



Full wwPDB EM Validation Report ⓘ

Jun 19, 2026 – 02:02 am BST

PDB ID : 9GMO / pdb_00009gmo
EMDB ID : EMD-51452
Title : eIF6-bound pre-60S large ribosomal subunit incorporating mutant uL16
Authors : Bothe, A.; Ban, N.; Kostova, K.
Deposited on : 2024-08-29
Resolution : 2.59 Å(reported)
Based on initial model : 8a3d

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:

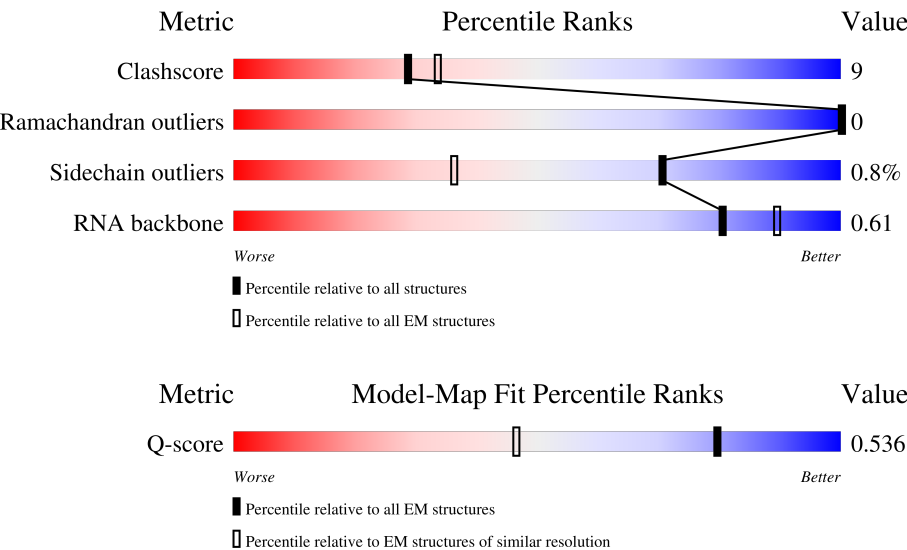
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal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

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

The reported resolution of this entry is 2.59 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.



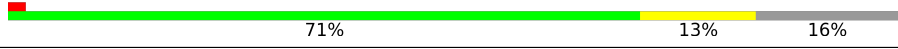
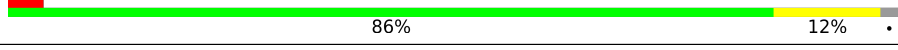
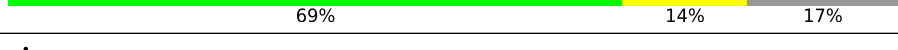
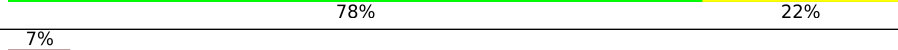
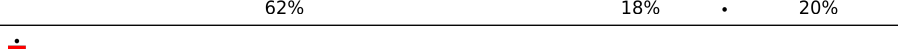
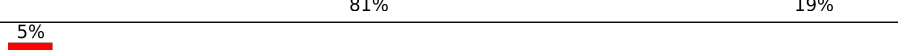
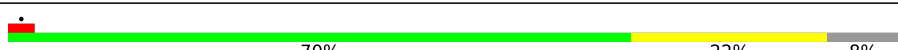
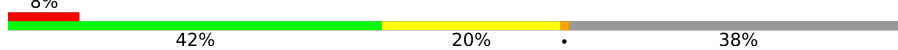
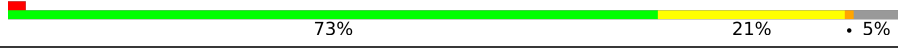
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7741 (2.09 - 3.09)

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	A	5064	33% 30% • 33%
2	B	119	57% 39% • •
3	C	157	48% 43% • 6%

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Mol	Chain	Length	Quality of chain
4	D	257	
5	E	403	
6	F	427	
7	G	297	
8	H	288	
9	I	203	
10	J	184	
11	K	188	
12	L	196	
13	M	176	
14	N	160	
15	O	128	
16	P	140	
17	Q	157	
18	R	156	
19	S	145	
20	T	136	
21	U	148	
22	V	159	
23	W	115	
24	X	125	
25	Y	135	
26	Z	110	
27	a	117	
28	b	123	

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Mol	Chain	Length	Quality of chain
29	c	105	
30	d	97	
31	e	70	
32	f	51	
33	g	128	
34	h	245	
35	i	106	
36	j	92	
37	k	137	
38	l	204	
39	m	248	
40	n	266	
41	o	192	
42	p	204	
43	q	178	
44	r	211	
45	s	215	
46	0	477	

2 Entry composition [i](#)

There are 53 unique types of molecules in this entry. The entry contains 132746 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3394	Total	C	N	O	P	1	0
			72870	32489	13334	23652	3395		

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	118	Total	C	N	O	P	0	0
			2518	1122	449	829	118		

- Molecule 3 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	148	Total	C	N	O	P	0	0
			3156	1408	563	1037	148		

- Molecule 4 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	246	Total	C	N	O	S	0	0
			1887	1183	387	311	6		

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	395	Total	C	N	O	S	1	0
			3194	2034	600	545	15		

- Molecule 6 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	360	Total	C	N	O	S	0	0
			2860	1800	572	475	13		

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	292	Total	C	N	O	S	0	0
			2372	1503	431	424	14		

- Molecule 8 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	218	Total	C	N	O	S	0	0
			1752	1128	333	287	4		

- Molecule 9 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	199	Total	C	N	O	S	0	0
			1634	1053	319	257	5		

- Molecule 10 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	152	Total	C	N	O	S	0	0
			1233	771	240	213	9		

- Molecule 11 is a protein called 60S ribosomal protein L18.

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

- Molecule 12 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	157	Total	C	N	O	S	0	0
			1304	813	280	202	9		

- Molecule 13 is a protein called 60S ribosomal protein L18a.

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

- Molecule 14 is a protein called 60S ribosomal protein L21.

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

- Molecule 15 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	99	Total	C	N	O	S	0	0
			804	516	140	146	2		

- Molecule 16 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	132	Total	C	N	O	S	0	0
			985	621	185	174	5		

- Molecule 17 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	62	Total	C	N	O	S	0	0
			519	332	101	83	3		

- Molecule 18 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	119	Total	C	N	O	S	0	0
			976	624	183	168	1		

- Molecule 19 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 20 is a protein called 60S ribosomal protein L27.

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

- Molecule 21 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 22 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	99	Total	C	N	O	S	0	0
			806	500	177	125	4		

- Molecule 23 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	100	Total	C	N	O	S	0	0
			772	490	136	139	7		

- Molecule 24 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	106	Total	C	N	O	S	0	0
			868	551	170	145	2		

- Molecule 25 is a protein called 60S ribosomal protein L32.

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

- Molecule 26 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	109	Total	C	N	O	S	1	0
			879	557	174	144	4		

- Molecule 27 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	111	Total	C	N	O	S	0	0
			882	552	182	142	6		

- Molecule 28 is a protein called 60S ribosomal protein L35.

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

- Molecule 29 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 30 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	86	Total	C	N	O	S	1	0
			713	442	155	111	5		

- Molecule 31 is a protein called 60S ribosomal protein L38.

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

- Molecule 32 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 33 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 34 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	225	Total	C	N	O	S	0	0
			1712	1065	295	340	12		

- Molecule 35 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	103	Total	C	N	O	S	0	0
			842	528	172	136	6		

- Molecule 36 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	92	Total	C	N	O	S	0	0
			716	450	137	121	8		

- Molecule 37 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	k	124	Total	C	N	O	S	0	0
			992	615	206	167	4		

- Molecule 38 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	203	Total	C	N	O	S	1	0
			1708	1077	360	267	4		

- Molecule 39 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	m	224	Total	C	N	O	S	0	0
			1856	1192	356	299	9		

- Molecule 40 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	223	Total	C	N	O	S	0	0
			1809	1153	349	303	4		

- Molecule 41 is a protein called 60S ribosomal protein L9.

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

- Molecule 42 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	p	203	Total	C	N	O	S	0	0
			1647	1045	318	272	12		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
p	?	-	MET	deletion	UNP P27635
p	?	-	LEU	deletion	UNP P27635
p	?	-	SER	deletion	UNP P27635
p	?	-	CYS	deletion	UNP P27635
p	?	-	ALA	deletion	UNP P27635
p	?	-	GLY	deletion	UNP P27635
p	?	-	ALA	deletion	UNP P27635
p	?	-	ASP	deletion	UNP P27635
p	?	-	ARG	deletion	UNP P27635
p	?	-	LEU	deletion	UNP P27635

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	q	170	Total	C	N	O	S	0	0
			1358	858	253	241	6		

- Molecule 44 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	r	206	Total	C	N	O	S	0	0
			1664	1041	345	274	4		

- Molecule 45 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	s	139	Total	C	N	O	S	0	0
			1138	730	218	183	7		

- Molecule 46 is a protein called Cytoplasmic 60S subunit biogenesis factor ZNF622.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	0	43	Total	C	N	O	S	0	0
			363	226	72	59	6		

- Molecule 47 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
47	A	213	Total 213	Mg 213	0
47	B	3	Total 3	Mg 3	0
47	C	6	Total 6	Mg 6	0
47	L	1	Total 1	Mg 1	0
47	P	1	Total 1	Mg 1	0
47	U	1	Total 1	Mg 1	0
47	i	1	Total 1	Mg 1	0
47	p	1	Total 1	Mg 1	0

- Molecule 48 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
48	A	139	Total 139	K 139	0
48	B	1	Total 1	K 1	0
48	D	3	Total 3	K 3	0
48	F	1	Total 1	K 1	0
48	J	1	Total 1	K 1	0
48	N	1	Total 1	K 1	0
48	V	1	Total 1	K 1	0
48	Y	1	Total 1	K 1	0
48	Z	1	Total 1	K 1	0
48	f	1	Total 1	K 1	0
48	i	1	Total 1	K 1	0
48	l	2	Total 2	K 2	0

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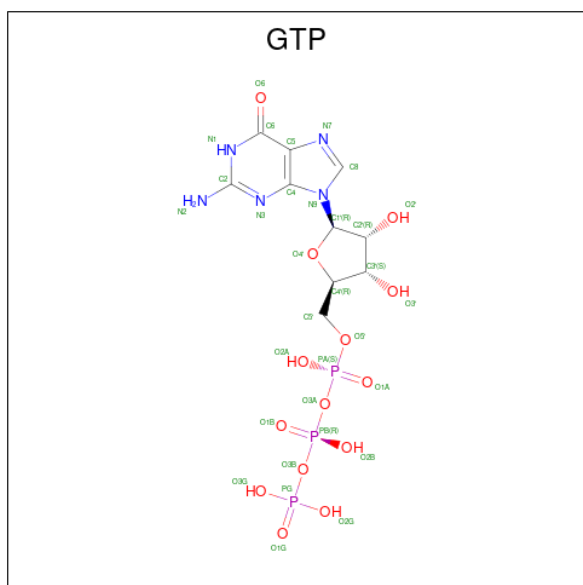
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Mol	Chain	Residues	Atoms		AltConf
48	o	1	Total	K	0
			1	1	
48	p	1	Total	K	0
			1	1	

- Molecule 49 is SODIUM ION (CCD ID: NA) (formula: Na).

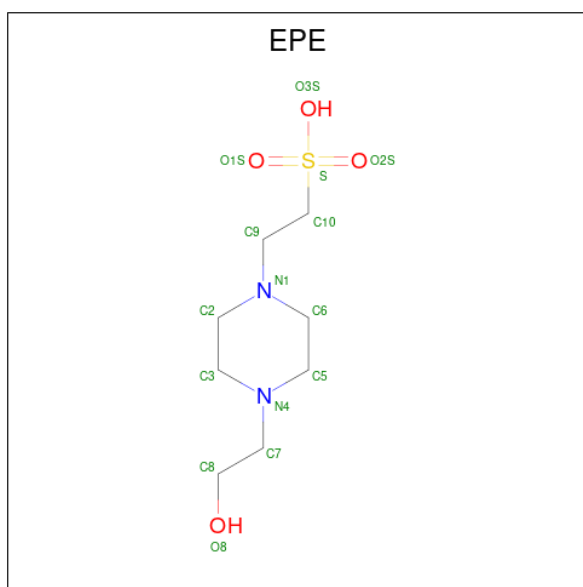
Mol	Chain	Residues	Atoms		AltConf
49	A	2	Total	Na	0
			2	2	

- Molecule 50 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

- Molecule 51 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					AltConf
51	M	1	Total	C	N	O	S	0
			15	8	2	4	1	

- Molecule 52 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
52	a	1	Total	Zn	0
			1	1	
52	d	1	Total	Zn	0
			1	1	
52	g	1	Total	Zn	0
			1	1	
52	i	1	Total	Zn	0
			1	1	
52	j	1	Total	Zn	0
			1	1	

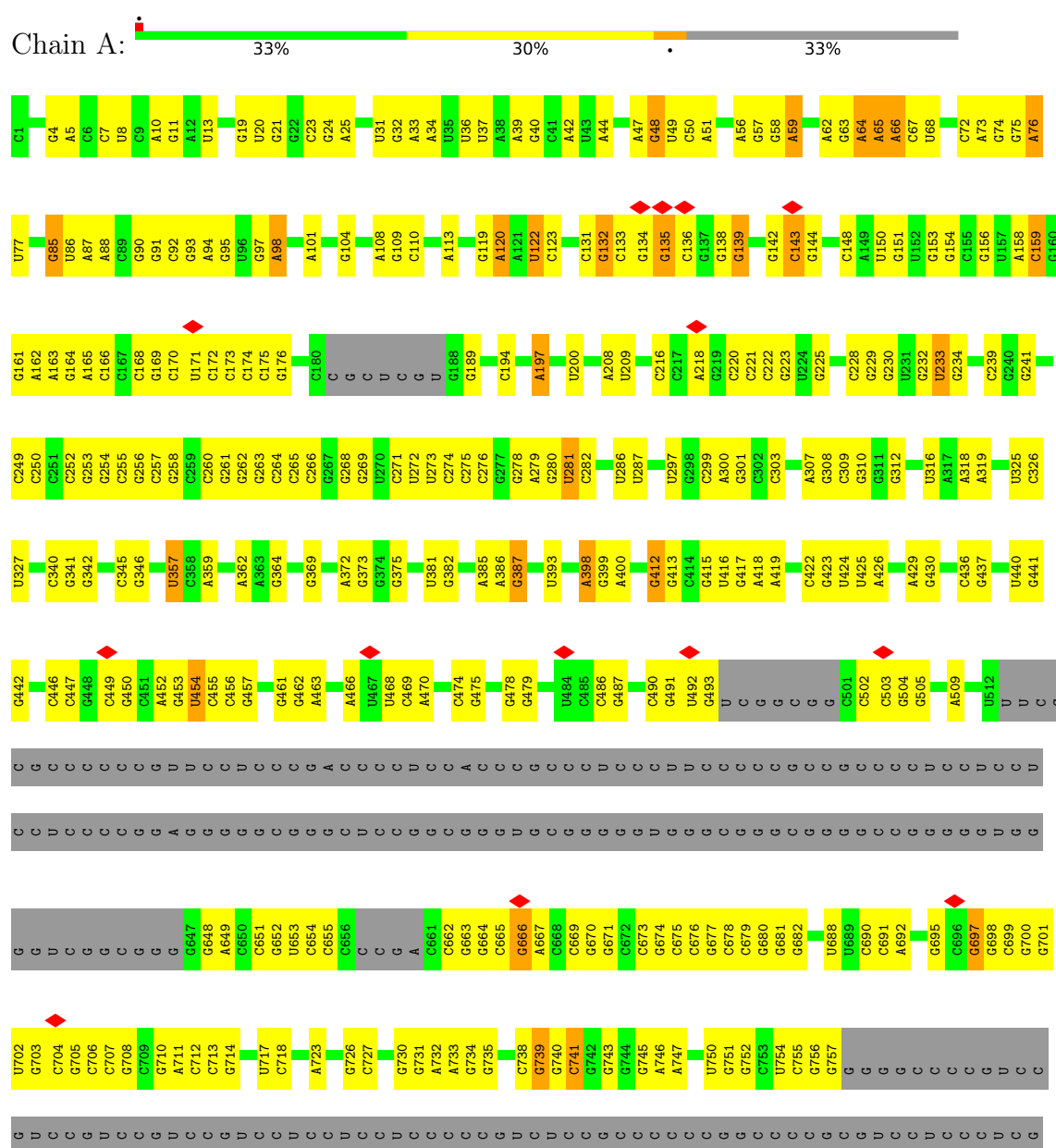
- Molecule 53 is water.

Mol	Chain	Residues	Atoms		AltConf
53	A	4	Total	O	0
			4	4	
53	G	1	Total	O	0
			1	1	

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: 28S rRNA





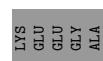
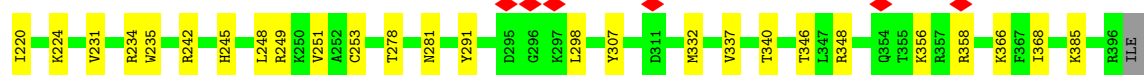
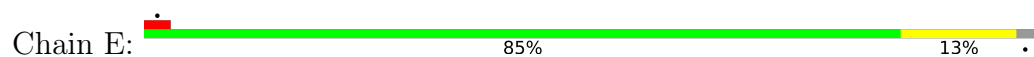


G4228	G4150	C4080	G	PSU	G3888	A3816	G3661	C	U	G	G
U4229	G4151	G4081	U	A	C3893	A3817	A3662	G			G
A4233	G4152	G4084	C	G	A3894	U13818	A3663	C			G
A4234	C4153	G4084	C	A	A3894	G3819	G3664	C			G
G4237	C4154	C4088	G	A	C3895	G3820	G3665	U			G
G4238	C4155	C4088	C	U	C3896		C3666	A			G
A4239	C4156	G4089	C	A	G3897	G3823	C3667	G			G
G4240	A4158	G4090	G	A	C3898	A3824	C3668	C3598			G
G4246	C4159	G4093	G	G	C3899	A3825	A3599	C3599			G
G4247	C4160	G	U	U	G3900	C3826	C3670	C3600			G
A4251	G4161	G	C	G	A3901	G3827	G3671				G
C4252	C4162	G	C	G	A3905	A3828	G3672	G3603			G
A4253	C4165	A	U	A	A3906	G3829	C3673	A3604			G
G4254	G4168	G	G	G	A3907	A3830		C3605			G
A4255	C4169	C	C	C	G3908	U3831	G3681	U3607			G
U4260	C4170	C	G	C	C3909		A3682	A3608			G
C4261	A4171	C	G	C	C3910	A3836	C3683	A3609			G
C4262	C4172	C	C	C	C3911	C3837	G3684	G3609			G
G4263	C4173	C	C	C	U3912	U3838	G3685	A3610			G
U4265	A4174	G	G	G		G3839	G3686	A3611			G
G4266	C4175	G	C	C	U3915	U3840	U3687	C3612			G
G4267	C4176	G	C	C	G3916		U3688	G3613			G
A4268	A4177	C	C	C	A3917	U3844	A3692	G3614			G
A4272	C4178	U	G	C	G3918	C3843		G3615			G
A4273	A4179	C	C	C	C3919	U3844		U3616			G
G4275	U4180	C	C	C	U3920			G3617			G
G4277	C4191	C	C	C	A3923	U3848	U3695	C3618			G
A4281	A4192	U	A	C	C3924	A3849	C3696	G3619			G
A4282	C4193	C	C	C	U3925	C3850	U3697	G3620			G
U4285	G4194	C	C	C	C3926	U3851	C3698	A3621			G
C4286	C4196	U	C	C	U3927	A3852	G3699	C3622			G
G4287	A4197	G	C	C	A3928	U3853	C3700	C3623			G
G4291	C4198	G	C	C		C3854	A3624	G3624			G
A4292	G4199	C	C	C	U3932	A3856	A3702	C3625			G
U4296	A4203	C	C	C	G3933		U3707	G3626			G
G4297	C4209	C	C	C	C3934	A3861	C3708	G3627			G
A4298	U4212	C	C	C	U3937	A3862	U3709	G3628			G
U4299	A4213	G	C	C			G3709	C3629			G
U4300	A4214	G	A	C	C3940	A3865	G3710				G
U4301	C4072	C	C	C	G3941	C3866	A3711	G3634			G
U4302	A4073	C	C	C	A3942	A3867	A3712	A3635			G
A4303	C4074	C	C	C	A3943	G3868	U3713	C3636			G
A4304	U4075	C	C	C	G3944	C3769	G3714	U3637			G
G4305	A4076	G	C	C	A3945	U3790	U3715	G3638			G
U4306	G4077	G	C	C	C3946	C3791	C3716	U3639			G
A4307	C4148	C	C	C	A3947	A3871	U3640	U3640			G
					C3948	A3717	A3641				G
					A	C3794	A3642				G
					U	A3795					G
					C	A3799	A3723	A3646			G
					C	C3877	A3724	A3647			G
					C	C3878	G3725	A3648			G
					C	G3879	A3726				G
					C	G3880	A3727				G
					C	G3881	A3728	A3653			G
					C	C3882	U3729	A3656			G
					C	U3883	U3730	U3657			G
					C	G3884	C3731	C3658			G
					C	U3884	A3732	G3659			G
					C	C3887	A3733	C3660			G

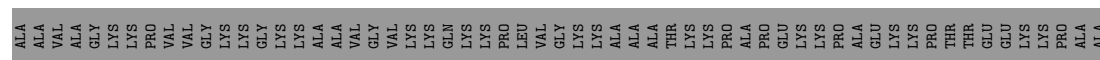
- Molecule 4: 60S ribosomal protein L8



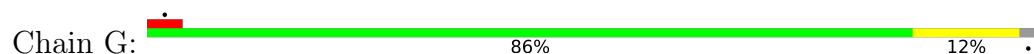
- Molecule 5: 60S ribosomal protein L3

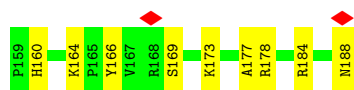


- Molecule 6: 60S ribosomal protein L4

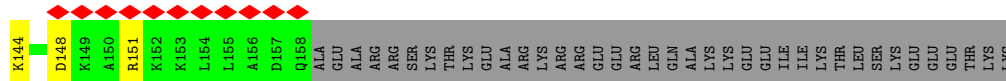
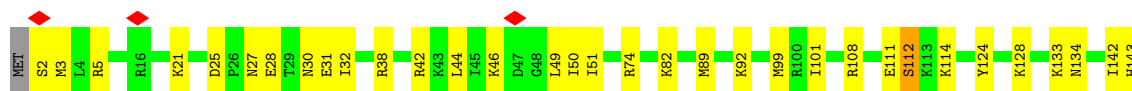


- Molecule 7: 60S ribosomal protein L5

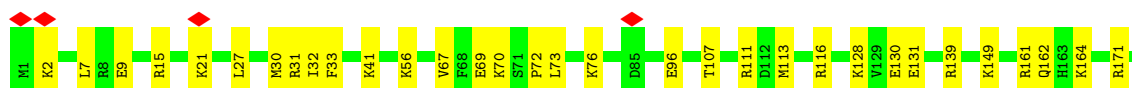
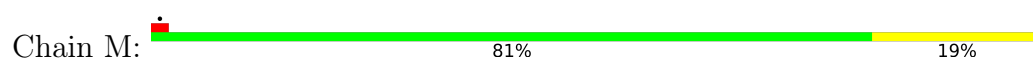




- Molecule 12: 60S ribosomal protein L19



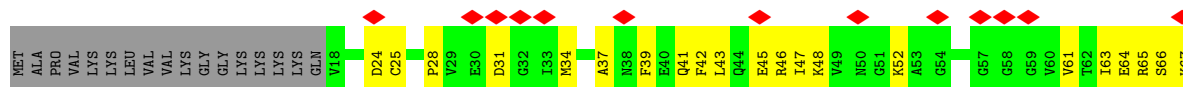
- Molecule 13: 60S ribosomal protein L18a



- Molecule 14: 60S ribosomal protein L21

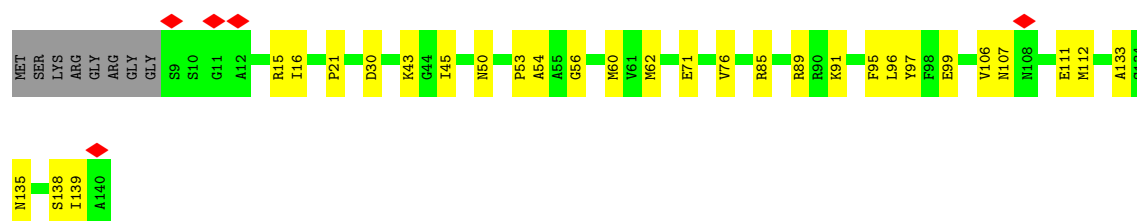


- Molecule 15: 60S ribosomal protein L22



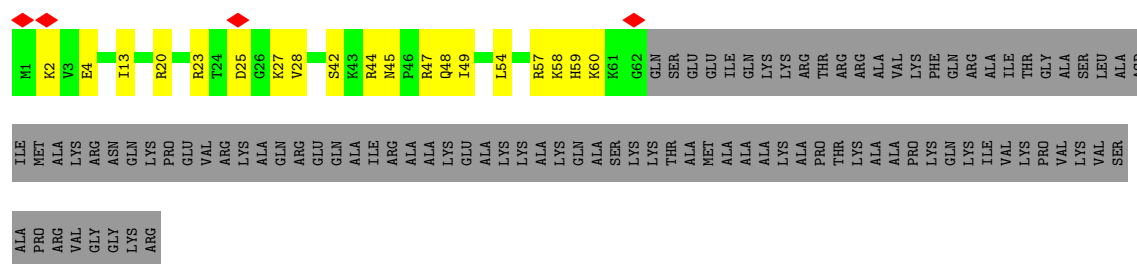
- Molecule 16: 60S ribosomal protein L23

Chain P: 



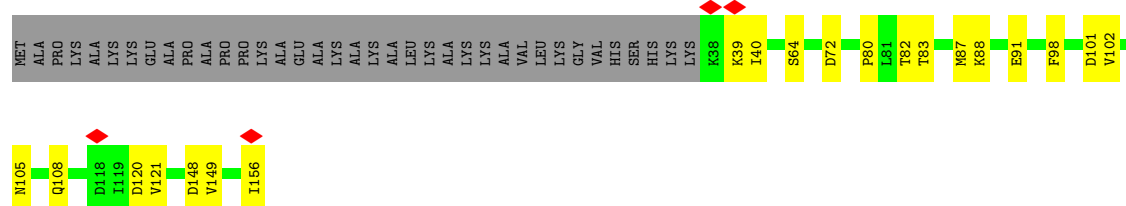
- Molecule 17: 60S ribosomal protein L24

Chain Q: 



- Molecule 18: 60S ribosomal protein L23a

Chain R: 



- Molecule 19: Large ribosomal subunit protein uL24

Chain S: 



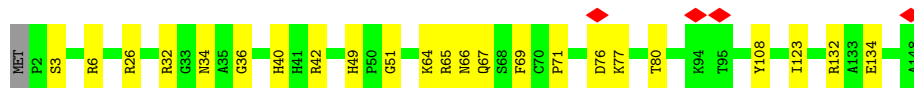
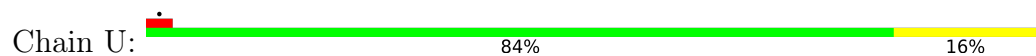
- Molecule 20: 60S ribosomal protein L27

Chain T: 

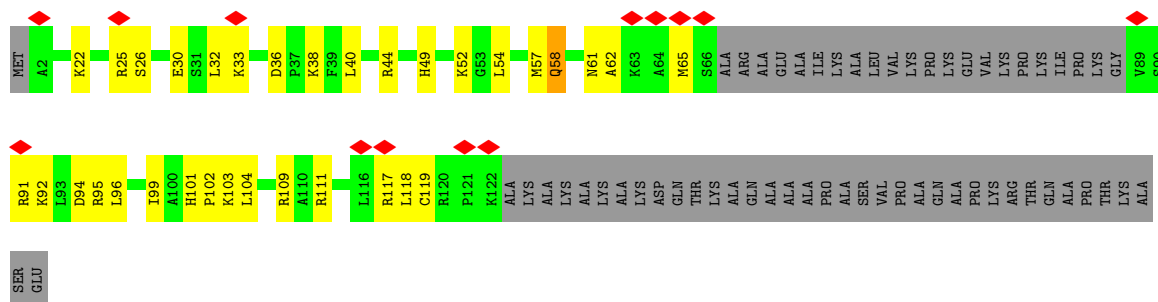




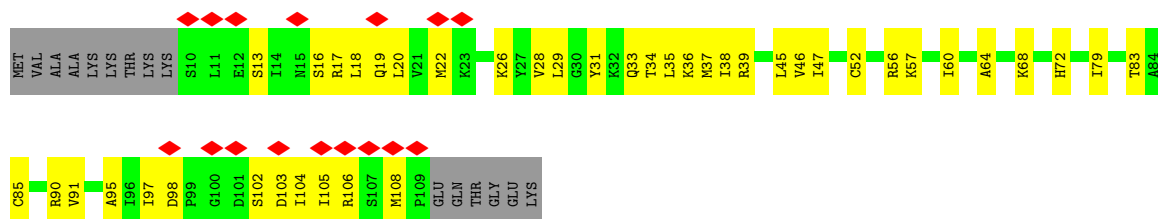
- Molecule 21: 60S ribosomal protein L27a



- Molecule 22: 60S ribosomal protein L29



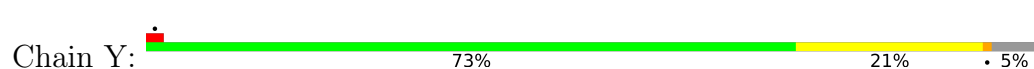
- Molecule 23: 60S ribosomal protein L30



- Molecule 24: 60S ribosomal protein L31



- Molecule 25: 60S ribosomal protein L32



GLU
ASN
GLU

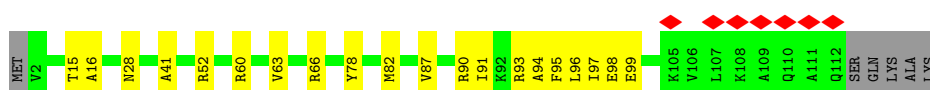
- Molecule 26: 60S ribosomal protein L35a

Chain Z:  83% 16% .



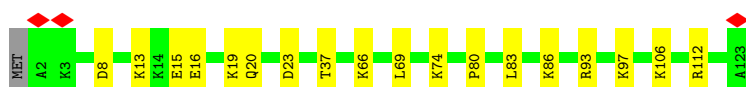
- Molecule 27: 60S ribosomal protein L34

Chain a:  6% 78% 17% 5%



- Molecule 28: 60S ribosomal protein L35

Chain b:  85% 15% .



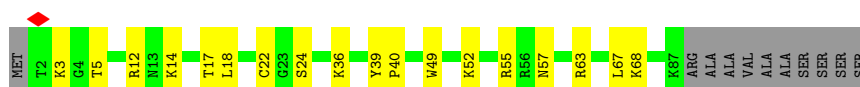
- Molecule 29: 60S ribosomal protein L36

Chain c:  6% 82% 15% .



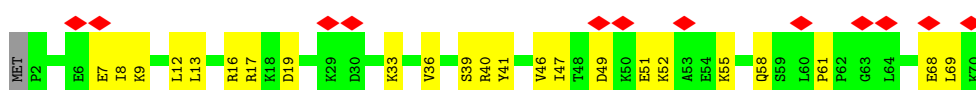
- Molecule 30: 60S ribosomal protein L37

Chain d:  70% 19% 11% .



- Molecule 31: 60S ribosomal protein L38

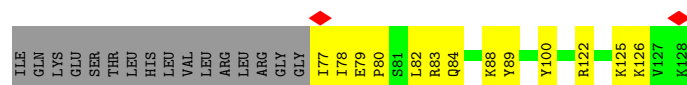
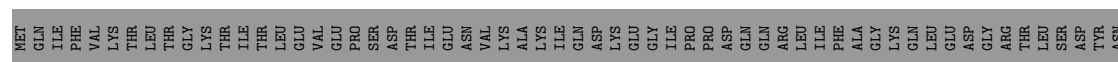
Chain e:  17% 66% 33% .



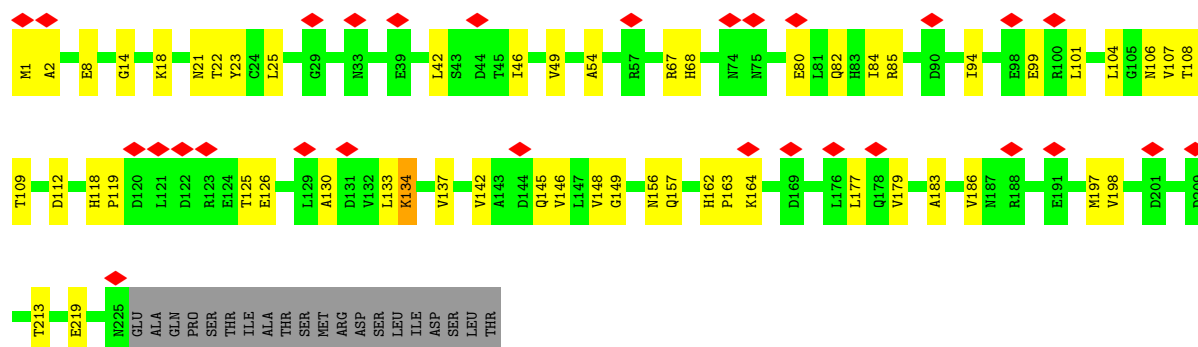
- Molecule 32: 60S ribosomal protein L39



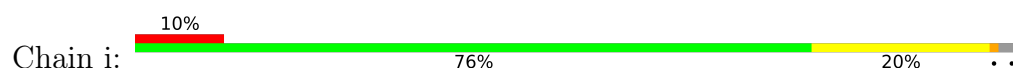
- Molecule 33: Ubiquitin-60S ribosomal protein L40



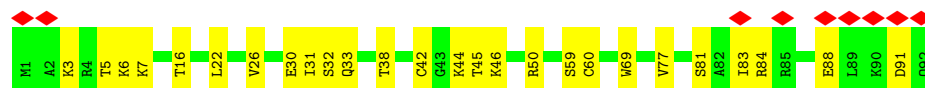
- Molecule 34: Eukaryotic translation initiation factor 6



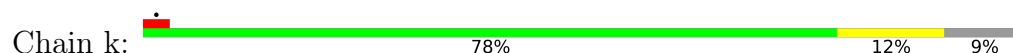
- Molecule 35: 60S ribosomal protein L36a



- Molecule 36: 60S ribosomal protein L37a



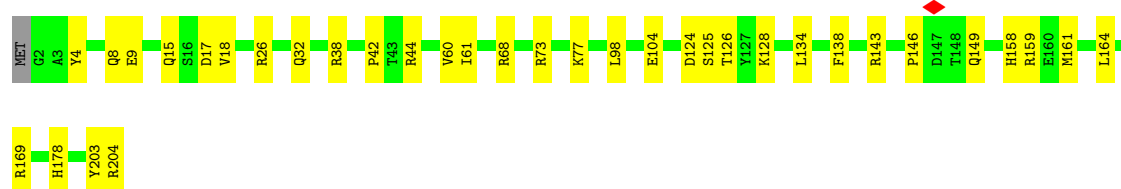
- Molecule 37: 60S ribosomal protein L28





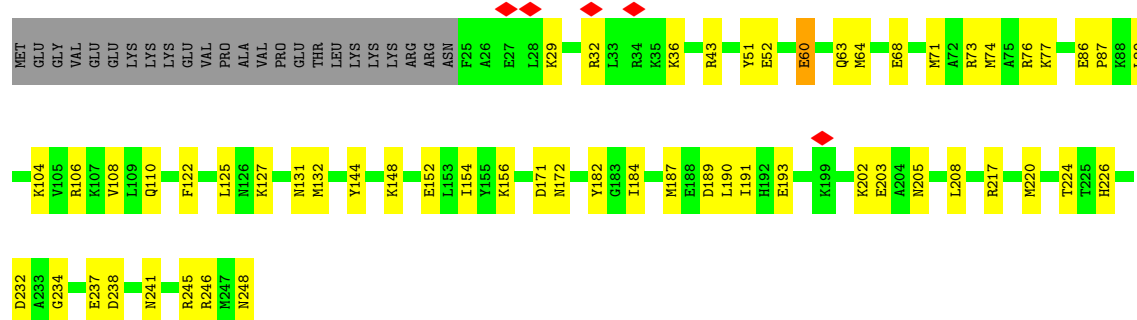
- Molecule 38: 60S ribosomal protein L15

Chain l: 82% 17%



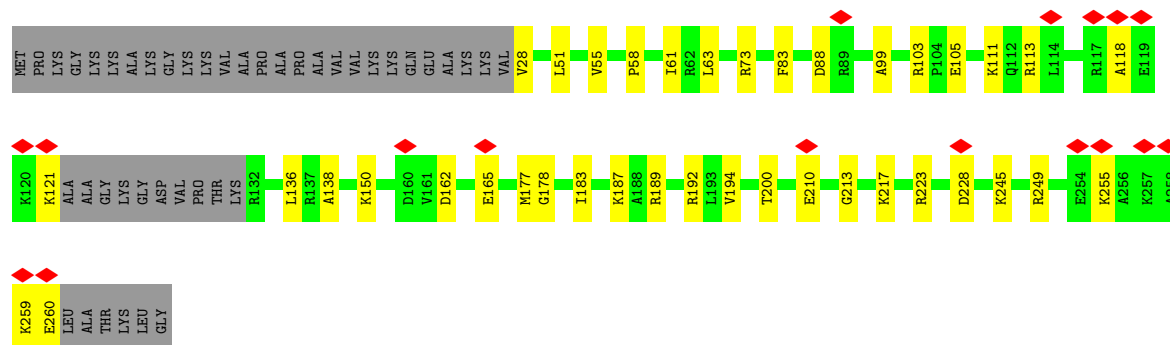
- Molecule 39: Large ribosomal subunit protein uL30

Chain m: 67% 23% 10%



- Molecule 40: 60S ribosomal protein L7a

Chain n: 6% 69% 15% 16%



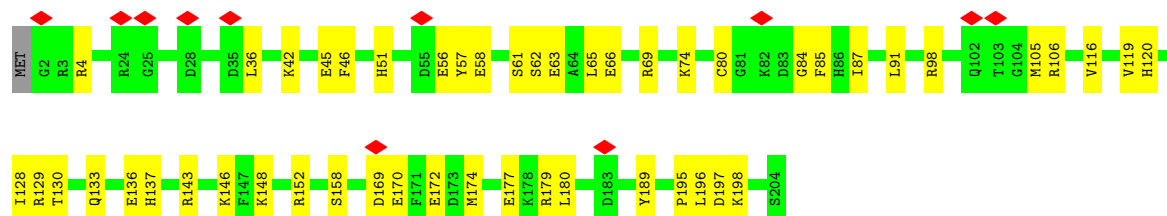
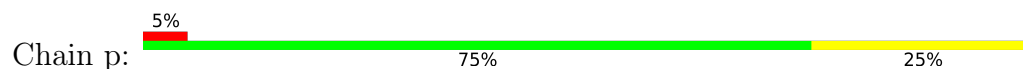
- Molecule 41: 60S ribosomal protein L9

Chain o: 6% 77% 22%

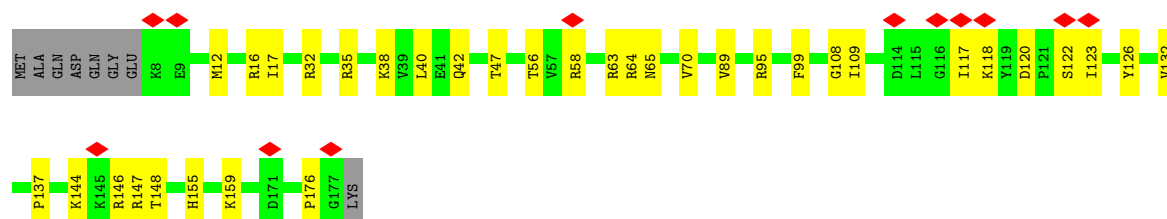
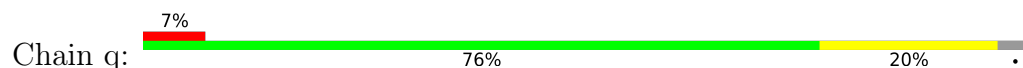




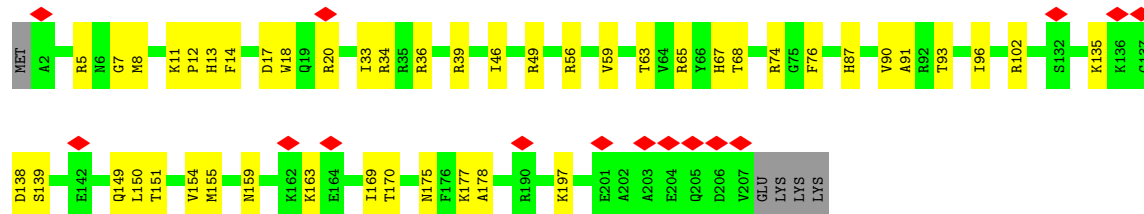
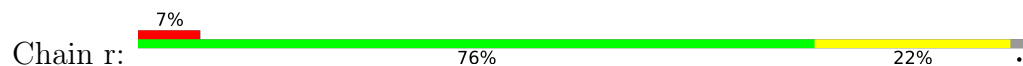
- Molecule 42: Large ribosomal subunit protein uL16



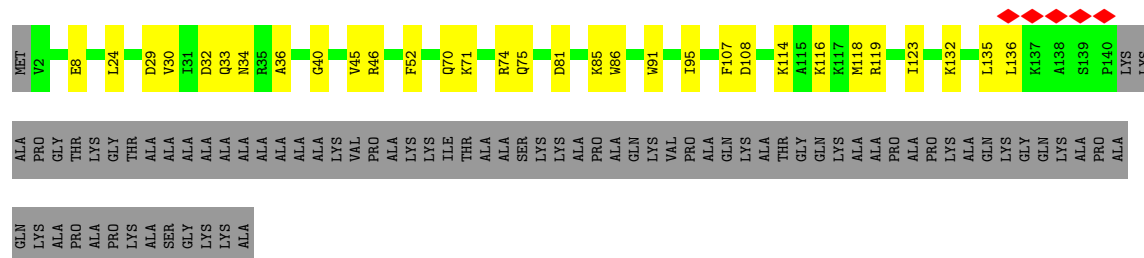
- Molecule 43: 60S ribosomal protein L11



- Molecule 44: 60S ribosomal protein L13



- Molecule 45: 60S ribosomal protein L14



Chain 0: 91%

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	193000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.487	Depositor
Minimum map value	-0.586	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	593.6, 593.6, 593.6	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, K, OMG, ZN, 5MC, 6MZ, UR3, NA, GTP, EPE, A2M, OMU, PSU, UY1, 1MA, MG

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	A	0.12	4/78643 (0.0%)	0.21	0/122654
2	B	0.08	0/2813	0.19	0/4384
3	C	0.08	0/3453	0.20	0/5376
4	D	0.10	0/1925	0.28	0/2581
5	E	0.08	0/3265	0.22	0/4369
6	F	0.09	0/2914	0.24	0/3915
7	G	0.08	0/2418	0.24	0/3239
8	H	0.11	0/1786	0.28	0/2395
9	I	0.12	0/1666	0.33	0/2228
10	J	0.12	0/1259	0.36	0/1689
11	K	0.11	0/1537	0.27	0/2052
12	L	0.13	0/1320	0.40	0/1749
13	M	0.11	0/1501	0.30	0/2013
14	N	0.16	0/1326	0.43	0/1770
15	O	0.22	0/818	0.61	0/1098
16	P	0.11	0/999	0.32	0/1340
17	Q	0.17	0/532	0.47	0/708
18	R	0.12	0/993	0.32	0/1334
19	S	0.13	0/1132	0.34	0/1504
20	T	0.12	0/1130	0.35	0/1507
21	U	0.09	0/1191	0.26	0/1591
22	V	0.15	0/819	0.42	0/1081
23	W	0.19	0/783	0.51	0/1052
24	X	0.12	0/883	0.31	0/1190
25	Y	0.11	0/1071	0.31	0/1429
26	Z	0.10	0/901	0.26	0/1206
27	a	0.09	0/892	0.23	0/1189
28	b	0.13	0/1023	0.39	0/1351
29	c	0.13	0/843	0.37	0/1115
30	d	0.07	0/732	0.22	0/968
31	e	0.15	0/575	0.42	0/761
32	f	0.12	0/454	0.30	0/599

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.11	0/435	0.34	0/575
34	h	0.13	0/1736	0.36	0/2362
35	i	0.11	0/855	0.35	0/1128
36	j	0.10	0/726	0.35	0/963
37	k	0.08	0/1007	0.24	0/1351
38	l	0.08	0/1753	0.21	0/2348
39	m	0.11	0/1890	0.28	0/2519
40	n	0.09	0/1840	0.23	0/2476
41	o	0.16	0/1537	0.40	0/2066
42	p	0.13	0/1686	0.35	0/2252
43	q	0.10	0/1381	0.30	0/1848
44	r	0.10	0/1695	0.27	0/2270
45	s	0.12	0/1161	0.36	0/1554
46	0	0.08	0/368	0.26	0/484
All	All	0.12	4/139667 (0.0%)	0.25	0/205633

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4523	A2M	O3'-P	5.06	1.61	1.56
1	A	3785	A2M	O3'-P	5.03	1.61	1.56
1	A	398	A2M	O3'-P	5.02	1.61	1.56
1	A	3718	A2M	O3'-P	5.00	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	72870	0	36883	1229	0
2	B	2518	0	1273	40	0
3	C	3156	0	1602	56	0
4	D	1887	0	1983	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	3194	0	3335	41	0
6	F	2860	0	3026	50	0
7	G	2372	0	2403	30	0
8	H	1752	0	1904	28	0
9	I	1634	0	1779	23	0
10	J	1233	0	1263	19	0
11	K	1513	0	1628	38	0
12	L	1304	0	1433	30	0
13	M	1461	0	1502	26	0
14	N	1298	0	1366	37	0
15	O	804	0	825	28	0
16	P	985	0	1044	27	0
17	Q	519	0	533	17	0
18	R	976	0	1053	15	0
19	S	1115	0	1205	28	0
20	T	1107	0	1182	32	0
21	U	1162	0	1213	19	0
22	V	806	0	865	26	0
23	W	772	0	808	34	0
24	X	868	0	912	11	0
25	Y	1053	0	1147	22	0
26	Z	879	0	915	13	0
27	a	882	0	972	14	0
28	b	1015	0	1148	19	0
29	c	832	0	917	11	0
30	d	713	0	746	15	0
31	e	569	0	637	19	0
32	f	444	0	482	12	0
33	g	429	0	465	13	0
34	h	1712	0	1689	40	0
35	i	842	0	912	15	0
36	j	716	0	768	22	0
37	k	992	0	1052	12	0
38	l	1708	0	1757	28	0
39	m	1856	0	1983	47	0
40	n	1809	0	1941	28	0
41	o	1518	0	1600	34	0
42	p	1647	0	1694	39	0
43	q	1358	0	1388	24	0
44	r	1664	0	1773	35	0
45	s	1138	0	1204	21	0
46	0	363	0	377	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	A	213	0	0	0	0
47	B	3	0	0	0	0
47	C	6	0	0	0	0
47	L	1	0	0	0	0
47	P	1	0	0	0	0
47	U	1	0	0	0	0
47	i	1	0	0	0	0
47	p	1	0	0	0	0
48	A	139	0	0	0	0
48	B	1	0	0	0	0
48	D	3	0	0	0	0
48	F	1	0	0	0	0
48	J	1	0	0	0	0
48	N	1	0	0	0	0
48	V	1	0	0	0	0
48	Y	1	0	0	0	0
48	Z	1	0	0	0	0
48	f	1	0	0	0	0
48	i	1	0	0	0	0
48	l	2	0	0	0	0
48	o	1	0	0	0	0
48	p	1	0	0	0	0
49	A	2	0	0	0	0
50	B	32	0	11	1	0
51	M	15	0	17	1	0
52	a	1	0	0	0	0
52	d	1	0	0	0	0
52	g	1	0	0	0	0
52	i	1	0	0	0	0
52	j	1	0	0	0	0
53	A	4	0	0	0	0
53	G	1	0	0	1	0
All	All	132746	0	96615	2108	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 9.

All (2108) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2845:A:H61	1:A:3843:C:H42	1.06	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:102:ARG:H	20:T:102:ARG:HE	1.20	0.87
1:A:2845:A:H61	1:A:3843:C:N4	1.75	0.84
1:A:2520:C:O2	1:A:2640:G:N2	2.11	0.84
1:A:3723:A:H2'	1:A:3724:A2M:H8	1.59	0.83
1:A:1870:C:H2'	1:A:1871:A2M:H8	1.61	0.82
1:A:2845:A:N6	1:A:3843:C:H42	1.81	0.79
12:L:3:MET:HE1	12:L:5:ARG:HG2	1.66	0.77
19:S:1:MET:HE3	19:S:2:LYS:H	1.49	0.77
17:Q:2:LYS:HA	17:Q:2:LYS:HE2	1.67	0.77
2:B:28:C:H1'	2:B:54:A:H61	1.51	0.76
1:A:33:A:OP2	1:A:48:G:N2	2.19	0.76
4:D:14:SER:OG	4:D:15:VAL:N	2.19	0.76
6:F:334:THR:HG1	39:m:51:TYR:HH	1.31	0.76
12:L:44:LEU:HD22	12:L:49:LEU:HD12	1.68	0.76
11:K:76:GLU:N	11:K:76:GLU:OE2	2.19	0.75
1:A:3700:C:O2'	1:A:3774:A:N3	2.20	0.74
41:o:51:LYS:HG2	41:o:52:LYS:HG3	1.67	0.74
1:A:2483:G:H1	1:A:2495:U:H3	1.36	0.74
1:A:2611:A:H5'	1:A:2688:G:H4'	1.70	0.74
1:A:4620:OMU:OP2	1:A:4670:C:N4	2.21	0.73
20:T:12:LEU:HB2	20:T:81:MET:HB3	1.69	0.73
17:Q:44:ARG:HH21	17:Q:49:ILE:HD12	1.54	0.72
42:p:56:GLU:OE1	42:p:56:GLU:N	2.23	0.72
1:A:3672:G:OP2	1:A:3672:G:N2	2.22	0.72
1:A:308:G:OP2	1:A:308:G:N2	2.19	0.72
1:A:2362:U:H2'	1:A:2363:A2M:H8	1.70	0.72
25:Y:11:LYS:HA	25:Y:11:LYS:HE3	1.72	0.72
39:m:203:GLU:N	39:m:203:GLU:OE2	2.22	0.72
1:A:4670:C:O2'	1:A:4672:A:OP2	2.07	0.71
1:A:3774:A:H2'	1:A:3775:A:C8	2.25	0.71
1:A:1633:G:O6	1:A:3918:G:O2'	2.09	0.71
16:P:71:GLU:OE2	16:P:71:GLU:N	2.18	0.71
15:O:105:ASN:HB3	15:O:111:GLU:HG2	1.73	0.71
1:A:3641:U:OP2	1:A:3646:A:N6	2.22	0.71
40:n:58:PRO:HD2	40:n:61:ILE:HD12	1.73	0.71
14:N:152:GLU:OE1	14:N:152:GLU:N	2.24	0.70
1:A:1802:A:H5''	1:A:1803:G:H5'	1.73	0.70
11:K:36:ALA:HB1	11:K:45:GLN:HG3	1.72	0.70
19:S:31:SER:HA	19:S:48:PRO:HA	1.72	0.70
8:H:41:LYS:HD3	8:H:42:PRO:HD2	1.72	0.70
1:A:3776:G:OP2	1:A:3776:G:N2	2.18	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:s:40:GLY:HA3	45:s:45:VAL:HB	1.73	0.70
14:N:94:GLU:N	14:N:94:GLU:OE2	2.25	0.70
1:A:3697:U:H5''	1:A:3698:G:H5'	1.72	0.70
9:I:186:GLU:OE2	9:I:186:GLU:N	2.21	0.69
17:Q:57:ARG:NH1	17:Q:57:ARG:HA	2.07	0.69
1:A:67:C:OP2	1:A:312:G:N2	2.26	0.69
12:L:31:GLU:OE1	12:L:31:GLU:N	2.25	0.69
1:A:2407:G:N2	1:A:2407:G:OP2	2.25	0.69
4:D:102:LEU:HB2	4:D:107:MET:HE3	1.74	0.69
10:J:94:MET:HG2	10:J:148:MET:HE1	1.74	0.69
11:K:94:GLU:N	11:K:94:GLU:OE2	2.25	0.69
1:A:3662:A:OP2	4:D:156:LYS:NZ	2.25	0.69
19:S:54:GLU:HB2	19:S:108:ARG:HB2	1.73	0.69
7:G:83:LEU:HB3	7:G:88:VAL:HB	1.74	0.69
12:L:89:MET:HE2	12:L:89:MET:HA	1.73	0.69
1:A:1332:C:H2'	1:A:1333:A:H8	1.58	0.68
3:C:82:A:N1	19:S:50:ARG:NH2	2.41	0.68
1:A:4520:G:N2	5:E:253:CYS:SG	2.66	0.68
22:V:30:GLU:N	22:V:30:GLU:OE2	2.26	0.68
16:P:111:GLU:N	16:P:111:GLU:OE2	2.27	0.68
1:A:4967:A:H2'	1:A:4968:A:H8	1.58	0.68
1:A:3823:G:N2	1:A:3823:G:OP2	2.27	0.67
1:A:1818:G:N2	1:A:1818:G:OP2	2.24	0.67
1:A:1940:G:H22	1:A:4434:C:H5''	1.59	0.67
42:p:80:CYS:HG	42:p:137:HIS:HD1	1.39	0.67
1:A:4527:G:N2	1:A:4527:G:OP2	2.25	0.67
11:K:70:MET:HE2	11:K:80:ALA:HB2	1.76	0.67
1:A:3870:C:H2'	1:A:3871:A:H8	1.60	0.66
14:N:137:GLU:OE2	14:N:137:GLU:N	2.28	0.66
1:A:393:U:O2'	10:J:96:LYS:NZ	2.29	0.66
1:A:375:G:OP2	30:d:52:LYS:NZ	2.29	0.66
34:h:157:GLN:N	34:h:157:GLN:OE1	2.29	0.66
1:A:956:A:H1'	1:A:2076:G:H5''	1.78	0.66
44:r:63:THR:HG22	44:r:65:ARG:H	1.61	0.66
1:A:194:C:O2	19:S:121:ARG:NH2	2.29	0.66
1:A:2745:A:H2'	1:A:2746:A:H8	1.61	0.66
1:A:5053:U:OP1	1:A:5054:C:N4	2.29	0.66
7:G:223:PHE:HB3	7:G:226:TYR:HB2	1.77	0.66
1:A:1364:U:OP2	44:r:36:ARG:NH2	2.29	0.65
1:A:2485:U:H2'	1:A:2486:G:C8	2.30	0.65
1:A:1457:G:O2'	11:K:75:ARG:NH2	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:46:VAL:HG11	23:W:60:ILE:HG21	1.78	0.65
1:A:381:U:H4'	1:A:415:G:H5'	1.78	0.65
1:A:924:C:H3'	1:A:925:C:H5''	1.78	0.65
3:C:71:A:N1	3:C:81:C:O2'	2.28	0.65
36:j:88:GLU:OE2	36:j:88:GLU:N	2.21	0.65
1:A:1573:G:OP1	12:L:92:LYS:NZ	2.29	0.65
1:A:1866:U:OP1	42:p:4:ARG:NH1	2.30	0.65
3:C:110:U:H5'	32:f:8:ARG:HH12	1.60	0.65
39:m:184:ILE:HG23	39:m:189:ASP:HB2	1.78	0.65
1:A:723:A:OP2	1:A:934:C:N4	2.29	0.65
1:A:3809:G:OP2	1:A:3809:G:N2	2.22	0.65
19:S:64:GLY:HA3	19:S:66:GLN:HE22	1.60	0.65
23:W:37:MET:HA	23:W:37:MET:HE3	1.79	0.65
1:A:223:G:N3	6:F:223:ASN:ND2	2.45	0.65
1:A:2557:G:H1	1:A:2570:U:H3	1.43	0.65
34:h:1:MET:HE2	34:h:1:MET:HA	1.79	0.64
1:A:2674:A:O4'	23:W:56:ARG:NH1	2.23	0.64
23:W:47:ILE:HG23	23:W:72:HIS:HD2	1.61	0.64
1:A:2837:OMU:HM22	1:A:2838:G:H5'	1.80	0.64
10:J:133:HIS:O	46:O:468:GLN:NE2	2.31	0.64
34:h:99:GLU:HB2	34:h:125:THR:HG21	1.78	0.64
35:i:74:GLU:HG3	35:i:77:CYS:HB3	1.77	0.64
1:A:2579:G:N2	1:A:2582:A:OP2	2.24	0.64
1:A:3946:G:H1	1:A:4067:U:H3	1.46	0.64
7:G:62:CYS:HB3	7:G:105:LEU:HD22	1.80	0.64
42:p:87:ILE:HG12	42:p:128:ILE:HG12	1.78	0.64
9:I:190:ASP:OD1	9:I:191:LYS:N	2.30	0.64
1:A:505:G:H1	1:A:653:U:H3	1.45	0.64
1:A:4541:G:N2	1:A:4544:A:OP2	2.23	0.64
2:B:92:C:H2'	2:B:93:G:H8	1.61	0.64
14:N:93:ILE:HG22	14:N:96:ILE:HD11	1.80	0.64
1:A:2520:C:H2'	1:A:2521:G:H8	1.63	0.64
1:A:4933:C:H2'	1:A:4934:A:C8	2.33	0.64
1:A:1855:G:O6	1:A:1880:G:N2	2.31	0.64
1:A:2759:G:O2'	1:A:2762:G:N2	2.31	0.64
1:A:3944:OMG:HN1	1:A:4069:U:H3	1.46	0.64
1:A:4566:U:O2'	5:E:234:ARG:NH1	2.29	0.64
1:A:4992:G:H2'	1:A:4993:G:C8	2.32	0.64
34:h:1:MET:HE1	34:h:219:GLU:HG2	1.80	0.64
1:A:1365:C:O2'	44:r:36:ARG:NH2	2.31	0.64
9:I:54:TYR:OH	9:I:73:PHE:O	2.16	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:16:LYS:O	11:K:33:ARG:NH2	2.30	0.64
19:S:37:GLU:OE2	19:S:37:GLU:N	2.21	0.64
1:A:4174:U:H2'	1:A:4175:G:H8	1.63	0.63
1:A:2631:U:OP2	15:O:48:LYS:NZ	2.32	0.63
1:A:4594:U:H2'	1:A:4595:G:H8	1.63	0.63
8:H:132:PRO:HG2	8:H:135:GLN:HG3	1.80	0.63
1:A:4722:G:OP2	1:A:4722:G:N2	2.25	0.63
10:J:138:PRO:HB3	10:J:140:MET:HE3	1.80	0.63
1:A:2411:C:H2'	1:A:2412:A:H8	1.63	0.63
1:A:257:C:H2'	1:A:258:G:H8	1.64	0.63
1:A:2777:G:H5'	1:A:2778:G:H5'	1.80	0.63
3:C:67:U:H2'	3:C:68:G:H8	1.64	0.63
1:A:1703:C:O2'	39:m:43:ARG:NH2	2.32	0.63
1:A:3717:A:H2'	1:A:3718:A2M:H8	1.81	0.63
6:F:146:GLU:N	6:F:146:GLU:OE2	2.32	0.62
1:A:419:A:N3	1:A:1332:C:O2'	2.30	0.62
1:A:4403:PSU:HN3	1:A:4440:G:H1	1.47	0.62
25:Y:24:GLN:HG2	25:Y:27:ARG:HD3	1.80	0.62
1:A:1933:G:H2'	1:A:1934:A:C8	2.35	0.62
1:A:2258:C:O2	8:H:91:THR:N	2.32	0.62
13:M:96:GLU:HG3	13:M:139:ARG:HG2	1.81	0.62
15:O:66:SER:OG	15:O:67:LYS:NZ	2.32	0.62
1:A:20:U:H3'	1:A:21:G:H8	1.63	0.62
1:A:937:U:OP1	45:s:46:ARG:NH1	2.33	0.62
7:G:65:ALA:HB2	7:G:74:ILE:HD13	1.82	0.62
1:A:1601:A:OP1	30:d:5:THR:OG1	2.17	0.62
1:A:1802:A:N3	14:N:130:ARG:NH2	2.45	0.62
20:T:81:MET:HE3	20:T:82:PRO:HD2	1.81	0.62
1:A:2804:OMC:HM22	1:A:2805:C:H5'	1.79	0.62
1:A:4199:C:H42	42:p:106:ARG:HH12	1.46	0.62
12:L:30:ASN:OD1	12:L:31:GLU:N	2.32	0.62
13:M:113:MET:HA	13:M:113:MET:HE2	1.80	0.62
1:A:4694:G:OP1	1:A:4694:G:N2	2.30	0.62
2:B:57:C:H2'	2:B:58:A:H8	1.65	0.62
22:V:32:LEU:HD23	22:V:40:LEU:HD11	1.82	0.62
1:A:3688:U:H2'	1:A:3689:G:H8	1.65	0.62
4:D:6:ARG:HH12	4:D:199:VAL:H	1.48	0.62
1:A:1930:U:OP2	9:I:49:ARG:NH1	2.27	0.62
1:A:3669:G:N2	1:A:3672:G:OP2	2.33	0.62
38:l:158:HIS:HB3	38:l:161:MET:HG3	1.80	0.62
45:s:33:GLN:OE1	45:s:33:GLN:N	2.22	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2495:U:H2'	1:A:2496:G:H8	1.65	0.61
4:D:30:ARG:HG2	4:D:74:GLU:HG3	1.81	0.61
39:m:60:GLU:OE1	39:m:60:GLU:N	2.34	0.61
1:A:5063:G:H2'	1:A:5064:G:H8	1.65	0.61
35:i:59:LYS:NZ	35:i:61:LYS:O	2.33	0.61
1:A:255:C:H2'	1:A:256:G:C8	2.36	0.61
41:o:107:GLU:OE2	41:o:111:LEU:HB3	1.99	0.61
1:A:62:A:N3	1:A:77:U:O2'	2.27	0.61
31:e:19:ASP:HB2	31:e:39:SER:HB3	1.82	0.61
1:A:4286:C:H2'	1:A:4287:G:H8	1.66	0.61
1:A:4537:C:H2'	1:A:4538:G:H8	1.66	0.61
1:A:327:U:O2'	29:c:30:ARG:NH1	2.34	0.61
19:S:67:ILE:O	19:S:84:ARG:NH2	2.33	0.61
43:q:35:ARG:HD2	43:q:123:ILE:HA	1.83	0.61
1:A:2705:G:O6	12:L:46:LYS:NZ	2.30	0.61
1:A:3848:U:H2'	1:A:3849:A:H8	1.65	0.61
1:A:4277:G:H5'	14:N:17:ARG:HG2	1.83	0.61
1:A:4954:G:H2'	1:A:4955:A:C8	2.36	0.61
15:O:43:LEU:O	15:O:47:ILE:HD12	2.00	0.61
20:T:10:VAL:O	20:T:83:THR:OG1	2.18	0.61
30:d:22:CYS:SG	30:d:24:SER:OG	2.58	0.61
1:A:153:G:H2'	1:A:154:G:H8	1.65	0.60
17:Q:4:GLU:O	17:Q:13:ILE:N	2.26	0.60
34:h:21:ASN:ND2	34:h:112:ASP:OD2	2.34	0.60
1:A:2706:G:O6	12:L:46:LYS:NZ	2.34	0.60
20:T:5:MET:HG3	20:T:77:TYR:CE1	2.36	0.60
26:Z:35:ALA:HB3	26:Z:38:GLU:HG3	1.83	0.60
1:A:1332:C:H2'	1:A:1333:A:C8	2.36	0.60
1:A:1707:C:OP2	22:V:103:LYS:NZ	2.33	0.60
1:A:2485:U:H2'	1:A:2486:G:H8	1.66	0.60
1:A:2758:G:O2'	1:A:2765:A:N3	2.31	0.60
3:C:141:C:OP1	38:l:38:ARG:NH1	2.35	0.60
25:Y:78:LEU:HD23	25:Y:98:GLU:HB3	1.82	0.60
1:A:943:A:H5'	1:A:945:U:H5'	1.82	0.60
1:A:4358:U:H4'	44:r:197:LYS:HD2	1.84	0.60
2:B:110:G:H2'	2:B:111:C:C6	2.36	0.60
9:I:81:TRP:HB2	9:I:104:VAL:HG21	1.83	0.60
1:A:757:G:O3'	41:o:52:LYS:NZ	2.34	0.60
1:A:1779:U:H2'	1:A:1780:A:C8	2.36	0.60
34:h:18:LYS:HB3	34:h:25:LEU:HB2	1.82	0.60
1:A:4967:A:H2'	1:A:4968:A:C8	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:752:G:H1	1:A:911:U:H3	1.50	0.60
1:A:4076:G:OP1	40:n:73:ARG:NE	2.35	0.60
1:A:1335:G:H21	6:F:95:MET:HB2	1.67	0.60
1:A:2770:C:H2'	1:A:2771:G:H8	1.66	0.60
1:A:4729:A:H5''	1:A:4965:U:H1'	1.83	0.60
3:C:30:U:H2'	3:C:31:G:C8	2.37	0.60
1:A:74:G:H5'	44:r:59:VAL:HB	1.83	0.60
15:O:61:VAL:HG22	15:O:74:SER:HB2	1.83	0.60
1:A:1613:A:H5'	4:D:183:GLY:HA2	1.82	0.59
1:A:2601:A:N6	1:A:2744:A:OP2	2.32	0.59
1:A:4319:C:H2'	1:A:4320:G:H8	1.65	0.59
1:A:1940:G:N2	1:A:4434:C:OP1	2.35	0.59
1:A:2318:G:N2	1:A:2321:G:OP2	2.24	0.59
34:h:118:HIS:CE1	34:h:146:VAL:HB	2.38	0.59
1:A:2495:U:H2'	1:A:2496:G:C8	2.37	0.59
2:B:119:U:H2'	7:G:261:VAL:HG11	1.84	0.59
1:A:239:C:OP1	19:S:46:SER:OG	2.20	0.59
1:A:2431:A:OP1	32:f:41:ARG:NH1	2.21	0.59
1:A:4314:C:H2'	1:A:4315:A:H8	1.67	0.59
6:F:116:ASN:HB2	6:F:119:GLN:HG3	1.84	0.59
9:I:125:LYS:HG3	9:I:129:LEU:HD12	1.83	0.59
41:o:51:LYS:H	41:o:51:LYS:HD3	1.67	0.59
1:A:440:U:H2'	1:A:441:G:H8	1.67	0.59
15:O:83:LEU:O	15:O:87:THR:OG1	2.20	0.59
1:A:417:G:OP1	1:A:2329:U:O2'	2.20	0.59
1:A:982:U:O2	8:H:70:LYS:NZ	2.32	0.59
1:A:1541:C:H5''	4:D:21:LYS:HG2	1.85	0.59
1:A:2300:A:N7	6:F:143:ARG:NH1	2.51	0.59
1:A:3880:G:H2'	1:A:3881:G:C8	2.37	0.59
4:D:116:LEU:HB3	4:D:126:LEU:HB2	1.85	0.59
12:L:99:MET:HE1	12:L:128:LYS:HA	1.85	0.59
1:A:1517:G:H22	6:F:103:ALA:HA	1.67	0.59
1:A:3718:A2M:HM'2	1:A:3719:A:H5'	1.84	0.59
1:A:4246:G:H2'	1:A:4247:G:H8	1.68	0.59
1:A:4935:C:H2'	1:A:4936:G:C8	2.38	0.59
1:A:1864:G:H21	42:p:105:MET:HE2	1.68	0.59
1:A:2735:G:H2'	1:A:2736:G:H8	1.66	0.59
1:A:3873:G:H2'	1:A:3874:G:C8	2.38	0.59
14:N:133:ALA:HB3	39:m:127:LYS:HB2	1.84	0.59
41:o:137:SER:HB3	41:o:143:GLU:HB3	1.83	0.59
1:A:3689:G:O2'	1:A:3818:UY1:OP2	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:65:GLU:HG3	6:F:80:ARG:HD3	1.84	0.59
42:p:136:GLU:N	42:p:136:GLU:OE2	2.34	0.59
1:A:164:G:H2'	1:A:165:A:H8	1.68	0.58
1:A:309:C:OP2	29:c:32:ARG:NH1	2.36	0.58
1:A:1268:G:N7	22:V:111:ARG:NH2	2.48	0.58
28:b:15:GLU:OE2	28:b:15:GLU:N	2.22	0.58
42:p:45:GLU:OE2	42:p:45:GLU:N	2.33	0.58
1:A:1093:C:H2'	1:A:1094:G:H8	1.67	0.58
1:A:1399:G:H2'	1:A:1400:G:H8	1.67	0.58
1:A:4353:PSU:H5'	1:A:4354:U:H5'	1.84	0.58
1:A:4763:U:O2'	13:M:174:THR:OG1	2.18	0.58
23:W:20:LEU:HD21	23:W:102:SER:HB2	1.85	0.58
28:b:13:LYS:NZ	28:b:16:GLU:OE1	2.35	0.58
31:e:51:GLU:OE1	31:e:51:GLU:N	2.25	0.58
35:i:34:TYR:O	35:i:39:ARG:NH1	2.36	0.58
1:A:364:G:O6	30:d:55:ARG:NH2	2.35	0.58
19:S:1:MET:HE3	19:S:2:LYS:N	2.18	0.58
1:A:1100:U:H3	1:A:1195:G:H1	1.52	0.58
1:A:1645:C:H2'	1:A:1646:A:C8	2.38	0.58
10:J:22:LEU:HD12	10:J:146:ILE:HD12	1.84	0.58
29:c:79:THR:HG22	29:c:82:ARG:H	1.68	0.58
42:p:172:GLU:OE1	42:p:172:GLU:N	2.25	0.58
1:A:3792:OMG:HM22	1:A:3793:U:H5'	1.83	0.58
8:H:199:THR:HG21	45:s:107:PHE:HB2	1.85	0.58
22:V:58:GLN:OE1	22:V:58:GLN:N	2.36	0.58
34:h:21:ASN:HB2	34:h:67:ARG:HB3	1.86	0.58
1:A:169:G:N2	1:A:169:G:OP2	2.36	0.58
1:A:369:G:N2	1:A:372:A:OP2	2.25	0.58
20:T:83:THR:HG22	27:a:95:PHE:CZ	2.38	0.58
1:A:1725:U:H2'	1:A:1726:U:H6	1.69	0.58
1:A:4472:G:O2'	33:g:100:TYR:O	2.22	0.58
16:P:62:MET:HE2	16:P:76:VAL:HG12	1.86	0.58
5:E:92:TYR:HB2	5:E:159:VAL:HB	1.85	0.58
9:I:10:ASP:OD2	9:I:37:ARG:NH2	2.37	0.58
11:K:93:GLN:OE1	11:K:93:GLN:N	2.34	0.58
42:p:133:GLN:OE1	42:p:133:GLN:N	2.22	0.58
42:p:195:PRO:HD2	42:p:198:LYS:HE2	1.85	0.58
41:o:47:LEU:HB3	41:o:53:LYS:HE3	1.86	0.58
1:A:651:C:H2'	1:A:652:G:H8	1.68	0.57
1:A:1316:OMG:HM22	1:A:1317:U:H5'	1.86	0.57
1:A:1872:G:O2'	1:A:4219:A:N3	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2723:U:H2'	1:A:2724:G:C8	2.38	0.57
1:A:4456:OMC:HM22	1:A:4457:PSU:H5''	1.85	0.57
6:F:71:ARG:NH2	46:O:465:ALA:O	2.36	0.57
23:W:102:SER:OG	23:W:103:ASP:N	2.34	0.57
1:A:3893:C:H2'	1:A:3894:A:H8	1.69	0.57
1:A:4535:A:H2'	1:A:4536:OMC:H6	1.69	0.57
9:I:39:GLU:OE2	9:I:39:GLU:N	2.22	0.57
1:A:4274:A:H2'	1:A:4275:G:H8	1.69	0.57
36:j:38:THR:HA	36:j:45:THR:HA	1.87	0.57
1:A:3785:A2M:HM'1	1:A:4537:C:H1'	1.85	0.57
31:e:58:GLN:OE1	31:e:58:GLN:N	2.32	0.57
36:j:3:LYS:NZ	36:j:5:THR:O	2.37	0.57
1:A:32:G:OP1	38:l:73:ARG:NH1	2.37	0.57
1:A:93:G:H2'	1:A:94:A:C8	2.40	0.57
1:A:2764:A:H2'	1:A:2765:A:H8	1.69	0.57
1:A:4184:G:H5'	4:D:233:ARG:HB2	1.85	0.57
1:A:4537:C:H2'	1:A:4538:G:C8	2.40	0.57
43:q:144:LYS:O	43:q:148:THR:OG1	2.22	0.57
1:A:713:C:O2	8:H:130:LYS:NZ	2.37	0.57
1:A:1074:G:H2'	1:A:1075:G:H8	1.70	0.57
6:F:328:LEU:HD13	39:m:187:MET:HE2	1.86	0.57
19:S:56:GLN:HB3	19:S:105:VAL:HG12	1.87	0.57
35:i:69:ARG:HH12	35:i:80:LYS:HD3	1.69	0.57
1:A:1399:G:H2'	1:A:1400:G:C8	2.39	0.57
1:A:2486:G:H2'	1:A:2487:G:C8	2.39	0.57
2:B:39:C:H4'	43:q:47:THR:HG23	1.86	0.57
31:e:16:ARG:HE	31:e:61:PRO:HG3	1.70	0.57
1:A:3659:G:OP1	4:D:241:ARG:NH1	2.37	0.57
6:F:56:GLU:OE1	6:F:56:GLU:N	2.21	0.57
11:K:157:GLY:O	11:K:188:ASN:ND2	2.37	0.57
11:K:178:ARG:H	21:U:51:GLY:HA2	1.69	0.57
1:A:2083:C:OP2	11:K:14:ARG:NH2	2.36	0.57
1:A:4286:C:H2'	1:A:4287:G:C8	2.40	0.57
1:A:4960:G:H2'	1:A:4961:G:H8	1.70	0.57
4:D:180:LEU:HD11	36:j:26:VAL:HG11	1.87	0.56
1:A:4934:A:H2'	1:A:4935:C:C6	2.40	0.56
3:C:39:G:OP1	28:b:86:LYS:NZ	2.38	0.56
10:J:16:LYS:HG2	10:J:149:ILE:HG12	1.86	0.56
35:i:71:GLU:OE2	35:i:78:ARG:NH2	2.39	0.56
42:p:42:LYS:N	42:p:45:GLU:OE1	2.38	0.56
1:A:1188:C:H2'	1:A:1189:G:H8	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1604:G:H2'	1:A:1605:G:C8	2.40	0.56
1:A:3653:A:H4'	4:D:179:ILE:HB	1.87	0.56
1:A:3732:A:H2'	1:A:3733:A:H8	1.70	0.56
6:F:212:ASN:HD22	6:F:255:SER:HB3	1.70	0.56
9:I:113:ASP:OD1	9:I:113:ASP:N	2.38	0.56
1:A:951:G:H2'	1:A:952:G:H8	1.70	0.56
1:A:1890:G:OP2	1:A:1890:G:N2	2.32	0.56
1:A:2303:C:H5''	25:Y:104:SER:HB3	1.87	0.56
1:A:4725:C:H2'	1:A:4726:G:H8	1.71	0.56
20:T:99:ASP:HA	20:T:102:ARG:NH2	2.21	0.56
7:G:200:MET:HA	7:G:200:MET:HE3	1.88	0.56
1:A:257:C:H2'	1:A:258:G:C8	2.41	0.56
1:A:3620:G:OP1	1:A:3622:C:N4	2.38	0.56
23:W:36:LYS:NZ	23:W:36:LYS:HB3	2.20	0.56
33:g:80:PRO:HA	33:g:83:ARG:HB3	1.88	0.56
1:A:1333:A:H2'	1:A:1334:A:H8	1.68	0.56
1:A:1468:C:OP1	21:U:132:ARG:NH2	2.34	0.56
14:N:159:MET:HA	14:N:159:MET:HE3	1.87	0.56
1:A:64:A:N1	1:A:108:A:O2'	2.34	0.56
1:A:651:C:H2'	1:A:652:G:C8	2.41	0.56
1:A:1695:U:H2'	1:A:1696:C:C6	2.41	0.56
1:A:4153:C:H2'	1:A:4154:G:C8	2.41	0.56
1:A:4598:C:H2'	1:A:4611:A:H61	1.71	0.56
27:a:41:ALA:O	27:a:52:ARG:NH1	2.34	0.56
38:l:146:PRO:HA	38:l:149:GLN:HG3	1.87	0.56
1:A:949:G:H2'	1:A:950:G:H8	1.71	0.56
1:A:2643:G:H2'	1:A:2644:G:H8	1.69	0.56
1:A:4145:C:H2'	1:A:4146:G:H8	1.70	0.56
1:A:4153:C:H2'	1:A:4154:G:H8	1.69	0.56
1:A:4471:PSU:H2'	1:A:4472:G:H8	1.71	0.56
1:A:4473:A:O2'	33:g:122:ARG:NH2	2.39	0.56
7:G:211:LEU:HB3	7:G:219:TYR:HB2	1.88	0.56
42:p:36:LEU:HD13	42:p:69:ARG:HH11	1.71	0.56
1:A:3661:G:H4'	1:A:3662:A:H5'	1.87	0.56
1:A:4274:A:H2'	1:A:4275:G:C8	2.41	0.56
16:P:43:LYS:HG3	16:P:60:MET:HG2	1.86	0.56
20:T:5:MET:HE1	20:T:82:PRO:HB3	1.88	0.55
34:h:22:THR:HG23	34:h:23:TYR:HD1	1.69	0.55
1:A:436:C:H2'	1:A:437:G:H8	1.70	0.55
1:A:1696:C:O2'	1:A:1719:A:N6	2.39	0.55
1:A:1876:U:H2'	1:A:1877:G:C8	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2764:A:H2'	1:A:2765:A:C8	2.41	0.55
1:A:3861:A:H2'	1:A:3862:A:H8	1.71	0.55
8:H:191:GLN:OE1	8:H:191:GLN:N	2.22	0.55
34:h:107:VAL:HG23	34:h:108:THR:HG23	1.88	0.55
1:A:2651:C:O2'	1:A:2653:C:OP1	2.21	0.55
1:A:3607:U:H2'	1:A:3608:A:H8	1.70	0.55
1:A:3887:OMC:HM22	1:A:3888:G:H5'	1.87	0.55
42:p:197:ASP:OD2	42:p:198:LYS:N	2.39	0.55
1:A:65:A:N6	1:A:75:G:H1'	2.22	0.55
1:A:3732:A:H2'	1:A:3733:A:C8	2.41	0.55
1:A:3786:U:OP1	1:A:4550:G:O2'	2.18	0.55
27:a:93:ARG:O	27:a:97:ILE:HG13	2.07	0.55
1:A:461:G:H2'	1:A:462:G:H8	1.71	0.55
1:A:2101:C:H2'	1:A:2102:G:C8	2.42	0.55
1:A:2525:U:OP1	12:L:42:ARG:NH2	2.37	0.55
1:A:4146:G:H2'	1:A:4147:G:H8	1.71	0.55
12:L:148:ASP:OD1	12:L:148:ASP:N	2.38	0.55
25:Y:66:THR:HA	25:Y:69:MET:HE2	1.88	0.55
1:A:1681:G:H2'	1:A:1682:A:H8	1.71	0.55
1:A:2413:U:H2'	1:A:2414:G:H8	1.71	0.55
1:A:4196:OMG:HM22	1:A:4197:G:H5'	1.88	0.55
1:A:4618:OMG:H5''	16:P:15:ARG:HB2	1.87	0.55
1:A:4991:U:H2'	1:A:4992:G:C8	2.41	0.55
1:A:4991:U:H2'	1:A:4992:G:H8	1.72	0.55
1:A:5057:C:H2'	1:A:5058:A:C8	2.41	0.55
22:V:49:HIS:HB3	22:V:52:LYS:HE2	1.88	0.55
1:A:1656:U:OP2	21:U:26:ARG:NH2	2.29	0.55
1:A:2539:C:H2'	1:A:2540:C:C6	2.41	0.55
1:A:3771:C:H2'	1:A:3772:U:C6	2.42	0.55
1:A:3911:C:H2'	1:A:3912:U:H6	1.71	0.55
3:C:57:C:OP2	30:d:68:LYS:NZ	2.39	0.55
40:n:165:GLU:OE2	40:n:165:GLU:N	2.37	0.55
1:A:1326:A2M:OP2	1:A:4445:U:O2'	2.23	0.55
1:A:2414:G:H2'	1:A:2415:OMU:H6	1.88	0.55
1:A:4474:A:OP2	1:A:4476:C:N4	2.39	0.55
1:A:85:G:N2	1:A:98:A:OP2	2.37	0.55
1:A:299:C:H2'	1:A:300:A:H8	1.72	0.55
1:A:2045:G:O6	1:A:3870:C:O2'	2.25	0.55
1:A:3598:C:H2'	1:A:3599:A:C8	2.42	0.55
1:A:4134:C:H2'	1:A:4135:G:H8	1.72	0.55
1:A:4761:G:H2'	1:A:4762:A:H8	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:m:171:ASP:OD2	39:m:172:ASN:N	2.39	0.55
41:o:93:ARG:HD2	41:o:143:GLU:OE2	2.06	0.55
1:A:718:C:OP1	39:m:217:ARG:NH1	2.40	0.55
1:A:1315:C:H2'	1:A:1316:OMG:H8	1.71	0.55
1:A:4088:C:H2'	1:A:4089:G:H8	1.71	0.55
1:A:64:A:H1'	1:A:76:A:H1'	1.88	0.54
1:A:171:U:H5''	44:r:135:LYS:HE2	1.88	0.54
1:A:653:U:H2'	1:A:654:C:C6	2.42	0.54
1:A:1645:C:H2'	1:A:1646:A:H8	1.71	0.54
1:A:1750:G:H22	1:A:1780:A:H2	1.55	0.54
1:A:1847:C:H2'	1:A:1848:C:C6	2.42	0.54
1:A:2520:C:H2'	1:A:2521:G:C8	2.42	0.54
3:C:75:OMG:OP2	19:S:74:TYR:OH	2.24	0.54
4:D:5:ILE:HG12	4:D:8:GLN:HG3	1.88	0.54
1:A:90:G:OP2	1:A:92:C:N4	2.39	0.54
1:A:255:C:H2'	1:A:256:G:H8	1.70	0.54
1:A:1743:A:N1	1:A:1789:C:O2'	2.38	0.54
1:A:1906:U:H2'	1:A:1907:A:H8	1.71	0.54
1:A:2459:G:N2	1:A:2462:C:OP2	2.39	0.54
1:A:3607:U:H2'	1:A:3608:A:C8	2.42	0.54
1:A:3698:G:OP2	4:D:247:ARG:NH1	2.41	0.54
4:D:80:GLU:HB2	4:D:170:ALA:HA	1.89	0.54
20:T:33:THR:HG23	20:T:40:HIS:HE1	1.72	0.54
20:T:64:LYS:HA	20:T:67:LYS:HE3	1.88	0.54
1:A:2485:U:H3	1:A:2493:G:H1	1.56	0.54
1:A:4622:A:H4'	5:E:13:SER:HB2	1.87	0.54
2:B:87:G:N2	2:B:90:A:OP2	2.35	0.54
31:e:68:GLU:N	31:e:68:GLU:OE2	2.40	0.54
1:A:7:C:H2'	1:A:8:U:C6	2.43	0.54
1:A:662:C:H2'	1:A:663:G:H8	1.72	0.54
1:A:4272:G:OP2	1:A:4272:G:N2	2.24	0.54
1:A:4448:G:H5''	1:A:4449:A:H5''	1.88	0.54
1:A:4734:A:H2'	1:A:4735:G:C8	2.42	0.54
19:S:54:GLU:N	19:S:54:GLU:OE2	2.40	0.54
34:h:163:PRO:HA	34:h:183:ALA:HB1	1.90	0.54
40:n:103:ARG:NH2	40:n:192:ARG:O	2.40	0.54
1:A:418:A:C2	3:C:17:A:H1'	2.43	0.54
1:A:2477:A:O2'	1:A:2479:G:OP1	2.24	0.54
7:G:41:LYS:NZ	14:N:32:ARG:O	2.34	0.54
18:R:120:ASP:OD2	18:R:121:VAL:N	2.40	0.54
31:e:9:LYS:HA	31:e:12:LEU:HD23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:n:210:GLU:OE2	40:n:210:GLU:N	2.33	0.54
41:o:183:GLU:OE2	41:o:185:GLY:N	2.41	0.54
1:A:1199:G:N3	14:N:144:ASN:ND2	2.55	0.54
5:E:356:LYS:HD3	5:E:358:ARG:H	1.71	0.54
18:R:64:SER:HB2	28:b:69:LEU:HD13	1.89	0.54
19:S:28:LYS:O	19:S:31:SER:OG	2.25	0.54
24:X:18:ASN:OD1	24:X:20:VAL:N	2.37	0.54
1:A:1290:G:H5'	8:H:219:LYS:HD2	1.90	0.54
1:A:1876:U:H2'	1:A:1877:G:H8	1.73	0.54
1:A:4084:G:O6	4:D:72:ARG:NH2	2.41	0.54
1:A:4265:U:N3	7:G:17:GLN:O	2.38	0.54
8:H:117:PRO:O	37:k:112:ARG:NH1	2.37	0.54
21:U:134:GLU:OE1	44:r:178:ALA:N	2.38	0.54
1:A:161:G:H2'	1:A:162:A:H8	1.72	0.54
1:A:4299:PSU:P	11:K:160:HIS:HE1	2.31	0.54
1:A:4389:C:H2'	1:A:4390:A:C8	2.43	0.54
3:C:30:U:H2'	3:C:31:G:H8	1.72	0.54
7:G:193:GLU:OE2	7:G:197:LYS:NZ	2.40	0.54
14:N:42:ILE:HD11	14:N:74:ILE:HG21	1.90	0.54
18:R:148:ASP:OD1	18:R:149:VAL:N	2.41	0.54
20:T:136:PHE:OXT	27:a:90:ARG:NH2	2.41	0.54
39:m:148:LYS:HE3	39:m:245:ARG:HH21	1.73	0.54
1:A:36:U:OP1	1:A:1651:G:N2	2.41	0.54
1:A:1097:C:H2'	1:A:1098:G:H8	1.72	0.54
1:A:1699:A:O2'	6:F:306:ARG:NH2	2.41	0.54
1:A:4458:C:H2'	1:A:4459:U:C6	2.43	0.54
27:a:94:ALA:O	27:a:98:GLU:HG2	2.07	0.54
32:f:42:ARG:HG3	32:f:47:THR:HG23	1.90	0.54
33:g:125:LYS:O	41:o:173:ARG:NH1	2.40	0.54
40:n:178:GLY:O	40:n:223:ARG:NH2	2.41	0.54
1:A:2411:C:H2'	1:A:2412:A:C8	2.42	0.54
1:A:2699:C:H2'	1:A:2700:G:H8	1.72	0.54
23:W:102:SER:OG	23:W:104:ILE:HG12	2.08	0.54
36:j:84:ARG:NH1	36:j:84:ARG:O	2.40	0.54
1:A:3748:A:O2'	4:D:223:SER:OG	2.16	0.53
1:A:4642:U:H2'	1:A:4643:G:H8	1.73	0.53
10:J:30:ARG:HD2	10:J:63:TYR:HE1	1.73	0.53
25:Y:78:LEU:O	37:k:20:ARG:NH1	2.40	0.53
1:A:300:A:H2'	1:A:301:G:H8	1.73	0.53
1:A:462:G:H2'	1:A:463:A:C8	2.42	0.53
1:A:4145:C:H2'	1:A:4146:G:C8	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:h:126:GLU:HG3	34:h:137:VAL:HG11	1.90	0.53
1:A:909:A:H2'	1:A:910:G:H8	1.72	0.53
1:A:4993:G:H1	1:A:5058:A:H2	1.54	0.53
6:F:337:ARG:NH1	8:H:55:GLY:O	2.41	0.53
23:W:13:SER:O	23:W:17:ARG:HG2	2.08	0.53
1:A:65:A:H61	1:A:75:G:H1'	1.74	0.53
1:A:2815:A2M:HM'2	1:A:2816:G:H5'	1.90	0.53
1:A:2897:G:H2'	1:A:2898:G:C8	2.44	0.53
1:A:4336:A:H5''	1:A:4337:C:H5'	1.90	0.53
1:A:4871:C:N4	13:M:171:ARG:O	2.41	0.53
3:C:8:U:H2'	3:C:9:A:C8	2.44	0.53
14:N:136:ARG:N	39:m:86:GLU:OE2	2.40	0.53
16:P:16:ILE:HD11	16:P:56:GLY:HA3	1.91	0.53
1:A:4303:C:H3'	1:A:4305:G:H21	1.73	0.53
4:D:112:ILE:H	36:j:83:ILE:HD11	1.73	0.53
6:F:230:LEU:HD11	6:F:239:LYS:HB2	1.91	0.53
20:T:89:ILE:HG21	20:T:117:LYS:HB3	1.91	0.53
1:A:1245:C:H2'	1:A:1246:G:H8	1.74	0.53
1:A:1333:A:H2'	1:A:1334:A:C8	2.43	0.53
1:A:2363:A2M:HM'2	1:A:2364:OMG:H5'	1.90	0.53
10:J:40:HIS:NE2	10:J:110:ASP:O	2.38	0.53
31:e:7:GLU:OE1	31:e:9:LYS:N	2.40	0.53
39:m:87:PRO:HG2	39:m:144:TYR:CG	2.44	0.53
1:A:1433:A:H3'	1:A:1434:G:H8	1.74	0.53
1:A:1440:U:H2'	1:A:1441:C:H6	1.72	0.53
1:A:1942:A:H2'	1:A:1943:A:C8	2.43	0.53
1:A:3848:U:H2'	1:A:3849:A:C8	2.43	0.53
1:A:3937:C:H1'	38:l:125:SER:HB3	1.91	0.53
6:F:108:TRP:O	38:l:204:ARG:NH2	2.41	0.53
20:T:94:THR:O	20:T:97:ASN:ND2	2.42	0.53
40:n:228:ASP:OD1	40:n:228:ASP:N	2.35	0.53
42:p:177:GLU:OE2	42:p:179:ARG:HG3	2.08	0.53
1:A:32:G:O2'	1:A:50:C:N4	2.42	0.53
1:A:2756:G:H2'	1:A:2757:A:C8	2.44	0.53
1:A:2884:G:H2'	1:A:2885:A:H8	1.73	0.53
3:C:82:A:H5''	3:C:86:U:H4'	1.91	0.53
4:D:140:ASN:ND2	4:D:143:THR:OG1	2.41	0.53
15:O:42:PHE:O	15:O:46:ARG:HG2	2.09	0.53
45:s:71:LYS:O	45:s:75:GLN:HG2	2.09	0.53
1:A:679:C:H2'	1:A:680:G:C8	2.44	0.53
1:A:1241:C:H1'	22:V:119:CYS:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:A:H4'	43:q:155:HIS:HB2	1.91	0.53
9:I:177:LEU:O	9:I:181:ALA:N	2.42	0.53
21:U:69:PHE:CG	44:r:65:ARG:HD3	2.44	0.53
44:r:49:ARG:O	44:r:149:GLN:NE2	2.42	0.53
1:A:10:A:H2'	1:A:11:G:H8	1.74	0.53
13:M:9:GLU:HB3	13:M:67:VAL:HB	1.91	0.53
21:U:71:PRO:HG2	21:U:108:TYR:HA	1.91	0.53
25:Y:99:ILE:HG21	25:Y:108:ARG:HG2	1.90	0.53
31:e:12:LEU:O	31:e:16:ARG:HG2	2.09	0.53
34:h:162:HIS:CE1	34:h:164:LYS:HG2	2.44	0.53
1:A:150:U:OP2	40:n:200:THR:OG1	2.23	0.52
1:A:963:G:H2'	1:A:964:A:O4'	2.09	0.52
44:r:138:ASP:OD2	44:r:139:SER:N	2.42	0.52
1:A:256:G:H2'	1:A:257:C:H6	1.73	0.52
1:A:440:U:H2'	1:A:441:G:C8	2.44	0.52
3:C:67:U:H2'	3:C:68:G:C8	2.44	0.52
13:M:76:LYS:HB3	13:M:131:GLU:HG2	1.92	0.52
17:Q:47:ARG:HH12	17:Q:54:LEU:HD13	1.74	0.52
24:X:64:ILE:HG23	24:X:68:LEU:HD23	1.91	0.52
25:Y:8:VAL:HG23	25:Y:10:PRO:HD3	1.89	0.52
1:A:265:C:O2'	28:b:112:ARG:NH2	2.32	0.52
1:A:1248:C:H2'	1:A:1249:C:H6	1.74	0.52
1:A:2351:OMC:HM22	1:A:2352:U:H5'	1.90	0.52
1:A:2897:G:H2'	1:A:2898:G:H8	1.74	0.52
1:A:3606:U:H2'	1:A:3607:U:H6	1.73	0.52
1:A:4088:C:H2'	1:A:4089:G:C8	2.44	0.52
17:Q:58:LYS:HG2	17:Q:59:HIS:HD2	1.73	0.52
25:Y:86:GLU:CD	25:Y:86:GLU:H	2.16	0.52
34:h:133:LEU:C	34:h:134:LYS:HD3	2.34	0.52
39:m:108:VAL:HG13	39:m:132:MET:HE3	1.91	0.52
1:A:1645:C:OP1	6:F:80:ARG:NH2	2.42	0.52
1:A:2498:C:H2'	1:A:2499:C:C6	2.45	0.52
1:A:2517:A:O2'	27:a:66:ARG:NH1	2.42	0.52
1:A:3599:A:H2'	1:A:3600:G:C8	2.43	0.52
1:A:3606:U:H2'	1:A:3607:U:C6	2.45	0.52
30:d:57:ASN:OD1	30:d:57:ASN:O	2.27	0.52
38:l:42:PRO:HG3	38:l:61:ILE:HG13	1.92	0.52
1:A:2765:A:H2'	1:A:2766:A:C8	2.45	0.52
1:A:4988:U:OP1	5:E:123:HIS:ND1	2.36	0.52
1:A:4321:U:H2'	1:A:4322:G:C8	2.45	0.52
1:A:4392:OMG:HM21	1:A:4394:A:H2'	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:j:46:LYS:HD3	36:j:59:SER:HB3	1.91	0.52
1:A:133:C:H41	28:b:74:LYS:HG3	1.75	0.52
1:A:1730:U:H2'	1:A:1731:C:H6	1.74	0.52
1:A:2483:G:H2'	1:A:2484:A:C8	2.44	0.52
1:A:2643:G:H2'	1:A:2644:G:C8	2.45	0.52
1:A:164:G:H2'	1:A:165:A:C8	2.45	0.52
1:A:1824:G:H2'	1:A:1825:A:C8	2.45	0.52
1:A:2568:C:H2'	1:A:2569:G:H8	1.75	0.52
1:A:3893:C:H2'	1:A:3894:A:C8	2.45	0.52
1:A:4227:OMU:HM21	1:A:4336:A:H1'	1.92	0.52
17:Q:48:GLN:OE1	17:Q:48:GLN:N	2.42	0.52
1:A:4146:G:H2'	1:A:4147:G:C8	2.45	0.52
1:A:4723:A:H2'	1:A:4724:A:H8	1.74	0.52
1:A:4725:C:H2'	1:A:4726:G:C8	2.45	0.52
13:M:130:GLU:N	13:M:130:GLU:OE1	2.43	0.52
20:T:91:LEU:HD12	20:T:96:VAL:HG21	1.92	0.52
23:W:47:ILE:HG23	23:W:72:HIS:CD2	2.42	0.52
27:a:15:THR:HG22	27:a:16:ALA:H	1.75	0.52
34:h:1:MET:SD	34:h:2:ALA:N	2.82	0.52
1:A:422:C:H2'	1:A:423:G:H8	1.74	0.52
1:A:1298:C:H2'	1:A:1299:G:C8	2.45	0.52
4:D:3:ARG:HG2	4:D:207:VAL:HG22	1.90	0.52
6:F:35:ASP:OD1	6:F:35:ASP:N	2.43	0.52
24:X:19:GLU:H	24:X:19:GLU:CD	2.18	0.52
28:b:8:ASP:OD2	28:b:8:ASP:N	2.35	0.52
38:l:32:GLN:HB2	40:n:63:LEU:HD12	1.92	0.52
1:A:34:A:O2'	1:A:1526:G:N3	2.43	0.51
1:A:441:G:H2'	1:A:442:G:H8	1.75	0.51
1:A:1097:C:H2'	1:A:1098:G:C8	2.44	0.51
1:A:1178:G:O2'	7:G:286:SER:OG	2.28	0.51
1:A:2089:G:OP2	6:F:294:LYS:NZ	2.39	0.51
1:A:2295:C:H2'	1:A:2296:G:H8	1.74	0.51
1:A:2357:G:H2'	1:A:2358:G:C8	2.45	0.51
1:A:2570:U:H2'	1:A:2571:C:C6	2.45	0.51
1:A:4619:U:H2'	1:A:4620:OMU:H6	1.92	0.51
1:A:5002:U:OP2	5:E:385:LYS:NZ	2.40	0.51
1:A:5030:U:H2'	1:A:5031:G:H8	1.75	0.51
2:B:26:C:O2'	43:q:147:ARG:NH1	2.43	0.51
19:S:2:LYS:NZ	19:S:7:VAL:O	2.34	0.51
1:A:727:C:OP1	39:m:73:ARG:NH2	2.38	0.51
1:A:1270:A:H1'	1:A:1440:U:H1'	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1779:U:H2'	1:A:1780:A:H8	1.74	0.51
1:A:1879:C:H2'	1:A:1880:G:O4'	2.10	0.51
1:A:2588:C:OP1	1:A:2768:C:O2'	2.21	0.51
1:A:3855:C:H2'	1:A:3856:A:H8	1.76	0.51
1:A:4503:A:H2'	1:A:4504:C:C6	2.45	0.51
1:A:4638:U:H3'	1:A:4639:G:H21	1.75	0.51
22:V:58:GLN:O	22:V:62:ALA:N	2.38	0.51
1:A:156:G:OP2	28:b:106:LYS:NZ	2.38	0.51
1:A:307:A:N3	1:A:310:G:O2'	2.41	0.51
1:A:362:A:N6	32:f:37:TYR:O	2.43	0.51
1:A:1692:C:H5''	11:K:53:MET:HE2	1.92	0.51
1:A:3772:U:H2'	1:A:3773:U:H2'	1.90	0.51
5:E:156:TYR:O	5:E:158:GLN:NE2	2.43	0.51
6:F:209:ILE:HB	6:F:229:LEU:HD23	1.92	0.51
12:L:133:LYS:NZ	12:L:134:ASN:HD22	2.09	0.51
15:O:64:GLU:OE2	15:O:64:GLU:N	2.44	0.51
23:W:26:LYS:N	23:W:26:LYS:HE2	2.25	0.51
1:A:4188:U:H2'	1:A:4189:U:C6	2.46	0.51
1:A:4282:A:N1	14:N:49:GLN:NE2	2.58	0.51
1:A:4591:U:H2'	1:A:4592:C:C6	2.45	0.51
15:O:25:CYS:HB3	15:O:112:LEU:HD13	1.92	0.51
36:j:50:ARG:HG3	36:j:50:ARG:HH11	1.75	0.51
1:A:162:A:H2'	1:A:163:A:H8	1.75	0.51
1:A:425:U:H2'	1:A:426:A:H8	1.75	0.51
1:A:1511:U:H2'	1:A:1512:G:H8	1.75	0.51
1:A:4251:A:H5''	43:q:108:GLY:HA3	1.93	0.51
1:A:4508:C:H5''	16:P:43:LYS:HD3	1.93	0.51
1:A:4625:C:OP1	5:E:224:LYS:HG3	2.11	0.51
2:B:23:A:N3	2:B:118:C:O2'	2.36	0.51
1:A:662:C:H2'	1:A:663:G:C8	2.46	0.51
1:A:2262:G:OP2	37:k:98:ARG:NH2	2.44	0.51
1:A:4583:C:O2'	1:A:4718:G:N2	2.43	0.51
2:B:6:C:H4'	7:G:52:ILE:HD13	1.91	0.51
19:S:30:MET:HE2	19:S:101:PRO:HG3	1.92	0.51
20:T:77:TYR:HD1	23:W:39:ARG:HD3	1.75	0.51
34:h:42:LEU:HD22	34:h:46:ILE:HD11	1.92	0.51
44:r:150:LEU:HD23	44:r:154:VAL:HG22	1.91	0.51
1:A:1298:C:H2'	1:A:1299:G:H8	1.75	0.51
1:A:2412:A:H2'	1:A:2413:U:C6	2.46	0.51
1:A:3598:C:H2'	1:A:3599:A:H8	1.74	0.51
1:A:3664:G:H2'	1:A:3665:G:H8	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4178:A:H2'	1:A:4179:G:H8	1.76	0.51
1:A:4691:A:OP1	41:o:75:SER:OG	2.27	0.51
1:A:4946:U:O2'	26:Z:2:SER:OG	2.26	0.51
2:B:92:C:H2'	2:B:93:G:C8	2.45	0.51
3:C:5:U:H2'	3:C:6:C:H6	1.75	0.51
3:C:58:G:N7	30:d:63:ARG:NH2	2.48	0.51
3:C:102:G:OP2	3:C:104:A:O2'	2.24	0.51
6:F:218:ILE:HG23	6:F:229:LEU:HD13	1.93	0.51
14:N:143:THR:O	14:N:146:LYS:NZ	2.44	0.51
41:o:143:GLU:OE2	41:o:143:GLU:HA	2.11	0.51
1:A:1390:G:N2	1:A:1393:G:OP2	2.31	0.51
1:A:1516:G:O2'	44:r:18:TRP:NE1	2.36	0.51
1:A:3789:C:OP2	1:A:3790:U:O2'	2.25	0.51
1:A:4964:C:H2'	1:A:4965:U:C6	2.46	0.51
9:I:130:LYS:HB2	9:I:133:ARG:HG2	1.90	0.51
18:R:91:GLU:N	18:R:91:GLU:OE2	2.42	0.51
21:U:76:ASP:N	21:U:76:ASP:OD1	2.42	0.51
1:A:168:C:H3'	1:A:169:G:H21	1.75	0.51
1:A:1335:G:N2	6:F:95:MET:HB2	2.25	0.51
1:A:1548:G:O2'	1:A:2812:A:N3	2.35	0.51
1:A:1749:A:H2'	1:A:1750:G:C8	2.46	0.51
1:A:2685:C:H2'	1:A:2686:G:O4'	2.10	0.51
1:A:4592:C:H2'	1:A:4593:C:C6	2.46	0.51
25:Y:100:ALA:O	25:Y:108:ARG:NH2	2.44	0.51
43:q:16:ARG:CZ	43:q:137:PRO:HG3	2.41	0.51
1:A:253:G:H2'	1:A:254:G:H8	1.76	0.51
1:A:697:G:H2'	1:A:698:G:H8	1.75	0.51
1:A:3787:G:H1'	1:A:3789:C:H41	1.76	0.51
4:D:2:GLY:HA2	4:D:207:VAL:HG23	1.92	0.51
30:d:17:THR:OG1	30:d:18:LEU:N	2.44	0.51
42:p:80:CYS:SG	42:p:137:HIS:ND1	2.69	0.51
1:A:679:C:H2'	1:A:680:G:H8	1.77	0.50
1:A:3924:C:H2'	1:A:3925:OMU:H6	1.94	0.50
3:C:19:C:H2'	3:C:20:A:C8	2.46	0.50
4:D:30:ARG:HG3	4:D:76:PHE:HZ	1.75	0.50
11:K:151:HIS:ND1	11:K:164:LYS:O	2.43	0.50
18:R:83:THR:O	18:R:87:MET:HG2	2.12	0.50
1:A:1646:A:O2'	30:d:49:TRP:O	2.23	0.50
1:A:1669:A:N3	1:A:1852:U:O2'	2.40	0.50
1:A:1840:G:OP2	39:m:202:LYS:NZ	2.41	0.50
1:A:2274:C:H2'	1:A:2275:G:H8	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2474:G:N2	1:A:2503:G:H5''	2.26	0.50
1:A:3731:C:H2'	1:A:3732:A:H8	1.76	0.50
3:C:153:C:H2'	3:C:154:G:H8	1.75	0.50
41:o:113:GLU:HA	41:o:113:GLU:OE2	2.12	0.50
1:A:63:G:OP1	38:l:169:ARG:NH2	2.38	0.50
1:A:2087:C:OP2	11:K:37:ARG:NH1	2.42	0.50
1:A:2891:U:OP2	12:L:74:ARG:NE	2.44	0.50
1:A:4743:G:H2'	1:A:4744:A:C8	2.46	0.50
1:A:4906:C:H2'	1:A:4907:G:C8	2.46	0.50
35:i:101:GLY:HA2	43:q:65:ASN:HD22	1.77	0.50
44:r:154:VAL:HG12	44:r:155:MET:HG3	1.92	0.50
1:A:3754:G:H1	1:A:3770:PSU:HN3	1.59	0.50
1:A:4594:U:H2'	1:A:4595:G:C8	2.45	0.50
11:K:178:ARG:N	21:U:51:GLY:HA2	2.26	0.50
19:S:2:LYS:HD3	19:S:7:VAL:HB	1.93	0.50
19:S:66:GLN:H	19:S:66:GLN:CD	2.19	0.50
23:W:29:LEU:HD12	23:W:91:VAL:HG11	1.94	0.50
42:p:51:HIS:CD2	42:p:158:SER:HB3	2.46	0.50
1:A:68:U:OP1	38:l:178:HIS:ND1	2.42	0.50
1:A:1089:G:H2'	1:A:1090:G:H8	1.77	0.50
1:A:4457:PSU:OP1	16:P:50:ASN:ND2	2.29	0.50
1:A:5004:C:H2'	1:A:5005:G:O4'	2.11	0.50
1:A:5063:G:H2'	1:A:5064:G:C8	2.44	0.50
2:B:38:U:N3	2:B:41:G:OP2	2.37	0.50
15:O:39:PHE:O	15:O:43:LEU:HD23	2.12	0.50
22:V:54:LEU:HA	22:V:57:MET:HB2	1.92	0.50
34:h:14:GLY:HA2	34:h:198:VAL:HG13	1.93	0.50
43:q:40:LEU:HD12	43:q:70:VAL:HG22	1.94	0.50
1:A:1074:G:H2'	1:A:1075:G:C8	2.46	0.50
1:A:3713:U:O2'	1:A:3715:PSU:OP2	2.28	0.50
1:A:3911:C:H2'	1:A:3912:U:C6	2.46	0.50
1:A:4523:A2M:H5''	1:A:4524:G:H5'	1.92	0.50
7:G:152:ARG:O	7:G:157:ASN:ND2	2.44	0.50
11:K:124:ASP:OD1	11:K:124:ASP:N	2.44	0.50
13:M:72:PRO:HG2	13:M:73:LEU:HD22	1.92	0.50
19:S:100:HIS:ND1	19:S:102:SER:OG	2.37	0.50
42:p:63:GLU:H	42:p:63:GLU:CD	2.18	0.50
1:A:10:A:H2'	1:A:11:G:C8	2.47	0.50
1:A:86:U:H2'	1:A:87:A:H8	1.77	0.50
1:A:710:G:H2'	1:A:711:A:H8	1.76	0.50
1:A:1440:U:H2'	1:A:1441:C:C6	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1881:OMC:HM21	1:A:1882:U:H5	1.77	0.50
1:A:1914:C:H4'	9:I:89:PRO:HD3	1.92	0.50
1:A:2374:A:H2'	1:A:2375:A:H8	1.76	0.50
1:A:3610:A:H2'	1:A:3611:A:H8	1.76	0.50
6:F:284:MET:HE2	6:F:287:THR:HA	1.94	0.50
16:P:96:LEU:HD12	16:P:97:TYR:N	2.25	0.50
17:Q:27:LYS:HD2	17:Q:28:VAL:H	1.77	0.50
1:A:175:C:H2'	1:A:176:G:H8	1.76	0.50
1:A:490:C:H2'	1:A:491:G:H8	1.76	0.50
1:A:717:U:H2'	1:A:718:C:C6	2.46	0.50
1:A:1094:G:H2'	1:A:1095:A:H8	1.76	0.50
1:A:1293:G:N2	1:A:1293:G:OP2	2.45	0.50
1:A:2809:G:O2'	1:A:4644:G:OP1	2.27	0.50
1:A:3610:A:H2'	1:A:3611:A:C8	2.47	0.50
1:A:4478:G:N2	1:A:4608:G:O2'	2.45	0.50
1:A:4567:G:OP1	5:E:19:ARG:N	2.45	0.50
8:H:190:HIS:HB3	8:H:193:PHE:HD2	1.76	0.50
23:W:28:VAL:HB	23:W:33:GLN:HE21	1.76	0.50
1:A:131:C:H2'	1:A:132:G:H4'	1.94	0.50
1:A:4344:U:H3	1:A:4368:G:H1	1.60	0.50
1:A:4347:G:H2'	1:A:4348:A:C8	2.47	0.50
3:C:153:C:H2'	3:C:154:G:C8	2.46	0.50
24:X:56:GLU:N	24:X:56:GLU:OE2	2.44	0.50
43:q:95:ARG:NH2	43:q:176:PRO:O	2.45	0.50
1:A:94:A:OP2	44:r:11:LYS:NZ	2.43	0.49
1:A:2083:C:P	11:K:14:ARG:HH22	2.35	0.49
1:A:4346:U:O2'	35:i:80:LYS:O	2.27	0.49
20:T:22:LYS:NZ	20:T:129:TRP:O	2.41	0.49
20:T:91:LEU:O	20:T:93:LYS:NZ	2.43	0.49
34:h:118:HIS:ND1	34:h:119:PRO:HD2	2.27	0.49
41:o:111:LEU:HD12	41:o:126:VAL:C	2.37	0.49
1:A:673:C:H2'	1:A:674:G:H8	1.75	0.49
1:A:1617:G:H1'	1:A:2513:A:N6	2.26	0.49
1:A:4126:C:H5''	1:A:4127:A:H5''	1.93	0.49
1:A:4507:A:H2'	1:A:4508:C:C6	2.47	0.49
1:A:5006:U:H4'	1:A:5007:A:H5'	1.92	0.49
3:C:9:A:H2'	3:C:10:G:H8	1.76	0.49
8:H:161:ARG:O	8:H:182:ASN:ND2	2.46	0.49
33:g:79:GLU:OE2	33:g:80:PRO:HD2	2.12	0.49
38:l:60[B]:VAL:HG23	38:l:134:LEU:HB2	1.93	0.49
41:o:91:LYS:HB3	41:o:143:GLU:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1070:G:O2'	1:A:1071:C:H5'	2.13	0.49
1:A:1514:U:H2'	1:A:1515:A:C8	2.48	0.49
1:A:1845:U:H2'	1:A:1846:G:H8	1.77	0.49
1:A:3628:G:H2'	1:A:3629:A:H8	1.76	0.49
1:A:3687:A:H3'	4:D:198:ARG:HH21	1.77	0.49
1:A:3688:U:H2'	1:A:3689:G:C8	2.45	0.49
1:A:4918:C:H2'	1:A:4919:G:C8	2.47	0.49
7:G:186:GLU:OE1	7:G:186:GLU:N	2.36	0.49
14:N:113:ASP:OD1	14:N:113:ASP:N	2.45	0.49
25:Y:86:GLU:OE2	25:Y:86:GLU:N	2.41	0.49
43:q:38:LYS:HE2	43:q:123:ILE:HD13	1.94	0.49
1:A:676:C:H2'	1:A:677:G:H8	1.77	0.49
1:A:1503:A:H4'	1:A:1504:G:H5'	1.94	0.49
1:A:1734:G:N2	1:A:1735:U:O4	2.33	0.49
1:A:1824:G:H2'	1:A:1825:A:H8	1.78	0.49
1:A:1846:G:H2'	1:A:1847:C:C6	2.47	0.49
1:A:4229:U:H4'	35:i:89:LYS:HE2	1.95	0.49
8:H:46:ARG:HB2	8:H:62:MET:HE1	1.93	0.49
39:m:217:ARG:O	39:m:246:ARG:NH1	2.39	0.49
41:o:63:ASN:N	41:o:66:GLU:OE1	2.46	0.49
42:p:91:LEU:HD11	42:p:119:VAL:HB	1.93	0.49
1:A:1308:C:H2'	1:A:1309:C:C6	2.48	0.49
1:A:1355:G:OP1	11:K:108:ARG:NH2	2.45	0.49
1:A:2751:G:H2'	1:A:2752:G:H8	1.76	0.49
1:A:3684:G:H2'	1:A:3685:C:C6	2.47	0.49
1:A:4596:C:H4'	34:h:8:GLU:HB3	1.94	0.49
1:A:4736:C:H2'	1:A:4737:G:H8	1.76	0.49
1:A:4876:U:H5'	51:M:201:EPE:H52	1.94	0.49
1:A:4906:C:H2'	1:A:4907:G:H8	1.77	0.49
16:P:62:MET:HA	16:P:62:MET:HE3	1.94	0.49
22:V:117:ARG:HG3	22:V:118:LEU:HD12	1.95	0.49
1:A:3861:A:H2'	1:A:3862:A:C8	2.48	0.49
1:A:4730:C:O2	1:A:4732:G:H1'	2.13	0.49
13:M:161:ARG:HE	13:M:164:LYS:HB2	1.77	0.49
42:p:169:ASP:OD1	42:p:170:GLU:N	2.45	0.49
1:A:208:A:N3	1:A:232:G:O2'	2.46	0.49
1:A:478:G:H2'	1:A:479:G:H8	1.78	0.49
1:A:1339:U:H2'	1:A:1340:OMC:C6	2.47	0.49
1:A:1475:G:H2'	1:A:1476:C:C6	2.47	0.49
1:A:1728:U:H2'	1:A:1729:A:C8	2.48	0.49
1:A:1875:C:H2'	1:A:1876:U:C6	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:7:U:H2'	3:C:8:U:C6	2.47	0.49
16:P:138:SER:HB3	34:h:101:LEU:HA	1.95	0.49
33:g:89:TYR:OH	41:o:181:VAL:O	2.28	0.49
37:k:85:ASN:O	37:k:89:THR:HG23	2.13	0.49
1:A:279:A:OP2	38:l:8:GLN:NE2	2.45	0.49
1:A:1327:C:H2'	1:A:1328:G:C8	2.48	0.49
1:A:4389:C:H2'	1:A:4390:A:H8	1.78	0.49
4:D:53:GLY:O	4:D:192:LYS:NZ	2.41	0.49
5:E:291:TYR:HB3	5:E:298:LEU:HD11	1.94	0.49
32:f:30:LYS:HB2	32:f:33:ASN:HB2	1.94	0.49
34:h:112:ASP:OD2	34:h:156:ASN:ND2	2.32	0.49
39:m:71:MET:HA	39:m:74:MET:HE3	1.95	0.49
1:A:1517:G:H1	6:F:104:PRO:HD2	1.77	0.49
1:A:4642:U:H2'	1:A:4643:G:C8	2.48	0.49
7:G:116:ASP:OD1	7:G:116:ASP:N	2.46	0.49
22:V:101:HIS:O	22:V:109:ARG:NH1	2.45	0.49
24:X:65:ASP:OD1	24:X:66:THR:N	2.46	0.49
34:h:68:HIS:ND1	34:h:134:LYS:HE2	2.28	0.49
34:h:163:PRO:HG2	34:h:164:LYS:HD2	1.94	0.49
1:A:56:A:H2'	1:A:57:G:C8	2.48	0.49
1:A:423:G:OP1	10:J:62:ARG:NH1	2.44	0.49
1:A:1741:G:O6	2:B:103:A:O2'	2.24	0.49
1:A:4075:U:OP1	40:n:249:ARG:NH2	2.46	0.49
1:A:4314:C:H5'	14:N:68:THR:HB	1.95	0.49
1:A:4638:U:H2'	1:A:4639:G:N3	2.28	0.49
1:A:4723:A:H2'	1:A:4724:A:C8	2.48	0.49
1:A:4935:C:H2'	1:A:4936:G:H8	1.76	0.49
8:H:180:VAL:HG11	8:H:258:LEU:HD11	1.95	0.49
1:A:1082:C:H2'	1:A:1083:U:O4'	2.13	0.48
1:A:1345:A:H2'	1:A:1346:C:C6	2.48	0.48
1:A:4237:C:H1'	1:A:4321:U:H1'	1.94	0.48
10:J:29:THR:HG21	10:J:146:ILE:HD11	1.95	0.48
18:R:82:THR:HG21	28:b:37:THR:HG22	1.95	0.48
24:X:55:LYS:HE2	24:X:56:GLU:OE2	2.13	0.48
41:o:113:GLU:OE2	41:o:125:ARG:HG2	2.13	0.48
1:A:272:U:H2'	1:A:273:U:C6	2.48	0.48
1:A:2745:A:H2'	1:A:2746:A:C8	2.44	0.48
1:A:3917:A:H2'	1:A:3918:G:H8	1.78	0.48
18:R:87:MET:HA	18:R:87:MET:HE3	1.95	0.48
38:l:138:PHE:HA	38:l:143:ARG:HD2	1.94	0.48
1:A:33:A:H2'	1:A:34:A:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:C:H2'	1:A:491:G:C8	2.48	0.48
1:A:710:G:H2'	1:A:711:A:C8	2.48	0.48
1:A:732:A:H2'	1:A:733:A:O4'	2.13	0.48
1:A:1400:G:H2'	1:A:1401:C:C6	2.48	0.48
1:A:3663:A:N6	1:A:4168:G:O2'	2.47	0.48
1:A:4743:G:H2'	1:A:4744:A:H8	1.79	0.48
14:N:157:GLU:OE1	14:N:158:PHE:N	2.47	0.48
34:h:84:ILE:HD13	34:h:94:ILE:HD13	1.95	0.48
38:l:98:LEU:HD12	38:l:128:LYS:HD2	1.95	0.48
39:m:238:ASP:O	39:m:241:ASN:ND2	2.43	0.48
1:A:299:C:H2'	1:A:300:A:C8	2.47	0.48
1:A:711:A:H2'	1:A:712:C:C6	2.48	0.48
1:A:2049:G:H2'	1:A:2050:G:C8	2.49	0.48
1:A:2483:G:H2'	1:A:2484:A:H8	1.78	0.48
37:k:105:ASP:OD1	37:k:105:ASP:N	2.36	0.48
43:q:58:ARG:NH1	43:q:58:ARG:HA	2.28	0.48
1:A:3725:G:N2	1:A:3728:A:OP2	2.37	0.48
1:A:4322:G:N2	1:A:4325:A:OP2	2.30	0.48
1:A:4510:A:C6	1:A:4592:C:H4'	2.48	0.48
4:D:101:VAL:HG22	4:D:165:VAL:HG22	1.96	0.48
13:M:41:LYS:NZ	39:m:237:GLU:OE2	2.47	0.48
39:m:190:LEU:HD21	39:m:208:LEU:HD21	1.96	0.48
1:A:318:A:H2'	1:A:319:A:H8	1.78	0.48
1:A:678:C:H2'	1:A:679:C:C6	2.49	0.48
1:A:1248:C:H2'	1:A:1249:C:C6	2.48	0.48
1:A:1738:A:H2'	1:A:1739:G:H8	1.79	0.48
1:A:2275:G:H2'	1:A:2276:A:C8	2.48	0.48
1:A:4305:G:O5'	14:N:83:LYS:NZ	2.46	0.48
1:A:4458:C:OP1	5:E:11:HIS:NE2	2.46	0.48
2:B:107:G:OP1	7:G:277:LYS:NZ	2.40	0.48
9:I:199:HIS:CD2	45:s:108:ASP:HB3	2.49	0.48
12:L:28:GLU:HB3	12:L:31:GLU:OE2	2.13	0.48
12:L:28:GLU:O	12:L:32:ILE:HG13	2.14	0.48
31:e:47:ILE:HG22	31:e:49:ASP:H	1.79	0.48
1:A:260:C:H2'	1:A:261:G:C8	2.49	0.48
1:A:2079:G:H2'	1:A:2080:U:C6	2.48	0.48
1:A:2274:C:H2'	1:A:2275:G:C8	2.48	0.48
1:A:4174:U:H2'	1:A:4175:G:C8	2.45	0.48
1:A:4593:C:H2'	1:A:4594:U:H6	1.79	0.48
1:A:4730:C:H2'	1:A:4731:G:O4'	2.13	0.48
44:r:175:ASN:O	44:r:177:LYS:NZ	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:s:32:ASP:OD2	45:s:34:ASN:N	2.40	0.48
1:A:86:U:O2'	21:U:65:ARG:NH2	2.42	0.48
1:A:101:A:H1'	21:U:66:ASN:HD21	1.78	0.48
1:A:280:G:OP2	38:l:44:ARG:NH2	2.39	0.48
1:A:424:U:H2'	1:A:425:U:C6	2.49	0.48
1:A:2527:A:OP1	12:L:38:ARG:NH2	2.38	0.48
1:A:4522:G:O2'	1:A:4525:C:OP2	2.29	0.48
1:A:4960:G:H2'	1:A:4961:G:C8	2.49	0.48
16:P:15:ARG:HH11	16:P:15:ARG:HG3	1.78	0.48
1:A:691:C:H2'	1:A:692:A:C8	2.48	0.48
1:A:1359:G:H4'	38:l:203:TYR:HB2	1.95	0.48
1:A:1465:G:OP1	22:V:44:ARG:NH1	2.46	0.48
1:A:1693:U:H2'	1:A:1694:C:O4'	2.14	0.48
1:A:4089:G:H2'	1:A:4090:G:H8	1.79	0.48
3:C:119:C:H2'	3:C:120:G:H8	1.79	0.48
14:N:88:ARG:NH1	22:V:33:LYS:O	2.47	0.48
17:Q:23:ARG:NH1	17:Q:25:ASP:OD1	2.46	0.48
21:U:77:LYS:O	21:U:80:THR:OG1	2.31	0.48
40:n:83:PHE:HA	40:n:183:ILE:HD13	1.95	0.48
41:o:76:HIS:O	41:o:80:MET:HG3	2.14	0.48
45:s:81:ASP:OD1	45:s:85:LYS:HG3	2.14	0.48
1:A:1681:G:H2'	1:A:1682:A:C8	2.48	0.48
1:A:2672:C:O2'	1:A:2675:G:O2'	2.32	0.48
1:A:2878:G:OP2	1:A:2879:A:O2'	2.24	0.48
1:A:3941:G:H2'	1:A:3942:A:H8	1.79	0.48
1:A:4089:G:H2'	1:A:4090:G:C8	2.49	0.48
1:A:4572:U:H2'	1:A:4573:G:C8	2.49	0.48
3:C:144:U:H2'	3:C:145:C:C6	2.49	0.48
40:n:213:GLY:O	40:n:217:LYS:NZ	2.47	0.48
41:o:14:GLU:OE2	41:o:14:GLU:N	2.39	0.48
1:A:652:G:H2'	1:A:653:U:C6	2.49	0.47
1:A:2568:C:H2'	1:A:2569:G:C8	2.49	0.47
1:A:2730:U:H2'	1:A:2731:C:C6	2.49	0.47
1:A:3869:OMC:HM23	9:I:62:MET:HE1	1.96	0.47
1:A:4067:U:H2'	1:A:4068:U:C6	2.49	0.47
1:A:4637:OMG:HM22	1:A:4638:U:O4'	2.14	0.47
10:J:64:ASN:ND2	10:J:80:GLN:OE1	2.47	0.47
21:U:36:GLY:HA3	21:U:40:HIS:CE1	2.49	0.47
1:A:268:G:H2'	1:A:269:G:H8	1.79	0.47
1:A:678:C:H2'	1:A:679:C:H6	1.78	0.47
1:A:2063:G:H2'	1:A:2064:G:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:66:A:H2'	3:C:67:U:C6	2.48	0.47
4:D:142:GLU:H	4:D:142:GLU:CD	2.22	0.47
7:G:156:GLY:HA2	7:G:181:PRO:HG3	1.96	0.47
11:K:45:GLN:H	11:K:45:GLN:CD	2.21	0.47
1:A:260:C:H2'	1:A:261:G:H8	1.79	0.47
1:A:1443:A:H62	1:A:2102:G:H1	1.62	0.47
1:A:2374:A:H2'	1:A:2375:A:C8	2.49	0.47
1:A:2474:G:H22	1:A:2503:G:H5''	1.80	0.47
1:A:4727:A:H2'	1:A:4728:U:O4'	2.15	0.47
13:M:69:GLU:OE1	13:M:70:LYS:N	2.46	0.47
25:Y:102:ASN:OD1	25:Y:102:ASN:N	2.45	0.47
29:c:42:ASP:N	29:c:42:ASP:OD1	2.47	0.47
1:A:133:C:H2'	1:A:134:G:O4'	2.14	0.47
1:A:271:C:H2'	1:A:272:U:C6	2.50	0.47
1:A:673:C:H2'	1:A:674:G:C8	2.49	0.47
1:A:1173:G:H2'	1:A:1174:G:C8	2.49	0.47
1:A:1400:G:H2'	1:A:1401:C:H6	1.80	0.47
1:A:1662:C:H2'	1:A:1663:C:H6	1.79	0.47
1:A:2357:G:H2'	1:A:2358:G:H8	1.80	0.47
1:A:2607:C:H2'	1:A:2608:G:H8	1.79	0.47
1:A:3824:A:H2'	1:A:3825:A2M:H8	1.95	0.47
1:A:4317:A:H2'	1:A:4318:C:C6	2.48	0.47
1:A:4459:U:H2'	1:A:4460:U:C6	2.49	0.47
1:A:4759:C:H2'	1:A:4760:G:C8	2.49	0.47
1:A:4934:A:H2'	1:A:4935:C:H6	1.79	0.47
3:C:27:U:H2'	3:C:28:C:H6	1.79	0.47
12:L:50:ILE:C	12:L:51:ILE:HD13	2.38	0.47
16:P:45:ILE:HG21	16:P:53:PRO:HB3	1.95	0.47
1:A:20:U:H3'	1:A:21:G:C8	2.47	0.47
1:A:66:A:O2'	1:A:326:C:O2	2.28	0.47
1:A:745:G:H2'	1:A:746:A:C8	2.50	0.47
1:A:1309:C:H2'	1:A:1310:C:C6	2.50	0.47
1:A:1942:A:H2'	1:A:1943:A:H8	1.78	0.47
1:A:2097:U:H3'	1:A:2098:G:H4'	1.95	0.47
1:A:2555:G:H2'	1:A:2556:G:C8	2.50	0.47
1:A:4571:A2M:HM'2	1:A:4572:U:H5'	1.96	0.47
4:D:20:VAL:HG12	4:D:23:ARG:HD2	1.96	0.47
16:P:133:ALA:O	34:h:106:ASN:ND2	2.46	0.47
34:h:118:HIS:HE1	34:h:146:VAL:HB	1.77	0.47
39:m:122:PHE:O	39:m:205:ASN:ND2	2.46	0.47
1:A:1304:C:H2'	1:A:1305:C:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2049:G:H2'	1:A:2050:G:H8	1.79	0.47
1:A:2730:U:H2'	1:A:2731:C:H6	1.80	0.47
2:B:11:A:N1	2:B:66:G:O2'	2.44	0.47
5:E:17:LEU:HD21	5:E:235:TRP:HH2	1.78	0.47
8:H:241:GLU:OE2	8:H:241:GLU:N	2.48	0.47
14:N:27:LEU:O	14:N:31:MET:HE2	2.15	0.47
14:N:68:THR:OG1	14:N:71:ALA:O	2.30	0.47
15:O:93:LYS:HG3	15:O:94:ASN:OD1	2.14	0.47
15:O:111:GLU:OE2	15:O:113:ARG:NH1	2.48	0.47
29:c:93:VAL:O	29:c:97:MET:HG2	2.14	0.47
43:q:146:ARG:HG2	43:q:147:ARG:HG3	1.95	0.47
1:A:19:G:P	28:b:93:ARG:HE	2.37	0.47
1:A:387:G:N1	1:A:412:G:H1'	2.29	0.47
1:A:2540:C:H2'	1:A:2541:G:C8	2.50	0.47
1:A:2634:C:H2'	1:A:2635:U:H6	1.80	0.47
1:A:2683:C:H2'	1:A:2684:C:H6	1.80	0.47
1:A:2850:A:O3'	1:A:4495:G:H5''	2.15	0.47
1:A:4177:C:H2'	1:A:4178:A:H8	1.80	0.47
1:A:4194:U:O2'	42:p:106:ARG:NH2	2.48	0.47
1:A:4704:C:H2'	1:A:4705:A:H8	1.79	0.47
1:A:4742:G:H2'	1:A:4743:G:H8	1.79	0.47
1:A:4933:C:H2'	1:A:4934:A:H8	1.76	0.47
1:A:4973:U:H1'	1:A:4986:G:C2	2.50	0.47
2:B:37:G:N2	2:B:41:G:N3	2.63	0.47
4:D:147:ARG:HG2	4:D:157:VAL:HG22	1.96	0.47
8:H:161:ARG:NH1	8:H:273:SER:OG	2.47	0.47
16:P:85:ARG:HG2	16:P:85:ARG:HH11	1.79	0.47
20:T:11:VAL:HG12	20:T:82:PRO:HA	1.96	0.47
20:T:50:PRO:HD3	20:T:68:ILE:HG12	1.97	0.47
23:W:90:ARG:HH21	36:j:44:LYS:HZ3	1.62	0.47
42:p:62:SER:HA	42:p:65:LEU:HD12	1.96	0.47
1:A:58:G:H4'	1:A:59:A:H4'	1.96	0.47
1:A:256:G:H2'	1:A:257:C:C6	2.49	0.47
1:A:1178:G:HO2'	7:G:286:SER:HG	1.61	0.47
1:A:1818:G:H1'	1:A:1822:U:C2	2.50	0.47
1:A:2563:C:H3'	1:A:2564:G:H8	1.80	0.47
1:A:2683:C:H2'	1:A:2684:C:C6	2.50	0.47
12:L:142:ILE:HD12	12:L:143:HIS:N	2.30	0.47
29:c:73:ILE:O	29:c:77:VAL:HG22	2.14	0.47
31:e:46:VAL:C	31:e:47:ILE:HD13	2.39	0.47
31:e:58:GLN:H	31:e:58:GLN:CD	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:q:12:MET:HA	43:q:12:MET:HE3	1.95	0.47
44:r:33:ILE:HD12	44:r:34:ARG:N	2.29	0.47
45:s:132:LYS:O	45:s:135:LEU:HG	2.15	0.47
1:A:31:U:H2'	1:A:32:G:O4'	2.15	0.47
1:A:1279:A:O2'	1:A:1281:G:N7	2.46	0.47
1:A:2642:A:N6	1:A:2643:G:O6	2.48	0.47
5:E:161:ARG:HG2	5:E:184:GLN:HA	1.96	0.47
11:K:18:PRO:HG3	11:K:52:PHE:HD1	1.80	0.47
14:N:112:ASN:HD22	14:N:128:LEU:HB3	1.80	0.47
20:T:5:MET:O	20:T:28:ASN:ND2	2.48	0.47
1:A:143:C:OP1	40:n:111:LYS:NZ	2.41	0.47
1:A:1397:A:N1	1:A:1498:G:O2'	2.41	0.47
1:A:4563:U:H2'	1:A:4564:A:H8	1.79	0.47
7:G:258:LYS:HE3	7:G:258:LYS:HB3	1.71	0.47
14:N:75:VAL:HG22	14:N:88:ARG:HG2	1.96	0.47
17:Q:47:ARG:HB2	17:Q:47:ARG:CZ	2.45	0.47
22:V:91:ARG:O	22:V:95:ARG:NH1	2.47	0.47
33:g:82:LEU:HD21	41:o:93:ARG:CZ	2.44	0.47
41:o:44:GLU:HB2	41:o:58:ASP:HB2	1.97	0.47
42:p:66:GLU:OE1	42:p:69:ARG:NE	2.39	0.47
1:A:86:U:H2'	1:A:87:A:C8	2.50	0.46
1:A:319:A:H1'	1:A:3726:A:N3	2.30	0.46
1:A:699:C:H2'	1:A:700:G:C8	2.49	0.46
1:A:750:U:H1'	1:A:917:A:C8	2.49	0.46
1:A:1095:A:H2'	1:A:1096:C:C6	2.50	0.46
1:A:1916:G:O6	26:Z:18:LEU:HB2	2.15	0.46
1:A:2898:G:H2'	1:A:2899:C:C6	2.50	0.46
1:A:4592:C:H2'	1:A:4593:C:H6	1.79	0.46
24:X:37:GLY:O	24:X:41:ARG:HG3	2.15	0.46
41:o:117:PHE:O	41:o:120:GLU:HG3	2.15	0.46
45:s:24:LEU:HD11	45:s:86:TRP:CG	2.50	0.46
45:s:119:ARG:O	45:s:123:ILE:HG12	2.15	0.46
1:A:133:C:N4	28:b:74:LYS:HG3	2.30	0.46
1:A:162:A:H2'	1:A:163:A:C8	2.50	0.46
1:A:1094:G:H2'	1:A:1095:A:C8	2.50	0.46
1:A:1727:U:OP1	39:m:131:ASN:ND2	2.45	0.46
1:A:2458:C:H1'	1:A:3671:G:H21	1.80	0.46
1:A:2465:C:H2'	1:A:2466:G:O4'	2.15	0.46
1:A:2622:G:H2'	1:A:2623:A:H8	1.81	0.46
1:A:2830:G:H2'	1:A:2831:G:H8	1.79	0.46
1:A:4122:G:N7	27:a:97:ILE:HD12	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4238:G:H2'	1:A:4239:A:H8	1.80	0.46
1:A:4246:G:H2'	1:A:4247:G:C8	2.50	0.46
1:A:4584:A:H2'	1:A:4585:U:O4'	2.15	0.46
1:A:4589:A:N1	1:A:4621:C:O2'	2.46	0.46
9:I:175:MET:HE3	9:I:179:LYS:HD3	1.97	0.46
20:T:29:ILE:HG22	20:T:32:GLY:H	1.80	0.46
23:W:34:THR:HG23	23:W:95:ALA:HB2	1.97	0.46
38:l:143:ARG:O	38:l:149:GLN:NE2	2.45	0.46
41:o:137:SER:HB2	41:o:145:ILE:HG12	1.96	0.46
41:o:152:GLU:HA	41:o:152:GLU:OE2	2.14	0.46
1:A:429:A:H2'	1:A:430:G:C8	2.50	0.46
1:A:1431:C:H2'	1:A:1432:G:O4'	2.16	0.46
1:A:1591:U:OP2	1:A:2856:C:O2'	2.31	0.46
1:A:1854:G:N2	1:A:4394:A:O4'	2.49	0.46
1:A:2803:U:H2'	1:A:2804:OMC:H6	1.80	0.46
1:A:2848:G:O2'	1:A:3838:U:O4	2.29	0.46
1:A:3932:U:H2'	1:A:3933:G:H8	1.81	0.46
1:A:4739:C:N4	1:A:4740:G:O6	2.48	0.46
3:C:90:C:H2'	3:C:91:A:C8	2.49	0.46
3:C:96:C:H5''	28:b:66:LYS:HG2	1.96	0.46
14:N:93:ILE:HD12	14:N:94:GLU:OE2	2.15	0.46
23:W:17:ARG:HG2	23:W:17:ARG:HH11	1.81	0.46
1:A:1577:G:O2'	1:A:1612:G:H4'	2.14	0.46
1:A:1677:PSU:H4'	1:A:1680:G:C2	2.50	0.46
1:A:3656:A:H2'	1:A:3657:U:H6	1.81	0.46
1:A:4992:G:H2'	1:A:4993:G:H8	1.78	0.46
4:D:243:THR:OG1	4:D:244:GLY:N	2.48	0.46
19:S:112:ASP:OD2	19:S:114:ASP:N	2.48	0.46
23:W:64:ALA:O	23:W:68:LYS:N	2.49	0.46
28:b:80:PRO:HD2	28:b:83:LEU:HD12	1.97	0.46
1:A:86:U:OP1	11:K:169:SER:OG	2.26	0.46
1:A:120:A:N1	1:A:148:C:O2'	2.43	0.46
1:A:158:A:H5''	1:A:159:C:H2'	1.98	0.46
1:A:228:C:H2'	1:A:229:G:H8	1.81	0.46
1:A:318:A:H2'	1:A:319:A:C8	2.50	0.46
1:A:325:U:H2'	1:A:326:C:C6	2.51	0.46
1:A:1701:A:H61	39:m:36:LYS:NZ	2.13	0.46
1:A:2607:C:H2'	1:A:2608:G:C8	2.50	0.46
1:A:3723:A:OP2	29:c:68:ARG:NH2	2.39	0.46
1:A:4120:U:C4	27:a:97:ILE:HG12	2.50	0.46
1:A:4578:G:H2'	1:A:4579:PSU:H6	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:356:LYS:NZ	5:E:358:ARG:HE	2.13	0.46
7:G:63:GLN:NE2	53:G:301:HOH:O	2.47	0.46
14:N:144:ASN:HB2	14:N:146:LYS:NZ	2.31	0.46
15:O:63:ILE:HG13	15:O:72:VAL:HG22	1.97	0.46
23:W:45:LEU:HD21	23:W:108:MET:HE2	1.97	0.46
23:W:103:ASP:N	23:W:103:ASP:OD1	2.48	0.46
25:Y:124:ASN:N	25:Y:124:ASN:OD1	2.48	0.46
43:q:17:ILE:HG23	43:q:132:VAL:HG13	1.96	0.46
44:r:67:HIS:CD2	44:r:68:THR:HG23	2.51	0.46
45:s:132:LYS:O	45:s:136:LEU:HD12	2.16	0.46
1:A:44:A:N3	1:A:94:A:H2	2.13	0.46
1:A:175:C:H2'	1:A:176:G:C8	2.50	0.46
1:A:474:C:H2'	1:A:475:G:H8	1.80	0.46
1:A:1246:G:H2'	1:A:1247:U:C6	2.50	0.46
1:A:2413:U:H2'	1:A:2414:G:C8	2.50	0.46
1:A:3829:G:H2'	1:A:3830:A2M:H8	1.98	0.46
1:A:4475:G:O6	33:g:125:LYS:NZ	2.48	0.46
1:A:4569:U:OP1	1:A:4982:A:O2'	2.24	0.46
1:A:4704:C:H2'	1:A:4705:A:C8	2.51	0.46
2:B:6:C:O2'	7:G:50:ARG:NH2	2.48	0.46
3:C:130:C:H2'	3:C:131:G:C8	2.50	0.46
15:O:68:SER:O	15:O:68:SER:OG	2.32	0.46
33:g:88:LYS:HD3	33:g:89:TYR:CE1	2.50	0.46
34:h:67:ARG:HG3	34:h:68:HIS:HD2	1.80	0.46
38:l:159:ARG:HB3	38:l:164:LEU:HB2	1.96	0.46
40:n:99:ALA:HB1	40:n:136:LEU:HD11	1.97	0.46
1:A:1093:C:H2'	1:A:1094:G:C8	2.50	0.46
1:A:1101:C:O2'	1:A:1168:G:O4'	2.33	0.46
1:A:1507:C:H2'	1:A:1508:A:H8	1.81	0.46
1:A:1730:U:H2'	1:A:1731:C:C6	2.50	0.46
1:A:2844:A:O2'	1:A:4631:G:H4'	2.15	0.46
1:A:4077:A:N1	1:A:4171:C:N4	2.62	0.46
1:A:4260:U:H2'	1:A:4261:C:C6	2.51	0.46
1:A:4314:C:H5''	14:N:69:GLN:HG2	1.98	0.46
1:A:4504:C:H2'	1:A:4505:C:C6	2.50	0.46
1:A:4736:C:H4'	1:A:5068:G:C4	2.51	0.46
14:N:48:VAL:HG21	14:N:94:GLU:HG2	1.98	0.46
15:O:43:LEU:HD12	15:O:47:ILE:HD11	1.98	0.46
23:W:38:ILE:HD11	23:W:46:VAL:HG21	1.96	0.46
36:j:31:ILE:HD12	36:j:32:SER:N	2.31	0.46
44:r:17:ASP:OD1	44:r:20:ARG:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2640:G:H2'	1:A:2641:A:C8	2.51	0.46
1:A:3613:U:H2'	1:A:3614:G:C8	2.50	0.46
1:A:3942:A:H2'	1:A:3943:A:H8	1.80	0.46
1:A:4503:A:H2'	1:A:4504:C:H6	1.80	0.46
4:D:117:GLU:O	4:D:162:ASN:ND2	2.39	0.46
5:E:307:TYR:HD2	5:E:366:LYS:HA	1.81	0.46
7:G:152:ARG:HG3	7:G:154:THR:HG23	1.97	0.46
7:G:235:MET:C	7:G:235:MET:HE2	2.40	0.46
14:N:18:PRO:HB2	14:N:21:LYS:HD2	1.97	0.46
1:A:750:U:C2	1:A:751:G:C8	3.03	0.46
1:A:1494:U:H2'	1:A:1495:G:C8	2.51	0.46
1:A:2326:G:H5''	25:Y:127:ALA:HB2	1.97	0.46
1:A:2486:G:H2'	1:A:2487:G:H8	1.79	0.46
1:A:4129:G:O6	1:A:4156:G:N2	2.48	0.46
1:A:4149:C:OP1	20:T:59:LYS:N	2.43	0.46
2:B:28:C:O2'	2:B:54:A:N1	2.48	0.46
6:F:300:ARG:NH1	6:F:300:ARG:HB2	2.31	0.46
10:J:131:ARG:HG3	10:J:137:ASN:OD1	2.16	0.46
11:K:88:ASP:OD1	11:K:89:ASP:N	2.49	0.46
18:R:91:GLU:H	18:R:91:GLU:CD	2.24	0.46
34:h:84:ILE:HD12	34:h:85:ARG:N	2.31	0.46
42:p:36:LEU:HD13	42:p:69:ARG:NH1	2.30	0.46
42:p:56:GLU:HG2	42:p:58:GLU:OE2	2.16	0.46
42:p:63:GLU:OE2	42:p:63:GLU:N	2.32	0.46
1:A:416:U:H4'	1:A:2330:G:H4'	1.97	0.46
1:A:652:G:H2'	1:A:653:U:H6	1.80	0.46
1:A:1239:C:H2'	1:A:1240:G:C8	2.51	0.46
1:A:1245:C:H2'	1:A:1246:G:C8	2.51	0.46
1:A:1669:A:H4'	1:A:1685:G:N2	2.31	0.46
1:A:2539:C:H2'	1:A:2540:C:H6	1.80	0.46
1:A:4134:C:H2'	1:A:4135:G:C8	2.50	0.46
1:A:4233:A:H4'	35:i:98:LYS:HD2	1.97	0.46
1:A:4883:C:H2'	1:A:4884:G:C8	2.51	0.46
5:E:220:ILE:HG12	5:E:278:THR:HG23	1.97	0.46
5:E:248:LEU:HD12	5:E:249:ARG:HG3	1.98	0.46
12:L:151:ARG:HG2	12:L:151:ARG:HH11	1.81	0.46
14:N:102:ARG:O	14:N:106:LEU:HD22	2.16	0.46
26:Z:50:VAL:HG22	26:Z:69:VAL:HG22	1.97	0.46
34:h:49:VAL:HG11	34:h:84:ILE:HG22	1.98	0.46
1:A:381:U:H2'	1:A:382:G:O4'	2.16	0.45
1:A:1326:A2M:HM'3	1:A:1326:A2M:H1'	1.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1341:U:H2'	1:A:1342:A:H8	1.81	0.45
1:A:1681:G:OP2	1:A:1853:G:N1	2.47	0.45
1:A:2686:G:O2'	1:A:2688:G:N7	2.45	0.45
1:A:4192:A:H2'	1:A:4193:C:H6	1.81	0.45
1:A:4429:C:N3	42:p:148:LYS:NZ	2.63	0.45
2:B:15:C:H2'	2:B:16:A:H8	1.81	0.45
1:A:478:G:H2'	1:A:479:G:C8	2.50	0.45
1:A:3816:A:H2'	1:A:3819:G:H21	1.81	0.45
1:A:4178:A:H2'	1:A:4179:G:C8	2.51	0.45
1:A:4582:C:OP2	5:E:28:LYS:NZ	2.36	0.45
2:B:54:A:C5	43:q:12:MET:HG3	2.51	0.45
6:F:144:ILE:HD12	6:F:150:LEU:HD11	1.97	0.45
6:F:159:GLU:HA	6:F:217:ILE:HB	1.97	0.45
8:H:67:ALA:HA	8:H:69:TYR:CE1	2.51	0.45
22:V:92:LYS:O	22:V:96:LEU:HG	2.16	0.45
23:W:37:MET:HG3	23:W:97:ILE:HD11	1.97	0.45
27:a:60:ARG:HB2	27:a:63:VAL:HG23	1.97	0.45
30:d:14:LYS:NZ	32:f:51:LEU:OXT	2.42	0.45
36:j:3:LYS:NZ	36:j:5:THR:OG1	2.49	0.45
36:j:22:LEU:O	36:j:26:VAL:HG12	2.16	0.45
1:A:272:U:H2'	1:A:273:U:H6	1.82	0.45
1:A:492:U:H1'	6:F:268:ARG:HH11	1.81	0.45
1:A:1424:G:O6	1:A:1462:A:N6	2.49	0.45
8:H:178:PRO:HD2	8:H:181:LEU:HD12	1.97	0.45
22:V:25:ARG:HD3	22:V:26:SER:N	2.31	0.45
23:W:45:LEU:HD12	23:W:46:VAL:H	1.82	0.45
26:Z:87:LYS:HE3	26:Z:87:LYS:HB3	1.66	0.45
43:q:35:ARG:NH1	43:q:122:SER:O	2.37	0.45
1:A:221:C:H2'	1:A:222:C:C6	2.52	0.45
1:A:1378:C:N4	44:r:159:ASN:O	2.47	0.45
1:A:2362:U:H5''	10:J:66:GLY:HA3	1.98	0.45
1:A:2674:A:C6	36:j:42:CYS:HA	2.52	0.45
1:A:2857:A:H2'	1:A:2858:A:O4'	2.17	0.45
1:A:2891:U:H2'	1:A:2892:C:O4'	2.17	0.45
1:A:3718:A2M:H2	1:A:3934:G:O4'	2.16	0.45
1:A:3910:C:H2'	1:A:3911:C:H6	1.82	0.45
1:A:4680:G:H2'	1:A:4681:A:C8	2.51	0.45
10:J:126:ARG:HD3	10:J:140:MET:HE1	1.97	0.45
28:b:16:GLU:O	28:b:20:GLN:N	2.38	0.45
1:A:229:G:H5''	19:S:11:ARG:HG3	1.97	0.45
1:A:730:G:OP2	39:m:76:ARG:NE	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1391:A:N3	1:A:4364:G:O2'	2.44	0.45
1:A:2298:U:OP1	6:F:204:ARG:NH2	2.44	0.45
1:A:2479:G:OP2	1:A:2591:A:O2'	2.34	0.45
1:A:2519:U:H1'	1:A:2520:C:C6	2.52	0.45
1:A:2555:G:H2'	1:A:2556:G:H8	1.80	0.45
1:A:4536:OMC:HM22	1:A:4537:C:H5'	1.98	0.45
3:C:13:G:O2'	10:J:121:LYS:O	2.34	0.45
5:E:57:VAL:HG22	5:E:73:VAL:HG22	1.98	0.45
13:M:128:LYS:HE2	13:M:130:GLU:OE2	2.17	0.45
15:O:25:CYS:O	15:O:28:PRO:HD2	2.16	0.45
23:W:52:CYS:HB3	23:W:57:LYS:HZ3	1.80	0.45
28:b:23:ASP:OD2	28:b:23:ASP:N	2.41	0.45
37:k:27:THR:O	37:k:27:THR:OG1	2.30	0.45
1:A:37:U:H4'	21:U:32:ARG:HD2	1.99	0.45
1:A:150:U:N3	40:n:162:ASP:O	2.36	0.45
1:A:466:A:O2'	1:A:468:U:OP2	2.32	0.45
1:A:474:C:H2'	1:A:475:G:C8	2.51	0.45
1:A:1373:A:H2	6:F:234:LYS:HD3	1.81	0.45
1:A:1662:C:H2'	1:A:1663:C:C6	2.51	0.45
1:A:3940:U:H2'	1:A:3941:G:H8	1.82	0.45
1:A:161:G:H2'	1:A:162:A:C8	2.50	0.45
1:A:663:G:H2'	1:A:664:G:H8	1.82	0.45
1:A:1266:G:H5'	22:V:99:ILE:HD11	1.98	0.45
1:A:1346:C:H2'	1:A:1347:G:C8	2.51	0.45
1:A:1683:PSU:H2'	1:A:1684:A:H8	1.81	0.45
1:A:1738:A:H2'	1:A:1739:G:C8	2.51	0.45
1:A:1809:C:H2'	1:A:1810:G:H8	1.82	0.45
1:A:2535:G:H2'	1:A:2536:A:C8	2.52	0.45
1:A:3745:U:HO2'	4:D:243:THR:H	1.61	0.45
1:A:5066:U:H2'	1:A:5067:U:C6	2.52	0.45
15:O:31:ASP:OD1	15:O:114:TYR:OH	2.26	0.45
16:P:106:VAL:HG12	16:P:112:MET:HA	1.99	0.45
18:R:39:LYS:NZ	18:R:40:ILE:O	2.44	0.45
34:h:68:HIS:HB3	34:h:134:LYS:NZ	2.32	0.45
42:p:143:ARG:HA	42:p:146:LYS:HE2	1.99	0.45
1:A:135:G:O6	28:b:97:LYS:HD3	2.17	0.45
1:A:151:G:OP2	38:l:4:TYR:OH	2.27	0.45
1:A:173:C:H4'	28:b:112:ARG:HA	1.98	0.45
1:A:373:G:OP2	30:d:36:LYS:NZ	2.46	0.45
1:A:670:G:H2'	1:A:671:G:H8	1.81	0.45
1:A:1317:U:H2'	1:A:1318:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1346:C:H2'	1:A:1347:G:H8	1.82	0.45
1:A:1733:G:N3	1:A:4214:A:H2'	2.32	0.45
1:A:1739:G:H2'	1:A:1740:C:C6	2.51	0.45
1:A:2062:C:OP1	13:M:2:LYS:HG3	2.17	0.45
1:A:2620:G:H2'	1:A:2621:A:H8	1.80	0.45
1:A:3788:C:N4	1:A:3812:C:O4'	2.50	0.45
1:A:4345:C:O2'	35:i:82:MET:SD	2.73	0.45
9:I:144:GLU:OE1	9:I:144:GLU:N	2.50	0.45
14:N:117:LYS:HE3	14:N:117:LYS:HB3	1.85	0.45
23:W:37:MET:HE2	23:W:97:ILE:HD12	1.98	0.45
26:Z:36:ARG:HB2	26:Z:80:ASN:HA	1.98	0.45
41:o:136:VAL:O	41:o:138:GLN:NE2	2.50	0.45
1:A:441:G:H2'	1:A:442:G:C8	2.52	0.45
1:A:1296:G:H2'	1:A:1297:U:H6	1.82	0.45
1:A:1486:C:H2'	1:A:1487:G:H8	1.82	0.45
1:A:1569:U:H2'	1:A:1570:G:H8	1.81	0.45
1:A:1751:A:H2'	1:A:1752:G:H8	1.82	0.45
1:A:4320:G:H2'	1:A:4321:U:C6	2.52	0.45
1:A:4551:U:H2'	1:A:4552:PSU:H6	1.82	0.45
1:A:4688:C:HO2'	41:o:155:SER:HG	1.61	0.45
2:B:70:G:H2'	2:B:71:G:H8	1.81	0.45
11:K:80:ALA:HB3	11:K:100:VAL:HG12	1.98	0.45
13:M:9:GLU:HG2	13:M:33:PHE:CE1	2.52	0.45
15:O:111:GLU:OE2	15:O:113:ARG:HD3	2.17	0.45
24:X:19:GLU:O	24:X:90:ARG:NE	2.50	0.45
26:Z:18:LEU:HD13	26:Z:19:ARG:HG3	1.98	0.45
27:a:95:PHE:CD2	27:a:96:LEU:HD23	2.52	0.45
36:j:77:VAL:O	36:j:81:SER:OG	2.32	0.45
44:r:87:HIS:HB3	44:r:90:VAL:HG23	1.99	0.45
1:A:150:U:O4	40:n:187:LYS:NZ	2.40	0.45
1:A:262:G:H2'	1:A:263:G:C8	2.52	0.45
1:A:654:C:H5''	6:F:268:ARG:HB3	1.98	0.45
1:A:705:G:H2'	1:A:706:C:C6	2.51	0.45
1:A:1478:C:H2'	1:A:1479:G:H8	1.82	0.45
1:A:1683:PSU:H2'	1:A:1684:A:C8	2.52	0.45
1:A:3787:G:H1'	1:A:3789:C:N4	2.32	0.45
1:A:4220:6MZ:H8	1:A:4220:6MZ:O5'	2.17	0.45
1:A:4419:U:H5	1:A:4420:PSU:HN1	1.65	0.45
1:A:4760:G:H2'	1:A:4761:G:O4'	2.16	0.45
1:A:5003:U:H2'	1:A:5004:C:C6	2.52	0.45
3:C:46:G:H2'	3:C:47:C:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:140:MET:HE2	10:J:140:MET:N	2.31	0.45
14:N:140:PHE:HZ	39:m:71:MET:HG3	1.81	0.45
23:W:17:ARG:HA	23:W:20:LEU:HD22	1.99	0.45
37:k:81:THR:C	37:k:82:ILE:HD13	2.41	0.45
41:o:129:ARG:HB2	41:o:153:LEU:HB3	1.99	0.45
1:A:924:C:H3'	1:A:925:C:C5'	2.47	0.44
1:A:1339:U:H2'	1:A:1340:OMC:H6	1.81	0.44
1:A:2498:C:H2'	1:A:2499:C:H6	1.82	0.44
1:A:3667:C:H4'	4:D:8:GLN:HA	1.99	0.44
1:A:5018:C:H2'	1:A:5019:A:C8	2.52	0.44
1:A:5018:C:H2'	1:A:5019:A:H8	1.82	0.44
17:Q:45:ASN:ND2	17:Q:48:GLN:OE1	2.49	0.44
19:S:37:GLU:H	19:S:37:GLU:CD	2.20	0.44
32:f:16:LYS:HA	32:f:16:LYS:HD2	1.82	0.44
40:n:51:LEU:O	40:n:55:VAL:HG23	2.18	0.44
1:A:707:C:O2'	1:A:4943:A:N1	2.42	0.44
1:A:1246:G:H2'	1:A:1247:U:H6	1.82	0.44
1:A:2666:U:OP2	12:L:124:TYR:OH	2.32	0.44
1:A:3684:G:H2'	1:A:3685:C:H6	1.83	0.44
4:D:133:TYR:HB3	4:D:168:VAL:HG12	1.99	0.44
5:E:358:ARG:HD3	5:E:358:ARG:HA	1.76	0.44
6:F:60:HIS:NE2	6:F:100:ARG:HD3	2.31	0.44
38:l:17:ASP:OD1	38:l:18:VAL:N	2.50	0.44
39:m:226:HIS:CD2	39:m:234:GLY:HA3	2.52	0.44
43:q:32:ARG:HH21	43:q:126:TYR:HE1	1.66	0.44
1:A:983:C:H2'	1:A:984:C:H6	1.83	0.44
1:A:1362:G:H5''	44:r:39:ARG:CZ	2.46	0.44
1:A:2279:A:O2'	25:Y:48:ARG:NH1	2.50	0.44
1:A:4359:U:H2'	1:A:4360:U:H6	1.82	0.44
1:A:4769:G:H5''	9:I:176:ARG:HD3	1.99	0.44
1:A:4929:C:H5''	45:s:114:LYS:HD2	2.00	0.44
20:T:120:GLU:O	20:T:124:THR:HG23	2.18	0.44
35:i:69:ARG:NH1	35:i:80:LYS:HD3	2.32	0.44
41:o:94:SER:HA	41:o:179:ILE:HA	1.99	0.44
1:A:382:G:N1	1:A:385:A:OP2	2.45	0.44
1:A:1701:A:H5'	6:F:304:ALA:HB3	1.99	0.44
1:A:2484:A:H2'	1:A:2485:U:C6	2.52	0.44
1:A:2560:C:H2'	1:A:2561:C:C6	2.53	0.44
1:A:3599:A:H2'	1:A:3600:G:H8	1.82	0.44
1:A:3944:OMG:HM22	1:A:3945:A:H5'	2.00	0.44
1:A:4285:U:H2'	1:A:4286:C:H6	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4590:A2M:HM'2	1:A:4591:U:O4'	2.18	0.44
1:A:4966:A:H2'	1:A:4967:A:C8	2.52	0.44
3:C:141:C:H5''	38:l:60[B]:VAL:HG11	1.99	0.44
5:E:224:LYS:HG2	5:E:340:THR:HG22	1.99	0.44
6:F:56:GLU:H	6:F:56:GLU:CD	2.17	0.44
12:L:112:SER:OG	12:L:114:LYS:HG3	2.16	0.44
12:L:144:LYS:HA	12:L:144:LYS:HD3	1.78	0.44
18:R:87:MET:HE1	18:R:156:ILE:HG21	1.98	0.44
44:r:56:ARG:NH1	44:r:74:ARG:O	2.46	0.44
1:A:109:G:H2'	1:A:110:C:O4'	2.18	0.44
1:A:357:U:O2	1:A:359:A:N6	2.51	0.44
1:A:1341:U:H2'	1:A:1342:A:C8	2.52	0.44
1:A:1427:A:H2	11:K:138:LEU:HD23	1.82	0.44
1:A:2460:A:O2'	38:l:104:GLU:OE1	2.36	0.44
1:A:4074:C:H2'	1:A:4075:U:C6	2.53	0.44
1:A:4135:G:H2'	1:A:4136:G:H8	1.82	0.44
1:A:4208:U:H2'	1:A:4209:G:C8	2.53	0.44
1:A:4598:C:H2'	1:A:4611:A:N6	2.32	0.44
5:E:78:ILE:HD13	5:E:332:MET:HG3	1.99	0.44
19:S:88:GLU:OE1	19:S:88:GLU:HA	2.18	0.44
36:j:88:GLU:HA	36:j:91:ASP:HB2	2.00	0.44
41:o:51:LYS:H	41:o:51:LYS:CD	2.28	0.44
1:A:252:C:H2'	1:A:253:G:H8	1.83	0.44
1:A:1617:G:O3'	30:d:12:ARG:NH2	2.51	0.44
1:A:1626:G:OP2	38:l:77:LYS:NZ	2.39	0.44
1:A:2080:U:H2'	1:A:2081:C:C6	2.53	0.44
1:A:2376:A:H2'	1:A:2377:C:C6	2.52	0.44
1:A:2662:G:H2'	1:A:2663:G:C8	2.52	0.44
1:A:3923:A:H2'	1:A:3924:C:C6	2.53	0.44
2:B:57:C:H2'	2:B:58:A:C8	2.50	0.44
5:E:220:ILE:HB	5:E:346:THR:HB	2.00	0.44
6:F:60:HIS:HA	6:F:92:PHE:HE1	1.81	0.44
11:K:177:ALA:O	11:K:184:ARG:HB2	2.17	0.44
15:O:65:ARG:HD2	15:O:67:LYS:O	2.17	0.44
34:h:99:GLU:HG3	34:h:101:LEU:H	1.82	0.44
45:s:91:TRP:O	45:s:95:ILE:HG13	2.17	0.44
1:A:4:G:H2'	1:A:5:A:H8	1.82	0.44
1:A:113:A:OP2	1:A:156:G:N1	2.35	0.44
1:A:1095:A:H2'	1:A:1096:C:H6	1.82	0.44
1:A:1291:G:H2'	1:A:1292:C:C6	2.53	0.44
1:A:1797:G:OP1	39:m:104:LYS:NZ	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1912:G:N2	9:I:87:MET:SD	2.91	0.44
1:A:2034:G:H2'	1:A:2035:C:H6	1.83	0.44
1:A:2744:A:H2'	1:A:2745:A:C8	2.53	0.44
1:A:2890:C:H42	1:A:3611:A:H61	1.65	0.44
1:A:3910:C:H2'	1:A:3911:C:C6	2.53	0.44
1:A:4069:U:H2'	1:A:4070:U:C6	2.53	0.44
1:A:4291:G:H5'	1:A:4293:PSU:C6	2.51	0.44
1:A:4593:C:H2'	1:A:4594:U:C6	2.53	0.44
1:A:4930:C:C2	1:A:4931:G:C8	3.06	0.44
6:F:144:ILE:O	6:F:147:VAL:HG22	2.17	0.44
8:H:182:ASN:OD1	8:H:182:ASN:N	2.50	0.44
11:K:166:TYR:HB3	44:r:8:MET:HB2	2.00	0.44
12:L:142:ILE:HD12	12:L:143:HIS:H	1.83	0.44
14:N:111:GLU:HA	14:N:114:GLN:HE21	1.82	0.44
29:c:44:ILE:HG13	38:l:9:GLU:HB3	2.00	0.44
36:j:6:LYS:HG2	36:j:7:LYS:HG3	1.99	0.44
1:A:49:U:H2'	1:A:50:C:O2	2.18	0.44
1:A:655:C:P	6:F:268:ARG:HE	2.41	0.44
1:A:1075:G:H2'	1:A:1076:C:C6	2.53	0.44
1:A:1418:C:H2'	1:A:1419:G:O4'	2.17	0.44
1:A:1874:A:O4'	1:A:4213:A:N6	2.51	0.44
1:A:4621:C:H2'	1:A:4622:A:H8	1.82	0.44
1:A:4718:G:O2'	1:A:4719:G:N2	2.51	0.44
13:M:31:ARG:C	13:M:32:ILE:HD13	2.43	0.44
22:V:102:PRO:HA	22:V:109:ARG:HH12	1.83	0.44
31:e:51:GLU:O	31:e:55:LYS:HG2	2.18	0.44
1:A:138:G:H2'	1:A:139:G:H8	1.82	0.44
1:A:273:U:H2'	1:A:274:C:C6	2.53	0.44
1:A:425:U:H2'	1:A:426:A:C8	2.52	0.44
1:A:1823:G:H2'	1:A:1824:G:C8	2.53	0.44
1:A:2068:C:H5''	26:Z:15:LYS:HE3	1.99	0.44
1:A:2735:G:H2'	1:A:2736:G:C8	2.51	0.44
1:A:2749:C:H2'	1:A:2750:G:C8	2.53	0.44
1:A:2856:C:O2	5:E:242:ARG:NH2	2.41	0.44
1:A:4263:C:H2'	1:A:4264:G:O4'	2.17	0.44
1:A:4415:A:H4'	42:p:74:LYS:HD2	2.00	0.44
2:B:111:C:H2'	2:B:112:U:O4'	2.17	0.44
11:K:14:ARG:HE	11:K:16:LYS:NZ	2.16	0.44
13:M:164:LYS:HE2	26:Z:34:TYR:HB2	1.99	0.44
16:P:30:ASP:OD2	16:P:30:ASP:N	2.50	0.44
22:V:22:LYS:HA	22:V:22:LYS:HE3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:G:H2'	1:A:675:C:H6	1.82	0.43
1:A:1338:G:H4'	1:A:1339:U:H6	1.83	0.43
1:A:5019:A:H2'	1:A:5020:G:C8	2.53	0.43
2:B:83:A:H4'	39:m:224:THR:HB	2.00	0.43
3:C:130:C:H2'	3:C:131:G:H8	1.82	0.43
8:H:192:LYS:HG2	26:Z:107:PRO:HB3	1.99	0.43
8:H:252:ALA:O	8:H:255:SER:OG	2.35	0.43
15:O:52:LYS:HE2	15:O:52:LYS:HB3	1.85	0.43
17:Q:42:SER:O	17:Q:42:SER:OG	2.35	0.43
17:Q:58:LYS:HG2	17:Q:59:HIS:CD2	2.52	0.43
33:g:77:ILE:HB	33:g:78:ILE:H	1.67	0.43
1:A:25:A:C8	1:A:341:G:C8	3.06	0.43
1:A:398:A2M:H8	1:A:398:A2M:O5'	2.17	0.43
1:A:653:U:H2'	1:A:654:C:H6	1.83	0.43
1:A:743:G:O6	1:A:922:C:N4	2.51	0.43
1:A:949:G:H2'	1:A:950:G:C8	2.51	0.43
1:A:1324:A:O2'	1:A:1326:A2M:OP1	2.27	0.43
1:A:2429:A:H5''	32:f:43:HIS:HE2	1.82	0.43
1:A:2684:C:H2'	1:A:2685:C:C6	2.53	0.43
1:A:2734:U:H2'	1:A:2735:G:C8	2.53	0.43
1:A:2770:C:H2'	1:A:2771:G:C8	2.50	0.43
1:A:3619:G:H22	1:A:3624:A:H1'	1.83	0.43
1:A:3870:C:H2'	1:A:3871:A:C8	2.47	0.43
1:A:4080:C:H2'	1:A:4081:G:H8	1.83	0.43
1:A:4304:A:OP2	1:A:4305:G:N2	2.51	0.43
1:A:4417:C:H2'	1:A:4418:G:O4'	2.17	0.43
1:A:4471:PSU:H2'	1:A:4472:G:C8	2.52	0.43
1:A:4582:C:H4'	5:E:99:LEU:HB2	1.99	0.43
4:D:24:LYS:HG3	4:D:49:ILE:HD12	1.99	0.43
9:I:192:TYR:CZ	45:s:118:MET:HG2	2.52	0.43
29:c:12:ASN:O	29:c:16:LYS:NZ	2.51	0.43
34:h:107:VAL:HB	34:h:118:HIS:HB2	1.99	0.43
41:o:106:GLN:N	41:o:106:GLN:OE1	2.50	0.43
1:A:271:C:H2'	1:A:272:U:H6	1.82	0.43
1:A:1217:G:H2'	1:A:1218:G:H8	1.82	0.43
1:A:1616:U:H2'	1:A:1617:G:H8	1.83	0.43
1:A:2078:C:H2'	1:A:2079:G:C8	2.53	0.43
1:A:2335:C:H2'	1:A:2336:G:H8	1.82	0.43
1:A:4070:U:H2'	1:A:4071:U:H6	1.83	0.43
1:A:4070:U:H2'	1:A:4071:U:C6	2.53	0.43
1:A:4072:C:C2	1:A:4073:A:C8	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4239:A:H2'	1:A:4240:G:H8	1.83	0.43
1:A:4454:G:H1	1:A:4526:U:H3	1.66	0.43
22:V:104:LEU:H	22:V:104:LEU:HD12	1.83	0.43
30:d:67:LEU:HD23	30:d:67:LEU:HA	1.84	0.43
34:h:142:VAL:HG23	34:h:148:VAL:HG12	2.00	0.43
1:A:666:G:O4'	37:k:67:ARG:NH2	2.45	0.43
1:A:1728:U:H2'	1:A:1729:A:H8	1.82	0.43
1:A:1848:C:H2'	1:A:1849:U:O4'	2.18	0.43
1:A:2037:C:H2'	1:A:2038:U:C6	2.54	0.43
1:A:4238:G:H2'	1:A:4239:A:C8	2.53	0.43
1:A:4748:U:H5''	26:Z:54:LYS:HE2	2.00	0.43
17:Q:60:LYS:HE2	17:Q:60:LYS:HB2	1.76	0.43
20:T:68:ILE:O	20:T:115:LYS:NZ	2.41	0.43
22:V:36:ASP:OD1	22:V:38:LYS:N	2.51	0.43
35:i:12:CYS:HB3	35:i:15:CYS:HB2	2.00	0.43
35:i:45:GLN:HE22	35:i:51:GLN:HA	1.82	0.43
39:m:77:LYS:HE2	39:m:77:LYS:HB3	1.91	0.43
39:m:220:MET:HG3	39:m:232:ASP:OD2	2.19	0.43
1:A:40:G:N2	1:A:4380:A:H62	2.16	0.43
1:A:1486:C:H2'	1:A:1487:G:C8	2.54	0.43
1:A:2643:G:H1	1:A:2691:U:H3	1.67	0.43
1:A:3634:G:N2	1:A:3636:C:H5''	2.34	0.43
1:A:4239:A:H2'	1:A:4240:G:C8	2.54	0.43
1:A:4676:G:OP1	5:E:281:ASN:ND2	2.48	0.43
1:A:4716:C:H2'	1:A:4717:A:H8	1.84	0.43
2:B:58:A:H2'	2:B:59:G:H8	1.83	0.43
15:O:31:ASP:OD2	15:O:31:ASP:N	2.37	0.43
15:O:80:LYS:HG2	15:O:110:TYR:CE2	2.53	0.43
35:i:99:ARG:HA	35:i:99:ARG:NE	2.33	0.43
41:o:147:GLU:OE2	41:o:147:GLU:HA	2.19	0.43
42:p:57:TYR:HD1	42:p:120:HIS:HA	1.83	0.43
1:A:1247:U:H2'	1:A:1248:C:C6	2.53	0.43
1:A:1435:G:O2'	1:A:1436:C:H5'	2.19	0.43
1:A:1687:U:H2'	1:A:1688:G:C8	2.54	0.43
1:A:1950:U:O2'	13:M:116:ARG:NH1	2.51	0.43
1:A:2417:A:C4	46:O:445:MET:HE3	2.53	0.43
1:A:2448:G:H2'	1:A:2449:A:C8	2.54	0.43
1:A:2540:C:H2'	1:A:2541:G:H8	1.83	0.43
1:A:4892:A:H2'	1:A:4893:A:O4'	2.17	0.43
3:C:66:A:H2'	3:C:67:U:H6	1.83	0.43
4:D:208:GLU:H	4:D:208:GLU:HG2	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:77:THR:HG21	5:E:337:VAL:HG22	2.00	0.43
6:F:230:LEU:HD21	6:F:239:LYS:HG3	1.99	0.43
31:e:40:ARG:HD3	31:e:41:TYR:CE1	2.54	0.43
31:e:69:LEU:HD23	31:e:69:LEU:HA	1.82	0.43
39:m:29:LYS:HG2	39:m:32:ARG:HH22	1.83	0.43
41:o:107:GLU:OE1	41:o:107:GLU:N	2.52	0.43
45:s:29:ASP:OD2	45:s:30:VAL:N	2.50	0.43
1:A:197:A:N1	1:A:225:G:O2'	2.50	0.43
1:A:385:A:H4'	1:A:386:A:H5'	2.00	0.43
1:A:1290:G:H2'	1:A:1291:G:C8	2.53	0.43
1:A:1307:A:H2'	1:A:1308:C:C6	2.54	0.43
1:A:1509:C:H2'	1:A:1510:G:C8	2.54	0.43
1:A:2275:G:H2'	1:A:2276:A:H8	1.84	0.43
1:A:3830:A2M:HM'2	1:A:3831:U:O4'	2.19	0.43
1:A:4208:U:H2'	1:A:4209:G:H8	1.84	0.43
5:E:356:LYS:HZ2	5:E:358:ARG:HB2	1.83	0.43
8:H:164:PHE:HA	8:H:175:VAL:HG12	1.99	0.43
15:O:37:ALA:HA	15:O:65:ARG:HH22	1.83	0.43
22:V:65:MET:HE3	22:V:65:MET:HB3	1.75	0.43
24:X:26:THR:OG1	24:X:85:ARG:NH1	2.36	0.43
28:b:13:LYS:HE2	28:b:15:GLU:OE1	2.19	0.43
39:m:51:TYR:HD1	39:m:52:GLU:OE1	2.01	0.43
41:o:17:ASP:OD1	41:o:17:ASP:N	2.51	0.43
42:p:174:MET:HB2	42:p:180:LEU:HD13	2.01	0.43
1:A:1089:G:H2'	1:A:1090:G:C8	2.54	0.43
1:A:1096:C:H2'	1:A:1097:C:C6	2.54	0.43
1:A:2340:C:H2'	1:A:2341:A:H8	1.84	0.43
1:A:2849:A:O2'	1:A:2855:G:N7	2.52	0.43
1:A:2897:G:C2	1:A:3603:G:C2	3.07	0.43
1:A:3794:C:H2'	1:A:3795:A:H8	1.83	0.43
3:C:27:U:H2'	3:C:28:C:C6	2.54	0.43
11:K:155:ALA:HB3	11:K:158:THR:HG23	2.00	0.43
23:W:22:MET:HG3	23:W:85:CYS:O	2.19	0.43
25:Y:35:TRP:CZ2	25:Y:56:PRO:HD2	2.54	0.43
37:k:33:LYS:HD2	37:k:40:TYR:CZ	2.53	0.43
38:l:124:ASP:OD1	38:l:126:THR:OG1	2.32	0.43
42:p:196:LEU:HD12	42:p:196:LEU:HA	1.88	0.43
1:A:7:C:H2'	1:A:8:U:H6	1.83	0.43
1:A:252:C:H2'	1:A:253:G:C8	2.54	0.43
1:A:1204:C:H2'	1:A:1205:G:C8	2.53	0.43
1:A:2072:C:C2	1:A:2073:C:C5	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2275:G:OP1	6:F:312:ARG:NH1	2.51	0.43
1:A:2689:C:H2'	1:A:2690:C:C6	2.54	0.43
1:A:2728:U:H2'	1:A:2729:C:H6	1.84	0.43
1:A:3667:C:H2'	1:A:3668:C:H6	1.84	0.43
1:A:3942:A:H2'	1:A:3943:A:C8	2.54	0.43
1:A:4306:OMU:HM22	1:A:4307:A:H5'	2.01	0.43
8:H:112:MET:HE3	8:H:113:PRO:HD2	2.00	0.43
8:H:261:ILE:HA	8:H:267:LEU:HD23	2.00	0.43
34:h:109:THR:HB	34:h:149:GLY:HA2	2.00	0.43
40:n:88:ASP:OD2	40:n:88:ASP:C	2.61	0.43
1:A:387:G:C6	1:A:412:G:H1'	2.53	0.43
1:A:670:G:H2'	1:A:671:G:C8	2.54	0.43
1:A:734:G:C2	1:A:735:G:C8	3.06	0.43
1:A:1209:U:O2'	1:A:1211:G:H5'	2.17	0.43
1:A:1666:C:H2'	1:A:1667:G:O4'	2.19	0.43
1:A:1703:C:H2'	1:A:1704:C:O4'	2.19	0.43
1:A:2514:G:O2'	1:A:2743:A:N6	2.52	0.43
1:A:3664:G:C2	1:A:3665:G:N7	2.87	0.43
1:A:3707:U:H3	1:A:3743:G:H1	1.67	0.43
1:A:3748:A:O5'	4:D:243:THR:OG1	2.37	0.43
1:A:4254:G:H2'	1:A:4254:G:N3	2.33	0.43
1:A:4376:A:O2'	21:U:42:ARG:NH1	2.52	0.43
1:A:4404:U:O2'	1:A:4406:U:O4	2.36	0.43
1:A:4618:OMG:HM22	1:A:4619:U:H5'	2.01	0.43
1:A:4688:C:H2'	1:A:4689:PSU:C6	2.53	0.43
1:A:4761:G:H2'	1:A:4762:A:C8	2.54	0.43
1:A:5019:A:H2'	1:A:5020:G:H8	1.84	0.43
5:E:94:GLU:H	5:E:94:GLU:CD	2.26	0.43
20:T:102:ARG:H	20:T:102:ARG:NE	2.01	0.43
30:d:39:TYR:CG	30:d:40:PRO:HA	2.54	0.43
33:g:80:PRO:O	33:g:84:GLN:HG3	2.19	0.43
34:h:99:GLU:HG3	34:h:101:LEU:N	2.34	0.43
41:o:138:GLN:CD	41:o:138:GLN:N	2.77	0.43
1:A:263:G:H2'	1:A:264:C:C6	2.54	0.42
1:A:648:G:H2'	1:A:649:A:H8	1.84	0.42
1:A:1629:G:N2	4:D:208:GLU:OE1	2.50	0.42
1:A:1748:U:H2'	1:A:1749:A:C8	2.54	0.42
1:A:1777:C:H2'	1:A:1778:C:H6	1.84	0.42
1:A:3702:A:H1'	1:A:3774:A:C8	2.53	0.42
1:A:4071:U:H2'	1:A:4072:C:H6	1.83	0.42
1:A:4159:C:H2'	1:A:4160:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4173:G:H2'	1:A:4174:U:C6	2.54	0.42
1:A:4929:C:H2'	1:A:4930:C:H6	1.82	0.42
16:P:112:MET:HE2	16:P:135:ASN:HD22	1.83	0.42
23:W:79:ILE:O	23:W:83:THR:HG23	2.18	0.42
34:h:177:LEU:HB2	34:h:179:VAL:HG12	2.01	0.42
39:m:64:MET:O	39:m:68:GLU:HG2	2.19	0.42
39:m:156:LYS:HD3	39:m:248:ASN:OD1	2.19	0.42
42:p:84:GLY:O	42:p:130:THR:OG1	2.31	0.42
1:A:341:G:C2	1:A:342:G:C8	3.07	0.42
1:A:469:C:H2'	1:A:470:A:H8	1.84	0.42
1:A:907:C:H2'	1:A:908:G:C8	2.54	0.42
1:A:1249:C:H2'	1:A:1250:C:H6	1.84	0.42
1:A:2338:C:C2	1:A:2339:G:C8	3.07	0.42
1:A:2634:C:H2'	1:A:2635:U:C6	2.55	0.42
1:A:3826:C:H2'	1:A:3827:G:C8	2.54	0.42
1:A:3927:U:H2'	1:A:3928:A:C8	2.53	0.42
1:A:4736:C:H2'	1:A:4737:G:C8	2.54	0.42
1:A:5053:U:H3'	1:A:5054:C:C6	2.54	0.42
2:B:24:C:H2'	2:B:25:G:O4'	2.18	0.42
3:C:7:U:H2'	3:C:8:U:H6	1.84	0.42
5:E:90:VAL:HG13	5:E:161:ARG:HB2	2.01	0.42
38:l:124:ASP:OD1	38:l:126:THR:N	2.41	0.42
39:m:89:LEU:HD11	39:m:122:PHE:HB3	2.01	0.42
39:m:154:ILE:HD12	39:m:191:ILE:HG12	2.00	0.42
44:r:90:VAL:O	44:r:93:THR:OG1	2.35	0.42
1:A:436:C:H2'	1:A:437:G:C8	2.53	0.42
1:A:922:C:H2'	1:A:923:C:C6	2.54	0.42
1:A:1361:G:H2'	1:A:1362:G:C8	2.54	0.42
1:A:1366:G:N2	44:r:33:ILE:HG21	2.34	0.42
1:A:1932:A:H2'	1:A:1933:G:C8	2.54	0.42
1:A:2396:A:N7	1:A:2814:C:H2'	2.34	0.42
1:A:2518:G:H1'	1:A:2539:C:H1'	1.99	0.42
1:A:2671:C:H2'	1:A:2672:C:C6	2.54	0.42
1:A:3717:A:P	1:A:3735:G:H21	2.41	0.42
1:A:3906:A:H5''	6:F:69:THR:OG1	2.19	0.42
1:A:4266:G:H2'	1:A:4266:G:N3	2.34	0.42
2:B:16:A:H2'	2:B:17:C:C6	2.55	0.42
3:C:28:C:H2'	3:C:29:G:H8	1.85	0.42
15:O:34:MET:HE3	15:O:34:MET:O	2.20	0.42
16:P:15:ARG:HG3	16:P:15:ARG:NH1	2.34	0.42
21:U:64:LYS:HE3	21:U:67:GLN:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:105:ILE:HD12	23:W:106:ARG:N	2.34	0.42
25:Y:89:LEU:HD13	25:Y:118:LEU:HG	1.99	0.42
36:j:26:VAL:HG22	36:j:30:GLU:HG3	2.01	0.42
40:n:189:ARG:HG2	40:n:192:ARG:HH12	1.84	0.42
1:A:23:C:H2'	1:A:24:G:O4'	2.20	0.42
1:A:253:G:H2'	1:A:254:G:C8	2.54	0.42
1:A:423:G:H2'	1:A:424:U:C6	2.54	0.42
1:A:663:G:H2'	1:A:664:G:C8	2.54	0.42
1:A:1472:C:H2'	1:A:1473:U:C6	2.54	0.42
1:A:1509:C:H2'	1:A:1510:G:H8	1.84	0.42
1:A:1603:C:H2'	1:A:1604:G:H8	1.84	0.42
1:A:1727:U:H2'	1:A:1728:U:H6	1.84	0.42
1:A:1795:A:N3	2:B:79:U:O2'	2.51	0.42
1:A:2079:G:H2'	1:A:2080:U:H6	1.84	0.42
1:A:2456:G:H2'	1:A:2457:G:C8	2.54	0.42
1:A:2863:G:O2'	12:L:82:LYS:O	2.32	0.42
1:A:3707:U:H2'	1:A:3708:C:C6	2.54	0.42
1:A:4454:G:H2'	1:A:4455:G:H8	1.85	0.42
20:T:57:MET:HG3	20:T:62:ILE:HG13	2.02	0.42
25:Y:58:ILE:HD12	25:Y:58:ILE:HA	1.91	0.42
39:m:60:GLU:HA	39:m:63:GLN:HB2	2.01	0.42
44:r:63:THR:HG22	44:r:65:ARG:N	2.32	0.42
1:A:163:A:H2'	1:A:164:G:H8	1.83	0.42
1:A:963:G:H3'	1:A:963:G:N3	2.34	0.42
1:A:1828:C:H1'	22:V:57:MET:HE3	2.01	0.42
1:A:2480:G:H2'	1:A:2481:G:H8	1.84	0.42
1:A:2694:G:H5'	1:A:2695:A:C2	2.55	0.42
1:A:2803:U:H2'	1:A:2804:OMC:C6	2.55	0.42
1:A:3670:C:N4	1:A:3671:G:O6	2.52	0.42
1:A:3774:A:H2'	1:A:3775:A:H8	1.77	0.42
1:A:3941:G:H2'	1:A:3942:A:C8	2.54	0.42
1:A:4272:G:O2'	1:A:4273:A:H8	2.02	0.42
1:A:4453:C:H2'	1:A:4454:G:O4'	2.19	0.42
3:C:75:OMG:HM22	3:C:76:C:O4'	2.19	0.42
14:N:107:LYS:HE3	14:N:107:LYS:HB3	1.84	0.42
21:U:49:HIS:NE2	44:r:7:GLY:O	2.40	0.42
42:p:56:GLU:OE2	42:p:152:ARG:N	2.40	0.42
42:p:85:PHE:HD2	42:p:87:ILE:HG13	1.85	0.42
43:q:42:GLN:NE2	43:q:117:ILE:HG23	2.34	0.42
1:A:169:G:H2'	1:A:170:C:O4'	2.20	0.42
1:A:1283:G:N1	1:A:2076:G:OP1	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1338:G:H4'	1:A:1339:U:C6	2.55	0.42
1:A:1392:A:H2'	1:A:1393:G:C8	2.55	0.42
1:A:1802:A:H4'	14:N:105:PHE:CE1	2.55	0.42
1:A:2295:C:H2'	1:A:2296:G:C8	2.54	0.42
1:A:2611:A:H2'	1:A:2612:G:C8	2.54	0.42
1:A:2844:A:N6	1:A:3839:G:O2'	2.51	0.42
1:A:2897:G:N3	1:A:3603:G:N2	2.67	0.42
1:A:3808:OMC:H3'	1:A:3809:G:C2	2.54	0.42
1:A:4071:U:H2'	1:A:4072:C:C6	2.55	0.42
1:A:4359:U:H2'	1:A:4360:U:C6	2.54	0.42
1:A:4460:U:H2'	1:A:4461:C:C6	2.55	0.42
1:A:4577:U:H2'	1:A:4578:G:C8	2.53	0.42
1:A:4970:C:C2	1:A:4971:A:C8	3.08	0.42
3:C:6:C:H2'	3:C:7:U:H6	1.84	0.42
3:C:119:C:H2'	3:C:120:G:C8	2.54	0.42
4:D:57:PRO:HG2	4:D:78:ALA:HB3	2.00	0.42
4:D:176:ASP:OD2	4:D:176:ASP:C	2.62	0.42
21:U:123:ILE:HD11	44:r:169:ILE:HG13	2.01	0.42
23:W:31:TYR:CZ	23:W:35:LEU:HD11	2.55	0.42
42:p:46:PHE:HB2	42:p:129:ARG:HH11	1.84	0.42
43:q:56:THR:OG1	43:q:64:ARG:N	2.52	0.42
44:r:12:PRO:HB2	44:r:14:PHE:HD2	1.84	0.42
45:s:70:GLN:HE21	45:s:74:ARG:NH2	2.16	0.42
1:A:274:C:H2'	1:A:275:C:C6	2.54	0.42
1:A:681:G:H2'	1:A:682:G:H8	1.85	0.42
1:A:1204:C:H2'	1:A:1205:G:H8	1.83	0.42
1:A:1368:A:H2'	1:A:1369:C:O4'	2.19	0.42
1:A:1724:G:N2	1:A:1876:U:OP1	2.53	0.42
1:A:1879:C:O2'	1:A:1891:A:N3	2.46	0.42
1:A:2822:G:OP2	12:L:21:LYS:NZ	2.51	0.42
1:A:3927:U:H2'	1:A:3928:A:H8	1.84	0.42
1:A:4135:G:H2'	1:A:4136:G:C8	2.54	0.42
1:A:4896:G:H2'	1:A:4897:G:H8	1.85	0.42
1:A:4959:U:H2'	1:A:4960:G:H8	1.85	0.42
1:A:4967:A:P	5:E:126:LYS:H	2.43	0.42
2:B:7:G:H2'	2:B:8:G:H8	1.85	0.42
2:B:62:U:O2'	2:B:64:G:O4'	2.37	0.42
11:K:8:ASN:O	11:K:9:LYS:HE2	2.19	0.42
19:S:47:MET:HE2	19:S:47:MET:HB2	1.69	0.42
20:T:92:ASP:OD2	20:T:92:ASP:C	2.63	0.42
1:A:94:A:H5''	21:U:34:ASN:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1330:A:H5''	1:A:3865:A:H5''	2.02	0.42
1:A:1725:U:H2'	1:A:1726:U:C6	2.50	0.42
1:A:1865:G:OP2	42:p:98:ARG:NH2	2.44	0.42
1:A:4069:U:H2'	1:A:4070:U:H6	1.84	0.42
1:A:4080:C:H2'	1:A:4081:G:C8	2.55	0.42
1:A:4968:A:H2'	1:A:4969:C:H6	1.85	0.42
2:B:73:U:OP2	2:B:74:A:O2'	2.35	0.42
17:Q:57:ARG:HA	17:Q:57:ARG:CZ	2.49	0.42
22:V:36:ASP:OD1	22:V:36:ASP:C	2.63	0.42
33:g:126:LYS:HD2	33:g:126:LYS:N	2.35	0.42
34:h:104:LEU:O	34:h:108:THR:OG1	2.30	0.42
1:A:1273:G:C6	8:H:73:TYR:HB2	2.54	0.42
1:A:1361:G:H2'	1:A:1362:G:H8	1.85	0.42
1:A:1473:U:H2'	1:A:1474:C:C6	2.55	0.42
1:A:1817:U:H2'	1:A:1818:G:O4'	2.20	0.42
1:A:2313:A:H5'	1:A:2314:G:OP2	2.19	0.42
1:A:2456:G:H2'	1:A:2457:G:H8	1.85	0.42
1:A:2610:G:H2'	1:A:2611:A:H8	1.85	0.42
1:A:2869:U:O2'	1:A:2881:A:N7	2.36	0.42
1:A:3681:G:C6	4:D:125:LYS:HB3	2.55	0.42
1:A:4192:A:H2'	1:A:4193:C:C6	2.55	0.42
1:A:4708:A:N3	1:A:4709:U:H5'	2.34	0.42
1:A:4881:U:O4	45:s:116:LYS:NZ	2.42	0.42
1:A:4909:A:OP1	9:I:163:LYS:NZ	2.53	0.42
1:A:4957:C:H2'	1:A:4958:C:C6	2.55	0.42
3:C:44:A:H2'	3:C:45:C:C6	2.55	0.42
3:C:141:C:H2'	3:C:142:U:C6	2.55	0.42
4:D:117:GLU:HG2	4:D:122:ASP:OD1	2.20	0.42
5:E:94:GLU:OE1	5:E:158:GLN:HB2	2.19	0.42
5:E:307:TYR:CD2	5:E:366:LYS:HG2	2.54	0.42
10:J:117:ILE:HG13	10:J:148:MET:HB3	2.01	0.42
11:K:122:THR:OG1	11:K:124:ASP:OD1	2.24	0.42
31:e:9:LYS:O	31:e:13:LEU:HD22	2.20	0.42
31:e:47:ILE:HG21	31:e:52:LYS:HB2	2.01	0.42
35:i:74:GLU:OE1	35:i:75:PRO:HD2	2.19	0.42
1:A:97:G:N7	44:r:13:HIS:NE2	2.60	0.42
1:A:131:C:N3	1:A:132:G:H1'	2.35	0.42
1:A:676:C:H2'	1:A:677:G:C8	2.54	0.42
1:A:705:G:H2'	1:A:706:C:H6	1.85	0.42
1:A:942:G:H3'	39:m:148:LYS:HD3	2.02	0.42
1:A:1806:G:H2'	1:A:1807:C:H6	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1867:A:H2'	1:A:1868:A:C8	2.54	0.42
1:A:2412:A:H2'	1:A:2413:U:H6	1.84	0.42
1:A:2684:C:H2'	1:A:2685:C:H6	1.84	0.42
1:A:2757:A:H2'	1:A:2758:G:C8	2.55	0.42
1:A:2838:G:H2'	1:A:2839:PSU:C6	2.55	0.42
1:A:3707:U:H2'	1:A:3708:C:H6	1.84	0.42
1:A:4297:G:H22	1:A:4313:A:H2	1.68	0.42
1:A:4712:C:C2	1:A:4713:G:C8	3.08	0.42
1:A:5039:U:OP2	1:A:5040:U:O2'	2.38	0.42
2:B:2:U:H2'	2:B:3:C:C6	2.55	0.42
13:M:7:LEU:H	13:M:107:THR:CG2	2.32	0.42
13:M:161:ARG:HA	13:M:161:ARG:HD2	1.86	0.42
39:m:106:ARG:O	39:m:110:GLN:HG3	2.20	0.42
42:p:179:ARG:HE	42:p:189:TYR:HE1	1.68	0.42
1:A:303:C:OP2	38:l:68:ARG:NH2	2.48	0.41
1:A:1351:G:H2'	1:A:1352:C:C6	2.55	0.41
1:A:1449:C:H2'	1:A:1450:C:H6	1.85	0.41
1:A:2620:G:H1	1:A:2636:U:H3	1.68	0.41
1:A:3662:A:O4'	1:A:3664:G:C8	2.73	0.41
1:A:3724:A2M:H2'	1:A:3725:G:C8	2.55	0.41
1:A:3727:A:H2'	1:A:3728:A:C8	2.56	0.41
1:A:4323:A:C6	7:G:153:THR:HG21	2.55	0.41
1:A:4420:PSU:O4	1:A:4420:PSU:H2'	2.19	0.41
1:A:4525:C:H5''	5:E:245:HIS:HB3	2.02	0.41
1:A:4750:G:H2'	1:A:4751:G:C8	2.54	0.41
1:A:5030:U:H2'	1:A:5031:G:C8	2.54	0.41
2:B:85:G:H2'	2:B:86:G:H8	1.85	0.41
3:C:28:C:C2	3:C:29:G:C8	3.08	0.41
3:C:133:G:H2'	3:C:134:G:H8	1.85	0.41
7:G:208:MET:HB3	7:G:219:TYR:HE1	1.85	0.41
7:G:236:MET:O	7:G:239:MET:HG3	2.20	0.41
14:N:158:PHE:C	14:N:158:PHE:CD2	2.98	0.41
15:O:100:LEU:HD23	15:O:100:LEU:HA	1.88	0.41
23:W:26:LYS:H	23:W:98:ASP:HB3	1.84	0.41
27:a:82:MET:HE2	27:a:82:MET:HB2	1.94	0.41
40:n:138:ALA:HB2	40:n:194:VAL:HG11	2.01	0.41
1:A:233:U:O2'	1:A:2304:U:O4	2.34	0.41
1:A:462:G:H2'	1:A:463:A:H8	1.85	0.41
1:A:674:G:H2'	1:A:675:C:C6	2.54	0.41
1:A:959:G:C8	8:H:123:ARG:HG2	2.55	0.41
1:A:1523:A:N3	1:A:4389:C:O2'	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1524:A2M:HM'3	1:A:3916:G:O2'	2.20	0.41
1:A:2078:C:H2'	1:A:2079:G:H8	1.84	0.41
1:A:4356:G:H2'	1:A:4357:G:H8	1.84	0.41
1:A:4538:G:H2'	1:A:4539:U:C6	2.55	0.41
1:A:4622:A:H2'	1:A:4623:OMG:H8	1.86	0.41
3:C:68:G:H2'	3:C:69:PSU:O4'	2.20	0.41
3:C:76:C:H2'	3:C:77:A:C8	2.56	0.41
5:E:56:ILE:HG22	5:E:368:ILE:HA	2.01	0.41
6:F:141:GLY:O	6:F:182:LYS:NZ	2.45	0.41
9:I:185:VAL:O	9:I:189:ILE:HG12	2.20	0.41
18:R:72:ASP:C	18:R:72:ASP:OD1	2.62	0.41
32:f:34:LYS:HE3	32:f:34:LYS:HB2	1.79	0.41
34:h:130:ALA:O	34:h:134:LYS:HA	2.21	0.41
1:A:299:C:C2	1:A:300:A:C8	3.08	0.41
1:A:345:C:H2'	1:A:346:G:H8	1.85	0.41
1:A:461:G:H2'	1:A:462:G:C8	2.54	0.41
1:A:1309:C:H2'	1:A:1310:C:H6	1.85	0.41
1:A:2743:A:H2'	1:A:2744:A:C8	2.55	0.41
1:A:2870:A:H2'	1:A:2871:A:C8	2.55	0.41
1:A:3731:C:H2'	1:A:3732:A:C8	2.54	0.41
1:A:4872:G:H4'	1:A:4873:G:H5''	2.01	0.41
1:A:4918:C:H2'	1:A:4919:G:H8	1.86	0.41
6:F:66:SER:HA	6:F:77:PRO:HA	2.02	0.41
12:L:25:ASP:C	12:L:25:ASP:OD2	2.63	0.41
13:M:107:THR:O	13:M:111:ARG:HG2	2.20	0.41
18:R:101:ASP:OD1	18:R:102:VAL:N	2.53	0.41
19:S:49:ILE:HD12	19:S:49:ILE:HA	1.86	0.41
23:W:79:ILE:HG13	23:W:90:ARG:HG2	2.02	0.41
24:X:44:ARG:O	24:X:48:GLU:HG2	2.20	0.41
27:a:87:VAL:O	27:a:91:ILE:HG13	2.21	0.41
40:n:259:LYS:HD2	40:n:260:GLU:HB2	2.02	0.41
45:s:36:ALA:HB2	45:s:52:PHE:CZ	2.56	0.41
1:A:31:U:H3	1:A:51:A:H61	1.67	0.41
1:A:268:G:H2'	1:A:269:G:C8	2.54	0.41
1:A:446:C:H2'	1:A:447:C:C6	2.55	0.41
1:A:690:C:H2'	1:A:691:C:C6	2.55	0.41
1:A:1207:C:H2'	1:A:1208:G:H8	1.85	0.41
1:A:1308:C:H2'	1:A:1309:C:H6	1.83	0.41
1:A:1538:U:H2'	1:A:1539:G:H8	1.85	0.41
1:A:4406:U:C2	1:A:4407:G:C8	3.08	0.41
1:A:4575:G:H2'	1:A:4576:PSU:H6	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4670:C:H2'	16:P:15:ARG:NH2	2.36	0.41
1:A:5002:U:H2'	1:A:5003:U:C6	2.56	0.41
2:B:112:U:H2'	2:B:113:G:H8	1.85	0.41
3:C:45:C:OP1	32:f:15:LYS:HD2	2.21	0.41
4:D:206:PRO:HG3	4:D:213:GLY:HA3	2.03	0.41
8:H:46:ARG:O	8:H:65:ARG:NH2	2.53	0.41
11:K:8:ASN:OD1	11:K:9:LYS:HG2	2.19	0.41
16:P:138:SER:C	16:P:139:ILE:HD13	2.45	0.41
31:e:8:ILE:HD12	31:e:8:ILE:N	2.34	0.41
1:A:122:U:H2'	1:A:123:C:H6	1.85	0.41
1:A:281:U:H2'	1:A:282:C:H6	1.85	0.41
1:A:429:A:H2'	1:A:430:G:H8	1.85	0.41
1:A:701:G:H2'	1:A:702:U:C6	2.56	0.41
1:A:1075:G:H2'	1:A:1076:C:H6	1.85	0.41
1:A:1191:C:H2'	1:A:1192:C:C6	2.54	0.41
1:A:2034:G:H1'	13:M:116:ARG:O	2.20	0.41
1:A:3866:C:H2'	1:A:3867:A2M:O4'	2.21	0.41
1:A:3908:A:N7	1:A:4449:A:N6	2.68	0.41
1:A:4165:C:OP1	40:n:245:LYS:NZ	2.49	0.41
1:A:4188:U:H2'	1:A:4189:U:H6	1.85	0.41
1:A:5029:C:H2'	1:A:5030:U:H6	1.86	0.41
7:G:211:LEU:HD23	7:G:211:LEU:HA	1.83	0.41
9:I:118:MET:HE3	9:I:118:MET:HB3	1.97	0.41
12:L:2:SER:OG	12:L:3:MET:N	2.52	0.41
17:Q:20:ARG:HE	17:Q:20:ARG:HB2	1.64	0.41
19:S:40:GLN:OE1	19:S:41:LYS:N	2.53	0.41
22:V:61:ASN:O	22:V:65:MET:HG2	2.20	0.41
23:W:16:SER:O	23:W:19:GLN:HG3	2.21	0.41
24:X:36:VAL:HG21	24:X:44:ARG:HG2	2.02	0.41
26:Z:14:TYR:OH	26:Z:92:LEU:O	2.28	0.41
36:j:59:SER:OG	36:j:60:CYS:N	2.53	0.41
37:k:97:ILE:HD12	37:k:107:ARG:HA	2.01	0.41
39:m:148:LYS:O	39:m:152:GLU:HG2	2.20	0.41
42:p:61:SER:HA	42:p:116:VAL:HG12	2.03	0.41
43:q:89:VAL:HG11	43:q:109:ILE:HG23	2.02	0.41
1:A:165:A:H2'	1:A:166:C:C6	2.55	0.41
1:A:228:C:H2'	1:A:229:G:C8	2.55	0.41
1:A:454:U:O2'	25:Y:5:ARG:NE	2.49	0.41
1:A:739:G:N7	1:A:926:G:C6	2.89	0.41
1:A:1920:C:H3'	1:A:1921:C:H5''	2.02	0.41
1:A:2034:G:H2'	1:A:2035:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2375:A:H2'	1:A:2376:A:H8	1.85	0.41
1:A:2402:G:C2	1:A:2403:A:C8	3.08	0.41
1:A:2789:A:H1'	32:f:45:ARG:HH22	1.86	0.41
1:A:3883:U:H2'	1:A:3884:PSU:C6	2.56	0.41
6:F:11:TYR:CZ	6:F:148:PRO:HB2	2.55	0.41
6:F:138:MET:HB3	6:F:138:MET:HE3	1.74	0.41
11:K:75:ARG:N	11:K:76:GLU:OE2	2.54	0.41
14:N:140:PHE:CZ	39:m:71:MET:HG3	2.55	0.41
15:O:41:GLN:O	15:O:45:GLU:HG2	2.21	0.41
16:P:16:ILE:C	16:P:16:ILE:HD12	2.45	0.41
20:T:103:ASP:OD2	20:T:103:ASP:C	2.63	0.41
22:V:91:ARG:HB2	22:V:94:ASP:HB3	2.01	0.41
43:q:56:THR:HG23	43:q:63:ARG:HA	2.02	0.41
44:r:46:ILE:HD12	44:r:49:ARG:HB2	2.02	0.41
46:0:442:GLU:O	46:0:446:GLN:HG3	2.21	0.41
1:A:173:C:H2'	1:A:174:C:C6	2.56	0.41
1:A:928:C:H2'	1:A:929:A:C8	2.55	0.41
1:A:1098:G:H2'	1:A:1099:C:C6	2.56	0.41
1:A:1368:A:H1'	19:S:1:MET:HE2	2.01	0.41
1:A:2372:U:H2'	1:A:2373:C:C6	2.55	0.41
1:A:2407:G:O6	32:f:2:SER:N	2.53	0.41
1:A:2897:G:H5'	12:L:101:ILE:HG21	2.01	0.41
1:A:3819:G:H2'	1:A:3820:G:H8	1.84	0.41
1:A:4088:C:OP1	4:D:37:ARG:NH2	2.45	0.41
2:B:15:C:H2'	2:B:16:A:C8	2.56	0.41
3:C:6:C:H2'	3:C:7:U:C6	2.55	0.41
6:F:298:ILE:O	6:F:302:LEU:HG	2.19	0.41
7:G:37:VAL:HB	7:G:67:ALA:HB2	2.02	0.41
11:K:18:PRO:HG2	11:K:29:VAL:HG21	2.03	0.41
20:T:92:ASP:OD2	20:T:94:THR:N	2.53	0.41
25:Y:98:GLU:HG3	25:Y:123:THR:OG1	2.21	0.41
28:b:19:LYS:HE3	28:b:19:LYS:HB3	1.78	0.41
34:h:186:VAL:HG21	34:h:197:MET:HB3	2.01	0.41
37:k:90:LEU:HD13	37:k:111:ILE:HG23	2.02	0.41
1:A:726:G:H2'	1:A:727:C:C6	2.56	0.41
1:A:1177:U:H2'	1:A:1178:G:C8	2.56	0.41
1:A:1912:G:H2'	1:A:1913:C:C6	2.56	0.41
1:A:2340:C:H2'	1:A:2341:A:C8	2.56	0.41
1:A:2384:U:H2'	1:A:2385:U:C6	2.56	0.41
1:A:2505:C:H4'	1:A:2506:G:O4'	2.21	0.41
1:A:2521:G:H2'	1:A:2522:G:H8	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3711:A:H2'	1:A:3712:A:O4'	2.20	0.41
1:A:4878:C:H2'	1:A:4879:C:H6	1.86	0.41
1:A:4962:C:H2'	1:A:4963:G:H8	1.85	0.41
2:B:63:C:H5'	2:B:64:G:H5''	2.03	0.41
6:F:183:VAL:HG22	6:F:204:ARG:HG3	2.03	0.41
13:M:30:MET:HB2	13:M:30:MET:HE2	1.82	0.41
16:P:21:PRO:HA	16:P:54:ALA:HA	2.02	0.41
17:Q:25:ASP:C	17:Q:25:ASP:OD2	2.62	0.41
21:U:3:SER:HA	21:U:6:ARG:HG3	2.03	0.41
31:e:17:ARG:NH2	31:e:19:ASP:OD2	2.54	0.41
1:A:88:A:N7	11:K:173:LYS:NZ	2.69	0.41
1:A:158:A:N1	1:A:276:C:O2'	2.45	0.41
1:A:223:G:H4'	1:A:225:G:N7	2.36	0.41
1:A:225:G:OP1	6:F:222:ARG:NE	2.53	0.41
1:A:229:G:H2'	1:A:230:G:H8	1.86	0.41
1:A:422:C:H2'	1:A:423:G:C8	2.54	0.41
1:A:664:G:H2'	1:A:665:C:C6	2.56	0.41
1:A:669:C:OP1	37:k:69:GLY:N	2.43	0.41
1:A:754:U:H2'	1:A:755:C:C6	2.56	0.41
1:A:755:C:H2'	1:A:756:G:C8	2.55	0.41
1:A:1084:C:H2'	1:A:1085:C:C6	2.56	0.41
1:A:1086:C:H2'	1:A:1087:A:H8	1.85	0.41
1:A:1809:C:H2'	1:A:1810:G:C8	2.56	0.41
1:A:1818:G:H2'	1:A:1820:C:OP2	2.21	0.41
1:A:1825:A:H2'	1:A:1826:G:C8	2.56	0.41
1:A:1849:U:H3'	44:r:5:ARG:HH12	1.86	0.41
1:A:2072:C:OP1	11:K:2:GLY:N	2.53	0.41
1:A:2727:C:H2'	1:A:2728:U:C6	2.56	0.41
1:A:2876:OMG:C8	36:j:16:THR:HG22	2.56	0.41
1:A:3734:PSU:H2'	1:A:3735:G:C8	2.56	0.41
1:A:4151:G:H2'	1:A:4152:G:H8	1.84	0.41
1:A:4155:C:H2'	1:A:4156:G:O4'	2.20	0.41
1:A:4285:U:H2'	1:A:4286:C:C6	2.55	0.41
1:A:4327:C:OP1	14:N:70:HIS:NE2	2.54	0.41
1:A:4481:U:H2'	1:A:4482:U:H6	1.85	0.41
1:A:4538:G:H2'	1:A:4539:U:H6	1.86	0.41
1:A:4551:U:H2'	1:A:4552:PSU:C6	2.55	0.41
1:A:4573:G:H21	1:A:4722:G:H22	1.68	0.41
1:A:4596:C:C4	1:A:4597:U:C4	3.09	0.41
1:A:4627:U:O2'	5:E:55:HIS:ND1	2.42	0.41
1:A:4726:G:H2'	1:A:4727:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4928:C:O2	45:s:118:MET:HE1	2.20	0.41
2:B:2:U:O4'	50:B:205:GTP:H2'	2.21	0.41
3:C:60:G:O6	3:C:96:C:O2'	2.33	0.41
3:C:92:U:H2'	3:C:93:C:O4'	2.21	0.41
5:E:119:TYR:OH	5:E:129:ALA:N	2.54	0.41
6:F:218:ILE:HA	6:F:229:LEU:HD13	2.03	0.41
6:F:348:LYS:HE2	6:F:348:LYS:HB3	1.92	0.41
9:I:128:ARG:NH1	13:M:162:GLN:OE1	2.51	0.41
16:P:85:ARG:NH1	16:P:99:GLU:O	2.54	0.41
18:R:88:LYS:HA	18:R:88:LYS:HD3	1.82	0.41
20:T:103:ASP:OD2	20:T:105:ALA:N	2.52	0.41
36:j:30:GLU:HA	36:j:33:GLN:HG2	2.02	0.41
40:n:118:ALA:O	40:n:121:LYS:HG3	2.21	0.41
40:n:259:LYS:HB3	40:n:259:LYS:HE3	1.73	0.41
43:q:99:PHE:O	43:q:159:LYS:NZ	2.54	0.41
43:q:120:ASP:OD2	43:q:120:ASP:C	2.64	0.41
1:A:249:C:H2'	1:A:250:C:H6	1.85	0.41
1:A:967:C:N4	1:A:2094:G:H22	2.19	0.41
1:A:1449:C:H2'	1:A:1450:C:C6	2.56	0.41
1:A:1460:C:H5''	11:K:144:LYS:HG2	2.03	0.41
1:A:1751:A:H2'	1:A:1752:G:C8	2.56	0.41
1:A:2610:G:H2'	1:A:2611:A:C8	2.56	0.41
1:A:2675:G:O6	23:W:33:GLN:HG3	2.21	0.41
1:A:2898:G:H2'	1:A:2899:C:H6	1.85	0.41
1:A:2899:C:P	12:L:108:ARG:HH22	2.44	0.41
1:A:3636:C:H4'	1:A:3825:A2M:H2	2.02	0.41
1:A:3642:A:C4	30:d:3:LYS:HB3	2.56	0.41
1:A:3682:A:H5''	4:D:132:ASN:OD1	2.20	0.41
1:A:3799:A:N3	1:A:4506:C:O2'	2.46	0.41
1:A:3835:C:H2'	1:A:3836:A:C8	2.56	0.41
1:A:4392:OMG:N3	1:A:4447:5MC:HM52	2.36	0.41
1:A:4426:C:H2'	1:A:4427:G:O4'	2.21	0.41
1:A:4474:A:H5''	33:g:125:LYS:HB2	2.03	0.41
1:A:4572:U:H5''	3:C:1:C:H41	1.86	0.41
3:C:71:A:H4'	3:C:72:A:O5'	2.21	0.41
4:D:74:GLU:OE2	4:D:74:GLU:HA	2.21	0.41
6:F:334:THR:OG1	39:m:51:TYR:OH	2.16	0.41
7:G:211:LEU:HD12	7:G:223:PHE:HE2	1.86	0.41
13:M:15:ARG:HB3	13:M:27:LEU:HD13	2.02	0.41
15:O:24:ASP:OD1	15:O:24:ASP:C	2.64	0.41
16:P:91:LYS:HD3	16:P:91:LYS:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:54:THR:H	20:T:57:MET:HE3	1.86	0.41
40:n:105:GLU:OE2	40:n:113:ARG:NH1	2.54	0.41
44:r:76:PHE:HA	44:r:102:ARG:HH21	1.86	0.41
45:s:8:GLU:OE1	45:s:8:GLU:N	2.54	0.41
46:0:457:LEU:O	46:0:461:MET:N	2.54	0.41
1:A:965:G:O2'	39:m:29:LYS:NZ	2.40	0.40
1:A:1084:C:H2'	1:A:1085:C:H6	1.85	0.40
1:A:2459:G:H2'	1:A:2461:G:OP2	2.21	0.40
1:A:2478:C:H4'	1:A:2479:G:H5''	2.02	0.40
1:A:2641:A:H2'	1:A:2642:A:O4'	2.22	0.40
1:A:2861:OMC:HM22	1:A:2862:G:H5'	2.03	0.40
1:A:3726:A:N6	1:A:4359:U:O2'	2.45	0.40
2:B:110:G:H2'	2:B:111:C:H6	1.85	0.40
4:D:5:ILE:HG13	4:D:7:GLY:H	1.86	0.40
4:D:173:GLY:O	36:j:69:TRP:NE1	2.48	0.40
12:L:111:GLU:OE1	12:L:111:GLU:C	2.64	0.40
15:O:43:LEU:HD23	15:O:43:LEU:H	1.85	0.40
18:R:105:ASN:OD1	18:R:108:GLN:HG3	2.21	0.40
31:e:33:LYS:HG2	31:e:46:VAL:HG22	2.03	0.40
34:h:54:ALA:N	34:h:80:GLU:OE1	2.43	0.40
44:r:163:LYS:HE3	44:r:163:LYS:HB2	1.92	0.40
1:A:385:A:O2'	1:A:387:G:H5'	2.21	0.40
1:A:907:C:H2'	1:A:908:G:H8	1.85	0.40
1:A:1374:G:H2'	1:A:1375:C:H6	1.86	0.40
1:A:1806:G:H2'	1:A:1807:C:C6	2.56	0.40
1:A:1811:G:H2'	1:A:1812:C:C6	2.56	0.40
1:A:2288:G:O2'	1:A:2290:C:O5'	2.31	0.40
1:A:2728:U:H2'	1:A:2729:C:C6	2.56	0.40
1:A:3867:A2M:H1'	1:A:3867:A2M:HM'3	1.67	0.40
1:A:3883:U:H2'	1:A:3884:PSU:H6	1.86	0.40
1:A:4156:G:OP2	1:A:4157:A:O2'	2.25	0.40
2:B:23:A:H2'	2:B:24:C:C6	2.55	0.40
3:C:79:G:H2'	3:C:80:A:C8	2.56	0.40
3:C:96:C:H2'	3:C:97:A:C8	2.56	0.40
10:J:126:ARG:HB3	46:0:453:SER:HB2	2.02	0.40
16:P:107:ASN:OD1	16:P:111:GLU:N	2.54	0.40
19:S:2:LYS:HB3	19:S:2:LYS:HE3	1.75	0.40
39:m:182:TYR:CZ	39:m:203:GLU:HG2	2.56	0.40
39:m:193:GLU:HA	39:m:193:GLU:OE2	2.22	0.40
40:n:150:LYS:NZ	40:n:177:MET:O	2.54	0.40
40:n:255:LYS:HE3	40:n:255:LYS:HB3	1.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:G:H2'	1:A:757:G:C8	2.57	0.40
1:A:1327:C:H5''	1:A:4449:A:OP1	2.21	0.40
1:A:2761:U:H4'	1:A:2762:G:O4'	2.21	0.40
1:A:2765:A:H2'	1:A:2766:A:H8	1.86	0.40
1:A:4068:U:H2'	1:A:4069:U:C6	2.56	0.40
1:A:4219:A:H2'	1:A:4220:6MZ:C8	2.51	0.40
1:A:4323:A:N6	7:G:153:THR:HG21	2.36	0.40
1:A:4454:G:O2'	1:A:4500:PSU:O2'	2.16	0.40
1:A:4486:C:H2'	1:A:4487:A:O4'	2.22	0.40
1:A:4523:A2M:HM'3	1:A:4559:A:N7	2.36	0.40
1:A:4957:C:H2'	1:A:4958:C:H6	1.85	0.40
3:C:64:U:C2	3:C:65:A:C8	3.09	0.40
3:C:154:G:H2'	3:C:155:C:C6	2.56	0.40
5:E:45:ALA:HB3	5:E:183:ILE:HG23	2.02	0.40
16:P:89:ARG:HB2	16:P:95:PHE:CE2	2.57	0.40
18:R:80:PRO:HA	18:R:98:PHE:HA	2.04	0.40
29:c:97:MET:HE2	29:c:97:MET:HB3	1.89	0.40
36:j:50:ARG:HG3	36:j:50:ARG:NH1	2.35	0.40
39:m:226:HIS:NE2	39:m:234:GLY:HA3	2.36	0.40
1:A:286:U:H2'	1:A:287:U:C6	2.57	0.40
1:A:713:C:H2'	1:A:714:G:H8	1.87	0.40
1:A:1191:C:H2'	1:A:1192:C:H6	1.87	0.40
1:A:1502:G:H1	11:K:89:ASP:HA	1.86	0.40
1:A:1504:G:H2'	1:A:1505:C:C6	2.57	0.40
1:A:1656:U:H2'	1:A:1657:G:H8	1.86	0.40
1:A:1895:G:H2'	1:A:1896:A:O4'	2.21	0.40
1:A:2029:A:H2'	1:A:2030:A:C8	2.56	0.40
1:A:2273:G:H2'	1:A:2274:C:C6	2.56	0.40
1:A:2273:G:H2'	1:A:2274:C:H6	1.87	0.40
1:A:2292:C:H2'	1:A:2293:U:C6	2.57	0.40
1:A:4961:G:H2'	1:A:4962:C:H6	1.86	0.40
5:E:29:VAL:HG13	5:E:348:ARG:HD3	2.03	0.40
13:M:21:LYS:HE2	13:M:21:LYS:HB2	1.90	0.40
25:Y:81:ASN:OD1	25:Y:84:GLU:HG3	2.21	0.40
29:c:94:LEU:HD23	29:c:94:LEU:HA	1.91	0.40
38:l:26:ARG:NH1	40:n:165:GLU:OE1	2.54	0.40
1:A:122:U:H2'	1:A:123:C:C6	2.56	0.40
1:A:142:G:H2'	1:A:144:G:H8	1.86	0.40
1:A:153:G:H2'	1:A:154:G:C8	2.52	0.40
1:A:454:U:H2'	1:A:455:C:O4'	2.20	0.40
1:A:740:G:O2'	1:A:741:C:H5'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1068:G:H2'	1:A:1069:G:H8	1.85	0.40
1:A:1199:G:O6	13:M:15:ARG:NH1	2.55	0.40
1:A:1355:G:H2'	1:A:1356:U:C6	2.57	0.40
1:A:1442:C:H2'	1:A:1443:A:N3	2.36	0.40
1:A:2484:A:H2'	1:A:2485:U:H6	1.87	0.40
1:A:2574:G:H5'	1:A:2575:U:OP1	2.21	0.40
1:A:2636:U:H2'	1:A:2637:U:C6	2.57	0.40
1:A:4300:U:H2'	1:A:4301:U:C6	2.56	0.40
5:E:231:VAL:HG21	5:E:251:VAL:HG23	2.03	0.40
8:H:119:GLU:HB3	25:Y:7:LEU:HD22	2.02	0.40
10:J:25:HIS:O	10:J:29:THR:OG1	2.34	0.40
11:K:129:ASP:OD2	11:K:129:ASP:C	2.65	0.40
20:T:136:PHE:O	27:a:78:TYR:OH	2.28	0.40
26:Z:94:ALA:O	26:Z:97:ILE:HG13	2.22	0.40
39:m:125:LEU:HD23	39:m:125:LEU:HA	1.90	0.40
44:r:91:ALA:HB1	44:r:96:ILE:HB	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
4	D	244/257 (95%)	235 (96%)	9 (4%)	0	100	100
5	E	394/403 (98%)	390 (99%)	4 (1%)	0	100	100
6	F	358/427 (84%)	353 (99%)	5 (1%)	0	100	100
7	G	290/297 (98%)	286 (99%)	4 (1%)	0	100	100
8	H	212/288 (74%)	206 (97%)	6 (3%)	0	100	100
9	I	197/203 (97%)	196 (100%)	1 (0%)	0	100	100
10	J	150/184 (82%)	150 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	185/188 (98%)	183 (99%)	2 (1%)	0	100	100
12	L	155/196 (79%)	154 (99%)	1 (1%)	0	100	100
13	M	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
14	N	157/160 (98%)	156 (99%)	1 (1%)	0	100	100
15	O	97/128 (76%)	92 (95%)	5 (5%)	0	100	100
16	P	130/140 (93%)	129 (99%)	1 (1%)	0	100	100
17	Q	60/157 (38%)	60 (100%)	0	0	100	100
18	R	117/156 (75%)	115 (98%)	2 (2%)	0	100	100
19	S	132/145 (91%)	130 (98%)	2 (2%)	0	100	100
20	T	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
21	U	145/148 (98%)	144 (99%)	1 (1%)	0	100	100
22	V	95/159 (60%)	94 (99%)	1 (1%)	0	100	100
23	W	98/115 (85%)	98 (100%)	0	0	100	100
24	X	104/125 (83%)	104 (100%)	0	0	100	100
25	Y	126/135 (93%)	126 (100%)	0	0	100	100
26	Z	108/110 (98%)	108 (100%)	0	0	100	100
27	a	109/117 (93%)	108 (99%)	1 (1%)	0	100	100
28	b	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
29	c	100/105 (95%)	100 (100%)	0	0	100	100
30	d	85/97 (88%)	85 (100%)	0	0	100	100
31	e	67/70 (96%)	67 (100%)	0	0	100	100
32	f	48/51 (94%)	48 (100%)	0	0	100	100
33	g	50/128 (39%)	50 (100%)	0	0	100	100
34	h	223/245 (91%)	218 (98%)	5 (2%)	0	100	100
35	i	101/106 (95%)	98 (97%)	3 (3%)	0	100	100
36	j	90/92 (98%)	87 (97%)	3 (3%)	0	100	100
37	k	122/137 (89%)	121 (99%)	1 (1%)	0	100	100
38	l	202/204 (99%)	200 (99%)	2 (1%)	0	100	100
39	m	222/248 (90%)	217 (98%)	5 (2%)	0	100	100
40	n	219/266 (82%)	216 (99%)	3 (1%)	0	100	100
41	o	188/192 (98%)	186 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	p	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
43	q	168/178 (94%)	167 (99%)	1 (1%)	0	100	100
44	r	204/211 (97%)	201 (98%)	3 (2%)	0	100	100
45	s	137/215 (64%)	136 (99%)	1 (1%)	0	100	100
46	o	41/477 (9%)	41 (100%)	0	0	100	100
All	All	6558/7899 (83%)	6472 (99%)	86 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	189/199 (95%)	187 (99%)	2 (1%)	65	84
5	E	345/349 (99%)	345 (100%)	0	100	100
6	F	297/348 (85%)	296 (100%)	1 (0%)	86	94
7	G	245/250 (98%)	244 (100%)	1 (0%)	84	93
8	H	193/252 (77%)	191 (99%)	2 (1%)	68	86
9	I	171/174 (98%)	171 (100%)	0	100	100
10	J	133/163 (82%)	133 (100%)	0	100	100
11	K	164/165 (99%)	164 (100%)	0	100	100
12	L	138/175 (79%)	136 (99%)	2 (1%)	59	81
13	M	157/157 (100%)	155 (99%)	2 (1%)	61	82
14	N	139/140 (99%)	136 (98%)	3 (2%)	45	72
15	O	88/115 (76%)	88 (100%)	0	100	100
16	P	102/107 (95%)	102 (100%)	0	100	100
17	Q	54/126 (43%)	54 (100%)	0	100	100
18	R	107/133 (80%)	107 (100%)	0	100	100
19	S	124/135 (92%)	123 (99%)	1 (1%)	73	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	T	117/118 (99%)	113 (97%)	4 (3%)	32	60
21	U	120/121 (99%)	120 (100%)	0	100	100
22	V	82/126 (65%)	81 (99%)	1 (1%)	63	83
23	W	84/97 (87%)	83 (99%)	1 (1%)	63	83
24	X	93/110 (84%)	93 (100%)	0	100	100
25	Y	114/121 (94%)	112 (98%)	2 (2%)	51	76
26	Z	89/89 (100%)	89 (100%)	0	100	100
27	a	95/100 (95%)	93 (98%)	2 (2%)	47	73
28	b	109/110 (99%)	109 (100%)	0	100	100
29	c	86/89 (97%)	84 (98%)	2 (2%)	44	71
30	d	74/80 (92%)	74 (100%)	0	100	100
31	e	64/65 (98%)	63 (98%)	1 (2%)	55	79
32	f	47/48 (98%)	45 (96%)	2 (4%)	26	51
33	g	48/116 (41%)	48 (100%)	0	100	100
34	h	195/213 (92%)	191 (98%)	4 (2%)	47	73
35	i	91/94 (97%)	88 (97%)	3 (3%)	33	61
36	j	75/75 (100%)	75 (100%)	0	100	100
37	k	107/121 (88%)	107 (100%)	0	100	100
38	l	172/172 (100%)	171 (99%)	1 (1%)	78	91
39	m	192/215 (89%)	191 (100%)	1 (0%)	81	92
40	n	193/223 (86%)	192 (100%)	1 (0%)	81	92
41	o	169/171 (99%)	166 (98%)	3 (2%)	51	76
42	p	173/174 (99%)	173 (100%)	0	100	100
43	q	142/149 (95%)	141 (99%)	1 (1%)	76	89
44	r	172/177 (97%)	170 (99%)	2 (1%)	63	83
45	s	118/161 (73%)	118 (100%)	0	100	100
46	0	38/404 (9%)	37 (97%)	1 (3%)	40	68
All	All	5705/6727 (85%)	5659 (99%)	46 (1%)	70	88

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	8	GLN

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Mol	Chain	Res	Type
4	D	159	SER
6	F	138	MET
7	G	37	VAL
8	H	93	THR
8	H	199	THR
12	L	27	ASN
12	L	112	SER
13	M	56	LYS
13	M	149	LYS
14	N	41	ASP
14	N	69	GLN
14	N	104	SER
19	S	82	ILE
20	T	26	VAL
20	T	54	THR
20	T	57	MET
20	T	119	GLU
22	V	58	GLN
23	W	18	LEU
25	Y	87	VAL
25	Y	118	LEU
27	a	28	ASN
27	a	99	GLU
29	c	18	THR
29	c	91	SER
31	e	36	VAL
32	f	9	ILE
32	f	47	THR
34	h	82	GLN
34	h	134	LYS
34	h	145	GLN
34	h	213	THR
35	i	25	GLN
35	i	76	ASN
35	i	82	MET
38	l	15	GLN
39	m	60	GLU
40	n	28	VAL
41	o	11	ASP
41	o	92	MET
41	o	112	VAL
43	q	118	LYS

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Mol	Chain	Res	Type
44	r	151	THR
44	r	170	THR
46	0	456	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	215	ASN
5	E	68	ASN
5	E	376	HIS
6	F	48	ASN
6	F	236	ASN
6	F	329	ASN
6	F	347	HIS
7	G	81	HIS
7	G	250	ASN
9	I	42	ASN
9	I	167	HIS
10	J	21	ASN
10	J	56	GLN
11	K	160	HIS
12	L	134	ASN
12	L	143	HIS
13	M	50	GLN
15	O	55	ASN
16	P	135	ASN
18	R	93	ASN
19	S	66	GLN
22	V	60	ASN
23	W	72	HIS
24	X	34	HIS
24	X	69	ASN
24	X	79	ASN
24	X	100	ASN
25	Y	117	GLN
28	b	30	GLN
28	b	98	HIS
29	c	36	HIS
30	d	48	ASN
34	h	162	HIS
35	i	45	GLN
37	k	41	ASN

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Mol	Chain	Res	Type
39	m	63	GLN
39	m	116	GLN
40	n	43	GLN
40	n	64	GLN
40	n	82	GLN
40	n	100	HIS
40	n	141	ASN
40	n	153	GLN
40	n	208	ASN
41	o	39	ASN
41	o	98	HIS
41	o	189	GLN
42	p	73	ASN
43	q	46	GLN
43	q	71	HIS
43	q	97	ASN
44	r	15	HIS
44	r	149	GLN
45	s	34	ASN
45	s	44	GLN
45	s	48	GLN
45	s	70	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	3366/5064 (66%)	457 (13%)	3 (0%)
2	B	117/119 (98%)	7 (5%)	0
3	C	145/157 (92%)	13 (8%)	0
All	All	3628/5340 (67%)	477 (13%)	3 (0%)

All (477) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	U
1	A	39	A
1	A	42	A
1	A	47	A
1	A	48	G
1	A	59	A
1	A	64	A

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Mol	Chain	Res	Type
1	A	65	A
1	A	66	A
1	A	72	C
1	A	73	A
1	A	76	A
1	A	85	G
1	A	91	G
1	A	95	G
1	A	98	A
1	A	104	G
1	A	119	G
1	A	120	A
1	A	122	U
1	A	132	G
1	A	135	G
1	A	136	C
1	A	139	G
1	A	143	C
1	A	159	C
1	A	172	C
1	A	189	G
1	A	197	A
1	A	200	U
1	A	209	U
1	A	216	C
1	A	218	A
1	A	220	C
1	A	233	U
1	A	234	G
1	A	241	G
1	A	266	C
1	A	278	G
1	A	281	U
1	A	297	U
1	A	316	U
1	A	340	C
1	A	357	U
1	A	387	G
1	A	399	G
1	A	412	G
1	A	413	G
1	A	449	C

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Mol	Chain	Res	Type
1	A	450	G
1	A	452	A
1	A	453	G
1	A	454	U
1	A	456	C
1	A	457	G
1	A	487	G
1	A	493	G
1	A	502	C
1	A	503	C
1	A	504	G
1	A	509	A
1	A	666	G
1	A	667	A
1	A	688	U
1	A	695	G
1	A	697	G
1	A	703	G
1	A	704	C
1	A	708	G
1	A	731	G
1	A	738	C
1	A	739	G
1	A	741	C
1	A	747	A
1	A	915	A
1	A	916	C
1	A	917	A
1	A	918	G
1	A	925	C
1	A	926	G
1	A	927	G
1	A	932	A
1	A	933	G
1	A	934	C
1	A	935	A
1	A	936	C
1	A	941	C
1	A	943	A
1	A	944	A
1	A	945	U
1	A	956	A

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Mol	Chain	Res	Type
1	A	957	G
1	A	959	G
1	A	960	A
1	A	961	G
1	A	962	C
1	A	964	A
1	A	965	G
1	A	966	A
1	A	967	C
1	A	971	U
1	A	982	U
1	A	1068	G
1	A	1071	C
1	A	1182	C
1	A	1185	G
1	A	1194	G
1	A	1198	G
1	A	1199	G
1	A	1200	G
1	A	1210	C
1	A	1211	G
1	A	1216	C
1	A	1266	G
1	A	1269	G
1	A	1273	G
1	A	1277	G
1	A	1280	C
1	A	1281	G
1	A	1284	G
1	A	1287	G
1	A	1293	G
1	A	1294	A
1	A	1295	C
1	A	1301	C
1	A	1314	C
1	A	1326	A2M
1	A	1354	A
1	A	1359	G
1	A	1365	C
1	A	1366	G
1	A	1379	C
1	A	1387	A

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Mol	Chain	Res	Type
1	A	1397	A
1	A	1420	A
1	A	1435	G
1	A	1436	C
1	A	1438	U
1	A	1439	C
1	A	1444	G
1	A	1457	G
1	A	1483	C
1	A	1497	A
1	A	1498	G
1	A	1502	G
1	A	1516	G
1	A	1523	A
1	A	1525	A
1	A	1534	A2M
1	A	1547	A
1	A	1553	A
1	A	1574	G
1	A	1578	U
1	A	1591	U
1	A	1596	U
1	A	1612	G
1	A	1613	A
1	A	1624	G
1	A	1625	OMG
1	A	1631	A
1	A	1633	G
1	A	1638	A
1	A	1641	G
1	A	1650	A
1	A	1654	G
1	A	1661	C
1	A	1676	C
1	A	1677	PSU
1	A	1678	C
1	A	1691	G
1	A	1694	C
1	A	1699	A
1	A	1700	G
1	A	1701	A
1	A	1705	G

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Mol	Chain	Res	Type
1	A	1707	C
1	A	1720	C
1	A	1722	C
1	A	1724	G
1	A	1787	A
1	A	1789	C
1	A	1794	A
1	A	1804	A
1	A	1806	G
1	A	1815	G
1	A	1821	G
1	A	1822	U
1	A	1834	U
1	A	1836	G
1	A	1837	A
1	A	1842	G
1	A	1855	G
1	A	1869	G
1	A	1881	OMC
1	A	1888	A
1	A	1897	A
1	A	1916	G
1	A	1917	A
1	A	1918	U
1	A	1921	C
1	A	1922	G
1	A	1931	C
1	A	1932	A
1	A	1935	C
1	A	1938	C
1	A	1940	G
1	A	1948	G
1	A	1955	G
1	A	2043	A
1	A	2044	U
1	A	2046	G
1	A	2048	U
1	A	2052	G
1	A	2055	G
1	A	2056	G
1	A	2069	A
1	A	2084	C

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Mol	Chain	Res	Type
1	A	2091	C
1	A	2092	G
1	A	2093	A
1	A	2095	A
1	A	2096	G
1	A	2097	U
1	A	2098	G
1	A	2258	C
1	A	2259	G
1	A	2261	G
1	A	2289	C
1	A	2300	A
1	A	2301	G
1	A	2306	G
1	A	2313	A
1	A	2316	G
1	A	2322	G
1	A	2331	G
1	A	2347	A
1	A	2348	G
1	A	2351	OMC
1	A	2360	A
1	A	2391	G
1	A	2395	A
1	A	2397	G
1	A	2402	G
1	A	2410	C
1	A	2417	A
1	A	2421	G
1	A	2425	U
1	A	2428	A
1	A	2441	C
1	A	2450	G
1	A	2469	C
1	A	2471	G
1	A	2474	G
1	A	2475	G
1	A	2479	G
1	A	2493	G
1	A	2502	G
1	A	2504	C
1	A	2505	C

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Mol	Chain	Res	Type
1	A	2513	A
1	A	2519	U
1	A	2520	C
1	A	2529	A
1	A	2554	U
1	A	2555	G
1	A	2573	A
1	A	2586	G
1	A	2587	A
1	A	2602	G
1	A	2618	G
1	A	2627	C
1	A	2653	C
1	A	2658	G
1	A	2662	G
1	A	2669	C
1	A	2675	G
1	A	2687	U
1	A	2694	G
1	A	2695	A
1	A	2696	A
1	A	2711	G
1	A	2725	A
1	A	2726	G
1	A	2743	A
1	A	2760	G
1	A	2763	U
1	A	2764	A
1	A	2787	A2M
1	A	2788	U
1	A	2790	U
1	A	2806	A
1	A	2814	C
1	A	2826	U
1	A	2827	G
1	A	2835	A
1	A	2855	G
1	A	2897	G
1	A	3605	C
1	A	3606	U
1	A	3615	G
1	A	3616	U

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Mol	Chain	Res	Type
1	A	3618	C
1	A	3626	G
1	A	3635	A
1	A	3648	A
1	A	3662	A
1	A	3664	G
1	A	3673	C
1	A	3692	A
1	A	3696	C
1	A	3709	U
1	A	3710	G
1	A	3713	U
1	A	3714	G
1	A	3734	PSU
1	A	3735	G
1	A	3753	G
1	A	3773	U
1	A	3774	A
1	A	3777	G
1	A	3778	U
1	A	3784	A
1	A	3811	G
1	A	3814	U
1	A	3817	A
1	A	3819	G
1	A	3838	U
1	A	3839	G
1	A	3840	U
1	A	3850	C
1	A	3877	A
1	A	3878	C
1	A	3879	G
1	A	3895	G
1	A	3897	G
1	A	3901	A
1	A	3905	A
1	A	3906	A
1	A	3907	G
1	A	3908	A
1	A	3915	U
1	A	4076	G
1	A	4084	G

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Mol	Chain	Res	Type
1	A	4093	G
1	A	4119	C
1	A	4122	G
1	A	4127	A
1	A	4128	A
1	A	4162	C
1	A	4170	A
1	A	4183	G
1	A	4184	G
1	A	4191	G
1	A	4203	A
1	A	4212	A
1	A	4225	G
1	A	4229	U
1	A	4233	A
1	A	4234	A
1	A	4251	A
1	A	4253	A
1	A	4254	G
1	A	4255	A
1	A	4266	G
1	A	4268	A
1	A	4273	A
1	A	4281	A
1	A	4304	A
1	A	4305	G
1	A	4306	OMU
1	A	4329	G
1	A	4330	G
1	A	4332	C
1	A	4354	U
1	A	4373	G
1	A	4377	G
1	A	4378	A
1	A	4379	A
1	A	4387	C
1	A	4394	A
1	A	4420	PSU
1	A	4421	C
1	A	4422	A
1	A	4430	G
1	A	4433	G

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Mol	Chain	Res	Type
1	A	4437	U
1	A	4444	C
1	A	4448	G
1	A	4464	A
1	A	4466	C
1	A	4475	G
1	A	4488	A
1	A	4500	PSU
1	A	4512	U
1	A	4513	A
1	A	4518	A
1	A	4524	G
1	A	4528	G
1	A	4548	A
1	A	4549	G
1	A	4560	C
1	A	4567	G
1	A	4569	U
1	A	4574	U
1	A	4575	G
1	A	4581	G
1	A	4590	A2M
1	A	4617	G
1	A	4627	U
1	A	4635	A
1	A	4636	U
1	A	4637	OMG
1	A	4656	A
1	A	4670	C
1	A	4672	A
1	A	4687	A
1	A	4700	A
1	A	4708	A
1	A	4709	U
1	A	4730	C
1	A	4731	G
1	A	4741	C
1	A	4742	G
1	A	4754	G
1	A	4757	C
1	A	4759	C
1	A	4765	G

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Mol	Chain	Res	Type
1	A	4870	G
1	A	4871	C
1	A	4877	G
1	A	4882	U
1	A	4883	C
1	A	4895	C
1	A	4900	C
1	A	4901	G
1	A	4910	A
1	A	4912	G
1	A	4913	G
1	A	4914	C
1	A	4937	C
1	A	4938	A
1	A	4943	A
1	A	4944	C
1	A	4947	U
1	A	4951	G
1	A	4976	U
1	A	4987	C
1	A	4988	U
1	A	5006	U
1	A	5014	A
1	A	5017	G
1	A	5034	A
1	A	5041	G
1	A	5050	C
1	A	5054	C
1	A	5062	G
1	A	5069	U
2	B	7	G
2	B	22	A
2	B	33	U
2	B	53	U
2	B	54	A
2	B	64	G
2	B	110	G
3	C	23	C
3	C	34	U
3	C	35	C
3	C	39	G
3	C	59	A

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Mol	Chain	Res	Type
3	C	62	A
3	C	63	U
3	C	80	A
3	C	94	G
3	C	103	A
3	C	105	C
3	C	110	U
3	C	114	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	486	C
1	A	964	A
1	A	3734	PSU

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

123 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	$\# Z > 2$
1	PSU	A	3844	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	OMC	A	4456	1	19,22,23	0.83	0	26,31,34	0.98	1 (3%)
1	A2M	A	2401	1,47	22,25,26	1.46	4 (18%)	31,36,39	2.13	10 (32%)
1	PSU	A	3734	1	18,21,22	1.34	2 (11%)	22,30,33	1.98	4 (18%)
1	PSU	A	4299	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	A	3637	48,1	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
1	PSU	A	3695	48,1	18,21,22	1.34	2 (11%)	22,30,33	1.88	4 (18%)
1	PSU	A	4576	48,1	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
1	PSU	A	1860	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	OMG	A	1522	1	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMC	A	2804	1	19,22,23	0.81	0	26,31,34	0.77	0
1	A2M	A	3724	1	22,25,26	1.48	4 (18%)	31,36,39	2.09	8 (25%)
1	OMU	A	4498	48,1	19,22,23	1.20	2 (10%)	26,31,34	1.69	5 (19%)
1	OMU	A	4620	1	19,22,23	1.23	3 (15%)	26,31,34	1.69	4 (15%)
1	PSU	A	3715	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	4 (18%)
1	PSU	A	4420	1	18,21,22	1.40	3 (16%)	22,30,33	1.81	4 (18%)
1	OMG	A	4637	1	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
1	OMG	A	4499	1	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
1	PSU	A	5001	48,1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	A	4353	48,1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	A2M	A	400	1	22,25,26	1.46	4 (18%)	31,36,39	2.10	10 (32%)
1	PSU	A	4521	48,1,47	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
1	A2M	A	3718	1	22,25,26	1.48	4 (18%)	31,36,39	2.05	9 (29%)
1	PSU	A	1536	1	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
1	A2M	A	1871	1,47	22,25,26	1.47	4 (18%)	31,36,39	2.09	9 (29%)
1	PSU	A	1677	48,1	18,21,22	1.33	2 (11%)	22,30,33	1.86	3 (13%)
1	OMC	A	2824	1	19,22,23	0.82	0	26,31,34	0.84	0
1	UY1	A	3818	48,1	19,22,23	0.87	0	22,31,34	1.76	4 (18%)
1	OMC	A	1881	1	19,22,23	0.83	0	26,31,34	1.09	2 (7%)
1	OMU	A	4306	1	19,22,23	1.23	3 (15%)	26,31,34	1.70	4 (15%)
1	PSU	A	4500	1	18,21,22	1.37	2 (11%)	22,30,33	1.81	3 (13%)
1	5MC	A	3782	1,47	18,22,23	0.96	2 (11%)	26,32,35	1.16	3 (11%)
1	A2M	A	1323	1	22,25,26	1.48	4 (18%)	31,36,39	2.08	8 (25%)
1	PSU	A	5010	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	OMU	A	3925	1	19,22,23	1.20	2 (10%)	26,31,34	1.69	5 (19%)
1	OMG	A	4623	1	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
1	A2M	A	4523	1,47	22,25,26	1.46	4 (18%)	31,36,39	2.13	10 (32%)
1	PSU	A	4579	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	OMC	A	2365	1,47	19,22,23	0.81	0	26,31,34	0.79	0
1	PSU	A	1683	48,1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	A	4532	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	OMG	A	3944	1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
1	PSU	A	4689	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	A	4972	48,1	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	A	1781	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	A	398	1	22,25,26	1.46	4 (18%)	31,36,39	2.17	10 (32%)
1	PSU	A	1582	48,1	18,21,22	1.34	2 (11%)	22,30,33	1.91	4 (18%)
1	A2M	A	1534	1,47	22,25,26	1.46	4 (18%)	31,36,39	2.09	9 (29%)
1	OMC	A	3701	48,1	19,22,23	0.79	0	26,31,34	0.73	0
1	OMC	A	3869	1	19,22,23	0.82	0	26,31,34	0.86	1 (3%)
1	OMG	A	4392	1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
1	OMG	A	3744	1	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
1	OMC	A	1340	1	19,22,23	0.83	0	26,31,34	0.88	1 (3%)
1	PSU	A	2508	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	A	4361	48,1	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	A	1792	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	4 (18%)
1	A2M	A	3785	1	22,25,26	1.44	4 (18%)	31,36,39	2.22	11 (35%)
3	PSU	C	55	3	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	A	1782	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	A2M	A	2787	1,47	22,25,26	1.45	4 (18%)	31,36,39	2.18	9 (29%)
1	OMG	A	2876	1	23,26,27	1.20	3 (13%)	33,38,41	1.97	6 (18%)
1	PSU	A	3768	1	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
1	PSU	A	3920	1,47	18,21,22	1.34	2 (11%)	22,30,33	1.91	4 (18%)
1	A2M	A	3867	1	22,25,26	1.47	4 (18%)	31,36,39	2.08	8 (25%)
1	PSU	A	3884	1	18,21,22	1.33	2 (11%)	22,30,33	1.90	3 (13%)
1	OMG	A	2364	1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
1	OMG	A	4370	1	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
1	PSU	A	4431	48,1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	A2M	A	1524	1	22,25,26	1.47	4 (18%)	31,36,39	2.12	8 (25%)
1	OMC	A	2861	1	19,22,23	0.82	0	26,31,34	0.93	1 (3%)
1	OMU	A	2415	1	19,22,23	1.25	4 (21%)	26,31,34	1.71	5 (19%)
1	OMC	A	3887	1	19,22,23	0.82	0	26,31,34	0.86	1 (3%)
1	OMG	A	4618	48,1	23,26,27	1.19	3 (13%)	33,38,41	1.95	6 (18%)
1	PSU	A	4552	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	A2M	A	4571	1	22,25,26	1.47	4 (18%)	31,36,39	2.10	10 (32%)
1	1MA	A	1322	1,47	21,25,26	1.38	4 (19%)	31,37,40	1.68	5 (16%)
1	OMG	A	4494	1	23,26,27	1.20	3 (13%)	33,38,41	1.96	6 (18%)
1	OMU	A	2837	1	19,22,23	1.24	3 (15%)	26,31,34	1.71	5 (19%)
1	PSU	A	3851	1	18,21,22	1.37	2 (11%)	22,30,33	1.85	4 (18%)
1	PSU	A	3770	1	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	A	1744	48,1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	A	4403	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	4 (18%)
1	5MC	A	4447	48,1	18,22,23	0.99	2 (11%)	26,32,35	1.19	2 (7%)
1	OMU	A	4227	1	19,22,23	1.22	3 (15%)	26,31,34	1.70	4 (15%)
1	OMG	A	3627	1	23,26,27	1.19	3 (13%)	33,38,41	1.95	6 (18%)
1	PSU	A	4312	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	A	1862	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	A	2632	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	A	4442	1	18,21,22	1.36	2 (11%)	22,30,33	1.90	4 (18%)
1	OMG	A	3899	1	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
1	A2M	A	1326	1	22,25,26	1.46	4 (18%)	31,36,39	2.09	8 (25%)
1	OMG	A	2424	1	23,26,27	1.20	3 (13%)	33,38,41	1.91	6 (18%)
1	OMC	A	3841	1	19,22,23	0.80	0	26,31,34	0.78	0
1	PSU	A	4296	1	18,21,22	1.33	2 (11%)	22,30,33	1.93	4 (18%)
1	OMG	A	1625	48,1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
1	OMC	A	4536	1,47	19,22,23	0.84	0	26,31,34	0.97	1 (3%)
1	OMG	A	4196	1	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
1	PSU	A	4293	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	A	4457	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	4 (18%)
1	A2M	A	3830	1	22,25,26	1.47	4 (18%)	31,36,39	2.10	10 (32%)
1	PSU	A	4471	48,1	18,21,22	1.34	2 (11%)	22,30,33	1.90	4 (18%)
1	A2M	A	2363	1,47	22,25,26	1.47	4 (18%)	31,36,39	2.11	9 (29%)
3	OMG	C	75	3	23,26,27	1.21	3 (13%)	33,38,41	1.94	6 (18%)
1	6MZ	A	4220	1	22,25,26	1.43	4 (18%)	30,36,39	2.18	9 (30%)
1	PSU	A	3639	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	OMG	A	4228	1	23,26,27	1.18	3 (13%)	33,38,41	1.93	6 (18%)
1	OMC	A	2351	1,47	19,22,23	0.82	0	26,31,34	0.87	1 (3%)
1	PSU	A	3730	1	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
1	OMC	A	3808	48,1	19,22,23	0.83	0	26,31,34	0.94	1 (3%)
1	PSU	A	4493	48,1	18,21,22	1.34	2 (11%)	22,30,33	1.89	4 (18%)
3	PSU	C	69	3	18,21,22	1.35	2 (11%)	22,30,33	1.88	4 (18%)
1	A2M	A	2815	48,1	22,25,26	1.47	4 (18%)	31,36,39	2.12	8 (25%)
1	OMG	A	1316	48,1	23,26,27	1.21	3 (13%)	33,38,41	1.95	6 (18%)
1	PSU	A	2839	1	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	A	4423	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	A	3853	1,47	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
1	OMG	A	3792	1	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
1	A2M	A	3825	1	22,25,26	1.48	4 (18%)	31,36,39	2.07	8 (25%)
1	UR3	A	4530	1	19,22,23	1.00	1 (5%)	26,32,35	1.41	1 (3%)
1	PSU	A	4628	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	OMC	A	2422	1,47	19,22,23	0.82	0	26,31,34	0.84	1 (3%)
1	PSU	A	4673	48,1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	A2M	A	4590	1	22,25,26	1.47	4 (18%)	31,36,39	2.09	8 (25%)

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
1	PSU	A	3844	1	-	1/7/25/26	0/2/2/2
1	OMC	A	4456	1	-	2/9/27/28	0/2/2/2
1	A2M	A	2401	1,47	-	0/9/27/28	0/3/3/3
1	PSU	A	3734	1	-	4/7/25/26	0/2/2/2
1	PSU	A	4299	1	-	0/7/25/26	0/2/2/2
1	PSU	A	3637	48,1	-	0/7/25/26	0/2/2/2
1	PSU	A	3695	48,1	-	0/7/25/26	0/2/2/2
1	PSU	A	4576	48,1	-	0/7/25/26	0/2/2/2
1	PSU	A	1860	1	-	0/7/25/26	0/2/2/2
1	OMG	A	1522	1	-	0/9/27/28	0/3/3/3
1	OMC	A	2804	1	-	0/9/27/28	0/2/2/2
1	A2M	A	3724	1	-	0/9/27/28	0/3/3/3
1	OMU	A	4498	48,1	-	0/9/27/28	0/2/2/2
1	OMU	A	4620	1	-	0/9/27/28	0/2/2/2
1	PSU	A	3715	1	-	0/7/25/26	0/2/2/2
1	PSU	A	4420	1	-	3/7/25/26	0/2/2/2
1	OMG	A	4637	1	-	0/9/27/28	0/3/3/3
1	OMG	A	4499	1	-	0/9/27/28	0/3/3/3
1	PSU	A	5001	48,1	-	0/7/25/26	0/2/2/2
1	PSU	A	4353	48,1	-	0/7/25/26	0/2/2/2
1	A2M	A	400	1	-	0/9/27/28	0/3/3/3
1	PSU	A	4521	48,1,47	-	0/7/25/26	0/2/2/2
1	A2M	A	3718	1	-	0/9/27/28	0/3/3/3
1	PSU	A	1536	1	-	0/7/25/26	0/2/2/2
1	A2M	A	1871	1,47	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A	1677	48,1	-	4/7/25/26	0/2/2/2
1	OMC	A	2824	1	-	2/9/27/28	0/2/2/2
1	UY1	A	3818	48,1	-	5/9/27/28	0/2/2/2
1	OMC	A	1881	1	-	5/9/27/28	0/2/2/2
1	OMU	A	4306	1	-	0/9/27/28	0/2/2/2
1	PSU	A	4500	1	-	2/7/25/26	0/2/2/2
1	5MC	A	3782	1,47	-	0/7/25/26	0/2/2/2
1	A2M	A	1323	1	-	0/9/27/28	0/3/3/3
1	PSU	A	5010	1	-	0/7/25/26	0/2/2/2
1	OMU	A	3925	1	-	0/9/27/28	0/2/2/2
1	OMG	A	4623	1	-	0/9/27/28	0/3/3/3
1	A2M	A	4523	1,47	-	2/9/27/28	0/3/3/3
1	PSU	A	4579	1	-	0/7/25/26	0/2/2/2
1	OMC	A	2365	1,47	-	0/9/27/28	0/2/2/2
1	PSU	A	1683	48,1	-	0/7/25/26	0/2/2/2
1	PSU	A	4532	1	-	0/7/25/26	0/2/2/2
1	OMG	A	3944	1	-	0/9/27/28	0/3/3/3
1	PSU	A	4689	1	-	0/7/25/26	0/2/2/2
1	PSU	A	4972	48,1	-	0/7/25/26	0/2/2/2
1	PSU	A	1781	1	-	0/7/25/26	0/2/2/2
1	A2M	A	398	1	-	2/9/27/28	0/3/3/3
1	PSU	A	1582	48,1	-	0/7/25/26	0/2/2/2
1	A2M	A	1534	1,47	-	2/9/27/28	0/3/3/3
1	OMC	A	3701	48,1	-	5/9/27/28	0/2/2/2
1	OMC	A	3869	1	-	0/9/27/28	0/2/2/2
1	OMG	A	4392	1	-	0/9/27/28	0/3/3/3
1	OMG	A	3744	1	-	0/9/27/28	0/3/3/3
1	OMC	A	1340	1	-	0/9/27/28	0/2/2/2
1	PSU	A	2508	1	-	0/7/25/26	0/2/2/2
1	PSU	A	4361	48,1	-	0/7/25/26	0/2/2/2
1	PSU	A	1792	1	-	0/7/25/26	0/2/2/2
1	A2M	A	3785	1	-	2/9/27/28	0/3/3/3
3	PSU	C	55	3	-	0/7/25/26	0/2/2/2
1	PSU	A	1782	1	-	0/7/25/26	0/2/2/2
1	A2M	A	2787	1,47	-	3/9/27/28	0/3/3/3
1	OMG	A	2876	1	-	1/9/27/28	0/3/3/3
1	PSU	A	3768	1	-	0/7/25/26	0/2/2/2
1	PSU	A	3920	1,47	-	0/7/25/26	0/2/2/2
1	A2M	A	3867	1	-	1/9/27/28	0/3/3/3
1	PSU	A	3884	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	A	2364	1	-	2/9/27/28	0/3/3/3
1	OMG	A	4370	1	-	0/9/27/28	0/3/3/3
1	PSU	A	4431	48,1	-	0/7/25/26	0/2/2/2
1	A2M	A	1524	1	-	0/9/27/28	0/3/3/3
1	OMC	A	2861	1	-	1/9/27/28	0/2/2/2
1	OMU	A	2415	1	-	2/9/27/28	0/2/2/2
1	OMC	A	3887	1	-	2/9/27/28	0/2/2/2
1	OMG	A	4618	48,1	-	0/9/27/28	0/3/3/3
1	PSU	A	4552	1	-	0/7/25/26	0/2/2/2
1	A2M	A	4571	1	-	1/9/27/28	0/3/3/3
1	1MA	A	1322	1,47	-	0/7/25/26	0/3/3/3
1	OMG	A	4494	1	-	0/9/27/28	0/3/3/3
1	OMU	A	2837	1	-	0/9/27/28	0/2/2/2
1	PSU	A	3851	1	-	1/7/25/26	0/2/2/2
1	PSU	A	3770	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1744	48,1	-	0/7/25/26	0/2/2/2
1	PSU	A	4403	1	-	0/7/25/26	0/2/2/2
1	5MC	A	4447	48,1	-	4/7/25/26	0/2/2/2
1	OMU	A	4227	1	-	0/9/27/28	0/2/2/2
1	OMG	A	3627	1	-	0/9/27/28	0/3/3/3
1	PSU	A	4312	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1862	1	-	0/7/25/26	0/2/2/2
1	PSU	A	2632	1	-	0/7/25/26	0/2/2/2
1	PSU	A	4442	1	-	0/7/25/26	0/2/2/2
1	OMG	A	3899	1	-	0/9/27/28	0/3/3/3
1	A2M	A	1326	1	-	1/9/27/28	0/3/3/3
1	OMG	A	2424	1	-	0/9/27/28	0/3/3/3
1	OMC	A	3841	1	-	0/9/27/28	0/2/2/2
1	PSU	A	4296	1	-	0/7/25/26	0/2/2/2
1	OMG	A	1625	48,1	-	1/9/27/28	0/3/3/3
1	OMC	A	4536	1,47	-	3/9/27/28	0/2/2/2
1	OMG	A	4196	1	-	0/9/27/28	0/3/3/3
1	PSU	A	4293	1	-	0/7/25/26	0/2/2/2
1	PSU	A	4457	1	-	0/7/25/26	0/2/2/2
1	A2M	A	3830	1	-	0/9/27/28	0/3/3/3
1	PSU	A	4471	48,1	-	0/7/25/26	0/2/2/2
1	A2M	A	2363	1,47	-	0/9/27/28	0/3/3/3
3	OMG	C	75	3	-	0/9/27/28	0/3/3/3
1	6MZ	A	4220	1	-	0/9/27/28	0/3/3/3
1	PSU	A	3639	1	-	0/7/25/26	0/2/2/2
1	OMG	A	4228	1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	A	2351	1,47	-	1/9/27/28	0/2/2/2
1	PSU	A	3730	1	-	0/7/25/26	0/2/2/2
1	OMC	A	3808	48,1	-	0/9/27/28	0/2/2/2
1	PSU	A	4493	48,1	-	0/7/25/26	0/2/2/2
3	PSU	C	69	3	-	0/7/25/26	0/2/2/2
1	A2M	A	2815	48,1	-	0/9/27/28	0/3/3/3
1	OMG	A	1316	48,1	-	0/9/27/28	0/3/3/3
1	PSU	A	2839	1	-	0/7/25/26	0/2/2/2
1	PSU	A	4423	1	-	0/7/25/26	0/2/2/2
1	PSU	A	3853	1,47	-	0/7/25/26	0/2/2/2
1	OMG	A	3792	1	-	0/9/27/28	0/3/3/3
1	A2M	A	3825	1	-	0/9/27/28	0/3/3/3
1	UR3	A	4530	1	-	0/7/25/26	0/2/2/2
1	PSU	A	4628	1	-	0/7/25/26	0/2/2/2
1	OMC	A	2422	1,47	-	0/9/27/28	0/2/2/2
1	PSU	A	4673	48,1	-	0/7/25/26	0/2/2/2
1	A2M	A	4590	1	-	1/9/27/28	0/3/3/3

All (285) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3718	A2M	C5-C4	4.57	1.47	1.39
1	A	3724	A2M	C5-C4	4.56	1.47	1.39
1	A	2815	A2M	C5-C4	4.55	1.47	1.39
1	A	1524	A2M	C5-C4	4.55	1.47	1.39
1	A	3825	A2M	C5-C4	4.54	1.47	1.39
1	A	4590	A2M	C5-C4	4.52	1.47	1.39
1	A	3867	A2M	C5-C4	4.52	1.47	1.39
1	A	1323	A2M	C5-C4	4.51	1.47	1.39
1	A	2787	A2M	C5-C4	4.51	1.47	1.39
1	A	2363	A2M	C5-C4	4.50	1.47	1.39
1	A	3830	A2M	C5-C4	4.50	1.47	1.39
1	A	2401	A2M	C5-C4	4.50	1.47	1.39
1	A	398	A2M	C5-C4	4.49	1.47	1.39
1	A	400	A2M	C5-C4	4.49	1.47	1.39
1	A	1326	A2M	C5-C4	4.49	1.47	1.39
1	A	4571	A2M	C5-C4	4.49	1.47	1.39
1	A	4220	6MZ	C5-C4	4.49	1.47	1.39
1	A	1871	A2M	C5-C4	4.47	1.47	1.39
1	A	4523	A2M	C5-C4	4.47	1.47	1.39
1	A	1534	A2M	C5-C4	4.45	1.47	1.39
1	A	3785	A2M	C5-C4	4.39	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4420	PSU	C6-C5	3.32	1.39	1.35
1	A	3734	PSU	C6-C5	3.22	1.39	1.35
1	A	3768	PSU	C6-C5	3.20	1.39	1.35
1	A	3851	PSU	C6-C5	3.19	1.39	1.35
1	A	3770	PSU	C6-C5	3.19	1.39	1.35
1	A	1322	1MA	C6-N6	3.18	1.35	1.28
1	A	4500	PSU	C6-C5	3.17	1.39	1.35
1	A	4532	PSU	C6-C5	3.17	1.39	1.35
1	A	3715	PSU	C6-C5	3.17	1.39	1.35
1	A	1860	PSU	C6-C5	3.16	1.39	1.35
1	A	3844	PSU	C6-C5	3.16	1.39	1.35
1	A	2632	PSU	C6-C5	3.16	1.39	1.35
1	A	4312	PSU	C6-C5	3.15	1.39	1.35
1	A	5010	PSU	C6-C5	3.15	1.39	1.35
1	A	4423	PSU	C6-C5	3.15	1.39	1.35
1	A	1792	PSU	C6-C5	3.15	1.39	1.35
1	A	1744	PSU	C6-C5	3.14	1.39	1.35
1	A	5001	PSU	C6-C5	3.14	1.39	1.35
3	C	69	PSU	C6-C5	3.14	1.39	1.35
1	A	1683	PSU	C6-C5	3.13	1.39	1.35
1	A	3853	PSU	C6-C5	3.13	1.39	1.35
1	A	4442	PSU	C6-C5	3.13	1.39	1.35
1	A	4576	PSU	C6-C5	3.13	1.39	1.35
1	A	4361	PSU	C6-C5	3.13	1.39	1.35
1	A	3792	OMG	C5-C4	3.13	1.47	1.38
1	A	4431	PSU	C6-C5	3.12	1.39	1.35
1	A	3944	OMG	C5-C4	3.12	1.47	1.38
3	C	55	PSU	C6-C5	3.12	1.39	1.35
1	A	1862	PSU	C6-C5	3.12	1.39	1.35
1	A	4196	OMG	C5-C4	3.12	1.47	1.38
1	A	4628	PSU	C6-C5	3.11	1.39	1.35
1	A	3695	PSU	C6-C5	3.11	1.38	1.35
3	C	75	OMG	C5-C4	3.11	1.47	1.38
1	A	4521	PSU	C6-C5	3.11	1.38	1.35
1	A	1782	PSU	C6-C5	3.11	1.38	1.35
1	A	2876	OMG	C5-C4	3.11	1.47	1.38
1	A	2364	OMG	C5-C4	3.10	1.47	1.38
1	A	3744	OMG	C5-C4	3.10	1.47	1.38
1	A	4673	PSU	C6-C5	3.10	1.38	1.35
1	A	2508	PSU	C6-C5	3.10	1.38	1.35
1	A	4972	PSU	C6-C5	3.10	1.38	1.35
1	A	1625	OMG	C5-C4	3.10	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1781	PSU	C6-C5	3.10	1.38	1.35
1	A	3639	PSU	C6-C5	3.10	1.38	1.35
1	A	4299	PSU	C6-C5	3.09	1.38	1.35
1	A	4353	PSU	C6-C5	3.09	1.38	1.35
1	A	1322	1MA	C5-C4	3.09	1.47	1.38
1	A	1582	PSU	C6-C5	3.09	1.38	1.35
1	A	1536	PSU	C6-C5	3.09	1.38	1.35
1	A	4623	OMG	C5-C4	3.09	1.47	1.38
1	A	3730	PSU	C6-C5	3.08	1.38	1.35
1	A	2424	OMG	C5-C4	3.08	1.47	1.38
1	A	4471	PSU	C6-C5	3.08	1.38	1.35
1	A	4296	PSU	C6-C5	3.08	1.38	1.35
1	A	3920	PSU	C6-C5	3.07	1.38	1.35
1	A	4499	OMG	C5-C4	3.07	1.47	1.38
1	A	4370	OMG	C5-C4	3.07	1.47	1.38
1	A	4493	PSU	C6-C5	3.07	1.38	1.35
1	A	4552	PSU	C6-C5	3.07	1.38	1.35
1	A	2839	PSU	C6-C5	3.07	1.38	1.35
1	A	4457	PSU	C6-C5	3.07	1.38	1.35
1	A	4637	OMG	C5-C4	3.07	1.47	1.38
1	A	1316	OMG	C5-C4	3.07	1.47	1.38
1	A	4494	OMG	C5-C4	3.06	1.47	1.38
1	A	4579	PSU	C6-C5	3.06	1.38	1.35
1	A	4392	OMG	C5-C4	3.06	1.47	1.38
1	A	4293	PSU	C6-C5	3.06	1.38	1.35
1	A	4618	OMG	C5-C4	3.05	1.47	1.38
1	A	1522	OMG	C5-C4	3.05	1.47	1.38
1	A	3899	OMG	C5-C4	3.05	1.47	1.38
1	A	3884	PSU	C6-C5	3.05	1.38	1.35
1	A	3627	OMG	C5-C4	3.04	1.47	1.38
1	A	4689	PSU	C6-C5	3.04	1.38	1.35
1	A	4228	OMG	C5-C4	3.03	1.47	1.38
1	A	3637	PSU	C6-C5	3.03	1.38	1.35
1	A	4403	PSU	C6-C5	3.02	1.38	1.35
1	A	1677	PSU	C6-C5	2.94	1.38	1.35
1	A	4447	5MC	C6-C5	2.82	1.39	1.34
1	A	3782	5MC	C6-C5	2.74	1.39	1.34
1	A	3637	PSU	C4-N3	-2.71	1.33	1.38
1	A	4590	A2M	C5-C6	2.71	1.48	1.41
1	A	4471	PSU	C4-N3	-2.70	1.33	1.38
1	A	3867	A2M	C5-C6	2.70	1.48	1.41
1	A	1781	PSU	C4-N3	-2.70	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4689	PSU	C4-N3	-2.69	1.33	1.38
1	A	4296	PSU	C4-N3	-2.69	1.33	1.38
1	A	1534	A2M	C5-C6	2.69	1.48	1.41
1	A	3724	A2M	C5-C6	2.69	1.48	1.41
1	A	2815	A2M	C5-C6	2.69	1.48	1.41
1	A	1582	PSU	C4-N3	-2.69	1.33	1.38
1	A	3830	A2M	C5-C6	2.69	1.48	1.41
1	A	4293	PSU	C4-N3	-2.69	1.33	1.38
1	A	398	A2M	C5-C6	2.69	1.48	1.41
1	A	3639	PSU	C4-N3	-2.68	1.33	1.38
1	A	2401	A2M	C5-C6	2.68	1.48	1.41
1	A	1683	PSU	C4-N3	-2.68	1.33	1.38
1	A	4521	PSU	C4-N3	-2.68	1.33	1.38
1	A	3920	PSU	C4-N3	-2.68	1.33	1.38
1	A	400	A2M	C5-C6	2.68	1.48	1.41
1	A	1536	PSU	C4-N3	-2.68	1.33	1.38
1	A	2508	PSU	C4-N3	-2.68	1.33	1.38
1	A	4361	PSU	C4-N3	-2.68	1.33	1.38
1	A	4571	A2M	C5-C6	2.67	1.48	1.41
1	A	3825	A2M	C5-C6	2.67	1.48	1.41
1	A	4353	PSU	C4-N3	-2.67	1.33	1.38
1	A	4579	PSU	C4-N3	-2.67	1.33	1.38
1	A	1524	A2M	C5-C6	2.67	1.48	1.41
1	A	4493	PSU	C4-N3	-2.67	1.33	1.38
1	A	3844	PSU	C4-N3	-2.67	1.33	1.38
1	A	4552	PSU	C4-N3	-2.67	1.33	1.38
1	A	3718	A2M	C5-C6	2.67	1.48	1.41
1	A	4431	PSU	C4-N3	-2.67	1.33	1.38
1	A	4523	A2M	C5-C6	2.66	1.48	1.41
1	A	1782	PSU	C4-N3	-2.66	1.33	1.38
1	A	4673	PSU	C4-N3	-2.66	1.33	1.38
1	A	1326	A2M	C5-C6	2.66	1.48	1.41
1	A	1323	A2M	C5-C6	2.66	1.48	1.41
1	A	4457	PSU	C4-N3	-2.66	1.33	1.38
1	A	3853	PSU	C4-N3	-2.66	1.33	1.38
1	A	3884	PSU	C4-N3	-2.66	1.33	1.38
1	A	4403	PSU	C4-N3	-2.66	1.33	1.38
1	A	1862	PSU	C4-N3	-2.65	1.33	1.38
1	A	2632	PSU	C4-N3	-2.65	1.33	1.38
1	A	4628	PSU	C4-N3	-2.65	1.33	1.38
1	A	1677	PSU	C4-N3	-2.65	1.33	1.38
1	A	4299	PSU	C4-N3	-2.65	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4312	PSU	C4-N3	-2.65	1.33	1.38
1	A	3695	PSU	C4-N3	-2.65	1.33	1.38
1	A	1744	PSU	C4-N3	-2.64	1.33	1.38
1	A	4423	PSU	C4-N3	-2.64	1.33	1.38
1	A	5010	PSU	C4-N3	-2.64	1.33	1.38
1	A	4532	PSU	C4-N3	-2.64	1.33	1.38
1	A	1792	PSU	C4-N3	-2.64	1.33	1.38
3	C	55	PSU	C4-N3	-2.64	1.33	1.38
1	A	2363	A2M	C5-C6	2.64	1.48	1.41
1	A	4442	PSU	C4-N3	-2.64	1.33	1.38
1	A	1860	PSU	C4-N3	-2.63	1.33	1.38
1	A	3734	PSU	C4-N3	-2.63	1.34	1.38
1	A	2787	A2M	C5-C6	2.63	1.48	1.41
1	A	4972	PSU	C4-N3	-2.63	1.34	1.38
1	A	1871	A2M	C5-C6	2.63	1.48	1.41
1	A	2839	PSU	C4-N3	-2.63	1.34	1.38
1	A	3851	PSU	C4-N3	-2.62	1.34	1.38
1	A	3770	PSU	C4-N3	-2.62	1.34	1.38
1	A	5001	PSU	C4-N3	-2.62	1.34	1.38
1	A	3715	PSU	C4-N3	-2.62	1.34	1.38
3	C	69	PSU	C4-N3	-2.62	1.34	1.38
1	A	3730	PSU	C4-N3	-2.62	1.34	1.38
1	A	4576	PSU	C4-N3	-2.62	1.34	1.38
1	A	3768	PSU	C4-N3	-2.61	1.34	1.38
1	A	3785	A2M	C5-C6	2.61	1.48	1.41
1	A	4500	PSU	C4-N3	-2.59	1.34	1.38
1	A	1316	OMG	C6-N1	-2.55	1.34	1.38
1	A	2364	OMG	C6-N1	-2.54	1.34	1.38
1	A	2837	OMU	C4-N3	-2.54	1.34	1.38
1	A	4306	OMU	C4-N3	-2.54	1.34	1.38
1	A	4620	OMU	C4-N3	-2.53	1.34	1.38
1	A	2415	OMU	C4-N3	-2.53	1.34	1.38
1	A	4420	PSU	C4-N3	-2.52	1.34	1.38
1	A	4637	OMG	C6-N1	-2.52	1.34	1.38
1	A	4392	OMG	C6-N1	-2.52	1.34	1.38
1	A	4623	OMG	C6-N1	-2.51	1.34	1.38
3	C	75	OMG	C6-N1	-2.51	1.34	1.38
1	A	3899	OMG	C6-N1	-2.51	1.34	1.38
1	A	4227	OMU	C4-N3	-2.51	1.34	1.38
1	A	4196	OMG	C6-N1	-2.50	1.34	1.38
1	A	4494	OMG	C6-N1	-2.50	1.34	1.38
1	A	3925	OMU	C4-N3	-2.50	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2876	OMG	C6-N1	-2.50	1.34	1.38
1	A	2424	OMG	C6-N1	-2.49	1.34	1.38
1	A	1522	OMG	C6-N1	-2.49	1.34	1.38
1	A	3792	OMG	C6-N1	-2.49	1.34	1.38
1	A	3744	OMG	C6-N1	-2.49	1.34	1.38
1	A	4370	OMG	C6-N1	-2.48	1.34	1.38
1	A	4498	OMU	C4-N3	-2.47	1.34	1.38
1	A	4220	6MZ	C5-C6	2.47	1.48	1.41
1	A	3944	OMG	C6-N1	-2.47	1.34	1.38
1	A	1625	OMG	C6-N1	-2.47	1.34	1.38
1	A	3627	OMG	C6-N1	-2.46	1.34	1.38
1	A	4499	OMG	C6-N1	-2.44	1.34	1.38
1	A	3830	A2M	C8-N7	2.43	1.36	1.31
1	A	1534	A2M	C8-N7	2.43	1.36	1.31
1	A	4618	OMG	C6-N1	-2.43	1.34	1.38
1	A	4228	OMG	C6-N1	-2.42	1.34	1.38
1	A	3867	A2M	C8-N7	2.41	1.36	1.31
1	A	4523	A2M	C8-N7	2.41	1.36	1.31
1	A	4590	A2M	C8-N7	2.41	1.36	1.31
1	A	398	A2M	C8-N7	2.41	1.36	1.31
1	A	400	A2M	C8-N7	2.40	1.36	1.31
1	A	4571	A2M	C8-N7	2.40	1.36	1.31
1	A	2401	A2M	C8-N7	2.40	1.36	1.31
1	A	3785	A2M	C8-N7	2.39	1.36	1.31
1	A	1323	A2M	C8-N7	2.38	1.36	1.31
1	A	1326	A2M	C8-N7	2.37	1.36	1.31
1	A	3724	A2M	C8-N7	2.37	1.36	1.31
1	A	1524	A2M	C8-N7	2.36	1.36	1.31
1	A	1871	A2M	C8-N7	2.36	1.36	1.31
1	A	2815	A2M	C8-N7	2.36	1.36	1.31
1	A	2415	OMU	C2-N1	2.35	1.42	1.38
1	A	3825	A2M	C8-N7	2.35	1.36	1.31
1	A	2363	A2M	C8-N7	2.35	1.36	1.31
1	A	3718	A2M	C8-N7	2.34	1.36	1.31
1	A	2787	A2M	C8-N7	2.33	1.36	1.31
1	A	4220	6MZ	C8-N7	2.27	1.35	1.31
1	A	1316	OMG	C5-N7	-2.27	1.34	1.39
1	A	4447	5MC	C6-N1	-2.26	1.34	1.38
1	A	4220	6MZ	C5-N7	-2.25	1.34	1.39
1	A	3825	A2M	C5-N7	-2.25	1.34	1.39
1	A	1524	A2M	C5-N7	-2.24	1.34	1.39
1	A	3718	A2M	C5-N7	-2.24	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2363	A2M	C5-N7	-2.24	1.34	1.39
1	A	3782	5MC	C6-N1	-2.24	1.34	1.38
1	A	3724	A2M	C5-N7	-2.23	1.34	1.39
1	A	1323	A2M	C5-N7	-2.22	1.34	1.39
1	A	2424	OMG	C5-N7	-2.21	1.34	1.39
1	A	2787	A2M	C5-N7	-2.21	1.34	1.39
1	A	2815	A2M	C5-N7	-2.21	1.34	1.39
1	A	1871	A2M	C5-N7	-2.21	1.34	1.39
1	A	2364	OMG	C5-N7	-2.21	1.34	1.39
1	A	1326	A2M	C5-N7	-2.21	1.34	1.39
1	A	1322	1MA	C2-N3	2.20	1.34	1.30
1	A	3792	OMG	C5-N7	-2.20	1.34	1.39
1	A	2837	OMU	C2-N1	2.19	1.42	1.38
1	A	3867	A2M	C5-N7	-2.19	1.34	1.39
1	A	2876	OMG	C5-N7	-2.19	1.34	1.39
1	A	4196	OMG	C5-N7	-2.18	1.34	1.39
1	A	4623	OMG	C5-N7	-2.18	1.34	1.39
1	A	1625	OMG	C5-N7	-2.18	1.34	1.39
1	A	4637	OMG	C5-N7	-2.17	1.34	1.39
1	A	1534	A2M	C5-N7	-2.17	1.34	1.39
1	A	4590	A2M	C5-N7	-2.17	1.34	1.39
1	A	4392	OMG	C5-N7	-2.17	1.34	1.39
1	A	3785	A2M	C5-N7	-2.17	1.34	1.39
1	A	3899	OMG	C5-N7	-2.17	1.34	1.39
1	A	3744	OMG	C5-N7	-2.17	1.34	1.39
1	A	4571	A2M	C5-N7	-2.17	1.34	1.39
1	A	398	A2M	C5-N7	-2.17	1.34	1.39
1	A	2401	A2M	C5-N7	-2.17	1.34	1.39
1	A	4523	A2M	C5-N7	-2.17	1.34	1.39
3	C	75	OMG	C5-N7	-2.17	1.34	1.39
1	A	400	A2M	C5-N7	-2.16	1.34	1.39
1	A	4227	OMU	C2-N3	-2.16	1.34	1.38
1	A	1322	1MA	C5-N7	-2.16	1.34	1.39
1	A	3830	A2M	C5-N7	-2.16	1.34	1.39
1	A	4494	OMG	C5-N7	-2.15	1.34	1.39
1	A	4306	OMU	C2-N3	-2.15	1.34	1.38
1	A	3925	OMU	C2-N3	-2.14	1.34	1.38
1	A	1522	OMG	C5-N7	-2.14	1.34	1.39
1	A	2837	OMU	C2-N3	-2.14	1.34	1.38
1	A	4370	OMG	C5-N7	-2.14	1.34	1.39
1	A	4620	OMU	C2-N3	-2.14	1.34	1.38
1	A	4499	OMG	C5-N7	-2.13	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4498	OMU	C2-N3	-2.13	1.34	1.38
1	A	3944	OMG	C5-N7	-2.13	1.35	1.39
1	A	4618	OMG	C5-N7	-2.12	1.35	1.39
1	A	3627	OMG	C5-N7	-2.11	1.35	1.39
1	A	4228	OMG	C5-N7	-2.10	1.35	1.39
1	A	4306	OMU	C2-N1	2.06	1.41	1.38
1	A	4620	OMU	C2-N1	2.05	1.41	1.38
1	A	4420	PSU	C4-C5	2.05	1.50	1.44
1	A	2415	OMU	C2-N3	-2.04	1.34	1.38
1	A	4530	UR3	C2-N1	2.04	1.41	1.38
1	A	4227	OMU	C2-N1	2.03	1.41	1.38
1	A	2415	OMU	C5-C4	-2.02	1.39	1.43

All (551) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2815	A2M	C5-C4-N3	-6.51	118.25	126.75
1	A	3724	A2M	C5-C4-N3	-6.43	118.36	126.75
1	A	1524	A2M	C5-C4-N3	-6.41	118.39	126.75
1	A	2876	OMG	C5-C4-N3	-6.35	118.16	128.46
1	A	3825	A2M	C5-C4-N3	-6.33	118.49	126.75
1	A	4590	A2M	C5-C4-N3	-6.32	118.50	126.75
1	A	4220	6MZ	C5-C4-N3	-6.29	118.54	126.75
1	A	3718	A2M	C5-C4-N3	-6.29	118.54	126.75
1	A	2363	A2M	C5-C4-N3	-6.28	118.56	126.75
1	A	3830	A2M	C5-C4-N3	-6.27	118.56	126.75
1	A	4196	OMG	C5-C4-N3	-6.26	118.30	128.46
1	A	1316	OMG	C5-C4-N3	-6.26	118.31	128.46
3	C	75	OMG	C5-C4-N3	-6.25	118.32	128.46
1	A	1323	A2M	C5-C4-N3	-6.25	118.59	126.75
1	A	2364	OMG	C5-C4-N3	-6.25	118.33	128.46
1	A	2401	A2M	C5-C4-N3	-6.25	118.60	126.75
1	A	3792	OMG	C5-C4-N3	-6.24	118.33	128.46
1	A	3867	A2M	C5-C4-N3	-6.24	118.61	126.75
1	A	4637	OMG	C5-C4-N3	-6.21	118.38	128.46
1	A	1326	A2M	C5-C4-N3	-6.21	118.65	126.75
1	A	1871	A2M	C5-C4-N3	-6.19	118.67	126.75
1	A	400	A2M	C5-C4-N3	-6.19	118.67	126.75
1	A	398	A2M	C5-C4-N3	-6.19	118.68	126.75
1	A	2787	A2M	C5-C4-N3	-6.18	118.69	126.75
1	A	3944	OMG	C5-C4-N3	-6.17	118.45	128.46
1	A	1534	A2M	C5-C4-N3	-6.17	118.71	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1625	OMG	C5-C4-N3	-6.16	118.47	128.46
1	A	3744	OMG	C5-C4-N3	-6.16	118.47	128.46
1	A	4623	OMG	C5-C4-N3	-6.15	118.49	128.46
1	A	4392	OMG	C5-C4-N3	-6.14	118.50	128.46
1	A	4494	OMG	C5-C4-N3	-6.12	118.53	128.46
1	A	4523	A2M	C5-C4-N3	-6.12	118.76	126.75
1	A	3899	OMG	C5-C4-N3	-6.12	118.53	128.46
1	A	4571	A2M	C5-C4-N3	-6.12	118.77	126.75
1	A	2424	OMG	C5-C4-N3	-6.10	118.56	128.46
1	A	1522	OMG	C5-C4-N3	-6.10	118.57	128.46
1	A	4370	OMG	C5-C4-N3	-6.07	118.61	128.46
1	A	3785	A2M	C5-C4-N3	-6.07	118.83	126.75
1	A	4296	PSU	N1-C2-N3	6.06	121.99	115.13
1	A	3637	PSU	N1-C2-N3	6.06	121.99	115.13
1	A	1536	PSU	N1-C2-N3	6.05	121.99	115.13
1	A	4499	OMG	C5-C4-N3	-6.05	118.65	128.46
1	A	1582	PSU	N1-C2-N3	6.03	121.96	115.13
1	A	3920	PSU	N1-C2-N3	6.02	121.95	115.13
1	A	3627	OMG	C5-C4-N3	-6.02	118.70	128.46
1	A	4618	OMG	C5-C4-N3	-6.01	118.70	128.46
1	A	4471	PSU	N1-C2-N3	6.01	121.94	115.13
1	A	4299	PSU	N1-C2-N3	6.01	121.94	115.13
1	A	4628	PSU	N1-C2-N3	6.01	121.93	115.13
1	A	4521	PSU	N1-C2-N3	6.00	121.93	115.13
1	A	4673	PSU	N1-C2-N3	6.00	121.93	115.13
1	A	3884	PSU	N1-C2-N3	5.99	121.92	115.13
1	A	1781	PSU	N1-C2-N3	5.99	121.92	115.13
1	A	3853	PSU	N1-C2-N3	5.99	121.92	115.13
1	A	4552	PSU	N1-C2-N3	5.99	121.92	115.13
1	A	4312	PSU	N1-C2-N3	5.99	121.92	115.13
1	A	1744	PSU	N1-C2-N3	5.99	121.92	115.13
1	A	1860	PSU	N1-C2-N3	5.99	121.91	115.13
1	A	4423	PSU	N1-C2-N3	5.99	121.91	115.13
1	A	4353	PSU	N1-C2-N3	5.99	121.91	115.13
1	A	2508	PSU	N1-C2-N3	5.98	121.91	115.13
1	A	4579	PSU	N1-C2-N3	5.98	121.91	115.13
1	A	4493	PSU	N1-C2-N3	5.98	121.91	115.13
1	A	4689	PSU	N1-C2-N3	5.98	121.91	115.13
1	A	1683	PSU	N1-C2-N3	5.98	121.90	115.13
1	A	4431	PSU	N1-C2-N3	5.98	121.90	115.13
1	A	3639	PSU	N1-C2-N3	5.97	121.90	115.13
1	A	1862	PSU	N1-C2-N3	5.97	121.90	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3770	PSU	N1-C2-N3	5.97	121.90	115.13
1	A	1677	PSU	N1-C2-N3	5.97	121.89	115.13
1	A	1782	PSU	N1-C2-N3	5.97	121.89	115.13
1	A	4442	PSU	N1-C2-N3	5.97	121.89	115.13
1	A	5010	PSU	N1-C2-N3	5.97	121.89	115.13
1	A	4532	PSU	N1-C2-N3	5.96	121.89	115.13
3	C	55	PSU	N1-C2-N3	5.95	121.88	115.13
1	A	2632	PSU	N1-C2-N3	5.95	121.88	115.13
1	A	4293	PSU	N1-C2-N3	5.95	121.87	115.13
1	A	3715	PSU	N1-C2-N3	5.94	121.86	115.13
1	A	5001	PSU	N1-C2-N3	5.94	121.86	115.13
1	A	3730	PSU	N1-C2-N3	5.94	121.86	115.13
1	A	2839	PSU	N1-C2-N3	5.93	121.85	115.13
1	A	4972	PSU	N1-C2-N3	5.93	121.85	115.13
1	A	3695	PSU	N1-C2-N3	5.93	121.85	115.13
1	A	3844	PSU	N1-C2-N3	5.93	121.85	115.13
1	A	4361	PSU	N1-C2-N3	5.92	121.83	115.13
1	A	4228	OMG	C5-C4-N3	-5.91	118.87	128.46
1	A	4457	PSU	N1-C2-N3	5.91	121.82	115.13
3	C	69	PSU	N1-C2-N3	5.91	121.82	115.13
1	A	4403	PSU	N1-C2-N3	5.90	121.82	115.13
1	A	4576	PSU	N1-C2-N3	5.90	121.81	115.13
1	A	3768	PSU	N1-C2-N3	5.89	121.81	115.13
1	A	3851	PSU	N1-C2-N3	5.88	121.79	115.13
1	A	1792	PSU	N1-C2-N3	5.88	121.79	115.13
1	A	3734	PSU	N1-C2-N3	5.82	121.72	115.13
1	A	4500	PSU	N1-C2-N3	5.78	121.67	115.13
1	A	4530	UR3	C4-N3-C2	-5.74	119.16	124.56
1	A	4420	PSU	N1-C2-N3	5.55	121.42	115.13
1	A	1322	1MA	C5-C4-N3	-5.29	119.37	127.26
1	A	2815	A2M	N3-C4-N9	5.07	135.44	127.08
1	A	2876	OMG	C2-N3-C4	5.04	121.28	112.30
1	A	3818	UY1	N1-C2-N3	5.03	120.83	115.13
1	A	4220	6MZ	N3-C4-N9	4.99	135.31	127.08
1	A	3724	A2M	N3-C4-N9	4.96	135.26	127.08
1	A	4196	OMG	C2-N3-C4	4.95	121.11	112.30
1	A	1524	A2M	N3-C4-N9	4.94	135.22	127.08
1	A	4637	OMG	C2-N3-C4	4.93	121.08	112.30
3	C	75	OMG	C2-N3-C4	4.92	121.07	112.30
1	A	3792	OMG	C2-N3-C4	4.91	121.05	112.30
1	A	2364	OMG	C2-N3-C4	4.91	121.04	112.30
1	A	1522	OMG	C2-N3-C4	4.90	121.04	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1625	OMG	C2-N3-C4	4.90	121.04	112.30
1	A	4618	OMG	C2-N3-C4	4.90	121.04	112.30
1	A	3899	OMG	C2-N3-C4	4.90	121.03	112.30
1	A	3944	OMG	C2-N3-C4	4.89	121.02	112.30
1	A	4494	OMG	C2-N3-C4	4.89	121.01	112.30
1	A	3825	A2M	N3-C4-N9	4.89	135.14	127.08
1	A	4590	A2M	N3-C4-N9	4.88	135.13	127.08
1	A	3627	OMG	C2-N3-C4	4.88	121.00	112.30
1	A	3744	OMG	C2-N3-C4	4.88	120.99	112.30
1	A	4392	OMG	C2-N3-C4	4.88	120.99	112.30
1	A	1316	OMG	C2-N3-C4	4.88	120.99	112.30
1	A	2363	A2M	N3-C4-N9	4.88	135.12	127.08
1	A	3830	A2M	N3-C4-N9	4.87	135.11	127.08
1	A	4623	OMG	C2-N3-C4	4.87	120.97	112.30
1	A	4499	OMG	C2-N3-C4	4.87	120.97	112.30
1	A	2787	A2M	N3-C4-N9	4.87	135.10	127.08
1	A	4370	OMG	C2-N3-C4	4.86	120.96	112.30
1	A	2401	A2M	N3-C4-N9	4.85	135.07	127.08
1	A	2424	OMG	C2-N3-C4	4.84	120.93	112.30
1	A	3718	A2M	N3-C4-N9	4.84	135.06	127.08
1	A	1871	A2M	N3-C4-N9	4.84	135.05	127.08
1	A	4228	OMG	C2-N3-C4	4.84	120.92	112.30
1	A	1323	A2M	N3-C4-N9	4.83	135.04	127.08
1	A	1326	A2M	N3-C4-N9	4.83	135.04	127.08
1	A	400	A2M	N3-C4-N9	4.81	135.01	127.08
1	A	3785	A2M	N3-C4-N9	4.80	134.99	127.08
1	A	398	A2M	N3-C4-N9	4.79	134.97	127.08
1	A	3867	A2M	N3-C4-N9	4.78	134.95	127.08
1	A	4571	A2M	N3-C4-N9	4.76	134.93	127.08
1	A	2876	OMG	N9-C4-N3	4.75	135.49	125.94
1	A	4523	A2M	N3-C4-N9	4.74	134.90	127.08
1	A	3792	OMG	N9-C4-N3	4.74	135.46	125.94
1	A	1316	OMG	N9-C4-N3	4.72	135.41	125.94
1	A	4196	OMG	N9-C4-N3	4.72	135.41	125.94
1	A	1534	A2M	N3-C4-N9	4.71	134.84	127.08
3	C	75	OMG	N9-C4-N3	4.68	135.34	125.94
1	A	2364	OMG	N9-C4-N3	4.67	135.31	125.94
1	A	1322	1MA	C2-N3-C4	4.64	121.53	112.41
1	A	1625	OMG	N9-C4-N3	4.61	135.20	125.94
1	A	3944	OMG	N9-C4-N3	4.61	135.19	125.94
1	A	4623	OMG	N9-C4-N3	4.61	135.19	125.94
1	A	2424	OMG	N9-C4-N3	4.60	135.18	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4637	OMG	N9-C4-N3	4.60	135.18	125.94
1	A	3744	OMG	N9-C4-N3	4.59	135.16	125.94
1	A	4392	OMG	N9-C4-N3	4.58	135.14	125.94
1	A	4494	OMG	N9-C4-N3	4.58	135.14	125.94
1	A	3899	OMG	N9-C4-N3	4.55	135.07	125.94
1	A	4370	OMG	N9-C4-N3	4.55	135.07	125.94
1	A	1522	OMG	N9-C4-N3	4.53	135.03	125.94
1	A	4499	OMG	N9-C4-N3	4.53	135.03	125.94
1	A	4498	OMU	C4-N3-C2	-4.48	120.67	126.58
1	A	4227	OMU	C4-N3-C2	-4.46	120.70	126.58
1	A	3925	OMU	C4-N3-C2	-4.45	120.71	126.58
1	A	3627	OMG	N9-C4-N3	4.45	134.87	125.94
1	A	4618	OMG	N9-C4-N3	4.44	134.85	125.94
1	A	4306	OMU	C4-N3-C2	-4.38	120.81	126.58
1	A	4620	OMU	C4-N3-C2	-4.37	120.81	126.58
1	A	4228	OMG	N9-C4-N3	4.34	134.66	125.94
1	A	2837	OMU	C4-N3-C2	-4.25	120.97	126.58
1	A	2415	OMU	C4-N3-C2	-4.13	121.14	126.58
1	A	4498	OMU	N3-C2-N1	4.11	120.34	114.89
1	A	3925	OMU	N3-C2-N1	4.08	120.31	114.89
1	A	4620	OMU	N3-C2-N1	4.08	120.31	114.89
1	A	4306	OMU	N3-C2-N1	4.08	120.30	114.89
1	A	4227	OMU	N3-C2-N1	4.07	120.29	114.89
1	A	4296	PSU	C4-N3-C2	-4.06	120.49	126.34
1	A	3818	UY1	C4-N3-C2	-4.04	120.51	126.34
1	A	2415	OMU	N3-C2-N1	4.04	120.25	114.89
1	A	2837	OMU	N3-C2-N1	4.04	120.25	114.89
1	A	1677	PSU	C4-N3-C2	-4.00	120.57	126.34
1	A	4471	PSU	C4-N3-C2	-3.99	120.59	126.34
1	A	1582	PSU	C4-N3-C2	-3.98	120.60	126.34
1	A	3920	PSU	C4-N3-C2	-3.98	120.61	126.34
1	A	2815	A2M	C2-N3-C4	3.97	121.14	111.75
1	A	4493	PSU	C4-N3-C2	-3.97	120.62	126.34
1	A	1781	PSU	C4-N3-C2	-3.96	120.63	126.34
1	A	4353	PSU	C4-N3-C2	-3.96	120.64	126.34
1	A	1536	PSU	C4-N3-C2	-3.95	120.64	126.34
1	A	4521	PSU	C4-N3-C2	-3.95	120.64	126.34
1	A	4447	5MC	C5-C6-N1	-3.95	119.27	123.34
1	A	4673	PSU	C4-N3-C2	-3.95	120.65	126.34
1	A	3637	PSU	C4-N3-C2	-3.95	120.65	126.34
1	A	4403	PSU	C4-N3-C2	-3.95	120.65	126.34
1	A	1782	PSU	C4-N3-C2	-3.94	120.66	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2508	PSU	C4-N3-C2	-3.94	120.66	126.34
1	A	4299	PSU	C4-N3-C2	-3.94	120.66	126.34
1	A	4312	PSU	C4-N3-C2	-3.93	120.68	126.34
1	A	1744	PSU	C4-N3-C2	-3.93	120.68	126.34
1	A	4590	A2M	C2-N3-C4	3.93	121.03	111.75
1	A	3770	PSU	C4-N3-C2	-3.93	120.68	126.34
1	A	3884	PSU	C4-N3-C2	-3.93	120.68	126.34
1	A	4579	PSU	C4-N3-C2	-3.93	120.68	126.34
1	A	4552	PSU	C4-N3-C2	-3.93	120.68	126.34
1	A	1683	PSU	C4-N3-C2	-3.92	120.68	126.34
1	A	1860	PSU	C4-N3-C2	-3.91	120.70	126.34
1	A	4293	PSU	C4-N3-C2	-3.91	120.70	126.34
1	A	4628	PSU	C4-N3-C2	-3.91	120.70	126.34
1	A	3639	PSU	C4-N3-C2	-3.91	120.71	126.34
1	A	1862	PSU	C4-N3-C2	-3.91	120.71	126.34
1	A	3724	A2M	C2-N3-C4	3.91	120.98	111.75
3	C	55	PSU	C4-N3-C2	-3.90	120.72	126.34
1	A	4457	PSU	C4-N3-C2	-3.90	120.72	126.34
1	A	5010	PSU	C4-N3-C2	-3.90	120.72	126.34
1	A	4431	PSU	C4-N3-C2	-3.89	120.73	126.34
1	A	4532	PSU	C4-N3-C2	-3.89	120.73	126.34
1	A	1534	A2M	C2-N3-C4	3.89	120.95	111.75
1	A	4442	PSU	C4-N3-C2	-3.88	120.74	126.34
1	A	4361	PSU	C4-N3-C2	-3.88	120.74	126.34
1	A	4972	PSU	C4-N3-C2	-3.88	120.74	126.34
1	A	3830	A2M	C2-N3-C4	3.88	120.92	111.75
1	A	3730	PSU	C4-N3-C2	-3.88	120.75	126.34
1	A	2363	A2M	C2-N3-C4	3.88	120.91	111.75
1	A	2839	PSU	C4-N3-C2	-3.88	120.75	126.34
1	A	2401	A2M	C2-N3-C4	3.87	120.90	111.75
1	A	3695	PSU	C4-N3-C2	-3.87	120.77	126.34
1	A	4423	PSU	C4-N3-C2	-3.86	120.77	126.34
1	A	400	A2M	C2-N3-C4	3.86	120.88	111.75
1	A	2632	PSU	C4-N3-C2	-3.86	120.77	126.34
1	A	1323	A2M	C2-N3-C4	3.86	120.87	111.75
1	A	1524	A2M	C2-N3-C4	3.86	120.87	111.75
1	A	1871	A2M	C2-N3-C4	3.86	120.87	111.75
1	A	1326	A2M	C2-N3-C4	3.86	120.87	111.75
3	C	69	PSU	C4-N3-C2	-3.86	120.78	126.34
1	A	398	A2M	C2-N3-C4	3.86	120.86	111.75
1	A	1792	PSU	C4-N3-C2	-3.85	120.78	126.34
1	A	3825	A2M	C2-N3-C4	3.85	120.85	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3785	A2M	C2-N3-C4	3.85	120.84	111.75
1	A	4523	A2M	C2-N3-C4	3.85	120.84	111.75
1	A	4220	6MZ	C2-N3-C4	3.85	120.84	111.75
1	A	4571	A2M	C2-N3-C4	3.84	120.83	111.75
1	A	4689	PSU	C4-N3-C2	-3.83	120.82	126.34
1	A	3853	PSU	C4-N3-C2	-3.83	120.82	126.34
1	A	2787	A2M	C2-N3-C4	3.83	120.79	111.75
1	A	5001	PSU	C4-N3-C2	-3.83	120.83	126.34
1	A	3715	PSU	C4-N3-C2	-3.82	120.83	126.34
1	A	3844	PSU	C4-N3-C2	-3.80	120.86	126.34
1	A	4576	PSU	C4-N3-C2	-3.79	120.88	126.34
1	A	3768	PSU	C4-N3-C2	-3.78	120.89	126.34
1	A	3718	A2M	C2-N3-C4	3.78	120.68	111.75
1	A	3867	A2M	C2-N3-C4	3.78	120.67	111.75
1	A	3734	PSU	C4-N3-C2	-3.77	120.90	126.34
1	A	398	A2M	C2'-C1'-N9	-3.75	107.22	113.53
1	A	3851	PSU	C4-N3-C2	-3.68	121.03	126.34
1	A	4227	OMU	C5-C4-N3	3.59	120.21	114.84
1	A	4498	OMU	C5-C4-N3	3.57	120.19	114.84
1	A	3925	OMU	C5-C4-N3	3.56	120.17	114.84
1	A	1536	PSU	O2-C2-N1	-3.55	118.88	122.79
1	A	4306	OMU	C5-C4-N3	3.53	120.11	114.84
1	A	4620	OMU	C5-C4-N3	3.52	120.10	114.84
1	A	4500	PSU	C4-N3-C2	-3.52	121.27	126.34
1	A	2837	OMU	C5-C4-N3	3.50	120.07	114.84
1	A	4689	PSU	O2-C2-N1	-3.49	118.94	122.79
1	A	3884	PSU	O2-C2-N1	-3.49	118.94	122.79
1	A	4220	6MZ	C9-N6-C6	-3.47	119.88	122.87
1	A	4628	PSU	O2-C2-N1	-3.45	118.99	122.79
3	C	55	PSU	O2-C2-N1	-3.44	119.00	122.79
1	A	4296	PSU	O2-C2-N1	-3.43	119.01	122.79
1	A	1860	PSU	O2-C2-N1	-3.43	119.02	122.79
1	A	4673	PSU	O2-C2-N1	-3.42	119.02	122.79
1	A	3920	PSU	O2-C2-N1	-3.42	119.03	122.79
1	A	4532	PSU	O2-C2-N1	-3.42	119.03	122.79
1	A	4423	PSU	O2-C2-N1	-3.41	119.03	122.79
1	A	1677	PSU	O2-C2-N1	-3.41	119.03	122.79
1	A	4312	PSU	O2-C2-N1	-3.41	119.04	122.79
1	A	4299	PSU	O2-C2-N1	-3.41	119.04	122.79
1	A	5001	PSU	O2-C2-N1	-3.41	119.04	122.79
1	A	1683	PSU	O2-C2-N1	-3.41	119.04	122.79
1	A	4579	PSU	O2-C2-N1	-3.41	119.04	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4442	PSU	O2-C2-N1	-3.40	119.04	122.79
1	A	3853	PSU	O2-C2-N1	-3.40	119.05	122.79
1	A	1744	PSU	O2-C2-N1	-3.40	119.05	122.79
1	A	1862	PSU	O2-C2-N1	-3.40	119.05	122.79
1	A	4431	PSU	O2-C2-N1	-3.39	119.05	122.79
1	A	4552	PSU	O2-C2-N1	-3.39	119.06	122.79
1	A	2839	PSU	O2-C2-N1	-3.39	119.06	122.79
1	A	4493	PSU	O2-C2-N1	-3.39	119.06	122.79
1	A	4972	PSU	O2-C2-N1	-3.39	119.06	122.79
3	C	69	PSU	O2-C2-N1	-3.38	119.06	122.79
1	A	4576	PSU	O2-C2-N1	-3.38	119.07	122.79
1	A	2415	OMU	C5-C4-N3	3.38	119.90	114.84
1	A	4521	PSU	O2-C2-N1	-3.38	119.07	122.79
1	A	1534	A2M	C4-C5-N7	-3.37	106.51	110.62
1	A	1582	PSU	O2-C2-N1	-3.37	119.08	122.79
1	A	3639	PSU	O2-C2-N1	-3.37	119.08	122.79
1	A	5010	PSU	O2-C2-N1	-3.37	119.08	122.79
1	A	3730	PSU	O2-C2-N1	-3.37	119.08	122.79
1	A	3715	PSU	O2-C2-N1	-3.36	119.09	122.79
1	A	3770	PSU	O2-C2-N1	-3.36	119.09	122.79
1	A	2508	PSU	O2-C2-N1	-3.36	119.09	122.79
1	A	4353	PSU	O2-C2-N1	-3.36	119.10	122.79
1	A	3851	PSU	O2-C2-N1	-3.35	119.10	122.79
1	A	1782	PSU	O2-C2-N1	-3.35	119.10	122.79
1	A	3867	A2M	C4-C5-N7	-3.35	106.54	110.62
1	A	3637	PSU	O2-C2-N1	-3.35	119.10	122.79
1	A	2632	PSU	O2-C2-N1	-3.35	119.11	122.79
1	A	4293	PSU	O2-C2-N1	-3.35	119.11	122.79
1	A	4403	PSU	O2-C2-N1	-3.35	119.11	122.79
1	A	3768	PSU	O2-C2-N1	-3.34	119.11	122.79
1	A	4457	PSU	O2-C2-N1	-3.34	119.12	122.79
1	A	3844	PSU	O2-C2-N1	-3.33	119.12	122.79
1	A	4228	OMG	C6-C5-N7	3.33	136.44	130.25
1	A	4590	A2M	C4-C5-N7	-3.33	106.57	110.62
1	A	3724	A2M	C4-C5-N7	-3.32	106.57	110.62
1	A	3782	5MC	C5-C6-N1	-3.32	119.92	123.34
1	A	398	A2M	C4-C5-N7	-3.32	106.57	110.62
1	A	4420	PSU	C4-N3-C2	-3.32	121.56	126.34
1	A	3830	A2M	C4-C5-N7	-3.31	106.58	110.62
1	A	4523	A2M	C4-C5-N7	-3.31	106.59	110.62
1	A	1781	PSU	O2-C2-N1	-3.30	119.15	122.79
1	A	1792	PSU	O2-C2-N1	-3.30	119.15	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2787	A2M	C2'-C1'-N9	-3.30	107.97	113.53
1	A	2401	A2M	C4-C5-N7	-3.30	106.60	110.62
1	A	4471	PSU	O2-C2-N1	-3.30	119.16	122.79
1	A	3825	A2M	C4-C5-N7	-3.29	106.61	110.62
1	A	3695	PSU	O2-C2-N1	-3.29	119.17	122.79
1	A	1524	A2M	C4-C5-N7	-3.29	106.61	110.62
1	A	4500	PSU	O2-C2-N1	-3.29	119.17	122.79
1	A	3734	PSU	C3'-C2'-C1'	3.29	105.47	101.64
1	A	400	A2M	C4-C5-N7	-3.28	106.62	110.62
1	A	4618	OMG	C6-C5-N7	3.28	136.34	130.25
1	A	4571	A2M	C4-C5-N7	-3.28	106.63	110.62
1	A	2815	A2M	C4-C5-N7	-3.27	106.63	110.62
1	A	1323	A2M	C4-C5-N7	-3.27	106.64	110.62
1	A	3627	OMG	C6-C5-N7	3.27	136.33	130.25
1	A	3718	A2M	C4-C5-N7	-3.27	106.64	110.62
1	A	1326	A2M	C4-C5-N7	-3.26	106.65	110.62
1	A	2363	A2M	C4-C5-N7	-3.26	106.65	110.62
1	A	4361	PSU	O2-C2-N1	-3.25	119.21	122.79
1	A	4420	PSU	O2-C2-N1	-3.25	119.22	122.79
1	A	3734	PSU	O2-C2-N1	-3.25	119.22	122.79
1	A	1871	A2M	C4-C5-N7	-3.23	106.69	110.62
1	A	1522	OMG	C6-C5-N7	3.22	136.23	130.25
1	A	1322	1MA	N9-C4-N3	3.20	134.41	126.94
1	A	4499	OMG	C6-C5-N7	3.18	136.17	130.25
1	A	4523	A2M	C2'-C1'-N9	-3.18	108.18	113.53
1	A	3785	A2M	C4-C5-N7	-3.18	106.75	110.62
1	A	3785	A2M	N3-C2-N1	-3.17	123.64	128.60
1	A	3899	OMG	C6-C5-N7	3.17	136.15	130.25
1	A	1534	A2M	N3-C2-N1	-3.17	123.64	128.60
1	A	2787	A2M	C4-C5-N7	-3.17	106.76	110.62
1	A	4370	OMG	C6-C5-N7	3.17	136.14	130.25
1	A	3785	A2M	C2'-C1'-N9	-3.16	108.21	113.53
1	A	4637	OMG	C6-C5-N7	3.15	136.10	130.25
1	A	4523	A2M	N3-C2-N1	-3.15	123.68	128.60
1	A	4494	OMG	C6-C5-N7	3.15	136.10	130.25
1	A	4571	A2M	N3-C2-N1	-3.15	123.68	128.60
1	A	4590	A2M	N3-C2-N1	-3.14	123.69	128.60
1	A	1871	A2M	N3-C2-N1	-3.13	123.70	128.60
1	A	4392	OMG	C6-C5-N7	3.13	136.07	130.25
1	A	400	A2M	N3-C2-N1	-3.13	123.71	128.60
1	A	398	A2M	N3-C2-N1	-3.12	123.72	128.60
1	A	2363	A2M	N3-C2-N1	-3.12	123.72	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1326	A2M	N3-C2-N1	-3.12	123.72	128.60
1	A	3944	OMG	C6-C5-N7	3.11	136.04	130.25
1	A	2787	A2M	N3-C2-N1	-3.11	123.74	128.60
1	A	3744	OMG	C6-C5-N7	3.11	136.03	130.25
1	A	3830	A2M	N3-C2-N1	-3.11	123.75	128.60
1	A	2401	A2M	N3-C2-N1	-3.10	123.75	128.60
1	A	2815	A2M	N3-C2-N1	-3.10	123.75	128.60
1	A	1323	A2M	N3-C2-N1	-3.10	123.75	128.60
1	A	4623	OMG	C6-C5-N7	3.09	135.99	130.25
1	A	1625	OMG	C6-C5-N7	3.09	135.99	130.25
1	A	4220	6MZ	N1-C2-N3	-3.07	123.80	128.60
1	A	4220	6MZ	C4-C5-N7	-3.07	106.89	110.62
1	A	3724	A2M	N3-C2-N1	-3.06	123.82	128.60
3	C	75	OMG	C6-C5-N7	3.06	135.93	130.25
1	A	2364	OMG	C6-C5-N7	3.05	135.92	130.25
1	A	2876	OMG	C6-C5-N7	3.04	135.90	130.25
1	A	4196	OMG	C6-C5-N7	3.04	135.90	130.25
1	A	3825	A2M	N3-C2-N1	-3.01	123.89	128.60
1	A	2424	OMG	C6-C5-N7	3.01	135.85	130.25
1	A	2401	A2M	C2'-C1'-N9	-3.01	108.47	113.53
1	A	4220	6MZ	C6-C5-N7	3.01	135.64	132.39
1	A	1316	OMG	C6-C5-N7	3.00	135.83	130.25
1	A	3925	OMU	O4-C4-C5	-2.99	119.90	125.16
1	A	3792	OMG	C6-C5-N7	2.99	135.81	130.25
1	A	1524	A2M	N3-C2-N1	-2.97	123.96	128.60
1	A	4498	OMU	O4-C4-C5	-2.97	119.94	125.16
1	A	4227	OMU	O4-C4-C5	-2.95	119.97	125.16
1	A	4306	OMU	O4-C4-C5	-2.95	119.97	125.16
1	A	2415	OMU	C1'-N1-C2	2.95	122.91	117.57
1	A	2363	A2M	C2'-C1'-N9	-2.94	108.58	113.53
1	A	4620	OMU	O4-C4-C5	-2.94	120.00	125.16
1	A	3818	UY1	O2-C2-N1	-2.93	119.57	122.79
1	A	2837	OMU	O4-C4-C5	-2.92	120.03	125.16
1	A	2415	OMU	O4-C4-C5	-2.91	120.03	125.16
1	A	3718	A2M	N3-C2-N1	-2.88	124.10	128.60
1	A	3867	A2M	N3-C2-N1	-2.86	124.13	128.60
1	A	4590	A2M	C5-N7-C8	2.79	107.47	103.51
1	A	398	A2M	C5-N7-C8	2.78	107.46	103.51
1	A	3830	A2M	C5-N7-C8	2.78	107.46	103.51
1	A	4523	A2M	C5-N7-C8	2.78	107.46	103.51
1	A	3724	A2M	C5-N7-C8	2.78	107.45	103.51
1	A	2401	A2M	C5-N7-C8	2.77	107.44	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2815	A2M	C5-N7-C8	2.77	107.44	103.51
1	A	1534	A2M	C5-N7-C8	2.77	107.44	103.51
1	A	3867	A2M	C5-N7-C8	2.76	107.44	103.51
1	A	400	A2M	C5-N7-C8	2.76	107.43	103.51
1	A	4571	A2M	C5-N7-C8	2.75	107.42	103.51
1	A	3785	A2M	C4-N9-C8	2.75	108.70	105.73
1	A	4420	PSU	C6-C5-C4	-2.75	116.28	118.20
1	A	1323	A2M	C5-N7-C8	2.73	107.39	103.51
1	A	1326	A2M	C5-N7-C8	2.73	107.39	103.51
1	A	3785	A2M	C5-N7-C8	2.72	107.38	103.51
1	A	2363	A2M	C5-N7-C8	2.71	107.35	103.51
1	A	3825	A2M	C5-N7-C8	2.69	107.33	103.51
1	A	1524	A2M	C5-N7-C8	2.68	107.32	103.51
1	A	1871	A2M	C5-N7-C8	2.68	107.32	103.51
1	A	2787	A2M	C5-N7-C8	2.67	107.31	103.51
1	A	1871	A2M	C2'-C1'-N9	-2.67	109.03	113.53
1	A	4228	OMG	C4-C5-N7	-2.66	106.50	110.72
1	A	3627	OMG	C4-C5-N7	-2.65	106.53	110.72
1	A	4618	OMG	C4-C5-N7	-2.65	106.53	110.72
1	A	4637	OMG	C4-C5-N7	-2.65	106.53	110.72
1	A	1522	OMG	C4-C5-N7	-2.64	106.55	110.72
1	A	3718	A2M	C5-N7-C8	2.63	107.25	103.51
1	A	3785	A2M	O4'-C1'-N9	2.62	113.23	108.06
1	A	3899	OMG	C4-C5-N7	-2.61	106.58	110.72
1	A	4370	OMG	C4-C5-N7	-2.60	106.60	110.72
1	A	3944	OMG	C4-C5-N7	-2.60	106.60	110.72
1	A	4571	A2M	C4-N9-C8	2.60	108.55	105.73
1	A	4392	OMG	C4-C5-N7	-2.60	106.61	110.72
1	A	3744	OMG	C4-C5-N7	-2.59	106.62	110.72
1	A	4220	6MZ	C5-N7-C8	2.59	107.19	103.51
1	A	1322	1MA	C4-C5-N7	-2.59	106.62	110.72
1	A	4499	OMG	C4-C5-N7	-2.59	106.62	110.72
1	A	1316	OMG	C4-C5-N7	-2.59	106.62	110.72
1	A	4523	A2M	C4-N9-C8	2.59	108.53	105.73
1	A	4494	OMG	C4-C5-N7	-2.58	106.63	110.72
1	A	2364	OMG	C4-C5-N7	-2.58	106.64	110.72
3	C	75	OMG	C4-C5-N7	-2.58	106.64	110.72
1	A	4623	OMG	C4-C5-N7	-2.57	106.65	110.72
1	A	2876	OMG	C4-C5-N7	-2.57	106.65	110.72
1	A	1625	OMG	C4-C5-N7	-2.56	106.67	110.72
1	A	4196	OMG	C4-C5-N7	-2.55	106.68	110.72
1	A	4536	OMC	O2-C2-N3	-2.55	118.18	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	400	A2M	C4-N9-C8	2.55	108.49	105.73
1	A	4456	OMC	O2-C2-N3	-2.54	118.20	122.33
1	A	3830	A2M	C4-N9-C8	2.54	108.48	105.73
1	A	3782	5MC	C5-C4-N3	-2.54	118.94	121.67
1	A	398	A2M	C4-N9-C8	2.53	108.47	105.73
1	A	2787	A2M	C4-N9-C8	2.52	108.46	105.73
1	A	2401	A2M	C4-N9-C8	2.52	108.45	105.73
1	A	3792	OMG	C4-C5-N7	-2.51	106.74	110.72
1	A	1871	A2M	C4-N9-C8	2.50	108.44	105.73
1	A	1326	A2M	C4-N9-C8	2.49	108.42	105.73
1	A	4447	5MC	C5-C4-N3	-2.48	118.99	121.67
1	A	1534	A2M	C4-N9-C8	2.48	108.42	105.73
1	A	2424	OMG	C4-C5-N7	-2.47	106.82	110.72
1	A	3718	A2M	C2'-C1'-N9	-2.45	109.40	113.53
1	A	4590	A2M	C4-N9-C8	2.44	108.37	105.73
1	A	3867	A2M	C4-N9-C8	2.43	108.36	105.73
1	A	4220	6MZ	C4-N9-C8	2.41	108.34	105.73
1	A	2363	A2M	C4-N9-C8	2.41	108.34	105.73
1	A	1323	A2M	C4-N9-C8	2.40	108.33	105.73
1	A	1881	OMC	O4'-C1'-N1	2.39	113.83	108.36
1	A	3808	OMC	O2-C2-N3	-2.35	118.50	122.33
1	A	2815	A2M	C4-N9-C8	2.35	108.28	105.73
1	A	400	A2M	C2'-C1'-N9	-2.34	109.59	113.53
1	A	2861	OMC	O2-C2-N3	-2.34	118.52	122.33
1	A	3825	A2M	C4-N9-C8	2.33	108.25	105.73
1	A	3724	A2M	C4-N9-C8	2.33	108.25	105.73
1	A	1534	A2M	C6-C5-N7	2.30	136.30	132.02
1	A	1524	A2M	C4-N9-C8	2.28	108.20	105.73
1	A	3718	A2M	C4-N9-C8	2.27	108.19	105.73
1	A	3782	5MC	O2-C2-N3	-2.25	118.67	122.33
1	A	3785	A2M	C6-C5-N7	2.23	136.18	132.02
1	A	4523	A2M	C6-C5-N7	2.22	136.16	132.02
1	A	4571	A2M	C6-C5-N7	2.21	136.14	132.02
1	A	398	A2M	C6-C5-N7	2.21	136.13	132.02
1	A	4442	PSU	O4'-C1'-C2'	2.20	108.25	105.14
1	A	4590	A2M	C6-C5-N7	2.20	136.12	132.02
1	A	400	A2M	C6-C5-N7	2.19	136.10	132.02
1	A	4403	PSU	O4'-C1'-C2'	2.17	108.21	105.14
1	A	1322	1MA	C6-C5-N7	2.17	136.15	132.20
1	A	2351	OMC	O2-C2-N3	-2.17	118.80	122.33
1	A	2401	A2M	C6-C5-N7	2.17	136.06	132.02
1	A	4571	A2M	C2'-C1'-N9	-2.16	109.89	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3867	A2M	C6-C5-N7	2.16	136.05	132.02
1	A	3830	A2M	C6-C5-N7	2.16	136.04	132.02
1	A	2424	OMG	O6-C6-C5	-2.16	120.87	126.60
1	A	1871	A2M	C6-C5-N7	2.16	136.04	132.02
1	A	1326	A2M	C6-C5-N7	2.15	136.03	132.02
1	A	4494	OMG	O6-C6-C5	-2.15	120.90	126.60
1	A	3818	UY1	C6-N1-C2	-2.14	120.49	122.68
1	A	2876	OMG	O6-C6-C5	-2.14	120.92	126.60
1	A	3785	A2M	N9-C8-N7	-2.14	110.98	113.91
1	A	1323	A2M	C6-C5-N7	2.14	136.00	132.02
1	A	3792	OMG	O6-C6-C5	-2.14	120.93	126.60
1	A	4499	OMG	O6-C6-C5	-2.13	120.94	126.60
1	A	1625	OMG	O6-C6-C5	-2.13	120.94	126.60
1	A	1316	OMG	O6-C6-C5	-2.13	120.96	126.60
1	A	4196	OMG	O6-C6-C5	-2.13	120.96	126.60
1	A	4498	OMU	O2-C2-N1	-2.13	119.96	122.79
1	A	4618	OMG	O6-C6-C5	-2.13	120.96	126.60
1	A	3830	A2M	C2'-C1'-N9	-2.12	109.96	113.53
1	A	4392	OMG	O6-C6-C5	-2.12	120.98	126.60
1	A	2363	A2M	C6-C5-N7	2.12	135.96	132.02
1	A	4623	OMG	O6-C6-C5	-2.11	120.99	126.60
1	A	3627	OMG	O6-C6-C5	-2.11	120.99	126.60
1	A	3695	PSU	O4'-C1'-C2'	2.11	108.12	105.14
1	A	4228	OMG	O6-C6-C5	-2.11	121.00	126.60
1	A	4370	OMG	O6-C6-C5	-2.11	121.00	126.60
1	A	2837	OMU	C1'-N1-C2	2.11	121.39	117.57
1	A	1522	OMG	O6-C6-C5	-2.11	121.01	126.60
1	A	3899	OMG	O6-C6-C5	-2.11	121.01	126.60
1	A	4296	PSU	C5-C6-N1	-2.11	118.95	122.11
1	A	3944	OMG	O6-C6-C5	-2.11	121.01	126.60
3	C	75	OMG	O6-C6-C5	-2.10	121.02	126.60
1	A	3744	OMG	O6-C6-C5	-2.10	121.03	126.60
3	C	69	PSU	O4'-C1'-C2'	2.10	108.10	105.14
1	A	4637	OMG	O6-C6-C5	-2.10	121.04	126.60
1	A	3825	A2M	C6-C5-N7	2.09	135.92	132.02
1	A	2364	OMG	O6-C6-C5	-2.09	121.06	126.60
1	A	3887	OMC	O2-C2-N3	-2.09	118.94	122.33
1	A	4457	PSU	O4'-C1'-C2'	2.09	108.08	105.14
1	A	1340	OMC	O2-C2-N3	-2.09	118.94	122.33
1	A	2422	OMC	O2-C2-N3	-2.08	118.95	122.33
1	A	3724	A2M	C6-C5-N7	2.08	135.89	132.02
1	A	2787	A2M	C6-C5-N7	2.07	135.89	132.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2815	A2M	C6-C5-N7	2.07	135.88	132.02
1	A	4523	A2M	N9-C8-N7	-2.07	111.08	113.91
1	A	1524	A2M	C6-C5-N7	2.06	135.85	132.02
1	A	4571	A2M	N9-C8-N7	-2.05	111.11	113.91
1	A	1582	PSU	C5-C6-N1	-2.05	119.03	122.11
1	A	3718	A2M	C6-C5-N7	2.05	135.84	132.02
1	A	3920	PSU	O4'-C1'-C2'	2.04	108.02	105.14
1	A	3925	OMU	O2-C2-N1	-2.04	120.08	122.79
1	A	3715	PSU	O4'-C1'-C2'	2.03	108.01	105.14
1	A	4471	PSU	C5-C6-N1	-2.03	119.06	122.11
1	A	1881	OMC	O2-C2-N3	-2.03	119.03	122.33
1	A	3830	A2M	N9-C8-N7	-2.02	111.15	113.91
1	A	398	A2M	N9-C8-N7	-2.02	111.15	113.91
1	A	400	A2M	N9-C8-N7	-2.02	111.15	113.91
1	A	3869	OMC	O2-C2-N3	-2.02	119.04	122.33
1	A	1781	PSU	C5-C6-N1	-2.01	119.09	122.11
1	A	3851	PSU	O4'-C1'-C2'	2.01	107.98	105.14
1	A	2401	A2M	N9-C8-N7	-2.01	111.17	113.91
1	A	4493	PSU	C5-C6-N1	-2.00	119.10	122.11
1	A	1792	PSU	O4'-C1'-C2'	2.00	107.97	105.14
1	A	1534	A2M	N9-C8-N7	-2.00	111.18	113.91

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1326	A2M	C1'-C2'-O2'-CM'
1	A	1677	PSU	C2'-C1'-C5-C4
1	A	1881	OMC	O4'-C1'-N1-C2
1	A	1881	OMC	O4'-C1'-N1-C6
1	A	1881	OMC	C3'-C4'-C5'-O5'
1	A	1881	OMC	O4'-C4'-C5'-O5'
1	A	3701	OMC	C2'-C1'-N1-C2
1	A	3701	OMC	C2'-C1'-N1-C6
1	A	3701	OMC	O4'-C4'-C5'-O5'
1	A	3734	PSU	O4'-C1'-C5-C4
1	A	3734	PSU	O4'-C1'-C5-C6
1	A	3785	A2M	O4'-C4'-C5'-O5'
1	A	3818	UY1	O4'-C1'-C5-C4
1	A	3818	UY1	O4'-C1'-C5-C6
1	A	3867	A2M	C1'-C2'-O2'-CM'
1	A	4420	PSU	C2'-C1'-C5-C4

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Mol	Chain	Res	Type	Atoms
1	A	4420	PSU	C2'-C1'-C5-C6
1	A	4447	5MC	C2'-C1'-N1-C6
1	A	4500	PSU	C2'-C1'-C5-C4
1	A	4590	A2M	C4'-C5'-O5'-P
1	A	3734	PSU	O4'-C4'-C5'-O5'
1	A	3785	A2M	C3'-C4'-C5'-O5'
1	A	4447	5MC	C2'-C1'-N1-C2
1	A	3734	PSU	C3'-C4'-C5'-O5'
1	A	3851	PSU	C4'-C5'-O5'-P
1	A	4500	PSU	C4'-C5'-O5'-P
1	A	1534	A2M	O4'-C4'-C5'-O5'
1	A	2824	OMC	C1'-C2'-O2'-CM2
1	A	4536	OMC	C1'-C2'-O2'-CM2
1	A	398	A2M	O4'-C4'-C5'-O5'
1	A	2364	OMG	O4'-C4'-C5'-O5'
1	A	2787	A2M	C2'-C1'-N9-C8
1	A	3818	UY1	C1'-C2'-O2'-CM2
1	A	3818	UY1	C3'-C2'-O2'-CM2
1	A	4447	5MC	O4'-C1'-N1-C6
1	A	1625	OMG	C4'-C5'-O5'-P
1	A	3818	UY1	C4'-C5'-O5'-P
1	A	3844	PSU	C4'-C5'-O5'-P
1	A	4447	5MC	O4'-C1'-N1-C2
1	A	4523	A2M	O4'-C4'-C5'-O5'
1	A	1881	OMC	C3'-C2'-O2'-CM2
1	A	4456	OMC	C3'-C2'-O2'-CM2
1	A	3887	OMC	C4'-C5'-O5'-P
1	A	3701	OMC	O4'-C1'-N1-C6
1	A	1677	PSU	O4'-C1'-C5-C4
1	A	4420	PSU	O4'-C1'-C5-C4
1	A	2824	OMC	C3'-C2'-O2'-CM2
1	A	2876	OMG	C3'-C2'-O2'-CM2
1	A	4536	OMC	C3'-C2'-O2'-CM2
1	A	2787	A2M	C2'-C1'-N9-C4
1	A	4571	A2M	O4'-C4'-C5'-O5'
1	A	2787	A2M	O4'-C1'-N9-C8
1	A	2415	OMU	C2'-C1'-N1-C2
1	A	2861	OMC	C2'-C1'-N1-C2
1	A	4456	OMC	C2'-C1'-N1-C2
1	A	4536	OMC	C2'-C1'-N1-C2
1	A	1677	PSU	O4'-C4'-C5'-O5'
1	A	1677	PSU	O4'-C1'-C5-C6

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Mol	Chain	Res	Type	Atoms
1	A	3701	OMC	O4'-C1'-N1-C2
1	A	1534	A2M	C3'-C4'-C5'-O5'
1	A	2351	OMC	O4'-C4'-C5'-O5'
1	A	2415	OMU	C2'-C1'-N1-C6
1	A	3887	OMC	C3'-C2'-O2'-CM2
1	A	398	A2M	C3'-C4'-C5'-O5'
1	A	2364	OMG	C3'-C4'-C5'-O5'
1	A	4523	A2M	C3'-C4'-C5'-O5'

There are no ring outliers.

65 monomers are involved in 89 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	4456	OMC	1	0
1	A	3734	PSU	1	0
1	A	4299	PSU	1	0
1	A	4576	PSU	1	0
1	A	2804	OMC	3	0
1	A	3724	A2M	2	0
1	A	4620	OMU	2	0
1	A	3715	PSU	1	0
1	A	4420	PSU	2	0
1	A	4637	OMG	1	0
1	A	4353	PSU	1	0
1	A	3718	A2M	3	0
1	A	1871	A2M	1	0
1	A	1677	PSU	1	0
1	A	3818	UY1	1	0
1	A	1881	OMC	1	0
1	A	4306	OMU	1	0
1	A	4500	PSU	1	0
1	A	3925	OMU	1	0
1	A	4623	OMG	1	0
1	A	4523	A2M	2	0
1	A	4579	PSU	1	0
1	A	1683	PSU	2	0
1	A	3944	OMG	2	0
1	A	4689	PSU	1	0
1	A	398	A2M	1	0
1	A	3869	OMC	1	0
1	A	4392	OMG	2	0
1	A	1340	OMC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	3785	A2M	1	0
1	A	2876	OMG	1	0
1	A	3867	A2M	2	0
1	A	3884	PSU	2	0
1	A	2364	OMG	1	0
1	A	1524	A2M	1	0
1	A	2861	OMC	1	0
1	A	2415	OMU	1	0
1	A	3887	OMC	1	0
1	A	4618	OMG	2	0
1	A	4552	PSU	2	0
1	A	4571	A2M	1	0
1	A	2837	OMU	1	0
1	A	3770	PSU	1	0
1	A	4403	PSU	1	0
1	A	4447	5MC	1	0
1	A	4227	OMU	1	0
1	A	1326	A2M	3	0
1	A	4536	OMC	2	0
1	A	4196	OMG	1	0
1	A	4293	PSU	1	0
1	A	4457	PSU	2	0
1	A	3830	A2M	2	0
1	A	4471	PSU	2	0
1	A	2363	A2M	2	0
3	C	75	OMG	2	0
1	A	4220	6MZ	2	0
1	A	2351	OMC	1	0
1	A	3808	OMC	1	0
3	C	69	PSU	1	0
1	A	2815	A2M	1	0
1	A	1316	OMG	2	0
1	A	2839	PSU	1	0
1	A	3792	OMG	1	0
1	A	3825	A2M	2	0
1	A	4590	A2M	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 391 ligands modelled in this entry, 389 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
50	GTP	B	205	2	30,34,34	0.50	0	46,54,54	0.53	0
51	EPE	M	201	-	15,15,15	0.81	1 (6%)	18,20,20	1.73	6 (33%)

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
50	GTP	B	205	2	-	0/22/38/38	0/3/3/3
51	EPE	M	201	-	-	5/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	M	201	EPE	C10-S	2.74	1.81	1.77

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	M	201	EPE	C5-N4-C3	4.20	118.28	108.83
51	M	201	EPE	C7-N4-C3	2.74	118.23	111.23
51	M	201	EPE	C7-N4-C5	2.63	117.96	111.23
51	M	201	EPE	O3S-S-C10	2.33	109.53	105.77
51	M	201	EPE	O2S-S-C10	2.20	109.56	106.92
51	M	201	EPE	O1S-S-C10	2.01	109.33	106.92

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
51	M	201	EPE	C10-C9-N1-C2
51	M	201	EPE	C9-C10-S-O1S
51	M	201	EPE	C9-C10-S-O3S
51	M	201	EPE	C9-C10-S-O2S
51	M	201	EPE	C8-C7-N4-C5

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	B	205	GTP	1	0
51	M	201	EPE	1	0

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.

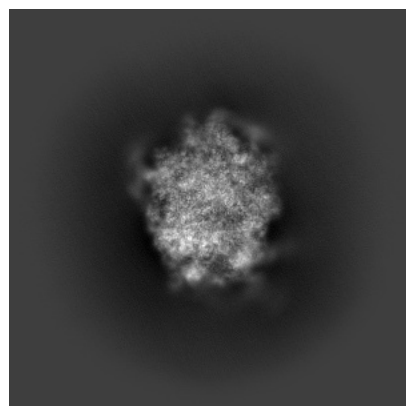
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51452. These allow visual inspection of the internal detail of the map and identification of artifacts.

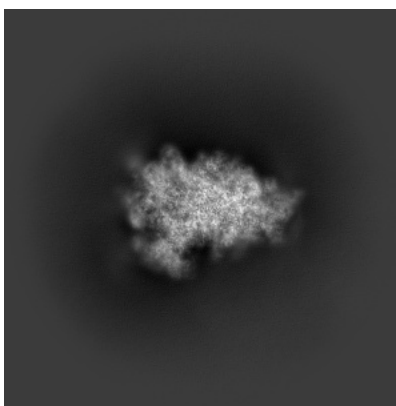
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

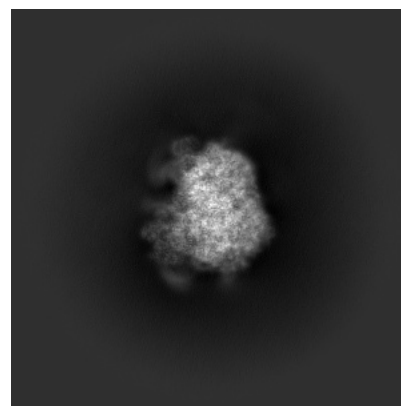
6.1.1 Primary map



X

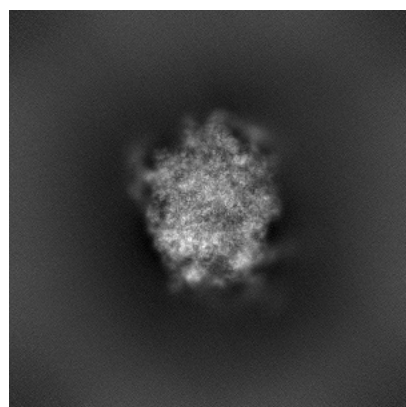


Y

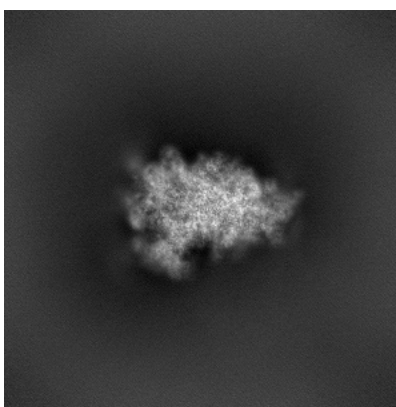


Z

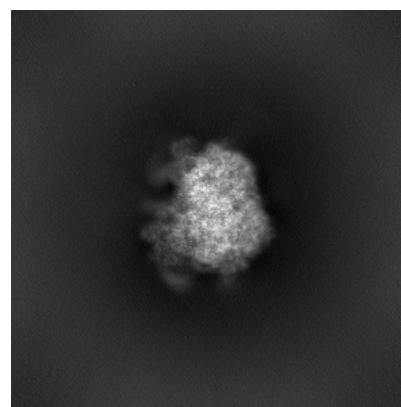
6.1.2 Raw map



X



Y

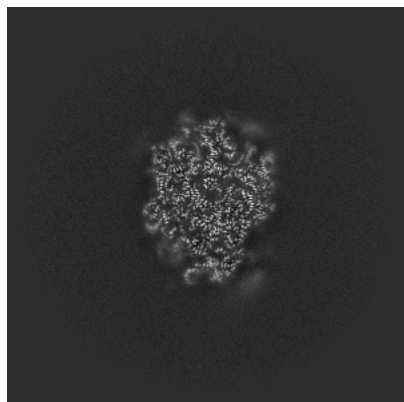


Z

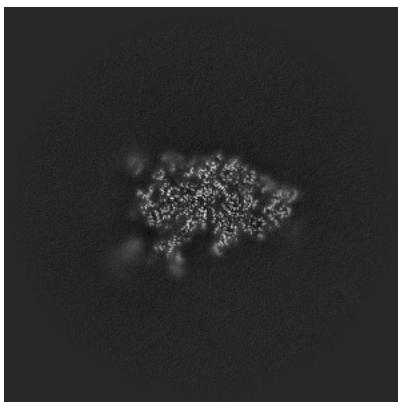
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

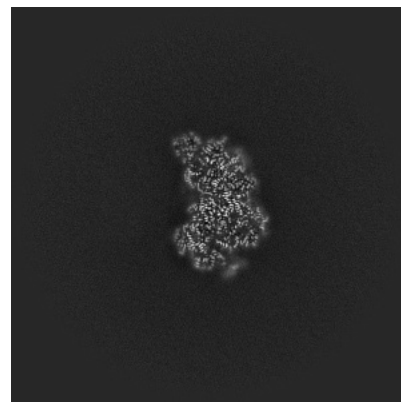
6.2.1 Primary map



X Index: 280

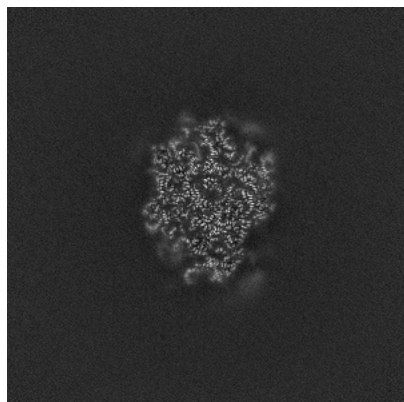


Y Index: 280

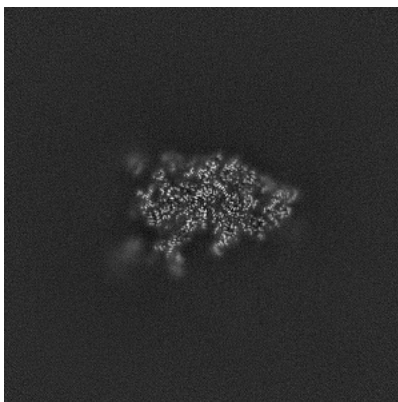


Z Index: 280

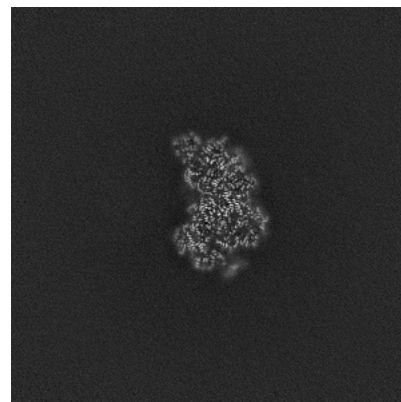
6.2.2 Raw map



X Index: 280



Y Index: 280

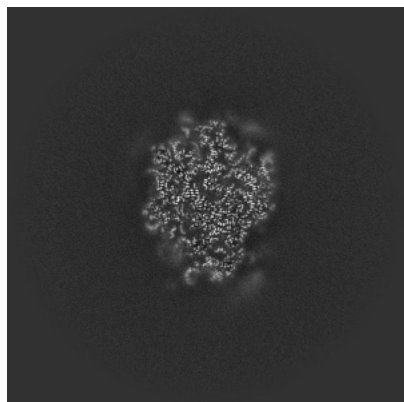


Z Index: 280

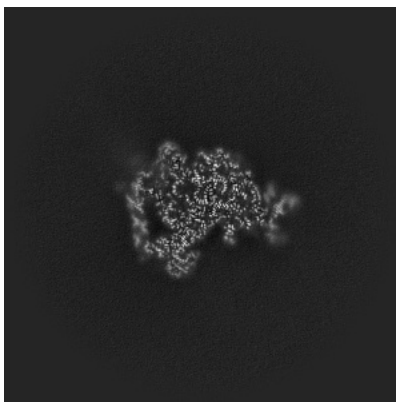
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

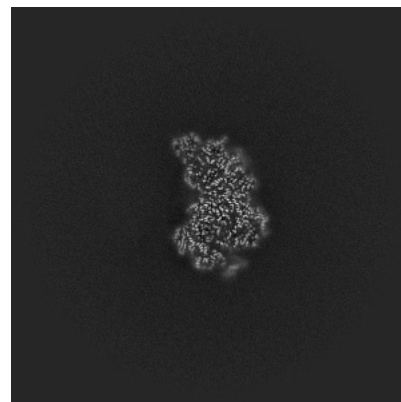
6.3.1 Primary map



X Index: 281

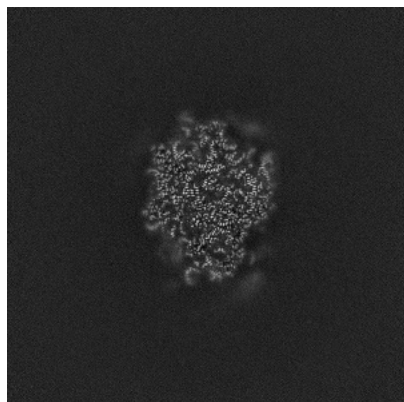


Y Index: 252

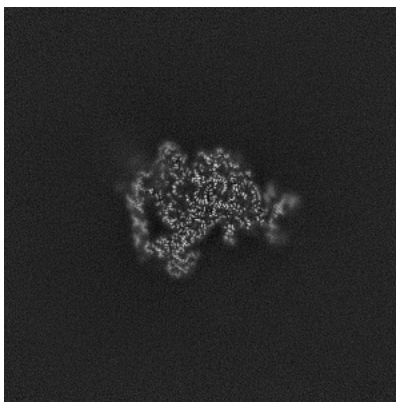


Z Index: 279

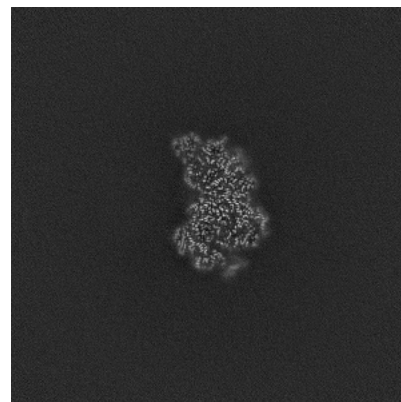
6.3.2 Raw map



X Index: 282



Y Index: 252

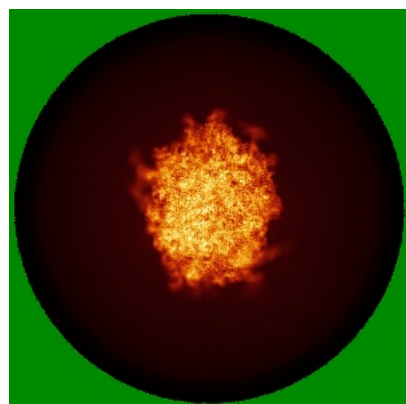


Z Index: 279

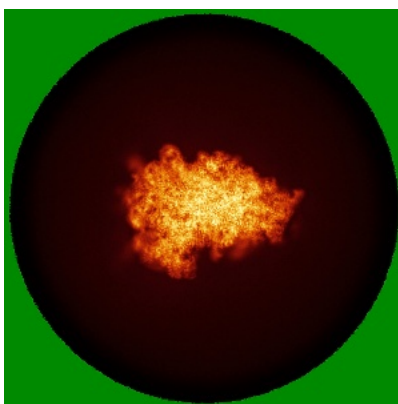
The images above show the largest variance slices of the map in three orthogonal directions.

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

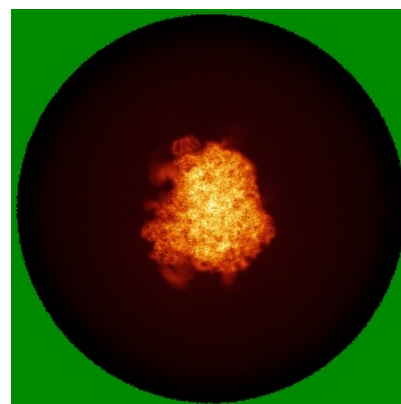
6.4.1 Primary map



X

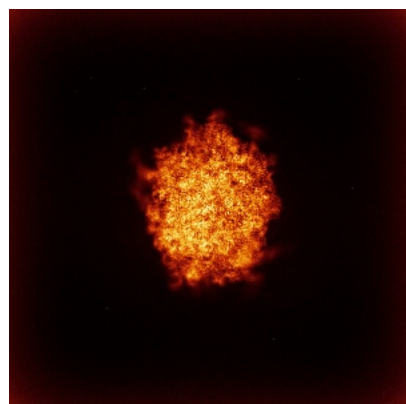


Y

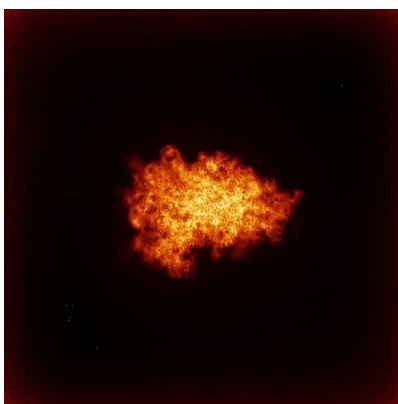


Z

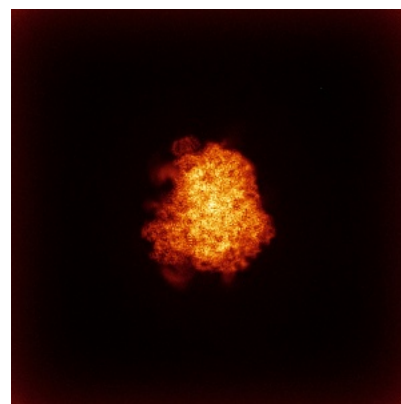
6.4.2 Raw map



X



Y



Z

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

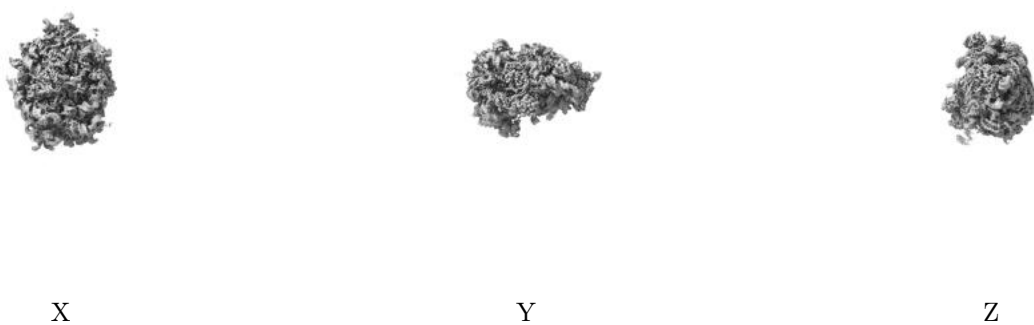
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

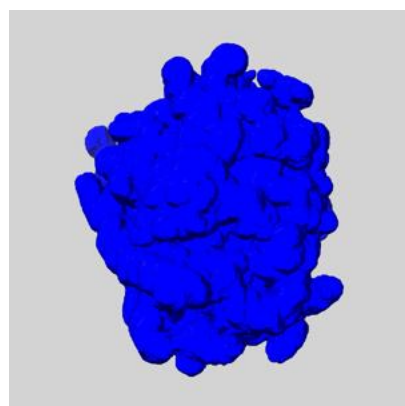
6.6 Mask visualisation [i](#)

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

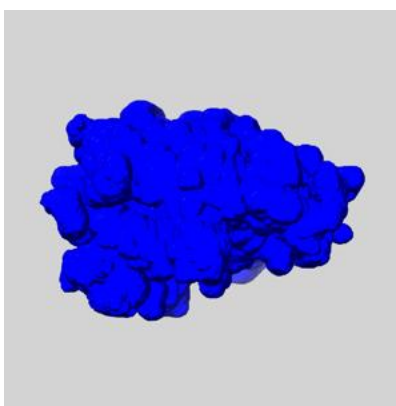
A mask typically either:

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

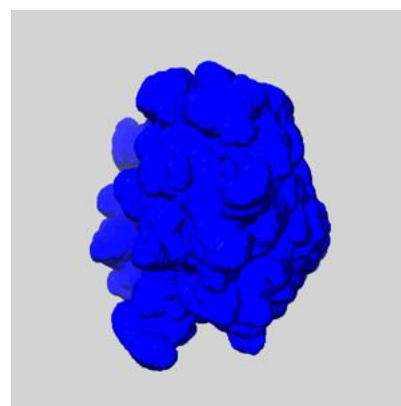
6.6.1 emd_51452_msk_1.map [i](#)



X



Y

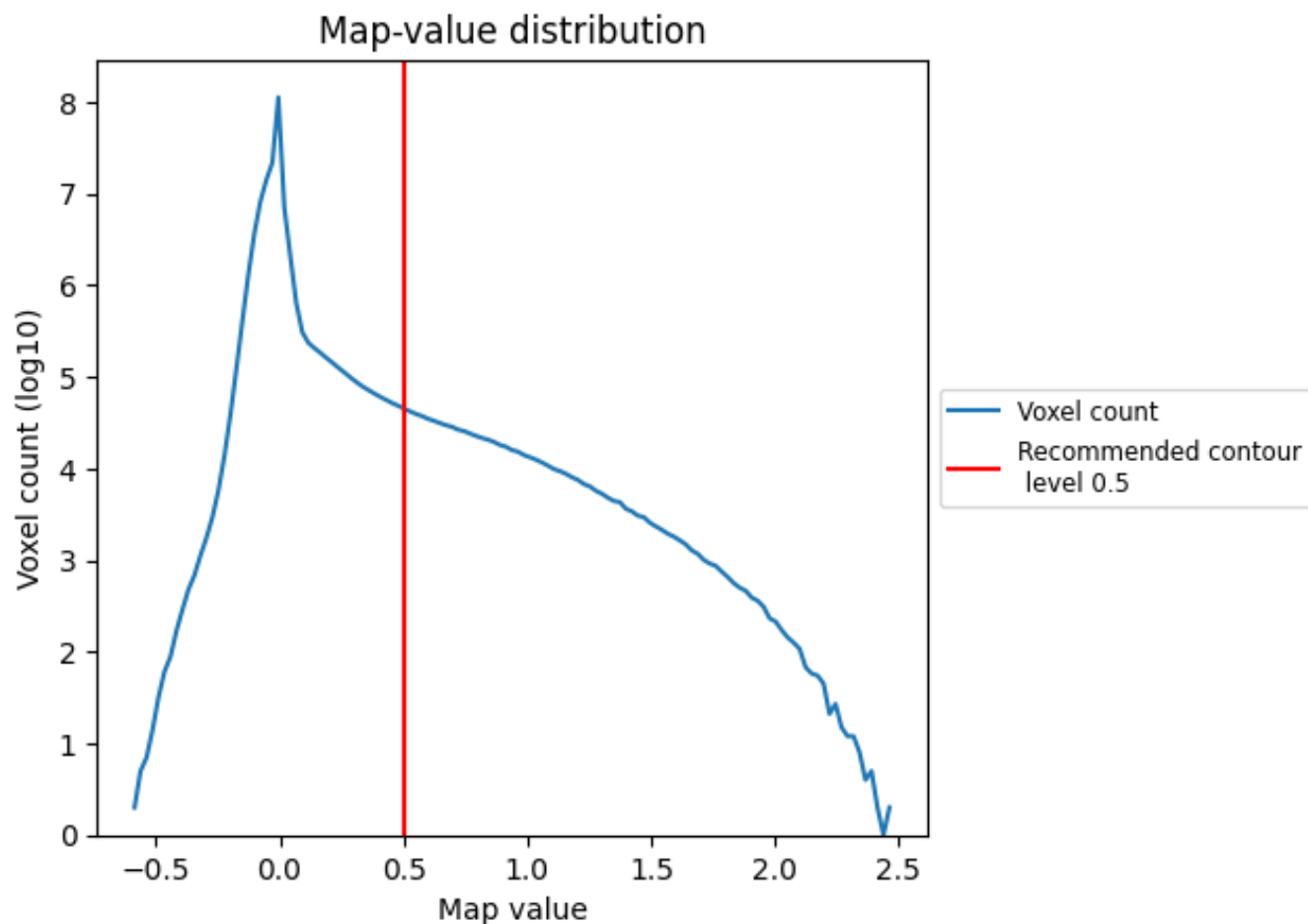


Z

7 Map analysis [i](#)

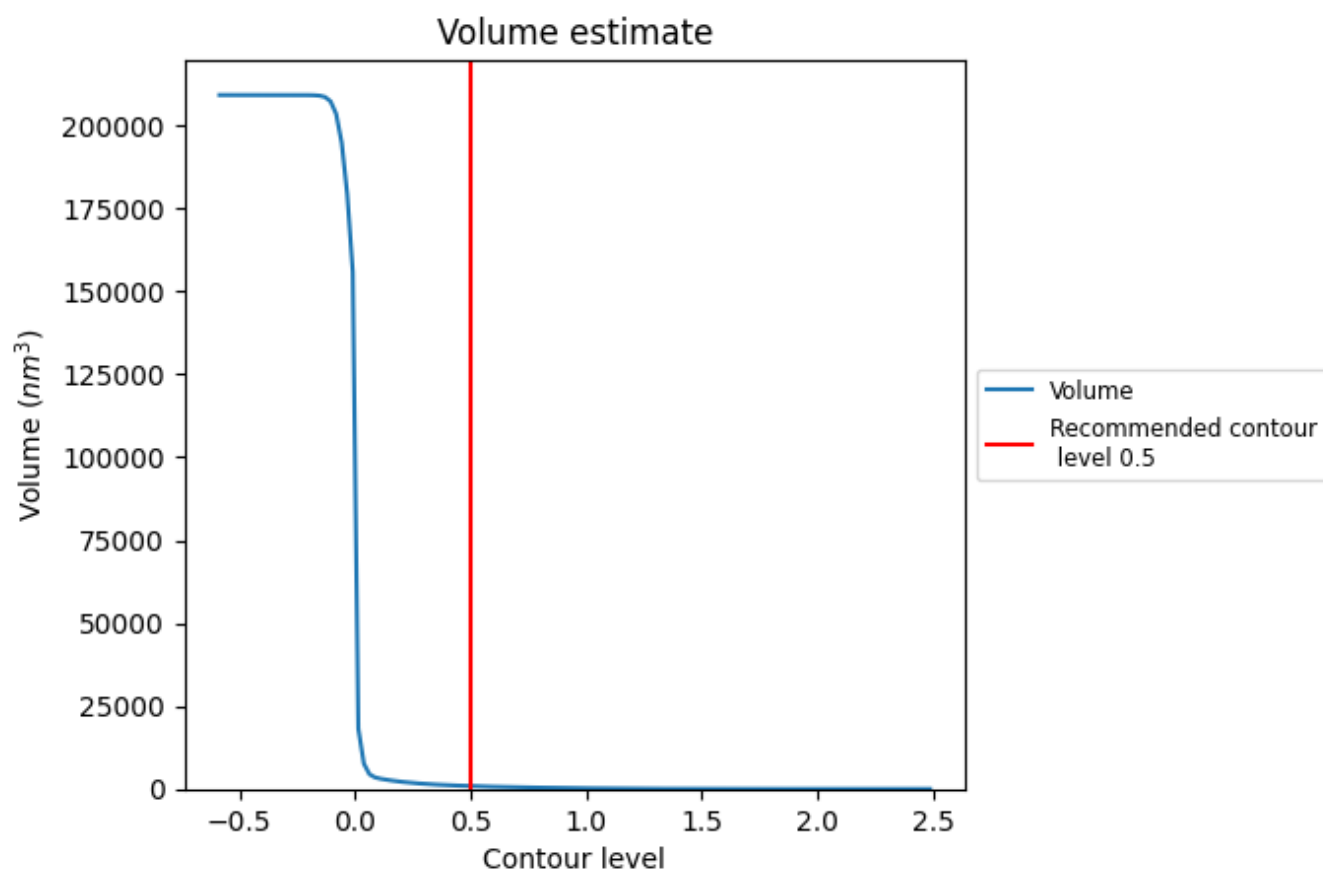
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

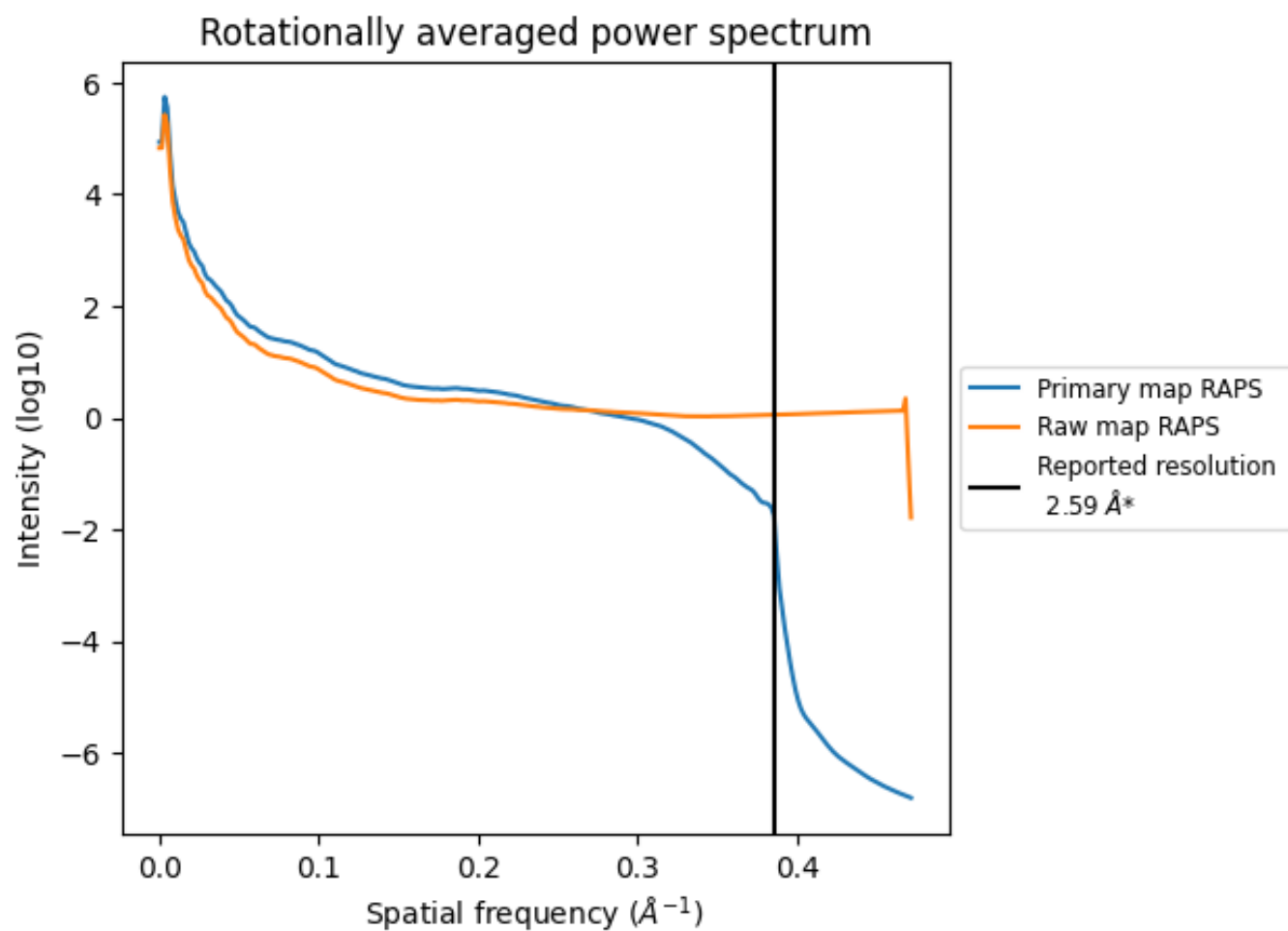
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 877 nm^3 ; this corresponds to an approximate mass of 792 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 ⓘ

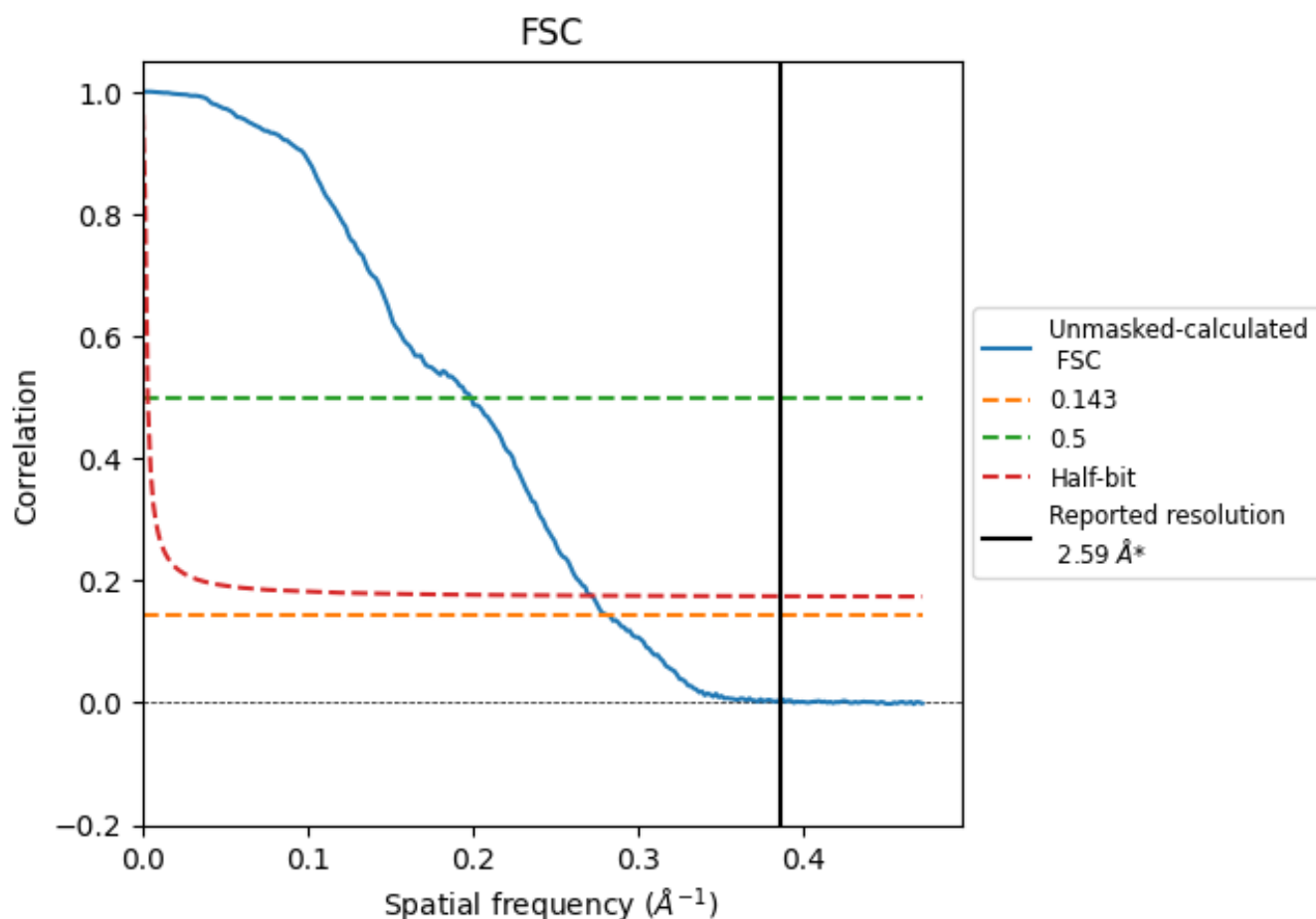


*Reported resolution corresponds to spatial frequency of 0.386 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.386 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

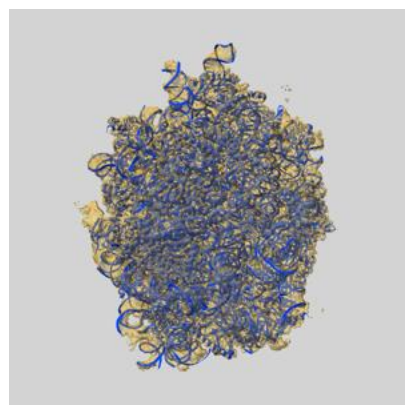
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.59	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.55	5.03	3.68

*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 3.55 differs from the reported value 2.59 by more than 10 %

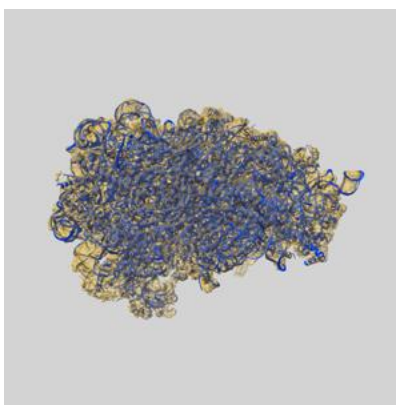
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51452 and PDB model 9GMO. Per-residue inclusion information can be found in section [3](#) on page [15](#).

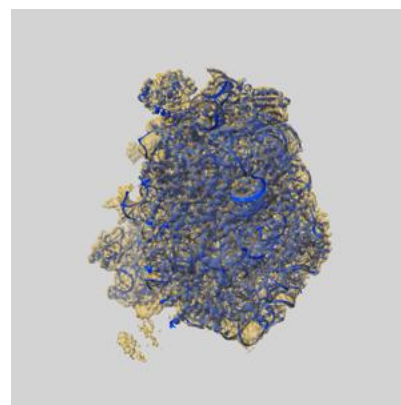
9.1 Map-model overlay [i](#)



X



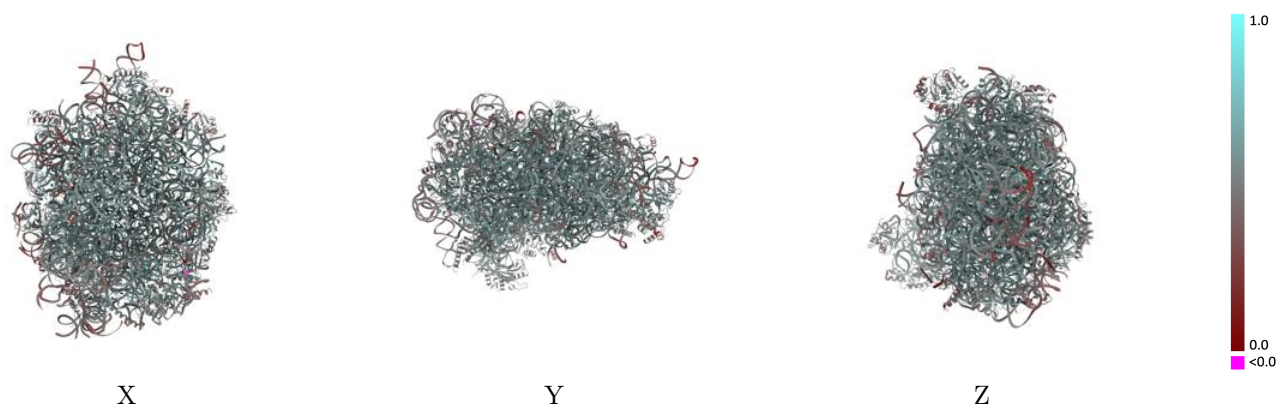
Y



Z

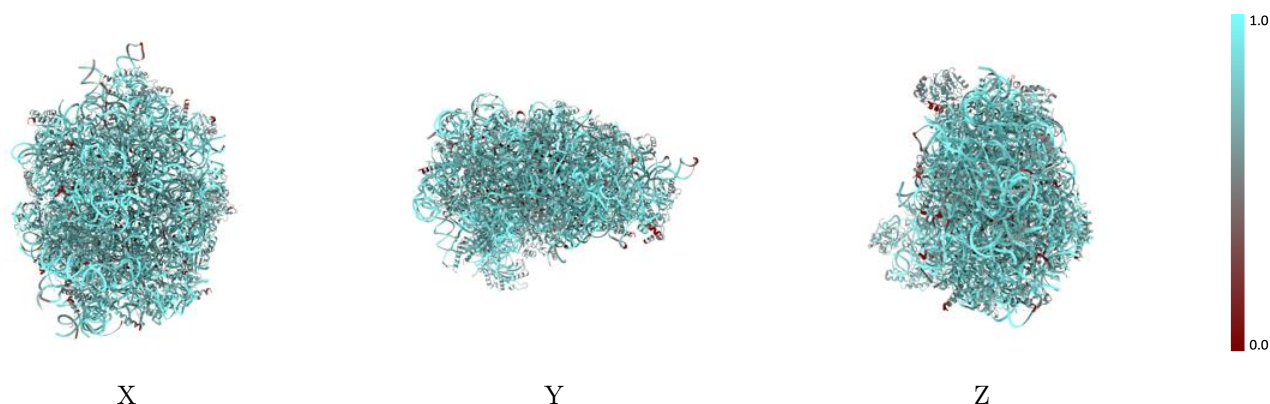
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



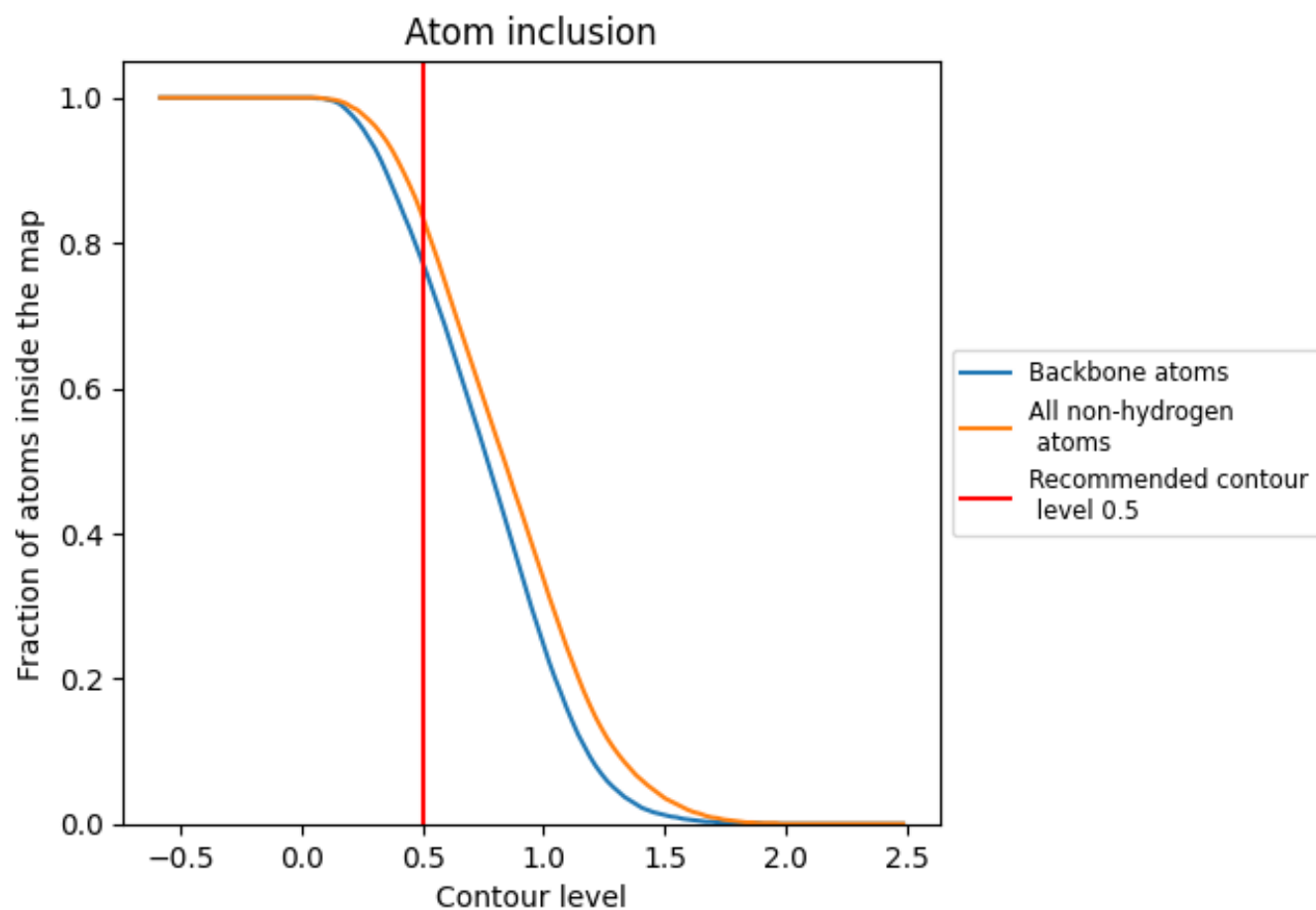
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 84% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8350	 0.5360
0	 0.1820	 0.4420
A	 0.9040	 0.5330
B	 0.9550	 0.5510
C	 0.9280	 0.5480
D	 0.7890	 0.5740
E	 0.7780	 0.5540
F	 0.7800	 0.5590
G	 0.7650	 0.5170
H	 0.7490	 0.5260
I	 0.7740	 0.5560
J	 0.7930	 0.5540
K	 0.7670	 0.5670
L	 0.7590	 0.5250
M	 0.7870	 0.5620
N	 0.7480	 0.5390
O	 0.6480	 0.4540
P	 0.7450	 0.5570
Q	 0.7260	 0.5410
R	 0.7620	 0.5430
S	 0.7790	 0.5420
T	 0.7160	 0.5190
U	 0.8070	 0.5700
V	 0.6970	 0.5170
W	 0.6460	 0.4960
X	 0.7500	 0.5460
Y	 0.7790	 0.5700
Z	 0.8230	 0.5860
a	 0.7200	 0.5470
b	 0.7530	 0.5200
c	 0.7030	 0.5030
d	 0.8290	 0.5770
e	 0.6300	 0.4860
f	 0.7550	 0.5690
g	 0.7670	 0.5460



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Chain	Atom inclusion	Q-score
h	 0.5910	 0.4670
i	 0.7010	 0.5510
j	 0.7040	 0.5300
k	 0.8100	 0.5620
l	 0.8260	 0.5830
m	 0.7680	 0.5520
n	 0.7030	 0.5060
o	 0.7300	 0.5290
p	 0.7540	 0.5430
q	 0.6960	 0.4860
r	 0.7390	 0.5340
s	 0.7860	 0.5300