:Bs:187:LEU:HB2	2.02	0.41
52:A2:1183:A:H5'	86:Ah:11:ARG:HH11	1.84	0.41
52:A2:1328:OMG:HM22	52:A2:1329:U:H5'	2.03	0.41
53:AA:88:LEU:HD23	53:AA:98:PRO:HB2	2.02	0.41
61:AI:88:ASN:ND2	61:AI:205:ARG:HH21	2.18	0.41
69:AQ:76:GLY:H	69:AQ:79:ALA:HB3	1.84	0.41
85:Ag:230:LEU:HD13	85:Ag:259:TRP:CG	2.56	0.41
4:B5:1198:G:N7	25:BT:142:ARG:HD3	2.35	0.41
4:B5:1401:C:H2'	4:B5:1402:G:H8	1.85	0.41
4:B5:1941:A:N6	4:B5:2038:G:H2'	2.35	0.41
6:B8:127:U:H2'	6:B8:128:C:C6	2.55	0.41
53:AA:197:VAL:HG13	53:AA:201:LEU:HD22	2.02	0.41
4:B5:453:G:H4'	4:B5:454:U:H5'	2.02	0.41
4:B5:1297:C:H2'	4:B5:1298:G:C8	2.56	0.41
4:B5:4106:G:H2'	4:B5:4107:G:C8	2.55	0.41
4:B5:4735:C:H2'	4:B5:4736:G:H8	1.85	0.41
15:BI:61:SER:HA	15:BI:126:VAL:HG12	2.03	0.41
17:BL:12:PRO:HB2	17:BL:15:HIS:CE1	2.55	0.41
49:Bt:137:GLN:HB3	49:Bt:148:PRO:HG2	2.02	0.41
52:A2:404:G:H2'	52:A2:405:G:H8	1.86	0.41
53:AA:141:ASN:ND2	55:AC:87:PRO:HD3	2.35	0.41
63:AK:16:PHE:HE2	63:AK:89:ILE:HG22	1.84	0.41
4:B5:175:C:H2'	4:B5:176:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B5:4139:C:H2'	4:B5:4140:G:O4'	2.20	0.41
4:B5:4741:G:H2'	4:B5:4742:G:C8	2.56	0.41
6:B8:140:C:H2'	6:B8:141:C:C6	2.55	0.41
50:Bu:94:VAL:HG23	50:Bu:109:PRO:HG3	2.03	0.41
50:Bu:96:ILE:HB	50:Bu:104:PHE:HB2	2.03	0.41
52:A2:159:A2M:HM'3	52:A2:468:A2M:HM'1	2.03	0.41
52:A2:748:C:H2'	52:A2:749:U:C6	2.55	0.41
52:A2:1787:G:H2'	52:A2:1788:A:C8	2.56	0.41
57:AE:73:ASP:HA	57:AE:164:LEU:HD13	2.02	0.41
72:AT:28:LEU:HD23	72:AT:54:TYR:HD1	1.85	0.41
72:AT:76:THR:HG22	72:AT:94:ARG:HB3	2.03	0.41
4:B5:1457:C:H2'	4:B5:1458:A:O4'	2.21	0.41
4:B5:1884:G:H5''	37:Bf:20:ASN:HD21	1.86	0.41
4:B5:2082:C:H5''	4:B5:2083:C:OP2	2.21	0.41
4:B5:2413:G:H2'	4:B5:2414:OMU:H6	2.02	0.41
4:B5:4148:C:H2'	4:B5:4149:G:C8	2.56	0.41
4:B5:4219:6MZ:H8	4:B5:4219:6MZ:O5'	2.20	0.41
6:B8:15:G:C6	6:B8:16:G:N1	2.89	0.41
6:B8:70:G:H5''	30:BY:27:ARG:CZ	2.50	0.41
10:BD:53:VAL:HG11	10:BD:159:VAL:HA	2.03	0.41
25:BT:42:ILE:HD11	25:BT:74:ILE:HG21	2.02	0.41
33:Bb:101:HIS:CE1	33:Bb:104:LEU:HD13	2.55	0.41
51:Bv:105:GLU:HB2	51:Bv:117:HIS:CE1	2.45	0.41
52:A2:1414:A:H62	52:A2:1422:G:N2	2.18	0.41
52:A2:1507:G:C5	84:Af:89:LYS:HG3	2.55	0.41
52:A2:1819:A:H4'	86:Ah:13:LEU:HD21	2.03	0.41
55:AC:253:PRO:HA	55:AC:256:TRP:CE2	2.55	0.41
80:Ab:62:VAL:HG11	80:Ab:65:GLN:NE2	2.36	0.41
4:B5:699:C:H2'	4:B5:700:G:H8	1.85	0.41
4:B5:727:C:H5''	12:BF:69:ILE:HG21	2.03	0.41
4:B5:4096:G:H2'	4:B5:4097:A:C8	2.56	0.41
4:B5:4437:U:H2'	4:B5:4438:U:O4'	2.21	0.41
32:Ba:132:ARG:HA	32:Ba:135:GLU:HG2	2.03	0.41
40:Bi:73:ILE:O	40:Bi:77:VAL:HG22	2.21	0.41
52:A2:59:U:H3	52:A2:61:A:H3'	1.85	0.41
52:A2:158:A:H2'	52:A2:159:A2M:O4'	2.21	0.41
52:A2:318:A:H5'	52:A2:319:C:H5'	2.03	0.41
52:A2:493:A:H1'	52:A2:574:A:H5'	2.03	0.41
52:A2:551:U:H2'	52:A2:552:G:C8	2.56	0.41
52:A2:610:G:H2'	52:A2:611:G:H8	1.85	0.41
52:A2:940:U:H3	52:A2:1002:U:H3	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:A2:1029:G:H2'	52:A2:1030:A:C8	2.56	0.41
52:A2:1125:C:H2'	52:A2:1126:G:C8	2.56	0.41
52:A2:1622:U:H3'	52:A2:1623:A:H4'	2.01	0.41
54:AB:113:MET:HB3	54:AB:142:PHE:CE2	2.55	0.41
54:AB:168:MET:HG2	54:AB:197:ILE:HG21	2.03	0.41
56:AD:48:ILE:HB	56:AD:86:LEU:HD22	2.03	0.41
57:AE:80:ILE:HG13	57:AE:81:THR:HG23	2.03	0.41
62:AJ:117:LEU:HD21	62:AJ:154:GLN:HE21	1.85	0.41
78:AZ:74:SER:HB2	78:AZ:79:ILE:O	2.21	0.41
85:Ag:164:ILE:HD13	85:Ag:164:ILE:HA	1.90	0.41
4:B5:99:A:H4'	19:BN:181:HIS:CD2	2.56	0.41
4:B5:4374:C:H5'	4:B5:4376:G:H5'	2.01	0.41
4:B5:4576:U:H2'	4:B5:4577:G:C8	2.56	0.41
26:BU:60:VAL:HG23	26:BU:61:VAL:HG23	2.02	0.41
45:Bo:35:ALA:O	45:Bo:39:ARG:HG3	2.21	0.41
52:A2:83:A:H2	77:AY:120:THR:HG22	1.86	0.41
52:A2:1103:C:H2'	52:A2:1104:G:C8	2.55	0.41
4:B5:509:A:H5''	17:BL:163:LYS:HG3	2.03	0.40
4:B5:962:G:H21	4:B5:963:A:N6	2.19	0.40
4:B5:3771:U:H3	4:B5:3775:G:H22	1.69	0.40
4:B5:4990:U:H2'	4:B5:4991:G:C8	2.56	0.40
12:BF:241:ASN:O	12:BF:245:ARG:HG2	2.20	0.40
37:Bf:36:ARG:HB2	37:Bf:80:ASN:HA	2.03	0.40
52:A2:969:U:H2'	54:AB:10:THR:HB	2.03	0.40
75:AW:11:LEU:HD12	75:AW:74:VAL:HB	2.03	0.40
4:B5:275:C:H5''	40:Bi:36:HIS:HB2	2.03	0.40
4:B5:499:G:H3'	4:B5:500:G:H8	1.86	0.40
6:B8:67:U:H2'	6:B8:68:G:C8	2.56	0.40
12:BF:92:VAL:O	12:BF:120:GLY:HA2	2.21	0.40
18:BM:100:ARG:HA	18:BM:103:LYS:HE2	2.04	0.40
23:BR:105:LEU:HD12	23:BR:135:LYS:HE3	2.03	0.40
34:Bc:5:LYS:HA	34:Bc:8:LYS:HE2	2.04	0.40
34:Bc:32:LYS:HE2	34:Bc:32:LYS:HB3	1.94	0.40
52:A2:67:C:N3	59:AG:164:LYS:HB2	2.35	0.40
52:A2:1822:A:H2'	52:A2:1823:A:C8	2.56	0.40
75:AW:6:VAL:HG13	75:AW:29:PRO:HD2	2.02	0.40
85:Ag:36:ARG:HG2	85:Ag:65:PHE:HB3	2.03	0.40
4:B5:691:C:H2'	4:B5:692:A:C8	2.56	0.40
4:B5:1092:C:H2'	4:B5:1093:G:C8	2.56	0.40
4:B5:1364:C:O2'	4:B5:1365:G:H3'	2.20	0.40
4:B5:2072:C:H5''	12:BF:212:LYS:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BV:112:MET:HE2	27:BV:112:MET:HB3	1.93	0.40
28:BW:102:LYS:HA	28:BW:105:ARG:HG2	2.03	0.40
48:Bs:125:ALA:HA	48:Bs:154:ILE:HB	2.03	0.40
52:A2:85:A:H2'	52:A2:86:C:C6	2.57	0.40
52:A2:99:A2M:H8	52:A2:99:A2M:O5'	2.21	0.40
52:A2:1136:PSU:H2'	52:A2:1137:U:C6	2.57	0.40
52:A2:1610:G:H2'	52:A2:1611:G:C8	2.55	0.40
73:AU:20:ILE:HD12	73:AU:98:VAL:HG21	2.04	0.40
85:Ag:101:PHE:CD2	85:Ag:136:GLY:HA2	2.56	0.40
2:B2:37:T6A:H152	2:B2:38:A:N3	2.37	0.40
4:B5:1396:A:N7	32:Ba:114:LYS:HD2	2.37	0.40
4:B5:1697:C:H2'	4:B5:1698:A:C8	2.56	0.40
4:B5:2567:C:H2'	4:B5:2568:G:H8	1.85	0.40
4:B5:4645:U:H5	23:BR:62:ARG:HH21	1.70	0.40
4:B5:4759:G:H2'	4:B5:4760:G:O4'	2.22	0.40
8:BB:90:VAL:HG13	8:BB:161:ARG:HB2	2.02	0.40
19:BN:5:LYS:HG3	40:Bi:40:VAL:HG11	2.04	0.40
19:BN:27:CYS:SG	19:BN:124:ASP:HB3	2.62	0.40
23:BR:82:LYS:HA	23:BR:82:LYS:HD2	1.98	0.40
41:Bj:39:TYR:CG	41:Bj:40:PRO:HA	2.56	0.40
52:A2:752:G:H2'	52:A2:753:C:C6	2.56	0.40
52:A2:1655:C:H2'	52:A2:1656:G:H8	1.86	0.40
53:AA:136:GLU:HA	53:AA:139:TYR:HD2	1.86	0.40
56:AD:16:ILE:HG21	82:Ad:22:ARG:HH11	1.87	0.40
58:AF:100:ILE:HA	58:AF:178:ILE:HD11	2.03	0.40
79:Aa:31:PRO:HG2	79:Aa:34:LYS:HB3	2.04	0.40
79:Aa:37:LYS:HB2	79:Aa:37:LYS:HE2	1.86	0.40
4:B5:760:G:H2'	4:B5:761:G:C8	2.56	0.40
4:B5:1729:U:H1'	25:BT:101:SER:HB3	2.03	0.40
4:B5:3839:U:H2'	4:B5:3840:OMC:O4'	2.21	0.40
4:B5:4624:C:OP1	8:BB:224:LYS:HG3	2.21	0.40
17:BL:61:CYS:HA	17:BL:62:PRO:HD3	1.92	0.40
42:Bk:34:PHE:HE1	42:Bk:47:ILE:HD11	1.86	0.40
43:Bl:23:ILE:HG23	43:Bl:38:ASN:HB2	2.03	0.40
50:Bu:94:VAL:HB	50:Bu:106:ILE:HB	2.04	0.40
52:A2:430:C:H2'	52:A2:431:G:H8	1.86	0.40
52:A2:831:G:H2'	52:A2:832:G:H8	1.87	0.40
52:A2:1446:A:O2'	52:A2:1447:OMG:H8	2.04	0.40
52:A2:1844:U:H2'	52:A2:1845:A:C8	2.57	0.40
68:AP:115:TYR:HB2	68:AP:118:GLU:HG3	2.04	0.40
85:Ag:107:ASP:HB2	85:Ag:125:ARG:HH11	1.86	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	B1	32/184 (17%)	31 (97%)	1 (3%)	0	100	100
7	BA	245/257 (95%)	235 (96%)	10 (4%)	0	100	100
8	BB	399/403 (99%)	396 (99%)	3 (1%)	0	100	100
9	BC	365/427 (86%)	360 (99%)	5 (1%)	0	100	100
10	BD	291/297 (98%)	286 (98%)	5 (2%)	0	100	100
11	BE	215/288 (75%)	210 (98%)	5 (2%)	0	100	100
12	BF	224/248 (90%)	218 (97%)	6 (3%)	0	100	100
13	BG	238/266 (90%)	237 (100%)	1 (0%)	0	100	100
14	BH	188/192 (98%)	187 (100%)	1 (0%)	0	100	100
15	BI	201/214 (94%)	198 (98%)	3 (2%)	0	100	100
16	BJ	169/178 (95%)	168 (99%)	1 (1%)	0	100	100
17	BL	208/211 (99%)	202 (97%)	6 (3%)	0	100	100
18	BM	134/215 (62%)	130 (97%)	4 (3%)	0	100	100
19	BN	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
20	BO	199/203 (98%)	197 (99%)	2 (1%)	0	100	100
21	BP	151/184 (82%)	149 (99%)	2 (1%)	0	100	100
22	BQ	185/188 (98%)	182 (98%)	3 (2%)	0	100	100
23	BR	185/196 (94%)	185 (100%)	0	0	100	100
24	BS	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
25	BT	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
26	BU	102/128 (80%)	100 (98%)	2 (2%)	0	100	100
27	BV	129/140 (92%)	127 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	BW	120/157 (76%)	116 (97%)	4 (3%)	0	100	100
29	BX	124/156 (80%)	124 (100%)	0	0	100	100
30	BY	130/145 (90%)	129 (99%)	1 (1%)	0	100	100
31	BZ	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
32	Ba	144/148 (97%)	139 (96%)	4 (3%)	1 (1%)	18	41
33	Bb	94/159 (59%)	92 (98%)	2 (2%)	0	100	100
34	Bc	104/115 (90%)	104 (100%)	0	0	100	100
35	Bd	105/125 (84%)	104 (99%)	1 (1%)	0	100	100
36	Be	126/135 (93%)	125 (99%)	1 (1%)	0	100	100
37	Bf	107/110 (97%)	107 (100%)	0	0	100	100
38	Bg	107/117 (92%)	107 (100%)	0	0	100	100
39	Bh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
40	Bi	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
41	Bj	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
42	Bk	66/70 (94%)	66 (100%)	0	0	100	100
43	Bl	49/51 (96%)	49 (100%)	0	0	100	100
44	Bm	49/128 (38%)	49 (100%)	0	0	100	100
45	Bo	100/106 (94%)	97 (97%)	3 (3%)	0	100	100
46	Bp	86/92 (94%)	85 (99%)	1 (1%)	0	100	100
47	Br	122/137 (89%)	121 (99%)	1 (1%)	0	100	100
48	Bs	194/317 (61%)	188 (97%)	6 (3%)	0	100	100
49	Bt	154/165 (93%)	153 (99%)	1 (1%)	0	100	100
50	Bu	64/215 (30%)	61 (95%)	3 (5%)	0	100	100
51	Bv	107/206 (52%)	102 (95%)	5 (5%)	0	100	100
53	AA	215/295 (73%)	213 (99%)	2 (1%)	0	100	100
54	AB	219/264 (83%)	218 (100%)	1 (0%)	0	100	100
55	AC	216/293 (74%)	216 (100%)	0	0	100	100
56	AD	223/243 (92%)	222 (100%)	1 (0%)	0	100	100
57	AE	260/263 (99%)	253 (97%)	7 (3%)	0	100	100
58	AF	190/204 (93%)	182 (96%)	8 (4%)	0	100	100
59	AG	238/249 (96%)	237 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
60	AH	186/194 (96%)	183 (98%)	3 (2%)	0	100	100
61	AI	201/208 (97%)	198 (98%)	3 (2%)	0	100	100
62	AJ	178/194 (92%)	177 (99%)	1 (1%)	0	100	100
63	AK	95/165 (58%)	94 (99%)	1 (1%)	0	100	100
64	AL	149/158 (94%)	147 (99%)	2 (1%)	0	100	100
65	AM	121/132 (92%)	118 (98%)	3 (2%)	0	100	100
66	AN	147/151 (97%)	146 (99%)	1 (1%)	0	100	100
67	AO	131/151 (87%)	129 (98%)	2 (2%)	0	100	100
68	AP	125/145 (86%)	124 (99%)	1 (1%)	0	100	100
69	AQ	140/146 (96%)	138 (99%)	2 (1%)	0	100	100
70	AR	132/135 (98%)	132 (100%)	0	0	100	100
71	AS	144/152 (95%)	141 (98%)	3 (2%)	0	100	100
72	AT	141/145 (97%)	141 (100%)	0	0	100	100
73	AU	99/119 (83%)	98 (99%)	1 (1%)	0	100	100
74	AV	82/84 (98%)	82 (100%)	0	0	100	100
75	AW	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
76	AX	139/143 (97%)	138 (99%)	1 (1%)	0	100	100
77	AY	122/133 (92%)	122 (100%)	0	0	100	100
78	AZ	70/125 (56%)	68 (97%)	2 (3%)	0	100	100
79	Aa	99/115 (86%)	99 (100%)	0	0	100	100
80	Ab	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
81	Ac	63/69 (91%)	62 (98%)	1 (2%)	0	100	100
82	Ad	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
83	Ae	55/133 (41%)	53 (96%)	2 (4%)	0	100	100
84	Af	72/156 (46%)	68 (94%)	4 (6%)	0	100	100
85	Ag	312/317 (98%)	301 (96%)	11 (4%)	0	100	100
86	Ah	23/25 (92%)	23 (100%)	0	0	100	100
All	All	11826/13850 (85%)	11645 (98%)	180 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	Ba	15	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	B1	32/151 (21%)	32 (100%)	0	100	100
7	BA	189/198 (96%)	187 (99%)	2 (1%)	65	85
8	BB	347/348 (100%)	344 (99%)	3 (1%)	70	87
9	BC	305/348 (88%)	305 (100%)	0	100	100
10	BD	247/250 (99%)	245 (99%)	2 (1%)	73	88
11	BE	195/252 (77%)	193 (99%)	2 (1%)	68	86
12	BF	195/215 (91%)	195 (100%)	0	100	100
13	BG	205/223 (92%)	205 (100%)	0	100	100
14	BH	169/171 (99%)	169 (100%)	0	100	100
15	BI	175/181 (97%)	173 (99%)	2 (1%)	65	85
16	BJ	144/149 (97%)	142 (99%)	2 (1%)	59	82
17	BL	176/177 (99%)	174 (99%)	2 (1%)	65	85
18	BM	116/161 (72%)	116 (100%)	0	100	100
19	BN	171/172 (99%)	171 (100%)	0	100	100
20	BO	173/174 (99%)	172 (99%)	1 (1%)	78	91
21	BP	134/163 (82%)	132 (98%)	2 (2%)	57	81
22	BQ	164/165 (99%)	163 (99%)	1 (1%)	78	91
23	BR	166/175 (95%)	165 (99%)	1 (1%)	78	91
24	BS	157/157 (100%)	153 (98%)	4 (2%)	42	71
25	BT	139/140 (99%)	138 (99%)	1 (1%)	76	90
26	BU	94/115 (82%)	92 (98%)	2 (2%)	47	75
27	BV	101/107 (94%)	100 (99%)	1 (1%)	68	86
28	BW	101/126 (80%)	100 (99%)	1 (1%)	68	86
29	BX	113/133 (85%)	111 (98%)	2 (2%)	51	78
30	BY	123/135 (91%)	123 (100%)	0	100	100
31	BZ	117/118 (99%)	116 (99%)	1 (1%)	70	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	Ba	119/120 (99%)	118 (99%)	1 (1%)	73	88
33	Bb	82/125 (66%)	82 (100%)	0	100	100
34	Bc	90/97 (93%)	87 (97%)	3 (3%)	33	63
35	Bd	96/110 (87%)	96 (100%)	0	100	100
36	Be	114/121 (94%)	114 (100%)	0	100	100
37	Bf	88/89 (99%)	88 (100%)	0	100	100
38	Bg	94/100 (94%)	91 (97%)	3 (3%)	34	64
39	Bh	109/110 (99%)	109 (100%)	0	100	100
40	Bi	85/89 (96%)	83 (98%)	2 (2%)	43	72
41	Bj	73/80 (91%)	72 (99%)	1 (1%)	59	82
42	Bk	63/65 (97%)	62 (98%)	1 (2%)	55	80
43	Bl	48/48 (100%)	47 (98%)	1 (2%)	47	75
44	Bm	47/116 (40%)	47 (100%)	0	100	100
45	Bo	90/93 (97%)	89 (99%)	1 (1%)	65	85
46	Bp	71/75 (95%)	69 (97%)	2 (3%)	38	68
47	Br	107/120 (89%)	105 (98%)	2 (2%)	50	77
48	Bs	164/258 (64%)	159 (97%)	5 (3%)	36	66
49	Bt	128/137 (93%)	122 (95%)	6 (5%)	23	51
50	Bu	59/183 (32%)	58 (98%)	1 (2%)	53	79
51	Bv	93/165 (56%)	86 (92%)	7 (8%)	12	31
53	AA	180/242 (74%)	178 (99%)	2 (1%)	65	85
54	AB	202/231 (87%)	201 (100%)	1 (0%)	81	92
55	AC	184/225 (82%)	183 (100%)	1 (0%)	81	92
56	AD	189/202 (94%)	188 (100%)	1 (0%)	81	92
57	AE	224/225 (100%)	223 (100%)	1 (0%)	84	93
58	AF	162/170 (95%)	160 (99%)	2 (1%)	63	84
59	AG	209/218 (96%)	208 (100%)	1 (0%)	81	92
60	AH	168/174 (97%)	168 (100%)	0	100	100
61	AI	177/180 (98%)	173 (98%)	4 (2%)	44	73
62	AJ	160/168 (95%)	158 (99%)	2 (1%)	61	83
63	AK	88/136 (65%)	86 (98%)	2 (2%)	44	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
64	AL	135/142 (95%)	135 (100%)	0	100	100
65	AM	104/108 (96%)	101 (97%)	3 (3%)	37	67
66	AN	130/131 (99%)	127 (98%)	3 (2%)	44	73
67	AO	104/118 (88%)	104 (100%)	0	100	100
68	AP	113/130 (87%)	113 (100%)	0	100	100
69	AQ	117/121 (97%)	116 (99%)	1 (1%)	70	87
70	AR	121/122 (99%)	121 (100%)	0	100	100
71	AS	126/131 (96%)	123 (98%)	3 (2%)	43	72
72	AT	113/114 (99%)	113 (100%)	0	100	100
73	AU	93/107 (87%)	92 (99%)	1 (1%)	65	85
74	AV	67/67 (100%)	65 (97%)	2 (3%)	36	66
75	AW	112/113 (99%)	109 (97%)	3 (3%)	39	69
76	AX	113/114 (99%)	110 (97%)	3 (3%)	39	69
77	AY	108/115 (94%)	108 (100%)	0	100	100
78	AZ	64/103 (62%)	63 (98%)	1 (2%)	55	80
79	Aa	88/98 (90%)	88 (100%)	0	100	100
80	Ab	75/76 (99%)	75 (100%)	0	100	100
81	Ac	58/62 (94%)	58 (100%)	0	100	100
82	Ad	48/49 (98%)	48 (100%)	0	100	100
83	Ae	46/104 (44%)	46 (100%)	0	100	100
84	Af	67/140 (48%)	67 (100%)	0	100	100
85	Ag	272/275 (99%)	269 (99%)	3 (1%)	65	85
86	Ah	24/24 (100%)	24 (100%)	0	100	100
All	All	10309/11740 (88%)	10201 (99%)	108 (1%)	65	86

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	BA	32	VAL
7	BA	208	GLU
8	BB	114	CYS
8	BB	190	VAL
8	BB	344	VAL
10	BD	93	THR

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Mol	Chain	Res	Type
10	BD	259	LYS
11	BE	71	ARG
11	BE	239	LYS
15	BI	31	ILE
15	BI	121	LYS
16	BJ	58	ARG
16	BJ	128	LEU
17	BL	67	HIS
17	BL	163	LYS
20	BO	126	VAL
21	BP	2	VAL
21	BP	131	ARG
22	BQ	82	VAL
23	BR	162	ARG
24	BS	82	LEU
24	BS	157	ARG
24	BS	158	VAL
24	BS	160	ARG
25	BT	76	VAL
26	BU	22	THR
26	BU	73	THR
27	BV	131	ARG
28	BW	1	MET
29	BX	36	LYS
29	BX	40	ILE
31	BZ	24	VAL
32	Ba	117	LEU
34	Bc	17	ARG
34	Bc	106	ARG
34	Bc	108	MET
38	Bg	28	ASN
38	Bg	48	VAL
38	Bg	73	HIS
40	Bi	29	ARG
40	Bi	34	THR
41	Bj	82	THR
42	Bk	36	VAL
43	Bl	47	THR
45	Bo	73	VAL
46	Bp	52	VAL
46	Bp	60	CYS
47	Br	26	SER

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Mol	Chain	Res	Type
47	Br	46	ARG
48	Bs	44	ARG
48	Bs	52	VAL
48	Bs	54	LEU
48	Bs	59	THR
48	Bs	191	GLN
49	Bt	12	VAL
49	Bt	15	LEU
49	Bt	22	VAL
49	Bt	35	LEU
49	Bt	60	VAL
49	Bt	73	VAL
50	Bu	80	MET
51	Bv	53	GLU
51	Bv	59	GLN
51	Bv	77	VAL
51	Bv	80	THR
51	Bv	89	GLN
51	Bv	94	LYS
51	Bv	97	VAL
53	AA	110	ASN
53	AA	112	ILE
54	AB	38	MET
55	AC	91	SER
56	AD	143	ARG
57	AE	45	ILE
58	AF	41	VAL
58	AF	187	SER
59	AG	5	ILE
61	AI	56	ARG
61	AI	119	LEU
61	AI	133	GLU
61	AI	158	ILE
62	AJ	3	VAL
62	AJ	174	LYS
63	AK	47	LYS
63	AK	93	THR
65	AM	52	LEU
65	AM	62	VAL
65	AM	104	VAL
66	AN	22	VAL
66	AN	55	ARG

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Mol	Chain	Res	Type
66	AN	145	THR
69	AQ	100	VAL
71	AS	98	VAL
71	AS	131	VAL
71	AS	144	ARG
73	AU	68	THR
74	AV	22	ARG
74	AV	47	ASN
75	AW	25	VAL
75	AW	105	THR
75	AW	121	THR
76	AX	105	PHE
76	AX	119	ARG
76	AX	125	VAL
78	AZ	69	THR
85	Ag	102	VAL
85	Ag	113	PHE
85	Ag	132	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (132) such sidechains are listed below:

Mol	Chain	Res	Type
1	B1	166	GLN
7	BA	50	HIS
8	BB	25	HIS
8	BB	184	GLN
8	BB	203	GLN
8	BB	208	ASN
8	BB	275	HIS
9	BC	310	HIS
10	BD	202	GLN
10	BD	225	GLN
10	BD	250	ASN
10	BD	275	GLN
11	BE	135	GLN
12	BF	24	ASN
12	BF	39	GLN
12	BF	119	ASN
12	BF	172	ASN
12	BF	205	ASN
12	BF	239	GLN
15	BI	166	HIS

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Mol	Chain	Res	Type
16	BJ	42	GLN
16	BJ	71	HIS
16	BJ	97	ASN
16	BJ	110	GLN
16	BJ	167	GLN
17	BL	15	HIS
17	BL	19	GLN
18	BM	20	HIS
20	BO	5	GLN
20	BO	199	HIS
21	BP	34	GLN
21	BP	97	ASN
22	BQ	77	ASN
23	BR	40	GLN
24	BS	50	GLN
24	BS	125	GLN
24	BS	173	ASN
26	BU	105	ASN
28	BW	63	GLN
28	BW	68	GLN
29	BX	35	HIS
29	BX	93	ASN
29	BX	107	HIS
30	BY	14	ASN
30	BY	43	ASN
30	BY	96	HIS
32	Ba	28	HIS
33	Bb	11	ASN
34	Bc	33	GLN
35	Bd	79	ASN
35	Bd	116	ASN
37	Bf	20	ASN
39	Bh	98	HIS
40	Bi	15	HIS
40	Bi	26	HIS
41	Bj	16	HIS
41	Bj	57	ASN
43	Bl	25	GLN
44	Bm	117	HIS
45	Bo	25	GLN
45	Bo	76	ASN
47	Br	30	ASN

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Mol	Chain	Res	Type
48	Bs	34	ASN
48	Bs	81	HIS
48	Bs	127	ASN
48	Bs	179	ASN
48	Bs	191	GLN
48	Bs	195	ASN
51	Bv	59	GLN
51	Bv	117	HIS
51	Bv	124	GLN
53	AA	9	GLN
53	AA	110	ASN
53	AA	113	GLN
53	AA	141	ASN
53	AA	169	HIS
54	AB	53	GLN
54	AB	76	ASN
54	AB	118	GLN
54	AB	177	GLN
54	AB	179	ASN
54	AB	186	ASN
54	AB	202	GLN
54	AB	208	HIS
55	AC	172	ASN
55	AC	235	ASN
57	AE	17	HIS
57	AE	138	HIS
57	AE	161	GLN
57	AE	197	ASN
58	AF	203	ASN
59	AG	65	GLN
60	AH	112	ASN
60	AH	186	ASN
61	AI	52	ASN
61	AI	88	ASN
61	AI	165	GLN
62	AJ	27	GLN
64	AL	19	ASN
65	AM	19	GLN
65	AM	28	HIS
66	AN	62	GLN
66	AN	105	ASN
66	AN	138	ASN

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Mol	Chain	Res	Type
67	AO	103	ASN
69	AQ	48	GLN
69	AQ	86	GLN
70	AR	127	ASN
71	AS	72	GLN
71	AS	135	HIS
72	AT	10	ASN
72	AT	12	GLN
72	AT	42	HIS
74	AV	29	HIS
74	AV	49	GLN
75	AW	70	ASN
77	AY	85	ASN
79	Aa	17	HIS
79	Aa	86	ASN
80	Ab	9	HIS
82	Ad	10	HIS
82	Ad	26	ASN
83	Ae	111	GLN
84	Af	93	HIS
84	Af	111	ASN
85	Ag	4	GLN
85	Ag	15	ASN
85	Ag	26	GLN
85	Ag	64	HIS
85	Ag	178	ASN
85	Ag	188	HIS
85	Ag	222	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B2	75/76 (98%)	16 (21%)	0
3	B4	5/6 (83%)	1 (20%)	0
4	B5	3628/5069 (71%)	553 (15%)	21 (0%)
5	B7	118/120 (98%)	9 (7%)	1 (0%)
52	A2	1773/1869 (94%)	233 (13%)	4 (0%)
6	B8	155/157 (98%)	21 (13%)	1 (0%)
All	All	5754/7297 (78%)	833 (14%)	27 (0%)

All (833) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B2	13	C
2	B2	16	H2U
2	B2	17	A
2	B2	18	G
2	B2	19	G
2	B2	20	H2U
2	B2	21	A
2	B2	22	G
2	B2	23	C
2	B2	42	G
2	B2	46	G7M
2	B2	47	H2U
2	B2	48	5MC
2	B2	59	U
2	B2	74	C
2	B2	76	A
3	B4	46	A
4	B5	25	A
4	B5	39	A
4	B5	42	A
4	B5	48	G
4	B5	56	A
4	B5	59	A
4	B5	64	A
4	B5	65	A
4	B5	72	C
4	B5	73	A
4	B5	91	G
4	B5	98	A
4	B5	108	A
4	B5	109	G
4	B5	119	G
4	B5	132	G
4	B5	133	C
4	B5	134	G
4	B5	135	G
4	B5	136	C
4	B5	139	G
4	B5	143	C
4	B5	144	G
4	B5	152	U
4	B5	159	C
4	B5	160	G

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Mol	Chain	Res	Type
4	B5	171	U
4	B5	173	C
4	B5	174	C
4	B5	182	G
4	B5	183	C
4	B5	185	C
4	B5	186	G
4	B5	187	U
4	B5	188	G
4	B5	189	G
4	B5	190	G
4	B5	191	G
4	B5	192	G
4	B5	200	U
4	B5	217	C
4	B5	218	A
4	B5	234	G
4	B5	246	G
4	B5	254	G
4	B5	255	C
4	B5	256	G
4	B5	264	C
4	B5	265	C
4	B5	280	G
4	B5	306	A
4	B5	315	G
4	B5	316	U
4	B5	340	C
4	B5	363	A
4	B5	373	G
4	B5	387	G
4	B5	407	A
4	B5	409	G
4	B5	410	A
4	B5	412	G
4	B5	413	G
4	B5	414	C
4	B5	449	C
4	B5	450	G
4	B5	453	G
4	B5	454	U
4	B5	467	U

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Mol	Chain	Res	Type
4	B5	468	U
4	B5	483	G
4	B5	484	U
4	B5	485	C
4	B5	492	U
4	B5	493	G
4	B5	498	C
4	B5	499	G
4	B5	500	G
4	B5	501	C
4	B5	502	C
4	B5	503	C
4	B5	509	A
4	B5	510	U
4	B5	513	U
4	B5	514	U
4	B5	666	G
4	B5	667	A
4	B5	668	C
4	B5	669	C
4	B5	682	G
4	B5	696	C
4	B5	704	C
4	B5	730	G
4	B5	731	G
4	B5	738	C
4	B5	739	G
4	B5	742	G
4	B5	746	A
4	B5	750	U
4	B5	912	U
4	B5	914	A
4	B5	915	C
4	B5	916	A
4	B5	925	G
4	B5	931	A
4	B5	932	G
4	B5	933	C
4	B5	934	A
4	B5	936	U
4	B5	938	G
4	B5	942	A

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Mol	Chain	Res	Type
4	B5	943	A
4	B5	944	U
4	B5	955	A
4	B5	957	G
4	B5	958	G
4	B5	959	A
4	B5	960	G
4	B5	961	C
4	B5	962	G
4	B5	963	A
4	B5	964	G
4	B5	965	A
4	B5	966	C
4	B5	967	C
4	B5	968	C
4	B5	969	G
4	B5	970	U
4	B5	971	C
4	B5	981	U
4	B5	1071	C
4	B5	1079	C
4	B5	1084	C
4	B5	1097	G
4	B5	1172	G
4	B5	1179	C
4	B5	1180	C
4	B5	1181	C
4	B5	1182	C
4	B5	1186	G
4	B5	1198	G
4	B5	1199	G
4	B5	1200	U
4	B5	1209	C
4	B5	1210	G
4	B5	1212	G
4	B5	1213	C
4	B5	1214	C
4	B5	1216	G
4	B5	1240	C
4	B5	1265	G
4	B5	1268	G
4	B5	1269	A

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Mol	Chain	Res	Type
4	B5	1271	C
4	B5	1272	G
4	B5	1283	G
4	B5	1284	U
4	B5	1286	G
4	B5	1292	G
4	B5	1301	U
4	B5	1302	A
4	B5	1303	C
4	B5	1323	A
4	B5	1325	A2M
4	B5	1336	A
4	B5	1353	A
4	B5	1357	G
4	B5	1358	G
4	B5	1378	C
4	B5	1380	U
4	B5	1386	A
4	B5	1393	G
4	B5	1396	A
4	B5	1397	A
4	B5	1398	G
4	B5	1410	C
4	B5	1438	C
4	B5	1442	A
4	B5	1456	G
4	B5	1481	G
4	B5	1482	C
4	B5	1485	C
4	B5	1496	A
4	B5	1497	G
4	B5	1500	C
4	B5	1501	G
4	B5	1533	A2M
4	B5	1546	A
4	B5	1573	G
4	B5	1576	G
4	B5	1577	U
4	B5	1590	U
4	B5	1595	U
4	B5	1623	G
4	B5	1624	OMG

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Mol	Chain	Res	Type
4	B5	1630	A
4	B5	1632	G
4	B5	1633	A
4	B5	1640	G
4	B5	1653	G
4	B5	1660	C
4	B5	1675	C
4	B5	1676	PSU
4	B5	1679	G
4	B5	1690	G
4	B5	1696	G
4	B5	1700	A
4	B5	1701	C
4	B5	1702	C
4	B5	1703	C
4	B5	1704	G
4	B5	1706	C
4	B5	1707	G
4	B5	1709	A
4	B5	1710	C
4	B5	1712	C
4	B5	1718	A
4	B5	1719	C
4	B5	1720	G
4	B5	1741	A
4	B5	1754	C
4	B5	1767	C
4	B5	1771	C
4	B5	1780	PSU
4	B5	1786	A
4	B5	1802	G
4	B5	1803	A
4	B5	1804	A
4	B5	1819	C
4	B5	1820	G
4	B5	1821	U
4	B5	1832	G
4	B5	1833	U
4	B5	1834	G
4	B5	1835	G
4	B5	1836	A
4	B5	1841	G

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Mol	Chain	Res	Type
4	B5	1854	G
4	B5	1868	G
4	B5	1896	A
4	B5	1915	G
4	B5	1917	U
4	B5	1918	G
4	B5	1920	C
4	B5	1921	G
4	B5	1930	C
4	B5	1931	A
4	B5	1934	C
4	B5	1939	G
4	B5	1944	G
4	B5	1946	U
4	B5	1958	U
4	B5	1960	G
4	B5	1971	G
4	B5	1975	G
4	B5	1976	C
4	B5	1982	A
4	B5	1983	A
4	B5	1984	G
4	B5	1985	U
4	B5	1986	C
4	B5	1996	U
4	B5	2000	G
4	B5	2002	G
4	B5	2003	U
4	B5	2023	G
4	B5	2025	A
4	B5	2045	G
4	B5	2047	U
4	B5	2054	G
4	B5	2055	G
4	B5	2068	A
4	B5	2084	G
4	B5	2088	G
4	B5	2090	C
4	B5	2091	G
4	B5	2093	G
4	B5	2094	A
4	B5	2096	U

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Mol	Chain	Res	Type
4	B5	2097	G
4	B5	2257	C
4	B5	2258	G
4	B5	2287	G
4	B5	2288	C
4	B5	2299	A
4	B5	2300	G
4	B5	2305	G
4	B5	2312	A
4	B5	2330	G
4	B5	2331	A
4	B5	2332	G
4	B5	2344	G
4	B5	2347	G
4	B5	2350	OMC
4	B5	2359	A
4	B5	2363	OMG
4	B5	2365	A
4	B5	2394	A
4	B5	2397	U
4	B5	2420	G
4	B5	2421	OMC
4	B5	2424	U
4	B5	2462	G
4	B5	2468	C
4	B5	2469	C
4	B5	2470	G
4	B5	2474	G
4	B5	2477	C
4	B5	2488	C
4	B5	2490	C
4	B5	2502	G
4	B5	2503	C
4	B5	2504	C
4	B5	2512	A
4	B5	2518	U
4	B5	2543	G
4	B5	2544	U
4	B5	2553	U
4	B5	2572	A
4	B5	2575	G
4	B5	2582	C

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Mol	Chain	Res	Type
4	B5	2586	A
4	B5	2588	C
4	B5	2600	A
4	B5	2626	C
4	B5	2651	G
4	B5	2657	G
4	B5	2661	G
4	B5	2668	C
4	B5	2674	G
4	B5	2675	A
4	B5	2686	U
4	B5	2687	G
4	B5	2693	G
4	B5	2694	A
4	B5	2695	A
4	B5	2696	A
4	B5	2702	G
4	B5	2704	G
4	B5	2705	G
4	B5	2706	U
4	B5	2708	C
4	B5	2709	C
4	B5	2710	G
4	B5	2711	G
4	B5	2725	G
4	B5	2742	A
4	B5	2753	G
4	B5	2758	G
4	B5	2759	G
4	B5	2760	U
4	B5	2762	U
4	B5	2763	A
4	B5	2768	U
4	B5	2786	A2M
4	B5	2787	U
4	B5	2789	U
4	B5	2813	C
4	B5	2814	A2M
4	B5	2825	U
4	B5	2826	G
4	B5	2828	U
4	B5	2829	G

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Mol	Chain	Res	Type
4	B5	2854	G
4	B5	2876	G
4	B5	3595	A
4	B5	3596	G
4	B5	3614	G
4	B5	3617	C
4	B5	3618	G
4	B5	3625	G
4	B5	3634	A
4	B5	3652	A
4	B5	3661	A
4	B5	3662	A
4	B5	3663	G
4	B5	3672	C
4	B5	3673	G
4	B5	3691	A
4	B5	3710	A
4	B5	3711	A
4	B5	3734	G
4	B5	3752	G
4	B5	3759	A
4	B5	3760	C
4	B5	3761	PSU
4	B5	3762	A
4	B5	3763	U
4	B5	3775	G
4	B5	3776	G
4	B5	3783	A
4	B5	3810	G
4	B5	3811	C
4	B5	3813	U
4	B5	3816	A
4	B5	3818	G
4	B5	3837	U
4	B5	3838	G
4	B5	3839	U
4	B5	3866	A2M
4	B5	3876	A
4	B5	3877	C
4	B5	3878	G
4	B5	3891	U
4	B5	3896	G

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Mol	Chain	Res	Type
4	B5	3900	A
4	B5	3904	A
4	B5	3905	A
4	B5	3906	G
4	B5	3907	A
4	B5	3914	U
4	B5	3937	G
4	B5	3938	G
4	B5	3948	A
4	B5	4057	U
4	B5	4063	C
4	B5	4075	G
4	B5	4096	G
4	B5	4104	A
4	B5	4105	G
4	B5	4106	G
4	B5	4115	C
4	B5	4118	C
4	B5	4119	U
4	B5	4120	G
4	B5	4126	A
4	B5	4141	C
4	B5	4142	G
4	B5	4143	C
4	B5	4144	C
4	B5	4161	C
4	B5	4162	U
4	B5	4169	A
4	B5	4182	G
4	B5	4183	G
4	B5	4190	G
4	B5	4203	C
4	B5	4228	U
4	B5	4232	A
4	B5	4250	A
4	B5	4254	A
4	B5	4255	A
4	B5	4256	A
4	B5	4265	G
4	B5	4267	A
4	B5	4270	A
4	B5	4280	A

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Mol	Chain	Res	Type
4	B5	4290	G
4	B5	4303	A
4	B5	4304	G
4	B5	4305	OMU
4	B5	4325	G
4	B5	4328	G
4	B5	4329	G
4	B5	4331	C
4	B5	4338	A
4	B5	4347	A
4	B5	4348	C
4	B5	4353	U
4	B5	4370	G
4	B5	4372	G
4	B5	4376	G
4	B5	4377	A
4	B5	4379	A
4	B5	4386	C
4	B5	4393	A
4	B5	4404	G
4	B5	4421	A
4	B5	4436	U
4	B5	4437	U
4	B5	4443	C
4	B5	4447	G
4	B5	4448	A
4	B5	4463	A
4	B5	4465	C
4	B5	4474	G
4	B5	4499	PSU
4	B5	4511	U
4	B5	4512	A
4	B5	4518	C
4	B5	4522	A2M
4	B5	4523	G
4	B5	4524	C
4	B5	4531	PSU
4	B5	4547	A
4	B5	4548	G
4	B5	4559	C
4	B5	4566	G
4	B5	4572	G

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Mol	Chain	Res	Type
4	B5	4574	G
4	B5	4589	A2M
4	B5	4599	G
4	B5	4626	U
4	B5	4634	A
4	B5	4635	PSU
4	B5	4653	C
4	B5	4655	A
4	B5	4656	U
4	B5	4657	G
4	B5	4669	C
4	B5	4670	C
4	B5	4671	A
4	B5	4693	G
4	B5	4699	A
4	B5	4707	A
4	B5	4708	U
4	B5	4729	C
4	B5	4730	G
4	B5	4731	G
4	B5	4733	A
4	B5	4740	C
4	B5	4741	G
4	B5	4753	G
4	B5	4757	U
4	B5	4758	C
4	B5	4764	G
4	B5	4869	G
4	B5	4870	C
4	B5	4871	G
4	B5	4874	G
4	B5	4876	G
4	B5	4881	U
4	B5	4882	C
4	B5	4894	C
4	B5	4896	G
4	B5	4900	G
4	B5	4909	A
4	B5	4911	G
4	B5	4912	G
4	B5	4913	C
4	B5	4925	C

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Mol	Chain	Res	Type
4	B5	4926	G
4	B5	4927	C
4	B5	4936	C
4	B5	4937	A
4	B5	4942	A
4	B5	4943	C
4	B5	4944	G
4	B5	4950	G
4	B5	4965	A
4	B5	4975	U
4	B5	5013	A
4	B5	5016	G
4	B5	5021	U
4	B5	5022	C
4	B5	5023	C
4	B5	5024	C
4	B5	5025	U
4	B5	5026	C
4	B5	5027	G
4	B5	5040	G
4	B5	5049	C
4	B5	5061	G
4	B5	5068	U
5	B7	7	G
5	B7	12	U
5	B7	22	A
5	B7	50	A
5	B7	53	U
5	B7	54	A
5	B7	63	C
5	B7	64	G
5	B7	110	G
6	B8	2	G
6	B8	23	C
6	B8	34	U
6	B8	35	C
6	B8	39	G
6	B8	59	A
6	B8	60	G
6	B8	62	A
6	B8	63	U
6	B8	83	C

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Mol	Chain	Res	Type
6	B8	84	A
6	B8	85	U
6	B8	86	U
6	B8	87	G
6	B8	94	G
6	B8	103	A
6	B8	105	C
6	B8	111	U
6	B8	112	G
6	B8	114	G
6	B8	150	C
52	A2	2	A
52	A2	4	C
52	A2	26	U
52	A2	33	G
52	A2	41	G
52	A2	46	A
52	A2	58	C
52	A2	64	A
52	A2	65	C
52	A2	67	C
52	A2	68	A
52	A2	75	G
52	A2	76	U
52	A2	79	A
52	A2	103	A
52	A2	113	G
52	A2	114	G
52	A2	115	U
52	A2	126	G
52	A2	128	U
52	A2	129	C
52	A2	130	G
52	A2	143	U
52	A2	155	G
52	A2	163	U
52	A2	168	C
52	A2	182	C
52	A2	184	G
52	A2	215	G
52	A2	226	A
52	A2	227	U

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Mol	Chain	Res	Type
52	A2	228	C
52	A2	280	G
52	A2	286	U
52	A2	294	U
52	A2	302	A
52	A2	305	U
52	A2	306	C
52	A2	307	G
52	A2	308	G
52	A2	312	G
52	A2	318	A
52	A2	319	C
52	A2	328	U
52	A2	329	G
52	A2	330	G
52	A2	347	G
52	A2	364	A
52	A2	369	C
52	A2	370	G
52	A2	385	G
52	A2	386	C
52	A2	400	C
52	A2	407	G
52	A2	409	C
52	A2	418	A
52	A2	426	A
52	A2	448	A
52	A2	450	C
52	A2	464	A
52	A2	472	C
52	A2	482	G
52	A2	485	A
52	A2	487	U
52	A2	492	C
52	A2	493	A
52	A2	508	A
52	A2	512	A2M
52	A2	516	A
52	A2	517	OMC
52	A2	525	A
52	A2	543	C
52	A2	548	C

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Mol	Chain	Res	Type
52	A2	549	C
52	A2	555	A
52	A2	556	U
52	A2	587	A
52	A2	588	G
52	A2	589	G
52	A2	591	U
52	A2	604	A
52	A2	606	G
52	A2	607	U
52	A2	608	C
52	A2	614	C
52	A2	627	OMU
52	A2	628	A
52	A2	643	A
52	A2	644	OMG
52	A2	655	A
52	A2	656	G
52	A2	660	C
52	A2	668	A2M
52	A2	669	A
52	A2	684	G
52	A2	688	U
52	A2	689	U
52	A2	690	G
52	A2	798	G
52	A2	799	OMU
52	A2	811	A
52	A2	821	G
52	A2	822	PSU
52	A2	827	A
52	A2	830	A
52	A2	831	G
52	A2	835	C
52	A2	836	G
52	A2	837	A
52	A2	839	C
52	A2	840	C
52	A2	841	G
52	A2	847	A
52	A2	851	C
52	A2	852	G

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Mol	Chain	Res	Type
52	A2	853	C
52	A2	861	A
52	A2	869	A
52	A2	870	A
52	A2	872	A
52	A2	891	G
52	A2	913	A
52	A2	919	A
52	A2	920	A
52	A2	922	A
52	A2	933	G
52	A2	943	U
52	A2	954	U
52	A2	955	A
52	A2	970	G
52	A2	971	G
52	A2	990	A
52	A2	992	A
52	A2	1023	A
52	A2	1061	U
52	A2	1062	A
52	A2	1083	A
52	A2	1085	C
52	A2	1086	G
52	A2	1138	C
52	A2	1144	A
52	A2	1149	A
52	A2	1154	U
52	A2	1171	G
52	A2	1195	A
52	A2	1207	G
52	A2	1215	C
52	A2	1217	A
52	A2	1224	G
52	A2	1242	U
52	A2	1250	A
52	A2	1251	A
52	A2	1253	A
52	A2	1256	G
52	A2	1257	G
52	A2	1259	A
52	A2	1274	G

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Mol	Chain	Res	Type
52	A2	1275	G
52	A2	1286	G
52	A2	1287	A
52	A2	1302	G
52	A2	1303	C
52	A2	1312	G
52	A2	1313	A
52	A2	1315	U
52	A2	1327	G
52	A2	1341	C
52	A2	1342	U
52	A2	1343	U
52	A2	1344	A
52	A2	1358	U
52	A2	1371	U
52	A2	1372	U
52	A2	1378	A
52	A2	1382	A
52	A2	1403	C
52	A2	1404	U
52	A2	1418	C
52	A2	1422	G
52	A2	1423	C
52	A2	1424	G
52	A2	1433	C
52	A2	1435	C
52	A2	1438	A
52	A2	1454	A
52	A2	1463	U
52	A2	1466	G
52	A2	1477	U
52	A2	1489	A
52	A2	1490	OMG
52	A2	1497	G
52	A2	1507	G
52	A2	1521	C
52	A2	1522	A
52	A2	1552	G
52	A2	1553	C
52	A2	1554	C
52	A2	1558	C
52	A2	1570	G

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Mol	Chain	Res	Type
52	A2	1579	A
52	A2	1580	A
52	A2	1585	U
52	A2	1601	A
52	A2	1606	G
52	A2	1621	U
52	A2	1623	A
52	A2	1632	G
52	A2	1639	G7M
52	A2	1665	G
52	A2	1671	G
52	A2	1675	A
52	A2	1680	G
52	A2	1699	A
52	A2	1721	U
52	A2	1722	G
52	A2	1744	G
52	A2	1765	C
52	A2	1767	C
52	A2	1777	G
52	A2	1783	C
52	A2	1784	G
52	A2	1829	G
52	A2	1831	A
52	A2	1835	A
52	A2	1836	G
52	A2	1838	U
52	A2	1849	G
52	A2	1851	MA6
52	A2	1861	G
52	A2	1862	G
52	A2	1863	A
52	A2	1865	C
52	A2	1869	A

All (27) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	B5	134	G
4	B5	245	C
4	B5	406	C
4	B5	452	A

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Mol	Chain	Res	Type
4	B5	667	A
4	B5	913	U
4	B5	966	C
4	B5	1632	G
4	B5	2674	G
4	B5	2710	G
4	B5	2759	G
4	B5	3662	A
4	B5	3751	C
4	B5	3904	A
4	B5	4056	C
4	B5	4141	C
4	B5	4255	A
4	B5	4347	A
4	B5	4652	C
4	B5	4698	U
4	B5	4895	G
5	B7	11	A
6	B8	82	A
52	A2	306	C
52	A2	688	U
52	A2	836	G
52	A2	1782	G

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

240 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	$\# Z > 2$
52	4AC	A2	1842	52	21,24,25	1.06	1 (4%)	29,34,37	1.26	3 (10%)
4	PSU	B5	5000	4	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
4	PSU	B5	4575	4	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
4	PSU	B5	4352	4	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OMG	B5	4227	4	23,26,27	1.18	3 (13%)	33,38,41	1.92	6 (18%)
4	OMG	B5	1521	4	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
4	OMG	B5	3791	4	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
52	OMG	A2	1328	87,52	23,26,27	1.18	3 (13%)	33,38,41	1.96	6 (18%)
52	PSU	A2	822	52	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
4	PSU	B5	4470	4	18,21,22	1.37	2 (11%)	22,30,33	1.87	3 (13%)
4	A2M	B5	3723	4	22,25,26	1.45	4 (18%)	31,36,39	2.10	9 (29%)
4	PSU	B5	1859	4	18,21,22	1.36	2 (11%)	22,30,33	1.93	3 (13%)
4	OMG	B5	1315	87,4	23,26,27	1.21	3 (13%)	33,38,41	1.91	6 (18%)
4	OMG	B5	4498	4	23,26,27	1.19	3 (13%)	33,38,41	1.95	6 (18%)
52	PSU	A2	218	52	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
52	OMU	A2	172	52	19,22,23	1.22	3 (15%)	26,31,34	1.74	5 (19%)
4	PSU	B5	4972	4	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
52	A2M	A2	1383	52	22,25,26	1.48	4 (18%)	31,36,39	2.12	10 (32%)
4	PSU	B5	3769	4	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
52	PSU	A2	1004	52	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
52	PSU	A2	1692	52	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
52	OMU	A2	1804	52	19,22,23	1.24	3 (15%)	26,31,34	1.66	5 (19%)
52	PSU	A2	1643	52	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
4	OMG	B5	3626	4	23,26,27	1.19	3 (13%)	33,38,41	1.95	6 (18%)
4	OMC	B5	4455	4	19,22,23	0.80	0	26,31,34	0.75	0
4	OMG	B5	3743	4	23,26,27	1.21	3 (13%)	33,38,41	1.93	6 (18%)
52	PSU	A2	1367	52	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
4	PSU	B5	4292	4	18,21,22	1.35	2 (11%)	22,30,33	1.87	4 (18%)
52	OMC	A2	517	52	19,22,23	0.83	0	26,31,34	0.93	1 (3%)
4	A2M	B5	2400	4	22,25,26	1.44	4 (18%)	31,36,39	2.13	10 (32%)
5	GTP	B7	1	5	30,34,34	0.50	0	46,54,54	0.51	0
4	PSU	B5	3883	4	18,21,22	1.38	2 (11%)	22,30,33	1.88	3 (13%)
52	PSU	A2	681	52	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
4	OMG	B5	2423	4	23,26,27	1.19	3 (13%)	33,38,41	1.95	7 (21%)
4	A2M	B5	400	4	22,25,26	1.46	4 (18%)	31,36,39	2.05	8 (25%)
52	OMG	A2	1447	52	23,26,27	1.19	3 (13%)	33,38,41	1.97	6 (18%)
52	OMG	A2	509	87,52	23,26,27	1.20	3 (13%)	33,38,41	1.97	6 (18%)
52	A2M	A2	166	52	22,25,26	1.47	4 (18%)	31,36,39	2.19	10 (32%)
4	PSU	B5	4402	4	18,21,22	1.34	2 (11%)	22,30,33	1.91	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	OMU	A2	116	52	19,22,23	1.21	2 (10%)	26,31,34	1.69	4 (15%)
2	H2U	B2	16	2	18,21,22	1.07	2 (11%)	21,30,33	2.07	1 (4%)
52	PSU	A2	609	52	18,21,22	1.34	2 (11%)	22,30,33	1.83	3 (13%)
2	1MA	B2	58	2	21,25,26	1.40	4 (19%)	31,37,40	1.73	5 (16%)
4	PSU	B5	1791	4	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
4	A2M	B5	3866	4	22,25,26	1.45	4 (18%)	31,36,39	2.11	10 (32%)
4	OMG	B5	3943	4	23,26,27	1.19	3 (13%)	33,38,41	1.95	6 (18%)
52	PSU	A2	36	52	18,21,22	1.36	2 (11%)	22,30,33	1.82	3 (13%)
52	PSU	A2	210	52	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
4	PSU	B5	4422	4	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
52	PSU	A2	34	52	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
52	OMU	A2	1288	52	19,22,23	1.22	3 (15%)	26,31,34	1.66	5 (19%)
4	PSU	B5	4295	4	18,21,22	1.32	2 (11%)	22,30,33	1.89	3 (13%)
4	PSU	B5	4311	4	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
4	PSU	B5	2842	4	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
52	PSU	A2	866	52	18,21,22	1.35	2 (11%)	22,30,33	1.83	3 (13%)
52	PSU	A2	1445	52	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
4	A2M	B5	4522	87,4	22,25,26	1.43	4 (18%)	31,36,39	2.19	10 (32%)
2	H2U	B2	20	2	18,21,22	1.00	2 (11%)	21,30,33	2.34	1 (4%)
4	OMU	B5	2414	4	19,22,23	1.24	3 (15%)	26,31,34	1.72	4 (15%)
2	2MG	B2	6	2	23,26,27	1.27	4 (17%)	32,38,41	2.19	6 (18%)
52	OMU	A2	627	52	19,22,23	1.19	3 (15%)	26,31,34	1.71	5 (19%)
2	PSU	B2	27	2	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
8	HIC	BB	245	8	10,11,12	0.60	0	8,14,16	0.40	0
52	MA6	A2	1850	52	23,26,27	2.25	5 (21%)	34,38,41	3.72	14 (41%)
45	MLZ	B _o	53	45	8,9,10	0.50	0	4,9,11	0.11	0
52	OMG	A2	644	52	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
6	PSU	B8	69	6	18,21,22	1.34	2 (11%)	22,30,33	1.88	4 (18%)
4	PSU	B5	2507	4	18,21,22	1.35	2 (11%)	22,30,33	1.90	4 (18%)
4	PSU	B5	3761	4	18,21,22	1.33	2 (11%)	22,30,33	1.90	5 (22%)
4	PSU	B5	4635	4	18,21,22	1.35	2 (11%)	22,30,33	1.93	4 (18%)
52	PSU	A2	966	52	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
4	A2M	B5	3784	4	22,25,26	1.42	4 (18%)	31,36,39	2.24	11 (35%)
4	A2M	B5	2786	87,4	22,25,26	1.43	4 (18%)	31,36,39	2.20	8 (25%)
2	OMC	B2	34	2,3	19,22,23	0.27	0	26,31,34	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PSU	B5	4360	4	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
4	PSU	B5	3636	4	18,21,22	1.36	3 (16%)	22,30,33	1.89	3 (13%)
52	OMC	A2	462	52	19,22,23	0.82	0	26,31,34	0.81	0
52	PSU	A2	572	52	18,21,22	1.36	2 (11%)	22,30,33	1.83	3 (13%)
4	PSU	B5	4578	4	18,21,22	1.37	2 (11%)	22,30,33	1.87	3 (13%)
4	OMU	B5	2836	4	19,22,23	1.23	2 (10%)	26,31,34	1.72	4 (15%)
4	OMC	B5	2421	87,4	19,22,23	0.81	0	26,31,34	0.85	1 (3%)
4	OMG	B5	3898	87,4	23,26,27	1.19	3 (13%)	33,38,41	1.97	7 (21%)
4	OMU	B5	4226	4	19,22,23	1.25	3 (15%)	26,31,34	1.71	4 (15%)
52	A2M	A2	668	87,52	22,25,26	1.47	4 (18%)	31,36,39	2.11	9 (29%)
52	PSU	A2	1177	52	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
52	4AC	A2	1337	52	21,24,25	1.08	2 (9%)	29,34,37	1.20	3 (10%)
2	5MC	B2	48	2	18,22,23	0.95	2 (11%)	26,32,35	1.16	2 (7%)
4	OMU	B5	4305	4	19,22,23	1.24	3 (15%)	26,31,34	1.67	4 (15%)
4	1MA	B5	1321	87,4	21,25,26	1.37	4 (19%)	31,37,40	1.69	6 (19%)
52	A2M	A2	1031	52	22,25,26	1.47	4 (18%)	31,36,39	2.09	9 (29%)
4	A2M	B5	4589	4	22,25,26	1.46	4 (18%)	31,36,39	2.08	9 (29%)
4	PSU	B5	1743	4	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
4	OMC	B5	2860	4	19,22,23	0.81	0	26,31,34	0.83	1 (3%)
33	MLZ	Bb	5	33	8,9,10	0.50	0	4,9,11	0.13	0
4	PSU	B5	4688	4	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
4	OMG	B5	4369	4	23,26,27	1.20	3 (13%)	33,38,41	1.90	6 (18%)
4	PSU	B5	1781	4	18,21,22	1.34	2 (11%)	22,30,33	1.89	4 (18%)
4	PSU	B5	3638	4	18,21,22	1.38	2 (11%)	22,30,33	1.87	3 (13%)
52	A2M	A2	27	52	22,25,26	1.48	4 (18%)	31,36,39	2.13	10 (32%)
52	A2M	A2	512	52	22,25,26	1.47	4 (18%)	31,36,39	2.12	9 (29%)
52	PSU	A2	105	52	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
52	MA6	A2	1851	52	23,26,27	2.25	5 (21%)	34,38,41	3.67	13 (38%)
52	OMG	A2	601	52	23,26,27	1.19	3 (13%)	33,38,41	1.92	6 (18%)
52	PSU	A2	651	52	18,21,22	1.33	2 (11%)	22,30,33	1.90	3 (13%)
52	A2M	A2	468	52	22,25,26	1.48	4 (18%)	31,36,39	2.09	9 (29%)
2	T6A	B2	37	2	31,34,35	0.47	0	44,49,52	0.60	1 (2%)
52	OMC	A2	1272	52	19,22,23	0.82	0	26,31,34	0.80	0
52	OMG	A2	867	52	23,26,27	1.19	3 (13%)	33,38,41	1.97	7 (21%)
4	PSU	B5	1861	4	18,21,22	1.34	2 (11%)	22,30,33	1.90	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OMG	B5	4636	4	23,26,27	1.19	3 (13%)	33,38,41	1.92	6 (18%)
52	PSU	A2	1056	52	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
52	PSU	A2	863	52	18,21,22	1.34	2 (11%)	22,30,33	1.84	3 (13%)
4	OMC	B5	2350	87,4	19,22,23	0.82	0	26,31,34	0.96	2 (7%)
4	OMG	B5	4195	2,4	23,26,27	1.20	3 (13%)	33,38,41	1.98	7 (21%)
4	A2M	B5	2362	87,4	22,25,26	1.45	4 (18%)	31,36,39	2.11	9 (29%)
4	PSU	B5	3694	4	18,21,22	1.36	2 (11%)	22,30,33	1.91	4 (18%)
4	OMC	B5	3886	4	19,22,23	0.81	0	26,31,34	0.88	0
4	A2M	B5	1325	4	22,25,26	1.44	4 (18%)	31,36,39	2.11	10 (32%)
4	PSU	B5	4551	4	18,21,22	1.35	2 (11%)	22,30,33	1.90	4 (18%)
52	PSU	A2	815	52	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
52	PSU	A2	1625	52	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
52	A2M	A2	484	52	22,25,26	1.48	4 (18%)	31,36,39	2.16	9 (29%)
4	OMC	B5	2364	4	19,22,23	0.80	0	26,31,34	0.77	0
4	PSU	B5	4520	87,4	18,21,22	1.35	2 (11%)	22,30,33	1.94	4 (18%)
6	OMU	B8	14	6,4	19,22,23	1.23	3 (15%)	26,31,34	1.72	5 (19%)
52	PSU	A2	1046	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
2	M2G	B2	26	2	24,27,28	1.31	4 (16%)	35,40,43	1.85	6 (17%)
4	OMG	B5	1624	4	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
52	OMC	A2	797	52	19,22,23	0.81	0	26,31,34	0.81	0
2	PSU	B2	55	2	18,21,22	1.34	2 (11%)	22,30,33	1.82	3 (13%)
52	OMC	A2	174	52	19,22,23	0.82	0	26,31,34	0.82	0
4	OMC	B5	3700	87,4	19,22,23	0.79	0	26,31,34	0.75	0
4	OMU	B5	3924	4	19,22,23	1.23	2 (10%)	26,31,34	1.71	4 (15%)
4	PSU	B5	4441	4	18,21,22	1.35	2 (11%)	22,30,33	1.92	4 (18%)
4	PSU	B5	4430	4	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
4	6MZ	B5	4219	4	22,25,26	1.46	4 (18%)	30,36,39	2.26	9 (30%)
4	PSU	B5	2631	4	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
2	H2U	B2	47	2	18,21,22	1.01	2 (11%)	21,30,33	1.94	1 (4%)
4	A2M	B5	1870	4	22,25,26	1.46	4 (18%)	31,36,39	2.12	10 (32%)
52	A2M	A2	99	87,52	22,25,26	1.48	4 (18%)	31,36,39	2.17	8 (25%)
52	A2M	A2	576	52	22,25,26	1.46	4 (18%)	31,36,39	2.12	10 (32%)
6	OMG	B8	75	6	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
52	OMC	A2	1391	52	19,22,23	0.82	0	26,31,34	0.81	0
52	PSU	A2	1174	52	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
4	UY1	B5	3817	87,4	19,22,23	1.35	3 (15%)	22,31,34	1.79	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OMG	B5	4617	4	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
4	A2M	B5	1523	4	22,25,26	1.45	4 (18%)	31,36,39	2.08	9 (29%)
52	PSU	A2	1136	52	18,21,22	1.33	2 (11%)	22,30,33	1.90	4 (18%)
52	A2M	A2	590	52	22,25,26	1.48	4 (18%)	31,36,39	2.19	7 (22%)
4	PSU	B5	1778	4	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
4	A2M	B5	3824	4	22,25,26	1.46	4 (18%)	31,36,39	2.11	10 (32%)
4	OMC	B5	2823	4	19,22,23	0.81	0	26,31,34	0.82	0
4	PSU	B5	3714	4	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
4	PSU	B5	4971	4	18,21,22	1.35	2 (11%)	22,30,33	1.91	4 (18%)
52	OMU	A2	1326	87,52	19,22,23	1.18	2 (10%)	26,31,34	1.71	5 (19%)
52	PSU	A2	1232	52	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
4	OMC	B5	1880	87,4	19,22,23	0.80	0	26,31,34	0.80	0
4	OMC	B5	3807	4	19,22,23	0.81	0	26,31,34	0.81	1 (3%)
4	PSU	B5	1682	4	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
4	PSU	B5	3767	4	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
52	OMU	A2	354	52	19,22,23	1.21	4 (21%)	26,31,34	1.68	5 (19%)
2	G7M	B2	46	2	23,26,27	3.09	8 (34%)	35,39,42	3.35	15 (42%)
4	PSU	B5	1535	4	18,21,22	1.37	2 (11%)	22,30,33	1.91	3 (13%)
4	A2M	B5	3829	4	22,25,26	1.46	4 (18%)	31,36,39	2.11	9 (29%)
52	PSU	A2	1045	52	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
4	PSU	B5	4627	4	18,21,22	1.35	2 (11%)	22,30,33	1.94	3 (13%)
4	5MC	B5	3781	87,4	18,22,23	0.95	2 (11%)	26,32,35	1.19	3 (11%)
4	PSU	B5	3843	4	18,21,22	1.39	2 (11%)	22,30,33	1.86	3 (13%)
67	IAS	AO	138	67	6,7,8	0.95	0	6,8,10	1.32	1 (16%)
52	PSU	A2	93	52	18,21,22	1.35	2 (11%)	22,30,33	1.83	3 (13%)
52	PSU	A2	109	52	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
4	PSU	B5	4492	87,4	18,21,22	1.33	2 (11%)	22,30,33	1.90	3 (13%)
76	HY3	AX	62	76	6,8,9	8.06	4 (66%)	5,10,12	1.09	0
52	PSU	A2	649	52	18,21,22	1.33	2 (11%)	22,30,33	1.86	3 (13%)
52	PSU	A2	1244	87,52	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
2	PSU	B2	39	2	18,21,22	0.90	1 (5%)	22,30,33	0.63	0
52	PSU	A2	1081	52	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
4	PSU	B5	5009	4	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
52	OMU	A2	121	52	19,22,23	1.21	3 (15%)	26,31,34	1.64	4 (15%)
4	PSU	B5	3729	4	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	PSU	A2	814	52	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
4	OMG	B5	2875	4	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
4	PSU	B5	1780	4	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
4	OMU	B5	4497	87,4	19,22,23	1.19	2 (10%)	26,31,34	1.74	5 (19%)
4	OMG	B5	4622	4	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
52	G7M	A2	1639	2,52	23,26,27	3.13	9 (39%)	35,39,42	3.31	13 (37%)
52	6MZ	A2	1832	87,52	22,25,26	1.48	4 (18%)	30,36,39	2.22	9 (30%)
4	OMG	B5	4493	4	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
4	OMC	B5	4535	4	19,22,23	0.82	0	26,31,34	0.83	0
52	PSU	A2	1347	52	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
52	B8N	A2	1248	52	24,29,30	1.30	3 (12%)	29,42,45	1.30	3 (10%)
6	PSU	B8	55	6	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
52	OMU	A2	799	52	19,22,23	1.21	4 (21%)	26,31,34	1.69	5 (19%)
52	OMG	A2	1490	87,52	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
52	PSU	A2	686	52	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
4	PSU	B5	3919	87,4	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
4	OMC	B5	3868	4	19,22,23	0.81	0	26,31,34	0.77	0
4	PSU	B5	4531	4	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
7	V5N	BA	216	7	9,11,12	2.07	2 (22%)	9,14,16	1.73	2 (22%)
4	PSU	B5	3821	4	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
4	PSU	B5	4456	4	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
32	V5N	Ba	39	32	9,11,12	2.07	2 (22%)	9,14,16	1.81	2 (22%)
4	A2M	B5	4570	4	22,25,26	1.46	4 (18%)	31,36,39	2.14	9 (29%)
4	OMG	B5	2363	87,4	23,26,27	1.18	3 (13%)	33,38,41	1.95	6 (18%)
52	A2M	A2	159	52	22,25,26	1.48	4 (18%)	31,36,39	2.09	9 (29%)
52	OMG	A2	436	52	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
52	OMU	A2	428	52	19,22,23	1.21	3 (15%)	26,31,34	1.72	5 (19%)
72	NMM	AT	67	72	9,11,12	0.60	0	6,12,14	0.48	0
2	5MU	B2	54	2	19,22,23	1.44	6 (31%)	28,32,35	2.00	6 (21%)
4	PSU	B5	1676	4	18,21,22	1.37	2 (11%)	22,30,33	1.85	4 (18%)
4	PSU	B5	3852	87,4	18,21,22	1.35	2 (11%)	22,30,33	1.91	4 (18%)
4	PSU	B5	2838	4	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
4	5MC	B5	4446	87,4	18,22,23	1.00	2 (11%)	26,32,35	1.21	2 (7%)
4	A2M	B5	2814	87,4	22,25,26	1.46	4 (18%)	31,36,39	2.13	9 (29%)
52	OMG	A2	683	52	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
4	PSU	B5	4298	4	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
4	A2M	B5	1322	4	22,25,26	1.46	4 (18%)	31,36,39	2.12	8 (25%)
4	PSU	B5	3850	4	18,21,22	1.38	2 (11%)	22,30,33	1.88	3 (13%)
4	PSU	B5	4499	4	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
4	PSU	B5	4672	4	18,21,22	1.39	2 (11%)	22,30,33	1.88	3 (13%)
52	OMU	A2	1442	87,52	19,22,23	1.21	3 (15%)	26,31,34	1.68	5 (19%)
4	OMC	B5	1339	4	19,22,23	0.82	0	26,31,34	0.78	0
4	OMG	B5	4391	4	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
52	PSU	A2	801	52	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
4	A2M	B5	1533	87,4	22,25,26	1.46	4 (18%)	31,36,39	2.08	8 (25%)
52	PSU	A2	406	52	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
4	PSU	B5	1581	4	18,21,22	1.38	2 (11%)	22,30,33	1.85	3 (13%)
4	A2M	B5	3717	4	22,25,26	1.48	4 (18%)	31,36,39	2.07	9 (29%)
2	PSU	B2	31	2	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
4	UR3	B5	4529	4	19,22,23	0.99	1 (5%)	26,32,35	1.43	1 (3%)
52	A2M	A2	1678	52	22,25,26	1.46	4 (18%)	31,36,39	2.26	10 (32%)
4	OMC	B5	3840	4	19,22,23	0.81	0	26,31,34	0.83	0
52	PSU	A2	296	52	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
52	OMC	A2	1703	52	19,22,23	0.82	0	26,31,34	0.83	1 (3%)
52	PSU	A2	119	52	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
52	PSU	A2	1238	52	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
4	A2M	B5	398	4	22,25,26	1.45	4 (18%)	31,36,39	2.16	9 (29%)
2	2MG	B2	10	2	23,26,27	1.27	4 (17%)	32,38,41	2.25	6 (18%)
4	OMC	B5	2803	4	19,22,23	0.83	0	26,31,34	0.81	0
4	OMU	B5	4619	4	19,22,23	1.22	3 (15%)	26,31,34	1.70	4 (15%)

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
52	4AC	A2	1842	52	-	4/11/29/30	0/2/2/2
4	PSU	B5	5000	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	4575	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	4352	4	-	0/7/25/26	0/2/2/2
4	OMG	B5	4227	4	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OMG	B5	1521	4	-	0/9/27/28	0/3/3/3
4	OMG	B5	3791	4	-	0/9/27/28	0/3/3/3
52	OMG	A2	1328	87,52	-	0/9/27/28	0/3/3/3
52	PSU	A2	822	52	-	1/7/25/26	0/2/2/2
4	PSU	B5	4470	4	-	0/7/25/26	0/2/2/2
4	A2M	B5	3723	4	-	0/9/27/28	0/3/3/3
4	PSU	B5	1859	4	-	0/7/25/26	0/2/2/2
4	OMG	B5	1315	87,4	-	2/9/27/28	0/3/3/3
4	OMG	B5	4498	4	-	0/9/27/28	0/3/3/3
52	PSU	A2	218	52	-	0/7/25/26	0/2/2/2
52	OMU	A2	172	52	-	0/9/27/28	0/2/2/2
4	PSU	B5	4972	4	-	0/7/25/26	0/2/2/2
52	A2M	A2	1383	52	-	0/9/27/28	0/3/3/3
4	PSU	B5	3769	4	-	0/7/25/26	0/2/2/2
52	PSU	A2	1004	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	1692	52	-	0/7/25/26	0/2/2/2
52	OMU	A2	1804	52	-	0/9/27/28	0/2/2/2
52	PSU	A2	1643	52	-	0/7/25/26	0/2/2/2
4	OMG	B5	3626	4	-	0/9/27/28	0/3/3/3
4	OMC	B5	4455	4	-	0/9/27/28	0/2/2/2
4	OMG	B5	3743	4	-	0/9/27/28	0/3/3/3
52	PSU	A2	1367	52	-	0/7/25/26	0/2/2/2
4	PSU	B5	4292	4	-	0/7/25/26	0/2/2/2
52	OMC	A2	517	52	-	1/9/27/28	0/2/2/2
4	A2M	B5	2400	4	-	0/9/27/28	0/3/3/3
5	GTP	B7	1	5	-	3/22/38/38	0/3/3/3
4	PSU	B5	3883	4	-	0/7/25/26	0/2/2/2
52	PSU	A2	681	52	-	0/7/25/26	0/2/2/2
4	OMG	B5	2423	4	-	0/9/27/28	0/3/3/3
4	A2M	B5	400	4	-	0/9/27/28	0/3/3/3
52	OMG	A2	1447	52	-	2/9/27/28	0/3/3/3
52	OMG	A2	509	87,52	-	3/9/27/28	0/3/3/3
52	A2M	A2	166	52	-	0/9/27/28	0/3/3/3
4	PSU	B5	4402	4	-	0/7/25/26	0/2/2/2
52	OMU	A2	116	52	-	1/9/27/28	0/2/2/2
2	H2U	B2	16	2	-	7/7/38/39	0/2/2/2
52	PSU	A2	609	52	-	0/7/25/26	0/2/2/2
2	1MA	B2	58	2	-	0/7/25/26	0/3/3/3
4	PSU	B5	1791	4	-	0/7/25/26	0/2/2/2
4	A2M	B5	3866	4	-	2/9/27/28	0/3/3/3
4	OMG	B5	3943	4	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	PSU	A2	36	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	210	52	-	0/7/25/26	0/2/2/2
4	PSU	B5	4422	4	-	0/7/25/26	0/2/2/2
52	PSU	A2	34	52	-	0/7/25/26	0/2/2/2
52	OMU	A2	1288	52	-	0/9/27/28	0/2/2/2
4	PSU	B5	4295	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	4311	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	2842	4	-	0/7/25/26	0/2/2/2
52	PSU	A2	866	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	1445	52	-	0/7/25/26	0/2/2/2
4	A2M	B5	4522	87,4	-	2/9/27/28	0/3/3/3
2	H2U	B2	20	2	-	5/7/38/39	0/2/2/2
4	OMU	B5	2414	4	-	0/9/27/28	0/2/2/2
2	2MG	B2	6	2	-	0/9/27/28	0/3/3/3
52	OMU	A2	627	52	-	2/9/27/28	0/2/2/2
2	PSU	B2	27	2	-	0/7/25/26	0/2/2/2
8	HIC	BB	245	8	-	2/5/6/8	0/1/1/1
52	MA6	A2	1850	52	-	3/11/29/30	0/3/3/3
45	MLZ	Bo	53	45	-	0/7/8/10	-
52	OMG	A2	644	52	-	4/9/27/28	0/3/3/3
6	PSU	B8	69	6	-	0/7/25/26	0/2/2/2
4	PSU	B5	2507	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	3761	4	-	2/7/25/26	0/2/2/2
4	PSU	B5	4635	4	-	2/7/25/26	0/2/2/2
52	PSU	A2	966	52	-	0/7/25/26	0/2/2/2
4	A2M	B5	3784	4	-	2/9/27/28	0/3/3/3
4	A2M	B5	2786	87,4	-	3/9/27/28	0/3/3/3
2	OMC	B2	34	2,3	-	0/9/27/28	0/2/2/2
4	PSU	B5	4360	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	3636	4	-	0/7/25/26	0/2/2/2
52	OMC	A2	462	52	-	0/9/27/28	0/2/2/2
52	PSU	A2	572	52	-	0/7/25/26	0/2/2/2
4	PSU	B5	4578	4	-	0/7/25/26	0/2/2/2
4	OMU	B5	2836	4	-	1/9/27/28	0/2/2/2
4	OMC	B5	2421	87,4	-	3/9/27/28	0/2/2/2
4	OMG	B5	3898	87,4	-	0/9/27/28	0/3/3/3
4	OMU	B5	4226	4	-	0/9/27/28	0/2/2/2
52	A2M	A2	668	87,52	-	2/9/27/28	0/3/3/3
52	PSU	A2	1177	52	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	4AC	A2	1337	52	-	4/11/29/30	0/2/2/2
2	5MC	B2	48	2	-	3/7/25/26	0/2/2/2
4	OMU	B5	4305	4	-	0/9/27/28	0/2/2/2
4	1MA	B5	1321	87,4	-	1/7/25/26	0/3/3/3
52	A2M	A2	1031	52	-	0/9/27/28	0/3/3/3
4	A2M	B5	4589	4	-	3/9/27/28	0/3/3/3
4	PSU	B5	1743	4	-	0/7/25/26	0/2/2/2
4	OMC	B5	2860	4	-	0/9/27/28	0/2/2/2
33	MLZ	Bb	5	33	-	0/7/8/10	-
4	PSU	B5	4688	4	-	0/7/25/26	0/2/2/2
4	OMG	B5	4369	4	-	0/9/27/28	0/3/3/3
4	PSU	B5	1781	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	3638	4	-	0/7/25/26	0/2/2/2
52	A2M	A2	27	52	-	1/9/27/28	0/3/3/3
52	A2M	A2	512	52	-	3/9/27/28	0/3/3/3
52	PSU	A2	105	52	-	0/7/25/26	0/2/2/2
52	MA6	A2	1851	52	-	2/11/29/30	0/3/3/3
52	OMG	A2	601	52	-	0/9/27/28	0/3/3/3
52	PSU	A2	651	52	-	0/7/25/26	0/2/2/2
52	A2M	A2	468	52	-	2/9/27/28	0/3/3/3
2	T6A	B2	37	2	-	8/23/41/42	0/3/3/3
52	OMC	A2	1272	52	-	1/9/27/28	0/2/2/2
52	OMG	A2	867	52	-	1/9/27/28	0/3/3/3
4	PSU	B5	1861	4	-	0/7/25/26	0/2/2/2
4	OMG	B5	4636	4	-	0/9/27/28	0/3/3/3
52	PSU	A2	1056	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	863	52	-	0/7/25/26	0/2/2/2
4	OMC	B5	2350	87,4	-	2/9/27/28	0/2/2/2
4	OMG	B5	4195	2,4	-	0/9/27/28	0/3/3/3
4	A2M	B5	2362	87,4	-	0/9/27/28	0/3/3/3
4	PSU	B5	3694	4	-	0/7/25/26	0/2/2/2
4	OMC	B5	3886	4	-	1/9/27/28	0/2/2/2
4	A2M	B5	1325	4	-	2/9/27/28	0/3/3/3
4	PSU	B5	4551	4	-	0/7/25/26	0/2/2/2
52	PSU	A2	815	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	1625	52	-	0/7/25/26	0/2/2/2
52	A2M	A2	484	52	-	0/9/27/28	0/3/3/3
4	OMC	B5	2364	4	-	0/9/27/28	0/2/2/2
4	PSU	B5	4520	87,4	-	0/7/25/26	0/2/2/2
6	OMU	B8	14	6,4	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	PSU	A2	1046	52	-	0/7/25/26	0/2/2/2
2	M2G	B2	26	2	-	0/11/29/30	0/3/3/3
4	OMG	B5	1624	4	-	1/9/27/28	0/3/3/3
52	OMC	A2	797	52	-	0/9/27/28	0/2/2/2
2	PSU	B2	55	2	-	0/7/25/26	0/2/2/2
52	OMC	A2	174	52	-	0/9/27/28	0/2/2/2
4	OMC	B5	3700	87,4	-	4/9/27/28	0/2/2/2
4	OMU	B5	3924	4	-	0/9/27/28	0/2/2/2
4	PSU	B5	4441	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	4430	4	-	0/7/25/26	0/2/2/2
4	6MZ	B5	4219	4	-	0/9/27/28	0/3/3/3
4	PSU	B5	2631	4	-	0/7/25/26	0/2/2/2
2	H2U	B2	47	2	-	7/7/38/39	0/2/2/2
4	A2M	B5	1870	4	-	1/9/27/28	0/3/3/3
52	A2M	A2	99	87,52	-	2/9/27/28	0/3/3/3
52	A2M	A2	576	52	-	2/9/27/28	0/3/3/3
6	OMG	B8	75	6	-	0/9/27/28	0/3/3/3
52	OMC	A2	1391	52	-	2/9/27/28	0/2/2/2
52	PSU	A2	1174	52	-	0/7/25/26	0/2/2/2
4	UY1	B5	3817	87,4	-	2/9/27/28	0/2/2/2
4	OMG	B5	4617	4	-	0/9/27/28	0/3/3/3
4	A2M	B5	1523	4	-	0/9/27/28	0/3/3/3
52	PSU	A2	1136	52	-	0/7/25/26	0/2/2/2
52	A2M	A2	590	52	-	3/9/27/28	0/3/3/3
4	PSU	B5	1778	4	-	0/7/25/26	0/2/2/2
4	A2M	B5	3824	4	-	0/9/27/28	0/3/3/3
4	OMC	B5	2823	4	-	1/9/27/28	0/2/2/2
4	PSU	B5	3714	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	4971	4	-	0/7/25/26	0/2/2/2
52	OMU	A2	1326	87,52	-	0/9/27/28	0/2/2/2
52	PSU	A2	1232	52	-	0/7/25/26	0/2/2/2
4	OMC	B5	1880	87,4	-	0/9/27/28	0/2/2/2
4	OMC	B5	3807	4	-	2/9/27/28	0/2/2/2
4	PSU	B5	1682	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	3767	4	-	0/7/25/26	0/2/2/2
52	OMU	A2	354	52	-	0/9/27/28	0/2/2/2
2	G7M	B2	46	2	-	3/7/25/26	0/3/3/3
4	PSU	B5	1535	4	-	0/7/25/26	0/2/2/2
4	A2M	B5	3829	4	-	0/9/27/28	0/3/3/3
52	PSU	A2	1045	52	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PSU	B5	4627	4	-	0/7/25/26	0/2/2/2
4	5MC	B5	3781	87,4	-	0/7/25/26	0/2/2/2
4	PSU	B5	3843	4	-	1/7/25/26	0/2/2/2
67	IAS	AO	138	67	-	1/7/7/8	-
52	PSU	A2	93	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	109	52	-	0/7/25/26	0/2/2/2
4	PSU	B5	4492	87,4	-	0/7/25/26	0/2/2/2
76	HY3	AX	62	76	-	1/1/12/14	0/1/1/1
52	PSU	A2	649	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	1244	87,52	-	0/7/25/26	0/2/2/2
2	PSU	B2	39	2	-	0/7/25/26	0/2/2/2
52	PSU	A2	1081	52	-	1/7/25/26	0/2/2/2
4	PSU	B5	5009	4	-	0/7/25/26	0/2/2/2
52	OMU	A2	121	52	-	0/9/27/28	0/2/2/2
4	PSU	B5	3729	4	-	0/7/25/26	0/2/2/2
52	PSU	A2	814	52	-	0/7/25/26	0/2/2/2
4	OMG	B5	2875	4	-	0/9/27/28	0/3/3/3
4	PSU	B5	1780	4	-	2/7/25/26	0/2/2/2
4	OMU	B5	4497	87,4	-	0/9/27/28	0/2/2/2
4	OMG	B5	4622	4	-	2/9/27/28	0/3/3/3
52	G7M	A2	1639	2,52	-	2/7/25/26	0/3/3/3
52	6MZ	A2	1832	87,52	-	0/9/27/28	0/3/3/3
4	OMG	B5	4493	4	-	0/9/27/28	0/3/3/3
4	OMC	B5	4535	4	-	0/9/27/28	0/2/2/2
52	PSU	A2	1347	52	-	0/7/25/26	0/2/2/2
52	B8N	A2	1248	52	-	0/16/34/35	0/2/2/2
6	PSU	B8	55	6	-	0/7/25/26	0/2/2/2
52	OMU	A2	799	52	-	3/9/27/28	0/2/2/2
52	OMG	A2	1490	87,52	-	0/9/27/28	0/3/3/3
52	PSU	A2	686	52	-	0/7/25/26	0/2/2/2
4	PSU	B5	3919	87,4	-	0/7/25/26	0/2/2/2
4	OMC	B5	3868	4	-	0/9/27/28	0/2/2/2
4	PSU	B5	4531	4	-	2/7/25/26	0/2/2/2
7	V5N	BA	216	7	-	3/9/10/12	0/1/1/1
4	PSU	B5	3821	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	4456	4	-	0/7/25/26	0/2/2/2
32	V5N	Ba	39	32	-	0/9/10/12	0/1/1/1
4	A2M	B5	4570	4	-	0/9/27/28	0/3/3/3
4	OMG	B5	2363	87,4	-	4/9/27/28	0/3/3/3
52	A2M	A2	159	52	-	0/9/27/28	0/3/3/3
52	OMG	A2	436	52	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	OMU	A2	428	52	-	2/9/27/28	0/2/2/2
72	NMM	AT	67	72	-	0/9/11/13	-
2	5MU	B2	54	2	-	0/7/25/26	0/2/2/2
4	PSU	B5	1676	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	3852	87,4	-	0/7/25/26	0/2/2/2
4	PSU	B5	2838	4	-	0/7/25/26	0/2/2/2
4	5MC	B5	4446	87,4	-	4/7/25/26	0/2/2/2
4	A2M	B5	2814	87,4	-	1/9/27/28	0/3/3/3
52	OMG	A2	683	52	-	0/9/27/28	0/3/3/3
4	PSU	B5	4298	4	-	0/7/25/26	0/2/2/2
4	A2M	B5	1322	4	-	2/9/27/28	0/3/3/3
4	PSU	B5	3850	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	4499	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	4672	4	-	0/7/25/26	0/2/2/2
52	OMU	A2	1442	87,52	-	0/9/27/28	0/2/2/2
4	OMC	B5	1339	4	-	0/9/27/28	0/2/2/2
4	OMG	B5	4391	4	-	1/9/27/28	0/3/3/3
52	PSU	A2	801	52	-	0/7/25/26	0/2/2/2
4	A2M	B5	1533	87,4	-	1/9/27/28	0/3/3/3
52	PSU	A2	406	52	-	0/7/25/26	0/2/2/2
4	PSU	B5	1581	4	-	2/7/25/26	0/2/2/2
4	A2M	B5	3717	4	-	0/9/27/28	0/3/3/3
2	PSU	B2	31	2	-	0/7/25/26	0/2/2/2
4	UR3	B5	4529	4	-	0/7/25/26	0/2/2/2
52	A2M	A2	1678	52	-	1/9/27/28	0/3/3/3
4	OMC	B5	3840	4	-	1/9/27/28	0/2/2/2
52	PSU	A2	296	52	-	0/7/25/26	0/2/2/2
52	OMC	A2	1703	52	-	3/9/27/28	0/2/2/2
52	PSU	A2	119	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	1238	52	-	0/7/25/26	0/2/2/2
4	A2M	B5	398	4	-	2/9/27/28	0/3/3/3
2	2MG	B2	10	2	-	0/9/27/28	0/3/3/3
4	OMC	B5	2803	4	-	0/9/27/28	0/2/2/2
4	OMU	B5	4619	4	-	0/9/27/28	0/2/2/2

All (571) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	AX	62	HY3	C3-CA	-18.71	1.36	1.55
52	A2	1639	G7M	C4-N9	7.83	1.58	1.38
2	B2	46	G7M	O6-C6	7.72	1.38	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	A2	1639	G7M	O6-C6	7.65	1.38	1.23
2	B2	46	G7M	C4-N9	7.46	1.57	1.38
52	A2	1850	MA6	C5-N7	6.84	1.51	1.39
52	A2	1851	MA6	C5-N7	6.82	1.51	1.39
52	A2	1639	G7M	C5-C4	6.21	1.54	1.38
2	B2	46	G7M	C5-C4	6.04	1.53	1.38
52	A2	1850	MA6	C8-N9	-5.34	1.28	1.37
52	A2	1851	MA6	C8-N9	-5.32	1.28	1.37
32	Ba	39	V5N	CG-ND1	-4.94	1.33	1.37
7	BA	216	V5N	CG-ND1	-4.89	1.33	1.37
52	A2	590	A2M	C5-C4	4.65	1.47	1.39
52	A2	99	A2M	C5-C4	4.63	1.47	1.39
52	A2	159	A2M	C5-C4	4.62	1.47	1.39
52	A2	484	A2M	C5-C4	4.61	1.47	1.39
52	A2	468	A2M	C5-C4	4.60	1.47	1.39
52	A2	1383	A2M	C5-C4	4.58	1.47	1.39
52	A2	512	A2M	C5-C4	4.58	1.47	1.39
4	B5	3717	A2M	C5-C4	4.57	1.47	1.39
52	A2	166	A2M	C5-C4	4.56	1.47	1.39
52	A2	27	A2M	C5-C4	4.56	1.47	1.39
52	A2	668	A2M	C5-C4	4.55	1.47	1.39
52	A2	1832	6MZ	C5-C4	4.53	1.47	1.39
52	A2	1031	A2M	C5-C4	4.52	1.47	1.39
4	B5	4570	A2M	C5-C4	4.52	1.47	1.39
52	A2	576	A2M	C5-C4	4.51	1.47	1.39
4	B5	4219	6MZ	C5-C4	4.49	1.47	1.39
4	B5	4589	A2M	C5-C4	4.49	1.47	1.39
4	B5	3723	A2M	C5-C4	4.49	1.47	1.39
4	B5	2814	A2M	C5-C4	4.46	1.47	1.39
4	B5	398	A2M	C5-C4	4.46	1.47	1.39
52	A2	1639	G7M	C2-N2	4.46	1.44	1.34
4	B5	400	A2M	C5-C4	4.45	1.47	1.39
4	B5	3829	A2M	C5-C4	4.45	1.47	1.39
52	A2	1678	A2M	C5-C4	4.45	1.47	1.39
4	B5	1533	A2M	C5-C4	4.43	1.47	1.39
4	B5	3824	A2M	C5-C4	4.43	1.47	1.39
4	B5	1523	A2M	C5-C4	4.42	1.47	1.39
4	B5	1322	A2M	C5-C4	4.41	1.47	1.39
2	B2	46	G7M	C2-N2	4.41	1.44	1.34
4	B5	1870	A2M	C5-C4	4.40	1.47	1.39
4	B5	3866	A2M	C5-C4	4.39	1.47	1.39
4	B5	2362	A2M	C5-C4	4.39	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B5	2400	A2M	C5-C4	4.37	1.47	1.39
4	B5	2786	A2M	C5-C4	4.37	1.47	1.39
4	B5	1325	A2M	C5-C4	4.34	1.47	1.39
4	B5	4522	A2M	C5-C4	4.31	1.47	1.39
4	B5	3784	A2M	C5-C4	4.25	1.47	1.39
2	B2	46	G7M	C2-N1	4.00	1.47	1.37
76	AX	62	HY3	C5-N	-3.94	1.34	1.49
52	A2	1639	G7M	C2-N1	3.85	1.47	1.37
76	AX	62	HY3	C4-C5	3.58	1.58	1.53
52	A2	1850	MA6	C4-N9	-3.57	1.29	1.37
4	B5	3817	UY1	C6-C5	3.53	1.39	1.35
2	B2	39	PSU	C6-C5	3.51	1.39	1.35
52	A2	1851	MA6	C4-N9	-3.50	1.29	1.37
52	A2	1851	MA6	C5-C4	3.43	1.45	1.39
52	A2	1639	G7M	C2-N3	3.32	1.41	1.33
52	A2	815	PSU	C6-C5	3.30	1.39	1.35
52	A2	1238	PSU	C6-C5	3.29	1.39	1.35
2	B2	55	PSU	C6-C5	3.29	1.39	1.35
52	A2	572	PSU	C6-C5	3.29	1.39	1.35
52	A2	866	PSU	C6-C5	3.28	1.39	1.35
52	A2	119	PSU	C6-C5	3.26	1.39	1.35
52	A2	36	PSU	C6-C5	3.26	1.39	1.35
52	A2	814	PSU	C6-C5	3.26	1.39	1.35
2	B2	31	PSU	C6-C5	3.26	1.39	1.35
52	A2	210	PSU	C6-C5	3.26	1.39	1.35
52	A2	1174	PSU	C6-C5	3.25	1.39	1.35
2	B2	58	1MA	C6-N6	3.25	1.36	1.28
52	A2	1347	PSU	C6-C5	3.25	1.39	1.35
4	B5	1778	PSU	C6-C5	3.24	1.39	1.35
52	A2	822	PSU	C6-C5	3.23	1.39	1.35
4	B5	4422	PSU	C6-C5	3.23	1.39	1.35
52	A2	1625	PSU	C6-C5	3.23	1.39	1.35
52	A2	296	PSU	C6-C5	3.23	1.39	1.35
4	B5	1781	PSU	C6-C5	3.22	1.39	1.35
52	A2	651	PSU	C6-C5	3.22	1.39	1.35
52	A2	1004	PSU	C6-C5	3.21	1.39	1.35
52	A2	1850	MA6	C5-C4	3.21	1.45	1.39
4	B5	3714	PSU	C6-C5	3.21	1.39	1.35
4	B5	1859	PSU	C6-C5	3.21	1.39	1.35
52	A2	801	PSU	C6-C5	3.21	1.39	1.35
52	A2	1056	PSU	C6-C5	3.21	1.39	1.35
4	B5	1780	PSU	C6-C5	3.20	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	A2	1136	PSU	C6-C5	3.20	1.39	1.35
52	A2	109	PSU	C6-C5	3.20	1.39	1.35
4	B5	4430	PSU	C6-C5	3.20	1.39	1.35
52	A2	1445	PSU	C6-C5	3.20	1.39	1.35
4	B5	1743	PSU	C6-C5	3.20	1.39	1.35
52	A2	34	PSU	C6-C5	3.20	1.39	1.35
52	A2	863	PSU	C6-C5	3.19	1.39	1.35
52	A2	218	PSU	C6-C5	3.19	1.39	1.35
52	A2	1232	PSU	C6-C5	3.19	1.39	1.35
52	A2	1177	PSU	C6-C5	3.19	1.39	1.35
4	B5	3850	PSU	C6-C5	3.19	1.39	1.35
52	A2	105	PSU	C6-C5	3.19	1.39	1.35
52	A2	93	PSU	C6-C5	3.18	1.39	1.35
4	B5	5009	PSU	C6-C5	3.18	1.39	1.35
52	A2	681	PSU	C6-C5	3.18	1.39	1.35
4	B5	4470	PSU	C6-C5	3.18	1.39	1.35
2	B2	27	PSU	C6-C5	3.17	1.39	1.35
52	A2	1367	PSU	C6-C5	3.17	1.39	1.35
52	A2	649	PSU	C6-C5	3.17	1.39	1.35
52	A2	1643	PSU	C6-C5	3.17	1.39	1.35
52	A2	686	PSU	C6-C5	3.17	1.39	1.35
52	A2	1244	PSU	C6-C5	3.17	1.39	1.35
52	A2	509	OMG	C5-C4	3.17	1.47	1.38
4	B5	3767	PSU	C6-C5	3.17	1.39	1.35
52	A2	966	PSU	C6-C5	3.17	1.39	1.35
4	B5	1676	PSU	C6-C5	3.16	1.39	1.35
4	B5	4688	PSU	C6-C5	3.16	1.39	1.35
52	A2	406	PSU	C6-C5	3.16	1.39	1.35
4	B5	3769	PSU	C6-C5	3.16	1.39	1.35
4	B5	1791	PSU	C6-C5	3.15	1.39	1.35
52	A2	1692	PSU	C6-C5	3.15	1.39	1.35
4	B5	4635	PSU	C6-C5	3.15	1.39	1.35
4	B5	3761	PSU	C6-C5	3.15	1.39	1.35
52	A2	644	OMG	C5-C4	3.14	1.47	1.38
4	B5	4499	PSU	C6-C5	3.14	1.39	1.35
2	B2	10	2MG	C5-C4	3.13	1.47	1.38
52	A2	1490	OMG	C5-C4	3.13	1.47	1.38
4	B5	3729	PSU	C6-C5	3.13	1.39	1.35
2	B2	6	2MG	C5-C4	3.13	1.47	1.38
4	B5	1321	1MA	C6-N6	3.13	1.35	1.28
2	B2	58	1MA	C5-C4	3.13	1.47	1.38
52	A2	436	OMG	C5-C4	3.12	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B5	1581	PSU	C6-C5	3.12	1.39	1.35
52	A2	609	PSU	C6-C5	3.11	1.38	1.35
2	B2	26	M2G	C5-C4	3.11	1.47	1.38
52	A2	1046	PSU	C6-C5	3.11	1.38	1.35
52	A2	1328	OMG	C5-C4	3.11	1.47	1.38
4	B5	4672	PSU	C6-C5	3.11	1.38	1.35
4	B5	4971	PSU	C6-C5	3.10	1.38	1.35
52	A2	1851	MA6	C6-N6	3.10	1.46	1.36
4	B5	4360	PSU	C6-C5	3.10	1.38	1.35
4	B5	3694	PSU	C6-C5	3.10	1.38	1.35
52	A2	867	OMG	C5-C4	3.10	1.47	1.38
6	B8	55	PSU	C6-C5	3.09	1.38	1.35
4	B5	4575	PSU	C6-C5	3.09	1.38	1.35
4	B5	3843	PSU	C6-C5	3.09	1.38	1.35
52	A2	1447	OMG	C5-C4	3.09	1.47	1.38
6	B8	75	OMG	C5-C4	3.09	1.47	1.38
4	B5	4578	PSU	C6-C5	3.09	1.38	1.35
52	A2	1248	B8N	C6-C5	3.08	1.39	1.34
4	B5	4369	OMG	C5-C4	3.08	1.47	1.38
4	B5	5000	PSU	C6-C5	3.08	1.38	1.35
52	A2	1081	PSU	C6-C5	3.08	1.38	1.35
4	B5	1682	PSU	C6-C5	3.08	1.38	1.35
52	A2	683	OMG	C5-C4	3.07	1.47	1.38
4	B5	1861	PSU	C6-C5	3.07	1.38	1.35
4	B5	3821	PSU	C6-C5	3.07	1.38	1.35
4	B5	4520	PSU	C6-C5	3.07	1.38	1.35
4	B5	4531	PSU	C6-C5	3.06	1.38	1.35
4	B5	2875	OMG	C5-C4	3.06	1.47	1.38
4	B5	3943	OMG	C5-C4	3.06	1.47	1.38
4	B5	1624	OMG	C5-C4	3.06	1.47	1.38
4	B5	2631	PSU	C6-C5	3.05	1.38	1.35
52	A2	601	OMG	C5-C4	3.05	1.47	1.38
4	B5	4195	OMG	C5-C4	3.05	1.47	1.38
4	B5	3791	OMG	C5-C4	3.05	1.47	1.38
6	B8	69	PSU	C6-C5	3.05	1.38	1.35
4	B5	4617	OMG	C5-C4	3.05	1.47	1.38
4	B5	4352	PSU	C6-C5	3.04	1.38	1.35
4	B5	4311	PSU	C6-C5	3.04	1.38	1.35
4	B5	4493	OMG	C5-C4	3.03	1.47	1.38
52	A2	1045	PSU	C6-C5	3.03	1.38	1.35
4	B5	3638	PSU	C6-C5	3.03	1.38	1.35
4	B5	3743	OMG	C5-C4	3.03	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B5	3626	OMG	C5-C4	3.02	1.47	1.38
4	B5	2838	PSU	C6-C5	3.02	1.38	1.35
4	B5	1321	1MA	C5-C4	3.02	1.47	1.38
4	B5	3883	PSU	C6-C5	3.02	1.38	1.35
4	B5	2423	OMG	C5-C4	3.02	1.47	1.38
4	B5	4498	OMG	C5-C4	3.01	1.47	1.38
4	B5	4292	PSU	C6-C5	3.01	1.38	1.35
4	B5	4636	OMG	C5-C4	3.01	1.47	1.38
4	B5	4402	PSU	C6-C5	3.01	1.38	1.35
4	B5	4492	PSU	C6-C5	3.01	1.38	1.35
4	B5	4456	PSU	C6-C5	3.00	1.38	1.35
4	B5	2842	PSU	C6-C5	3.00	1.38	1.35
4	B5	4972	PSU	C6-C5	3.00	1.38	1.35
52	A2	1850	MA6	C6-N6	2.99	1.45	1.36
4	B5	4441	PSU	C6-C5	2.99	1.38	1.35
4	B5	4551	PSU	C6-C5	2.99	1.38	1.35
4	B5	4298	PSU	C6-C5	2.99	1.38	1.35
4	B5	4391	OMG	C5-C4	2.99	1.47	1.38
4	B5	3919	PSU	C6-C5	2.98	1.38	1.35
4	B5	1535	PSU	C6-C5	2.98	1.38	1.35
4	B5	4227	OMG	C5-C4	2.98	1.47	1.38
4	B5	2363	OMG	C5-C4	2.96	1.47	1.38
4	B5	1521	OMG	C5-C4	2.96	1.47	1.38
52	A2	1248	B8N	C4-N3	-2.96	1.34	1.40
4	B5	4622	OMG	C5-C4	2.96	1.47	1.38
4	B5	4295	PSU	C6-C5	2.95	1.38	1.35
4	B5	3852	PSU	C6-C5	2.94	1.38	1.35
4	B5	4627	PSU	C6-C5	2.94	1.38	1.35
4	B5	1315	OMG	C5-C4	2.94	1.46	1.38
2	B2	46	G7M	C2-N3	2.93	1.40	1.33
52	A2	1337	4AC	C4-N4	-2.93	1.35	1.39
4	B5	3898	OMG	C5-C4	2.93	1.46	1.38
4	B5	2507	PSU	C6-C5	2.91	1.38	1.35
4	B5	3636	PSU	C6-C5	2.89	1.38	1.35
2	B2	26	M2G	C2-N2	2.88	1.40	1.35
32	Ba	39	V5N	CD2-NE2	-2.87	1.33	1.37
4	B5	3636	PSU	C4-N3	-2.84	1.33	1.38
7	BA	216	V5N	CD2-NE2	-2.83	1.33	1.37
4	B5	4672	PSU	C4-N3	-2.81	1.33	1.38
4	B5	4446	5MC	C6-C5	2.80	1.39	1.34
4	B5	2507	PSU	C4-N3	-2.80	1.33	1.38
4	B5	3852	PSU	C4-N3	-2.78	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B5	3919	PSU	C4-N3	-2.78	1.33	1.38
2	B2	54	5MU	C4-N3	-2.78	1.33	1.38
4	B5	3883	PSU	C4-N3	-2.78	1.33	1.38
52	A2	1842	4AC	C4-N4	-2.78	1.35	1.39
4	B5	1535	PSU	C4-N3	-2.77	1.33	1.38
4	B5	4551	PSU	C4-N3	-2.77	1.33	1.38
4	B5	4635	PSU	C4-N3	-2.77	1.33	1.38
4	B5	2842	PSU	C4-N3	-2.77	1.33	1.38
4	B5	3843	PSU	C4-N3	-2.76	1.33	1.38
4	B5	3821	PSU	C4-N3	-2.75	1.33	1.38
2	B2	48	5MC	C6-C5	2.75	1.39	1.34
4	B5	3638	PSU	C4-N3	-2.75	1.33	1.38
52	A2	1678	A2M	C5-C6	2.74	1.48	1.41
4	B5	4578	PSU	C4-N3	-2.74	1.33	1.38
4	B5	4456	PSU	C4-N3	-2.74	1.33	1.38
2	B2	16	H2U	C2-N3	-2.74	1.33	1.38
4	B5	1581	PSU	C4-N3	-2.74	1.33	1.38
4	B5	4971	PSU	C4-N3	-2.74	1.33	1.38
4	B5	3694	PSU	C4-N3	-2.73	1.33	1.38
52	A2	27	A2M	C5-C6	2.73	1.48	1.41
4	B5	4298	PSU	C4-N3	-2.73	1.33	1.38
52	A2	1383	A2M	C5-C6	2.73	1.48	1.41
52	A2	590	A2M	C5-C6	2.73	1.48	1.41
4	B5	4688	PSU	C4-N3	-2.72	1.33	1.38
4	B5	4627	PSU	C4-N3	-2.72	1.33	1.38
4	B5	4292	PSU	C4-N3	-2.72	1.33	1.38
4	B5	4520	PSU	C4-N3	-2.72	1.33	1.38
4	B5	3729	PSU	C4-N3	-2.72	1.33	1.38
2	B2	54	5MU	C6-C5	2.72	1.39	1.34
4	B5	1682	PSU	C4-N3	-2.72	1.33	1.38
4	B5	4575	PSU	C4-N3	-2.72	1.33	1.38
52	A2	468	A2M	C5-C6	2.71	1.48	1.41
52	A2	484	A2M	C5-C6	2.71	1.48	1.41
4	B5	5009	PSU	C4-N3	-2.71	1.33	1.38
4	B5	4311	PSU	C4-N3	-2.71	1.33	1.38
2	B2	20	H2U	C2-N3	-2.71	1.33	1.38
4	B5	1861	PSU	C4-N3	-2.71	1.33	1.38
52	A2	1136	PSU	C4-N3	-2.71	1.33	1.38
4	B5	4441	PSU	C4-N3	-2.70	1.33	1.38
4	B5	1859	PSU	C4-N3	-2.70	1.33	1.38
52	A2	159	A2M	C5-C6	2.70	1.48	1.41
4	B5	2838	PSU	C4-N3	-2.70	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B5	4352	PSU	C4-N3	-2.70	1.33	1.38
52	A2	681	PSU	C4-N3	-2.70	1.33	1.38
6	B8	69	PSU	C4-N3	-2.70	1.33	1.38
4	B5	4972	PSU	C4-N3	-2.70	1.33	1.38
6	B8	55	PSU	C4-N3	-2.69	1.33	1.38
4	B5	3850	PSU	C4-N3	-2.69	1.33	1.38
4	B5	3717	A2M	C5-C6	2.69	1.48	1.41
4	B5	398	A2M	C5-C6	2.69	1.48	1.41
52	A2	668	A2M	C5-C6	2.69	1.48	1.41
52	A2	512	A2M	C5-C6	2.69	1.48	1.41
4	B5	5000	PSU	C4-N3	-2.68	1.33	1.38
52	A2	99	A2M	C5-C6	2.68	1.48	1.41
4	B5	4295	PSU	C4-N3	-2.68	1.33	1.38
4	B5	4402	PSU	C4-N3	-2.68	1.33	1.38
4	B5	4531	PSU	C4-N3	-2.68	1.33	1.38
4	B5	4470	PSU	C4-N3	-2.68	1.33	1.38
4	B5	2631	PSU	C4-N3	-2.68	1.33	1.38
4	B5	1781	PSU	C4-N3	-2.67	1.33	1.38
4	B5	1791	PSU	C4-N3	-2.67	1.33	1.38
4	B5	3761	PSU	C4-N3	-2.67	1.33	1.38
4	B5	4360	PSU	C4-N3	-2.67	1.33	1.38
52	A2	166	A2M	C5-C6	2.67	1.48	1.41
52	A2	576	A2M	C5-C6	2.67	1.48	1.41
52	A2	1232	PSU	C4-N3	-2.66	1.33	1.38
52	A2	966	PSU	C4-N3	-2.66	1.33	1.38
4	B5	4492	PSU	C4-N3	-2.66	1.33	1.38
52	A2	406	PSU	C4-N3	-2.65	1.33	1.38
4	B5	4589	A2M	C5-C6	2.65	1.48	1.41
52	A2	1045	PSU	C4-N3	-2.65	1.33	1.38
52	A2	1031	A2M	C5-C6	2.65	1.48	1.41
4	B5	4391	OMG	C6-N1	-2.65	1.33	1.38
2	B2	31	PSU	C4-N3	-2.65	1.33	1.38
52	A2	1056	PSU	C4-N3	-2.65	1.33	1.38
4	B5	4570	A2M	C5-C6	2.65	1.48	1.41
52	A2	1177	PSU	C4-N3	-2.65	1.33	1.38
52	A2	1081	PSU	C4-N3	-2.64	1.33	1.38
52	A2	1004	PSU	C4-N3	-2.64	1.33	1.38
52	A2	105	PSU	C4-N3	-2.64	1.33	1.38
52	A2	1244	PSU	C4-N3	-2.64	1.33	1.38
52	A2	686	PSU	C4-N3	-2.63	1.33	1.38
52	A2	1174	PSU	C4-N3	-2.63	1.33	1.38
4	B5	2362	A2M	C5-C6	2.63	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	A2	1238	PSU	C4-N3	-2.63	1.34	1.38
52	A2	651	PSU	C4-N3	-2.63	1.34	1.38
52	A2	1347	PSU	C4-N3	-2.63	1.34	1.38
4	B5	1533	A2M	C5-C6	2.63	1.48	1.41
4	B5	4305	OMU	C4-N3	-2.63	1.33	1.38
4	B5	1676	PSU	C4-N3	-2.62	1.34	1.38
52	A2	609	PSU	C4-N3	-2.62	1.34	1.38
52	A2	815	PSU	C4-N3	-2.62	1.34	1.38
4	B5	2814	A2M	C5-C6	2.62	1.48	1.41
52	A2	801	PSU	C4-N3	-2.62	1.34	1.38
4	B5	3924	OMU	C4-N3	-2.62	1.33	1.38
52	A2	109	PSU	C4-N3	-2.62	1.34	1.38
4	B5	4422	PSU	C4-N3	-2.62	1.34	1.38
4	B5	1743	PSU	C4-N3	-2.62	1.34	1.38
4	B5	4430	PSU	C4-N3	-2.62	1.34	1.38
2	B2	46	G7M	C5-N7	2.62	1.42	1.39
52	A2	1367	PSU	C4-N3	-2.62	1.34	1.38
4	B5	3769	PSU	C4-N3	-2.61	1.34	1.38
52	A2	1046	PSU	C4-N3	-2.61	1.34	1.38
4	B5	1322	A2M	C5-C6	2.61	1.48	1.41
4	B5	1523	A2M	C5-C6	2.61	1.48	1.41
4	B5	1780	PSU	C4-N3	-2.61	1.34	1.38
52	A2	93	PSU	C4-N3	-2.61	1.34	1.38
52	A2	1692	PSU	C4-N3	-2.61	1.34	1.38
52	A2	296	PSU	C4-N3	-2.61	1.34	1.38
52	A2	1625	PSU	C4-N3	-2.60	1.34	1.38
52	A2	210	PSU	C4-N3	-2.60	1.34	1.38
4	B5	3781	5MC	C6-C5	2.60	1.38	1.34
4	B5	400	A2M	C5-C6	2.60	1.48	1.41
4	B5	3829	A2M	C5-C6	2.60	1.48	1.41
4	B5	3767	PSU	C4-N3	-2.60	1.34	1.38
52	A2	1643	PSU	C4-N3	-2.60	1.34	1.38
4	B5	3824	A2M	C5-C6	2.60	1.48	1.41
52	A2	863	PSU	C4-N3	-2.60	1.34	1.38
52	A2	34	PSU	C4-N3	-2.60	1.34	1.38
52	A2	866	PSU	C4-N3	-2.60	1.34	1.38
4	B5	3723	A2M	C5-C6	2.60	1.48	1.41
4	B5	3866	A2M	C5-C6	2.60	1.48	1.41
52	A2	1445	PSU	C4-N3	-2.59	1.34	1.38
52	A2	36	PSU	C4-N3	-2.59	1.34	1.38
4	B5	2414	OMU	C4-N3	-2.59	1.33	1.38
52	A2	649	PSU	C4-N3	-2.59	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	A2	814	PSU	C4-N3	-2.59	1.34	1.38
2	B2	16	H2U	C4-N3	-2.58	1.33	1.37
2	B2	27	PSU	C4-N3	-2.58	1.34	1.38
52	A2	119	PSU	C4-N3	-2.58	1.34	1.38
4	B5	4499	PSU	C4-N3	-2.58	1.34	1.38
4	B5	2836	OMU	C4-N3	-2.58	1.33	1.38
4	B5	1870	A2M	C5-C6	2.58	1.48	1.41
4	B5	1325	A2M	C5-C6	2.58	1.48	1.41
2	B2	55	PSU	C4-N3	-2.58	1.34	1.38
4	B5	4619	OMU	C4-N3	-2.57	1.33	1.38
2	B2	47	H2U	C2-N3	-2.57	1.33	1.38
4	B5	1778	PSU	C4-N3	-2.57	1.34	1.38
4	B5	3714	PSU	C4-N3	-2.57	1.34	1.38
4	B5	1315	OMG	C6-N1	-2.56	1.34	1.38
4	B5	2400	A2M	C5-C6	2.55	1.48	1.41
4	B5	4617	OMG	C6-N1	-2.55	1.34	1.38
4	B5	1521	OMG	C6-N1	-2.55	1.34	1.38
4	B5	3743	OMG	C6-N1	-2.55	1.34	1.38
4	B5	4522	A2M	C5-C6	2.55	1.48	1.41
4	B5	2875	OMG	C6-N1	-2.55	1.34	1.38
52	A2	218	PSU	C4-N3	-2.55	1.34	1.38
6	B8	14	OMU	C4-N3	-2.55	1.34	1.38
52	A2	572	PSU	C4-N3	-2.54	1.34	1.38
4	B5	3817	UY1	C2-N1	2.54	1.40	1.36
4	B5	4369	OMG	C6-N1	-2.53	1.34	1.38
4	B5	4622	OMG	C6-N1	-2.53	1.34	1.38
52	A2	822	PSU	C4-N3	-2.53	1.34	1.38
4	B5	3626	OMG	C6-N1	-2.52	1.34	1.38
2	B2	10	2MG	C6-N1	-2.52	1.34	1.38
4	B5	3784	A2M	C5-C6	2.52	1.48	1.41
4	B5	4226	OMU	C4-N3	-2.52	1.34	1.38
4	B5	4493	OMG	C6-N1	-2.51	1.34	1.38
2	B2	26	M2G	C6-N1	-2.51	1.34	1.38
6	B8	75	OMG	C6-N1	-2.51	1.34	1.38
4	B5	4195	OMG	C6-N1	-2.51	1.34	1.38
52	A2	116	OMU	C4-N3	-2.50	1.34	1.38
4	B5	4636	OMG	C6-N1	-2.50	1.34	1.38
4	B5	3898	OMG	C6-N1	-2.50	1.34	1.38
4	B5	2423	OMG	C6-N1	-2.49	1.34	1.38
52	A2	1832	6MZ	C5-C6	2.49	1.48	1.41
52	A2	1804	OMU	C4-N3	-2.49	1.34	1.38
4	B5	4219	6MZ	C5-C6	2.49	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B2	54	5MU	C2-N1	2.49	1.42	1.38
4	B5	1624	OMG	C6-N1	-2.48	1.34	1.38
52	A2	1490	OMG	C6-N1	-2.48	1.34	1.38
52	A2	601	OMG	C6-N1	-2.47	1.34	1.38
4	B5	4497	OMU	C4-N3	-2.47	1.34	1.38
4	B5	2786	A2M	C5-C6	2.47	1.48	1.41
52	A2	428	OMU	C4-N3	-2.47	1.34	1.38
4	B5	2363	OMG	C6-N1	-2.47	1.34	1.38
4	B5	3791	OMG	C6-N1	-2.46	1.34	1.38
52	A2	436	OMG	C6-N1	-2.46	1.34	1.38
52	A2	27	A2M	C8-N7	2.46	1.36	1.31
52	A2	509	OMG	C6-N1	-2.46	1.34	1.38
52	A2	172	OMU	C4-N3	-2.45	1.34	1.38
52	A2	121	OMU	C4-N3	-2.45	1.34	1.38
52	A2	668	A2M	C8-N7	2.45	1.36	1.31
52	A2	644	OMG	C6-N1	-2.44	1.34	1.38
52	A2	468	A2M	C8-N7	2.43	1.36	1.31
52	A2	867	OMG	C6-N1	-2.43	1.34	1.38
4	B5	3943	OMG	C6-N1	-2.43	1.34	1.38
52	A2	1248	B8N	C2-N3	-2.43	1.34	1.38
52	A2	1288	OMU	C4-N3	-2.43	1.34	1.38
52	A2	1442	OMU	C4-N3	-2.42	1.34	1.38
52	A2	1383	A2M	C8-N7	2.42	1.36	1.31
52	A2	1326	OMU	C4-N3	-2.42	1.34	1.38
52	A2	1447	OMG	C6-N1	-2.42	1.34	1.38
52	A2	159	A2M	C8-N7	2.41	1.36	1.31
52	A2	683	OMG	C6-N1	-2.41	1.34	1.38
52	A2	1639	G7M	C5-N7	2.41	1.42	1.39
4	B5	1533	A2M	C8-N7	2.40	1.36	1.31
2	B2	6	2MG	C6-N1	-2.40	1.34	1.38
4	B5	3717	A2M	C8-N7	2.40	1.36	1.31
4	B5	4446	5MC	C6-N1	-2.40	1.34	1.38
52	A2	627	OMU	C4-N3	-2.40	1.34	1.38
52	A2	1328	OMG	C6-N1	-2.39	1.34	1.38
4	B5	4498	OMG	C6-N1	-2.39	1.34	1.38
52	A2	354	OMU	C4-N3	-2.39	1.34	1.38
52	A2	512	A2M	C8-N7	2.39	1.36	1.31
52	A2	1678	A2M	C8-N7	2.39	1.36	1.31
4	B5	398	A2M	C8-N7	2.39	1.36	1.31
4	B5	4589	A2M	C8-N7	2.39	1.36	1.31
2	B2	58	1MA	C2-N3	2.38	1.35	1.30
4	B5	2400	A2M	C8-N7	2.38	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	A2	576	A2M	C8-N7	2.38	1.36	1.31
52	A2	1031	A2M	C8-N7	2.38	1.36	1.31
52	A2	99	A2M	C8-N7	2.38	1.36	1.31
52	A2	799	OMU	C4-N3	-2.37	1.34	1.38
4	B5	400	A2M	C8-N7	2.37	1.36	1.31
4	B5	4227	OMG	C6-N1	-2.37	1.34	1.38
4	B5	1870	A2M	C8-N7	2.37	1.36	1.31
4	B5	2786	A2M	C5-N7	-2.36	1.34	1.39
52	A2	166	A2M	C8-N7	2.36	1.36	1.31
4	B5	3723	A2M	C8-N7	2.36	1.36	1.31
52	A2	1804	OMU	C2-N1	2.35	1.42	1.38
4	B5	3784	A2M	C8-N7	2.35	1.36	1.31
52	A2	590	A2M	C8-N7	2.35	1.36	1.31
4	B5	3829	A2M	C8-N7	2.35	1.36	1.31
2	B2	47	H2U	C4-N3	-2.34	1.33	1.37
4	B5	4219	6MZ	C8-N7	2.33	1.36	1.31
52	A2	172	OMU	C2-N1	2.33	1.42	1.38
2	B2	46	G7M	C6-N1	2.33	1.43	1.38
2	B2	6	2MG	C2-N3	2.33	1.36	1.31
4	B5	4570	A2M	C8-N7	2.32	1.36	1.31
2	B2	20	H2U	C4-N3	-2.32	1.33	1.37
4	B5	3817	UY1	C6-N1	-2.31	1.32	1.36
4	B5	3824	A2M	C8-N7	2.31	1.36	1.31
4	B5	2362	A2M	C8-N7	2.31	1.36	1.31
4	B5	1523	A2M	C8-N7	2.31	1.36	1.31
52	A2	1832	6MZ	C8-N7	2.31	1.36	1.31
6	B8	14	OMU	C2-N3	-2.31	1.33	1.38
4	B5	4522	A2M	C8-N7	2.31	1.36	1.31
4	B5	3781	5MC	C6-N1	-2.30	1.34	1.38
2	B2	54	5MU	C4-C5	2.30	1.48	1.44
4	B5	2362	A2M	C5-N7	-2.30	1.34	1.39
4	B5	3866	A2M	C8-N7	2.30	1.35	1.31
4	B5	2814	A2M	C8-N7	2.29	1.35	1.31
4	B5	3829	A2M	C5-N7	-2.29	1.34	1.39
52	A2	484	A2M	C8-N7	2.28	1.35	1.31
76	AX	62	HY3	C4-C3	2.28	1.56	1.52
4	B5	1322	A2M	C5-N7	-2.27	1.34	1.39
4	B5	2814	A2M	C5-N7	-2.27	1.34	1.39
4	B5	1322	A2M	C8-N7	2.27	1.35	1.31
4	B5	2414	OMU	C2-N3	-2.27	1.33	1.38
4	B5	1325	A2M	C5-N7	-2.27	1.34	1.39
4	B5	1325	A2M	C8-N7	2.26	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B5	3824	A2M	C5-N7	-2.26	1.34	1.39
2	B2	48	5MC	C6-N1	-2.26	1.34	1.38
4	B5	4219	6MZ	C5-N7	-2.25	1.34	1.39
2	B2	10	2MG	C2-N3	2.25	1.36	1.31
52	A2	166	A2M	C5-N7	-2.24	1.34	1.39
52	A2	99	A2M	C5-N7	-2.24	1.34	1.39
4	B5	3866	A2M	C5-N7	-2.24	1.34	1.39
52	A2	1288	OMU	C2-N1	2.24	1.42	1.38
4	B5	1315	OMG	C5-N7	-2.24	1.34	1.39
52	A2	484	A2M	C5-N7	-2.23	1.34	1.39
4	B5	2875	OMG	C5-N7	-2.23	1.34	1.39
4	B5	1523	A2M	C5-N7	-2.23	1.34	1.39
4	B5	4305	OMU	C2-N3	-2.23	1.34	1.38
4	B5	2400	A2M	C5-N7	-2.23	1.34	1.39
4	B5	3784	A2M	C5-N7	-2.23	1.34	1.39
52	A2	1832	6MZ	C5-N7	-2.23	1.34	1.39
4	B5	2423	OMG	C5-N7	-2.22	1.34	1.39
4	B5	4497	OMU	C2-N3	-2.22	1.34	1.38
4	B5	4619	OMU	C2-N3	-2.22	1.34	1.38
4	B5	1321	1MA	C5-N7	-2.21	1.34	1.39
4	B5	1533	A2M	C5-N7	-2.21	1.34	1.39
4	B5	2786	A2M	C8-N7	2.21	1.35	1.31
4	B5	3924	OMU	C2-N3	-2.21	1.34	1.38
4	B5	1624	OMG	C5-N7	-2.21	1.34	1.39
4	B5	4195	OMG	C5-N7	-2.21	1.34	1.39
4	B5	1870	A2M	C5-N7	-2.20	1.34	1.39
4	B5	3743	OMG	C5-N7	-2.20	1.34	1.39
4	B5	4570	A2M	C5-N7	-2.20	1.34	1.39
52	A2	590	A2M	C5-N7	-2.20	1.34	1.39
4	B5	4226	OMU	C2-N1	2.20	1.42	1.38
4	B5	3791	OMG	C5-N7	-2.20	1.34	1.39
4	B5	4391	OMG	C5-N7	-2.20	1.34	1.39
4	B5	2836	OMU	C2-N3	-2.20	1.34	1.38
4	B5	400	A2M	C5-N7	-2.20	1.34	1.39
4	B5	3717	A2M	C5-N7	-2.19	1.34	1.39
4	B5	3723	A2M	C5-N7	-2.19	1.34	1.39
52	A2	799	OMU	C2-N1	2.19	1.42	1.38
4	B5	4493	OMG	C5-N7	-2.18	1.34	1.39
52	A2	436	OMG	C5-N7	-2.18	1.34	1.39
4	B5	4522	A2M	C5-N7	-2.18	1.34	1.39
52	A2	1031	A2M	C5-N7	-2.18	1.34	1.39
52	A2	1678	A2M	C5-N7	-2.18	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	A2	27	A2M	C5-N7	-2.18	1.34	1.39
4	B5	4226	OMU	C2-N3	-2.18	1.34	1.38
6	B8	75	OMG	C5-N7	-2.18	1.34	1.39
52	A2	668	A2M	C5-N7	-2.17	1.34	1.39
52	A2	116	OMU	C2-N3	-2.16	1.34	1.38
4	B5	4622	OMG	C5-N7	-2.16	1.34	1.39
4	B5	4589	A2M	C5-N7	-2.16	1.34	1.39
4	B5	4617	OMG	C5-N7	-2.16	1.34	1.39
4	B5	1521	OMG	C5-N7	-2.16	1.34	1.39
2	B2	54	5MU	C6-N1	-2.16	1.34	1.38
52	A2	428	OMU	C2-N1	2.16	1.41	1.38
4	B5	4498	OMG	C5-N7	-2.15	1.34	1.39
52	A2	576	A2M	C5-N7	-2.15	1.35	1.39
52	A2	644	OMG	C5-N7	-2.15	1.34	1.39
52	A2	512	A2M	C5-N7	-2.15	1.35	1.39
52	A2	468	A2M	C5-N7	-2.15	1.35	1.39
52	A2	1639	G7M	C4-N3	2.15	1.39	1.34
4	B5	398	A2M	C5-N7	-2.14	1.35	1.39
2	B2	10	2MG	C5-N7	-2.14	1.34	1.39
52	A2	159	A2M	C5-N7	-2.14	1.35	1.39
4	B5	1321	1MA	C2-N3	2.14	1.34	1.30
2	B2	58	1MA	C5-N7	-2.14	1.34	1.39
4	B5	4369	OMG	C5-N7	-2.13	1.34	1.39
52	A2	1442	OMU	C2-N1	2.13	1.41	1.38
4	B5	3626	OMG	C5-N7	-2.13	1.35	1.39
4	B5	3898	OMG	C5-N7	-2.13	1.35	1.39
2	B2	26	M2G	C5-N7	-2.13	1.35	1.39
4	B5	2363	OMG	C5-N7	-2.13	1.35	1.39
4	B5	4636	OMG	C5-N7	-2.12	1.35	1.39
52	A2	354	OMU	C2-N1	2.12	1.41	1.38
52	A2	1490	OMG	C5-N7	-2.12	1.35	1.39
52	A2	1383	A2M	C5-N7	-2.11	1.35	1.39
52	A2	509	OMG	C5-N7	-2.11	1.35	1.39
52	A2	428	OMU	C2-N3	-2.10	1.34	1.38
52	A2	627	OMU	C2-N1	2.10	1.41	1.38
4	B5	4227	OMG	C5-N7	-2.10	1.35	1.39
52	A2	121	OMU	C2-N3	-2.09	1.34	1.38
4	B5	3943	OMG	C5-N7	-2.09	1.35	1.39
52	A2	867	OMG	C5-N7	-2.09	1.35	1.39
4	B5	4619	OMU	C5-C4	-2.08	1.39	1.43
52	A2	1639	G7M	C6-N1	2.08	1.42	1.38
4	B5	4305	OMU	C5-C4	-2.08	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	A2	1288	OMU	C2-N3	-2.08	1.34	1.38
52	A2	1447	OMG	C5-N7	-2.07	1.35	1.39
52	A2	683	OMG	C5-N7	-2.07	1.35	1.39
52	A2	1326	OMU	C2-N3	-2.06	1.34	1.38
2	B2	6	2MG	C5-N7	-2.06	1.35	1.39
52	A2	601	OMG	C5-N7	-2.06	1.35	1.39
52	A2	1442	OMU	C2-N3	-2.05	1.34	1.38
52	A2	1328	OMG	C5-N7	-2.04	1.35	1.39
2	B2	54	5MU	C2-N3	-2.04	1.34	1.38
4	B5	2414	OMU	C2-N1	2.04	1.41	1.38
52	A2	121	OMU	C2-N1	2.04	1.41	1.38
52	A2	799	OMU	C2-N3	-2.04	1.34	1.38
6	B8	14	OMU	C5-C4	-2.04	1.39	1.43
4	B5	3636	PSU	C2-N3	-2.03	1.34	1.37
52	A2	1337	4AC	C7-N4	-2.03	1.33	1.37
52	A2	172	OMU	C5-C4	-2.02	1.39	1.43
52	A2	1804	OMU	C2-N3	-2.02	1.34	1.38
4	B5	4529	UR3	C2-N1	2.02	1.41	1.38
52	A2	354	OMU	C2-N3	-2.02	1.34	1.38
52	A2	627	OMU	C2-N3	-2.02	1.34	1.38
52	A2	799	OMU	C5-C4	-2.01	1.39	1.43
52	A2	354	OMU	C5-C4	-2.00	1.39	1.43

All (1039) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	A2	1850	MA6	C4-N9-C8	14.75	121.72	105.73
52	A2	1851	MA6	C4-N9-C8	14.40	121.33	105.73
2	B2	46	G7M	C8-N7-C5	11.45	122.10	107.78
52	A2	1639	G7M	C8-N7-C5	11.45	122.09	107.78
2	B2	20	H2U	C4-N3-C2	-9.87	117.60	125.79
2	B2	16	H2U	C4-N3-C2	-8.91	118.40	125.79
2	B2	47	H2U	C4-N3-C2	-8.26	118.94	125.79
2	B2	10	2MG	C2-N3-C4	7.52	121.36	112.04
2	B2	46	G7M	C6-C5-N7	7.29	141.06	132.25
2	B2	6	2MG	C2-N3-C4	7.28	121.06	112.04
52	A2	1850	MA6	N3-C4-N9	6.96	138.55	127.08
52	A2	1851	MA6	N3-C4-N9	6.84	138.35	127.08
52	A2	590	A2M	C5-C4-N3	-6.81	117.87	126.75
52	A2	1639	G7M	N9-C4-N3	6.58	139.15	125.94
52	A2	99	A2M	C5-C4-N3	-6.51	118.25	126.75
52	A2	1639	G7M	C6-C5-N7	6.46	140.06	132.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B5	1322	A2M	C5-C4-N3	-6.45	118.34	126.75
52	A2	166	A2M	C5-C4-N3	-6.42	118.37	126.75
52	A2	484	A2M	C5-C4-N3	-6.39	118.41	126.75
2	B2	46	G7M	CN7-N7-C5	-6.39	118.83	126.77
52	A2	1832	6MZ	C5-C4-N3	-6.37	118.44	126.75
52	A2	512	A2M	C5-C4-N3	-6.35	118.47	126.75
2	B2	10	2MG	C5-C4-N3	-6.31	118.22	128.46
4	B5	4195	OMG	C5-C4-N3	-6.31	118.23	128.46
52	A2	509	OMG	C5-C4-N3	-6.29	118.25	128.46
4	B5	2814	A2M	C5-C4-N3	-6.29	118.55	126.75
4	B5	4570	A2M	C5-C4-N3	-6.27	118.57	126.75
4	B5	2362	A2M	C5-C4-N3	-6.27	118.58	126.75
4	B5	3723	A2M	C5-C4-N3	-6.26	118.59	126.75
4	B5	2875	OMG	C5-C4-N3	-6.25	118.32	128.46
52	A2	1031	A2M	C5-C4-N3	-6.24	118.61	126.75
2	B2	26	M2G	C5-C4-N3	-6.24	118.34	128.46
6	B8	75	OMG	C5-C4-N3	-6.24	118.34	128.46
4	B5	398	A2M	C5-C4-N3	-6.22	118.63	126.75
52	A2	468	A2M	C5-C4-N3	-6.21	118.64	126.75
52	A2	867	OMG	C5-C4-N3	-6.21	118.38	128.46
52	A2	27	A2M	C5-C4-N3	-6.19	118.67	126.75
52	A2	1383	A2M	C5-C4-N3	-6.19	118.68	126.75
4	B5	3866	A2M	C5-C4-N3	-6.18	118.68	126.75
52	A2	576	A2M	C5-C4-N3	-6.18	118.68	126.75
52	A2	1447	OMG	C5-C4-N3	-6.18	118.43	128.46
4	B5	1533	A2M	C5-C4-N3	-6.18	118.69	126.75
52	A2	644	OMG	C5-C4-N3	-6.17	118.46	128.46
52	A2	159	A2M	C5-C4-N3	-6.16	118.72	126.75
52	A2	1490	OMG	C5-C4-N3	-6.16	118.47	128.46
4	B5	4627	PSU	N1-C2-N3	6.15	122.09	115.13
4	B5	400	A2M	C5-C4-N3	-6.15	118.73	126.75
4	B5	4520	PSU	N1-C2-N3	6.14	122.09	115.13
4	B5	2400	A2M	C5-C4-N3	-6.13	118.75	126.75
4	B5	4219	6MZ	C5-C4-N3	-6.13	118.76	126.75
4	B5	2786	A2M	C5-C4-N3	-6.12	118.76	126.75
4	B5	2423	OMG	C5-C4-N3	-6.12	118.53	128.46
4	B5	3717	A2M	C5-C4-N3	-6.12	118.77	126.75
52	A2	1328	OMG	C5-C4-N3	-6.11	118.54	128.46
4	B5	1859	PSU	N1-C2-N3	6.11	122.05	115.13
4	B5	3824	A2M	C5-C4-N3	-6.10	118.79	126.75
4	B5	3829	A2M	C5-C4-N3	-6.10	118.79	126.75
4	B5	3791	OMG	C5-C4-N3	-6.10	118.57	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B5	1325	A2M	C5-C4-N3	-6.10	118.79	126.75
4	B5	4522	A2M	C5-C4-N3	-6.09	118.80	126.75
4	B5	4589	A2M	C5-C4-N3	-6.09	118.81	126.75
52	A2	668	A2M	C5-C4-N3	-6.09	118.81	126.75
4	B5	4635	PSU	N1-C2-N3	6.08	122.02	115.13
52	A2	436	OMG	C5-C4-N3	-6.08	118.60	128.46
2	B2	6	2MG	C5-C4-N3	-6.08	118.60	128.46
4	B5	3636	PSU	N1-C2-N3	6.06	122.00	115.13
4	B5	3852	PSU	N1-C2-N3	6.06	122.00	115.13
52	A2	1232	PSU	N1-C2-N3	6.05	121.99	115.13
4	B5	4498	OMG	C5-C4-N3	-6.05	118.64	128.46
4	B5	4402	PSU	N1-C2-N3	6.05	121.98	115.13
52	A2	105	PSU	N1-C2-N3	6.05	121.98	115.13
52	A2	1678	A2M	C5-C4-N3	-6.05	118.86	126.75
52	A2	601	OMG	C5-C4-N3	-6.04	118.66	128.46
52	A2	406	PSU	N1-C2-N3	6.04	121.97	115.13
4	B5	1535	PSU	N1-C2-N3	6.04	121.97	115.13
4	B5	1624	OMG	C5-C4-N3	-6.03	118.67	128.46
4	B5	4972	PSU	N1-C2-N3	6.03	121.96	115.13
6	B8	55	PSU	N1-C2-N3	6.03	121.96	115.13
4	B5	4441	PSU	N1-C2-N3	6.03	121.96	115.13
4	B5	4352	PSU	N1-C2-N3	6.02	121.96	115.13
4	B5	2363	OMG	C5-C4-N3	-6.02	118.69	128.46
4	B5	1870	A2M	C5-C4-N3	-6.02	118.90	126.75
52	A2	1445	PSU	N1-C2-N3	6.02	121.95	115.13
4	B5	3694	PSU	N1-C2-N3	6.02	121.94	115.13
4	B5	3626	OMG	C5-C4-N3	-6.01	118.71	128.46
4	B5	4470	PSU	N1-C2-N3	6.01	121.94	115.13
4	B5	4688	PSU	N1-C2-N3	6.01	121.94	115.13
4	B5	5009	PSU	N1-C2-N3	6.01	121.94	115.13
4	B5	2842	PSU	N1-C2-N3	6.01	121.94	115.13
52	A2	109	PSU	N1-C2-N3	6.01	121.94	115.13
4	B5	3850	PSU	N1-C2-N3	6.01	121.93	115.13
4	B5	3638	PSU	N1-C2-N3	6.00	121.93	115.13
52	A2	801	PSU	N1-C2-N3	6.00	121.93	115.13
4	B5	3919	PSU	N1-C2-N3	6.00	121.93	115.13
4	B5	5000	PSU	N1-C2-N3	6.00	121.93	115.13
4	B5	1791	PSU	N1-C2-N3	6.00	121.92	115.13
52	A2	681	PSU	N1-C2-N3	5.99	121.92	115.13
4	B5	4492	PSU	N1-C2-N3	5.99	121.92	115.13
4	B5	4493	OMG	C5-C4-N3	-5.99	118.75	128.46
52	A2	1004	PSU	N1-C2-N3	5.99	121.91	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B5	1781	PSU	N1-C2-N3	5.98	121.91	115.13
4	B5	4422	PSU	N1-C2-N3	5.98	121.91	115.13
4	B5	1523	A2M	C5-C4-N3	-5.98	118.94	126.75
4	B5	3883	PSU	N1-C2-N3	5.98	121.91	115.13
4	B5	4311	PSU	N1-C2-N3	5.98	121.91	115.13
4	B5	3743	OMG	C5-C4-N3	-5.98	118.76	128.46
4	B5	3821	PSU	N1-C2-N3	5.98	121.90	115.13
4	B5	4971	PSU	N1-C2-N3	5.98	121.90	115.13
4	B5	3943	OMG	C5-C4-N3	-5.98	118.76	128.46
4	B5	4672	PSU	N1-C2-N3	5.98	121.90	115.13
52	A2	651	PSU	N1-C2-N3	5.97	121.90	115.13
4	B5	4430	PSU	N1-C2-N3	5.97	121.90	115.13
52	A2	1045	PSU	N1-C2-N3	5.97	121.89	115.13
52	A2	1046	PSU	N1-C2-N3	5.97	121.89	115.13
4	B5	3784	A2M	C5-C4-N3	-5.97	118.96	126.75
4	B5	1861	PSU	N1-C2-N3	5.97	121.89	115.13
52	A2	1174	PSU	N1-C2-N3	5.97	121.89	115.13
4	B5	4531	PSU	N1-C2-N3	5.97	121.89	115.13
4	B5	4578	PSU	N1-C2-N3	5.97	121.89	115.13
4	B5	4617	OMG	C5-C4-N3	-5.97	118.78	128.46
4	B5	4551	PSU	N1-C2-N3	5.97	121.89	115.13
52	A2	1367	PSU	N1-C2-N3	5.96	121.89	115.13
52	A2	1238	PSU	N1-C2-N3	5.96	121.89	115.13
4	B5	3843	PSU	N1-C2-N3	5.96	121.88	115.13
4	B5	4456	PSU	N1-C2-N3	5.96	121.88	115.13
4	B5	4391	OMG	C5-C4-N3	-5.96	118.80	128.46
4	B5	4295	PSU	N1-C2-N3	5.95	121.88	115.13
52	A2	1347	PSU	N1-C2-N3	5.95	121.88	115.13
52	A2	1643	PSU	N1-C2-N3	5.95	121.88	115.13
6	B8	69	PSU	N1-C2-N3	5.95	121.87	115.13
52	A2	34	PSU	N1-C2-N3	5.95	121.87	115.13
52	A2	966	PSU	N1-C2-N3	5.95	121.87	115.13
4	B5	3714	PSU	N1-C2-N3	5.95	121.87	115.13
52	A2	1081	PSU	N1-C2-N3	5.95	121.87	115.13
4	B5	3761	PSU	N1-C2-N3	5.95	121.87	115.13
4	B5	4636	OMG	C5-C4-N3	-5.95	118.81	128.46
52	A2	1136	PSU	N1-C2-N3	5.95	121.87	115.13
4	B5	4622	OMG	C5-C4-N3	-5.95	118.81	128.46
52	A2	1625	PSU	N1-C2-N3	5.95	121.87	115.13
52	A2	683	OMG	C5-C4-N3	-5.94	118.82	128.46
4	B5	4360	PSU	N1-C2-N3	5.94	121.86	115.13
52	A2	296	PSU	N1-C2-N3	5.94	121.86	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B5	1780	PSU	N1-C2-N3	5.94	121.86	115.13
52	A2	1056	PSU	N1-C2-N3	5.94	121.86	115.13
4	B5	4575	PSU	N1-C2-N3	5.94	121.86	115.13
52	A2	1244	PSU	N1-C2-N3	5.94	121.86	115.13
4	B5	1743	PSU	N1-C2-N3	5.94	121.86	115.13
4	B5	4369	OMG	C5-C4-N3	-5.94	118.83	128.46
52	A2	210	PSU	N1-C2-N3	5.94	121.86	115.13
4	B5	3729	PSU	N1-C2-N3	5.92	121.84	115.13
4	B5	1682	PSU	N1-C2-N3	5.92	121.83	115.13
4	B5	1676	PSU	N1-C2-N3	5.92	121.83	115.13
52	A2	1692	PSU	N1-C2-N3	5.91	121.83	115.13
4	B5	3898	OMG	C5-C4-N3	-5.91	118.87	128.46
2	B2	31	PSU	N1-C2-N3	5.91	121.83	115.13
52	A2	649	PSU	N1-C2-N3	5.91	121.83	115.13
4	B5	2507	PSU	N1-C2-N3	5.91	121.83	115.13
4	B5	2838	PSU	N1-C2-N3	5.90	121.81	115.13
52	A2	686	PSU	N1-C2-N3	5.90	121.81	115.13
4	B5	2631	PSU	N1-C2-N3	5.89	121.81	115.13
52	A2	218	PSU	N1-C2-N3	5.89	121.81	115.13
4	B5	3769	PSU	N1-C2-N3	5.89	121.81	115.13
52	A2	1850	MA6	N9-C8-N7	-5.89	105.86	113.91
4	B5	1778	PSU	N1-C2-N3	5.89	121.80	115.13
2	B2	27	PSU	N1-C2-N3	5.89	121.80	115.13
4	B5	4298	PSU	N1-C2-N3	5.89	121.80	115.13
52	A2	119	PSU	N1-C2-N3	5.89	121.80	115.13
52	A2	1177	PSU	N1-C2-N3	5.89	121.80	115.13
4	B5	3767	PSU	N1-C2-N3	5.88	121.79	115.13
52	A2	93	PSU	N1-C2-N3	5.87	121.79	115.13
52	A2	609	PSU	N1-C2-N3	5.87	121.78	115.13
4	B5	4529	UR3	C4-N3-C2	-5.86	119.04	124.56
52	A2	1851	MA6	C5-C4-N3	-5.86	119.11	126.75
52	A2	815	PSU	N1-C2-N3	5.86	121.76	115.13
52	A2	814	PSU	N1-C2-N3	5.85	121.76	115.13
52	A2	572	PSU	N1-C2-N3	5.85	121.76	115.13
52	A2	1851	MA6	C4-C5-N7	-5.85	103.49	110.62
52	A2	822	PSU	N1-C2-N3	5.85	121.76	115.13
52	A2	866	PSU	N1-C2-N3	5.85	121.75	115.13
4	B5	1581	PSU	N1-C2-N3	5.85	121.75	115.13
4	B5	4499	PSU	N1-C2-N3	5.83	121.74	115.13
52	A2	863	PSU	N1-C2-N3	5.83	121.73	115.13
4	B5	4292	PSU	N1-C2-N3	5.81	121.71	115.13
52	A2	36	PSU	N1-C2-N3	5.80	121.70	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B5	1521	OMG	C5-C4-N3	-5.78	119.08	128.46
52	A2	1851	MA6	N9-C8-N7	-5.77	106.02	113.91
2	B2	46	G7M	N9-C4-N3	5.76	137.51	125.94
4	B5	1315	OMG	C5-C4-N3	-5.76	119.12	128.46
52	A2	1850	MA6	C5-C4-N3	-5.75	119.25	126.75
2	B2	55	PSU	N1-C2-N3	5.66	121.55	115.13
52	A2	1639	G7M	CN7-N7-C5	-5.66	119.73	126.77
4	B5	4227	OMG	C5-C4-N3	-5.65	119.30	128.46
2	B2	58	1MA	C5-C4-N3	-5.56	118.97	127.26
52	A2	1850	MA6	C4-C5-N7	-5.54	103.87	110.62
52	A2	590	A2M	N3-C4-N9	5.36	135.91	127.08
4	B5	1321	1MA	C5-C4-N3	-5.31	119.33	127.26
4	B5	3817	UY1	C4-N3-C2	-5.21	118.84	126.34
52	A2	99	A2M	N3-C4-N9	5.08	135.46	127.08
4	B5	1322	A2M	N3-C4-N9	5.06	135.43	127.08
52	A2	1832	6MZ	N3-C4-N9	5.06	135.42	127.08
4	B5	4195	OMG	C2-N3-C4	5.03	121.27	112.30
52	A2	166	A2M	N3-C4-N9	5.02	135.36	127.08
52	A2	867	OMG	C2-N3-C4	5.01	121.23	112.30
4	B5	2875	OMG	C2-N3-C4	5.00	121.21	112.30
4	B5	2786	A2M	N3-C4-N9	5.00	135.31	127.08
52	A2	1328	OMG	C2-N3-C4	4.99	121.20	112.30
52	A2	484	A2M	N3-C4-N9	4.99	135.30	127.08
52	A2	512	A2M	N3-C4-N9	4.98	135.29	127.08
4	B5	2363	OMG	C2-N3-C4	4.98	121.17	112.30
52	A2	509	OMG	C2-N3-C4	4.98	121.17	112.30
4	B5	3791	OMG	C2-N3-C4	4.98	121.17	112.30
4	B5	2423	OMG	C2-N3-C4	4.97	121.16	112.30
52	A2	1447	OMG	C2-N3-C4	4.97	121.15	112.30
4	B5	3723	A2M	N3-C4-N9	4.97	135.26	127.08
4	B5	3898	OMG	C2-N3-C4	4.96	121.14	112.30
4	B5	4570	A2M	N3-C4-N9	4.96	135.26	127.08
6	B8	75	OMG	C2-N3-C4	4.95	121.12	112.30
4	B5	4498	OMG	C2-N3-C4	4.94	121.10	112.30
4	B5	3943	OMG	C2-N3-C4	4.91	121.04	112.30
4	B5	3866	A2M	N3-C4-N9	4.89	135.14	127.08
52	A2	436	OMG	C2-N3-C4	4.89	121.00	112.30
4	B5	3626	OMG	C2-N3-C4	4.88	121.00	112.30
52	A2	644	OMG	C2-N3-C4	4.88	120.99	112.30
4	B5	4522	A2M	N3-C4-N9	4.87	135.11	127.08
52	A2	1031	A2M	N3-C4-N9	4.87	135.10	127.08
52	A2	1490	OMG	C2-N3-C4	4.86	120.96	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	A2	601	OMG	C2-N3-C4	4.86	120.95	112.30
4	B5	4195	OMG	N9-C4-N3	4.85	135.68	125.94
4	B5	2814	A2M	N3-C4-N9	4.85	135.07	127.08
52	A2	576	A2M	N3-C4-N9	4.85	135.07	127.08
4	B5	4617	OMG	C2-N3-C4	4.85	120.94	112.30
4	B5	4636	OMG	C2-N3-C4	4.85	120.94	112.30
52	A2	683	OMG	C2-N3-C4	4.85	120.94	112.30
4	B5	1624	OMG	C2-N3-C4	4.84	120.92	112.30
4	B5	4622	OMG	C2-N3-C4	4.84	120.92	112.30
4	B5	2362	A2M	N3-C4-N9	4.83	135.05	127.08
4	B5	398	A2M	N3-C4-N9	4.83	135.04	127.08
2	B2	54	5MU	C4-N3-C2	-4.83	121.10	127.35
4	B5	4493	OMG	C2-N3-C4	4.82	120.89	112.30
52	A2	468	A2M	N3-C4-N9	4.82	135.02	127.08
2	B2	54	5MU	N3-C2-N1	4.81	121.28	114.89
52	A2	27	A2M	N3-C4-N9	4.81	135.01	127.08
4	B5	3743	OMG	C2-N3-C4	4.81	120.87	112.30
4	B5	4219	6MZ	N3-C4-N9	4.81	135.00	127.08
4	B5	1325	A2M	N3-C4-N9	4.81	135.00	127.08
52	A2	1383	A2M	N3-C4-N9	4.80	135.00	127.08
4	B5	4391	OMG	C2-N3-C4	4.79	120.84	112.30
4	B5	400	A2M	N3-C4-N9	4.79	134.98	127.08
4	B5	4369	OMG	C2-N3-C4	4.79	120.83	112.30
4	B5	1521	OMG	C2-N3-C4	4.78	120.82	112.30
4	B5	3829	A2M	N3-C4-N9	4.78	134.96	127.08
52	A2	668	A2M	N3-C4-N9	4.77	134.94	127.08
4	B5	2400	A2M	N3-C4-N9	4.77	134.93	127.08
2	B2	26	M2G	N9-C4-N3	4.76	135.50	125.94
4	B5	3824	A2M	N3-C4-N9	4.76	134.92	127.08
2	B2	10	2MG	N9-C4-N3	4.75	135.48	125.94
4	B5	1533	A2M	N3-C4-N9	4.75	134.90	127.08
4	B5	4589	A2M	N3-C4-N9	4.74	134.90	127.08
52	A2	509	OMG	N9-C4-N3	4.73	135.45	125.94
52	A2	159	A2M	N3-C4-N9	4.73	134.88	127.08
4	B5	1315	OMG	C2-N3-C4	4.72	120.71	112.30
4	B5	3717	A2M	N3-C4-N9	4.72	134.86	127.08
2	B2	58	1MA	C2-N3-C4	4.71	121.67	112.41
4	B5	3784	A2M	N3-C4-N9	4.71	134.84	127.08
52	A2	867	OMG	N9-C4-N3	4.70	135.37	125.94
4	B5	1321	1MA	C2-N3-C4	4.70	121.64	112.41
52	A2	1678	A2M	N3-C4-N9	4.70	134.82	127.08
4	B5	2875	OMG	N9-C4-N3	4.69	135.37	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B2	46	G7M	C2-N3-C4	4.69	120.66	112.30
4	B5	1523	A2M	N3-C4-N9	4.69	134.81	127.08
52	A2	1639	G7M	C2-N3-C4	4.69	120.65	112.30
4	B5	4227	OMG	C2-N3-C4	4.68	120.64	112.30
2	B2	26	M2G	C2-N3-C4	4.67	121.15	112.51
4	B5	1870	A2M	N3-C4-N9	4.67	134.78	127.08
6	B8	75	OMG	N9-C4-N3	4.64	135.26	125.94
52	A2	1490	OMG	N9-C4-N3	4.64	135.26	125.94
4	B5	2423	OMG	N9-C4-N3	4.63	135.23	125.94
4	B5	4497	OMU	C4-N3-C2	-4.62	120.48	126.58
4	B5	3791	OMG	N9-C4-N3	4.61	135.20	125.94
4	B5	2414	OMU	C4-N3-C2	-4.61	120.50	126.58
52	A2	1447	OMG	N9-C4-N3	4.61	135.19	125.94
52	A2	644	OMG	N9-C4-N3	4.59	135.15	125.94
52	A2	436	OMG	N9-C4-N3	4.58	135.14	125.94
4	B5	1624	OMG	N9-C4-N3	4.57	135.12	125.94
52	A2	1328	OMG	N9-C4-N3	4.55	135.08	125.94
4	B5	4498	OMG	N9-C4-N3	4.53	135.04	125.94
2	B2	6	2MG	N9-C4-N3	4.53	135.04	125.94
52	A2	1326	OMU	C4-N3-C2	-4.53	120.61	126.58
4	B5	2836	OMU	C4-N3-C2	-4.51	120.62	126.58
4	B5	3924	OMU	C4-N3-C2	-4.51	120.63	126.58
52	A2	601	OMG	N9-C4-N3	4.49	134.96	125.94
6	B8	14	OMU	C4-N3-C2	-4.49	120.66	126.58
4	B5	2363	OMG	N9-C4-N3	4.47	134.92	125.94
4	B5	4493	OMG	N9-C4-N3	4.46	134.90	125.94
4	B5	3743	OMG	N9-C4-N3	4.44	134.85	125.94
4	B5	4636	OMG	N9-C4-N3	4.43	134.84	125.94
4	B5	4369	OMG	N9-C4-N3	4.43	134.84	125.94
4	B5	3626	OMG	N9-C4-N3	4.43	134.83	125.94
4	B5	4391	OMG	N9-C4-N3	4.43	134.82	125.94
4	B5	4622	OMG	N9-C4-N3	4.41	134.80	125.94
4	B5	3943	OMG	N9-C4-N3	4.41	134.79	125.94
52	A2	683	OMG	N9-C4-N3	4.41	134.79	125.94
52	A2	116	OMU	C4-N3-C2	-4.39	120.79	126.58
4	B5	4226	OMU	C4-N3-C2	-4.39	120.79	126.58
4	B5	4617	OMG	N9-C4-N3	4.37	134.71	125.94
52	A2	1639	G7M	C5-C4-N3	-4.36	119.80	128.15
4	B5	4619	OMU	C4-N3-C2	-4.35	120.84	126.58
52	A2	1337	4AC	N4-C4-N3	4.34	121.14	113.85
4	B5	4497	OMU	N3-C2-N1	4.34	120.65	114.89
52	A2	1639	G7M	CN7-N7-C8	-4.32	118.18	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	A2	627	OMU	C4-N3-C2	-4.31	120.90	126.58
4	B5	3898	OMG	N9-C4-N3	4.30	134.57	125.94
52	A2	1842	4AC	N4-C4-N3	4.29	121.05	113.85
4	B5	1315	OMG	N9-C4-N3	4.27	134.51	125.94
52	A2	1442	OMU	C4-N3-C2	-4.26	120.95	126.58
2	B2	54	5MU	C5-C4-N3	4.26	118.95	115.31
4	B5	2414	OMU	N3-C2-N1	4.25	120.53	114.89
52	A2	428	OMU	C4-N3-C2	-4.24	120.98	126.58
52	A2	799	OMU	C4-N3-C2	-4.23	121.00	126.58
52	A2	1850	MA6	N1-C2-N3	-4.22	122.00	128.60
52	A2	354	OMU	C4-N3-C2	-4.22	121.02	126.58
4	B5	4305	OMU	C4-N3-C2	-4.21	121.02	126.58
4	B5	2836	OMU	N3-C2-N1	4.21	120.48	114.89
52	A2	1851	MA6	N1-C2-N3	-4.21	122.02	128.60
4	B5	1521	OMG	N9-C4-N3	4.20	134.38	125.94
52	A2	1678	A2M	C2'-C1'-N9	-4.18	106.48	113.53
6	B8	14	OMU	N3-C2-N1	4.16	120.41	114.89
52	A2	1288	OMU	C4-N3-C2	-4.14	121.11	126.58
52	A2	121	OMU	C4-N3-C2	-4.14	121.12	126.58
52	A2	590	A2M	C2-N3-C4	4.14	121.52	111.75
52	A2	1851	MA6	C2-N1-C6	4.13	121.51	111.75
4	B5	4446	5MC	C5-C6-N1	-4.12	119.10	123.34
4	B5	3924	OMU	N3-C2-N1	4.11	120.34	114.89
52	A2	116	OMU	N3-C2-N1	4.10	120.33	114.89
52	A2	428	OMU	N3-C2-N1	4.09	120.32	114.89
4	B5	4619	OMU	N3-C2-N1	4.09	120.32	114.89
52	A2	1804	OMU	C4-N3-C2	-4.09	121.19	126.58
4	B5	2507	PSU	C4-N3-C2	-4.08	120.46	126.34
4	B5	3817	UY1	N1-C2-N3	4.08	119.75	115.13
52	A2	172	OMU	C4-N3-C2	-4.07	121.21	126.58
52	A2	1136	PSU	C4-N3-C2	-4.07	120.48	126.34
4	B5	4520	PSU	C4-N3-C2	-4.05	120.50	126.34
4	B5	4627	PSU	C4-N3-C2	-4.05	120.51	126.34
4	B5	4226	OMU	N3-C2-N1	4.04	120.26	114.89
4	B5	4635	PSU	C4-N3-C2	-4.04	120.51	126.34
4	B5	4971	PSU	C4-N3-C2	-4.04	120.52	126.34
4	B5	4441	PSU	C4-N3-C2	-4.03	120.53	126.34
4	B5	3769	PSU	C4-N3-C2	-4.03	120.53	126.34
52	A2	1232	PSU	C4-N3-C2	-4.03	120.53	126.34
4	B5	4402	PSU	C4-N3-C2	-4.02	120.54	126.34
4	B5	4227	OMG	N9-C4-N3	4.02	134.02	125.94
4	B5	3761	PSU	C4-N3-C2	-4.02	120.55	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	A2	1850	MA6	C2-N1-C6	4.02	121.25	111.75
4	B5	4292	PSU	C4-N3-C2	-4.02	120.55	126.34
52	A2	651	PSU	C4-N3-C2	-4.02	120.55	126.34
4	B5	3694	PSU	C4-N3-C2	-4.01	120.56	126.34
52	A2	1326	OMU	N3-C2-N1	4.01	120.22	114.89
4	B5	4531	PSU	C4-N3-C2	-4.01	120.56	126.34
52	A2	1045	PSU	C4-N3-C2	-4.01	120.56	126.34
4	B5	4551	PSU	C4-N3-C2	-4.01	120.56	126.34
4	B5	4492	PSU	C4-N3-C2	-4.00	120.58	126.34
4	B5	1861	PSU	C4-N3-C2	-3.99	120.59	126.34
4	B5	4219	6MZ	C9-N6-C6	-3.99	119.43	122.87
4	B5	3852	PSU	C4-N3-C2	-3.99	120.59	126.34
4	B5	1781	PSU	C4-N3-C2	-3.98	120.60	126.34
4	B5	4352	PSU	C4-N3-C2	-3.98	120.60	126.34
4	B5	2842	PSU	C4-N3-C2	-3.98	120.61	126.34
4	B5	1535	PSU	C4-N3-C2	-3.98	120.61	126.34
4	B5	1859	PSU	C4-N3-C2	-3.98	120.61	126.34
4	B5	4295	PSU	C4-N3-C2	-3.97	120.62	126.34
4	B5	4305	OMU	N3-C2-N1	3.97	120.16	114.89
4	B5	3636	PSU	C4-N3-C2	-3.97	120.62	126.34
4	B5	4972	PSU	C4-N3-C2	-3.97	120.62	126.34
4	B5	1322	A2M	C2-N3-C4	3.97	121.12	111.75
4	B5	3821	PSU	C4-N3-C2	-3.97	120.62	126.34
52	A2	354	OMU	N3-C2-N1	3.96	120.14	114.89
52	A2	1442	OMU	N3-C2-N1	3.96	120.14	114.89
52	A2	681	PSU	C4-N3-C2	-3.95	120.64	126.34
52	A2	1244	PSU	C4-N3-C2	-3.95	120.65	126.34
52	A2	801	PSU	C4-N3-C2	-3.95	120.65	126.34
52	A2	1177	PSU	C4-N3-C2	-3.94	120.66	126.34
52	A2	686	PSU	C4-N3-C2	-3.94	120.66	126.34
52	A2	627	OMU	N3-C2-N1	3.94	120.12	114.89
52	A2	1367	PSU	C4-N3-C2	-3.94	120.67	126.34
52	A2	166	A2M	C2-N3-C4	3.93	121.03	111.75
4	B5	1780	PSU	C4-N3-C2	-3.93	120.68	126.34
6	B8	55	PSU	C4-N3-C2	-3.92	120.69	126.34
4	B5	4430	PSU	C4-N3-C2	-3.92	120.69	126.34
52	A2	512	A2M	C2-N3-C4	3.92	121.01	111.75
52	A2	1238	PSU	C4-N3-C2	-3.92	120.69	126.34
4	B5	1791	PSU	C4-N3-C2	-3.92	120.69	126.34
4	B5	4522	A2M	C2-N3-C4	3.92	121.00	111.75
4	B5	2814	A2M	C2-N3-C4	3.92	121.00	111.75
4	B5	5000	PSU	C4-N3-C2	-3.91	120.70	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B2	46	G7M	N9-C8-N7	-3.91	102.53	112.21
4	B5	4522	A2M	C2'-C1'-N9	-3.91	106.94	113.53
4	B5	1682	PSU	C4-N3-C2	-3.91	120.71	126.34
52	A2	1046	PSU	C4-N3-C2	-3.91	120.71	126.34
52	A2	1804	OMU	N3-C2-N1	3.90	120.07	114.89
52	A2	27	A2M	C2-N3-C4	3.90	120.97	111.75
4	B5	398	A2M	C2-N3-C4	3.90	120.97	111.75
4	B5	4456	PSU	C4-N3-C2	-3.90	120.72	126.34
52	A2	172	OMU	N3-C2-N1	3.89	120.06	114.89
52	A2	468	A2M	C2-N3-C4	3.89	120.94	111.75
4	B5	1533	A2M	C2-N3-C4	3.89	120.93	111.75
52	A2	484	A2M	C2-N3-C4	3.89	120.93	111.75
52	A2	1174	PSU	C4-N3-C2	-3.88	120.74	126.34
52	A2	119	PSU	C4-N3-C2	-3.88	120.74	126.34
6	B8	69	PSU	C4-N3-C2	-3.88	120.75	126.34
4	B5	3714	PSU	C4-N3-C2	-3.88	120.75	126.34
4	B5	3723	A2M	C2-N3-C4	3.88	120.92	111.75
4	B5	3784	A2M	C2-N3-C4	3.88	120.91	111.75
4	B5	1743	PSU	C4-N3-C2	-3.87	120.76	126.34
52	A2	121	OMU	N3-C2-N1	3.87	120.03	114.89
4	B5	4311	PSU	C4-N3-C2	-3.87	120.76	126.34
52	A2	576	A2M	C2-N3-C4	3.87	120.89	111.75
52	A2	966	PSU	C4-N3-C2	-3.87	120.77	126.34
52	A2	1004	PSU	C4-N3-C2	-3.87	120.77	126.34
52	A2	1383	A2M	C2-N3-C4	3.87	120.89	111.75
52	A2	34	PSU	C4-N3-C2	-3.86	120.77	126.34
4	B5	4422	PSU	C4-N3-C2	-3.86	120.77	126.34
52	A2	1692	PSU	C4-N3-C2	-3.86	120.77	126.34
52	A2	109	PSU	C4-N3-C2	-3.86	120.78	126.34
4	B5	4360	PSU	C4-N3-C2	-3.86	120.78	126.34
4	B5	3850	PSU	C4-N3-C2	-3.86	120.78	126.34
4	B5	2362	A2M	C2-N3-C4	3.86	120.87	111.75
4	B5	4570	A2M	C2-N3-C4	3.86	120.87	111.75
52	A2	1056	PSU	C4-N3-C2	-3.86	120.78	126.34
52	A2	799	OMU	N3-C2-N1	3.86	120.01	114.89
52	A2	1081	PSU	C4-N3-C2	-3.86	120.78	126.34
52	A2	1347	PSU	C4-N3-C2	-3.86	120.78	126.34
4	B5	4470	PSU	C4-N3-C2	-3.85	120.79	126.34
4	B5	5009	PSU	C4-N3-C2	-3.85	120.79	126.34
52	A2	1288	OMU	N3-C2-N1	3.85	120.00	114.89
52	A2	99	A2M	C2-N3-C4	3.85	120.84	111.75
4	B5	1325	A2M	C2-N3-C4	3.85	120.84	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	A2	1832	6MZ	C2-N3-C4	3.85	120.84	111.75
52	A2	649	PSU	C4-N3-C2	-3.85	120.80	126.34
4	B5	2400	A2M	C2-N3-C4	3.84	120.83	111.75
52	A2	105	PSU	C4-N3-C2	-3.84	120.80	126.34
52	A2	218	PSU	C4-N3-C2	-3.84	120.80	126.34
4	B5	3883	PSU	C4-N3-C2	-3.84	120.80	126.34
4	B5	4219	6MZ	C2-N3-C4	3.84	120.82	111.75
4	B5	3829	A2M	C2-N3-C4	3.84	120.82	111.75
4	B5	3729	PSU	C4-N3-C2	-3.84	120.81	126.34
52	A2	1031	A2M	C2-N3-C4	3.83	120.81	111.75
52	A2	1445	PSU	C4-N3-C2	-3.83	120.81	126.34
52	A2	815	PSU	C4-N3-C2	-3.83	120.82	126.34
52	A2	668	A2M	C2-N3-C4	3.83	120.80	111.75
4	B5	3866	A2M	C2-N3-C4	3.83	120.79	111.75
4	B5	3919	PSU	C4-N3-C2	-3.82	120.83	126.34
52	A2	406	PSU	C4-N3-C2	-3.82	120.83	126.34
4	B5	400	A2M	C2-N3-C4	3.82	120.78	111.75
4	B5	1870	A2M	C2-N3-C4	3.82	120.78	111.75
52	A2	1643	PSU	C4-N3-C2	-3.82	120.83	126.34
52	A2	863	PSU	C4-N3-C2	-3.82	120.84	126.34
2	B2	46	G7M	C5-C4-N3	-3.82	120.83	128.15
4	B5	2631	PSU	C4-N3-C2	-3.82	120.84	126.34
4	B5	2838	PSU	C4-N3-C2	-3.81	120.84	126.34
4	B5	4578	PSU	C4-N3-C2	-3.81	120.84	126.34
2	B2	46	G7M	C4-C5-N7	-3.81	101.43	107.67
52	A2	1678	A2M	C2-N3-C4	3.81	120.76	111.75
52	A2	210	PSU	C4-N3-C2	-3.81	120.85	126.34
4	B5	3824	A2M	C2-N3-C4	3.81	120.74	111.75
4	B5	4688	PSU	C4-N3-C2	-3.81	120.85	126.34
4	B5	4672	PSU	C4-N3-C2	-3.80	120.86	126.34
2	B2	31	PSU	C4-N3-C2	-3.80	120.86	126.34
4	B5	3767	PSU	C4-N3-C2	-3.80	120.86	126.34
4	B5	4589	A2M	C2-N3-C4	3.80	120.72	111.75
2	B2	55	PSU	C4-N3-C2	-3.79	120.88	126.34
4	B5	1523	A2M	C2-N3-C4	3.78	120.69	111.75
52	A2	159	A2M	C2-N3-C4	3.78	120.68	111.75
4	B5	3717	A2M	C2-N3-C4	3.78	120.68	111.75
52	A2	1625	PSU	C4-N3-C2	-3.78	120.89	126.34
52	A2	1639	G7M	C5-C6-N1	3.78	119.68	111.79
4	B5	4499	PSU	C4-N3-C2	-3.77	120.90	126.34
4	B5	4575	PSU	C4-N3-C2	-3.77	120.90	126.34
4	B5	1778	PSU	C4-N3-C2	-3.77	120.90	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B5	2786	A2M	C2-N3-C4	3.77	120.66	111.75
2	B2	27	PSU	C4-N3-C2	-3.77	120.91	126.34
52	A2	814	PSU	C4-N3-C2	-3.77	120.91	126.34
52	A2	866	PSU	C4-N3-C2	-3.76	120.92	126.34
52	A2	296	PSU	C4-N3-C2	-3.75	120.93	126.34
52	A2	1639	G7M	N9-C8-N7	-3.74	102.95	112.21
4	B5	4298	PSU	C4-N3-C2	-3.74	120.94	126.34
2	B2	46	G7M	CN7-N7-C8	-3.74	119.07	124.84
4	B5	3843	PSU	C4-N3-C2	-3.74	120.96	126.34
52	A2	609	PSU	C4-N3-C2	-3.73	120.97	126.34
4	B5	1581	PSU	C4-N3-C2	-3.73	120.97	126.34
4	B5	2786	A2M	C2'-C1'-N9	-3.71	107.29	113.53
52	A2	93	PSU	C4-N3-C2	-3.70	121.00	126.34
2	B2	54	5MU	O4-C4-C5	-3.70	120.62	124.90
4	B5	3638	PSU	C4-N3-C2	-3.68	121.03	126.34
52	A2	572	PSU	C4-N3-C2	-3.68	121.03	126.34
52	A2	36	PSU	C4-N3-C2	-3.67	121.06	126.34
52	A2	822	PSU	C4-N3-C2	-3.66	121.06	126.34
4	B5	1676	PSU	C4-N3-C2	-3.66	121.06	126.34
6	B8	14	OMU	C5-C4-N3	3.64	120.29	114.84
52	A2	1326	OMU	C5-C4-N3	3.63	120.28	114.84
4	B5	2414	OMU	C5-C4-N3	3.62	120.26	114.84
2	B2	46	G7M	C5-C6-N1	3.62	119.35	111.79
2	B2	48	5MC	C5-C6-N1	-3.62	119.61	123.34
52	A2	1639	G7M	C4-C5-N7	-3.62	101.76	107.67
4	B5	3924	OMU	C5-C4-N3	3.59	120.22	114.84
4	B5	4226	OMU	C5-C4-N3	3.58	120.20	114.84
4	B5	2836	OMU	C5-C4-N3	3.56	120.17	114.84
52	A2	799	OMU	C5-C4-N3	3.55	120.15	114.84
4	B5	3638	PSU	O2-C2-N1	-3.54	118.89	122.79
4	B5	4619	OMU	C5-C4-N3	3.53	120.13	114.84
52	A2	627	OMU	C5-C4-N3	3.53	120.13	114.84
52	A2	1442	OMU	C5-C4-N3	3.53	120.13	114.84
4	B5	4227	OMG	C6-C5-N7	3.53	136.82	130.25
52	A2	99	A2M	C2'-C1'-N9	-3.53	107.58	113.53
4	B5	4305	OMU	C5-C4-N3	3.53	120.12	114.84
4	B5	4497	OMU	C5-C4-N3	3.52	120.11	114.84
52	A2	1851	MA6	C1'-N9-C8	-3.52	119.18	127.14
52	A2	116	OMU	C5-C4-N3	3.52	120.11	114.84
52	A2	1288	OMU	C5-C4-N3	3.52	120.10	114.84
52	A2	296	PSU	O2-C2-N1	-3.52	118.92	122.79
4	B5	3784	A2M	O4'-C1'-N9	3.51	114.98	108.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	A2	1851	MA6	C2-N3-C4	3.51	120.03	111.75
4	B5	4627	PSU	O2-C2-N1	-3.50	118.94	122.79
4	B5	2838	PSU	O2-C2-N1	-3.49	118.94	122.79
52	A2	121	OMU	C5-C4-N3	3.49	120.06	114.84
4	B5	1535	PSU	O2-C2-N1	-3.48	118.96	122.79
52	A2	822	PSU	O2-C2-N1	-3.47	118.97	122.79
52	A2	1248	B8N	C4-N3-C2	-3.47	121.07	125.46
52	A2	354	OMU	C5-C4-N3	3.47	120.03	114.84
4	B5	1859	PSU	O2-C2-N1	-3.47	118.97	122.79
52	A2	1445	PSU	O2-C2-N1	-3.47	118.97	122.79
52	A2	1850	MA6	C2-N3-C4	3.46	119.94	111.75
4	B5	4520	PSU	O2-C2-N1	-3.46	118.98	122.79
52	A2	428	OMU	C5-C4-N3	3.46	120.02	114.84
52	A2	172	OMU	C5-C4-N3	3.45	120.01	114.84
4	B5	3898	OMG	C6-C5-N7	3.45	136.67	130.25
52	A2	681	PSU	O2-C2-N1	-3.45	118.99	122.79
52	A2	1851	MA6	C6-C5-N7	3.45	139.07	133.28
52	A2	1046	PSU	O2-C2-N1	-3.45	119.00	122.79
4	B5	4575	PSU	O2-C2-N1	-3.44	119.00	122.79
4	B5	4672	PSU	O2-C2-N1	-3.44	119.00	122.79
4	B5	1521	OMG	C6-C5-N7	3.44	136.65	130.25
52	A2	406	PSU	O2-C2-N1	-3.44	119.00	122.79
4	B5	1780	PSU	O2-C2-N1	-3.44	119.01	122.79
4	B5	3852	PSU	O2-C2-N1	-3.44	119.01	122.79
52	A2	1238	PSU	O2-C2-N1	-3.44	119.01	122.79
52	A2	1045	PSU	O2-C2-N1	-3.43	119.01	122.79
52	A2	1804	OMU	C5-C4-N3	3.43	119.97	114.84
52	A2	801	PSU	O2-C2-N1	-3.43	119.01	122.79
52	A2	1678	A2M	C4-C5-N7	-3.43	106.44	110.62
4	B5	1682	PSU	O2-C2-N1	-3.43	119.02	122.79
2	B2	27	PSU	O2-C2-N1	-3.43	119.02	122.79
52	A2	1056	PSU	O2-C2-N1	-3.42	119.02	122.79
4	B5	4402	PSU	O2-C2-N1	-3.42	119.02	122.79
52	A2	1850	MA6	C1'-N9-C8	-3.42	119.41	127.14
4	B5	4635	PSU	O2-C2-N1	-3.42	119.03	122.79
52	A2	1004	PSU	O2-C2-N1	-3.41	119.03	122.79
4	B5	4311	PSU	O2-C2-N1	-3.41	119.03	122.79
4	B5	4352	PSU	O2-C2-N1	-3.41	119.04	122.79
52	A2	1174	PSU	O2-C2-N1	-3.41	119.04	122.79
4	B5	3843	PSU	O2-C2-N1	-3.41	119.04	122.79
4	B5	1743	PSU	O2-C2-N1	-3.41	119.04	122.79
52	A2	1367	PSU	O2-C2-N1	-3.40	119.04	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	A2	1625	PSU	O2-C2-N1	-3.40	119.04	122.79
6	B8	69	PSU	O2-C2-N1	-3.40	119.04	122.79
4	B5	3850	PSU	O2-C2-N1	-3.40	119.05	122.79
4	B5	3883	PSU	O2-C2-N1	-3.40	119.05	122.79
4	B5	1778	PSU	O2-C2-N1	-3.40	119.05	122.79
4	B5	4441	PSU	O2-C2-N1	-3.39	119.05	122.79
4	B5	2631	PSU	O2-C2-N1	-3.39	119.06	122.79
4	B5	5000	PSU	O2-C2-N1	-3.39	119.06	122.79
4	B5	3694	PSU	O2-C2-N1	-3.38	119.06	122.79
4	B5	4971	PSU	O2-C2-N1	-3.38	119.07	122.79
52	A2	119	PSU	O2-C2-N1	-3.38	119.07	122.79
4	B5	1791	PSU	O2-C2-N1	-3.38	119.07	122.79
52	A2	1643	PSU	O2-C2-N1	-3.38	119.07	122.79
4	B5	4470	PSU	O2-C2-N1	-3.38	119.07	122.79
4	B5	2842	PSU	O2-C2-N1	-3.38	119.07	122.79
4	B5	3919	PSU	O2-C2-N1	-3.38	119.07	122.79
52	A2	649	PSU	O2-C2-N1	-3.37	119.08	122.79
32	Ba	39	V5N	CD2-CG-ND1	3.37	110.14	105.71
52	A2	109	PSU	O2-C2-N1	-3.37	119.08	122.79
4	B5	4430	PSU	O2-C2-N1	-3.37	119.08	122.79
4	B5	3729	PSU	O2-C2-N1	-3.37	119.08	122.79
4	B5	4688	PSU	O2-C2-N1	-3.37	119.08	122.79
4	B5	5009	PSU	O2-C2-N1	-3.37	119.08	122.79
7	BA	216	V5N	CD2-CG-ND1	3.37	110.13	105.71
2	B2	58	1MA	N9-C4-N3	3.36	134.78	126.94
52	A2	218	PSU	O2-C2-N1	-3.36	119.09	122.79
4	B5	4422	PSU	O2-C2-N1	-3.36	119.09	122.79
4	B5	4492	PSU	O2-C2-N1	-3.36	119.09	122.79
52	A2	1639	G7M	O6-C6-C5	-3.36	120.48	128.06
4	B5	1781	PSU	O2-C2-N1	-3.36	119.09	122.79
4	B5	4972	PSU	O2-C2-N1	-3.35	119.10	122.79
52	A2	34	PSU	O2-C2-N1	-3.35	119.10	122.79
52	A2	93	PSU	O2-C2-N1	-3.35	119.10	122.79
52	A2	572	PSU	O2-C2-N1	-3.35	119.11	122.79
4	B5	4219	6MZ	C6-C5-N7	3.35	136.01	132.39
4	B5	4456	PSU	O2-C2-N1	-3.35	119.11	122.79
4	B5	2507	PSU	O2-C2-N1	-3.34	119.11	122.79
52	A2	484	A2M	C4-C5-N7	-3.34	106.55	110.62
52	A2	651	PSU	O2-C2-N1	-3.34	119.12	122.79
2	B2	54	5MU	C5-C6-N1	-3.34	119.91	123.34
52	A2	36	PSU	O2-C2-N1	-3.33	119.12	122.79
4	B5	3943	OMG	C6-C5-N7	3.33	136.44	130.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	A2	1383	A2M	C4-C5-N7	-3.33	106.56	110.62
4	B5	3821	PSU	O2-C2-N1	-3.33	119.12	122.79
4	B5	2400	A2M	C2'-C1'-N9	-3.33	107.92	113.53
4	B5	3769	PSU	O2-C2-N1	-3.33	119.13	122.79
52	A2	166	A2M	C4-C5-N7	-3.33	106.57	110.62
4	B5	4295	PSU	O2-C2-N1	-3.33	119.13	122.79
52	A2	99	A2M	C4-C5-N7	-3.33	106.57	110.62
52	A2	159	A2M	C4-C5-N7	-3.32	106.57	110.62
52	A2	1177	PSU	O2-C2-N1	-3.32	119.13	122.79
4	B5	2814	A2M	C4-C5-N7	-3.32	106.57	110.62
52	A2	1081	PSU	O2-C2-N1	-3.32	119.13	122.79
4	B5	4499	PSU	O2-C2-N1	-3.32	119.13	122.79
4	B5	4360	PSU	O2-C2-N1	-3.32	119.13	122.79
4	B5	1861	PSU	O2-C2-N1	-3.32	119.14	122.79
4	B5	2362	A2M	C4-C5-N7	-3.32	106.58	110.62
52	A2	210	PSU	O2-C2-N1	-3.32	119.14	122.79
52	A2	1347	PSU	O2-C2-N1	-3.32	119.14	122.79
4	B5	4551	PSU	O2-C2-N1	-3.31	119.14	122.79
4	B5	4531	PSU	O2-C2-N1	-3.31	119.14	122.79
52	A2	966	PSU	O2-C2-N1	-3.31	119.14	122.79
52	A2	686	PSU	O2-C2-N1	-3.31	119.14	122.79
52	A2	468	A2M	C4-C5-N7	-3.31	106.59	110.62
4	B5	1870	A2M	C2'-C1'-N9	-3.31	107.96	113.53
4	B5	4298	PSU	O2-C2-N1	-3.31	119.15	122.79
4	B5	1533	A2M	C4-C5-N7	-3.31	106.59	110.62
4	B5	3829	A2M	C2'-C1'-N9	-3.31	107.97	113.53
4	B5	398	A2M	C4-C5-N7	-3.30	106.59	110.62
4	B5	398	A2M	C2'-C1'-N9	-3.30	107.97	113.53
52	A2	866	PSU	O2-C2-N1	-3.30	119.16	122.79
4	B5	4522	A2M	N3-C2-N1	-3.30	123.44	128.60
4	B5	1581	PSU	O2-C2-N1	-3.29	119.16	122.79
4	B5	4292	PSU	O2-C2-N1	-3.29	119.17	122.79
52	A2	683	OMG	C6-C5-N7	3.29	136.37	130.25
4	B5	4617	OMG	C6-C5-N7	3.29	136.37	130.25
52	A2	814	PSU	O2-C2-N1	-3.29	119.17	122.79
6	B8	55	PSU	O2-C2-N1	-3.29	119.17	122.79
4	B5	3767	PSU	O2-C2-N1	-3.29	119.17	122.79
52	A2	1244	PSU	O2-C2-N1	-3.29	119.17	122.79
52	A2	1692	PSU	O2-C2-N1	-3.29	119.17	122.79
52	A2	609	PSU	O2-C2-N1	-3.29	119.17	122.79
52	A2	105	PSU	O2-C2-N1	-3.28	119.17	122.79
4	B5	3824	A2M	C4-C5-N7	-3.28	106.62	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B5	2363	OMG	C6-C5-N7	3.28	136.35	130.25
4	B5	4570	A2M	C2'-C1'-N9	-3.28	108.00	113.53
4	B5	4578	PSU	O2-C2-N1	-3.28	119.18	122.79
4	B5	3761	PSU	O2-C2-N1	-3.28	119.18	122.79
4	B5	1315	OMG	C6-C5-N7	3.28	136.34	130.25
4	B5	2400	A2M	C4-C5-N7	-3.28	106.63	110.62
4	B5	3784	A2M	N3-C2-N1	-3.28	123.48	128.60
52	A2	27	A2M	C4-C5-N7	-3.27	106.63	110.62
2	B2	31	PSU	O2-C2-N1	-3.27	119.19	122.79
4	B5	3714	PSU	O2-C2-N1	-3.27	119.19	122.79
4	B5	3626	OMG	C6-C5-N7	3.27	136.33	130.25
4	B5	1870	A2M	N3-C2-N1	-3.26	123.50	128.60
52	A2	1232	PSU	O2-C2-N1	-3.26	119.20	122.79
4	B5	3781	5MC	C5-C6-N1	-3.26	119.99	123.34
4	B5	3717	A2M	C4-C5-N7	-3.25	106.66	110.62
4	B5	1325	A2M	C4-C5-N7	-3.25	106.66	110.62
52	A2	1031	A2M	C4-C5-N7	-3.25	106.66	110.62
52	A2	1328	OMG	C6-C5-N7	3.25	136.28	130.25
4	B5	4391	OMG	C6-C5-N7	3.24	136.28	130.25
4	B5	4622	OMG	C6-C5-N7	3.24	136.28	130.25
4	B5	1676	PSU	O2-C2-N1	-3.24	119.22	122.79
4	B5	1870	A2M	C4-C5-N7	-3.24	106.67	110.62
52	A2	1850	MA6	C4-N9-C1'	-3.24	118.87	126.59
52	A2	1850	MA6	C6-C5-N7	3.24	138.72	133.28
4	B5	1321	1MA	N9-C4-N3	3.24	134.48	126.94
4	B5	4636	OMG	C6-C5-N7	3.24	136.27	130.25
52	A2	863	PSU	O2-C2-N1	-3.23	119.23	122.79
2	B2	6	2MG	C6-C5-N7	3.23	136.26	130.25
2	B2	46	G7M	O6-C6-C5	-3.22	120.78	128.06
4	B5	400	A2M	C4-C5-N7	-3.22	106.69	110.62
4	B5	3743	OMG	C6-C5-N7	3.22	136.24	130.25
52	A2	576	A2M	C4-C5-N7	-3.22	106.70	110.62
4	B5	4589	A2M	C4-C5-N7	-3.22	106.70	110.62
52	A2	668	A2M	C4-C5-N7	-3.22	106.70	110.62
4	B5	1325	A2M	N3-C2-N1	-3.21	123.58	128.60
4	B5	4493	OMG	C6-C5-N7	3.21	136.22	130.25
4	B5	4498	OMG	C6-C5-N7	3.21	136.22	130.25
52	A2	1136	PSU	O2-C2-N1	-3.21	119.26	122.79
4	B5	4570	A2M	C4-C5-N7	-3.21	106.71	110.62
52	A2	590	A2M	N3-C2-N1	-3.21	123.59	128.60
52	A2	172	OMU	C1'-N1-C2	3.21	123.37	117.57
4	B5	3829	A2M	N3-C2-N1	-3.20	123.59	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B5	4369	OMG	C6-C5-N7	3.20	136.20	130.25
52	A2	815	PSU	O2-C2-N1	-3.20	119.27	122.79
4	B5	1322	A2M	N3-C2-N1	-3.20	123.60	128.60
4	B5	1322	A2M	C4-C5-N7	-3.20	106.72	110.62
52	A2	601	OMG	C6-C5-N7	3.19	136.19	130.25
52	A2	512	A2M	C4-C5-N7	-3.19	106.73	110.62
52	A2	27	A2M	N3-C2-N1	-3.18	123.63	128.60
4	B5	3829	A2M	C4-C5-N7	-3.18	106.75	110.62
4	B5	1533	A2M	N3-C2-N1	-3.18	123.63	128.60
4	B5	3784	A2M	C4-C5-N7	-3.18	106.75	110.62
52	A2	512	A2M	N3-C2-N1	-3.18	123.64	128.60
52	A2	1447	OMG	C6-C5-N7	3.18	136.15	130.25
4	B5	3636	PSU	O2-C2-N1	-3.16	119.31	122.79
52	A2	590	A2M	C4-C5-N7	-3.16	106.77	110.62
4	B5	3866	A2M	C4-C5-N7	-3.16	106.77	110.62
52	A2	576	A2M	N3-C2-N1	-3.16	123.66	128.60
4	B5	1523	A2M	N3-C2-N1	-3.16	123.66	128.60
4	B5	3791	OMG	C6-C5-N7	3.16	136.12	130.25
52	A2	644	OMG	C6-C5-N7	3.15	136.12	130.25
52	A2	468	A2M	N3-C2-N1	-3.15	123.67	128.60
4	B5	4219	6MZ	C4-C5-N7	-3.15	106.78	110.62
52	A2	1832	6MZ	C4-C5-N7	-3.15	106.78	110.62
4	B5	2814	A2M	N3-C2-N1	-3.15	123.68	128.60
4	B5	398	A2M	N3-C2-N1	-3.15	123.68	128.60
4	B5	2400	A2M	N3-C2-N1	-3.15	123.68	128.60
52	A2	867	OMG	C6-C5-N7	3.14	136.10	130.25
52	A2	576	A2M	C2'-C1'-N9	-3.14	108.24	113.53
4	B5	400	A2M	N3-C2-N1	-3.14	123.69	128.60
52	A2	668	A2M	N3-C2-N1	-3.14	123.69	128.60
52	A2	166	A2M	N3-C2-N1	-3.14	123.70	128.60
4	B5	4219	6MZ	N1-C2-N3	-3.13	123.70	128.60
4	B5	1523	A2M	C4-C5-N7	-3.13	106.80	110.62
52	A2	1678	A2M	N3-C2-N1	-3.13	123.71	128.60
2	B2	10	2MG	C6-C5-N7	3.13	136.06	130.25
52	A2	1383	A2M	N3-C2-N1	-3.11	123.74	128.60
4	B5	3723	A2M	C4-C5-N7	-3.11	106.83	110.62
52	A2	436	OMG	C6-C5-N7	3.11	136.03	130.25
4	B5	1624	OMG	C6-C5-N7	3.11	136.02	130.25
4	B5	3723	A2M	N3-C2-N1	-3.10	123.75	128.60
4	B5	2423	OMG	C6-C5-N7	3.09	136.00	130.25
6	B8	75	OMG	C6-C5-N7	3.09	136.00	130.25
2	B2	55	PSU	O2-C2-N1	-3.09	119.39	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	A2	1850	MA6	C5-C4-N9	-3.08	102.19	105.78
4	B5	3824	A2M	N3-C2-N1	-3.08	123.78	128.60
52	A2	1490	OMG	C6-C5-N7	3.08	135.98	130.25
4	B5	4570	A2M	N3-C2-N1	-3.08	123.78	128.60
4	B5	2875	OMG	C6-C5-N7	3.08	135.97	130.25
4	B5	2362	A2M	N3-C2-N1	-3.08	123.79	128.60
52	A2	354	OMU	O4-C4-C5	-3.08	119.75	125.16
4	B5	4522	A2M	C4-C5-N7	-3.07	106.87	110.62
52	A2	1326	OMU	O4-C4-C5	-3.07	119.76	125.16
52	A2	484	A2M	N3-C2-N1	-3.07	123.80	128.60
52	A2	1248	B8N	N3-C2-N1	3.07	121.09	116.76
4	B5	2786	A2M	N3-C2-N1	-3.06	123.81	128.60
52	A2	509	OMG	C6-C5-N7	3.06	135.94	130.25
4	B5	4589	A2M	N3-C2-N1	-3.06	123.82	128.60
52	A2	799	OMU	O4-C4-C5	-3.06	119.78	125.16
4	B5	3866	A2M	N3-C2-N1	-3.06	123.82	128.60
52	A2	27	A2M	C2'-C1'-N9	-3.06	108.38	113.53
52	A2	1031	A2M	N3-C2-N1	-3.06	123.82	128.60
52	A2	1442	OMU	O4-C4-C5	-3.05	119.79	125.16
4	B5	3717	A2M	N3-C2-N1	-3.04	123.84	128.60
52	A2	166	A2M	C2'-C1'-N9	-3.04	108.41	113.53
52	A2	1832	6MZ	N1-C2-N3	-3.02	123.87	128.60
52	A2	121	OMU	O4-C4-C5	-3.02	119.84	125.16
4	B5	3824	A2M	C2'-C1'-N9	-3.02	108.45	113.53
2	B2	26	M2G	C6-C5-N7	3.01	135.85	130.25
52	A2	1832	6MZ	C6-C5-N7	3.01	135.65	132.39
52	A2	1639	G7M	C2-N1-C6	-3.01	119.61	125.10
4	B5	4226	OMU	O4-C4-C5	-3.01	119.87	125.16
6	B8	14	OMU	O4-C4-C5	-3.00	119.88	125.16
52	A2	627	OMU	O4-C4-C5	-3.00	119.89	125.16
52	A2	1851	MA6	C4-N9-C1'	-2.98	119.48	126.59
52	A2	172	OMU	O4-C4-C5	-2.98	119.92	125.16
52	A2	1288	OMU	O4-C4-C5	-2.98	119.92	125.16
52	A2	1383	A2M	C2'-C1'-N9	-2.98	108.52	113.53
4	B5	3784	A2M	C2'-C1'-N9	-2.97	108.52	113.53
4	B5	3924	OMU	O4-C4-C5	-2.97	119.94	125.16
52	A2	1804	OMU	O4-C4-C5	-2.96	119.95	125.16
52	A2	1678	A2M	C5-N7-C8	2.95	107.70	103.51
52	A2	159	A2M	N3-C2-N1	-2.95	124.00	128.60
4	B5	4497	OMU	O4-C4-C5	-2.94	119.99	125.16
4	B5	2414	OMU	O4-C4-C5	-2.94	119.99	125.16
52	A2	116	OMU	O4-C4-C5	-2.94	119.99	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B5	4195	OMG	C6-C5-N7	2.94	135.71	130.25
4	B5	2786	A2M	C4-C5-N7	-2.93	107.05	110.62
4	B5	2836	OMU	O4-C4-C5	-2.93	120.01	125.16
52	A2	99	A2M	N3-C2-N1	-2.93	124.03	128.60
4	B5	4305	OMU	O4-C4-C5	-2.92	120.03	125.16
4	B5	3717	A2M	C2'-C1'-N9	-2.90	108.64	113.53
4	B5	4619	OMU	O4-C4-C5	-2.90	120.06	125.16
52	A2	428	OMU	O4-C4-C5	-2.88	120.09	125.16
4	B5	2362	A2M	C2'-C1'-N9	-2.88	108.68	113.53
52	A2	166	A2M	C5-N7-C8	2.88	107.60	103.51
4	B5	4589	A2M	C2'-C1'-N9	-2.87	108.69	113.53
4	B5	3866	A2M	C2'-C1'-N9	-2.85	108.73	113.53
52	A2	99	A2M	C5-N7-C8	2.81	107.51	103.51
4	B5	3784	A2M	C4-N9-C8	2.81	108.78	105.73
52	A2	484	A2M	C5-N7-C8	2.81	107.50	103.51
52	A2	1383	A2M	C5-N7-C8	2.80	107.49	103.51
4	B5	1325	A2M	C5-N7-C8	2.80	107.49	103.51
4	B5	2814	A2M	C5-N7-C8	2.79	107.47	103.51
4	B5	4522	A2M	C4-N9-C8	2.79	108.75	105.73
52	A2	1851	MA6	C5-C4-N9	-2.79	102.54	105.78
4	B5	398	A2M	C5-N7-C8	2.77	107.44	103.51
2	B2	46	G7M	C2-N1-C6	-2.77	120.05	125.10
4	B5	2362	A2M	C5-N7-C8	2.77	107.44	103.51
4	B5	2400	A2M	C5-N7-C8	2.77	107.44	103.51
52	A2	27	A2M	C5-N7-C8	2.77	107.44	103.51
52	A2	512	A2M	C2'-C1'-N9	-2.76	108.88	113.53
4	B5	3824	A2M	C5-N7-C8	2.75	107.41	103.51
4	B5	4227	OMG	C4-C5-N7	-2.75	106.37	110.72
52	A2	468	A2M	C5-N7-C8	2.75	107.41	103.51
52	A2	1678	A2M	C4-N9-C8	2.74	108.70	105.73
4	B5	3784	A2M	C5-N7-C8	2.74	107.40	103.51
4	B5	1533	A2M	C5-N7-C8	2.72	107.38	103.51
52	A2	1031	A2M	C5-N7-C8	2.72	107.38	103.51
52	A2	576	A2M	C5-N7-C8	2.72	107.37	103.51
2	B2	58	1MA	C4-C5-N7	-2.72	106.42	110.72
4	B5	2786	A2M	C4-N9-C8	2.71	108.67	105.73
52	A2	590	A2M	C5-N7-C8	2.70	107.35	103.51
4	B5	4570	A2M	C5-N7-C8	2.70	107.35	103.51
4	B5	1322	A2M	C5-N7-C8	2.70	107.34	103.51
52	A2	668	A2M	C5-N7-C8	2.69	107.34	103.51
52	A2	159	A2M	C5-N7-C8	2.69	107.33	103.51
4	B5	3829	A2M	C5-N7-C8	2.68	107.32	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B5	1870	A2M	C5-N7-C8	2.67	107.31	103.51
52	A2	1832	6MZ	C5-N7-C8	2.67	107.31	103.51
4	B5	3866	A2M	C5-N7-C8	2.67	107.30	103.51
52	A2	512	A2M	C5-N7-C8	2.67	107.30	103.51
52	A2	1842	4AC	C6-C5-C4	2.67	120.22	116.96
4	B5	1325	A2M	C4-N9-C8	2.67	108.62	105.73
4	B5	1521	OMG	C4-C5-N7	-2.66	106.51	110.72
4	B5	400	A2M	C5-N7-C8	2.66	107.28	103.51
52	A2	159	A2M	C2'-C1'-N9	-2.66	109.06	113.53
4	B5	3943	OMG	C4-C5-N7	-2.65	106.52	110.72
52	A2	644	OMG	C4-C5-N7	-2.65	106.52	110.72
4	B5	4522	A2M	C5-N7-C8	2.65	107.28	103.51
4	B5	3898	OMG	C4-C5-N7	-2.65	106.53	110.72
4	B5	4589	A2M	C5-N7-C8	2.65	107.27	103.51
4	B5	3866	A2M	C4-N9-C8	2.65	108.59	105.73
4	B5	2400	A2M	C4-N9-C8	2.64	108.59	105.73
4	B5	4617	OMG	C4-C5-N7	-2.64	106.54	110.72
52	A2	683	OMG	C4-C5-N7	-2.64	106.55	110.72
4	B5	3723	A2M	C5-N7-C8	2.64	107.25	103.51
4	B5	3717	A2M	C5-N7-C8	2.63	107.25	103.51
4	B5	4219	6MZ	C5-N7-C8	2.63	107.24	103.51
4	B5	2814	A2M	C2'-C1'-N9	-2.63	109.11	113.53
52	A2	1328	OMG	C4-C5-N7	-2.63	106.57	110.72
52	A2	1447	OMG	C4-C5-N7	-2.62	106.57	110.72
4	B5	1523	A2M	C5-N7-C8	2.61	107.22	103.51
52	A2	428	OMU	C1'-N1-C2	2.61	122.30	117.57
4	B5	3626	OMG	C4-C5-N7	-2.61	106.59	110.72
4	B5	3824	A2M	C4-N9-C8	2.61	108.56	105.73
2	B2	6	2MG	C4-C5-N7	-2.61	106.59	110.72
4	B5	4498	OMG	C4-C5-N7	-2.60	106.61	110.72
6	B8	75	OMG	C4-C5-N7	-2.60	106.61	110.72
4	B5	4622	OMG	C4-C5-N7	-2.59	106.61	110.72
4	B5	2363	OMG	C4-C5-N7	-2.59	106.62	110.72
4	B5	3781	5MC	C5-C4-N3	-2.59	118.88	121.67
52	A2	799	OMU	C1'-N1-C2	2.59	122.25	117.57
52	A2	601	OMG	C4-C5-N7	-2.58	106.63	110.72
4	B5	4493	OMG	C4-C5-N7	-2.58	106.63	110.72
4	B5	2786	A2M	C5-N7-C8	2.58	107.18	103.51
4	B5	1325	A2M	C2'-C1'-N9	-2.58	109.19	113.53
4	B5	3743	OMG	C4-C5-N7	-2.58	106.64	110.72
52	A2	668	A2M	C4-N9-C8	2.58	108.52	105.73
4	B5	1870	A2M	C4-N9-C8	2.58	108.52	105.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B5	4369	OMG	C4-C5-N7	-2.58	106.64	110.72
52	A2	576	A2M	C4-N9-C8	2.57	108.51	105.73
4	B5	2875	OMG	C4-C5-N7	-2.57	106.66	110.72
4	B5	4446	5MC	C5-C4-N3	-2.57	118.90	121.67
7	BA	216	V5N	O-C-CA	-2.57	118.05	124.78
4	B5	1315	OMG	C4-C5-N7	-2.56	106.66	110.72
52	A2	509	OMG	C4-C5-N7	-2.56	106.67	110.72
52	A2	867	OMG	C4-C5-N7	-2.56	106.68	110.72
4	B5	4589	A2M	C4-N9-C8	2.56	108.50	105.73
4	B5	400	A2M	C4-N9-C8	2.55	108.50	105.73
52	A2	627	OMU	C1'-N1-C2	2.55	122.19	117.57
4	B5	1321	1MA	C4-C5-N7	-2.55	106.69	110.72
52	A2	1490	OMG	C4-C5-N7	-2.55	106.69	110.72
4	B5	1523	A2M	C4-N9-C8	2.55	108.49	105.73
4	B5	4636	OMG	C4-C5-N7	-2.55	106.69	110.72
52	A2	1288	OMU	C1'-N1-C2	2.55	122.18	117.57
4	B5	4391	OMG	C4-C5-N7	-2.54	106.70	110.72
4	B5	3723	A2M	C4-N9-C8	2.54	108.48	105.73
32	Ba	39	V5N	O-C-CA	-2.54	118.12	124.78
4	B5	1624	OMG	C4-C5-N7	-2.54	106.70	110.72
4	B5	3829	A2M	C4-N9-C8	2.53	108.47	105.73
52	A2	1383	A2M	C4-N9-C8	2.53	108.47	105.73
52	A2	27	A2M	C4-N9-C8	2.53	108.47	105.73
4	B5	3723	A2M	C2'-C1'-N9	-2.53	109.27	113.53
67	AO	138	IAS	OD1-CG-CB	-2.53	118.05	125.43
2	B2	10	2MG	C4-C5-N7	-2.53	106.71	110.72
4	B5	4570	A2M	C4-N9-C8	2.53	108.47	105.73
52	A2	436	OMG	C4-C5-N7	-2.52	106.73	110.72
52	A2	1832	6MZ	C9-N6-C6	-2.52	120.70	122.87
4	B5	3791	OMG	C4-C5-N7	-2.52	106.74	110.72
4	B5	398	A2M	C4-N9-C8	2.51	108.45	105.73
52	A2	1031	A2M	C4-N9-C8	2.50	108.44	105.73
52	A2	1832	6MZ	C4-N9-C8	2.50	108.44	105.73
4	B5	4497	OMU	O2-C2-N1	-2.49	119.47	122.79
52	A2	484	A2M	C2'-C1'-N9	-2.48	109.36	113.53
52	A2	1031	A2M	C2'-C1'-N9	-2.48	109.36	113.53
2	B2	26	M2G	C4-C5-N7	-2.47	106.82	110.72
4	B5	1533	A2M	C4-N9-C8	2.47	108.40	105.73
52	A2	166	A2M	C4-N9-C8	2.46	108.40	105.73
4	B5	4219	6MZ	C4-N9-C8	2.46	108.39	105.73
52	A2	468	A2M	C4-N9-C8	2.46	108.39	105.73
4	B5	3817	UY1	C6-C5-C4	2.45	119.91	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	A2	99	A2M	C4-N9-C8	2.45	108.38	105.73
2	B2	48	5MC	C5-C4-N3	-2.45	119.03	121.67
4	B5	1322	A2M	C4-N9-C8	2.44	108.37	105.73
4	B5	2423	OMG	C4-C5-N7	-2.43	106.87	110.72
52	A2	1804	OMU	C1'-N1-C2	2.42	121.96	117.57
52	A2	159	A2M	C4-N9-C8	2.42	108.35	105.73
4	B5	2362	A2M	C4-N9-C8	2.42	108.35	105.73
4	B5	1523	A2M	C2'-C1'-N9	-2.41	109.48	113.53
4	B5	3781	5MC	O2-C2-N3	-2.40	118.42	122.33
4	B5	3717	A2M	C4-N9-C8	2.40	108.33	105.73
52	A2	1337	4AC	C5-C4-N4	-2.40	118.76	122.92
52	A2	512	A2M	C4-N9-C8	2.39	108.31	105.73
52	A2	484	A2M	C4-N9-C8	2.38	108.31	105.73
4	B5	4195	OMG	C4-C5-N7	-2.38	106.96	110.72
52	A2	1850	MA6	C5-C6-N6	-2.36	121.18	125.30
4	B5	4195	OMG	O6-C6-C5	-2.36	120.34	126.60
4	B5	2814	A2M	C4-N9-C8	2.36	108.28	105.73
4	B5	3784	A2M	C6-C5-N7	2.34	136.38	132.02
4	B5	2350	OMC	O2-C2-N3	-2.32	118.56	122.33
4	B5	3817	UY1	O2-C2-N1	-2.31	120.25	122.79
52	A2	1678	A2M	C6-C5-N7	2.31	136.32	132.02
52	A2	468	A2M	C2'-C1'-N9	-2.31	109.65	113.53
4	B5	2507	PSU	C5-C6-N1	-2.28	118.69	122.11
2	B2	37	T6A	C5-C6-N6	2.28	124.73	118.71
4	B5	2423	OMG	O6-C6-C5	-2.26	120.61	126.60
4	B5	1533	A2M	C6-C5-N7	2.26	136.22	132.02
52	A2	1678	A2M	N9-C8-N7	-2.25	110.84	113.91
52	A2	867	OMG	O6-C6-C5	-2.25	120.64	126.60
4	B5	2363	OMG	O6-C6-C5	-2.24	120.64	126.60
52	A2	517	OMC	O2-C2-N3	-2.24	118.68	122.33
52	A2	1326	OMU	O2-C2-N1	-2.23	119.82	122.79
52	A2	1337	4AC	C6-C5-C4	2.23	119.69	116.96
52	A2	1248	B8N	C5-C4-N3	2.22	120.29	116.17
4	B5	3784	A2M	N9-C8-N7	-2.22	110.87	113.91
52	A2	1383	A2M	C6-C5-N7	2.22	136.15	132.02
2	B2	54	5MU	C1'-N1-C2	2.22	121.58	117.57
52	A2	27	A2M	C6-C5-N7	2.21	136.15	132.02
4	B5	2814	A2M	C6-C5-N7	2.21	136.14	132.02
52	A2	468	A2M	C6-C5-N7	2.21	136.14	132.02
52	A2	1639	G7M	C5-C4-N9	-2.21	101.05	105.89
4	B5	3898	OMG	O6-C6-C5	-2.21	120.75	126.60
4	B5	398	A2M	C6-C5-N7	2.20	136.12	132.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B5	3791	OMG	O6-C6-C5	-2.20	120.77	126.60
52	A2	159	A2M	C6-C5-N7	2.20	136.11	132.02
52	A2	1851	MA6	C5-N7-C8	2.19	106.62	103.51
4	B5	1325	A2M	C6-C5-N7	2.18	136.09	132.02
4	B5	1870	A2M	C6-C5-N7	2.18	136.09	132.02
4	B5	2400	A2M	C6-C5-N7	2.18	136.09	132.02
4	B5	3824	A2M	C6-C5-N7	2.18	136.09	132.02
52	A2	668	A2M	C6-C5-N7	2.18	136.09	132.02
2	B2	26	M2G	O6-C6-C5	-2.18	120.81	126.60
4	B5	2362	A2M	C6-C5-N7	2.18	136.07	132.02
52	A2	1490	OMG	O6-C6-C5	-2.17	120.84	126.60
4	B5	4589	A2M	C6-C5-N7	2.17	136.06	132.02
52	A2	1447	OMG	O6-C6-C5	-2.17	120.85	126.60
52	A2	509	OMG	O6-C6-C5	-2.17	120.86	126.60
4	B5	1321	1MA	C6-C5-N7	2.16	136.12	132.20
52	A2	590	A2M	C4-N9-C8	2.16	108.06	105.73
4	B5	3829	A2M	C6-C5-N7	2.15	136.03	132.02
2	B2	10	2MG	O6-C6-C5	-2.15	120.89	126.60
4	B5	1523	A2M	C6-C5-N7	2.15	136.03	132.02
4	B5	4522	A2M	C6-C5-N7	2.15	136.02	132.02
4	B5	4498	OMG	O6-C6-C5	-2.15	120.91	126.60
52	A2	683	OMG	O6-C6-C5	-2.14	120.92	126.60
4	B5	1676	PSU	O4'-C1'-C2'	2.14	108.16	105.14
2	B2	58	1MA	C6-C5-N7	2.14	136.09	132.20
4	B5	4617	OMG	O6-C6-C5	-2.14	120.94	126.60
52	A2	1328	OMG	O6-C6-C5	-2.13	120.95	126.60
52	A2	668	A2M	C2'-C1'-N9	-2.13	109.94	113.53
4	B5	3717	A2M	C6-C5-N7	2.13	135.99	132.02
4	B5	4227	OMG	O6-C6-C5	-2.13	120.96	126.60
4	B5	4622	OMG	O6-C6-C5	-2.13	120.96	126.60
52	A2	1442	OMU	C1'-N1-C2	2.12	121.42	117.57
52	A2	436	OMG	O6-C6-C5	-2.12	120.97	126.60
52	A2	601	OMG	O6-C6-C5	-2.12	120.97	126.60
4	B5	4522	A2M	N9-C8-N7	-2.12	111.01	113.91
4	B5	3743	OMG	O6-C6-C5	-2.12	120.97	126.60
4	B5	2875	OMG	O6-C6-C5	-2.12	120.98	126.60
4	B5	2400	A2M	N9-C8-N7	-2.12	111.02	113.91
4	B5	1521	OMG	O6-C6-C5	-2.12	120.99	126.60
52	A2	1031	A2M	C6-C5-N7	2.11	135.96	132.02
4	B5	400	A2M	C6-C5-N7	2.11	135.96	132.02
52	A2	576	A2M	C6-C5-N7	2.11	135.96	132.02
52	A2	644	OMG	O6-C6-C5	-2.11	121.00	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B5	3626	OMG	O6-C6-C5	-2.11	121.00	126.60
4	B5	1325	A2M	N9-C8-N7	-2.11	111.03	113.91
52	A2	484	A2M	C6-C5-N7	2.11	135.95	132.02
4	B5	1624	OMG	O6-C6-C5	-2.11	121.01	126.60
4	B5	3943	OMG	O6-C6-C5	-2.10	121.02	126.60
6	B8	75	OMG	O6-C6-C5	-2.10	121.03	126.60
4	B5	3761	PSU	C5-C6-N1	-2.10	118.96	122.11
4	B5	4636	OMG	O6-C6-C5	-2.09	121.05	126.60
4	B5	3866	A2M	C6-C5-N7	2.09	135.92	132.02
2	B2	46	G7M	N2-C2-N1	2.09	121.17	116.71
52	A2	166	A2M	C6-C5-N7	2.09	135.91	132.02
4	B5	2421	OMC	O2-C2-N3	-2.08	118.94	122.33
4	B5	1315	OMG	O6-C6-C5	-2.08	121.08	126.60
4	B5	2860	OMC	O2-C2-N3	-2.08	118.95	122.33
4	B5	2350	OMC	C1'-N1-C2	2.07	123.05	118.42
4	B5	4493	OMG	O6-C6-C5	-2.07	121.11	126.60
4	B5	3723	A2M	C6-C5-N7	2.07	135.88	132.02
4	B5	4520	PSU	C5-C6-N1	-2.07	119.01	122.11
4	B5	4570	A2M	C6-C5-N7	2.07	135.87	132.02
4	B5	4369	OMG	O6-C6-C5	-2.07	121.12	126.60
2	B2	6	2MG	O6-C6-C5	-2.07	121.12	126.60
2	B2	46	G7M	C1'-N9-C4	-2.06	120.37	126.50
52	A2	512	A2M	C6-C5-N7	2.06	135.87	132.02
52	A2	1136	PSU	C5-C6-N1	-2.06	119.01	122.11
4	B5	1322	A2M	C6-C5-N7	2.06	135.86	132.02
4	B5	4971	PSU	C5-C6-N1	-2.06	119.02	122.11
4	B5	3761	PSU	O4'-C1'-C2'	2.06	108.05	105.14
4	B5	4441	PSU	C5-C6-N1	-2.05	119.03	122.11
4	B5	3824	A2M	N9-C8-N7	-2.04	111.12	113.91
4	B5	4391	OMG	O6-C6-C5	-2.04	121.18	126.60
4	B5	1321	1MA	N1-C2-N3	-2.04	123.57	126.00
4	B5	4635	PSU	C5-C6-N1	-2.04	119.05	122.11
4	B5	2423	OMG	C5-C6-N1	2.04	118.36	113.19
4	B5	1861	PSU	C5-C6-N1	-2.03	119.06	122.11
52	A2	354	OMU	C1'-N1-C2	2.03	121.25	117.57
52	A2	1703	OMC	O2-C2-N3	-2.03	119.03	122.33
52	A2	27	A2M	N9-C8-N7	-2.03	111.14	113.91
6	B8	69	PSU	O4'-C1'-C2'	2.03	108.00	105.14
4	B5	1781	PSU	C5-C6-N1	-2.03	119.07	122.11
4	B5	4195	OMG	C5-C6-N1	2.02	118.33	113.19
52	A2	1383	A2M	N9-C8-N7	-2.02	111.15	113.91
4	B5	3694	PSU	C5-C6-N1	-2.02	119.07	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B2	46	G7M	C8-N9-C4	2.02	112.28	107.16
4	B5	4292	PSU	C5-C6-N1	-2.02	119.08	122.11
52	A2	1842	4AC	C5-C4-N4	-2.02	119.41	122.92
6	B8	14	OMU	C1'-N1-C2	2.02	121.22	117.57
4	B5	3898	OMG	C5-C6-N1	2.02	118.31	113.19
4	B5	3866	A2M	N9-C8-N7	-2.01	111.16	113.91
4	B5	4402	PSU	C5-C6-N1	-2.01	119.09	122.11
52	A2	867	OMG	C5-C6-N1	2.01	118.30	113.19
52	A2	166	A2M	N9-C8-N7	-2.01	111.17	113.91
4	B5	3852	PSU	C5-C6-N1	-2.01	119.10	122.11
52	A2	1850	MA6	C5-N7-C8	2.01	106.36	103.51
4	B5	3807	OMC	O2-C2-N3	-2.01	119.07	122.33
4	B5	4551	PSU	C5-C6-N1	-2.00	119.10	122.11
52	A2	576	A2M	N9-C8-N7	-2.00	111.18	113.91
4	B5	1870	A2M	N9-C8-N7	-2.00	111.18	113.91

There are no chirality outliers.

All (165) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B7	1	GTP	C5'-O5'-PA-O3A
7	BA	216	V5N	O-C-CA-CB
76	AX	62	HY3	O-C-CA-C3
2	B2	16	H2U	O4'-C1'-N1-C6
2	B2	16	H2U	C2'-C1'-N1-C6
2	B2	20	H2U	O4'-C1'-N1-C6
2	B2	20	H2U	C2'-C1'-N1-C6
2	B2	37	T6A	O10-C10-N6-C6
2	B2	37	T6A	N11-C10-N6-C6
2	B2	37	T6A	C13-C12-C14-O14
2	B2	37	T6A	C13-C12-C14-C15
2	B2	47	H2U	O4'-C1'-N1-C2
2	B2	47	H2U	O4'-C1'-N1-C6
2	B2	48	5MC	O4'-C4'-C5'-O5'
4	B5	1581	PSU	O4'-C1'-C5-C4
4	B5	1581	PSU	O4'-C1'-C5-C6
4	B5	1780	PSU	C3'-C4'-C5'-O5'
4	B5	2363	OMG	O4'-C4'-C5'-O5'
4	B5	3700	OMC	C2'-C1'-N1-C2
4	B5	3700	OMC	C2'-C1'-N1-C6
4	B5	3817	UY1	C1'-C2'-O2'-CM2
4	B5	4589	A2M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	B5	4589	A2M	C3'-C4'-C5'-O5'
52	A2	512	A2M	O4'-C4'-C5'-O5'
52	A2	517	OMC	O4'-C4'-C5'-O5'
52	A2	644	OMG	O4'-C4'-C5'-O5'
52	A2	1337	4AC	N3-C4-N4-C7
52	A2	1337	4AC	C5-C4-N4-C7
52	A2	1337	4AC	O7-C7-N4-C4
52	A2	1337	4AC	CM7-C7-N4-C4
52	A2	1678	A2M	C1'-C2'-O2'-CM'
52	A2	1842	4AC	N3-C4-N4-C7
52	A2	1842	4AC	C5-C4-N4-C7
52	A2	1842	4AC	O7-C7-N4-C4
52	A2	1842	4AC	CM7-C7-N4-C4
52	A2	1850	MA6	C5-C6-N6-C9
52	A2	1850	MA6	C5-C6-N6-C10
2	B2	20	H2U	O4'-C1'-N1-C2
52	A2	428	OMU	O4'-C1'-N1-C2
2	B2	16	H2U	C2'-C1'-N1-C2
2	B2	20	H2U	C2'-C1'-N1-C2
2	B2	46	G7M	O4'-C4'-C5'-O5'
2	B2	46	G7M	C3'-C4'-C5'-O5'
2	B2	47	H2U	C3'-C4'-C5'-O5'
2	B2	48	5MC	C3'-C4'-C5'-O5'
4	B5	1780	PSU	O4'-C4'-C5'-O5'
4	B5	2363	OMG	C3'-C4'-C5'-O5'
4	B5	2814	A2M	O4'-C4'-C5'-O5'
4	B5	3784	A2M	O4'-C4'-C5'-O5'
4	B5	3784	A2M	C3'-C4'-C5'-O5'
4	B5	4531	PSU	C3'-C4'-C5'-O5'
4	B5	4531	PSU	O4'-C4'-C5'-O5'
4	B5	4635	PSU	C3'-C4'-C5'-O5'
52	A2	512	A2M	C3'-C4'-C5'-O5'
52	A2	644	OMG	C3'-C4'-C5'-O5'
52	A2	668	A2M	O4'-C4'-C5'-O5'
52	A2	668	A2M	C3'-C4'-C5'-O5'
52	A2	1639	G7M	C3'-C4'-C5'-O5'
4	B5	3817	UY1	C4'-C5'-O5'-P
2	B2	16	H2U	C3'-C4'-C5'-O5'
2	B2	47	H2U	O4'-C4'-C5'-O5'
4	B5	398	A2M	O4'-C4'-C5'-O5'
4	B5	1322	A2M	O4'-C4'-C5'-O5'
4	B5	3761	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	B5	4522	A2M	O4'-C4'-C5'-O5'
52	A2	468	A2M	O4'-C4'-C5'-O5'
52	A2	509	OMG	O4'-C4'-C5'-O5'
52	A2	576	A2M	O4'-C4'-C5'-O5'
52	A2	576	A2M	C3'-C4'-C5'-O5'
52	A2	1639	G7M	O4'-C4'-C5'-O5'
52	A2	1850	MA6	N1-C6-N6-C9
2	B2	37	T6A	N11-C12-C14-O14
2	B2	37	T6A	N11-C12-C14-C15
52	A2	428	OMU	O4'-C1'-N1-C6
4	B5	3866	A2M	C3'-C4'-C5'-O5'
4	B5	4446	5MC	C2'-C1'-N1-C6
2	B2	16	H2U	O4'-C4'-C5'-O5'
4	B5	4635	PSU	O4'-C4'-C5'-O5'
52	A2	99	A2M	O4'-C4'-C5'-O5'
52	A2	799	OMU	O4'-C4'-C5'-O5'
2	B2	47	H2U	C2'-C1'-N1-C6
52	A2	627	OMU	C3'-C4'-C5'-O5'
52	A2	1851	MA6	C5-C6-N6-C9
5	B7	1	GTP	C4'-C5'-O5'-PA
52	A2	867	OMG	C3'-C2'-O2'-CM2
52	A2	509	OMG	C3'-C4'-C5'-O5'
52	A2	627	OMU	O4'-C4'-C5'-O5'
4	B5	2786	A2M	C2'-C1'-N9-C8
52	A2	468	A2M	C3'-C4'-C5'-O5'
52	A2	799	OMU	C3'-C4'-C5'-O5'
4	B5	2421	OMC	C1'-C2'-O2'-CM2
2	B2	37	T6A	N11-C12-C13-ODB
4	B5	4446	5MC	O4'-C1'-N1-C6
52	A2	799	OMU	C4'-C5'-O5'-P
52	A2	1851	MA6	C4'-C5'-O5'-P
5	B7	1	GTP	C5'-O5'-PA-O1A
4	B5	2823	OMC	C3'-C2'-O2'-CM2
4	B5	4391	OMG	C3'-C2'-O2'-CM2
52	A2	116	OMU	C3'-C2'-O2'-CM2
52	A2	1447	OMG	C3'-C2'-O2'-CM2
2	B2	16	H2U	C4'-C5'-O5'-P
4	B5	3761	PSU	C3'-C4'-C5'-O5'
52	A2	1447	OMG	C3'-C4'-C5'-O5'
52	A2	1703	OMC	C3'-C4'-C5'-O5'
2	B2	48	5MC	C4'-C5'-O5'-P
4	B5	3843	PSU	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
4	B5	4446	5MC	O4'-C1'-N1-C2
4	B5	4589	A2M	C4'-C5'-O5'-P
4	B5	4446	5MC	C2'-C1'-N1-C2
2	B2	20	H2U	C4'-C5'-O5'-P
4	B5	3886	OMC	C4'-C5'-O5'-P
4	B5	3700	OMC	O4'-C1'-N1-C6
7	BA	216	V5N	O2-CB-CG-CD2
4	B5	3866	A2M	O4'-C4'-C5'-O5'
4	B5	4522	A2M	C3'-C4'-C5'-O5'
52	A2	590	A2M	C3'-C4'-C5'-O5'
4	B5	2836	OMU	C3'-C2'-O2'-CM2
52	A2	509	OMG	C3'-C2'-O2'-CM2
52	A2	512	A2M	C3'-C2'-O2'-CM'
52	A2	644	OMG	C3'-C2'-O2'-CM2
2	B2	16	H2U	O4'-C1'-N1-C2
2	B2	37	T6A	N11-C12-C13-ODA
52	A2	644	OMG	C4'-C5'-O5'-P
7	BA	216	V5N	O2-CB-CG-ND1
4	B5	2786	A2M	C2'-C1'-N9-C4
2	B2	47	H2U	C2'-C1'-N1-C2
2	B2	47	H2U	C4'-C5'-O5'-P
4	B5	2363	OMG	C3'-C2'-O2'-CM2
4	B5	2421	OMC	C3'-C2'-O2'-CM2
4	B5	3807	OMC	C3'-C2'-O2'-CM2
4	B5	3840	OMC	C3'-C2'-O2'-CM2
52	A2	27	A2M	C3'-C2'-O2'-CM'
52	A2	1272	OMC	C3'-C2'-O2'-CM2
52	A2	1703	OMC	C3'-C2'-O2'-CM2
4	B5	3700	OMC	O4'-C1'-N1-C2
4	B5	398	A2M	C3'-C4'-C5'-O5'
4	B5	1322	A2M	C3'-C4'-C5'-O5'
52	A2	590	A2M	O4'-C1'-N9-C8
52	A2	99	A2M	C3'-C4'-C5'-O5'
4	B5	1315	OMG	C1'-C2'-O2'-CM2
4	B5	2363	OMG	C1'-C2'-O2'-CM2
4	B5	3807	OMC	C1'-C2'-O2'-CM2
4	B5	4622	OMG	C1'-C2'-O2'-CM2
52	A2	1391	OMC	C1'-C2'-O2'-CM2
4	B5	4622	OMG	C3'-C2'-O2'-CM2
52	A2	1391	OMC	C3'-C2'-O2'-CM2
52	A2	822	PSU	C4'-C5'-O5'-P
52	A2	1703	OMC	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
8	BB	245	HIC	CA-CB-CG-ND1
4	B5	1325	A2M	C4'-C5'-O5'-P
4	B5	2786	A2M	O4'-C1'-N9-C8
4	B5	1533	A2M	O4'-C4'-C5'-O5'
4	B5	2350	OMC	O4'-C4'-C5'-O5'
4	B5	2350	OMC	C2'-C1'-N1-C2
52	A2	1081	PSU	C4'-C5'-O5'-P
67	AO	138	IAS	CA-CB-CG-OD1
4	B5	1315	OMG	C3'-C2'-O2'-CM2
4	B5	1325	A2M	C3'-C2'-O2'-CM'
4	B5	1870	A2M	C3'-C2'-O2'-CM'
4	B5	2421	OMC	O4'-C4'-C5'-O5'
52	A2	590	A2M	C2'-C1'-N9-C8
2	B2	46	G7M	C4'-C5'-O5'-P
4	B5	1624	OMG	C4'-C5'-O5'-P
8	BB	245	HIC	CA-CB-CG-CD2
4	B5	1321	1MA	C2'-C1'-N9-C8

There are no ring outliers.

76 monomers are involved in 93 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	A2	1842	4AC	1	0
4	B5	3791	OMG	1	0
52	A2	1328	OMG	1	0
4	B5	3723	A2M	1	0
4	B5	1315	OMG	1	0
52	A2	172	OMU	1	0
4	B5	3769	PSU	1	0
52	A2	1804	OMU	1	0
4	B5	4455	OMC	2	0
52	A2	1447	OMG	2	0
52	A2	166	A2M	2	0
52	A2	116	OMU	3	0
2	B2	16	H2U	2	0
2	B2	58	1MA	1	0
4	B5	3943	OMG	1	0
52	A2	36	PSU	1	0
4	B5	4295	PSU	2	0
4	B5	4311	PSU	1	0
4	B5	4522	A2M	1	0
4	B5	2414	OMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B2	27	PSU	1	0
8	BB	245	HIC	1	0
2	B2	34	OMC	2	0
52	A2	462	OMC	1	0
4	B5	4578	PSU	1	0
4	B5	4226	OMU	1	0
52	A2	1337	4AC	2	0
52	A2	1031	A2M	1	0
4	B5	4589	A2M	1	0
4	B5	2860	OMC	1	0
52	A2	27	A2M	1	0
52	A2	601	OMG	1	0
52	A2	468	A2M	3	0
2	B2	37	T6A	2	0
52	A2	1272	OMC	1	0
4	B5	2350	OMC	1	0
4	B5	2362	A2M	1	0
4	B5	3886	OMC	1	0
4	B5	1325	A2M	1	0
52	A2	484	A2M	1	0
4	B5	2364	OMC	1	0
2	B2	26	M2G	1	0
4	B5	4219	6MZ	1	0
4	B5	1870	A2M	2	0
52	A2	99	A2M	2	0
52	A2	576	A2M	1	0
52	A2	1391	OMC	1	0
4	B5	4617	OMG	1	0
52	A2	1136	PSU	1	0
4	B5	1778	PSU	2	0
4	B5	3824	A2M	1	0
4	B5	3807	OMC	1	0
4	B5	3829	A2M	2	0
52	A2	121	OMU	1	0
4	B5	2875	OMG	1	0
52	A2	1832	6MZ	1	0
4	B5	4535	OMC	1	0
52	A2	1248	B8N	1	0
52	A2	799	OMU	1	0
52	A2	1490	OMG	1	0
4	B5	4456	PSU	1	0
4	B5	4570	A2M	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	A2	159	A2M	4	0
52	A2	436	OMG	1	0
72	AT	67	NMM	2	0
2	B2	54	5MU	1	0
4	B5	4446	5MC	1	0
4	B5	2814	A2M	1	0
4	B5	4391	OMG	2	0
4	B5	3717	A2M	2	0
52	A2	1678	A2M	1	0
4	B5	3840	OMC	1	0
52	A2	1703	OMC	1	0
4	B5	398	A2M	1	0
4	B5	2803	OMC	1	0
4	B5	4619	OMU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 440 ligands modelled in this entry, 440 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

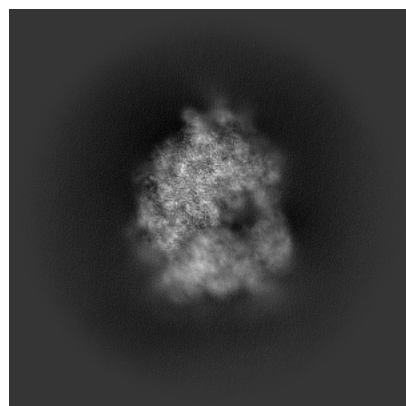
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56598. These allow visual inspection of the internal detail of the map and identification of artifacts.

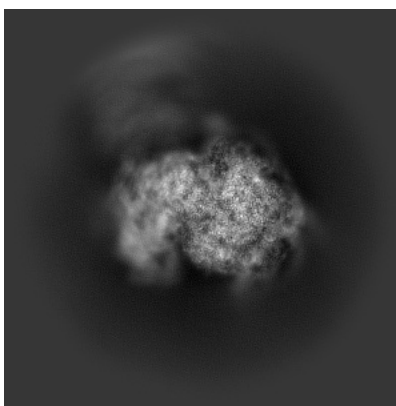
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

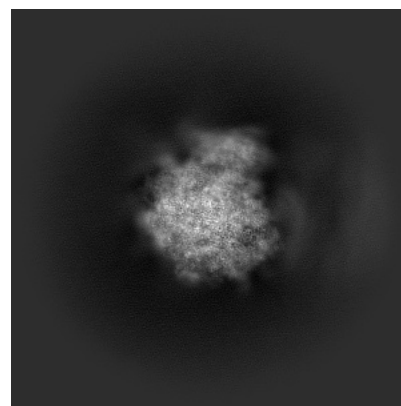
6.1.1 Primary map



X

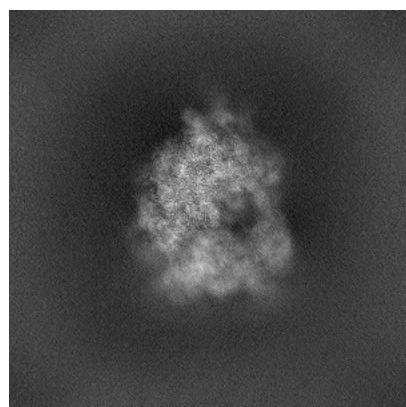


Y

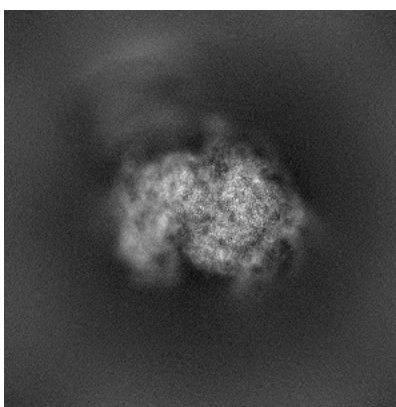


Z

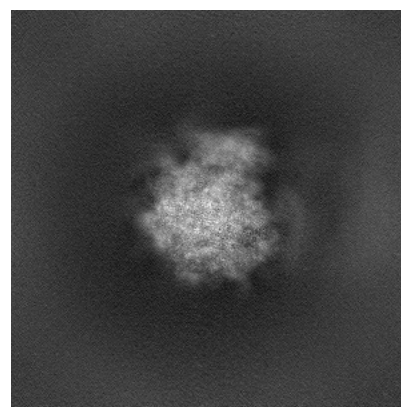
6.1.2 Raw map



X



Y

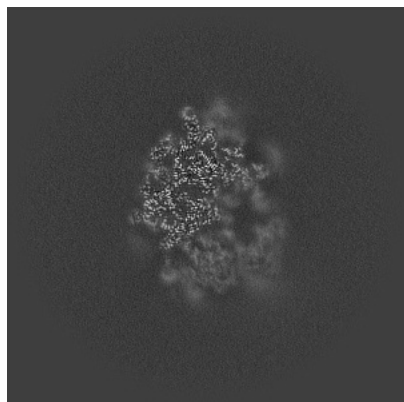


Z

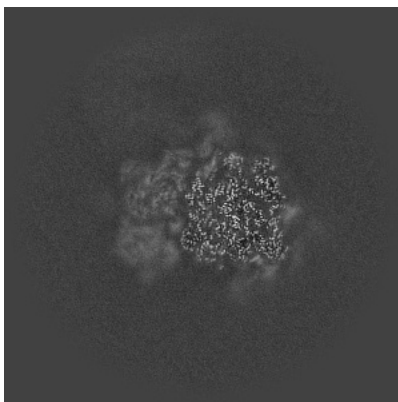
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

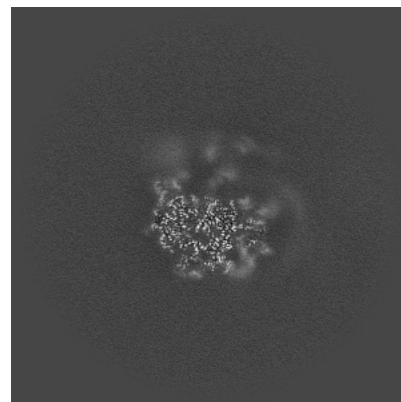
6.2.1 Primary map



X Index: 280

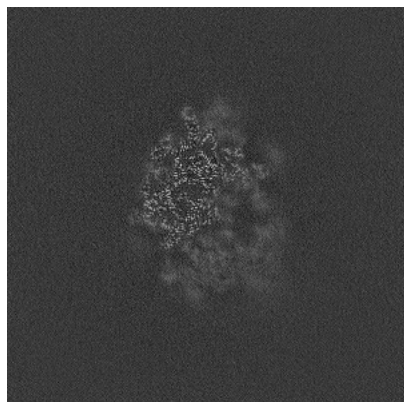


Y Index: 280

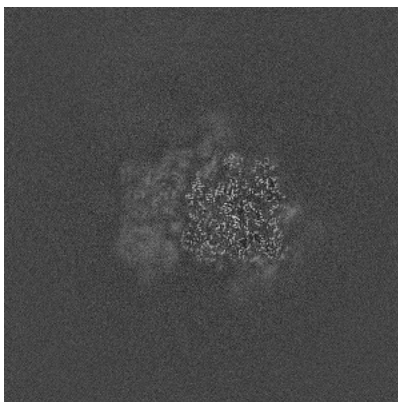


Z Index: 280

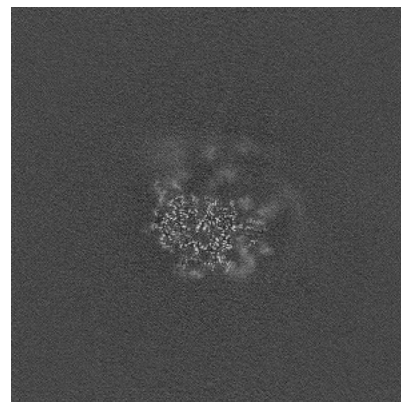
6.2.2 Raw map



X Index: 280



Y Index: 280

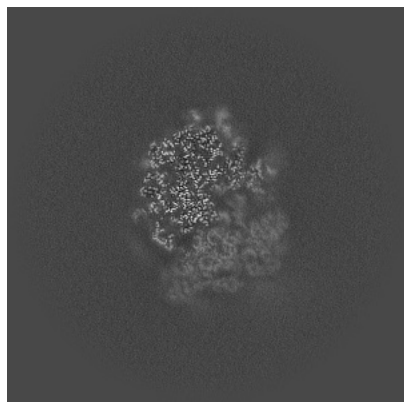


Z Index: 280

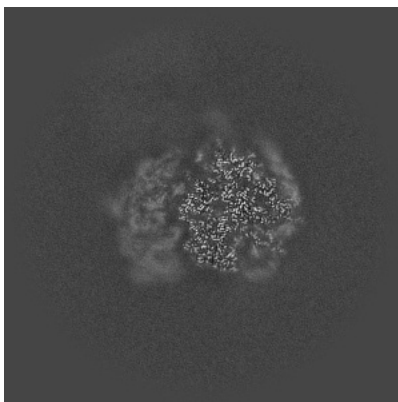
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

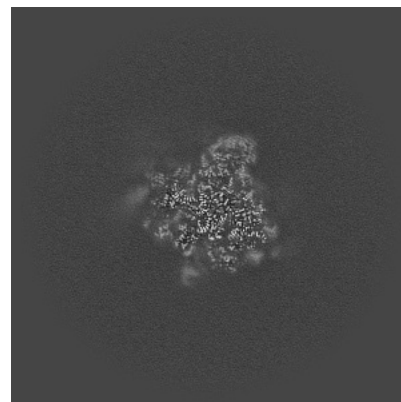
6.3.1 Primary map



X Index: 294

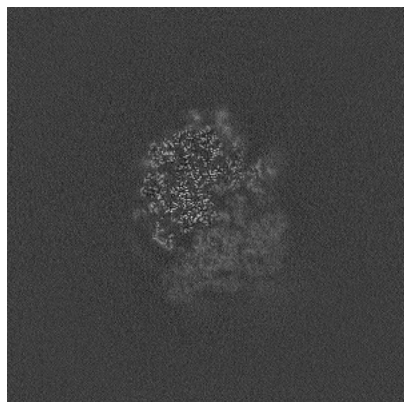


Y Index: 264

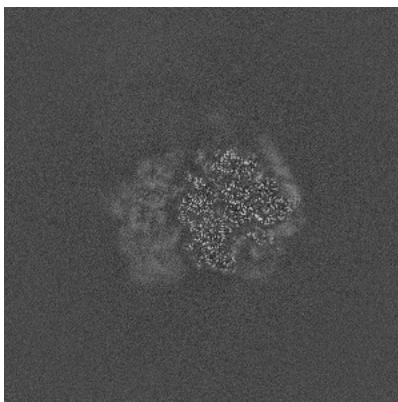


Z Index: 327

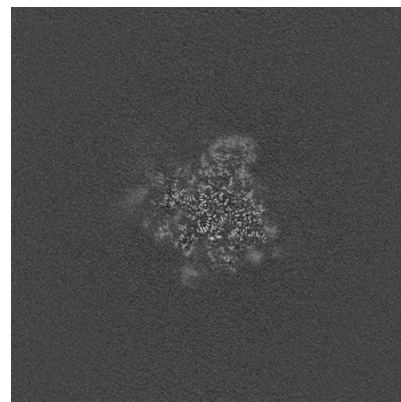
6.3.2 Raw map



X Index: 294



Y Index: 262

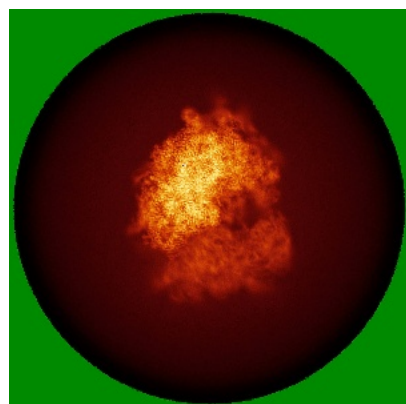


Z Index: 327

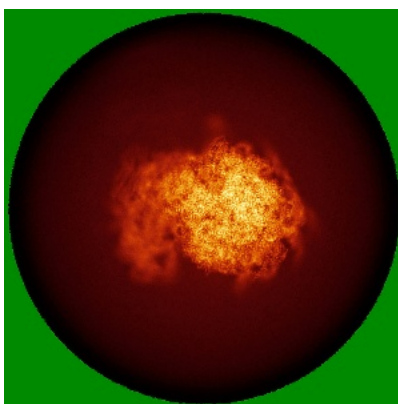
The images above show the largest variance slices of the map in three orthogonal directions.

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

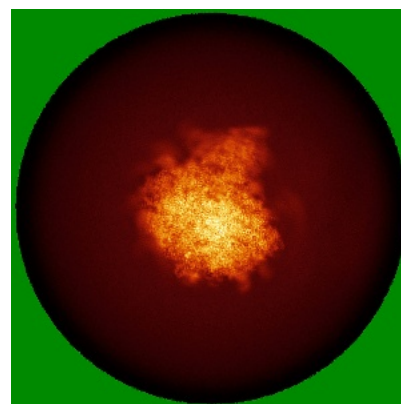
6.4.1 Primary map



X

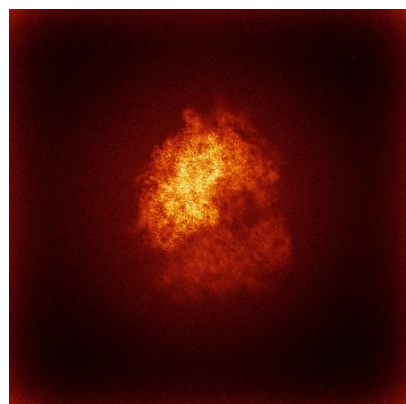


Y

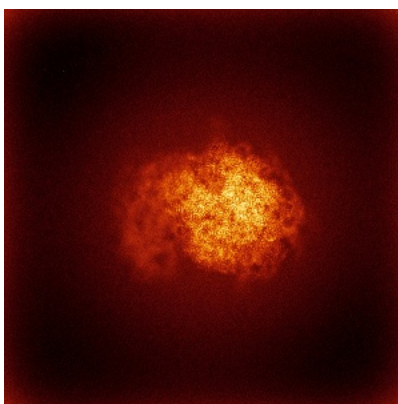


Z

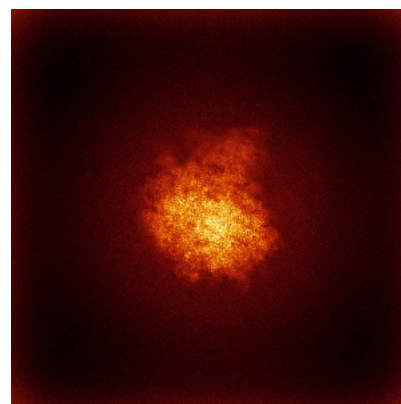
6.4.2 Raw map



X



Y

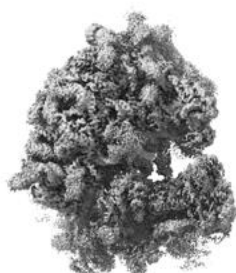


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



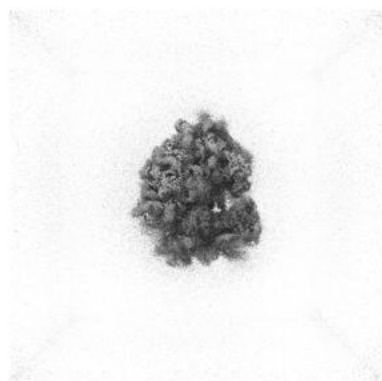
Y



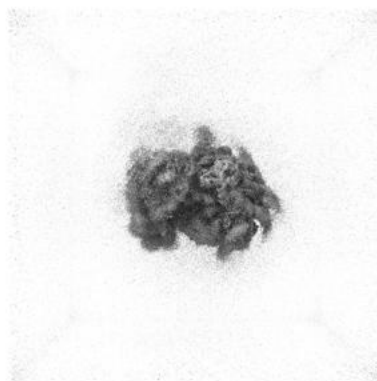
Z

The images above show the 3D surface view of the map at the recommended contour level 0.149. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

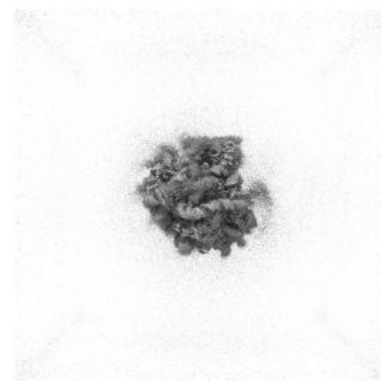
6.5.2 Raw map



X



Y



Z

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

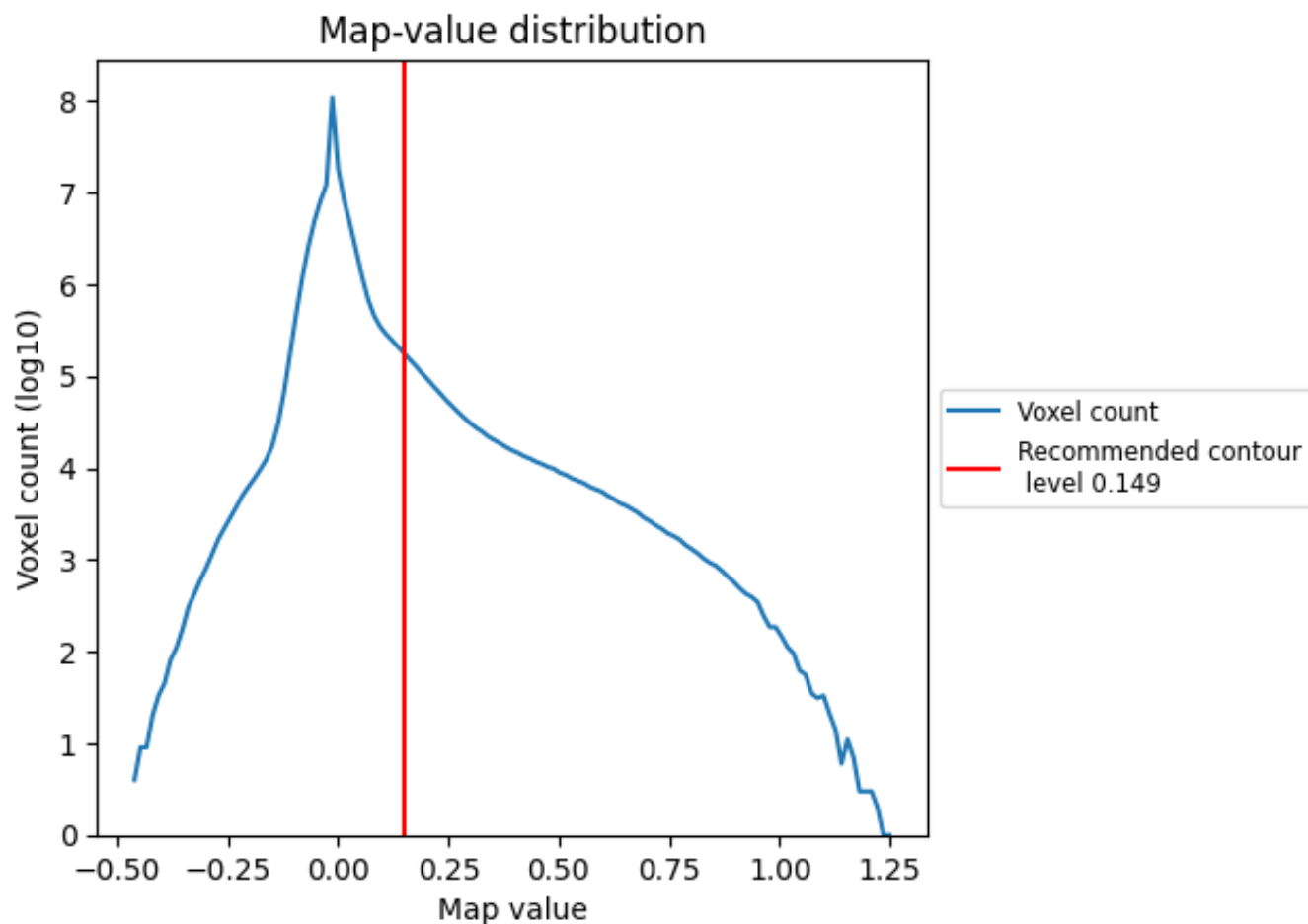
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

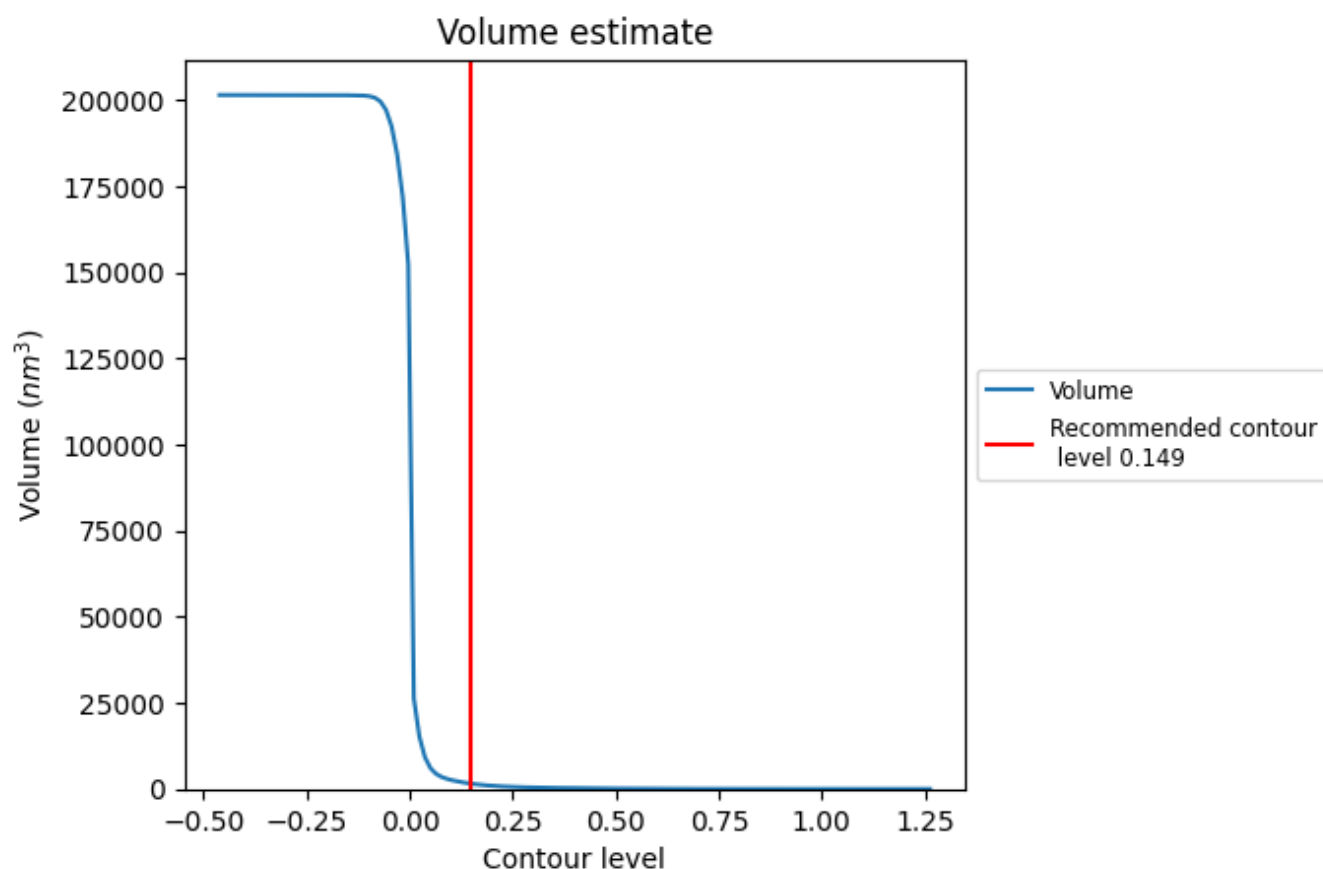
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

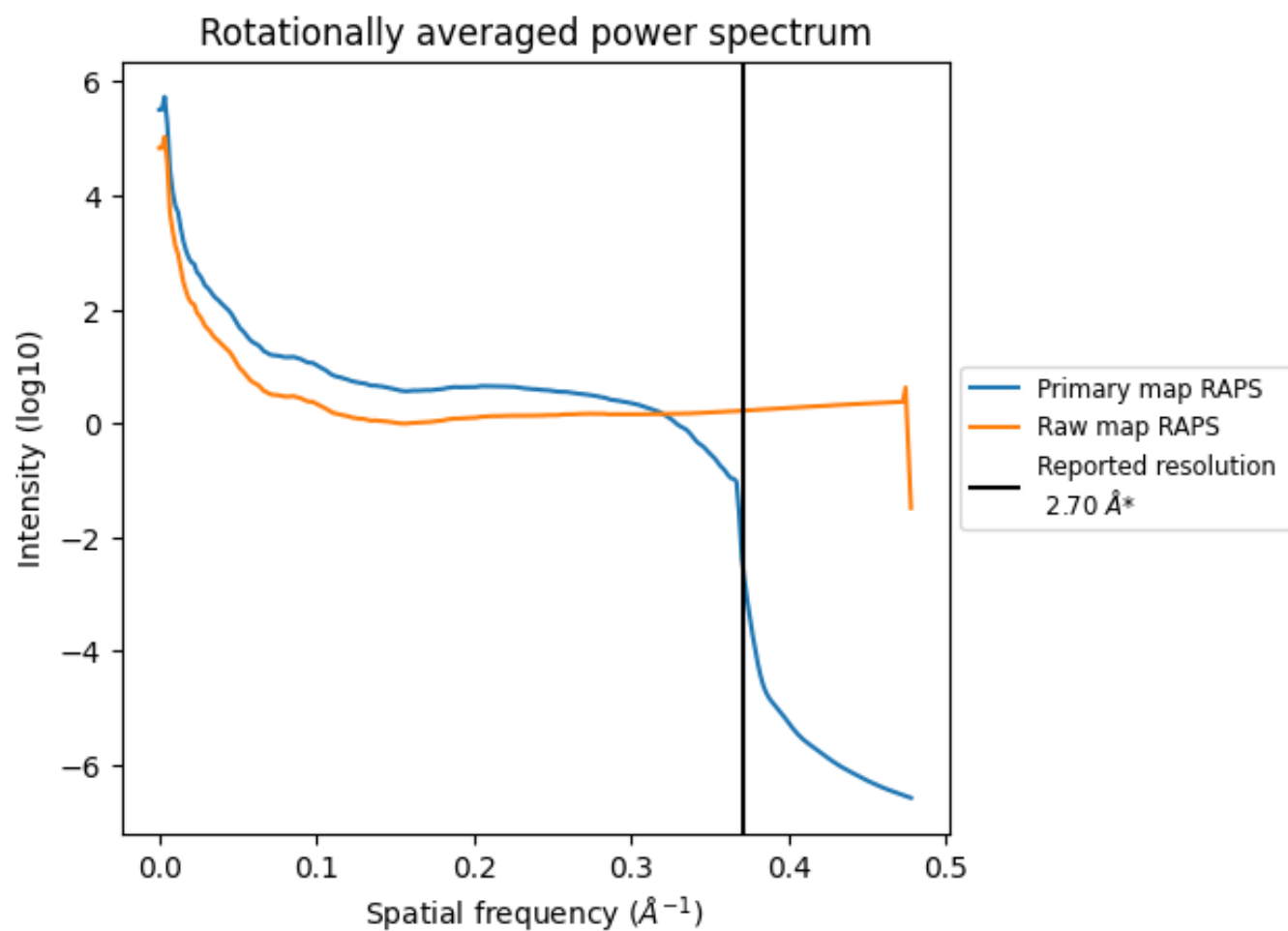
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1547 nm³; this corresponds to an approximate mass of 1397 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 ⓘ

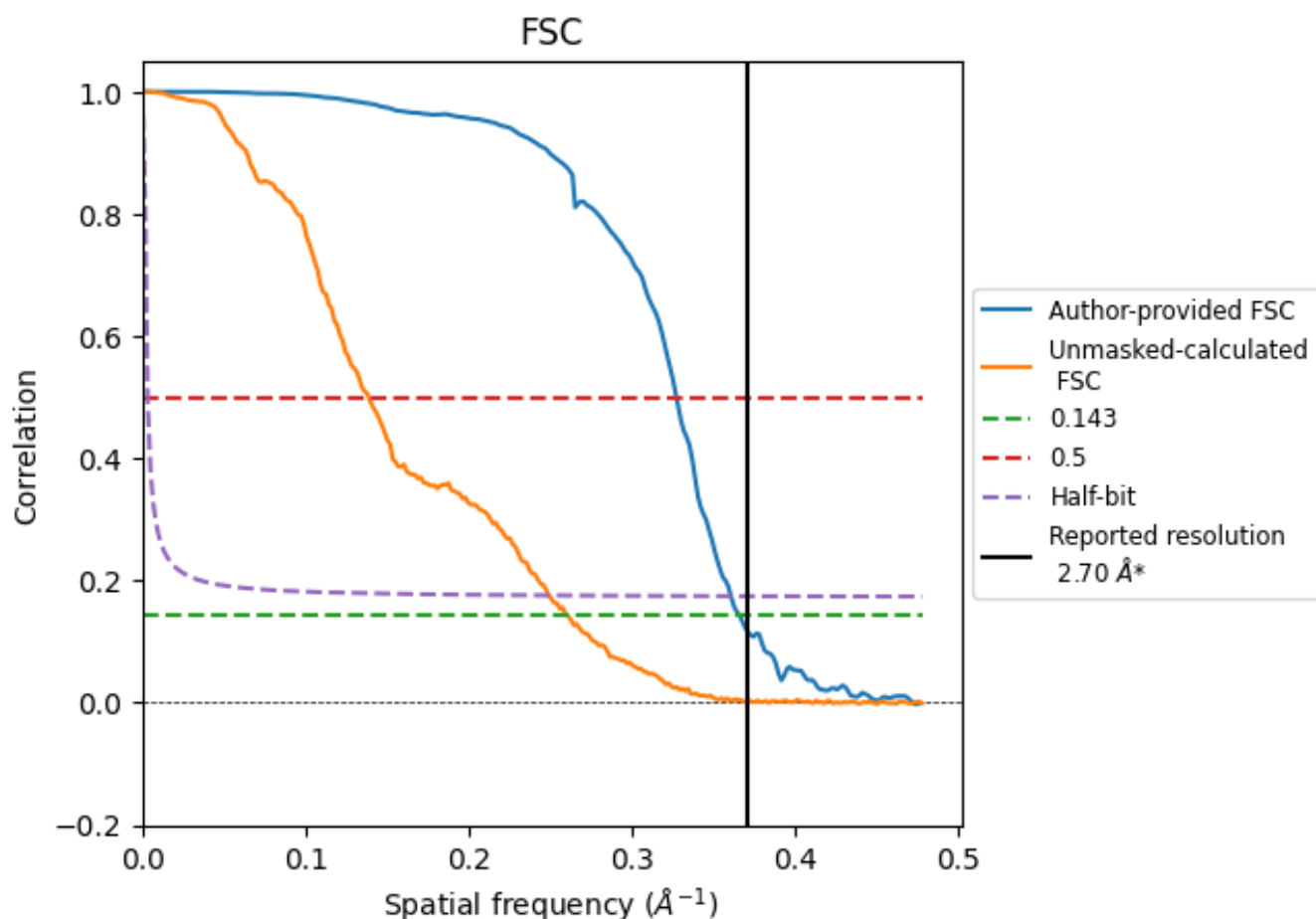


*Reported resolution corresponds to spatial frequency of 0.370 \AA^{-1}

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 0.370 \AA^{-1}

8.2 Resolution estimates [i](#)

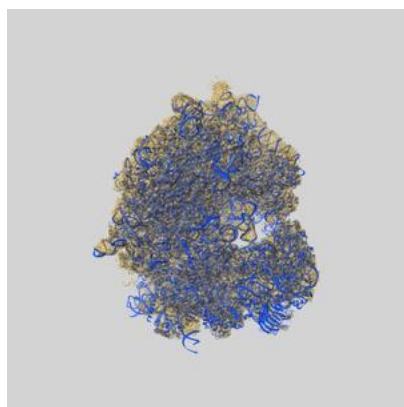
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.73	3.06	2.77
Unmasked-calculated*	3.84	7.21	4.02

*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 3.84 differs from the reported value 2.7 by more than 10 %

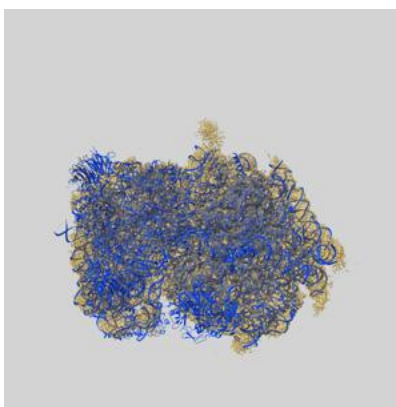
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-56598 and PDB model 28LN. Per-residue inclusion information can be found in section [3](#) on page [22](#).

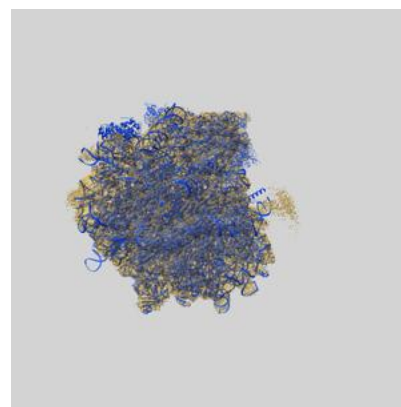
9.1 Map-model overlay [i](#)



X



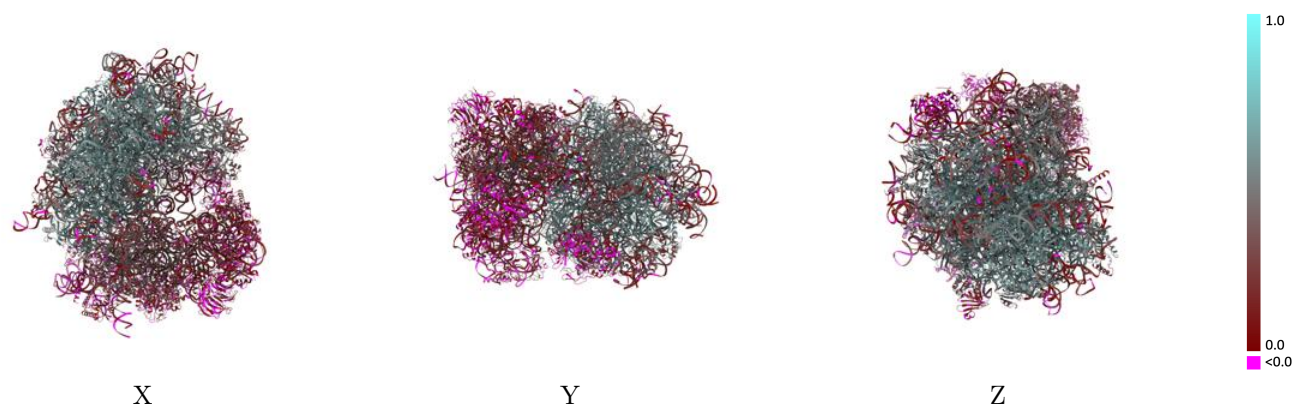
Y



Z

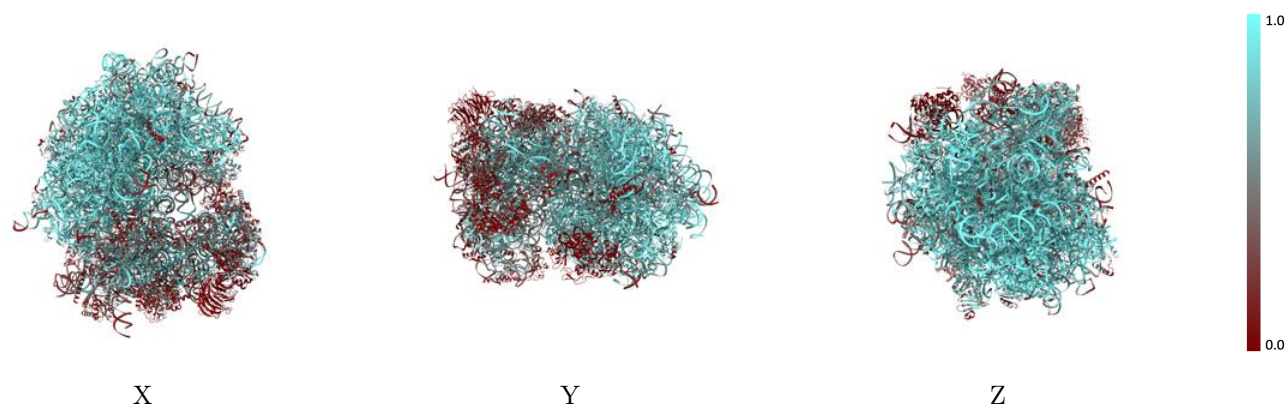
The images above show the 3D surface view of the map at the recommended contour level 0.149 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



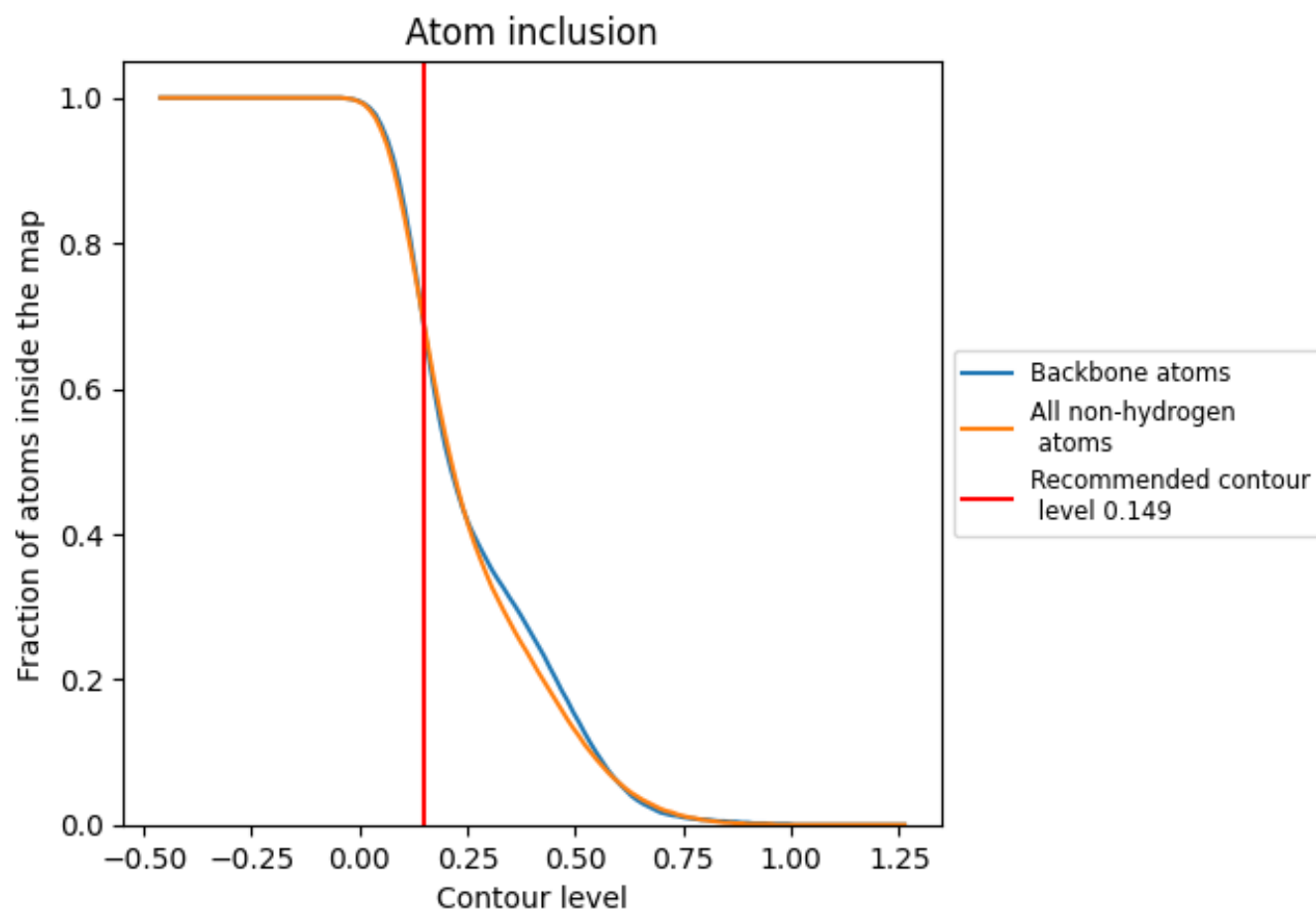
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.149).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 69% 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 (0.149) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6880	 0.3670
A2	 0.6480	 0.2030
AA	 0.2520	 0.2150
AB	 0.2870	 0.2610
AC	 0.2830	 0.2190
AD	 0.1750	 0.1620
AE	 0.2260	 0.1080
AF	 0.2650	 0.1620
AG	 0.1030	 0.0790
AH	 0.2430	 0.1730
AI	 0.1560	 0.1390
AJ	 0.2410	 0.1090
AK	 0.0850	 0.0810
AL	 0.2480	 0.1940
AM	 0.0050	 0.0240
AN	 0.4530	 0.3710
AO	 0.3660	 0.2830
AP	 0.2460	 0.1290
AQ	 0.2460	 0.1380
AR	 0.1770	 0.1480
AS	 0.3990	 0.1560
AT	 0.3160	 0.1500
AU	 0.2070	 0.1670
AV	 0.2400	 0.2100
AW	 0.4480	 0.2960
AX	 0.1430	 0.1550
AY	 0.1360	 0.0790
AZ	 0.1910	 0.1450
Aa	 0.3500	 0.2610
Ab	 0.3260	 0.2450
Ac	 0.2400	 0.1910
Ad	 0.3470	 0.1370
Ae	 0.1810	 0.1040
Af	 0.0100	 0.0210
Ag	 0.0150	 0.0660























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Chain	Atom inclusion	Q-score
Ah	 0.0830	 0.2060
B1	 0.4890	 0.3790
B2	 0.5400	 0.2290
B4	 0.7320	 0.2860
B5	 0.8690	 0.4610
B7	 0.9510	 0.4820
B8	 0.9450	 0.5280
BA	 0.9230	 0.5970
BB	 0.8910	 0.5620
BC	 0.9270	 0.5820
BD	 0.7060	 0.4140
BE	 0.8450	 0.5030
BF	 0.9120	 0.5670
BG	 0.7700	 0.4910
BH	 0.6950	 0.4190
BI	 0.3520	 0.2650
BJ	 0.6060	 0.3560
BL	 0.7610	 0.4970
BM	 0.8480	 0.5010
BN	 0.9340	 0.6040
BO	 0.8900	 0.5580
BP	 0.9100	 0.5750
BQ	 0.9150	 0.5900
BR	 0.7010	 0.4460
BS	 0.8500	 0.5340
BT	 0.8340	 0.5290
BU	 0.7890	 0.4720
BV	 0.8780	 0.5710
BW	 0.4310	 0.3030
BX	 0.8680	 0.5370
BY	 0.8870	 0.5530
BZ	 0.8550	 0.5230
Ba	 0.9060	 0.5710
Bb	 0.6100	 0.4200
Bc	 0.7550	 0.4600
Bd	 0.8840	 0.5490
Be	 0.9170	 0.5910
Bf	 0.9400	 0.5990
Bg	 0.8720	 0.5560
Bh	 0.8650	 0.5480
Bi	 0.6370	 0.4660
Bj	 0.8990	 0.5820

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Chain	Atom inclusion	Q-score
Bk	 0.6560	 0.4540
Bl	 0.8680	 0.5530
Bm	 0.0170	 0.0730
Bo	 0.4940	 0.4260
Bp	 0.8720	 0.5520
Br	 0.9450	 0.5800
Bs	 0.0070	 0.0400
Bt	 0.0010	 0.0380
Bu	 0.4550	 0.1120
Bv	 0.5520	 0.2470