



Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 03:37 PM UTC

PDB ID : 5AJ3 / pdb_00005aj3
EMDB ID : EMD-2913
Title : Structure of the small subunit of the mammalian mitoribosome
Authors : Greber, B.J.; Bieri, P.; Leibundgut, M.; Leitner, A.; Aebersold, R.; Boehringer, D.; Ban, N.
Deposited on : 2015-02-20
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

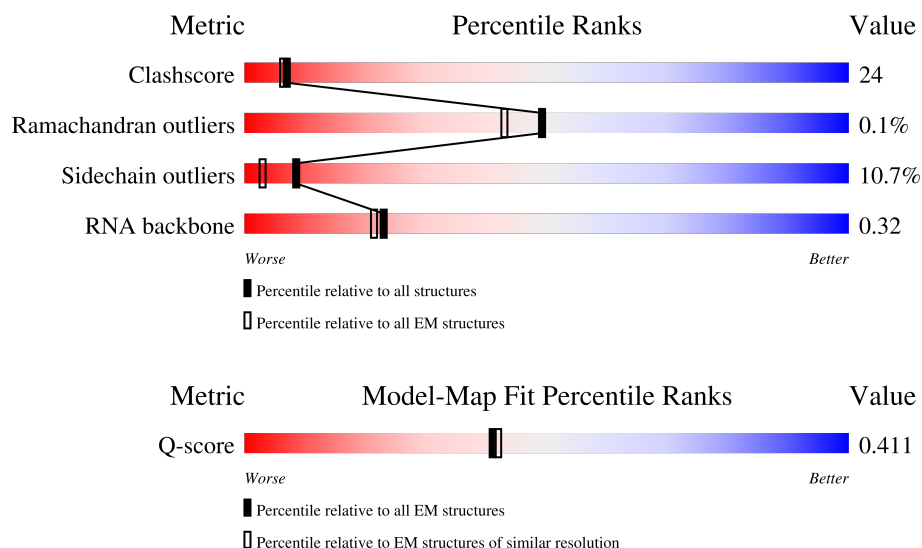
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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.



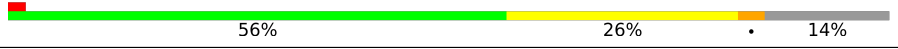
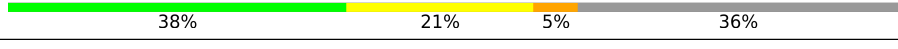
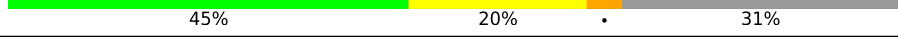
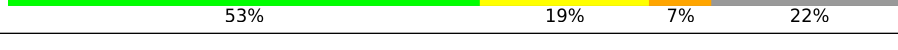
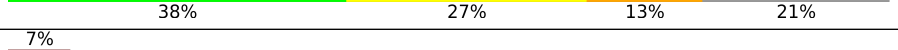
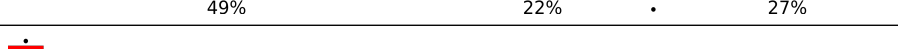
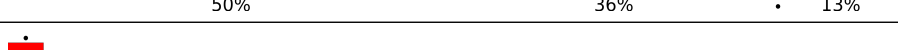
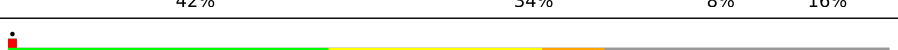
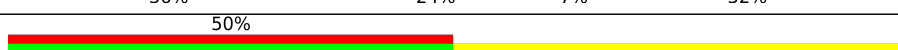
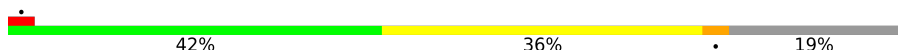
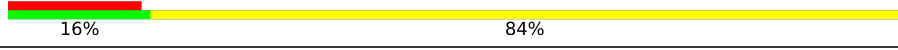
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	962	
2	B	289	
3	C	167	

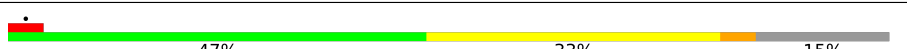
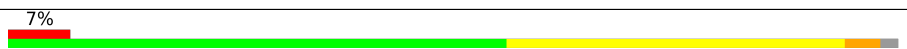
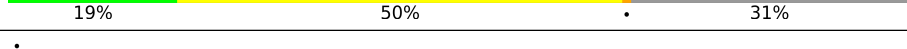
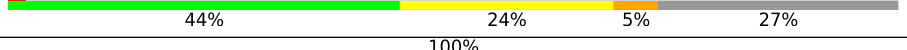
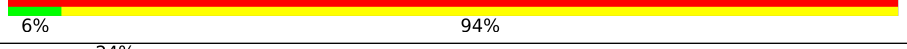
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Mol	Chain	Length	Quality of chain
4	E	430	
5	F	124	
6	G	242	
7	I	397	
8	J	201	
9	K	196	
10	L	139	
11	N	128	
12	O	239	
13	P	135	
14	Q	130	
15	R	143	
16	T	14	
17	U	87	
18	V	64	
18	Y	64	
19	X	13	
20	a	360	
21	b	190	
22	c	173	
23	d	205	
24	e	336	
25	f	188	
26	g	397	
27	h	387	

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Mol	Chain	Length	Quality of chain
28	i	106	
29	j	218	
30	k	325	
31	m	118	
32	n	199	
33	o	692	
34	p	258	
35	s	16	
36	z	17	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	Y5P	V	43	-	-	X	-
18	Y5P	Y	25	-	-	X	-
18	Y5P	Y	26	-	-	X	-
18	Y5P	Y	68	-	-	X	-

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 66363 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 MITORIBOSOMAL 12S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	960	Total	C	N	O	P	0	0
			20411	9162	3708	6581	960		

- Molecule 2 is a protein called MITORIBOSOMAL PROTEIN US2M, MRPS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	220	Total	C	N	O	S	0	0
			1762	1126	326	304	6		

- Molecule 3 is a protein called MITORIBOSOMAL PROTEIN US3M, MRPS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	132	Total	C	N	O	S	0	0
			1075	695	195	181	4		

- Molecule 4 is a protein called MITORIBOSOMAL PROTEIN US5M, MRPS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	328	Total	C	N	O	S	0	0
			2621	1641	498	471	11		

- Molecule 5 is a protein called MITORIBOSOMAL PROTEIN BS6M, MRPS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	123	Total	C	N	O	S	0	0
			990	626	180	178	6		

- Molecule 6 is a protein called MITORIBOSOMAL PROTEIN US7M, MRPS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	208	Total	C	N	O	S	0	0
			1721	1097	314	299	11		

- Molecule 7 is a protein called MITORIBOSOMAL PROTEIN US9M, MRPS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	311	Total	C	N	O	S	0	0
			2498	1586	450	449	13		

- Molecule 8 is a protein called MITORIBOSOMAL PROTEIN US10M, MRPS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	129	Total	C	N	O	S	0	0
			1067	690	182	192	3		

- Molecule 9 is a protein called MITORIBOSOMAL PROTEIN US11M, MRPS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	136	Total	C	N	O	S	0	0
			1001	628	192	178	3		

- Molecule 10 is a protein called MITORIBOSOMAL PROTEIN US12M, MRPS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	109	Total	C	N	O	S	0	0
			840	524	172	138	6		

- Molecule 11 is a protein called MITORIBOSOMAL PROTEIN US14M, MRPS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	101	Total	C	N	O	S	0	0
			858	534	174	144	6		

- Molecule 12 is a protein called MITORIBOSOMAL PROTEIN US15M, MRPS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	175	Total	C	N	O	S	0	0
			1448	919	272	248	9		

- Molecule 13 is a protein called MITORIBOSOMAL PROTEIN BS16M, MRPS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	117	Total	C	N	O	S	0	0
			932	588	184	155	5		

- Molecule 14 is a protein called MITORIBOSOMAL PROTEIN US17M, MRPS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	109	Total	C	N	O	S	0	0
			853	555	150	145	3		

- Molecule 15 is a protein called MITORIBOSOMAL PROTEIN BS18M, MRPS18C.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	97	Total	C	N	O	S	0	0
			784	507	132	138	7		

- Molecule 16 is a protein called MITORIBOSOMAL PROTEIN BL19M, MRPL19.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	T	14	Total	C	N	O	0	0
			84	56	14	14		

- Molecule 17 is a protein called MITORIBOSOMAL PROTEIN BS21M, MRPS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	86	Total	C	N	O	S	0	0
			734	453	148	125	8		

- Molecule 18 is a RNA chain called P-SITE AND A-SITE TRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	64	Total	C	N	O	P	0	0
			1158	579	134	382	63		
18	Y	64	Total	C	N	O	P	0	0
			1158	579	134	382	63		

- Molecule 19 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	13	Total	C	N	O	P	0	0
			231	117	26	76	12		

- Molecule 20 is a protein called MITORIBOSOMAL PROTEIN MS22, MRPS22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	a	292	Total	C	N	O	S	0	0
			2296	1476	394	417	9		

- Molecule 21 is a protein called MITORIBOSOMAL PROTEIN MS23, MRPS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	b	135	Total	C	N	O	S	0	0
			1101	709	199	192	1		

- Molecule 22 is a protein called MITORIBOSOMAL PROTEIN MS25, MRPS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	c	169	Total	C	N	O	S	0	0
			1367	876	236	245	10		

- Molecule 23 is a protein called MITORIBOSOMAL PROTEIN MS26, MRPS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	177	Total	C	N	O	S	0	0
			1467	904	288	273	2		

- Molecule 24 is a protein called MITORIBOSOMAL PROTEIN MS27, MRPS27.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	e	336	Total	C	N	O	0	0
			2016	1344	336	336		

- Molecule 25 is a protein called MITORIBOSOMAL PROTEIN MS28, MRPS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	f	99	Total	C	N	O	S	0	0
			778	494	134	146	4		

- Molecule 26 is a protein called MITORIBOSOMAL PROTEIN MS29, MRPS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	g	346	Total	C	N	O	S	0	0
			2774	1786	489	489	10		

- Molecule 27 is a protein called MITORIBOSOMAL PROTEIN MS31, MRPS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	h	103	Total	C	N	O	S	0	0
			876	569	145	159	3		

- Molecule 28 is a protein called MITORIBOSOMAL PROTEIN MS33, MRPS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	i	99	Total	C	N	O	S	0	0
			824	522	156	143	3		

- Molecule 29 is a protein called MITORIBOSOMAL PROTEIN MS34, MRPS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	j	213	Total	C	N	O	S	0	0
			1777	1123	339	308	7		

- Molecule 30 is a protein called MITORIBOSOMAL PROTEIN MS35, MRPS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	k	275	Total	C	N	O	S	0	0
			2222	1414	380	419	9		

- Molecule 31 is a protein called MITORIBOSOMAL PROTEIN MS37, MRPS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	m	116	Total	C	N	O	S	0	0
			930	577	185	160	8		

- Molecule 32 is a protein called MITORIBOSOMAL PROTEIN MS38, MRPS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	n	72	Total	C	N	O	S	0	0
			639	407	139	92	1		

- Molecule 33 is a protein called MITORIBOSOMAL PROTEIN MS39, MRPS39.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	o	476	Total	C	N	O	S	0	0
			3028	2007	500	519	2		

There are 525 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
o	153	UNK	SER	conflict	UNP K7GKS8
o	154	UNK	GLU	conflict	UNP K7GKS8
o	155	UNK	ALA	conflict	UNP K7GKS8
o	156	UNK	ALA	conflict	UNP K7GKS8
o	157	UNK	LEU	conflict	UNP K7GKS8
o	158	UNK	GLN	conflict	UNP K7GKS8

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Chain	Residue	Modelled	Actual	Comment	Reference
o	159	UNK	GLU	conflict	UNP K7GKS8
o	160	UNK	ARG	conflict	UNP K7GKS8
o	161	UNK	ILE	conflict	UNP K7GKS8
o	162	UNK	LYS	conflict	UNP K7GKS8
o	163	UNK	LEU	conflict	UNP K7GKS8
o	164	UNK	ARG	conflict	UNP K7GKS8
o	165	UNK	LYS	conflict	UNP K7GKS8
o	166	UNK	VAL	conflict	UNP K7GKS8
o	167	UNK	LYS	conflict	UNP K7GKS8
o	168	UNK	ALA	conflict	UNP K7GKS8
o	169	UNK	SER	conflict	UNP K7GKS8
o	170	UNK	VAL	conflict	UNP K7GKS8
o	171	UNK	ASP	conflict	UNP K7GKS8
o	172	UNK	MET	conflict	UNP K7GKS8
o	173	UNK	PHE	conflict	UNP K7GKS8
o	174	UNK	ASP	conflict	UNP K7GKS8
o	175	UNK	GLN	conflict	UNP K7GKS8
o	176	UNK	LEU	conflict	UNP K7GKS8
o	177	UNK	LEU	conflict	UNP K7GKS8
o	178	UNK	GLN	conflict	UNP K7GKS8
o	179	UNK	ALA	conflict	UNP K7GKS8
o	180	UNK	GLY	conflict	UNP K7GKS8
o	181	UNK	THR	conflict	UNP K7GKS8
o	182	UNK	THR	conflict	UNP K7GKS8
o	183	UNK	VAL	conflict	UNP K7GKS8
o	184	UNK	SER	conflict	UNP K7GKS8
o	185	UNK	LEU	conflict	UNP K7GKS8
o	186	UNK	GLU	conflict	UNP K7GKS8
o	187	UNK	THR	conflict	UNP K7GKS8
o	188	UNK	THR	conflict	UNP K7GKS8
o	189	UNK	ASN	conflict	UNP K7GKS8
o	190	UNK	SER	conflict	UNP K7GKS8
o	191	UNK	LEU	conflict	UNP K7GKS8
o	192	UNK	LEU	conflict	UNP K7GKS8
o	193	UNK	ASP	conflict	UNP K7GKS8
o	194	UNK	LEU	conflict	UNP K7GKS8
o	195	UNK	LEU	conflict	UNP K7GKS8
o	196	UNK	CYS	conflict	UNP K7GKS8
o	197	UNK	TYR	conflict	UNP K7GKS8
o	198	UNK	TYR	conflict	UNP K7GKS8
o	199	UNK	GLY	conflict	UNP K7GKS8
o	200	UNK	ASN	conflict	UNP K7GKS8

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Chain	Residue	Modelled	Actual	Comment	Reference
o	201	UNK	GLN	conflict	UNP K7GKS8
o	202	UNK	GLU	conflict	UNP K7GKS8
o	203	UNK	PRO	conflict	UNP K7GKS8
o	204	UNK	SER	conflict	UNP K7GKS8
o	205	UNK	ALA	conflict	UNP K7GKS8
o	206	UNK	ASN	conflict	UNP K7GKS8
o	207	UNK	TYR	conflict	UNP K7GKS8
o	208	UNK	ASN	conflict	UNP K7GKS8
o	209	UNK	PHE	conflict	UNP K7GKS8
o	210	UNK	GLN	conflict	UNP K7GKS8
o	211	UNK	GLN	conflict	UNP K7GKS8
o	212	UNK	ARG	conflict	UNP K7GKS8
o	213	UNK	GLU	conflict	UNP K7GKS8
o	214	UNK	GLN	conflict	UNP K7GKS8
o	215	UNK	SER	conflict	UNP K7GKS8
o	216	UNK	GLU	conflict	UNP K7GKS8
o	217	UNK	GLU	conflict	UNP K7GKS8
o	218	UNK	LEU	conflict	UNP K7GKS8
o	219	UNK	GLU	conflict	UNP K7GKS8
o	220	UNK	GLU	conflict	UNP K7GKS8
o	221	UNK	ALA	conflict	UNP K7GKS8
o	222	UNK	THR	conflict	UNP K7GKS8
o	223	UNK	GLU	conflict	UNP K7GKS8
o	224	UNK	ALA	conflict	UNP K7GKS8
o	225	UNK	ASP	conflict	UNP K7GKS8
o	226	UNK	ASN	conflict	UNP K7GKS8
o	227	UNK	GLU	conflict	UNP K7GKS8
o	228	UNK	LYS	conflict	UNP K7GKS8
o	229	UNK	SER	conflict	UNP K7GKS8
o	230	UNK	LYS	conflict	UNP K7GKS8
o	231	UNK	THR	conflict	UNP K7GKS8
o	232	UNK	LYS	conflict	UNP K7GKS8
o	233	UNK	ALA	conflict	UNP K7GKS8
o	234	UNK	GLY	conflict	UNP K7GKS8
o	235	UNK	HIS	conflict	UNP K7GKS8
o	236	UNK	HIS	conflict	UNP K7GKS8
o	237	UNK	LEU	conflict	UNP K7GKS8
o	238	UNK	GLY	conflict	UNP K7GKS8
o	239	UNK	VAL	conflict	UNP K7GKS8
o	240	UNK	THR	conflict	UNP K7GKS8
o	241	UNK	TRP	conflict	UNP K7GKS8
o	242	UNK	ARG	conflict	UNP K7GKS8

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Chain	Residue	Modelled	Actual	Comment	Reference
o	243	UNK	THR	conflict	UNP K7GKS8
o	244	UNK	LYS	conflict	UNP K7GKS8
o	245	UNK	ASN	conflict	UNP K7GKS8
o	246	UNK	ASN	conflict	UNP K7GKS8
o	247	UNK	ALA	conflict	UNP K7GKS8
o	248	UNK	GLU	conflict	UNP K7GKS8
o	249	UNK	ARG	conflict	UNP K7GKS8
o	250	UNK	ILE	conflict	UNP K7GKS8
o	251	UNK	PHE	conflict	UNP K7GKS8
o	252	UNK	ALA	conflict	UNP K7GKS8
o	253	UNK	LEU	conflict	UNP K7GKS8
o	254	UNK	MET	conflict	UNP K7GKS8
o	255	UNK	PRO	conflict	UNP K7GKS8
o	256	UNK	GLU	conflict	UNP K7GKS8
o	257	UNK	LYS	conflict	UNP K7GKS8
o	258	UNK	ASN	conflict	UNP K7GKS8
o	259	UNK	ALA	conflict	UNP K7GKS8
o	260	UNK	HIS	conflict	UNP K7GKS8
o	261	UNK	SER	conflict	UNP K7GKS8
o	262	UNK	TYR	conflict	UNP K7GKS8
o	263	UNK	CYS	conflict	UNP K7GKS8
o	264	UNK	THR	conflict	UNP K7GKS8
o	265	UNK	MET	conflict	UNP K7GKS8
o	266	UNK	ILE	conflict	UNP K7GKS8
o	267	UNK	ARG	conflict	UNP K7GKS8
o	268	UNK	GLY	conflict	UNP K7GKS8
o	269	UNK	MET	conflict	UNP K7GKS8
o	270	UNK	VAL	conflict	UNP K7GKS8
o	271	UNK	LYS	conflict	UNP K7GKS8
o	272	UNK	HIS	conflict	UNP K7GKS8
o	273	UNK	GLN	conflict	UNP K7GKS8
o	274	UNK	ALA	conflict	UNP K7GKS8
o	275	UNK	PRO	conflict	UNP K7GKS8
o	276	UNK	THR	conflict	UNP K7GKS8
o	277	UNK	GLN	conflict	UNP K7GKS8
o	278	UNK	ALA	conflict	UNP K7GKS8
o	279	UNK	LEU	conflict	UNP K7GKS8
o	280	UNK	ASN	conflict	UNP K7GKS8
o	281	UNK	LEU	conflict	UNP K7GKS8
o	282	UNK	TYR	conflict	UNP K7GKS8
o	283	UNK	THR	conflict	UNP K7GKS8
o	284	UNK	VAL	conflict	UNP K7GKS8

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Chain	Residue	Modelled	Actual	Comment	Reference
o	285	UNK	LEU	conflict	UNP K7GKS8
o	286	UNK	LEU	conflict	UNP K7GKS8
o	287	UNK	ASN	conflict	UNP K7GKS8
o	288	UNK	ASN	conflict	UNP K7GKS8
o	289	UNK	ARG	conflict	UNP K7GKS8
o	290	UNK	LEU	conflict	UNP K7GKS8
o	291	UNK	ARG	conflict	UNP K7GKS8
o	292	UNK	ALA	conflict	UNP K7GKS8
o	293	UNK	ASP	conflict	UNP K7GKS8
o	294	UNK	VAL	conflict	UNP K7GKS8
o	295	UNK	TYR	conflict	UNP K7GKS8
o	296	UNK	THR	conflict	UNP K7GKS8
o	297	UNK	PHE	conflict	UNP K7GKS8
o	298	UNK	ASN	conflict	UNP K7GKS8
o	299	UNK	SER	conflict	UNP K7GKS8
o	300	UNK	LEU	conflict	UNP K7GKS8
o	301	UNK	ILE	conflict	UNP K7GKS8
o	302	UNK	GLU	conflict	UNP K7GKS8
o	303	UNK	ALA	conflict	UNP K7GKS8
o	304	UNK	THR	conflict	UNP K7GKS8
o	305	UNK	ALA	conflict	UNP K7GKS8
o	306	UNK	LEU	conflict	UNP K7GKS8
o	307	UNK	VAL	conflict	UNP K7GKS8
o	308	UNK	VAL	conflict	UNP K7GKS8
o	309	UNK	ASN	conflict	UNP K7GKS8
o	310	UNK	GLU	conflict	UNP K7GKS8
o	311	UNK	LYS	conflict	UNP K7GKS8
o	312	UNK	PHE	conflict	UNP K7GKS8
o	313	UNK	GLU	conflict	UNP K7GKS8
o	314	UNK	GLU	conflict	UNP K7GKS8
o	315	UNK	LYS	conflict	UNP K7GKS8
o	316	UNK	TRP	conflict	UNP K7GKS8
o	317	UNK	ASN	conflict	UNP K7GKS8
o	318	UNK	ASN	conflict	UNP K7GKS8
o	319	UNK	ILE	conflict	UNP K7GKS8
o	320	UNK	LEU	conflict	UNP K7GKS8
o	321	UNK	ASP	conflict	UNP K7GKS8
o	322	UNK	LEU	conflict	UNP K7GKS8
o	323	UNK	LEU	conflict	UNP K7GKS8
o	324	UNK	LYS	conflict	UNP K7GKS8
o	325	UNK	GLN	conflict	UNP K7GKS8
o	326	UNK	MET	conflict	UNP K7GKS8

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Chain	Residue	Modelled	Actual	Comment	Reference
o	327	UNK	VAL	conflict	UNP K7GKS8
o	328	UNK	THR	conflict	UNP K7GKS8
o	329	UNK	GLN	conflict	UNP K7GKS8
o	330	UNK	ASN	conflict	UNP K7GKS8
o	331	UNK	VAL	conflict	UNP K7GKS8
o	332	UNK	LYS	conflict	UNP K7GKS8
o	333	UNK	PRO	conflict	UNP K7GKS8
o	334	UNK	ASN	conflict	UNP K7GKS8
o	335	UNK	LEU	conflict	UNP K7GKS8
o	336	UNK	GLN	conflict	UNP K7GKS8
o	337	UNK	THR	conflict	UNP K7GKS8
o	338	UNK	PHE	conflict	UNP K7GKS8
o	339	UNK	ASN	conflict	UNP K7GKS8
o	340	UNK	THR	conflict	UNP K7GKS8
o	341	UNK	ILE	conflict	UNP K7GKS8
o	342	UNK	LEU	conflict	UNP K7GKS8
o	343	UNK	LYS	conflict	UNP K7GKS8
o	344	UNK	CYS	conflict	UNP K7GKS8
o	345	UNK	LEU	conflict	UNP K7GKS8
o	346	UNK	ARG	conflict	UNP K7GKS8
o	347	UNK	ARG	conflict	UNP K7GKS8
o	348	UNK	PHE	conflict	UNP K7GKS8
o	349	UNK	TYR	conflict	UNP K7GKS8
o	350	UNK	ALA	conflict	UNP K7GKS8
o	351	UNK	PHE	conflict	UNP K7GKS8
o	352	UNK	GLY	conflict	UNP K7GKS8
o	353	UNK	LYS	conflict	UNP K7GKS8
o	354	UNK	LEU	conflict	UNP K7GKS8
o	355	UNK	PRO	conflict	UNP K7GKS8
o	356	UNK	ALA	conflict	UNP K7GKS8
o	357	UNK	LEU	conflict	UNP K7GKS8
o	358	UNK	GLN	conflict	UNP K7GKS8
o	359	UNK	THR	conflict	UNP K7GKS8
o	360	UNK	LEU	conflict	UNP K7GKS8
o	361	UNK	ARG	conflict	UNP K7GKS8
o	362	UNK	GLU	conflict	UNP K7GKS8
o	363	UNK	MET	conflict	UNP K7GKS8
o	364	UNK	LYS	conflict	UNP K7GKS8
o	365	UNK	ALA	conflict	UNP K7GKS8
o	366	UNK	ILE	conflict	UNP K7GKS8
o	367	UNK	GLY	conflict	UNP K7GKS8
o	368	UNK	ILE	conflict	UNP K7GKS8

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Chain	Residue	Modelled	Actual	Comment	Reference
o	369	UNK	GLU	conflict	UNP K7GKS8
o	370	UNK	PRO	conflict	UNP K7GKS8
o	371	UNK	SER	conflict	UNP K7GKS8
o	372	UNK	LEU	conflict	UNP K7GKS8
o	373	UNK	ALA	conflict	UNP K7GKS8
o	374	UNK	THR	conflict	UNP K7GKS8
o	375	UNK	TYR	conflict	UNP K7GKS8
o	376	UNK	HIS	conflict	UNP K7GKS8
o	377	UNK	TYR	conflict	UNP K7GKS8
o	378	UNK	VAL	conflict	UNP K7GKS8
o	379	UNK	ILE	conflict	UNP K7GKS8
o	380	UNK	GLN	conflict	UNP K7GKS8
o	381	UNK	LEU	conflict	UNP K7GKS8
o	382	UNK	PHE	conflict	UNP K7GKS8
o	383	UNK	TYR	conflict	UNP K7GKS8
o	384	UNK	GLN	conflict	UNP K7GKS8
o	385	UNK	HIS	conflict	UNP K7GKS8
o	386	UNK	GLU	conflict	UNP K7GKS8
o	387	UNK	SER	conflict	UNP K7GKS8
o	388	UNK	PRO	conflict	UNP K7GKS8
o	389	UNK	SER	conflict	UNP K7GKS8
o	390	UNK	LYS	conflict	UNP K7GKS8
o	391	UNK	GLY	conflict	UNP K7GKS8
o	392	UNK	SER	conflict	UNP K7GKS8
o	393	UNK	SER	conflict	UNP K7GKS8
o	394	UNK	LEU	conflict	UNP K7GKS8
o	395	UNK	ILE	conflict	UNP K7GKS8
o	396	UNK	ILE	conflict	UNP K7GKS8
o	397	UNK	TYR	conflict	UNP K7GKS8
o	398	UNK	ASP	conflict	UNP K7GKS8
o	399	UNK	ILE	conflict	UNP K7GKS8
o	400	UNK	MET	conflict	UNP K7GKS8
o	401	UNK	ASN	conflict	UNP K7GKS8
o	402	UNK	GLU	conflict	UNP K7GKS8
o	403	UNK	VAL	conflict	UNP K7GKS8
o	404	UNK	MET	conflict	UNP K7GKS8
o	405	UNK	GLY	conflict	UNP K7GKS8
o	406	UNK	LYS	conflict	UNP K7GKS8
o	407	UNK	ARG	conflict	UNP K7GKS8
o	408	UNK	PHE	conflict	UNP K7GKS8
o	409	UNK	SER	conflict	UNP K7GKS8
o	410	UNK	PRO	conflict	UNP K7GKS8

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Chain	Residue	Modelled	Actual	Comment	Reference
o	411	UNK	ARG	conflict	UNP K7GKS8
o	412	UNK	ASP	conflict	UNP K7GKS8
o	413	UNK	PRO	conflict	UNP K7GKS8
o	414	UNK	ASP	conflict	UNP K7GKS8
o	415	UNK	ASP	conflict	UNP K7GKS8
o	416	UNK	ASP	conflict	UNP K7GKS8
o	417	UNK	MET	conflict	UNP K7GKS8
o	418	UNK	PHE	conflict	UNP K7GKS8
o	419	UNK	PHE	conflict	UNP K7GKS8
o	420	UNK	GLN	conflict	UNP K7GKS8
o	421	UNK	SER	conflict	UNP K7GKS8
o	422	UNK	ALA	conflict	UNP K7GKS8
o	423	UNK	MET	conflict	UNP K7GKS8
o	424	UNK	ARG	conflict	UNP K7GKS8
o	425	UNK	VAL	conflict	UNP K7GKS8
o	426	UNK	CYS	conflict	UNP K7GKS8
o	427	UNK	SER	conflict	UNP K7GKS8
o	428	UNK	SER	conflict	UNP K7GKS8
o	429	UNK	LEU	conflict	UNP K7GKS8
o	430	UNK	ARG	conflict	UNP K7GKS8
o	431	UNK	ASP	conflict	UNP K7GKS8
o	432	UNK	LEU	conflict	UNP K7GKS8
o	433	UNK	GLU	conflict	UNP K7GKS8
o	434	UNK	LEU	conflict	UNP K7GKS8
o	435	UNK	ALA	conflict	UNP K7GKS8
o	436	UNK	TYR	conflict	UNP K7GKS8
o	437	UNK	GLN	conflict	UNP K7GKS8
o	438	UNK	VAL	conflict	UNP K7GKS8
o	439	UNK	HIS	conflict	UNP K7GKS8
o	440	UNK	GLY	conflict	UNP K7GKS8
o	441	UNK	LEU	conflict	UNP K7GKS8
o	442	UNK	LEU	conflict	UNP K7GKS8
o	443	UNK	ASN	conflict	UNP K7GKS8
o	444	UNK	THR	conflict	UNP K7GKS8
o	445	UNK	GLY	conflict	UNP K7GKS8
o	446	UNK	ASP	conflict	UNP K7GKS8
o	447	UNK	ASN	conflict	UNP K7GKS8
o	448	UNK	TRP	conflict	UNP K7GKS8
o	449	UNK	LYS	conflict	UNP K7GKS8
o	450	UNK	LEU	conflict	UNP K7GKS8
o	451	UNK	ILE	conflict	UNP K7GKS8
o	452	UNK	GLY	conflict	UNP K7GKS8

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Chain	Residue	Modelled	Actual	Comment	Reference
o	453	UNK	SER	conflict	UNP K7GKS8
o	454	UNK	ASP	conflict	UNP K7GKS8
o	455	UNK	HIS	conflict	UNP K7GKS8
o	456	UNK	ARG	conflict	UNP K7GKS8
o	457	UNK	ARG	conflict	UNP K7GKS8
o	458	UNK	ASN	conflict	UNP K7GKS8
o	459	UNK	PHE	conflict	UNP K7GKS8
o	460	UNK	TYR	conflict	UNP K7GKS8
o	461	UNK	TYR	conflict	UNP K7GKS8
o	462	UNK	SER	conflict	UNP K7GKS8
o	463	UNK	LYS	conflict	UNP K7GKS8
o	464	UNK	PHE	conflict	UNP K7GKS8
o	465	UNK	PHE	conflict	UNP K7GKS8
o	466	UNK	ASN	conflict	UNP K7GKS8
o	467	UNK	LEU	conflict	UNP K7GKS8
o	468	UNK	LEU	conflict	UNP K7GKS8
o	469	UNK	CYS	conflict	UNP K7GKS8
o	470	UNK	PHE	conflict	UNP K7GKS8
o	471	UNK	MET	conflict	UNP K7GKS8
o	472	UNK	GLU	conflict	UNP K7GKS8
o	473	UNK	GLN	conflict	UNP K7GKS8
o	474	UNK	ILE	conflict	UNP K7GKS8
o	475	UNK	ASP	conflict	UNP K7GKS8
o	476	UNK	VAL	conflict	UNP K7GKS8
o	477	UNK	THR	conflict	UNP K7GKS8
o	478	UNK	LEU	conflict	UNP K7GKS8
o	479	UNK	LYS	conflict	UNP K7GKS8
o	480	UNK	TRP	conflict	UNP K7GKS8
o	481	UNK	TYR	conflict	UNP K7GKS8
o	482	UNK	LYS	conflict	UNP K7GKS8
o	483	UNK	ASP	conflict	UNP K7GKS8
o	484	UNK	LEU	conflict	UNP K7GKS8
o	485	UNK	ILE	conflict	UNP K7GKS8
o	486	UNK	PRO	conflict	UNP K7GKS8
o	487	UNK	SER	conflict	UNP K7GKS8
o	488	UNK	VAL	conflict	UNP K7GKS8
o	489	UNK	PHE	conflict	UNP K7GKS8
o	490	UNK	PHE	conflict	UNP K7GKS8
o	491	UNK	PRO	conflict	UNP K7GKS8
o	492	UNK	HIS	conflict	UNP K7GKS8
o	493	UNK	SER	conflict	UNP K7GKS8
o	494	UNK	GLN	conflict	UNP K7GKS8

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Chain	Residue	Modelled	Actual	Comment	Reference
o	495	UNK	THR	conflict	UNP K7GKS8
o	496	UNK	MET	conflict	UNP K7GKS8
o	497	UNK	ILE	conflict	UNP K7GKS8
o	498	UNK	ASP	conflict	UNP K7GKS8
o	499	UNK	LEU	conflict	UNP K7GKS8
o	500	UNK	LEU	conflict	UNP K7GKS8
o	501	UNK	GLN	conflict	UNP K7GKS8
o	502	UNK	ALA	conflict	UNP K7GKS8
o	503	UNK	LEU	conflict	UNP K7GKS8
o	504	UNK	ASP	conflict	UNP K7GKS8
o	505	UNK	VAL	conflict	UNP K7GKS8
o	506	UNK	ALA	conflict	UNP K7GKS8
o	507	UNK	ASN	conflict	UNP K7GKS8
o	508	UNK	ARG	conflict	UNP K7GKS8
o	509	UNK	LEU	conflict	UNP K7GKS8
o	510	UNK	ASP	conflict	UNP K7GKS8
o	511	UNK	MET	conflict	UNP K7GKS8
o	512	UNK	VAL	conflict	UNP K7GKS8
o	513	UNK	PRO	conflict	UNP K7GKS8
o	514	UNK	GLN	conflict	UNP K7GKS8
o	515	UNK	ILE	conflict	UNP K7GKS8
o	516	UNK	TRP	conflict	UNP K7GKS8
o	517	UNK	LYS	conflict	UNP K7GKS8
o	518	UNK	ASP	conflict	UNP K7GKS8
o	519	UNK	SER	conflict	UNP K7GKS8
o	520	UNK	LYS	conflict	UNP K7GKS8
o	521	UNK	GLU	conflict	UNP K7GKS8
o	522	UNK	TYR	conflict	UNP K7GKS8
o	523	UNK	GLY	conflict	UNP K7GKS8
o	524	UNK	HIS	conflict	UNP K7GKS8
o	525	UNK	THR	conflict	UNP K7GKS8
o	526	UNK	PHE	conflict	UNP K7GKS8
o	527	UNK	ARG	conflict	UNP K7GKS8
o	528	UNK	ASN	conflict	UNP K7GKS8
o	529	UNK	GLU	conflict	UNP K7GKS8
o	530	UNK	LEU	conflict	UNP K7GKS8
o	531	UNK	LYS	conflict	UNP K7GKS8
o	532	UNK	GLU	conflict	UNP K7GKS8
o	533	UNK	GLU	conflict	UNP K7GKS8
o	534	UNK	ILE	conflict	UNP K7GKS8
o	535	UNK	LEU	conflict	UNP K7GKS8
o	536	UNK	MET	conflict	UNP K7GKS8

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Chain	Residue	Modelled	Actual	Comment	Reference
o	537	UNK	LEU	conflict	UNP K7GKS8
o	538	UNK	MET	conflict	UNP K7GKS8
o	539	UNK	ALA	conflict	UNP K7GKS8
o	540	UNK	ARG	conflict	UNP K7GKS8
o	541	UNK	ASP	conflict	UNP K7GKS8
o	542	UNK	GLN	conflict	UNP K7GKS8
o	543	UNK	HIS	conflict	UNP K7GKS8
o	544	UNK	PRO	conflict	UNP K7GKS8
o	545	UNK	PRO	conflict	UNP K7GKS8
o	546	UNK	GLU	conflict	UNP K7GKS8
o	547	UNK	LEU	conflict	UNP K7GKS8
o	548	UNK	GLN	conflict	UNP K7GKS8
o	549	UNK	VAL	conflict	UNP K7GKS8
o	550	UNK	ALA	conflict	UNP K7GKS8
o	551	UNK	PHE	conflict	UNP K7GKS8
o	552	UNK	ALA	conflict	UNP K7GKS8
o	553	UNK	ASP	conflict	UNP K7GKS8
o	554	UNK	CYS	conflict	UNP K7GKS8
o	555	UNK	ALA	conflict	UNP K7GKS8
o	556	UNK	ALA	conflict	UNP K7GKS8
o	557	UNK	ASP	conflict	UNP K7GKS8
o	558	UNK	ILE	conflict	UNP K7GKS8
o	559	UNK	LYS	conflict	UNP K7GKS8
o	560	UNK	SER	conflict	UNP K7GKS8
o	561	UNK	THR	conflict	UNP K7GKS8
o	562	UNK	TYR	conflict	UNP K7GKS8
o	563	UNK	GLU	conflict	UNP K7GKS8
o	564	UNK	SER	conflict	UNP K7GKS8
o	565	UNK	GLN	conflict	UNP K7GKS8
o	566	UNK	ASP	conflict	UNP K7GKS8
o	567	UNK	ALA	conflict	UNP K7GKS8
o	568	UNK	ARG	conflict	UNP K7GKS8
o	569	UNK	GLN	conflict	UNP K7GKS8
o	570	UNK	THR	conflict	UNP K7GKS8
o	571	UNK	ALA	conflict	UNP K7GKS8
o	572	UNK	PRO	conflict	UNP K7GKS8
o	573	UNK	GLU	conflict	UNP K7GKS8
o	574	UNK	TRP	conflict	UNP K7GKS8
o	575	UNK	PRO	conflict	UNP K7GKS8
o	576	UNK	ALA	conflict	UNP K7GKS8
o	577	UNK	SER	conflict	UNP K7GKS8
o	578	UNK	SER	conflict	UNP K7GKS8

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Chain	Residue	Modelled	Actual	Comment	Reference
o	579	UNK	LEU	conflict	UNP K7GKS8
o	580	UNK	ASN	conflict	UNP K7GKS8
o	581	UNK	TYR	conflict	UNP K7GKS8
o	582	UNK	VAL	conflict	UNP K7GKS8
o	583	UNK	ALA	conflict	UNP K7GKS8
o	584	UNK	VAL	conflict	UNP K7GKS8
o	585	UNK	LEU	conflict	UNP K7GKS8
o	586	UNK	PHE	conflict	UNP K7GKS8
o	587	UNK	LEU	conflict	UNP K7GKS8
o	588	UNK	ARG	conflict	UNP K7GKS8
o	589	UNK	ALA	conflict	UNP K7GKS8
o	590	UNK	GLY	conflict	UNP K7GKS8
o	591	UNK	ARG	conflict	UNP K7GKS8
o	592	UNK	THR	conflict	UNP K7GKS8
o	593	UNK	GLN	conflict	UNP K7GKS8
o	594	UNK	GLU	conflict	UNP K7GKS8
o	595	UNK	ALA	conflict	UNP K7GKS8
o	596	UNK	TRP	conflict	UNP K7GKS8
o	597	UNK	LYS	conflict	UNP K7GKS8
o	598	UNK	MET	conflict	UNP K7GKS8
o	599	UNK	LEU	conflict	UNP K7GKS8
o	600	UNK	GLY	conflict	UNP K7GKS8
o	601	UNK	LEU	conflict	UNP K7GKS8
o	602	UNK	PHE	conflict	UNP K7GKS8
o	603	UNK	ARG	conflict	UNP K7GKS8
o	604	UNK	LYS	conflict	UNP K7GKS8
o	605	UNK	HIS	conflict	UNP K7GKS8
o	606	UNK	ASN	conflict	UNP K7GKS8
o	607	UNK	LYS	conflict	UNP K7GKS8
o	608	UNK	ILE	conflict	UNP K7GKS8
o	609	UNK	PRO	conflict	UNP K7GKS8
o	610	UNK	ARG	conflict	UNP K7GKS8
o	611	UNK	ALA	conflict	UNP K7GKS8
o	612	UNK	GLU	conflict	UNP K7GKS8
o	613	UNK	LEU	conflict	UNP K7GKS8
o	614	UNK	LEU	conflict	UNP K7GKS8
o	615	UNK	ASN	conflict	UNP K7GKS8
o	616	UNK	GLU	conflict	UNP K7GKS8
o	617	UNK	PHE	conflict	UNP K7GKS8
o	618	UNK	LEU	conflict	UNP K7GKS8
o	619	UNK	ASP	conflict	UNP K7GKS8
o	620	UNK	SER	conflict	UNP K7GKS8

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Chain	Residue	Modelled	Actual	Comment	Reference
o	621	UNK	ALA	conflict	UNP K7GKS8
o	622	UNK	LYS	conflict	UNP K7GKS8
o	623	UNK	ALA	conflict	UNP K7GKS8
o	624	UNK	SER	conflict	UNP K7GKS8
o	625	UNK	SER	conflict	UNP K7GKS8
o	626	UNK	SER	conflict	UNP K7GKS8
o	627	UNK	PRO	conflict	UNP K7GKS8
o	628	UNK	ALA	conflict	UNP K7GKS8
o	629	UNK	GLN	conflict	UNP K7GKS8
o	630	UNK	ALA	conflict	UNP K7GKS8
o	631	UNK	ILE	conflict	UNP K7GKS8
o	632	UNK	GLU	conflict	UNP K7GKS8
o	633	UNK	LEU	conflict	UNP K7GKS8
o	634	UNK	VAL	conflict	UNP K7GKS8
o	635	UNK	LYS	conflict	UNP K7GKS8
o	636	UNK	LEU	conflict	UNP K7GKS8
o	637	UNK	ALA	conflict	UNP K7GKS8
o	638	UNK	SER	conflict	UNP K7GKS8
o	639	UNK	ALA	conflict	UNP K7GKS8
o	640	UNK	PHE	conflict	UNP K7GKS8
o	641	UNK	SER	conflict	UNP K7GKS8
o	642	UNK	LEU	conflict	UNP K7GKS8
o	643	UNK	PRO	conflict	UNP K7GKS8
o	644	UNK	VAL	conflict	UNP K7GKS8
o	645	UNK	CYS	conflict	UNP K7GKS8
o	646	UNK	GLU	conflict	UNP K7GKS8
o	647	UNK	GLY	conflict	UNP K7GKS8
o	648	UNK	LEU	conflict	UNP K7GKS8
o	649	UNK	THR	conflict	UNP K7GKS8
o	650	UNK	ARG	conflict	UNP K7GKS8
o	651	UNK	ARG	conflict	UNP K7GKS8
o	652	UNK	VAL	conflict	UNP K7GKS8
o	653	UNK	MET	conflict	UNP K7GKS8
o	654	UNK	ALA	conflict	UNP K7GKS8
o	655	UNK	GLU	conflict	UNP K7GKS8
o	656	UNK	PHE	conflict	UNP K7GKS8
o	657	UNK	THR	conflict	UNP K7GKS8
o	658	UNK	LEU	conflict	UNP K7GKS8
o	659	UNK	THR	conflict	UNP K7GKS8
o	660	UNK	GLN	conflict	UNP K7GKS8
o	661	UNK	GLU	conflict	UNP K7GKS8
o	662	UNK	GLN	conflict	UNP K7GKS8

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Chain	Residue	Modelled	Actual	Comment	Reference
o	663	UNK	ARG	conflict	UNP K7GKS8
o	664	UNK	GLU	conflict	UNP K7GKS8
o	665	UNK	ALA	conflict	UNP K7GKS8
o	666	UNK	LEU	conflict	UNP K7GKS8
o	667	UNK	GLY	conflict	UNP K7GKS8
o	668	UNK	GLU	conflict	UNP K7GKS8
o	669	UNK	LEU	conflict	UNP K7GKS8
o	670	UNK	THR	conflict	UNP K7GKS8
o	671	UNK	ALA	conflict	UNP K7GKS8
o	672	UNK	LEU	conflict	UNP K7GKS8
o	673	UNK	THR	conflict	UNP K7GKS8
o	674	UNK	SER	conflict	UNP K7GKS8
o	675	UNK	ASP	conflict	UNP K7GKS8
o	676	UNK	SER	conflict	UNP K7GKS8
o	677	UNK	SER	conflict	UNP K7GKS8

- Molecule 34 is a protein called MITORIBOSOMAL PROTEIN MS40, MRPS18B.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	p	188	Total	C	N	O	S	0	0
			1551	983	290	270	8		

- Molecule 35 is a protein called UNASSIGNED HELICES.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	s	16	Total	C	N	O	0	0
			96	64	16	16		

- Molecule 36 is a protein called UNASSIGNED HELICES.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	z	17	Total	C	N	O	0	0
			102	68	17	17		

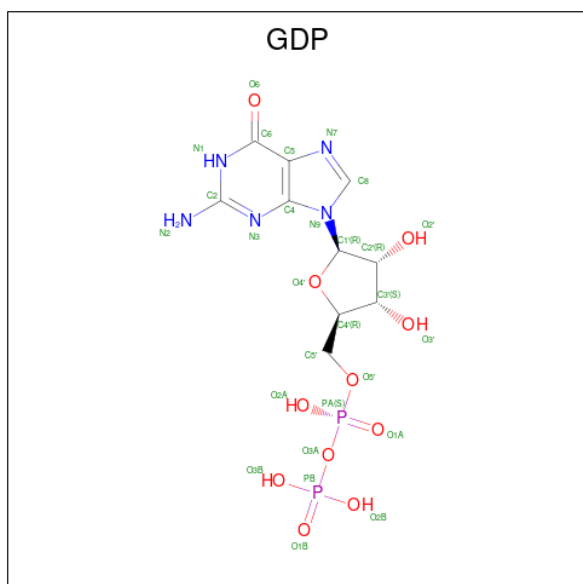
- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	A	143	Total	Mg	0
			143	143	
37	g	1	Total	Mg	0
			1	1	

- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
38	R	1	Total	Zn	0
			1	1	
38	c	1	Total	Zn	0
			1	1	
38	p	1	Total	Zn	0
			1	1	

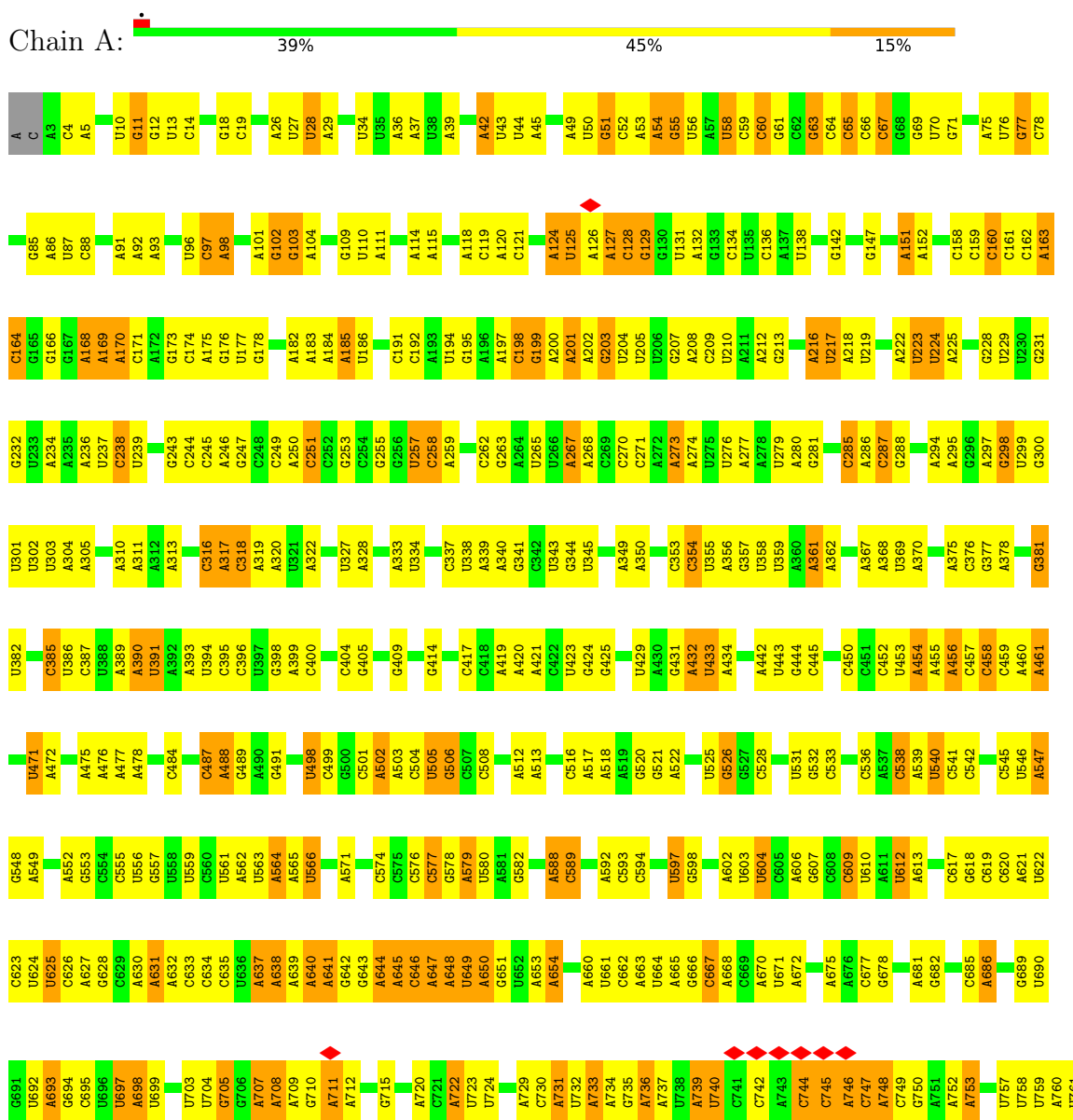
- Molecule 39 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

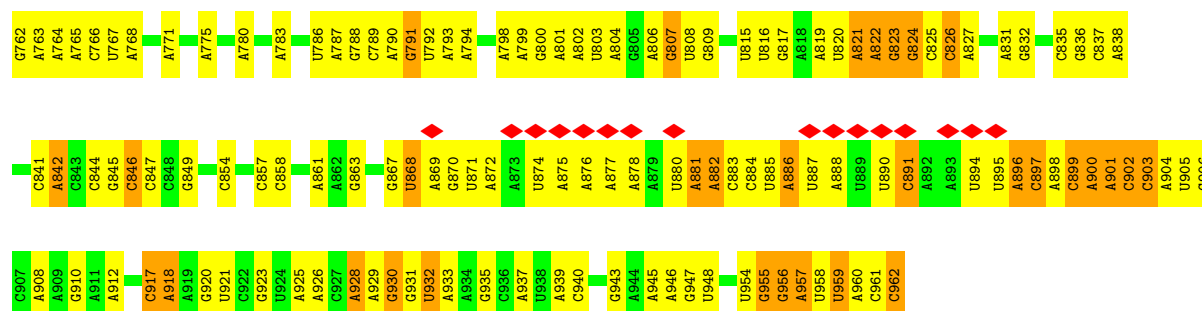


3 Residue-property plots

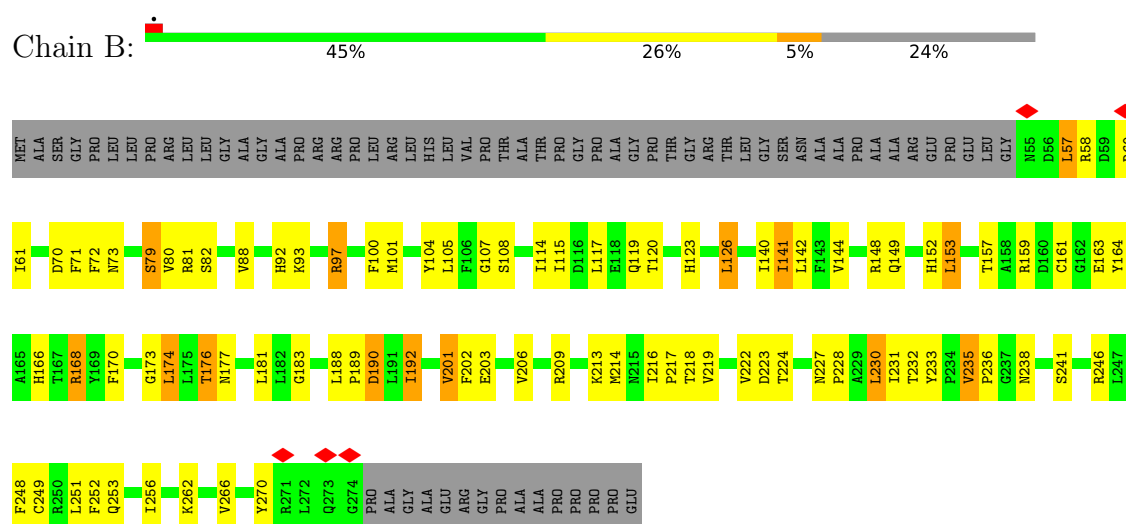
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: MITORIBOSOMAL 12S RRNA

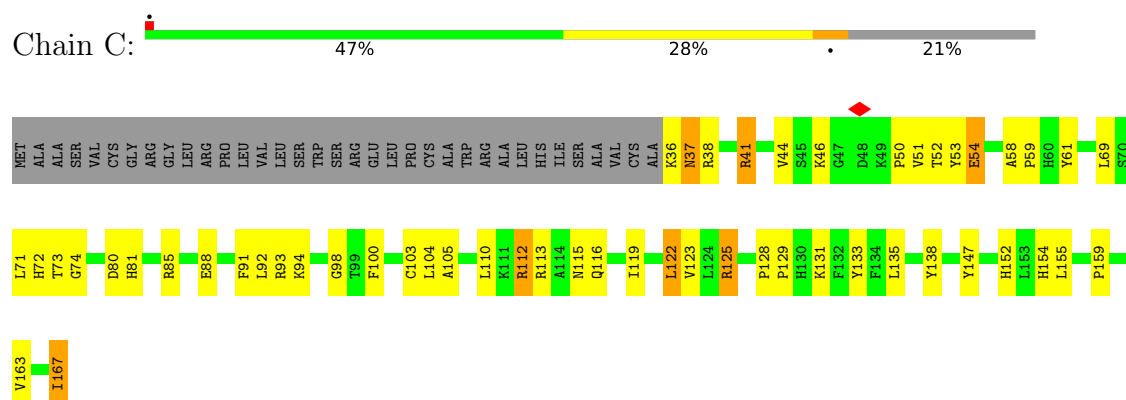




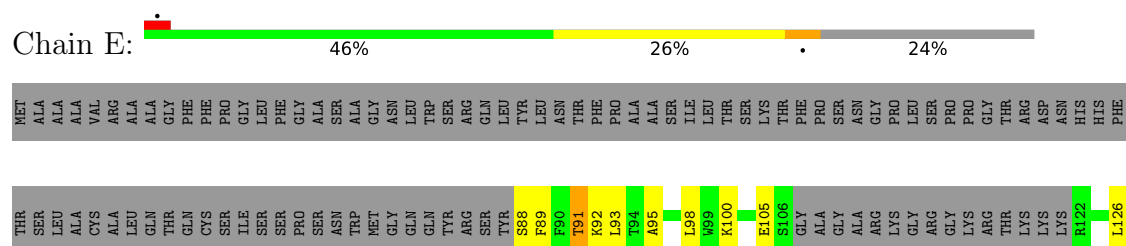
• Molecule 2: MITORIBOSOMAL PROTEIN US2M, MRPS2

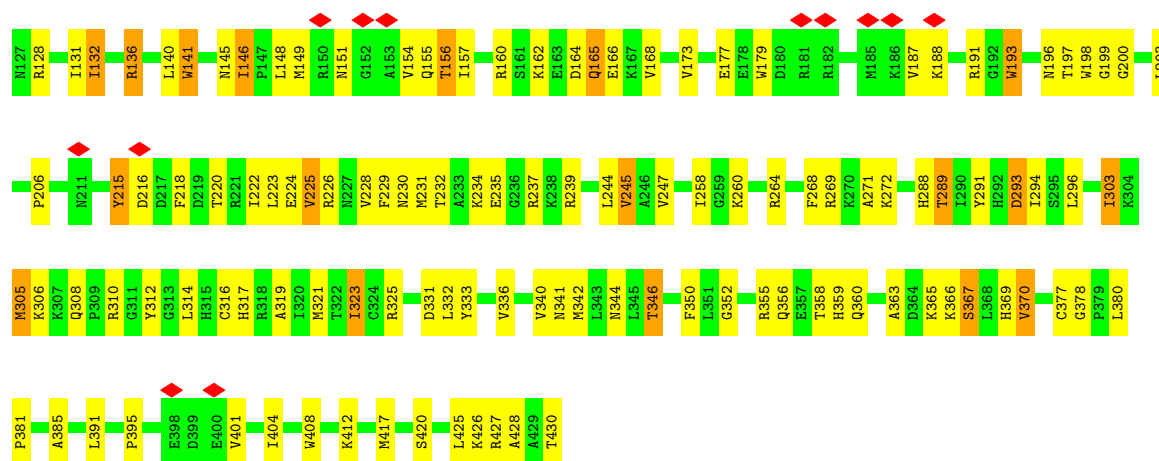


• Molecule 3: MITORIBOSOMAL PROTEIN US3M, MRPS24

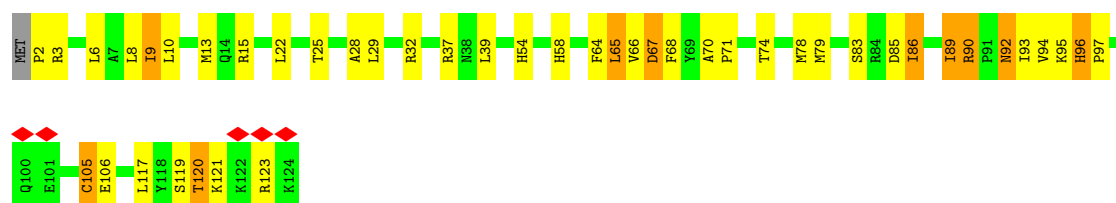


• Molecule 4: MITORIBOSOMAL PROTEIN US5M, MRPS5

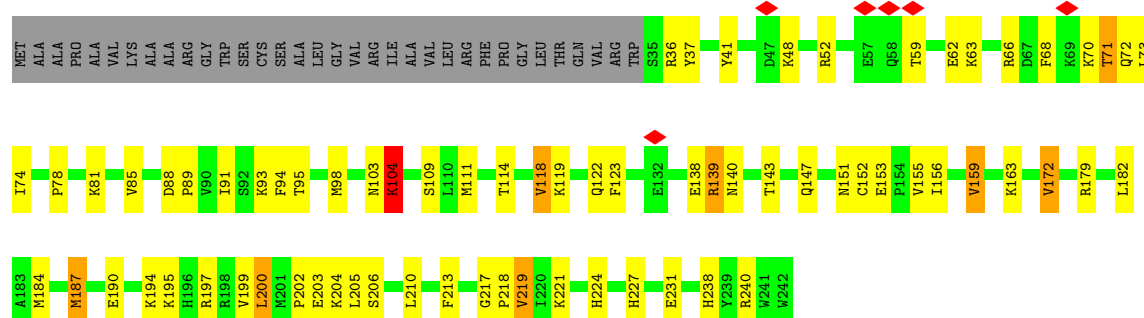




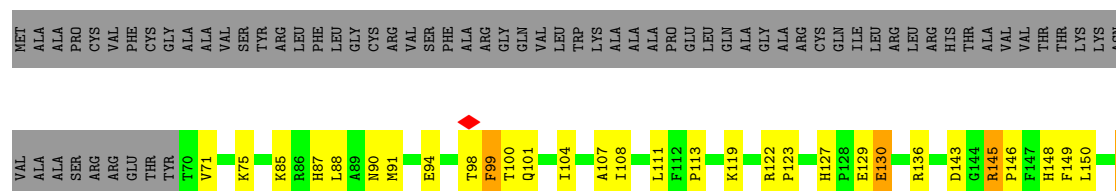
• Molecule 5: MITORIBOSOMAL PROTEIN BS6M, MRPS6

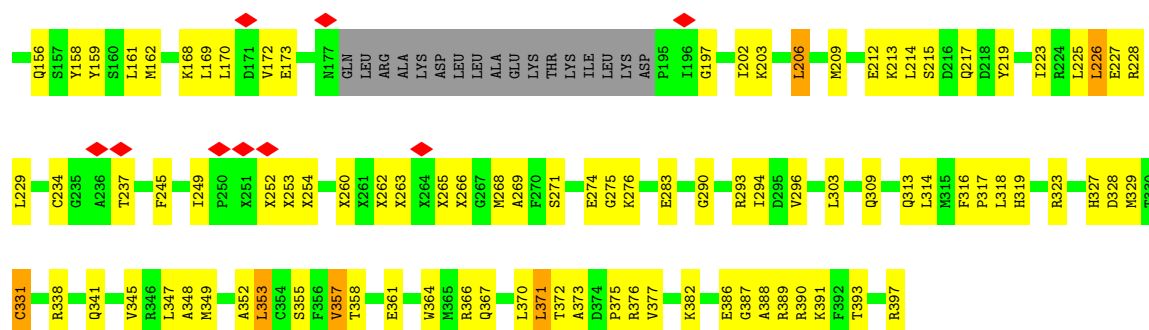


• Molecule 6: MITORIBOSOMAL PROTEIN US7M, MRPS7

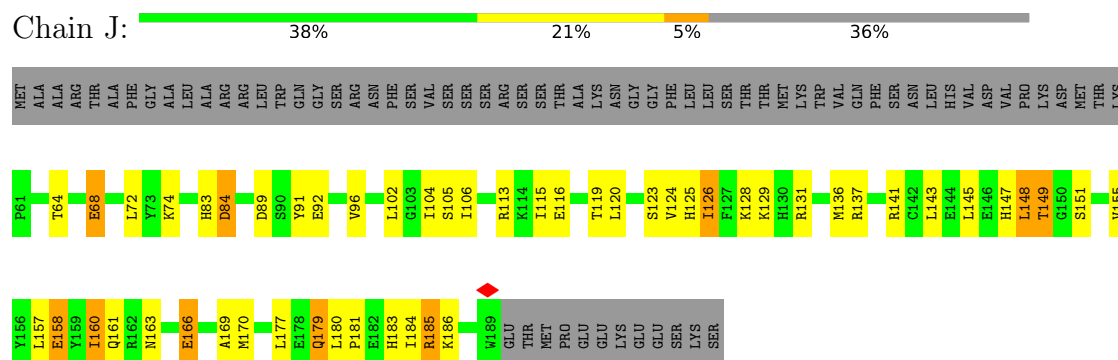


• Molecule 7: MITORIBOSOMAL PROTEIN US9M, MRPS9

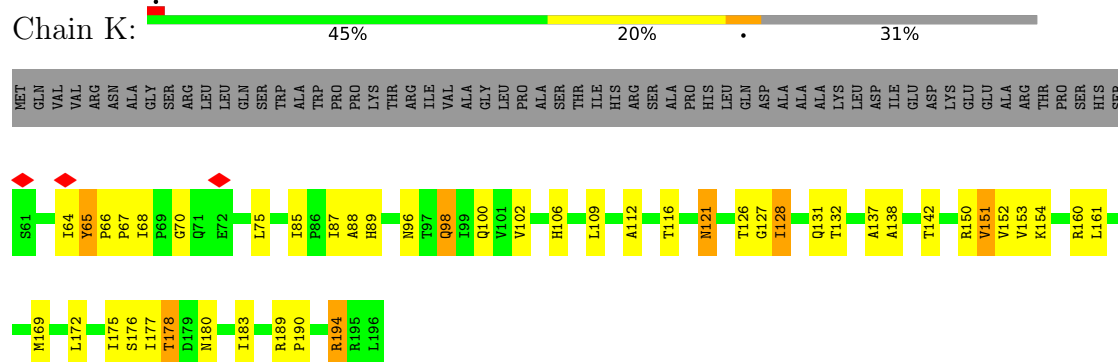




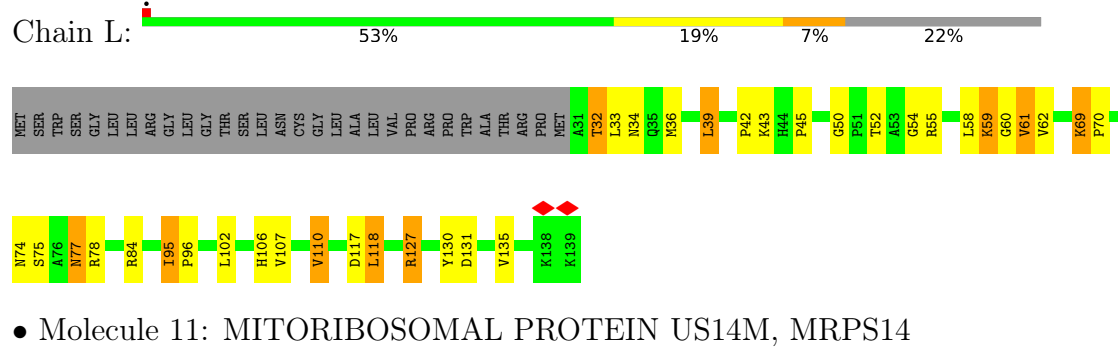
• Molecule 8: MITORIBOSOMAL PROTEIN US10M, MRPS10



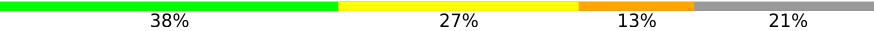
• Molecule 9: MITORIBOSOMAL PROTEIN US11M, MRPS11

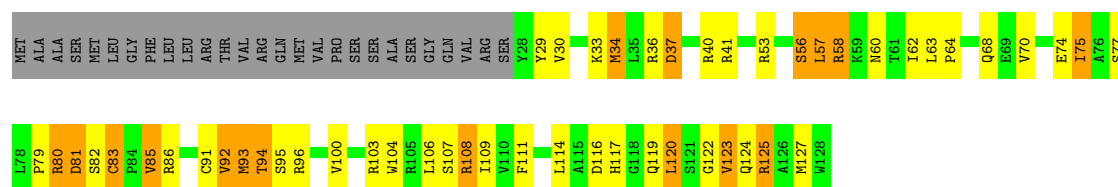


• Molecule 10: MITORIBOSOMAL PROTEIN US12M, MRPS12



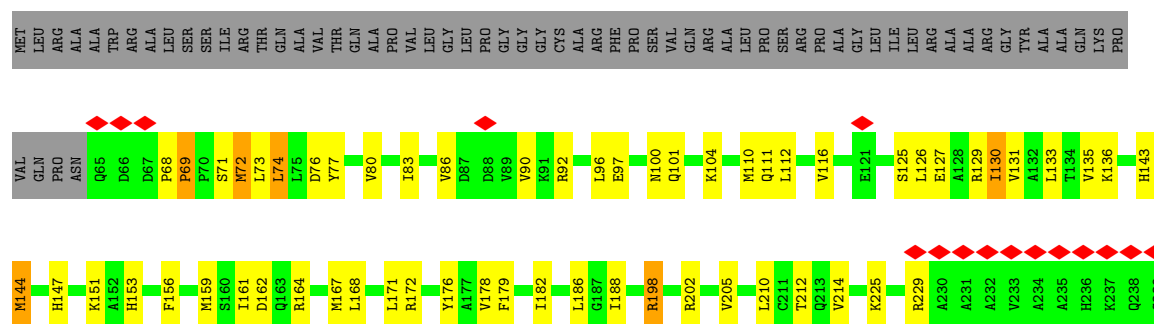
• Molecule 11: MITORIBOSOMAL PROTEIN US14M, MRPS14

Chain N: 



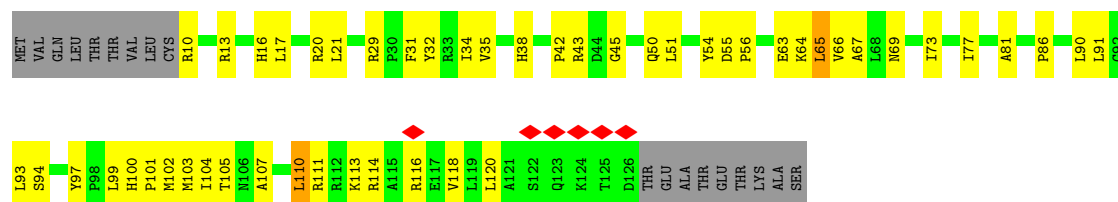
• Molecule 12: MITORIBOSOMAL PROTEIN US15M, MRPS15

Chain O: 



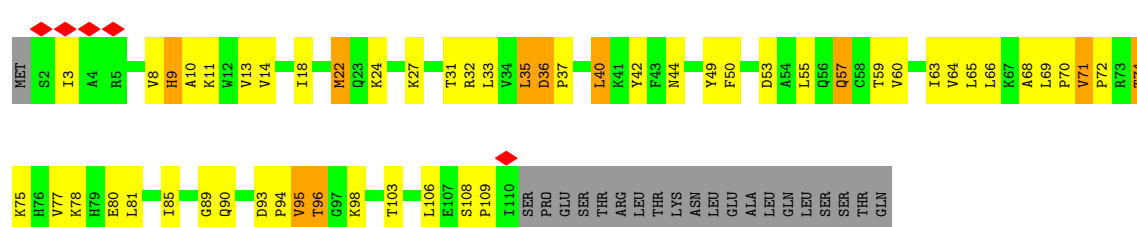
• Molecule 13: MITORIBOSOMAL PROTEIN BS16M, MRPS16

Chain P: 

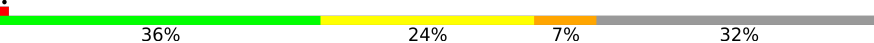


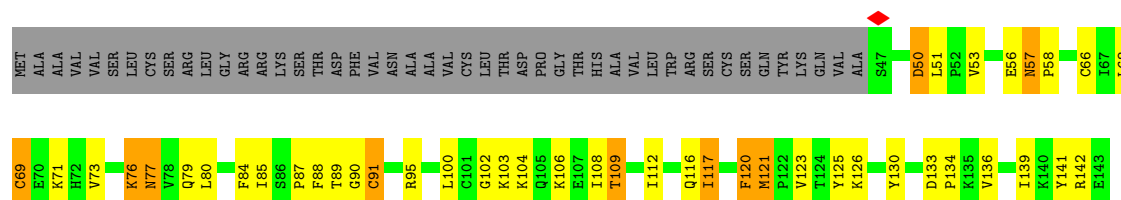
• Molecule 14: MITORIBOSOMAL PROTEIN US17M, MRPS17

Chain Q: 

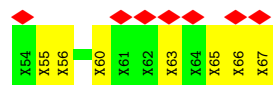


• Molecule 15: MITORIBOSOMAL PROTEIN BS18M, MRPS18C

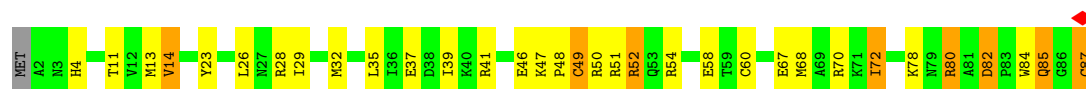
Chain R: 



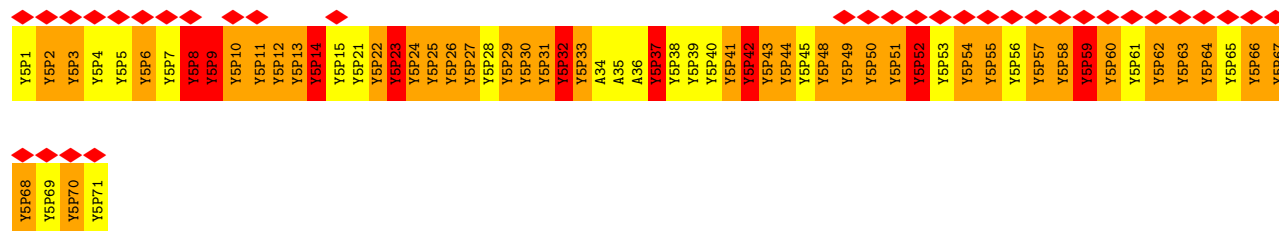
• Molecule 16: MITORIBOSOMAL PROTEIN BL19M, MRPL19



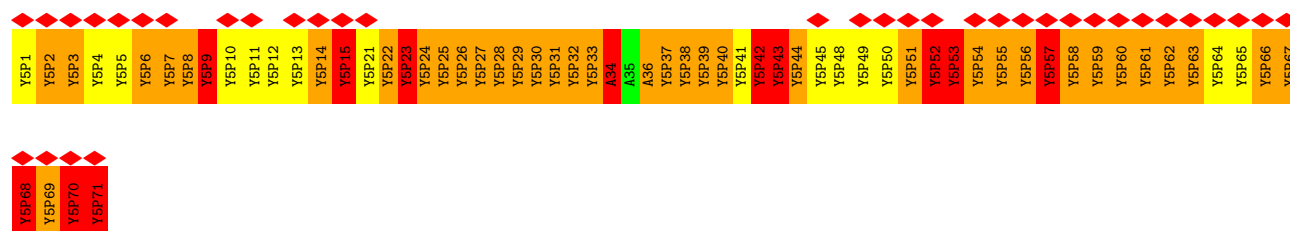
• Molecule 17: MITORIBOSOMAL PROTEIN BS21M, MRPS21



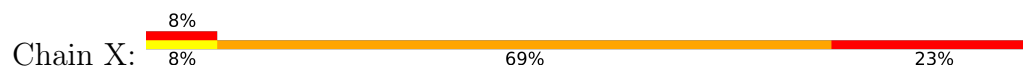
• Molecule 18: P-SITE AND A-SITE TRNA

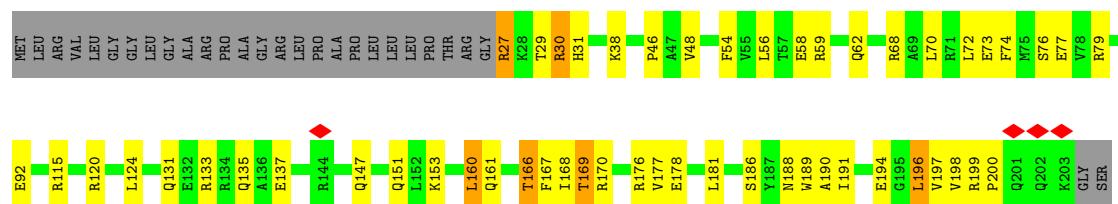


• Molecule 18: P-SITE AND A-SITE TRNA

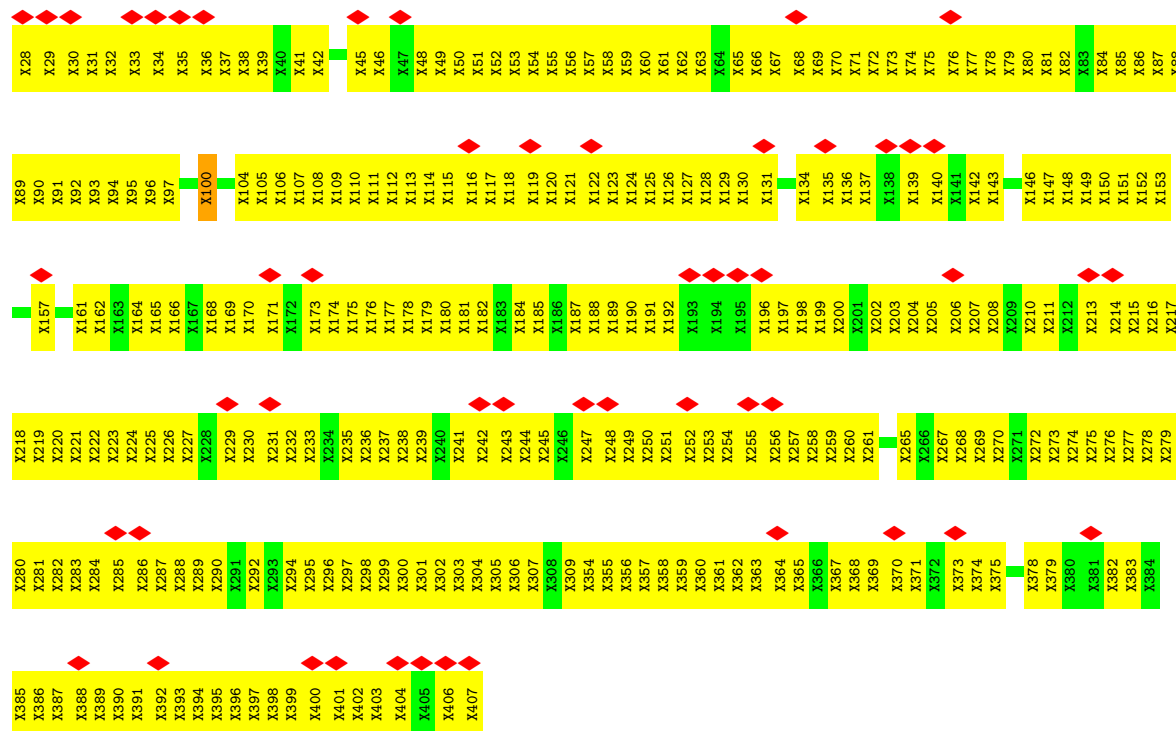


• Molecule 19: MRNA

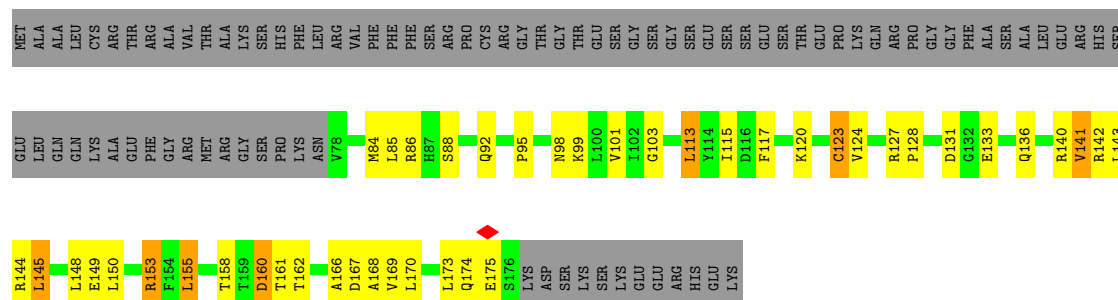
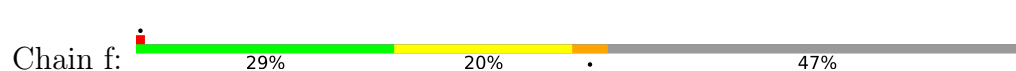




• Molecule 24: MITORIBOSOMAL PROTEIN MS27, MRPS27

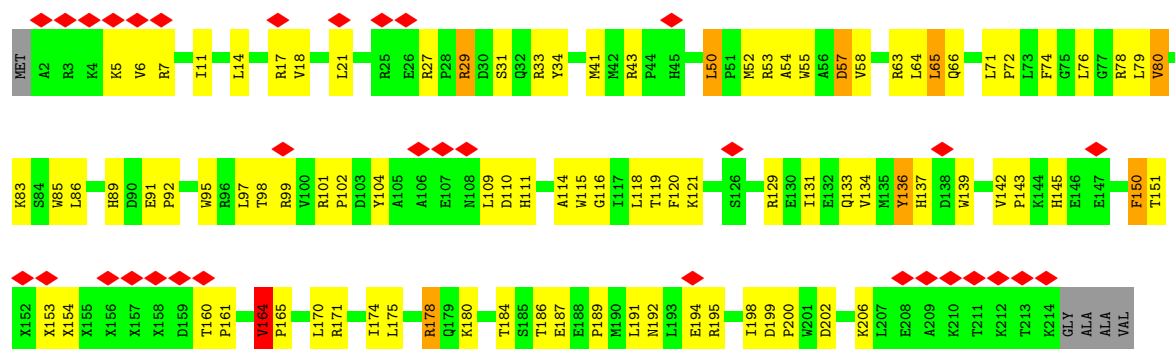


• Molecule 25: MITORIBOSOMAL PROTEIN MS28, MRPS28

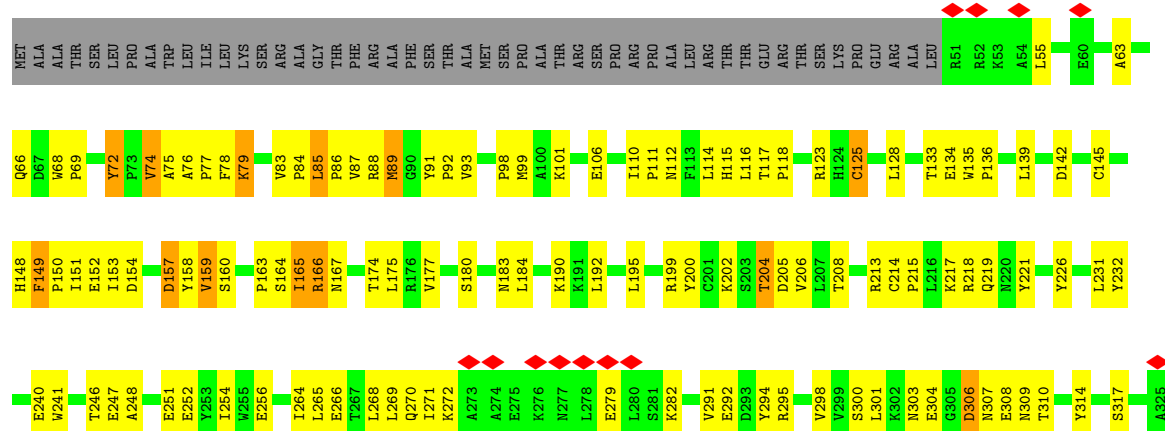


• Molecule 26: MITORIBOSOMAL PROTEIN MS29, MRPS29

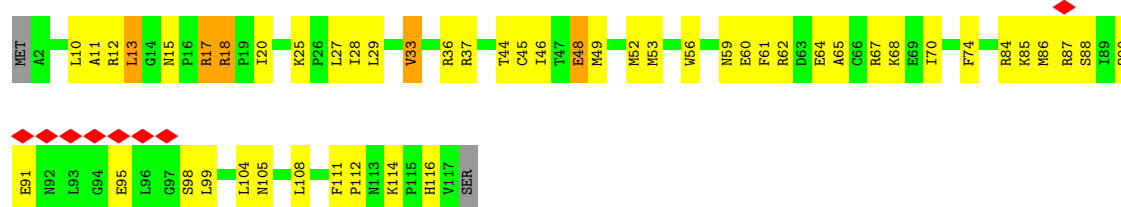




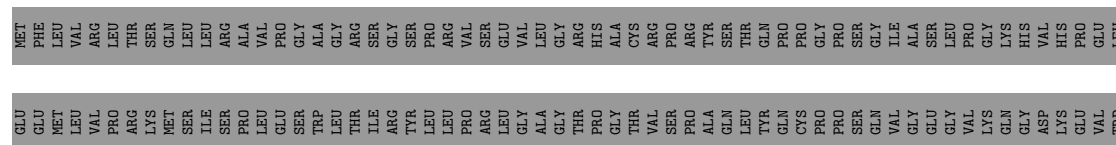
• Molecule 30: MITORIBOSOMAL PROTEIN MS35, MRPS35

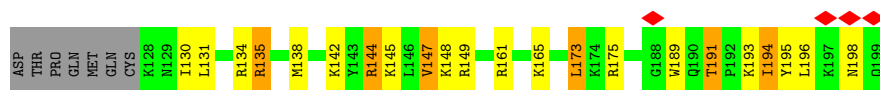


• Molecule 31: MITORIBOSOMAL PROTEIN MS37, MRPS37

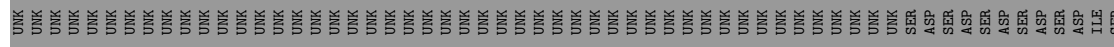
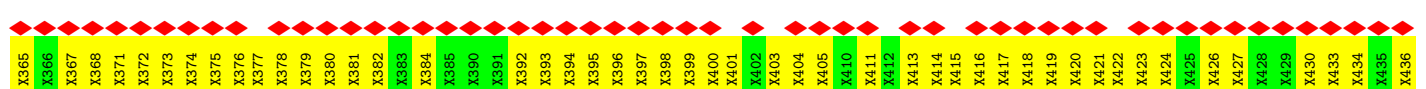
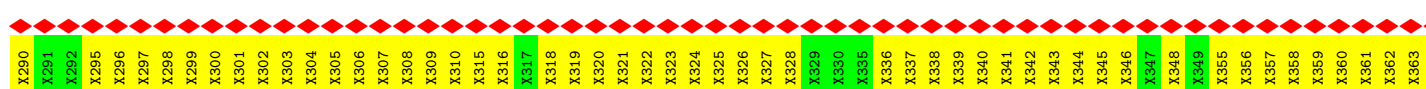
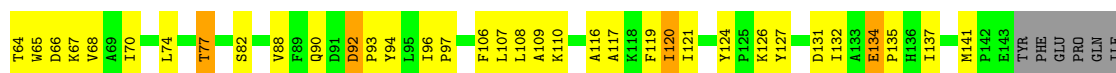
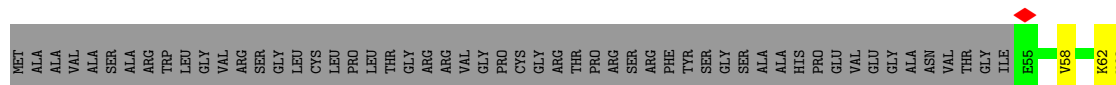
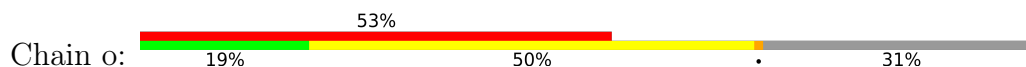


• Molecule 32: MITORIBOSOMAL PROTEIN MS38, MRPS38

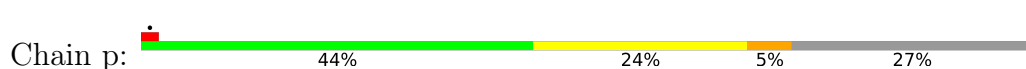




• Molecule 33: MITORIBOSOMAL PROTEIN MS39, MRPS39



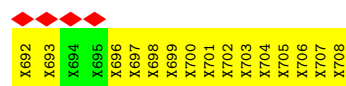
• Molecule 34: MITORIBOSOMAL PROTEIN MS40, MRPS18B



• Molecule 35: UNASSIGNED HELICES



- Molecule 36: UNASSIGNED HELICES



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	78783	Depositor
Resolution determination method	Not provided	
CTF correction method	PER DETECTOR FRAME	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	100000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.529	Depositor
Minimum map value	-0.250	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.06	Depositor
Map size ($\text{\AA}$)	300.24, 300.24, 300.24	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.39, 1.39, 1.39	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: Y5P, P5P, ZN, MG, GDP

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	0.34	0/22852	0.49	0/35580
2	B	0.62	0/1804	0.97	7/2445 (0.3%)
3	C	0.52	0/1105	0.99	1/1496 (0.1%)
4	E	0.59	1/2673 (0.0%)	0.96	6/3591 (0.2%)
5	F	0.54	0/1008	1.00	6/1358 (0.4%)
6	G	0.51	0/1763	0.90	4/2368 (0.2%)
7	I	0.47	0/2455	0.85	2/3291 (0.1%)
8	J	0.58	0/1091	1.03	4/1474 (0.3%)
9	K	0.62	0/1021	1.11	4/1381 (0.3%)
10	L	0.52	0/858	1.07	9/1152 (0.8%)
11	N	0.56	0/874	0.92	2/1171 (0.2%)
12	O	0.52	0/1473	0.92	4/1970 (0.2%)
13	P	0.57	0/954	0.95	1/1284 (0.1%)
14	Q	0.56	0/871	1.09	3/1181 (0.3%)
15	R	0.63	0/802	1.13	5/1079 (0.5%)
17	U	0.57	0/745	0.90	2/993 (0.2%)
20	a	0.45	0/2052	0.85	1/2774 (0.0%)
21	b	0.48	0/1126	0.96	4/1514 (0.3%)
22	c	0.53	0/1399	1.11	16/1881 (0.9%)
23	d	0.48	0/1490	0.79	0/2005
25	f	0.49	0/790	0.90	1/1064 (0.1%)
26	g	0.42	0/2731	0.91	8/3696 (0.2%)
27	h	0.39	0/903	0.85	2/1215 (0.2%)
28	i	0.44	0/841	0.90	2/1121 (0.2%)
29	j	0.44	0/1779	0.95	3/2404 (0.1%)
30	k	0.45	0/2268	0.93	7/3069 (0.2%)
31	m	0.53	0/947	0.95	2/1268 (0.2%)
32	n	0.63	0/650	0.91	0/858
33	o	0.45	0/726	0.97	6/988 (0.6%)
34	p	0.56	0/1602	1.08	8/2175 (0.4%)
All	All	0.46	1/61653 (0.0%)	0.80	120/87846 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
8	J	0	2
9	K	0	1
20	a	0	1
24	e	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	193	TRP	CA-C	-5.60	1.48	1.52

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	Q	36	ASP	CA-C-N	9.88	129.67	119.19
14	Q	36	ASP	C-N-CA	9.88	129.67	119.19
34	p	54	GLU	CA-C-N	9.16	131.28	119.84
34	p	54	GLU	C-N-CA	9.16	131.28	119.84
34	p	230	PRO	CA-C-N	8.74	129.38	120.38
34	p	230	PRO	C-N-CA	8.74	129.38	120.38
30	k	76	ALA	CA-C-N	8.62	128.27	119.82
30	k	76	ALA	C-N-CA	8.62	128.27	119.82
21	b	39	PRO	CA-C-N	8.61	128.47	120.21
21	b	39	PRO	C-N-CA	8.61	128.47	120.21
4	E	310	ARG	N-CA-C	8.18	120.28	111.36
31	m	15	ASN	CA-C-N	8.15	127.79	119.56
31	m	15	ASN	C-N-CA	8.15	127.79	119.56
2	B	227	ASN	CA-C-N	8.10	127.74	119.56
2	B	227	ASN	C-N-CA	8.10	127.74	119.56
5	F	105	CYS	N-CA-C	-7.84	98.27	109.96
15	R	90	GLY	N-CA-C	-7.81	104.24	115.64
29	j	164	VAL	CA-C-N	7.80	129.59	119.84
29	j	164	VAL	C-N-CA	7.80	129.59	119.84
7	I	145	ARG	CA-C-N	7.73	127.49	119.76
7	I	145	ARG	C-N-CA	7.73	127.49	119.76
8	J	68	GLU	CA-C-N	7.73	129.50	119.84
8	J	68	GLU	C-N-CA	7.73	129.50	119.84
34	p	229	GLY	CA-C-N	-7.57	112.59	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	p	229	GLY	C-N-CA	-7.57	112.59	120.38
33	o	92	ASP	CA-C-N	7.41	127.77	119.32
33	o	92	ASP	C-N-CA	7.41	127.77	119.32
2	B	216	ILE	CA-C-N	-7.34	113.11	120.31
2	B	216	ILE	C-N-CA	-7.34	113.11	120.31
9	K	85	ILE	CA-C-N	7.28	127.33	119.90
9	K	85	ILE	C-N-CA	7.28	127.33	119.90
4	E	141	TRP	CA-C-N	7.20	128.84	119.84
4	E	141	TRP	C-N-CA	7.20	128.84	119.84
4	E	378	GLY	CA-C-N	6.95	127.09	119.87
4	E	378	GLY	C-N-CA	6.95	127.09	119.87
22	c	141	CYS	N-CA-C	-6.95	103.71	111.28
22	c	7	PHE	CA-C-N	6.93	126.62	119.56
22	c	7	PHE	C-N-CA	6.93	126.62	119.56
34	p	235	MET	N-CA-C	6.87	121.55	112.35
9	K	194	ARG	N-CA-C	6.67	121.11	107.69
29	j	116	GLY	N-CA-C	6.67	122.01	112.81
2	B	183	GLY	CA-C-N	6.41	126.62	119.32
2	B	183	GLY	C-N-CA	6.41	126.62	119.32
5	F	106	GLU	N-CA-C	-6.40	104.95	112.89
22	c	73	SER	CA-C-N	6.39	126.15	119.76
22	c	73	SER	C-N-CA	6.39	126.15	119.76
15	R	121	MET	CA-C-N	-6.37	113.97	120.85
15	R	121	MET	C-N-CA	-6.37	113.97	120.85
30	k	83	VAL	CA-C-N	6.36	125.93	119.19
30	k	83	VAL	C-N-CA	6.36	125.93	119.19
12	O	68	PRO	CA-C-N	6.33	126.90	120.38
12	O	68	PRO	C-N-CA	6.33	126.90	120.38
12	O	69	PRO	CA-C-N	6.18	126.64	119.47
12	O	69	PRO	C-N-CA	6.18	126.64	119.47
28	i	99	GLY	N-CA-C	6.16	119.65	112.50
30	k	184	LEU	N-CA-C	6.11	118.85	110.24
8	J	119	THR	N-CA-C	6.09	119.05	108.76
11	N	96	ARG	CA-C-N	6.03	125.65	119.56
11	N	96	ARG	C-N-CA	6.03	125.65	119.56
26	g	340	ILE	CA-C-N	6.02	127.36	119.84
26	g	340	ILE	C-N-CA	6.02	127.36	119.84
27	h	353	ASN	CA-C-N	5.97	125.59	119.56
27	h	353	ASN	C-N-CA	5.97	125.59	119.56
6	G	217	GLY	CA-C-N	5.96	126.12	119.32
6	G	217	GLY	C-N-CA	5.96	126.12	119.32
34	p	86	PRO	O-C-N	5.92	123.93	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	g	82	LEU	N-CA-C	-5.91	101.95	110.40
22	c	144	GLU	N-CA-C	5.88	118.19	111.02
22	c	71	THR	CA-C-N	5.84	125.54	119.82
22	c	71	THR	C-N-CA	5.84	125.54	119.82
10	L	95	ILE	CA-C-N	5.83	126.32	120.14
10	L	95	ILE	C-N-CA	5.83	126.32	120.14
10	L	130	TYR	CB-CA-C	-5.82	109.31	117.23
17	U	82	ASP	CA-C-N	5.81	125.18	118.85
17	U	82	ASP	C-N-CA	5.81	125.18	118.85
22	c	125	HIS	CA-C-N	5.79	125.92	119.32
22	c	125	HIS	C-N-CA	5.79	125.92	119.32
10	L	69	LYS	CA-C-N	5.77	126.58	120.11
10	L	69	LYS	C-N-CA	5.77	126.58	120.11
33	o	141	MET	CA-C-N	5.75	125.73	120.21
33	o	141	MET	C-N-CA	5.75	125.73	120.21
6	G	71	THR	N-CA-C	-5.75	103.98	111.74
5	F	90	ARG	CA-C-N	5.67	127.66	120.51
5	F	90	ARG	C-N-CA	5.67	127.66	120.51
22	c	83	GLY	N-CA-C	-5.67	107.36	115.64
9	K	121	ASN	N-CA-C	5.64	118.16	111.33
22	c	149	CYS	CA-C-N	5.60	126.84	119.84
22	c	149	CYS	C-N-CA	5.60	126.84	119.84
22	c	141	CYS	CA-CB-SG	5.60	127.27	114.40
15	R	57	ASN	CA-C-N	5.55	126.78	119.84
15	R	57	ASN	C-N-CA	5.55	126.78	119.84
8	J	129	LYS	N-CA-C	-5.52	105.80	112.54
22	c	105	ILE	N-CA-C	5.49	115.58	110.42
6	G	104	LYS	N-CA-C	-5.46	104.98	111.69
21	b	39	PRO	O-C-N	5.43	123.70	121.15
26	g	323	LEU	CA-C-N	5.37	124.56	118.97
26	g	323	LEU	C-N-CA	5.37	124.56	118.97
22	c	5	GLY	N-CA-C	-5.33	105.04	112.18
30	k	149	PHE	CA-C-N	5.30	124.81	119.19
30	k	149	PHE	C-N-CA	5.30	124.81	119.19
26	g	386	ASN	CA-C-N	5.29	124.74	119.24
26	g	386	ASN	C-N-CA	5.29	124.74	119.24
14	Q	3	ILE	N-CA-C	5.18	114.20	106.85
28	i	68	LEU	N-CA-C	-5.17	106.94	113.20
3	C	51	VAL	N-CA-C	5.16	115.47	107.78
13	P	20	ARG	N-CA-C	5.16	115.05	108.24
10	L	50	GLY	CA-C-N	5.15	124.95	119.28
10	L	50	GLY	C-N-CA	5.15	124.95	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	216	ASP	N-CA-C	-5.13	107.07	113.38
10	L	45	PRO	CA-C-N	5.11	125.11	119.90
10	L	45	PRO	C-N-CA	5.11	125.11	119.90
33	o	124	TYR	CA-C-N	5.11	124.72	119.56
33	o	124	TYR	C-N-CA	5.11	124.72	119.56
25	f	141	VAL	N-CA-C	5.10	117.37	108.90
26	g	373	GLU	N-CA-C	-5.09	106.58	112.89
20	a	154	LYS	N-CA-C	5.08	117.40	110.24
2	B	174	LEU	N-CA-C	5.06	117.19	111.02
21	b	30	LEU	N-CA-C	5.05	116.47	110.97
5	F	96	HIS	CA-C-N	5.04	125.32	119.47
5	F	96	HIS	C-N-CA	5.04	125.32	119.47

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	J	185	ARG	Peptide
8	J	186	LYS	Peptide
9	K	194	ARG	Peptide
20	a	336	UNK	Peptide
24	e	100	UNK	Peptide

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	20411	0	10345	381	0
2	B	1762	0	1774	75	0
3	C	1075	0	1087	45	0
4	E	2621	0	2640	98	0
5	F	990	0	1025	36	0
6	G	1721	0	1747	57	0
7	I	2498	0	2475	102	0
8	J	1067	0	1101	40	0
9	K	1001	0	1037	37	0
10	L	840	0	890	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	N	858	0	883	40	0
12	O	1448	0	1536	40	0
13	P	932	0	951	38	0
14	Q	853	0	913	41	0
15	R	784	0	813	36	0
16	T	84	0	86	10	0
17	U	734	0	745	33	0
18	V	1158	0	765	61	0
18	Y	1158	0	766	68	0
19	X	231	0	157	8	0
20	a	2296	0	2318	190	0
21	b	1101	0	1118	21	0
22	c	1367	0	1385	52	0
23	d	1467	0	1466	46	0
24	e	2016	0	2028	573	0
25	f	778	0	791	32	0
26	g	2774	0	2810	126	0
27	h	876	0	832	33	0
28	i	824	0	842	33	0
29	j	1777	0	1789	98	0
30	k	2222	0	2270	100	0
31	m	930	0	959	42	0
32	n	639	0	709	22	0
33	o	3028	0	3081	570	0
34	p	1551	0	1519	64	0
35	s	96	0	98	21	0
36	z	102	0	104	33	0
37	A	143	0	0	0	0
37	g	1	0	0	0	0
38	R	1	0	0	0	0
38	c	1	0	0	0	0
38	p	1	0	0	0	0
39	g	28	0	12	1	0
40	A	114	0	0	8	0
40	g	4	0	0	1	0
All	All	66363	0	55867	2932	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 24.

All (2932) 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)
33:o:514:UNK:CG	33:o:541:UNK:HG1	1.40	1.52
33:o:514:UNK:HG1	33:o:541:UNK:CG	1.53	1.39
24:e:267:UNK:HG2	24:e:270:UNK:CG	1.53	1.39
24:e:68:UNK:HG2	24:e:71:UNK:CG	1.52	1.38
24:e:104:UNK:HG2	24:e:107:UNK:CG	1.54	1.37
7:I:253:UNK:CG	7:I:366:ARG:HH22	1.39	1.33
24:e:391:UNK:O	24:e:394:UNK:HG3	1.31	1.31
24:e:181:UNK:HG1	24:e:210:UNK:CG	1.59	1.30
24:e:68:UNK:CG	24:e:71:UNK:HG3	1.61	1.28
20:a:322:UNK:O	20:a:326:UNK:HG3	1.27	1.27
20:a:343:UNK:O	20:a:346:UNK:HG3	1.34	1.26
20:a:312:UNK:O	20:a:316:UNK:HG3	1.29	1.26
20:a:307:HIS:O	20:a:313:UNK:HG1	1.36	1.26
33:o:538:UNK:O	33:o:542:UNK:HG3	1.31	1.25
24:e:202:UNK:O	24:e:205:UNK:HG3	1.30	1.23
20:a:346:UNK:O	20:a:349:UNK:HG3	1.37	1.23
24:e:218:UNK:O	24:e:221:UNK:HG3	1.37	1.23
33:o:485:UNK:O	33:o:489:UNK:HG3	1.40	1.21
33:o:558:UNK:CG	33:o:576:UNK:HG1	1.72	1.20
33:o:226:UNK:O	33:o:229:UNK:HG3	1.37	1.20
20:a:310:UNK:CG	20:a:313:UNK:HG2	1.72	1.19
20:a:314:UNK:O	20:a:318:UNK:HG3	1.41	1.18
20:a:340:UNK:O	20:a:343:UNK:HG3	1.41	1.18
24:e:46:UNK:HG1	24:e:77:UNK:CG	1.71	1.18
33:o:558:UNK:HG1	33:o:576:UNK:CG	1.72	1.18
24:e:357:UNK:O	24:e:361:UNK:HG3	1.41	1.17
33:o:521:UNK:HG1	33:o:534:UNK:CG	1.72	1.17
33:o:360:UNK:O	33:o:363:UNK:HG3	1.43	1.17
33:o:427:UNK:HG2	33:o:466:UNK:HG1	1.25	1.17
24:e:398:UNK:O	24:e:401:UNK:HG3	1.39	1.16
20:a:337:UNK:HG2	20:a:340:UNK:CG	1.76	1.15
33:o:190:UNK:HG1	33:o:223:UNK:HB2	1.16	1.15
20:a:323:UNK:O	20:a:327:UNK:HG3	1.42	1.15
24:e:125:UNK:O	24:e:128:UNK:HG3	1.44	1.15
18:V:55:Y5P:C2'	18:V:57:Y5P:H5	1.77	1.15
24:e:143:UNK:O	24:e:147:UNK:HG2	1.45	1.14
24:e:181:UNK:CG	24:e:210:UNK:HG1	1.77	1.14
24:e:358:UNK:O	24:e:362:UNK:HG3	1.46	1.14
24:e:63:UNK:CG	24:e:65:UNK:HG3	1.77	1.14
24:e:389:UNK:O	24:e:392:UNK:HG3	1.44	1.13
18:V:25:Y5P:H4A	18:V:26:Y5P:H4	1.26	1.13
20:a:337:UNK:O	20:a:340:UNK:HG3	1.48	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:e:165:UNK:O	24:e:169:UNK:HG3	1.48	1.13
20:a:349:UNK:O	20:a:352:UNK:HG3	1.49	1.12
24:e:93:UNK:O	24:e:96:UNK:HG3	1.49	1.12
8:J:64:THR:HG22	33:o:64:THR:O	1.49	1.12
24:e:157:UNK:O	24:e:161:UNK:HG2	1.50	1.11
24:e:46:UNK:HG1	24:e:77:UNK:HG2	1.20	1.11
24:e:70:UNK:O	24:e:73:UNK:HG3	1.52	1.10
24:e:54:UNK:O	24:e:58:UNK:HG2	1.53	1.09
24:e:104:UNK:CG	24:e:107:UNK:HG3	1.82	1.09
24:e:75:UNK:O	24:e:79:UNK:HG3	1.51	1.08
24:e:181:UNK:HG1	24:e:210:UNK:HG3	1.12	1.08
26:g:52:UNK:HG2	26:g:66:UNK:HG3	1.32	1.08
26:g:63:UNK:O	26:g:64:UNK:HG3	1.53	1.08
24:e:181:UNK:CG	24:e:210:UNK:CG	2.29	1.08
20:a:337:UNK:HG2	20:a:340:UNK:HG3	1.32	1.08
24:e:38:UNK:O	24:e:41:UNK:HG3	1.51	1.07
24:e:361:UNK:O	24:e:364:UNK:HG3	1.53	1.07
18:Y:25:Y5P:H4A	18:Y:26:Y5P:H4	1.32	1.07
24:e:200:UNK:O	24:e:204:UNK:HG3	1.55	1.07
24:e:213:UNK:O	24:e:216:UNK:HG3	1.55	1.06
24:e:225:UNK:O	24:e:229:UNK:HG3	1.55	1.06
18:Y:9:Y5P:H4A	18:Y:22:Y5P:H4A	1.33	1.06
33:o:521:UNK:HG1	33:o:534:UNK:HG1	1.30	1.06
24:e:367:UNK:O	24:e:370:UNK:HG3	1.53	1.05
24:e:73:UNK:O	24:e:76:UNK:HG3	1.55	1.05
16:T:65:UNK:HB1	24:e:51:UNK:HG1	1.35	1.05
24:e:89:UNK:O	24:e:92:UNK:HG3	1.55	1.04
24:e:120:UNK:O	24:e:124:UNK:HG3	1.57	1.04
7:I:253:UNK:HG1	7:I:366:ARG:HH22	1.21	1.04
29:j:171:ARG:HH12	34:p:191:PRO:HD2	1.20	1.04
7:I:253:UNK:CG	7:I:366:ARG:NH2	2.20	1.04
24:e:267:UNK:CG	24:e:270:UNK:HG3	1.85	1.04
24:e:294:UNK:O	24:e:297:UNK:HG3	1.57	1.04
24:e:104:UNK:CG	24:e:107:UNK:CG	2.37	1.03
36:z:698:UNK:O	36:z:701:UNK:HG3	1.56	1.03
24:e:63:UNK:HG2	24:e:65:UNK:HG3	1.04	1.03
20:a:326:UNK:O	20:a:330:UNK:HG3	1.58	1.02
26:g:54:UNK:HG1	26:g:67:UNK:HA	1.40	1.02
24:e:277:UNK:O	24:e:281:UNK:HG3	1.57	1.02
24:e:181:UNK:HG2	24:e:210:UNK:HG1	1.41	1.02
24:e:247:UNK:HG2	24:e:247:UNK:O	1.58	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:e:170:UNK:HG2	24:e:170:UNK:O	1.60	1.01
24:e:69:UNK:O	24:e:72:UNK:HG3	1.61	1.01
20:a:315:UNK:O	20:a:319:UNK:HG3	1.58	1.01
24:e:230:UNK:O	24:e:231:UNK:HG3	1.60	1.01
24:e:170:UNK:HG1	29:j:78:ARG:NH2	1.76	1.00
23:d:59:ARG:NH1	34:p:202:TRP:O	1.94	1.00
33:o:225:UNK:O	33:o:228:UNK:HG3	1.61	1.00
24:e:208:UNK:O	24:e:211:UNK:HG3	1.58	0.99
24:e:46:UNK:CG	24:e:77:UNK:CG	2.40	0.99
20:a:88:LYS:NZ	20:a:260:LEU:O	1.94	0.99
24:e:273:UNK:O	24:e:277:UNK:HG3	1.61	0.99
20:a:347:UNK:O	20:a:350:UNK:HG3	1.61	0.99
24:e:208:UNK:HG2	24:e:220:UNK:HG1	1.42	0.99
33:o:458:UNK:O	33:o:461:UNK:HG3	1.63	0.99
24:e:46:UNK:CG	24:e:77:UNK:HG2	1.90	0.99
24:e:371:UNK:O	24:e:374:UNK:HG3	1.62	0.98
33:o:338:UNK:HG1	33:o:365:UNK:HG1	1.43	0.98
24:e:63:UNK:HG2	24:e:65:UNK:CG	1.94	0.98
24:e:175:UNK:O	24:e:179:UNK:HG2	1.61	0.97
24:e:68:UNK:CG	24:e:71:UNK:CG	2.27	0.97
24:e:178:UNK:O	24:e:182:UNK:HG2	1.65	0.97
33:o:538:UNK:O	33:o:542:UNK:CG	2.11	0.97
24:e:51:UNK:O	24:e:55:UNK:HG2	1.64	0.97
24:e:134:UNK:O	24:e:135:UNK:HG3	1.64	0.97
24:e:188:UNK:O	24:e:192:UNK:HG3	1.65	0.97
24:e:208:UNK:CG	24:e:220:UNK:HG1	1.93	0.97
24:e:385:UNK:O	24:e:388:UNK:HG3	1.65	0.97
24:e:267:UNK:CG	24:e:270:UNK:CG	2.42	0.96
18:V:55:Y5P:O2'	18:V:57:Y5P:H5	1.65	0.96
33:o:392:UNK:O	33:o:395:UNK:HG3	1.66	0.96
33:o:167:UNK:O	33:o:170:UNK:HG3	1.63	0.96
24:e:218:UNK:CG	24:e:296:UNK:HG1	1.96	0.95
33:o:414:UNK:O	33:o:417:UNK:HG3	1.67	0.95
2:B:238:ASN:OD1	25:f:120:LYS:NZ	2.00	0.95
24:e:400:UNK:O	24:e:403:UNK:HG3	1.66	0.94
24:e:219:UNK:O	24:e:223:UNK:HG3	1.68	0.94
18:Y:68:Y5P:H4A	18:Y:69:Y5P:H4	1.49	0.94
24:e:394:UNK:O	24:e:397:UNK:HG3	1.65	0.94
24:e:208:UNK:HG3	24:e:211:UNK:HG1	1.45	0.94
33:o:301:UNK:O	33:o:304:UNK:HG3	1.66	0.94
26:g:205:GLU:OE2	26:g:248:ARG:NH1	2.01	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:a:330:UNK:O	20:a:334:UNK:HG3	1.68	0.94
24:e:149:UNK:O	24:e:153:UNK:HG2	1.67	0.94
24:e:222:UNK:O	24:e:225:UNK:HG3	1.68	0.93
33:o:229:UNK:O	33:o:232:UNK:HG3	1.67	0.93
20:a:322:UNK:HG3	20:a:325:UNK:CG	1.97	0.93
1:A:287:C:N3	22:c:11:ARG:NH2	2.17	0.93
20:a:310:UNK:CG	20:a:313:UNK:CG	2.47	0.93
33:o:375:UNK:O	33:o:379:UNK:HG3	1.69	0.93
33:o:521:UNK:CG	33:o:534:UNK:HG1	1.98	0.93
33:o:338:UNK:CG	33:o:365:UNK:HG1	1.97	0.93
30:k:226:TYR:CD2	36:z:706:UNK:HG1	2.04	0.93
7:I:228:ARG:HD2	17:U:85:GLN:HE21	1.31	0.92
24:e:390:UNK:O	24:e:393:UNK:HG3	1.68	0.92
18:V:55:Y5P:H2'	18:V:57:Y5P:H5	1.47	0.92
18:Y:23:Y5P:H4A	18:Y:24:Y5P:H4	1.49	0.92
18:Y:9:Y5P:C4	18:Y:22:Y5P:H4A	1.99	0.92
18:V:8:Y5P:N3	18:V:14:Y5P:H5	1.85	0.92
23:d:27:ARG:HG2	23:d:27:ARG:HH11	1.33	0.92
33:o:415:UNK:O	33:o:418:UNK:HG3	1.69	0.92
20:a:344:UNK:O	20:a:347:UNK:HG3	1.69	0.91
24:e:34:UNK:O	24:e:37:UNK:HG3	1.68	0.91
24:e:213:UNK:O	24:e:216:UNK:CG	2.19	0.91
24:e:397:UNK:O	24:e:400:UNK:HG3	1.71	0.91
24:e:104:UNK:HG2	24:e:107:UNK:HG3	0.91	0.91
33:o:82:SER:O	33:o:446:UNK:HG1	1.72	0.90
20:a:310:UNK:HG2	20:a:313:UNK:HG2	1.54	0.90
18:Y:31:Y5P:H4A	18:Y:32:Y5P:H4	1.53	0.89
18:Y:51:Y5P:H4A	18:Y:52:Y5P:H4	1.53	0.89
1:A:60:C:OP1	29:j:43:ARG:NH1	2.06	0.89
24:e:267:UNK:HG2	24:e:270:UNK:HG3	0.89	0.89
10:L:78:ARG:HG3	10:L:118:LEU:HD21	1.54	0.89
24:e:81:UNK:O	24:e:82:UNK:HG3	1.73	0.89
33:o:427:UNK:CG	33:o:466:UNK:HG1	2.03	0.89
18:Y:54:Y5P:H4A	18:Y:55:Y5P:H4A	1.55	0.88
31:m:36:ARG:NH1	31:m:91:GLU:OE1	2.06	0.88
24:e:146:UNK:O	24:e:150:UNK:HG2	1.72	0.88
24:e:196:UNK:HG2	24:e:199:UNK:HG2	1.53	0.88
24:e:355:UNK:O	24:e:359:UNK:HG3	1.72	0.88
24:e:90:UNK:O	24:e:93:UNK:HG3	1.74	0.88
33:o:538:UNK:O	33:o:550:UNK:HG1	1.73	0.87
24:e:91:UNK:O	24:e:94:UNK:HG3	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:e:196:UNK:CG	24:e:199:UNK:HG2	2.05	0.87
33:o:521:UNK:HG1	33:o:534:UNK:HG2	1.52	0.87
33:o:172:UNK:O	33:o:175:UNK:HG3	1.75	0.87
33:o:225:UNK:HG1	33:o:263:UNK:HB1	1.56	0.86
33:o:194:UNK:HA	33:o:230:UNK:HG1	1.57	0.86
20:a:328:UNK:O	20:a:331:UNK:HG3	1.75	0.86
24:e:196:UNK:CG	24:e:199:UNK:CG	2.54	0.86
24:e:232:UNK:HG2	24:e:235:UNK:CG	2.05	0.86
35:s:2361:UNK:O	35:s:2364:UNK:HG3	1.76	0.86
33:o:167:UNK:O	33:o:170:UNK:CG	2.24	0.86
33:o:82:SER:O	33:o:446:UNK:CG	2.24	0.85
18:Y:9:Y5P:H4	18:Y:22:Y5P:H5	1.58	0.85
33:o:323:UNK:O	33:o:327:UNK:HG3	1.75	0.85
27:h:323:HIS:HD2	27:h:361:LYS:HZ1	1.23	0.85
24:e:118:UNK:O	24:e:119:UNK:HG3	1.76	0.85
15:R:112:ILE:HG23	15:R:121:MET:HE1	1.59	0.84
29:j:29:ARG:NH1	29:j:104:TYR:O	2.10	0.84
12:O:171:LEU:HB3	12:O:179:PHE:HB2	1.58	0.84
30:k:226:TYR:CE2	36:z:706:UNK:HG1	2.12	0.84
33:o:427:UNK:HG2	33:o:466:UNK:CG	2.05	0.84
33:o:235:UNK:HG1	33:o:237:UNK:HB2	1.57	0.84
17:U:49:CYS:SG	17:U:50:ARG:N	2.51	0.84
24:e:267:UNK:HG2	24:e:270:UNK:HG1	1.60	0.83
18:V:54:Y5P:N3	18:V:58:Y5P:H5	1.93	0.83
24:e:105:UNK:O	24:e:108:UNK:HG3	1.78	0.83
24:e:391:UNK:O	24:e:394:UNK:CG	2.23	0.83
20:a:346:UNK:O	20:a:349:UNK:CG	2.25	0.83
24:e:268:UNK:HG3	34:p:214:SER:OG	1.77	0.83
20:a:319:UNK:HG2	20:a:320:UNK:H	1.43	0.83
1:A:566:U:O2	1:A:686:A:N6	2.11	0.83
24:e:235:UNK:O	24:e:238:UNK:HG3	1.78	0.83
24:e:63:UNK:CG	24:e:65:UNK:CG	2.53	0.83
33:o:303:UNK:HA	33:o:306:UNK:HG3	1.58	0.83
20:a:337:UNK:HG2	20:a:340:UNK:HG1	1.60	0.82
7:I:150:LEU:O	7:I:153:THR:OG1	1.96	0.82
18:V:24:Y5P:H4A	18:V:25:Y5P:H4	1.61	0.82
33:o:158:UNK:O	33:o:161:UNK:HG3	1.80	0.82
33:o:379:UNK:HA	33:o:382:UNK:HG3	1.62	0.82
13:P:93:LEU:O	20:a:174:ARG:NH1	2.12	0.82
20:a:323:UNK:HG2	20:a:324:UNK:N	1.92	0.82
24:e:232:UNK:CG	24:e:235:UNK:CG	2.58	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:o:514:UNK:HB2	33:o:537:UNK:HG3	1.61	0.82
24:e:46:UNK:CG	24:e:77:UNK:HG1	2.10	0.82
24:e:110:UNK:O	24:e:114:UNK:HG3	1.78	0.82
24:e:401:UNK:O	24:e:404:UNK:HG3	1.80	0.81
7:I:263:UNK:HG3	7:I:268:MET:O	1.81	0.81
18:V:12:Y5P:H4A	18:V:13:Y5P:H4	1.62	0.81
18:V:49:Y5P:H4A	18:V:50:Y5P:H4	1.63	0.81
20:a:310:UNK:HG3	20:a:313:UNK:CG	2.09	0.81
24:e:108:UNK:O	24:e:111:UNK:HG3	1.79	0.81
33:o:481:UNK:O	33:o:484:UNK:HG3	1.80	0.81
33:o:397:UNK:O	33:o:400:UNK:HG3	1.81	0.81
6:G:68:PHE:HB3	7:I:367:GLN:HE21	1.44	0.81
33:o:244:UNK:O	33:o:247:UNK:HG3	1.80	0.81
33:o:394:UNK:HA	33:o:397:UNK:HG3	1.62	0.81
1:A:103:G:H4'	14:Q:8:VAL:HG13	1.63	0.81
24:e:398:UNK:O	24:e:401:UNK:CG	2.28	0.81
36:z:698:UNK:O	36:z:701:UNK:CG	2.28	0.81
7:I:253:UNK:HG3	7:I:366:ARG:HH22	1.43	0.81
26:g:59:UNK:HG2	26:g:62:UNK:HB2	1.62	0.81
33:o:157:UNK:CG	33:o:177:UNK:HG1	2.11	0.81
33:o:340:UNK:O	33:o:343:UNK:HG3	1.80	0.81
33:o:346:UNK:HG1	33:o:379:UNK:HB2	1.61	0.80
1:A:630:A:H2	1:A:654:A:H61	1.29	0.80
22:c:78:PHE:HB2	22:c:86:VAL:HB	1.62	0.80
24:e:120:UNK:O	24:e:124:UNK:CG	2.28	0.80
1:A:632:A:OP1	4:E:269:ARG:NH2	2.15	0.80
3:C:125:ARG:HH21	3:C:159:PRO:HD3	1.44	0.80
5:F:65:LEU:HD21	15:R:76:LYS:HD3	1.63	0.80
18:Y:25:Y5P:H2'	18:Y:26:Y5P:H6	1.64	0.80
18:Y:28:Y5P:H4A	18:Y:29:Y5P:H4	1.61	0.80
18:Y:30:Y5P:H4A	18:Y:31:Y5P:H4	1.63	0.80
33:o:266:UNK:O	33:o:269:UNK:HG3	1.82	0.80
15:R:87:PRO:HA	15:R:126:LYS:HB2	1.61	0.80
1:A:744:C:H3'	1:A:745:C:H4'	1.64	0.80
33:o:503:UNK:HB2	33:o:513:UNK:HG2	1.62	0.80
24:e:38:UNK:O	24:e:41:UNK:CG	2.28	0.80
24:e:46:UNK:HG1	24:e:77:UNK:HG1	1.63	0.80
24:e:218:UNK:HG1	24:e:296:UNK:HG1	1.64	0.79
24:e:232:UNK:CG	24:e:235:UNK:HG1	2.11	0.79
33:o:538:UNK:HG2	33:o:550:UNK:HB2	1.64	0.79
33:o:558:UNK:HG1	33:o:576:UNK:HG1	0.84	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:a:317:UNK:HG2	20:a:318:UNK:N	1.96	0.79
33:o:497:UNK:O	33:o:500:UNK:HG3	1.81	0.79
18:Y:9:Y5P:H4	18:Y:22:Y5P:C5	2.11	0.79
24:e:213:UNK:C	24:e:216:UNK:HG3	2.12	0.79
24:e:247:UNK:O	24:e:247:UNK:CG	2.28	0.79
24:e:394:UNK:O	24:e:397:UNK:CG	2.29	0.79
18:Y:25:Y5P:C4	18:Y:26:Y5P:H4	2.12	0.79
24:e:73:UNK:O	24:e:76:UNK:CG	2.29	0.79
4:E:215:TYR:HH	21:b:2:ALA:N	1.81	0.79
18:V:25:Y5P:C4	18:V:26:Y5P:H4	2.12	0.79
20:a:330:UNK:HA	20:a:333:UNK:HG3	1.65	0.79
24:e:296:UNK:HA	24:e:299:UNK:HG3	1.63	0.79
1:A:124:A:H1'	1:A:125:U:H5	1.47	0.78
33:o:521:UNK:CB	33:o:534:UNK:HG1	2.13	0.78
26:g:99:MET:HG3	39:g:500:GDP:HN21	1.48	0.78
1:A:300:G:N7	40:A:7098:HOH:O	2.14	0.78
7:I:253:UNK:HG3	7:I:366:ARG:NH2	1.96	0.78
24:e:38:UNK:C	24:e:41:UNK:HG3	2.13	0.78
24:e:170:UNK:CG	29:j:78:ARG:NH2	2.46	0.78
24:e:243:UNK:CG	24:e:245:UNK:HG3	2.12	0.78
24:e:378:UNK:O	24:e:382:UNK:HG2	1.83	0.78
33:o:396:UNK:O	33:o:399:UNK:HG3	1.83	0.78
24:e:232:UNK:HG2	24:e:235:UNK:HG3	1.64	0.78
18:V:26:Y5P:H4A	18:V:27:Y5P:H4	1.64	0.78
33:o:411:UNK:HG1	35:s:2360:UNK:HG1	1.66	0.78
1:A:273:A:OP1	34:p:92:LYS:NZ	2.16	0.78
22:c:36:THR:H	22:c:69:ASN:HD21	1.30	0.78
24:e:174:UNK:CG	24:e:176:UNK:CG	2.62	0.78
26:g:63:UNK:O	26:g:64:UNK:CG	2.31	0.78
32:n:196:LEU:O	32:n:198:ASN:ND2	2.16	0.78
33:o:341:UNK:O	33:o:344:UNK:HG3	1.82	0.78
26:g:284:GLU:OE2	26:g:293:ARG:NH1	2.16	0.78
33:o:420:UNK:HB2	33:o:459:UNK:HG1	1.66	0.78
4:E:215:TYR:HB3	4:E:218:PHE:HD2	1.49	0.78
20:a:323:UNK:O	20:a:327:UNK:CG	2.30	0.77
24:e:174:UNK:HG2	24:e:176:UNK:CG	2.14	0.77
24:e:218:UNK:C	24:e:221:UNK:HG3	2.13	0.77
18:Y:8:Y5P:N3	18:Y:14:Y5P:H5	1.99	0.77
22:c:125:HIS:HD2	22:c:127:ALA:H	1.31	0.77
33:o:336:UNK:HB1	33:o:372:UNK:HG1	1.66	0.77
24:e:395:UNK:HA	24:e:398:UNK:HG3	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:A:OP1	11:N:33:LYS:NZ	2.16	0.77
11:N:60:ASN:O	11:N:68:GLN:NE2	2.17	0.77
36:z:703:UNK:O	36:z:707:UNK:HG2	1.83	0.77
18:Y:9:Y5P:C4	18:Y:22:Y5P:C4	2.63	0.77
22:c:125:HIS:CD2	22:c:127:ALA:H	2.03	0.77
33:o:476:UNK:HB1	33:o:506:UNK:HG1	1.65	0.77
20:a:325:UNK:O	20:a:329:UNK:HG3	1.86	0.76
18:Y:25:Y5P:H4A	18:Y:26:Y5P:C4	2.13	0.76
18:Y:6:Y5P:H4A	18:Y:7:Y5P:H4	1.67	0.76
33:o:270:UNK:O	33:o:273:UNK:HG3	1.84	0.76
24:e:112:UNK:HA	24:e:115:UNK:HG3	1.65	0.76
26:g:68:UNK:HG2	26:g:96:ALA:O	1.86	0.76
24:e:299:UNK:O	24:e:303:UNK:HG3	1.85	0.76
18:V:9:Y5P:O2'	18:V:10:Y5P:C5	2.34	0.76
20:a:322:UNK:HG3	20:a:325:UNK:HG3	1.67	0.76
24:e:170:UNK:O	24:e:170:UNK:CG	2.32	0.76
33:o:339:UNK:O	33:o:342:UNK:HG3	1.86	0.76
24:e:215:UNK:O	24:e:219:UNK:HG3	1.87	0.75
20:a:348:UNK:O	20:a:351:UNK:HG3	1.86	0.75
24:e:71:UNK:HA	24:e:74:UNK:HG3	1.69	0.75
18:Y:14:Y5P:H4A	18:Y:15:Y5P:H4	1.68	0.75
2:B:97:ARG:HH22	21:b:60:VAL:HB	1.51	0.75
8:J:123:SER:O	11:N:108:ARG:NH2	2.19	0.75
24:e:127:UNK:O	24:e:131:UNK:HG3	1.87	0.75
24:e:52:UNK:O	24:e:56:UNK:HG2	1.86	0.75
24:e:104:UNK:CG	24:e:107:UNK:HG1	2.17	0.75
24:e:211:UNK:HB1	24:e:216:UNK:HG2	1.68	0.75
33:o:486:UNK:O	33:o:490:UNK:HG3	1.87	0.75
12:O:129:ARG:HB2	12:O:167:MET:HE1	1.66	0.75
20:a:312:UNK:O	20:a:316:UNK:CG	2.24	0.75
24:e:386:UNK:O	24:e:389:UNK:HG3	1.87	0.75
26:g:275:ARG:HE	26:g:281:ILE:HG22	1.51	0.75
21:b:28:LYS:HG3	21:b:32:LEU:HD23	1.67	0.75
24:e:221:UNK:O	24:e:224:UNK:HG3	1.87	0.75
26:g:259:VAL:HB	26:g:305:ILE:HG22	1.68	0.75
33:o:206:UNK:HA	33:o:209:UNK:HG3	1.67	0.75
40:A:7150:HOH:O	18:V:30:Y5P:H4A	1.86	0.75
4:E:160:ARG:HD2	4:E:165:GLN:HE22	1.49	0.75
24:e:224:UNK:O	24:e:227:UNK:HG3	1.85	0.75
24:e:387:UNK:O	24:e:391:UNK:HG3	1.87	0.75
20:a:346:UNK:C	20:a:349:UNK:HG3	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:e:198:UNK:O	24:e:202:UNK:HG2	1.87	0.74
33:o:318:UNK:HA	33:o:321:UNK:HG3	1.68	0.74
34:p:59:LEU:HD13	34:p:121:LYS:HB2	1.69	0.74
18:V:23:Y5P:H4A	18:V:24:Y5P:H4	1.66	0.74
24:e:248:UNK:HA	24:e:251:UNK:HG3	1.70	0.74
34:p:108:CYS:SG	34:p:146:GLN:HG3	2.27	0.74
33:o:243:UNK:HA	33:o:246:UNK:HG3	1.69	0.74
24:e:84:UNK:HG2	24:e:86:UNK:HG3	1.68	0.74
24:e:142:UNK:O	24:e:146:UNK:HG2	1.88	0.74
24:e:202:UNK:O	24:e:205:UNK:CG	2.23	0.74
24:e:402:UNK:O	24:e:406:UNK:HG3	1.88	0.74
26:g:57:UNK:CG	26:g:142:HIS:NE2	2.51	0.74
33:o:88:VAL:O	33:o:110:LYS:NZ	2.20	0.74
1:A:881:A:N3	24:e:66:UNK:HG1	2.02	0.74
24:e:69:UNK:C	24:e:72:UNK:HG3	2.18	0.74
28:i:13:ARG:NH2	36:z:692:UNK:HG2	2.00	0.74
1:A:249:C:N4	10:L:117:ASP:OD1	2.21	0.73
5:F:105:CYS:HB3	15:R:69:CYS:SG	2.28	0.73
1:A:343:U:OP2	9:K:96:ASN:ND2	2.21	0.73
33:o:360:UNK:C	33:o:363:UNK:HG3	2.18	0.73
24:e:268:UNK:CG	34:p:214:SER:OG	2.35	0.73
33:o:338:UNK:HA	33:o:341:UNK:HG3	1.70	0.73
1:A:124:A:HI'	1:A:125:U:C5	2.24	0.73
24:e:114:UNK:HA	24:e:117:UNK:HG3	1.69	0.73
24:e:218:UNK:O	24:e:221:UNK:CG	2.28	0.73
33:o:514:UNK:CG	33:o:541:UNK:CG	2.32	0.73
14:Q:95:VAL:HG11	23:d:120:ARG:HH12	1.53	0.73
24:e:72:UNK:O	24:e:75:UNK:HG3	1.88	0.73
33:o:476:UNK:HB2	33:o:513:UNK:HG1	1.68	0.73
24:e:130:UNK:O	24:e:134:UNK:HG2	1.89	0.73
14:Q:95:VAL:HG11	23:d:120:ARG:NH1	2.04	0.73
33:o:225:UNK:HB1	33:o:248:UNK:HG1	1.70	0.73
8:J:161:GLN:HG2	8:J:170:MET:HE1	1.71	0.72
24:e:67:UNK:O	24:e:100:UNK:HG1	1.88	0.72
24:e:357:UNK:O	24:e:361:UNK:CG	2.31	0.72
24:e:371:UNK:O	24:e:374:UNK:CG	2.35	0.72
33:o:204:UNK:HA	33:o:207:UNK:HG3	1.71	0.72
2:B:81:ARG:HA	25:f:84:MET:HE1	1.71	0.72
18:Y:27:Y5P:O5'	18:Y:27:Y5P:H6	1.87	0.72
20:a:324:UNK:O	20:a:328:UNK:HG3	1.88	0.72
33:o:167:UNK:C	33:o:170:UNK:HG3	2.17	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:o:501:UNK:O	33:o:504:UNK:HG3	1.90	0.72
24:e:273:UNK:O	24:e:277:UNK:CG	2.36	0.72
24:e:273:UNK:CG	24:e:276:UNK:HG3	2.18	0.72
24:e:176:UNK:O	24:e:180:UNK:HG2	1.88	0.72
24:e:218:UNK:HG2	24:e:296:UNK:HG1	1.72	0.72
33:o:241:UNK:HA	33:o:244:UNK:HG3	1.70	0.72
24:e:385:UNK:O	24:e:388:UNK:CG	2.38	0.72
33:o:374:UNK:O	33:o:378:UNK:HG3	1.89	0.72
9:K:68:ILE:HG22	9:K:70:GLY:H	1.54	0.72
15:R:95:ARG:HH12	15:R:102:GLY:HA2	1.55	0.72
33:o:514:UNK:O	33:o:517:UNK:HG3	1.90	0.72
1:A:177:U:H2'	1:A:178:G:H8	1.55	0.72
5:F:6:LEU:HB3	5:F:66:VAL:HB	1.72	0.72
13:P:67:ALA:HB1	20:a:160:ILE:HD12	1.70	0.72
18:V:43:Y5P:H2'	18:V:44:Y5P:H6	1.71	0.72
24:e:34:UNK:O	24:e:37:UNK:CG	2.37	0.72
26:g:57:UNK:HG2	26:g:142:HIS:NE2	2.05	0.72
26:g:386:ASN:HD22	26:g:389:GLN:HB2	1.54	0.72
28:i:13:ARG:NH1	36:z:692:UNK:HG2	2.05	0.72
4:E:203:LEU:HD13	4:E:222:ILE:HD11	1.72	0.71
25:f:160:ASP:N	25:f:160:ASP:OD1	2.23	0.71
26:g:120:ALA:HB3	26:g:298:ASN:HA	1.72	0.71
4:E:206:PRO:HA	4:E:272:LYS:HD2	1.71	0.71
20:a:322:UNK:O	20:a:326:UNK:CG	2.22	0.71
18:V:62:Y5P:H4A	18:V:63:Y5P:H4	1.71	0.71
20:a:311:UNK:HG2	20:a:312:UNK:N	2.03	0.71
24:e:70:UNK:O	24:e:73:UNK:CG	2.34	0.71
20:a:278:LYS:HE2	20:a:307:HIS:HE1	1.54	0.71
20:a:337:UNK:O	20:a:340:UNK:CG	2.35	0.71
20:a:341:UNK:HG2	20:a:342:UNK:N	2.05	0.71
1:A:630:A:H2	1:A:654:A:N6	1.87	0.71
1:A:759:U:H2'	1:A:760:A:H8	1.56	0.71
24:e:197:UNK:HG2	24:e:230:UNK:HG1	1.72	0.71
27:h:351:SER:OG	30:k:213:ARG:NH1	2.22	0.71
33:o:161:UNK:HB2	33:o:170:UNK:HB2	1.71	0.71
33:o:174:UNK:HA	33:o:177:UNK:HG3	1.71	0.71
33:o:546:UNK:O	33:o:550:UNK:HG3	1.90	0.71
1:A:724:U:OP1	6:G:195:LYS:NZ	2.24	0.71
8:J:89:ASP:OD1	8:J:141:ARG:NH2	2.22	0.71
26:g:211:LYS:HE3	26:g:212:ARG:HE	1.55	0.71
33:o:267:UNK:O	33:o:271:UNK:HG3	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:e:68:UNK:CG	24:e:71:UNK:HG1	2.20	0.71
1:A:887:U:OP2	29:j:101:ARG:NH1	2.24	0.70
24:e:74:UNK:HA	24:e:77:UNK:HG3	1.72	0.70
24:e:362:UNK:O	24:e:365:UNK:HG3	1.91	0.70
27:h:323:HIS:HD2	27:h:361:LYS:NZ	1.88	0.70
4:E:412:LYS:HG2	4:E:417:MET:HB2	1.74	0.70
14:Q:14:VAL:H	22:c:63:GLN:HE22	1.39	0.70
24:e:35:UNK:O	24:e:38:UNK:HG3	1.91	0.70
24:e:90:UNK:HG2	24:e:91:UNK:N	2.05	0.70
24:e:106:UNK:HB1	24:e:383:UNK:HB1	1.72	0.70
33:o:459:UNK:HA	33:o:462:UNK:HG3	1.73	0.70
24:e:355:UNK:O	24:e:358:UNK:CG	2.39	0.70
28:i:13:ARG:CZ	36:z:692:UNK:HG2	2.21	0.70
24:e:184:UNK:O	24:e:188:UNK:HG2	1.92	0.70
26:g:265:ASN:OD1	26:g:265:ASN:N	2.25	0.70
29:j:171:ARG:NH1	34:p:191:PRO:HD2	2.00	0.70
24:e:73:UNK:C	24:e:76:UNK:HG3	2.20	0.70
24:e:131:UNK:HB2	24:e:136:UNK:HB2	1.74	0.70
26:g:264:VAL:HG21	26:g:307:LEU:HB3	1.72	0.70
24:e:84:UNK:CG	24:e:86:UNK:HG3	2.21	0.70
24:e:196:UNK:HG2	24:e:199:UNK:CG	2.21	0.70
24:e:300:UNK:O	24:e:304:UNK:HG3	1.91	0.70
33:o:392:UNK:O	33:o:395:UNK:CG	2.39	0.70
26:g:52:UNK:HG2	26:g:66:UNK:CG	2.18	0.70
24:e:170:UNK:CG	29:j:78:ARG:HH22	2.04	0.70
29:j:11:ILE:HG23	29:j:14:LEU:HD23	1.73	0.70
33:o:267:UNK:HA	33:o:270:UNK:HG3	1.74	0.70
33:o:427:UNK:CG	33:o:466:UNK:CG	2.68	0.70
2:B:219:VAL:HG22	2:B:233:TYR:HB2	1.73	0.69
20:a:94:LEU:HB2	34:p:166:HIS:HB2	1.74	0.69
24:e:134:UNK:O	24:e:135:UNK:CG	2.39	0.69
1:A:54:A:OP2	23:d:27:ARG:NH1	2.23	0.69
1:A:96:U:H4'	13:P:17:LEU:HD13	1.72	0.69
18:V:54:Y5P:N3	18:V:58:Y5P:C5	2.55	0.69
20:a:300:VAL:HG21	20:a:330:UNK:HG1	1.72	0.69
1:A:744:C:HO2'	1:A:746:A:HO2'	1.38	0.69
24:e:273:UNK:HG3	24:e:276:UNK:HG3	1.74	0.69
33:o:295:UNK:HA	33:o:298:UNK:HG3	1.74	0.69
1:A:58:U:N3	29:j:57:ASP:OD2	2.25	0.69
3:C:163:VAL:HG21	3:C:167:ILE:HD12	1.73	0.69
5:F:3:ARG:NH1	5:F:70:ALA:O	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:e:232:UNK:HG1	24:e:235:UNK:HG1	1.74	0.69
33:o:507:UNK:HG1	33:o:541:UNK:HB1	1.73	0.69
1:A:697:U:H5''	1:A:698:A:C8	2.28	0.69
4:E:140:LEU:HD21	4:E:160:ARG:HE	1.58	0.69
1:A:954:U:H4'	1:A:955:G:H5'	1.73	0.69
4:E:149:MET:HG2	4:E:154:VAL:H	1.57	0.69
8:J:74:LYS:HB2	8:J:177:LEU:HD21	1.75	0.69
20:a:315:UNK:HG2	20:a:316:UNK:N	2.06	0.69
20:a:343:UNK:HG2	20:a:344:UNK:N	2.06	0.69
24:e:139:UNK:HG3	24:e:140:UNK:N	2.07	0.69
24:e:367:UNK:O	24:e:370:UNK:CG	2.36	0.69
2:B:218:THR:HG22	2:B:231:ILE:HG23	1.73	0.69
18:Y:8:Y5P:N3	18:Y:14:Y5P:C5	2.56	0.69
24:e:398:UNK:C	24:e:401:UNK:HG3	2.23	0.69
30:k:246:THR:HG22	30:k:248:ALA:H	1.59	0.69
33:o:191:UNK:HA	33:o:194:UNK:HG3	1.75	0.69
18:V:59:Y5P:H4A	18:V:60:Y5P:H4	1.74	0.68
24:e:77:UNK:O	24:e:80:UNK:HG3	1.92	0.68
30:k:166:ARG:NE	33:o:134:GLU:OE2	2.22	0.68
1:A:798:A:H2'	1:A:799:A:H8	1.58	0.68
5:F:67:ASP:OD1	5:F:67:ASP:N	2.26	0.68
24:e:75:UNK:O	24:e:78:UNK:HG3	1.92	0.68
28:i:61:LEU:HB2	33:o:127:TYR:HD2	1.56	0.68
33:o:274:UNK:HG2	33:o:275:UNK:N	2.09	0.68
33:o:504:UNK:HA	33:o:537:UNK:HG2	1.75	0.68
33:o:656:UNK:HB1	33:o:674:UNK:HG1	1.73	0.68
17:U:68:MET:HE3	31:m:33:VAL:HG23	1.74	0.68
18:V:54:Y5P:H4A	18:V:55:Y5P:H4	1.75	0.68
24:e:33:UNK:O	24:e:36:UNK:HG3	1.93	0.68
24:e:113:UNK:O	24:e:116:UNK:HG3	1.92	0.68
18:V:30:Y5P:H4A	18:V:31:Y5P:H4	1.75	0.68
24:e:361:UNK:O	24:e:364:UNK:CG	2.35	0.68
1:A:223:U:O2'	1:A:224:U:OP1	2.10	0.68
33:o:322:UNK:HA	33:o:325:UNK:HG3	1.76	0.68
24:e:197:UNK:CG	24:e:230:UNK:HG1	2.24	0.68
24:e:391:UNK:C	24:e:394:UNK:HG3	2.20	0.68
33:o:225:UNK:CG	33:o:263:UNK:HB1	2.23	0.68
20:a:311:UNK:O	20:a:315:UNK:HG3	1.94	0.68
24:e:77:UNK:C	24:e:80:UNK:HG3	2.23	0.68
24:e:208:UNK:HG3	24:e:211:UNK:CG	2.22	0.68
24:e:267:UNK:CG	24:e:270:UNK:HG1	2.21	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:o:194:UNK:CA	33:o:230:UNK:HG1	2.24	0.68
24:e:56:UNK:O	24:e:60:UNK:HG2	1.94	0.68
24:e:207:UNK:CG	24:e:219:UNK:HG2	2.24	0.68
34:p:120:VAL:HG13	34:p:163:LEU:HD12	1.76	0.68
1:A:506:G:H5''	32:n:144:ARG:HH22	1.58	0.67
16:T:66:UNK:HG3	16:T:66:UNK:O	1.93	0.67
20:a:309:UNK:HG2	20:a:309:UNK:O	1.92	0.67
29:j:171:ARG:HG3	29:j:189:PRO:HG3	1.76	0.67
33:o:239:UNK:HA	33:o:242:UNK:HG3	1.76	0.67
33:o:670:UNK:HA	33:o:673:UNK:HG3	1.75	0.67
33:o:300:UNK:HA	33:o:303:UNK:HG3	1.76	0.67
1:A:257:U:H4'	1:A:258:C:H5'	1.76	0.67
1:A:646:C:H4'	1:A:647:A:H5'	1.77	0.67
1:A:707:A:H3'	1:A:708:A:H5''	1.77	0.67
2:B:114:ILE:HG21	25:f:85:LEU:HD11	1.76	0.67
2:B:153:LEU:HD11	2:B:246:ARG:HG2	1.75	0.67
24:e:243:UNK:HG2	24:e:245:UNK:HG3	1.75	0.67
33:o:666:UNK:O	33:o:670:UNK:HG3	1.95	0.67
4:E:197:THR:HG22	4:E:199:GLY:H	1.59	0.67
20:a:316:UNK:HB2	20:a:329:UNK:HG1	1.75	0.67
24:e:174:UNK:HG2	24:e:176:UNK:HG2	1.75	0.67
6:G:153:GLU:HG3	6:G:179:ARG:HB3	1.76	0.67
24:e:355:UNK:O	24:e:358:UNK:HG3	1.93	0.67
33:o:480:UNK:O	33:o:483:UNK:HG3	1.95	0.67
13:P:29:ARG:NH2	22:c:140:MET:O	2.27	0.67
24:e:174:UNK:CG	24:e:176:UNK:HG2	2.23	0.67
27:h:379:LEU:HB3	27:h:386:LEU:HB2	1.77	0.67
35:s:2362:UNK:HA	35:s:2365:UNK:HG3	1.76	0.67
4:E:141:TRP:H	4:E:145:ASN:HD22	1.42	0.67
24:e:273:UNK:HG3	24:e:276:UNK:CG	2.24	0.67
33:o:189:UNK:HA	33:o:192:UNK:HG3	1.76	0.67
24:e:218:UNK:HB1	24:e:256:UNK:HG1	1.75	0.67
24:e:255:UNK:HA	24:e:258:UNK:HG3	1.76	0.67
27:h:309:ASN:O	30:k:166:ARG:NH1	2.26	0.67
33:o:242:UNK:O	33:o:245:UNK:HG3	1.95	0.67
33:o:358:UNK:O	33:o:362:UNK:HG3	1.95	0.67
2:B:203:GLU:HG3	31:m:114:LYS:HZ1	1.59	0.66
20:a:310:UNK:O	20:a:314:UNK:HG3	1.95	0.66
24:e:294:UNK:O	24:e:297:UNK:CG	2.40	0.66
26:g:52:UNK:HG2	26:g:66:UNK:N	2.11	0.66
29:j:178:ARG:NH2	29:j:187:GLU:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:o:404:UNK:HG2	33:o:405:UNK:N	2.08	0.66
35:s:2370:UNK:HA	35:s:2373:UNK:HG3	1.77	0.66
18:V:55:Y5P:O2'	18:V:57:Y5P:C5	2.41	0.66
24:e:269:UNK:HG1	34:p:211:ARG:HA	1.78	0.66
33:o:316:UNK:O	33:o:319:UNK:HG3	1.95	0.66
6:G:78:PRO:HG2	6:G:81:LYS:HB2	1.77	0.66
18:Y:31:Y5P:H4A	18:Y:32:Y5P:C4	2.23	0.66
24:e:222:UNK:HG1	24:e:299:UNK:CG	2.25	0.66
26:g:133:LYS:NZ	40:g:503:HOH:O	2.27	0.66
33:o:398:UNK:HA	33:o:401:UNK:HG3	1.76	0.66
33:o:420:UNK:CG	33:o:459:UNK:HG1	2.25	0.66
33:o:602:UNK:O	33:o:605:UNK:HG3	1.94	0.66
7:I:253:UNK:HG1	7:I:366:ARG:NH2	2.01	0.66
12:O:130:ILE:HG12	12:O:167:MET:HE2	1.76	0.66
14:Q:33:LEU:HB2	22:c:56:GLN:HE21	1.61	0.66
14:Q:96:THR:HB	14:Q:98:LYS:HE2	1.78	0.66
15:R:133:ASP:HB3	15:R:134:PRO:HD2	1.77	0.66
24:e:174:UNK:CG	24:e:176:UNK:HG3	2.25	0.66
20:a:96:GLU:HA	34:p:131:THR:HG23	1.77	0.66
24:e:287:UNK:O	24:e:290:UNK:HG3	1.96	0.66
25:f:150:LEU:HD21	25:f:167:ASP:HB2	1.78	0.66
9:K:64:ILE:HG22	9:K:66:PRO:HD2	1.76	0.66
18:V:2:Y5P:H4A	18:V:3:Y5P:H4	1.77	0.66
24:e:108:UNK:HG2	24:e:109:UNK:N	2.10	0.66
24:e:279:UNK:HG2	24:e:280:UNK:N	2.09	0.66
24:e:285:UNK:HA	24:e:288:UNK:HG3	1.77	0.66
24:e:203:UNK:HA	24:e:206:UNK:HG3	1.78	0.66
24:e:367:UNK:C	24:e:370:UNK:HG3	2.24	0.66
26:g:57:UNK:CG	26:g:142:HIS:CE1	2.79	0.66
33:o:392:UNK:C	33:o:395:UNK:HG3	2.24	0.66
3:C:128:PRO:HD2	3:C:131:LYS:HD2	1.78	0.66
20:a:193:GLN:HG3	20:a:203:ILE:HG12	1.77	0.66
20:a:198:ARG:NH2	34:p:171:GLU:O	2.29	0.66
23:d:68:ARG:HH11	29:j:198:ILE:HG12	1.61	0.66
24:e:68:UNK:HG2	24:e:71:UNK:HG3	0.73	0.66
33:o:433:UNK:HA	33:o:436:UNK:HG3	1.78	0.66
34:p:126:PHE:HE1	34:p:140:THR:HG21	1.60	0.66
33:o:460:UNK:HA	33:o:463:UNK:HG3	1.78	0.66
1:A:647:A:H3'	1:A:648:A:C5'	2.26	0.66
24:e:187:UNK:O	24:e:190:UNK:HG3	1.96	0.66
33:o:245:UNK:HA	33:o:248:UNK:HG3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:115:ILE:HG12	8:J:137:ARG:HG2	1.78	0.65
33:o:420:UNK:CB	33:o:459:UNK:HG1	2.25	0.65
33:o:539:UNK:HG2	33:o:583:UNK:HG1	1.76	0.65
35:s:2365:UNK:O	35:s:2368:UNK:HG3	1.96	0.65
24:e:134:UNK:C	24:e:135:UNK:HG3	2.26	0.65
33:o:439:UNK:O	33:o:442:UNK:HG3	1.95	0.65
1:A:826:C:H2'	1:A:827:A:H8	1.61	0.65
1:A:202:A:H5'	13:P:102:MET:HE3	1.78	0.65
1:A:317:A:H2	1:A:318:C:C5	2.15	0.65
18:V:8:Y5P:C4	18:V:14:Y5P:H5	2.27	0.65
18:V:25:Y5P:H4A	18:V:26:Y5P:C4	2.16	0.65
20:a:324:UNK:HG2	20:a:325:UNK:N	2.10	0.65
24:e:222:UNK:HG1	24:e:299:UNK:HG2	1.77	0.65
33:o:336:UNK:O	33:o:340:UNK:HG3	1.96	0.65
33:o:440:UNK:O	33:o:444:UNK:HG3	1.96	0.65
1:A:59:C:O2'	29:j:43:ARG:NH2	2.29	0.65
24:e:105:UNK:C	24:e:108:UNK:HG3	2.26	0.65
26:g:137:LEU:HD11	26:g:260:ALA:HB1	1.77	0.65
1:A:672:A:H2	11:N:127:MET:HE3	1.62	0.65
2:B:70:ASP:O	2:B:73:ASN:N	2.22	0.65
26:g:178:ASP:N	26:g:178:ASP:OD1	2.27	0.65
33:o:278:UNK:O	33:o:282:UNK:HG3	1.96	0.65
33:o:558:UNK:CB	33:o:576:UNK:HG1	2.27	0.65
7:I:290:GLY:HA2	7:I:328:ASP:HB2	1.77	0.65
24:e:58:UNK:O	24:e:62:UNK:HG3	1.96	0.65
24:e:200:UNK:O	24:e:204:UNK:CG	2.41	0.65
24:e:358:UNK:HG2	24:e:359:UNK:N	2.12	0.65
24:e:389:UNK:C	24:e:392:UNK:HG3	2.25	0.65
28:i:13:ARG:HH22	36:z:692:UNK:HG2	1.62	0.65
1:A:270:C:OP1	34:p:80:ASN:ND2	2.29	0.65
13:P:17:LEU:HD23	13:P:81:ALA:HB2	1.79	0.65
20:a:322:UNK:CG	20:a:325:UNK:HG3	2.25	0.65
24:e:123:UNK:O	24:e:127:UNK:HG3	1.97	0.65
24:e:230:UNK:O	24:e:230:UNK:HG2	1.95	0.65
24:e:379:UNK:O	24:e:383:UNK:HG2	1.95	0.65
33:o:514:UNK:HG2	33:o:541:UNK:HG1	1.68	0.65
1:A:316:C:H4'	1:A:317:A:OP2	1.95	0.64
20:a:340:UNK:O	20:a:343:UNK:CG	2.33	0.64
24:e:48:UNK:HG1	24:e:74:UNK:O	1.97	0.64
36:z:699:UNK:HG2	36:z:700:UNK:N	2.12	0.64
6:G:155:VAL:H	6:G:227:HIS:HE1	1.42	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:104:ILE:HG23	8:J:148:LEU:HD21	1.79	0.64
20:a:329:UNK:O	20:a:333:UNK:HG3	1.98	0.64
24:e:390:UNK:C	24:e:393:UNK:HG3	2.27	0.64
26:g:63:UNK:C	26:g:64:UNK:HG3	2.26	0.64
33:o:427:UNK:HG1	33:o:463:UNK:HA	1.79	0.64
18:Y:51:Y5P:H4A	18:Y:52:Y5P:C4	2.27	0.64
24:e:108:UNK:O	24:e:111:UNK:CG	2.45	0.64
15:R:130:TYR:OH	23:d:188:ASN:ND2	2.30	0.64
20:a:174:ARG:HH11	20:a:174:ARG:HG3	1.62	0.64
24:e:390:UNK:HA	24:e:393:UNK:HG3	1.80	0.64
33:o:265:UNK:HA	33:o:268:UNK:HG3	1.78	0.64
5:F:15:ARG:NH2	23:d:178:GLU:OE2	2.29	0.64
20:a:316:UNK:HB2	20:a:329:UNK:CG	2.28	0.64
20:a:334:UNK:O	20:a:334:UNK:HG2	1.96	0.64
31:m:17:ARG:HD3	31:m:18:ARG:H	1.63	0.64
33:o:321:UNK:HA	33:o:324:UNK:HG3	1.80	0.64
33:o:415:UNK:C	33:o:418:UNK:HG3	2.27	0.64
1:A:499:C:O2	40:A:7194:HOH:O	2.12	0.64
26:g:247:LYS:HB2	26:g:295:MET:HE1	1.80	0.64
1:A:285:C:HO2'	1:A:488:A:H2	1.44	0.64
1:A:356:A:H2'	1:A:357:G:H8	1.63	0.64
6:G:200:LEU:HB3	6:G:202:PRO:HD2	1.80	0.64
33:o:202:UNK:HA	33:o:205:UNK:HG3	1.79	0.64
33:o:340:UNK:C	33:o:343:UNK:HG3	2.27	0.64
33:o:343:UNK:HA	33:o:379:UNK:HG1	1.80	0.64
11:N:117:HIS:HB2	11:N:119:GLN:HG3	1.80	0.64
24:e:120:UNK:HG1	24:e:123:UNK:HG1	1.80	0.64
26:g:215:THR:HG23	26:g:219:ARG:HG3	1.80	0.64
8:J:151:SER:HB2	30:k:133:THR:HG22	1.80	0.64
24:e:224:UNK:C	24:e:227:UNK:HG3	2.28	0.64
33:o:193:UNK:HA	33:o:196:UNK:HG3	1.80	0.64
20:a:344:UNK:C	20:a:347:UNK:HG3	2.28	0.64
20:a:347:UNK:HG2	20:a:348:UNK:N	2.11	0.64
29:j:95:TRP:HE3	29:j:118:LEU:HD13	1.63	0.64
33:o:206:UNK:O	33:o:210:UNK:HG3	1.98	0.64
27:h:309:ASN:ND2	30:k:157:ASP:OD1	2.31	0.63
20:a:350:UNK:O	20:a:353:UNK:HG3	1.99	0.63
24:e:354:UNK:HG2	24:e:357:UNK:HG3	1.79	0.63
26:g:173:ASN:O	26:g:176:ARG:NH1	2.31	0.63
33:o:535:UNK:HA	33:o:538:UNK:HG3	1.79	0.63
24:e:120:UNK:CG	24:e:123:UNK:CG	2.76	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:e:230:UNK:C	24:e:231:UNK:HG3	2.28	0.63
20:a:317:UNK:CG	20:a:318:UNK:N	2.61	0.63
22:c:139:CYS:HB3	22:c:141:CYS:SG	2.38	0.63
24:e:92:UNK:CG	24:e:93:UNK:N	2.61	0.63
33:o:503:UNK:HA	33:o:506:UNK:HG3	1.79	0.63
2:B:228:PRO:HA	2:B:231:ILE:HD12	1.79	0.63
24:e:399:UNK:HG2	24:e:400:UNK:N	2.11	0.63
33:o:271:UNK:O	33:o:274:UNK:HG3	1.99	0.63
33:o:280:UNK:HA	33:o:283:UNK:HG3	1.81	0.63
33:o:485:UNK:O	33:o:489:UNK:CG	2.33	0.63
33:o:339:UNK:HG2	33:o:376:UNK:HB1	1.79	0.63
33:o:550:UNK:HA	33:o:553:UNK:HG3	1.79	0.63
33:o:555:UNK:HA	33:o:558:UNK:HG3	1.81	0.63
36:z:693:UNK:HG2	36:z:693:UNK:O	1.98	0.63
1:A:232:G:H5'	4:E:196:ASN:HD22	1.62	0.63
40:A:7154:HOH:O	18:V:29:Y5P:H4A	1.99	0.63
24:e:170:UNK:HG1	29:j:78:ARG:HH22	1.55	0.63
24:e:174:UNK:HG2	24:e:176:UNK:HG3	1.79	0.63
24:e:175:UNK:HG1	24:e:368:UNK:HG3	1.79	0.63
33:o:194:UNK:CB	33:o:230:UNK:HG1	2.28	0.63
2:B:119:GLN:O	2:B:123:HIS:ND1	2.30	0.63
3:C:53:TYR:HB2	30:k:99:MET:HE1	1.81	0.63
24:e:34:UNK:C	24:e:37:UNK:HG3	2.28	0.63
24:e:306:UNK:O	24:e:309:UNK:HG3	1.98	0.63
33:o:224:UNK:HA	33:o:227:UNK:HG3	1.80	0.63
24:e:125:UNK:C	24:e:128:UNK:HG3	2.29	0.62
24:e:166:UNK:O	24:e:171:UNK:HG3	1.99	0.62
24:e:221:UNK:C	24:e:224:UNK:HG3	2.29	0.62
33:o:157:UNK:HG1	33:o:177:UNK:HB1	1.80	0.62
23:d:27:ARG:HG2	23:d:27:ARG:NH1	2.04	0.62
33:o:411:UNK:HA	33:o:414:UNK:HG3	1.80	0.62
24:e:174:UNK:HG1	24:e:176:UNK:CG	2.28	0.62
24:e:361:UNK:C	24:e:364:UNK:HG3	2.28	0.62
33:o:580:UNK:HA	33:o:583:UNK:HG3	1.79	0.62
1:A:644:A:O2'	1:A:645:A:O5'	2.17	0.62
2:B:168:ARG:HG3	7:I:159:TYR:CZ	2.35	0.62
3:C:72:HIS:HD2	3:C:74:GLY:H	1.47	0.62
24:e:109:UNK:HA	24:e:112:UNK:HG3	1.82	0.62
33:o:504:UNK:CA	33:o:537:UNK:HG2	2.29	0.62
1:A:136:C:O2	12:O:198:ARG:NH2	2.32	0.62
16:T:55:UNK:O	16:T:55:UNK:HG2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:e:248:UNK:HA	24:e:251:UNK:CG	2.29	0.62
33:o:158:UNK:C	33:o:161:UNK:HG3	2.29	0.62
33:o:318:UNK:O	33:o:322:UNK:HG3	1.99	0.62
1:A:4:C:C4	4:E:427:ARG:HD3	2.35	0.62
3:C:100:PHE:HB3	3:C:103:CYS:SG	2.39	0.62
15:R:125:TYR:HE2	17:U:4:HIS:HB3	1.65	0.62
18:V:25:Y5P:H2'	18:V:26:Y5P:H6	1.82	0.62
33:o:197:UNK:HG1	33:o:230:UNK:HG2	1.81	0.62
24:e:48:UNK:HB2	24:e:53:UNK:CG	2.28	0.62
33:o:284:UNK:HA	33:o:287:UNK:HG3	1.81	0.62
22:c:51:ASN:ND2	22:c:95:ASN:OD1	2.33	0.62
24:e:232:UNK:CG	24:e:235:UNK:HG3	2.29	0.62
35:s:2366:UNK:HA	35:s:2369:UNK:HG3	1.81	0.62
9:K:178:THR:HB	17:U:11:THR:HG23	1.80	0.62
14:Q:69:LEU:HD12	14:Q:70:PRO:HD2	1.81	0.62
16:T:65:UNK:HB1	24:e:51:UNK:CG	2.20	0.62
24:e:208:UNK:HG2	24:e:220:UNK:CG	2.24	0.62
24:e:387:UNK:HA	24:e:390:UNK:HG3	1.81	0.62
33:o:514:UNK:HG1	33:o:541:UNK:CB	2.27	0.62
1:A:792:U:H2'	1:A:793:A:H8	1.65	0.62
1:A:794:A:OP1	7:I:390:ARG:NH1	2.32	0.62
1:A:747:C:N4	1:A:749:C:OP2	2.32	0.61
20:a:307:HIS:O	20:a:313:UNK:CG	2.30	0.61
1:A:633:C:OP1	4:E:269:ARG:NH1	2.32	0.61
14:Q:94:PRO:HB3	22:c:77:ARG:NH2	2.15	0.61
18:Y:68:Y5P:H4A	18:Y:69:Y5P:C4	2.26	0.61
20:a:300:VAL:CG2	20:a:330:UNK:HG1	2.30	0.61
16:T:60:UNK:HG2	16:T:60:UNK:O	1.99	0.61
33:o:287:UNK:O	33:o:290:UNK:HG3	2.00	0.61
33:o:436:UNK:O	33:o:439:UNK:HG3	2.00	0.61
17:U:48:PRO:O	17:U:52:ARG:HD2	1.99	0.61
20:a:337:UNK:CG	20:a:340:UNK:CG	2.67	0.61
24:e:137:UNK:HB2	29:j:72:PRO:HB3	1.82	0.61
24:e:289:UNK:O	24:e:292:UNK:HG3	2.00	0.61
26:g:66:UNK:HA	26:g:98:LEU:O	2.00	0.61
28:i:13:ARG:HH22	36:z:692:UNK:CG	2.14	0.61
8:J:83:HIS:CE1	11:N:122:GLY:HA3	2.36	0.61
12:O:172:ARG:NH1	14:Q:60:VAL:O	2.32	0.61
20:a:77:ILE:HG23	20:a:298:SER:HB3	1.82	0.61
24:e:280:UNK:HA	24:e:283:UNK:HG3	1.81	0.61
33:o:160:UNK:O	33:o:164:UNK:HG3	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:160:ARG:NH1	17:U:23:TYR:OH	2.34	0.61
26:g:52:UNK:CG	26:g:66:UNK:HG3	2.20	0.61
24:e:51:UNK:HA	24:e:54:UNK:HG3	1.83	0.61
24:e:274:UNK:HG2	24:e:275:UNK:N	2.15	0.61
29:j:180:LYS:HG3	34:p:181:HIS:HD2	1.65	0.61
1:A:767:U:H2'	1:A:768:A:H8	1.64	0.61
4:E:98:LEU:HD11	28:i:75:HIS:CD2	2.35	0.61
13:P:42:PRO:HG2	13:P:45:GLY:HA3	1.82	0.61
24:e:118:UNK:C	24:e:119:UNK:HG3	2.30	0.61
33:o:171:UNK:HA	33:o:174:UNK:HG3	1.83	0.61
33:o:514:UNK:HG1	33:o:541:UNK:HG1	0.66	0.61
24:e:296:UNK:HA	24:e:299:UNK:CG	2.31	0.61
1:A:353:C:H4'	1:A:354:C:H5'	1.83	0.61
1:A:512:A:H2'	1:A:513:A:H8	1.65	0.61
24:e:93:UNK:O	24:e:96:UNK:CG	2.37	0.61
24:e:390:UNK:HG2	24:e:391:UNK:N	2.16	0.61
26:g:122:ARG:HA	26:g:305:ILE:HG13	1.83	0.61
33:o:241:UNK:CG	33:o:270:UNK:HB2	2.30	0.61
33:o:298:UNK:HA	33:o:301:UNK:HG3	1.82	0.61
33:o:459:UNK:O	33:o:462:UNK:HG3	2.00	0.61
1:A:250:A:H2'	1:A:251:C:C6	2.36	0.60
1:A:533:C:H5''	31:m:37:ARG:NH1	2.16	0.60
7:I:275:GLY:H	7:I:348:ALA:HB2	1.65	0.60
13:P:93:LEU:HD21	13:P:103:MET:HE1	1.83	0.60
24:e:28:UNK:HA	24:e:31:UNK:HG3	1.83	0.60
24:e:93:UNK:C	24:e:96:UNK:HG3	2.29	0.60
18:V:23:Y5P:OP2	18:V:23:Y5P:H6	2.01	0.60
28:i:13:ARG:NH2	36:z:692:UNK:CG	2.63	0.60
33:o:222:UNK:HA	33:o:225:UNK:HG3	1.83	0.60
33:o:225:UNK:CB	33:o:248:UNK:HG1	2.32	0.60
33:o:458:UNK:C	33:o:461:UNK:HG3	2.31	0.60
1:A:59:C:H4'	29:j:50:LEU:HD13	1.82	0.60
29:j:95:TRP:HZ2	29:j:131:ILE:HA	1.65	0.60
33:o:476:UNK:HB2	33:o:513:UNK:CG	2.31	0.60
33:o:656:UNK:CB	33:o:674:UNK:HG1	2.31	0.60
36:z:706:UNK:HG2	36:z:707:UNK:N	2.15	0.60
1:A:868:U:O2'	1:A:900:A:N6	2.35	0.60
8:J:84:ASP:OD1	8:J:84:ASP:N	2.23	0.60
9:K:65:TYR:HB3	17:U:13:MET:H	1.66	0.60
27:h:375:LYS:HD3	27:h:378:ILE:HD12	1.84	0.60
33:o:371:UNK:HG2	33:o:372:UNK:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:767:U:H2'	1:A:768:A:C8	2.37	0.60
3:C:69:LEU:HD13	3:C:93:ARG:HH12	1.65	0.60
22:c:47:PHE:HA	22:c:51:ASN:HD22	1.65	0.60
33:o:375:UNK:O	33:o:379:UNK:CG	2.48	0.60
1:A:747:C:H2'	1:A:748:A:H5''	1.83	0.60
24:e:149:UNK:O	24:e:153:UNK:CG	2.45	0.60
1:A:177:U:H2'	1:A:178:G:C8	2.36	0.60
1:A:194:U:H5'	13:P:86:PRO:HG3	1.83	0.60
1:A:279:U:O2'	10:L:54:GLY:O	2.19	0.60
33:o:172:UNK:C	33:o:175:UNK:HG3	2.31	0.60
33:o:415:UNK:O	33:o:418:UNK:CG	2.47	0.60
1:A:338:U:H2'	1:A:339:A:C8	2.37	0.60
2:B:93:LYS:HE2	25:f:149:GLU:HG2	1.83	0.60
5:F:71:PRO:HG2	5:F:74:THR:OG1	2.02	0.60
7:I:262:UNK:HA	7:I:269:ALA:HA	1.84	0.60
11:N:29:TYR:CD1	28:i:55:HIS:HB2	2.37	0.60
14:Q:40:LEU:HD21	22:c:13:LEU:HG	1.84	0.60
9:K:183:ILE:HG12	17:U:39:ILE:HD11	1.84	0.60
15:R:116:GLN:HG3	15:R:121:MET:HE2	1.84	0.60
20:a:74:VAL:HG11	20:a:272:TRP:HE1	1.67	0.60
24:e:205:UNK:HG2	24:e:206:UNK:N	2.16	0.60
24:e:218:UNK:HG2	24:e:296:UNK:CG	2.32	0.60
24:e:230:UNK:O	24:e:231:UNK:CG	2.44	0.60
28:i:17:ARG:HH12	36:z:696:UNK:HG2	1.65	0.60
28:i:17:ARG:NH2	36:z:698:UNK:HG3	2.17	0.60
30:k:153:ILE:HG12	30:k:221:TYR:HE1	1.66	0.60
1:A:744:C:O2'	1:A:746:A:O2'	2.14	0.59
6:G:155:VAL:H	6:G:227:HIS:CE1	2.19	0.59
20:a:323:UNK:CG	20:a:324:UNK:N	2.63	0.59
22:c:30:MET:HG3	22:c:78:PHE:CE2	2.37	0.59
24:e:50:UNK:HG2	24:e:51:UNK:N	2.17	0.59
33:o:244:UNK:C	33:o:247:UNK:HG3	2.31	0.59
1:A:552:A:H2'	1:A:553:G:C8	2.37	0.59
20:a:331:UNK:HB2	20:a:341:UNK:CG	2.32	0.59
24:e:218:UNK:CG	24:e:296:UNK:CG	2.76	0.59
33:o:325:UNK:HA	33:o:328:UNK:HG3	1.84	0.59
25:f:113:LEU:HD21	25:f:127:ARG:HB2	1.83	0.59
33:o:157:UNK:HG1	33:o:177:UNK:HG1	1.84	0.59
1:A:59:C:H42	29:j:133:GLN:CG	2.15	0.59
24:e:224:UNK:HG2	24:e:249:UNK:HB1	1.84	0.59
33:o:242:UNK:C	33:o:245:UNK:HG3	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:o:297:UNK:HA	33:o:300:UNK:HG3	1.84	0.59
1:A:201:A:H2'	1:A:202:A:C8	2.37	0.59
1:A:663:A:H1'	11:N:127:MET:HE2	1.85	0.59
1:A:708:A:H4'	1:A:708:A:OP1	2.02	0.59
24:e:286:UNK:O	24:e:289:UNK:HG3	2.02	0.59
24:e:394:UNK:HG2	24:e:395:UNK:N	2.17	0.59
29:j:64:LEU:HD23	29:j:134:VAL:HG13	1.83	0.59
33:o:287:UNK:HA	33:o:290:UNK:HG3	1.84	0.59
34:p:91:ARG:NH2	34:p:103:ASN:O	2.36	0.59
20:a:211:GLU:HA	20:a:214:LEU:HD12	1.84	0.59
22:c:101:HIS:CE1	22:c:105:ILE:HD11	2.38	0.59
33:o:531:UNK:HA	33:o:534:UNK:HG3	1.84	0.59
24:e:69:UNK:O	24:e:72:UNK:CG	2.46	0.59
24:e:185:UNK:O	24:e:189:UNK:HG2	2.03	0.59
24:e:299:UNK:HA	24:e:302:UNK:HG3	1.85	0.59
29:j:114:ALA:HB3	29:j:131:ILE:HD12	1.85	0.59
33:o:188:UNK:O	33:o:192:UNK:HG3	2.02	0.59
33:o:263:UNK:HA	33:o:266:UNK:HB1	1.84	0.59
33:o:414:UNK:C	33:o:417:UNK:HG3	2.33	0.59
11:N:30:VAL:H	11:N:34:MET:HE2	1.66	0.59
20:a:315:UNK:CG	20:a:316:UNK:N	2.66	0.59
24:e:49:UNK:HG2	24:e:52:UNK:HG2	1.85	0.59
24:e:63:UNK:HG1	24:e:65:UNK:CG	2.32	0.59
24:e:365:UNK:O	24:e:365:UNK:HG2	2.03	0.59
1:A:185:A:O2'	1:A:213:G:N2	2.35	0.59
1:A:580:U:OP1	8:J:128:LYS:NZ	2.35	0.59
33:o:539:UNK:HA	33:o:550:UNK:HG2	1.84	0.59
1:A:28:U:H2'	1:A:29:A:H8	1.67	0.59
24:e:92:UNK:HG2	24:e:93:UNK:N	2.16	0.59
24:e:143:UNK:O	24:e:147:UNK:CG	2.37	0.59
24:e:222:UNK:C	24:e:225:UNK:HG3	2.33	0.59
25:f:98:ASN:HD22	25:f:144:ARG:HE	1.50	0.59
26:g:365:LEU:HD23	26:g:370:ALA:HB1	1.85	0.59
33:o:362:UNK:O	33:o:365:UNK:HG3	2.03	0.59
1:A:356:A:H2'	1:A:357:G:C8	2.38	0.58
12:O:69:PRO:HD2	12:O:72:MET:HG3	1.84	0.58
24:e:205:UNK:CG	24:e:206:UNK:N	2.65	0.58
27:h:301:LYS:HG2	33:o:137:ILE:HG21	1.83	0.58
33:o:226:UNK:C	33:o:229:UNK:HG3	2.25	0.58
33:o:411:UNK:CG	35:s:2360:UNK:HG1	2.32	0.58
33:o:420:UNK:HA	33:o:423:UNK:HG3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:o:514:UNK:CB	33:o:541:UNK:HG1	2.24	0.58
33:o:671:UNK:HA	33:o:674:UNK:HG3	1.84	0.58
6:G:218:PRO:HA	6:G:221:LYS:HE3	1.85	0.58
20:a:338:UNK:O	20:a:342:UNK:HG3	2.04	0.58
20:a:343:UNK:CG	20:a:344:UNK:N	2.67	0.58
27:h:323:HIS:CD2	27:h:361:LYS:NZ	2.70	0.58
33:o:476:UNK:HB1	33:o:506:UNK:CG	2.32	0.58
1:A:60:C:H4'	29:j:34:TYR:HE2	1.68	0.58
26:g:122:ARG:HH11	26:g:336:LEU:HD23	1.67	0.58
33:o:208:UNK:HA	33:o:211:UNK:HG3	1.85	0.58
33:o:341:UNK:O	33:o:345:UNK:HG3	2.03	0.58
24:e:72:UNK:HA	24:e:75:UNK:HG3	1.86	0.58
29:j:160:THR:HB	29:j:161:PRO:HD2	1.84	0.58
33:o:192:UNK:HA	33:o:195:UNK:HG3	1.85	0.58
4:E:154:VAL:HG13	33:o:108:LEU:HD11	1.86	0.58
13:P:69:ASN:ND2	20:a:160:ILE:O	2.37	0.58
20:a:337:UNK:HG2	20:a:337:UNK:O	2.03	0.58
33:o:161:UNK:O	33:o:165:UNK:HG3	2.03	0.58
1:A:202:A:N1	23:d:46:PRO:HG2	2.19	0.58
18:V:54:Y5P:C4	18:V:58:Y5P:H5	2.34	0.58
20:a:310:UNK:HG1	20:a:313:UNK:HG2	1.77	0.58
2:B:203:GLU:HG3	31:m:114:LYS:NZ	2.18	0.58
9:K:65:TYR:OH	15:R:142:ARG:HD2	2.04	0.58
9:K:175:ILE:HG13	9:K:176:SER:H	1.69	0.58
28:i:13:ARG:HH12	36:z:692:UNK:HG2	1.68	0.58
30:k:252:GLU:HA	30:k:303:ASN:HD21	1.67	0.58
2:B:79:SER:H	2:B:82:SER:HB3	1.68	0.58
6:G:62:GLU:CD	6:G:66:ARG:HH21	2.11	0.58
13:P:50:GLN:HE22	22:c:129:PHE:H	1.52	0.58
18:V:9:Y5P:O2'	18:V:10:Y5P:H5	2.02	0.58
24:e:89:UNK:HG2	24:e:90:UNK:N	2.17	0.58
24:e:399:UNK:O	24:e:402:UNK:CG	2.52	0.58
29:j:171:ARG:HA	29:j:174:ILE:HD12	1.86	0.58
33:o:157:UNK:HG1	33:o:177:UNK:CG	2.34	0.58
33:o:393:UNK:HA	33:o:396:UNK:HG3	1.86	0.58
33:o:436:UNK:HA	33:o:439:UNK:HG3	1.86	0.58
1:A:882:A:N3	1:A:886:A:N6	2.51	0.58
24:e:46:UNK:HG3	24:e:77:UNK:CG	2.33	0.58
33:o:394:UNK:HA	33:o:397:UNK:CG	2.31	0.58
36:z:705:UNK:CG	36:z:706:UNK:N	2.66	0.58
40:A:7150:HOH:O	18:V:30:Y5P:C4	2.48	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:263:UNK:N	7:I:268:MET:O	2.37	0.58
24:e:30:UNK:O	24:e:34:UNK:HG3	2.04	0.58
24:e:124:UNK:HA	24:e:127:UNK:HG3	1.85	0.58
24:e:215:UNK:O	24:e:218:UNK:HG3	2.04	0.58
25:f:133:GLU:O	25:f:136:GLN:NE2	2.36	0.58
33:o:461:UNK:O	33:o:464:UNK:HG3	2.04	0.58
33:o:596:UNK:HA	33:o:599:UNK:HG3	1.86	0.58
4:E:198:TRP:HB2	4:E:225:VAL:CG1	2.34	0.57
6:G:203:GLU:O	6:G:206:SER:OG	2.17	0.57
11:N:62:ILE:HG21	27:h:341:HIS:HB3	1.86	0.57
18:Y:59:Y5P:H4A	18:Y:60:Y5P:H4	1.86	0.57
24:e:105:UNK:O	24:e:109:UNK:HG3	2.03	0.57
24:e:235:UNK:C	24:e:238:UNK:HG3	2.34	0.57
29:j:64:LEU:HB2	29:j:139:TRP:CD1	2.39	0.57
33:o:411:UNK:HG1	35:s:2360:UNK:CG	2.33	0.57
1:A:54:A:C8	23:d:27:ARG:NH1	2.72	0.57
1:A:763:A:O3'	11:N:58:ARG:NH2	2.37	0.57
24:e:225:UNK:HB1	24:e:249:UNK:HB2	1.85	0.57
26:g:59:UNK:CG	26:g:62:UNK:HB2	2.32	0.57
33:o:82:SER:O	33:o:446:UNK:HG2	2.03	0.57
33:o:190:UNK:O	33:o:194:UNK:HG3	2.04	0.57
33:o:463:UNK:HA	33:o:466:UNK:HG3	1.86	0.57
1:A:625:U:O2'	1:A:626:C:OP2	2.22	0.57
4:E:203:LEU:HD23	4:E:272:LYS:HG3	1.85	0.57
6:G:240:ARG:NH2	31:m:44:THR:O	2.38	0.57
13:P:110:LEU:O	13:P:114:ARG:HG2	2.04	0.57
24:e:211:UNK:HB1	24:e:216:UNK:CG	2.33	0.57
30:k:145:CYS:O	30:k:149:PHE:N	2.37	0.57
33:o:378:UNK:HA	33:o:381:UNK:HG3	1.86	0.57
36:z:701:UNK:O	36:z:704:UNK:HG3	2.04	0.57
1:A:168:A:H2'	1:A:169:A:C8	2.40	0.57
1:A:232:G:H5''	4:E:196:ASN:ND2	2.19	0.57
1:A:285:C:O2'	1:A:488:A:H2	1.86	0.57
6:G:159:VAL:HB	6:G:172:VAL:HG21	1.86	0.57
24:e:378:UNK:O	24:e:382:UNK:CG	2.51	0.57
33:o:411:UNK:C	33:o:414:UNK:HG3	2.35	0.57
5:F:121:LYS:HD3	5:F:123:ARG:HH21	1.68	0.57
7:I:357:VAL:HG22	7:I:361:GLU:OE1	2.05	0.57
18:Y:70:Y5P:H4A	18:Y:71:Y5P:C5	2.35	0.57
20:a:329:UNK:HA	20:a:332:UNK:HG3	1.87	0.57
22:c:137:ARG:HH12	22:c:143:VAL:HG21	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:e:355:UNK:C	24:e:358:UNK:HG3	2.34	0.57
33:o:168:UNK:O	33:o:171:UNK:HG3	2.04	0.57
5:F:120:THR:HG22	31:m:116:HIS:HA	1.85	0.57
20:a:253:ASP:HB2	20:a:274:PHE:CZ	2.39	0.57
32:n:144:ARG:NH1	32:n:147:VAL:HG11	2.19	0.57
33:o:157:UNK:HG1	33:o:177:UNK:CB	2.34	0.57
33:o:280:UNK:C	33:o:283:UNK:HG3	2.35	0.57
33:o:303:UNK:HA	33:o:306:UNK:CG	2.34	0.57
1:A:59:C:H42	29:j:133:GLN:HG2	1.70	0.57
4:E:198:TRP:HB2	4:E:225:VAL:HG11	1.85	0.57
5:F:117:LEU:HD13	31:m:10:LEU:HD12	1.85	0.57
24:e:399:UNK:O	24:e:402:UNK:HG3	2.05	0.57
29:j:71:LEU:HD22	29:j:76:LEU:HD12	1.87	0.57
30:k:136:PRO:HG2	30:k:139:LEU:HD12	1.87	0.57
1:A:77:G:H8	1:A:77:G:OP2	1.88	0.57
33:o:655:UNK:HA	33:o:658:UNK:HG3	1.86	0.57
30:k:136:PRO:HB3	33:o:58:VAL:O	2.05	0.57
33:o:269:UNK:O	33:o:272:UNK:HG3	2.05	0.57
33:o:457:UNK:O	33:o:460:UNK:HG3	2.04	0.57
1:A:203:G:H2'	1:A:204:U:C6	2.39	0.57
24:e:390:UNK:O	24:e:393:UNK:CG	2.49	0.57
31:m:59:ASN:O	31:m:60:GLU:HG2	2.05	0.57
33:o:223:UNK:HA	33:o:226:UNK:HG3	1.86	0.57
33:o:301:UNK:C	33:o:304:UNK:HG3	2.33	0.57
18:V:43:Y5P:H4A	18:V:44:Y5P:H4	1.86	0.56
20:a:344:UNK:HA	20:a:347:UNK:HG3	1.85	0.56
24:e:235:UNK:HG2	24:e:236:UNK:N	2.19	0.56
33:o:186:UNK:HG2	33:o:223:UNK:HG1	1.86	0.56
1:A:212:A:N7	40:A:7163:HOH:O	2.32	0.56
12:O:92:ARG:HE	12:O:97:GLU:HG2	1.69	0.56
30:k:306:ASP:N	30:k:306:ASP:OD1	2.38	0.56
32:n:189:TRP:CD1	32:n:191:THR:HG1	2.22	0.56
33:o:157:UNK:HA	33:o:160:UNK:HG3	1.87	0.56
33:o:159:UNK:HA	33:o:162:UNK:HG3	1.87	0.56
33:o:659:UNK:HB2	33:o:670:UNK:CG	2.34	0.56
1:A:631:A:H5'	3:C:46:LYS:HE3	1.86	0.56
3:C:69:LEU:HB3	3:C:93:ARG:HH22	1.71	0.56
20:a:166:HIS:HA	20:a:169:ARG:HG3	1.86	0.56
23:d:199:ARG:HB3	23:d:200:PRO:HD2	1.86	0.56
24:e:113:UNK:C	24:e:116:UNK:HG3	2.34	0.56
24:e:215:UNK:HA	24:e:218:UNK:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:h:335:LYS:O	27:h:340:ARG:HG3	2.05	0.56
20:a:337:UNK:CG	20:a:340:UNK:HG1	2.33	0.56
24:e:147:UNK:O	24:e:151:UNK:HG2	2.04	0.56
24:e:169:UNK:O	24:e:170:UNK:HG3	2.04	0.56
24:e:284:UNK:HA	24:e:287:UNK:HG3	1.88	0.56
33:o:304:UNK:O	33:o:307:UNK:HG3	2.06	0.56
33:o:413:UNK:HA	33:o:416:UNK:HG3	1.87	0.56
20:a:81:MET:HB3	20:a:267:PHE:HE2	1.69	0.56
20:a:340:UNK:HG2	20:a:341:UNK:N	2.21	0.56
22:c:4:LYS:O	22:c:11:ARG:NH1	2.39	0.56
24:e:90:UNK:CG	24:e:91:UNK:N	2.68	0.56
1:A:59:C:C2	29:j:136:TYR:HB2	2.41	0.56
1:A:641:A:N7	4:E:260:LYS:NZ	2.52	0.56
4:E:232:THR:HG22	4:E:235:GLU:H	1.70	0.56
21:b:11:SER:O	21:b:14:SER:OG	2.20	0.56
24:e:280:UNK:O	24:e:283:UNK:HG3	2.06	0.56
24:e:294:UNK:C	24:e:297:UNK:HG3	2.34	0.56
33:o:240:UNK:HA	33:o:243:UNK:HG3	1.88	0.56
33:o:339:UNK:HG1	33:o:372:UNK:HB2	1.87	0.56
33:o:420:UNK:HG1	33:o:459:UNK:HG1	1.87	0.56
33:o:462:UNK:O	33:o:466:UNK:HG3	2.06	0.56
33:o:476:UNK:O	33:o:479:UNK:HG3	2.05	0.56
1:A:512:A:H2'	1:A:513:A:C8	2.40	0.56
1:A:641:A:OP1	4:E:230:ASN:HB2	2.05	0.56
24:e:75:UNK:C	24:e:78:UNK:HG3	2.36	0.56
33:o:531:UNK:C	33:o:534:UNK:HG3	2.35	0.56
34:p:90:THR:N	34:p:144:MET:HE3	2.21	0.56
6:G:94:PHE:HD1	6:G:184:MET:HG2	1.71	0.56
24:e:173:UNK:O	24:e:173:UNK:HG2	2.06	0.56
24:e:196:UNK:CG	24:e:199:UNK:HG1	2.34	0.56
24:e:202:UNK:C	24:e:205:UNK:HG3	2.25	0.56
33:o:376:UNK:O	33:o:380:UNK:HG3	2.05	0.56
33:o:418:UNK:O	33:o:421:UNK:HG3	2.05	0.56
33:o:496:UNK:HA	33:o:499:UNK:HG3	1.87	0.56
33:o:554:UNK:HG2	33:o:576:UNK:HB2	1.88	0.56
36:z:705:UNK:HG3	36:z:706:UNK:N	2.21	0.56
1:A:961:C:H2'	1:A:962:C:H5'	1.88	0.56
2:B:217:PRO:HG3	21:b:31:TRP:HB2	1.87	0.56
18:Y:9:Y5P:H4	18:Y:22:Y5P:C4	2.32	0.56
18:Y:54:Y5P:N3	18:Y:58:Y5P:H5	2.21	0.56
24:e:302:UNK:O	24:e:306:UNK:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:g:213:GLU:CB	26:g:231:ARG:HH12	2.19	0.56
33:o:497:UNK:C	33:o:500:UNK:HG3	2.35	0.56
1:A:318:C:H3'	15:R:106:LYS:HE2	1.88	0.56
8:J:166:GLU:H	8:J:166:GLU:CD	2.11	0.56
20:a:312:UNK:HB1	20:a:333:UNK:CG	2.36	0.56
20:a:324:UNK:CG	20:a:325:UNK:N	2.69	0.56
24:e:105:UNK:O	24:e:108:UNK:CG	2.53	0.56
24:e:164:UNK:O	24:e:168:UNK:HG2	2.06	0.56
26:g:265:ASN:ND2	26:g:310:SER:O	2.38	0.56
29:j:27:ARG:HH12	29:j:33:ARG:NH1	2.04	0.56
33:o:222:UNK:C	33:o:225:UNK:HG3	2.35	0.56
33:o:581:UNK:HA	33:o:584:UNK:HG3	1.87	0.56
2:B:104:TYR:HD2	2:B:236:PRO:HG3	1.71	0.55
18:Y:32:Y5P:H4A	18:Y:33:Y5P:H4	1.87	0.55
24:e:28:UNK:HA	24:e:31:UNK:CG	2.36	0.55
26:g:52:UNK:O	26:g:66:UNK:HG3	2.06	0.55
33:o:238:UNK:O	33:o:241:UNK:HG2	2.06	0.55
33:o:394:UNK:CA	33:o:397:UNK:HG3	2.35	0.55
33:o:411:UNK:O	33:o:414:UNK:HG3	2.05	0.55
17:U:67:GLU:HG3	25:f:155:LEU:HG	1.88	0.55
20:a:310:UNK:HG3	20:a:313:UNK:HG1	1.84	0.55
24:e:272:UNK:O	24:e:272:UNK:HG2	2.06	0.55
35:s:2371:UNK:O	35:s:2374:UNK:HG3	2.06	0.55
11:N:62:ILE:HG12	27:h:341:HIS:CD2	2.41	0.55
18:Y:31:Y5P:C4	18:Y:32:Y5P:H4	2.33	0.55
20:a:342:UNK:HA	20:a:345:UNK:HG3	1.87	0.55
24:e:114:UNK:HA	24:e:117:UNK:CG	2.35	0.55
24:e:125:UNK:O	24:e:128:UNK:CG	2.37	0.55
24:e:397:UNK:HG2	24:e:398:UNK:N	2.22	0.55
33:o:235:UNK:HG1	33:o:237:UNK:CB	2.35	0.55
35:s:2367:UNK:O	35:s:2371:UNK:HG3	2.06	0.55
1:A:13:U:H1'	1:A:640:A:N3	2.21	0.55
1:A:358:U:H2'	1:A:359:U:C6	2.41	0.55
28:i:46:LYS:HA	28:i:49:TYR:CE1	2.42	0.55
33:o:196:UNK:CG	33:o:206:UNK:HG1	2.36	0.55
33:o:398:UNK:O	33:o:401:UNK:HG3	2.07	0.55
33:o:499:UNK:O	33:o:503:UNK:HG3	2.06	0.55
33:o:536:UNK:O	33:o:540:UNK:HG3	2.07	0.55
24:e:46:UNK:HG3	24:e:77:UNK:HG1	1.87	0.55
24:e:389:UNK:O	24:e:392:UNK:CG	2.37	0.55
33:o:189:UNK:HA	33:o:192:UNK:CG	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:o:222:UNK:HA	33:o:225:UNK:CG	2.37	0.55
33:o:224:UNK:O	33:o:227:UNK:HG3	2.07	0.55
33:o:336:UNK:CB	33:o:372:UNK:HG1	2.33	0.55
10:L:61:VAL:HG23	10:L:84:ARG:HB2	1.88	0.55
23:d:168:ILE:HG12	23:d:176:ARG:HG3	1.88	0.55
27:h:302:LEU:HD22	27:h:303:TRP:H	1.70	0.55
1:A:160:C:H2'	1:A:163:A:H61	1.72	0.55
5:F:8:LEU:HB2	5:F:64:PHE:HB2	1.89	0.55
24:e:140:UNK:CG	24:e:174:UNK:HG1	2.37	0.55
24:e:273:UNK:HG2	24:e:276:UNK:HG3	1.88	0.55
33:o:338:UNK:HA	33:o:341:UNK:CG	2.36	0.55
33:o:459:UNK:C	33:o:462:UNK:HG3	2.37	0.55
36:z:702:UNK:O	36:z:705:UNK:HG3	2.06	0.55
2:B:58:ARG:O	2:B:61:ILE:HG22	2.07	0.55
12:O:153:HIS:HA	12:O:156:PHE:HD2	1.72	0.55
14:Q:8:VAL:HG12	14:Q:10:ALA:H	1.71	0.55
23:d:54:PHE:HD2	34:p:208:PRO:HB3	1.72	0.55
24:e:221:UNK:HG1	24:e:253:UNK:HB1	1.89	0.55
27:h:286:PHE:HD1	27:h:291:GLU:HG3	1.70	0.55
30:k:164:SER:HA	33:o:134:GLU:HB2	1.88	0.55
33:o:517:UNK:O	33:o:520:UNK:HG3	2.07	0.55
1:A:209:C:H4'	13:P:43:ARG:HH12	1.72	0.55
1:A:526:G:H1'	4:E:231:MET:HB3	1.88	0.55
1:A:887:U:H2'	1:A:888:A:C8	2.42	0.55
3:C:52:THR:HG22	3:C:54:GLU:H	1.72	0.55
20:a:311:UNK:CG	20:a:312:UNK:N	2.69	0.55
24:e:120:UNK:HG2	24:e:123:UNK:CG	2.36	0.55
24:e:196:UNK:HG3	24:e:199:UNK:CG	2.35	0.55
24:e:357:UNK:HG2	24:e:358:UNK:N	2.21	0.55
26:g:133:LYS:HZ3	26:g:310:SER:HA	1.72	0.55
33:o:516:UNK:HA	33:o:519:UNK:HG3	1.89	0.55
33:o:656:UNK:HB1	33:o:674:UNK:CG	2.36	0.55
1:A:733:A:C8	26:g:129:LYS:HE2	2.42	0.55
3:C:73:THR:HG21	30:k:160:SER:HB2	1.89	0.55
4:E:244:LEU:HD21	4:E:346:THR:HG21	1.89	0.55
4:E:316:CYS:HB2	4:E:321:MET:HG3	1.88	0.55
17:U:51:ARG:HG3	17:U:54:ARG:HH12	1.72	0.55
20:a:330:UNK:HA	20:a:333:UNK:CG	2.35	0.55
24:e:118:UNK:O	24:e:119:UNK:CG	2.53	0.55
30:k:63:ALA:HB3	30:k:66:GLN:HB2	1.88	0.55
33:o:340:UNK:HA	33:o:343:UNK:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:U:O2'	1:A:431:G:N7	2.34	0.54
7:I:316:PHE:HB3	7:I:317:PRO:HD3	1.89	0.54
24:e:70:UNK:HG2	24:e:71:UNK:N	2.23	0.54
24:e:208:UNK:O	24:e:211:UNK:CG	2.46	0.54
24:e:282:UNK:HA	24:e:285:UNK:HG3	1.88	0.54
24:e:385:UNK:HG2	24:e:386:UNK:N	2.21	0.54
33:o:283:UNK:O	33:o:287:UNK:HG3	2.06	0.54
33:o:601:UNK:CG	33:o:655:UNK:HB1	2.38	0.54
1:A:102:G:O3'	14:Q:78:LYS:NZ	2.40	0.54
1:A:819:A:P	6:G:93:LYS:HZ3	2.30	0.54
1:A:823:G:H5'	1:A:824:G:OP2	2.08	0.54
4:E:224:GLU:HB2	4:E:342:MET:HG2	1.90	0.54
17:U:37:GLU:O	17:U:41:ARG:HB2	2.07	0.54
24:e:174:UNK:HG3	24:e:177:UNK:HG3	1.88	0.54
24:e:219:UNK:HA	24:e:222:UNK:HG3	1.87	0.54
24:e:232:UNK:HG2	24:e:235:UNK:HG1	1.73	0.54
24:e:374:UNK:HG2	24:e:375:UNK:N	2.21	0.54
36:z:701:UNK:HG2	36:z:702:UNK:N	2.22	0.54
1:A:926:A:H4'	32:n:134:ARG:HH21	1.72	0.54
11:N:53:ARG:HE	27:h:364:HIS:HD2	1.56	0.54
33:o:381:UNK:HA	33:o:384:UNK:HG3	1.89	0.54
1:A:333:A:N7	1:A:361:A:H2	2.05	0.54
2:B:168:ARG:HH22	17:U:87:CYS:C	2.15	0.54
6:G:71:THR:HG23	7:I:253:UNK:HB2	1.88	0.54
15:R:80:LEU:HD22	23:d:189:TRP:HZ3	1.71	0.54
20:a:217:MET:HG3	20:a:222:GLN:HB2	1.89	0.54
24:e:131:UNK:O	24:e:136:UNK:N	2.40	0.54
24:e:296:UNK:CA	24:e:299:UNK:HG3	2.35	0.54
26:g:82:LEU:HD12	26:g:83:PRO:HD2	1.88	0.54
26:g:99:MET:HE1	26:g:354:SER:HB3	1.90	0.54
28:i:17:ARG:HH21	36:z:698:UNK:HG3	1.71	0.54
33:o:532:UNK:HA	33:o:535:UNK:HG3	1.88	0.54
9:K:112:ALA:HB3	9:K:137:ALA:HB2	1.88	0.54
20:a:160:ILE:O	20:a:160:ILE:HG12	2.07	0.54
20:a:261:LEU:HB2	20:a:270:MET:SD	2.48	0.54
24:e:215:UNK:C	24:e:218:UNK:HG3	2.38	0.54
33:o:173:UNK:HA	33:o:176:UNK:HG3	1.87	0.54
1:A:731:A:H5'	26:g:319:ARG:HB2	1.90	0.54
7:I:129:GLU:HG3	7:I:130:GLU:HG3	1.89	0.54
7:I:266:UNK:HG1	7:I:268:MET:HE2	1.90	0.54
18:Y:43:Y5P:OP1	18:Y:43:Y5P:HA	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:e:175:UNK:CG	24:e:368:UNK:HG3	2.37	0.54
26:g:161:VAL:HG22	26:g:289:ILE:HD11	1.89	0.54
33:o:191:UNK:HA	33:o:194:UNK:CG	2.36	0.54
33:o:260:UNK:O	33:o:263:UNK:CG	2.56	0.54
33:o:531:UNK:O	33:o:535:UNK:HG3	2.07	0.54
17:U:72:ILE:HD12	31:m:104:LEU:HD22	1.90	0.54
20:a:253:ASP:HB2	20:a:274:PHE:HZ	1.72	0.54
24:e:247:UNK:HG2	24:e:250:UNK:HG3	1.90	0.54
24:e:280:UNK:C	24:e:283:UNK:HG3	2.38	0.54
28:i:42:LEU:HD13	28:i:45:ARG:NH1	2.23	0.54
30:k:254:ILE:HG22	30:k:256:GLU:H	1.72	0.54
33:o:192:UNK:C	33:o:195:UNK:HG3	2.38	0.54
33:o:430:UNK:HB2	33:o:433:UNK:HG2	1.90	0.54
34:p:73:VAL:O	34:p:74:TRP:CG	2.61	0.54
1:A:821:A:H5'	1:A:822:A:OP2	2.08	0.54
3:C:91:PHE:HD1	4:E:89:PHE:CE2	2.26	0.54
14:Q:11:LYS:HA	14:Q:68:ALA:HB2	1.89	0.54
24:e:113:UNK:O	24:e:117:UNK:HG3	2.08	0.54
24:e:399:UNK:CG	24:e:400:UNK:N	2.70	0.54
25:f:153:ARG:NH2	25:f:158:THR:O	2.38	0.54
26:g:133:LYS:NZ	26:g:310:SER:HA	2.22	0.54
1:A:739:A:H4'	1:A:740:U:C2	2.43	0.54
1:A:891:C:H5	29:j:21:LEU:HD21	1.73	0.54
4:E:288:HIS:HD2	4:E:289:THR:OG1	1.90	0.54
5:F:119:SER:HB3	5:F:121:LYS:HE3	1.90	0.54
13:P:110:LEU:O	13:P:113:LYS:HG2	2.07	0.54
18:V:11:Y5P:H4A	18:V:12:Y5P:H4	1.90	0.54
24:e:67:UNK:HG3	24:e:68:UNK:N	2.23	0.54
24:e:279:UNK:O	24:e:282:UNK:HG3	2.08	0.54
24:e:371:UNK:C	24:e:374:UNK:HG3	2.35	0.54
26:g:213:GLU:HB3	26:g:231:ARG:HH12	1.73	0.54
33:o:190:UNK:HA	33:o:193:UNK:HG3	1.89	0.54
33:o:404:UNK:CG	33:o:405:UNK:N	2.71	0.54
33:o:419:UNK:HA	33:o:422:UNK:HG3	1.89	0.54
13:P:34:ILE:HG22	13:P:51:LEU:HB2	1.89	0.54
24:e:178:UNK:O	24:e:181:UNK:HG3	2.08	0.54
33:o:320:UNK:C	33:o:323:UNK:HG3	2.37	0.54
1:A:56:U:OP1	1:A:204:U:O2'	2.22	0.53
1:A:506:G:C5'	32:n:144:ARG:HH22	2.20	0.53
20:a:240:GLU:O	20:a:244:ILE:HG12	2.08	0.53
20:a:346:UNK:HG2	20:a:347:UNK:N	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:e:48:UNK:HB2	24:e:53:UNK:HG1	1.89	0.53
24:e:192:UNK:HG2	24:e:192:UNK:O	2.06	0.53
24:e:395:UNK:HA	24:e:398:UNK:CG	2.37	0.53
33:o:305:UNK:HA	33:o:308:UNK:HG3	1.89	0.53
33:o:341:UNK:C	33:o:344:UNK:HG3	2.38	0.53
35:s:2362:UNK:HA	35:s:2365:UNK:CG	2.39	0.53
11:N:125:ARG:HG2	11:N:125:ARG:HH11	1.73	0.53
12:O:210:LEU:HD22	32:n:173:LEU:HB3	1.90	0.53
24:e:39:UNK:HA	24:e:42:UNK:HG3	1.89	0.53
24:e:208:UNK:HG1	24:e:220:UNK:HG1	1.88	0.53
30:k:190:LYS:NZ	30:k:252:GLU:OE2	2.39	0.53
33:o:398:UNK:C	33:o:401:UNK:HG3	2.37	0.53
1:A:762:G:N2	1:A:764:A:H3'	2.24	0.53
2:B:79:SER:OG	2:B:80:VAL:N	2.39	0.53
7:I:275:GLY:HA2	7:I:347:LEU:HD23	1.90	0.53
11:N:103:ARG:HB3	11:N:104:TRP:CE3	2.43	0.53
22:c:24:LYS:HG3	22:c:107:GLY:O	2.09	0.53
26:g:52:UNK:O	26:g:66:UNK:CG	2.57	0.53
29:j:57:ASP:OD1	29:j:57:ASP:N	2.40	0.53
33:o:225:UNK:C	33:o:228:UNK:HG3	2.33	0.53
33:o:598:UNK:HB2	33:o:655:UNK:HB2	1.91	0.53
20:a:81:MET:HE2	20:a:267:PHE:CE2	2.43	0.53
26:g:64:UNK:HG1	26:g:350:LYS:HD2	1.91	0.53
29:j:63:ARG:NH1	29:j:110:ASP:OD2	2.41	0.53
1:A:134:C:H5'	14:Q:22:MET:HE3	1.89	0.53
1:A:344:G:H1	9:K:121:ASN:CB	2.21	0.53
1:A:545:C:H1'	1:A:820:U:H1'	1.89	0.53
5:F:105:CYS:CB	15:R:69:CYS:SG	2.94	0.53
8:J:166:GLU:OE1	8:J:166:GLU:N	2.32	0.53
18:V:24:Y5P:C4	18:V:25:Y5P:H4	2.37	0.53
18:Y:25:Y5P:C5	18:Y:26:Y5P:H5	2.38	0.53
33:o:238:UNK:O	33:o:241:UNK:CG	2.56	0.53
33:o:344:UNK:HG2	33:o:345:UNK:N	2.23	0.53
34:p:104:PRO:HB2	34:p:109:ARG:HB3	1.91	0.53
1:A:67:C:N3	23:d:27:ARG:HB2	2.24	0.53
1:A:939:A:H2'	1:A:940:C:C6	2.44	0.53
11:N:63:LEU:HD22	11:N:64:PRO:HD2	1.90	0.53
23:d:30:ARG:HB3	23:d:31:HIS:CD2	2.43	0.53
33:o:339:UNK:HG3	33:o:340:UNK:N	2.23	0.53
33:o:492:UNK:O	33:o:496:UNK:HG3	2.09	0.53
33:o:579:UNK:HA	33:o:582:UNK:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:p:136:HIS:CD2	34:p:138:PRO:HD2	2.43	0.53
1:A:217:U:H2'	1:A:218:A:C8	2.43	0.53
11:N:81:ASP:OD1	11:N:81:ASP:N	2.42	0.53
23:d:194:GLU:HB2	23:d:196:LEU:HG	1.90	0.53
24:e:84:UNK:O	24:e:87:UNK:HG3	2.09	0.53
24:e:85:UNK:O	24:e:88:UNK:HG3	2.08	0.53
29:j:31:SER:HA	29:j:111:HIS:HD2	1.73	0.53
30:k:300:SER:O	30:k:304:GLU:HB3	2.09	0.53
31:m:86:MET:O	31:m:90:GLN:HB2	2.09	0.53
33:o:229:UNK:CG	33:o:230:UNK:N	2.72	0.53
33:o:265:UNK:HA	33:o:268:UNK:CG	2.39	0.53
1:A:390:A:O2'	12:O:153:HIS:HE1	1.92	0.53
1:A:640:A:OP2	4:E:260:LYS:NZ	2.40	0.53
10:L:96:PRO:O	10:L:127:ARG:NH1	2.41	0.53
24:e:72:UNK:C	24:e:75:UNK:HG3	2.37	0.53
33:o:156:UNK:HA	33:o:159:UNK:HG3	1.90	0.53
33:o:260:UNK:O	33:o:263:UNK:HG2	2.09	0.53
33:o:320:UNK:HA	33:o:323:UNK:HG3	1.90	0.53
33:o:514:UNK:C	33:o:517:UNK:HG3	2.39	0.53
2:B:101:MET:HA	2:B:101:MET:HE2	1.90	0.53
2:B:223:ASP:OD1	2:B:224:THR:N	2.39	0.53
4:E:193:TRP:CE3	4:E:199:GLY:HA3	2.44	0.53
6:G:91:ILE:O	6:G:95:THR:OG1	2.19	0.53
14:Q:35:LEU:HB2	14:Q:42:TYR:CZ	2.44	0.53
15:R:116:GLN:HG2	15:R:123:VAL:HG22	1.91	0.53
22:c:89:ASP:OD2	23:d:120:ARG:NH2	2.42	0.53
24:e:394:UNK:C	24:e:397:UNK:HG3	2.37	0.53
30:k:55:LEU:O	33:o:93:PRO:HB3	2.09	0.53
33:o:229:UNK:C	33:o:232:UNK:HG3	2.37	0.53
33:o:245:UNK:O	33:o:249:UNK:HG3	2.09	0.53
33:o:304:UNK:HA	33:o:307:UNK:HG3	1.90	0.53
33:o:486:UNK:O	33:o:490:UNK:CG	2.55	0.53
33:o:550:UNK:O	33:o:553:UNK:HG3	2.08	0.53
1:A:838:A:C4	32:n:131:LEU:HD11	2.43	0.53
1:A:931:G:H4'	1:A:932:U:H5''	1.90	0.53
4:E:341:ASN:OD1	4:E:344:ASN:HB2	2.09	0.53
24:e:92:UNK:O	24:e:95:UNK:CG	2.57	0.53
24:e:235:UNK:HA	24:e:238:UNK:HG3	1.90	0.53
26:g:155:PRO:O	26:g:262:ASP:HB3	2.08	0.53
28:i:15:SER:OG	30:k:195:LEU:O	2.24	0.53
33:o:186:UNK:HG1	33:o:220:UNK:HB1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:o:190:UNK:CG	33:o:223:UNK:HB2	2.11	0.53
33:o:400:UNK:CG	33:o:401:UNK:N	2.72	0.53
33:o:659:UNK:HB2	33:o:670:UNK:HG2	1.91	0.53
1:A:357:G:H21	9:K:100:GLN:HE22	1.56	0.52
1:A:904:A:H2'	1:A:905:U:C6	2.43	0.52
18:V:67:Y5P:H4A	18:V:68:Y5P:H4	1.90	0.52
20:a:81:MET:HE2	20:a:267:PHE:HE2	1.72	0.52
20:a:331:UNK:HB2	20:a:341:UNK:HG1	1.90	0.52
24:e:120:UNK:CG	24:e:123:UNK:HG1	2.40	0.52
26:g:338:PRO:HD3	30:k:294:TYR:OH	2.09	0.52
33:o:398:UNK:HA	33:o:401:UNK:CG	2.39	0.52
1:A:103:G:H1'	14:Q:9:HIS:HE1	1.73	0.52
13:P:65:LEU:HB3	20:a:195:TYR:OH	2.08	0.52
20:a:314:UNK:C	20:a:317:UNK:HG3	2.38	0.52
24:e:135:UNK:HG2	24:e:135:UNK:O	2.07	0.52
33:o:306:UNK:HA	33:o:309:UNK:HG3	1.90	0.52
33:o:379:UNK:HA	33:o:382:UNK:CG	2.37	0.52
1:A:670:A:N3	6:G:36:ARG:NH1	2.57	0.52
1:A:791:G:C8	7:I:376:ARG:HB3	2.45	0.52
24:e:360:UNK:HA	24:e:363:UNK:HG3	1.91	0.52
29:j:41:MET:HG3	29:j:50:LEU:HB2	1.91	0.52
3:C:112:ARG:HH11	3:C:112:ARG:HB2	1.74	0.52
9:K:175:ILE:HG13	9:K:176:SER:N	2.25	0.52
14:Q:32:ARG:NH2	14:Q:49:TYR:OH	2.43	0.52
20:a:281:ASP:OD2	20:a:337:UNK:HG3	2.09	0.52
24:e:282:UNK:O	24:e:285:UNK:HG3	2.09	0.52
24:e:302:UNK:O	24:e:305:UNK:HG3	2.10	0.52
29:j:89:HIS:CE1	29:j:121:LYS:HD3	2.45	0.52
30:k:123:ARG:HB3	33:o:77:THR:HG21	1.91	0.52
30:k:183:ASN:HB3	30:k:232:TYR:OH	2.09	0.52
33:o:463:UNK:O	33:o:467:UNK:HG3	2.10	0.52
1:A:168:A:O2'	1:A:170:A:N1	2.39	0.52
1:A:667:C:H3'	1:A:668:A:H8	1.73	0.52
1:A:800:G:H2'	1:A:801:A:C8	2.44	0.52
8:J:163:ASN:HB3	30:k:116:LEU:HD11	1.90	0.52
14:Q:74:THR:HG22	14:Q:75:LYS:H	1.75	0.52
18:V:31:Y5P:H4A	18:V:32:Y5P:H4	1.92	0.52
20:a:174:ARG:NH1	20:a:174:ARG:HG3	2.25	0.52
24:e:71:UNK:HA	24:e:74:UNK:CG	2.37	0.52
25:f:115:ILE:HG21	25:f:143:LEU:HD11	1.91	0.52
29:j:171:ARG:HH12	34:p:191:PRO:CD	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:k:175:LEU:O	30:k:208:THR:HA	2.10	0.52
33:o:280:UNK:O	33:o:283:UNK:HG3	2.08	0.52
33:o:295:UNK:HA	33:o:298:UNK:CG	2.40	0.52
34:p:73:VAL:HG12	34:p:106:PRO:HB2	1.91	0.52
1:A:43:U:H2'	1:A:44:U:O4'	2.10	0.52
1:A:375:A:H62	31:m:17:ARG:HH22	1.57	0.52
1:A:826:C:H2'	1:A:827:A:C8	2.42	0.52
12:O:116:VAL:HG21	12:O:186:LEU:HD21	1.92	0.52
18:V:43:Y5P:H2'	18:V:44:Y5P:C6	2.39	0.52
24:e:32:UNK:HA	24:e:35:UNK:HG3	1.92	0.52
24:e:54:UNK:O	24:e:58:UNK:CG	2.42	0.52
24:e:385:UNK:C	24:e:388:UNK:HG3	2.39	0.52
26:g:196:HIS:CD2	26:g:196:HIS:H	2.28	0.52
29:j:171:ARG:HE	29:j:175:LEU:HD11	1.73	0.52
30:k:84:PRO:HG2	30:k:85:LEU:HG	1.92	0.52
33:o:599:UNK:HA	33:o:602:UNK:HG3	1.91	0.52
7:I:225:LEU:HD12	7:I:228:ARG:HD3	1.91	0.52
7:I:265:UNK:HG2	7:I:266:UNK:N	2.24	0.52
7:I:386:GLU:HB3	7:I:390:ARG:HG3	1.92	0.52
12:O:143:HIS:HD2	12:O:144:MET:HE2	1.74	0.52
24:e:207:UNK:HG1	24:e:219:UNK:HG2	1.90	0.52
24:e:242:UNK:O	24:e:242:UNK:HG2	2.08	0.52
24:e:243:UNK:O	24:e:244:UNK:CG	2.56	0.52
33:o:241:UNK:HG2	33:o:270:UNK:HB2	1.90	0.52
1:A:835:C:H2'	1:A:836:G:C8	2.44	0.52
1:A:899:C:H2'	1:A:900:A:H4'	1.90	0.52
1:A:947:G:H2'	1:A:948:U:C6	2.44	0.52
2:B:100:PHE:CE1	21:b:47:ARG:HD2	2.45	0.52
4:E:93:LEU:H	28:i:75:HIS:CD2	2.27	0.52
8:J:64:THR:CG2	33:o:64:THR:HB	2.40	0.52
10:L:60:GLY:HA2	10:L:84:ARG:O	2.10	0.52
24:e:108:UNK:C	24:e:111:UNK:HG3	2.40	0.52
24:e:196:UNK:HG3	24:e:199:UNK:HG1	1.91	0.52
24:e:252:UNK:HA	24:e:255:UNK:HG3	1.92	0.52
29:j:91:GLU:HG2	29:j:92:PRO:HD2	1.92	0.52
33:o:196:UNK:HG2	33:o:206:UNK:HG1	1.91	0.52
33:o:202:UNK:HA	33:o:205:UNK:CG	2.39	0.52
33:o:287:UNK:C	33:o:290:UNK:HG3	2.40	0.52
33:o:363:UNK:CG	33:o:364:UNK:N	2.71	0.52
33:o:519:UNK:HA	33:o:522:UNK:HG3	1.92	0.52
34:p:136:HIS:HD2	34:p:138:PRO:HD2	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:V:66:Y5P:H4A	18:V:67:Y5P:H4	1.92	0.52
24:e:387:UNK:O	24:e:390:UNK:HG3	2.09	0.52
33:o:232:UNK:HB2	33:o:241:UNK:HG1	1.92	0.52
33:o:283:UNK:HA	33:o:286:UNK:HG3	1.92	0.52
33:o:357:UNK:HA	33:o:360:UNK:HG3	1.92	0.52
1:A:124:A:H5'	1:A:125:U:OP1	2.09	0.52
1:A:164:C:C2	29:j:14:LEU:HD21	2.45	0.52
4:E:296:LEU:HB3	4:E:303:ILE:HG22	1.91	0.52
7:I:260:UNK:HG3	7:I:355:SER:HB3	1.92	0.52
18:V:41:Y5P:H4A	18:V:42:Y5P:C5	2.40	0.52
33:o:459:UNK:CA	33:o:462:UNK:HG3	2.40	0.52
1:A:667:C:H3'	1:A:668:A:C8	2.45	0.51
7:I:127:HIS:CD2	7:I:129:GLU:HG2	2.45	0.51
7:I:228:ARG:HD2	17:U:85:GLN:NE2	2.14	0.51
24:e:107:UNK:HA	24:e:110:UNK:HG3	1.92	0.51
24:e:175:UNK:HB2	24:e:368:UNK:CG	2.40	0.51
24:e:223:UNK:O	24:e:226:UNK:HG2	2.10	0.51
24:e:282:UNK:C	24:e:285:UNK:HG3	2.40	0.51
33:o:271:UNK:C	33:o:274:UNK:HG3	2.40	0.51
33:o:282:UNK:O	33:o:286:UNK:HG3	2.10	0.51
33:o:655:UNK:HG2	33:o:674:UNK:CB	2.40	0.51
3:C:154:HIS:CD2	30:k:77:PRO:HG3	2.45	0.51
24:e:220:UNK:HA	24:e:223:UNK:CG	2.40	0.51
33:o:176:UNK:HA	33:o:179:UNK:HG3	1.92	0.51
4:E:325:ARG:HH21	4:E:430:THR:C	2.17	0.51
5:F:22:LEU:HD11	5:F:64:PHE:CE2	2.45	0.51
7:I:111:LEU:HD22	30:k:114:LEU:HD23	1.92	0.51
24:e:75:UNK:HA	24:e:78:UNK:HG3	1.92	0.51
24:e:304:UNK:HA	24:e:307:UNK:HG3	1.91	0.51
24:e:304:UNK:O	24:e:307:UNK:HG3	2.10	0.51
24:e:365:UNK:HG2	24:e:368:UNK:HG2	1.92	0.51
24:e:395:UNK:HG2	24:e:396:UNK:N	2.26	0.51
26:g:301:GLN:NE2	30:k:270:GLN:OE1	2.42	0.51
1:A:42:A:O2'	1:A:43:U:OP2	2.27	0.51
6:G:59:THR:HG22	6:G:63:LYS:HE3	1.92	0.51
11:N:53:ARG:O	11:N:56:SER:OG	2.27	0.51
19:X:20:Y5P:H4A	19:X:21:Y5P:H4	1.92	0.51
20:a:70:MET:HA	20:a:75:GLN:HE21	1.75	0.51
20:a:78:LEU:HD13	20:a:268:GLY:HA2	1.91	0.51
20:a:338:UNK:O	20:a:341:UNK:HG3	2.09	0.51
20:a:348:UNK:HA	20:a:351:UNK:HG3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:e:70:UNK:C	24:e:73:UNK:HG3	2.37	0.51
24:e:166:UNK:HB1	24:e:171:UNK:HG1	1.91	0.51
31:m:95:GLU:HB3	31:m:98:SER:HB3	1.92	0.51
33:o:361:UNK:HA	33:o:364:UNK:HG3	1.93	0.51
1:A:737:A:H5'	26:g:165:ARG:CZ	2.41	0.51
4:E:291:TYR:H	4:E:356:GLN:NE2	2.08	0.51
18:Y:67:Y5P:H4A	18:Y:68:Y5P:H4	1.92	0.51
26:g:191:LYS:HZ1	26:g:198:LEU:HD12	1.75	0.51
26:g:311:GLN:OE1	26:g:312:THR:HG23	2.11	0.51
33:o:575:UNK:O	33:o:579:UNK:HG3	2.09	0.51
1:A:63:G:H5'	1:A:64:C:OP2	2.11	0.51
1:A:216:A:C6	1:A:274:A:N7	2.78	0.51
1:A:317:A:H2	1:A:318:C:C6	2.28	0.51
1:A:722:A:C2	1:A:749:C:H4'	2.45	0.51
2:B:141:ILE:HB	2:B:163:GLU:CD	2.35	0.51
19:X:20:Y5P:H4	18:Y:36:P5P:N1	2.25	0.51
23:d:58:GLU:O	23:d:62:GLN:HG2	2.11	0.51
24:e:302:UNK:C	24:e:305:UNK:HG3	2.40	0.51
26:g:201:ILE:O	26:g:220:PRO:HA	2.10	0.51
27:h:330:LEU:O	27:h:340:ARG:NH2	2.44	0.51
31:m:33:VAL:N	31:m:105:ASN:OD1	2.44	0.51
33:o:232:UNK:HG2	33:o:233:UNK:N	2.25	0.51
33:o:263:UNK:O	33:o:267:UNK:HG3	2.11	0.51
33:o:539:UNK:HB2	33:o:551:UNK:HB1	1.91	0.51
1:A:729:A:H2'	1:A:730:C:O4'	2.10	0.51
1:A:881:A:O2'	24:e:66:UNK:HG2	2.10	0.51
6:G:238:HIS:HE1	9:K:127:GLY:H	1.59	0.51
6:G:238:HIS:CE1	9:K:127:GLY:H	2.29	0.51
7:I:253:UNK:HG2	7:I:366:ARG:HH22	1.58	0.51
18:Y:23:Y5P:H2'	18:Y:24:Y5P:H6	1.93	0.51
20:a:146:ILE:HD11	34:p:203:TYR:HD1	1.75	0.51
20:a:312:UNK:HB1	20:a:333:UNK:HB2	1.91	0.51
24:e:35:UNK:HA	24:e:38:UNK:HG3	1.92	0.51
24:e:123:UNK:HG2	24:e:124:UNK:N	2.26	0.51
25:f:173:LEU:HD23	25:f:173:LEU:H	1.76	0.51
27:h:352:LYS:O	27:h:354:PRO:HD3	2.11	0.51
33:o:228:UNK:HA	33:o:231:UNK:HG3	1.91	0.51
33:o:320:UNK:O	33:o:323:UNK:HG3	2.10	0.51
13:P:118:VAL:HG22	34:p:237:GLU:HG3	1.91	0.51
20:a:344:UNK:O	20:a:347:UNK:CG	2.50	0.51
24:e:171:UNK:O	24:e:171:UNK:HG2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:h:326:LEU:HB2	27:h:347:THR:HG23	1.93	0.51
28:i:11:MET:HE3	30:k:241:TRP:HH2	1.75	0.51
30:k:268:LEU:O	30:k:272:LYS:HG2	2.10	0.51
33:o:436:UNK:C	33:o:439:UNK:HG3	2.41	0.51
1:A:752:A:H3'	1:A:753:A:H5'	1.92	0.51
2:B:141:ILE:HD12	2:B:256:ILE:HD11	1.92	0.51
7:I:197:GLY:O	7:I:249:ILE:HG12	2.11	0.51
22:c:35:ASN:OD1	22:c:69:ASN:ND2	2.44	0.51
23:d:68:ARG:NH1	29:j:198:ILE:HG12	2.25	0.51
23:d:73:GLU:O	23:d:76:SER:OG	2.25	0.51
24:e:390:UNK:CG	24:e:391:UNK:N	2.73	0.51
24:e:390:UNK:CA	24:e:393:UNK:HG3	2.40	0.51
27:h:310:GLU:OE2	30:k:217:LYS:N	2.43	0.51
31:m:11:ALA:O	31:m:12:ARG:NH1	2.33	0.51
33:o:158:UNK:HA	33:o:161:UNK:HG3	1.93	0.51
33:o:242:UNK:O	33:o:245:UNK:CG	2.59	0.51
33:o:398:UNK:CA	33:o:401:UNK:HG3	2.40	0.51
33:o:414:UNK:O	33:o:417:UNK:CG	2.52	0.51
1:A:103:G:H1'	14:Q:9:HIS:CE1	2.46	0.51
5:F:29:LEU:HG	5:F:78:MET:HE3	1.93	0.51
24:e:148:UNK:O	24:e:152:UNK:HG2	2.11	0.51
24:e:173:UNK:HA	24:e:177:UNK:CG	2.41	0.51
24:e:197:UNK:HG2	24:e:230:UNK:CG	2.40	0.51
26:g:56:UNK:HB2	26:g:146:LYS:HZ1	1.75	0.51
27:h:296:TRP:CZ3	27:h:301:LYS:HD2	2.45	0.51
1:A:528:C:O2'	1:A:928:A:N1	2.39	0.50
4:E:288:HIS:CD2	4:E:289:THR:H	2.29	0.50
11:N:120:LEU:HD23	11:N:123:VAL:HG21	1.92	0.50
24:e:91:UNK:HG2	24:e:92:UNK:N	2.27	0.50
24:e:162:UNK:O	24:e:166:UNK:HG2	2.11	0.50
24:e:369:UNK:O	24:e:373:UNK:HG2	2.11	0.50
29:j:6:VAL:O	29:j:7:ARG:HG2	2.11	0.50
1:A:59:C:H1'	29:j:136:TYR:CD1	2.46	0.50
4:E:291:TYR:H	4:E:356:GLN:HE21	1.59	0.50
22:c:27:VAL:HA	22:c:80:LEU:HD23	1.94	0.50
24:e:48:UNK:HB2	24:e:53:UNK:HG2	1.92	0.50
24:e:203:UNK:O	24:e:206:UNK:HG3	2.10	0.50
24:e:224:UNK:HA	24:e:227:UNK:HG3	1.92	0.50
26:g:52:UNK:HB2	26:g:65:UNK:HG3	1.93	0.50
26:g:290:HIS:CE1	26:g:294:LYS:HE3	2.46	0.50
28:i:17:ARG:CZ	36:z:697:UNK:HA	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:j:151:THR:O	29:j:154:UNK:HG3	2.10	0.50
30:k:91:TYR:CD1	30:k:92:PRO:HD2	2.46	0.50
33:o:225:UNK:O	33:o:266:UNK:HG1	2.10	0.50
33:o:228:UNK:HB2	33:o:244:UNK:CG	2.41	0.50
33:o:269:UNK:CG	33:o:270:UNK:N	2.73	0.50
33:o:533:UNK:HA	33:o:536:UNK:HG3	1.94	0.50
1:A:317:A:C2	1:A:318:C:C5	2.98	0.50
1:A:455:A:N7	1:A:935:G:O2'	2.41	0.50
4:E:140:LEU:HB3	4:E:146:ILE:HD13	1.92	0.50
4:E:321:MET:HE2	4:E:325:ARG:NH2	2.26	0.50
7:I:382:LYS:HD2	7:I:388:ALA:HA	1.93	0.50
11:N:58:ARG:HG3	11:N:75:ILE:HD11	1.92	0.50
18:Y:52:Y5P:H4A	18:Y:53:Y5P:H4	1.93	0.50
20:a:81:MET:HB3	20:a:267:PHE:CE2	2.46	0.50
24:e:302:UNK:HA	24:e:305:UNK:HG3	1.94	0.50
29:j:171:ARG:HH12	34:p:190:ALA:HA	1.77	0.50
33:o:416:UNK:HA	33:o:419:UNK:HG3	1.94	0.50
1:A:12:G:H5'	4:E:229:PHE:HD2	1.77	0.50
1:A:645:A:H5'	1:A:646:C:H5	1.77	0.50
1:A:675:A:OP1	3:C:41:ARG:NH1	2.45	0.50
5:F:68:PHE:CE1	5:F:78:MET:HE1	2.46	0.50
18:V:43:Y5P:N3	18:V:44:Y5P:H4	2.27	0.50
18:Y:62:Y5P:N3	18:Y:63:Y5P:H4	2.26	0.50
24:e:29:UNK:HB2	24:e:148:UNK:HG2	1.93	0.50
24:e:265:UNK:HG3	24:e:265:UNK:O	2.11	0.50
33:o:227:UNK:HA	33:o:230:UNK:HG3	1.94	0.50
33:o:602:UNK:C	33:o:605:UNK:HG3	2.41	0.50
1:A:270:C:H2'	1:A:271:C:C6	2.47	0.50
4:E:408:TRP:NE1	4:E:412:LYS:HE3	2.27	0.50
18:Y:25:Y5P:C6	18:Y:26:Y5P:H5	2.41	0.50
30:k:301:LEU:HA	30:k:310:THR:HG21	1.94	0.50
33:o:503:UNK:HB2	33:o:513:UNK:CG	2.38	0.50
1:A:475:A:OP2	5:F:123:ARG:NH2	2.45	0.50
1:A:634:C:O2'	1:A:650:A:N1	2.41	0.50
18:Y:66:Y5P:H4A	18:Y:67:Y5P:H4	1.94	0.50
21:b:29:PRO:O	21:b:32:LEU:HB3	2.11	0.50
33:o:315:UNK:HA	33:o:318:UNK:HG3	1.94	0.50
33:o:338:UNK:HG2	33:o:365:UNK:HG1	1.89	0.50
1:A:164:C:H4'	29:j:18:VAL:HG11	1.93	0.50
1:A:707:A:H3'	1:A:708:A:C5'	2.42	0.50
1:A:846:C:H2'	1:A:847:C:O4'	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:60:UNK:O	16:T:60:UNK:CG	2.59	0.50
24:e:54:UNK:HA	24:e:57:UNK:HG3	1.94	0.50
24:e:120:UNK:O	24:e:120:UNK:HG2	2.10	0.50
24:e:243:UNK:C	24:e:244:UNK:HG3	2.41	0.50
1:A:577:C:OP2	8:J:128:LYS:HD3	2.12	0.50
4:E:156:THR:HG22	4:E:157:ILE:H	1.76	0.50
6:G:119:LYS:NZ	26:g:364:TRP:O	2.45	0.50
16:T:56:UNK:O	16:T:56:UNK:HG2	2.11	0.50
18:Y:68:Y5P:H2'	18:Y:69:Y5P:H6	1.94	0.50
26:g:93:PHE:C	26:g:95:GLU:H	2.20	0.50
29:j:63:ARG:HB3	29:j:137:HIS:HD2	1.76	0.50
33:o:191:UNK:CA	33:o:194:UNK:HG3	2.42	0.50
33:o:598:UNK:O	33:o:601:UNK:HG3	2.12	0.50
33:o:672:UNK:HA	33:o:675:UNK:HG3	1.92	0.50
34:p:74:TRP:HB3	34:p:106:PRO:HG3	1.93	0.50
1:A:565:A:HO2'	1:A:589:C:HO2'	1.60	0.50
13:P:111:ARG:HG2	34:p:235:MET:SD	2.51	0.50
18:V:8:Y5P:H6	18:V:8:Y5P:O5'	2.12	0.50
20:a:343:UNK:O	20:a:346:UNK:CG	2.29	0.50
24:e:81:UNK:C	24:e:82:UNK:HG3	2.39	0.50
24:e:221:UNK:HA	24:e:224:UNK:HG3	1.94	0.50
24:e:357:UNK:CG	24:e:358:UNK:N	2.75	0.50
24:e:398:UNK:HG2	24:e:399:UNK:N	2.26	0.50
27:h:292:GLU:HG3	27:h:296:TRP:NE1	2.27	0.50
33:o:229:UNK:HG2	33:o:230:UNK:N	2.27	0.50
33:o:232:UNK:CG	33:o:233:UNK:N	2.75	0.50
1:A:857:C:H2'	1:A:858:C:C6	2.47	0.49
3:C:50:PRO:HB3	3:C:167:ILE:HD11	1.93	0.49
7:I:226:LEU:HD11	7:I:245:PHE:CD2	2.47	0.49
18:Y:51:Y5P:H4A	18:Y:52:Y5P:C5	2.41	0.49
20:a:224:VAL:HG22	20:a:261:LEU:HD23	1.93	0.49
24:e:77:UNK:O	24:e:80:UNK:CG	2.58	0.49
26:g:138:CYS:HA	26:g:141:LEU:HB2	1.94	0.49
33:o:303:UNK:CA	33:o:306:UNK:HG3	2.37	0.49
33:o:420:UNK:HB2	33:o:459:UNK:CG	2.40	0.49
1:A:807:G:C6	1:A:809:G:C2	3.00	0.49
3:C:94:LYS:HZ1	4:E:92:LYS:HB2	1.78	0.49
7:I:253:UNK:O	7:I:254:UNK:HG2	2.13	0.49
10:L:70:PRO:HG3	10:L:78:ARG:HE	1.77	0.49
18:Y:54:Y5P:H4A	18:Y:55:Y5P:C4	2.36	0.49
20:a:349:UNK:HG2	20:a:350:UNK:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:c:125:HIS:HD2	22:c:127:ALA:N	2.07	0.49
22:c:129:PHE:CE2	22:c:140:MET:HB2	2.47	0.49
24:e:112:UNK:HA	24:e:115:UNK:CG	2.38	0.49
24:e:386:UNK:O	24:e:389:UNK:CG	2.58	0.49
33:o:274:UNK:CG	33:o:275:UNK:N	2.74	0.49
33:o:310:UNK:HG1	33:o:348:UNK:HB1	1.93	0.49
33:o:481:UNK:C	33:o:484:UNK:HG3	2.40	0.49
1:A:432:A:H4'	1:A:433:U:H5''	1.95	0.49
4:E:160:ARG:NH1	4:E:168:VAL:HG21	2.28	0.49
8:J:91:TYR:OH	8:J:160:ILE:HG23	2.13	0.49
18:V:49:Y5P:O5'	18:V:49:Y5P:H6	2.11	0.49
24:e:35:UNK:C	24:e:38:UNK:HG3	2.41	0.49
24:e:218:UNK:CB	24:e:256:UNK:HG1	2.43	0.49
26:g:122:ARG:HH11	26:g:336:LEU:CD2	2.25	0.49
26:g:191:LYS:NZ	26:g:198:LEU:HD12	2.28	0.49
26:g:286:LEU:HD12	26:g:289:ILE:HD12	1.93	0.49
26:g:356:ILE:HG21	26:g:376:LYS:HD2	1.94	0.49
33:o:278:UNK:HA	33:o:281:UNK:HG3	1.93	0.49
33:o:379:UNK:CA	33:o:382:UNK:HG3	2.38	0.49
33:o:433:UNK:HA	33:o:436:UNK:CG	2.41	0.49
23:d:166:THR:O	23:d:176:ARG:NH2	2.46	0.49
24:e:51:UNK:HA	24:e:54:UNK:CG	2.41	0.49
24:e:243:UNK:CG	24:e:245:UNK:CG	2.88	0.49
24:e:243:UNK:HG1	24:e:245:UNK:HG3	1.91	0.49
33:o:237:UNK:O	33:o:241:UNK:HG3	2.12	0.49
33:o:318:UNK:HA	33:o:321:UNK:CG	2.37	0.49
33:o:411:UNK:CA	33:o:414:UNK:HG3	2.43	0.49
33:o:554:UNK:HG3	33:o:555:UNK:N	2.28	0.49
2:B:238:ASN:ND2	2:B:241:SER:HB3	2.28	0.49
5:F:54:HIS:NE2	5:F:85:ASP:O	2.45	0.49
20:a:264:THR:HG22	20:a:266:HIS:H	1.78	0.49
20:a:314:UNK:O	20:a:317:UNK:HG3	2.13	0.49
20:a:342:UNK:HA	20:a:345:UNK:CG	2.43	0.49
27:h:292:GLU:HG3	27:h:296:TRP:HE1	1.77	0.49
29:j:175:LEU:HA	29:j:178:ARG:HD3	1.94	0.49
1:A:97:C:H5'	1:A:98:A:OP2	2.13	0.49
3:C:37:ASN:H	3:C:37:ASN:HD22	1.60	0.49
3:C:110:LEU:HD22	3:C:119:ILE:HG12	1.94	0.49
20:a:190:ARG:HG3	20:a:191:MET:HE2	1.94	0.49
24:e:73:UNK:HG2	24:e:74:UNK:N	2.26	0.49
24:e:108:UNK:CG	24:e:109:UNK:N	2.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:e:235:UNK:CG	24:e:236:UNK:N	2.76	0.49
24:e:355:UNK:O	24:e:358:UNK:HG2	2.11	0.49
29:j:114:ALA:C	29:j:115:TRP:HD1	2.20	0.49
33:o:359:UNK:O	33:o:363:UNK:HB1	2.12	0.49
5:F:9:ILE:HB	5:F:89:ILE:HG22	1.95	0.49
11:N:37:ASP:O	11:N:41:ARG:HG2	2.12	0.49
18:Y:54:Y5P:N3	18:Y:58:Y5P:C5	2.76	0.49
24:e:49:UNK:CG	24:e:52:UNK:HG2	2.43	0.49
29:j:118:LEU:HD12	29:j:119:THR:N	2.28	0.49
33:o:228:UNK:HB2	33:o:244:UNK:HG1	1.95	0.49
33:o:337:UNK:HG2	33:o:338:UNK:N	2.27	0.49
33:o:514:UNK:HA	33:o:517:UNK:HG3	1.95	0.49
33:o:654:UNK:HA	33:o:657:UNK:HG3	1.94	0.49
34:p:208:PRO:HG2	34:p:213:LEU:HD21	1.93	0.49
1:A:28:U:H2'	1:A:29:A:C8	2.46	0.49
1:A:579:A:H8	1:A:579:A:OP1	1.95	0.49
6:G:152:CYS:SG	6:G:219:VAL:HB	2.53	0.49
6:G:231:GLU:HA	31:m:53:MET:SD	2.52	0.49
7:I:316:PHE:CE1	7:I:370:LEU:HD21	2.48	0.49
16:T:65:UNK:HG2	16:T:67:UNK:HB1	1.93	0.49
18:V:54:Y5P:H4A	18:V:55:Y5P:C4	2.43	0.49
24:e:61:UNK:HG1	24:e:94:UNK:HB2	1.93	0.49
24:e:287:UNK:HA	24:e:290:UNK:HG3	1.93	0.49
24:e:301:UNK:HA	24:e:304:UNK:HG3	1.95	0.49
29:j:31:SER:HA	29:j:111:HIS:CD2	2.47	0.49
29:j:64:LEU:HD13	29:j:80:VAL:HG11	1.93	0.49
29:j:192:ASN:HB3	29:j:194:GLU:HG3	1.94	0.49
33:o:197:UNK:HG1	33:o:230:UNK:CG	2.43	0.49
3:C:125:ARG:NH1	33:o:94:TYR:HB2	2.28	0.49
7:I:71:VAL:HG12	7:I:75:LYS:HE3	1.95	0.49
9:K:65:TYR:O	9:K:67:PRO:HD3	2.12	0.49
14:Q:14:VAL:HG12	22:c:29:VAL:HG11	1.95	0.49
20:a:319:UNK:HG2	20:a:320:UNK:N	2.20	0.49
20:a:346:UNK:CG	20:a:347:UNK:N	2.76	0.49
21:b:35:TYR:OH	21:b:43:GLU:OE1	2.30	0.49
24:e:59:UNK:HA	24:e:62:UNK:HG3	1.95	0.49
24:e:248:UNK:CA	24:e:251:UNK:HG3	2.41	0.49
24:e:392:UNK:O	24:e:395:UNK:HG3	2.12	0.49
26:g:122:ARG:NH1	26:g:336:LEU:HD23	2.27	0.49
33:o:280:UNK:HA	33:o:283:UNK:CG	2.42	0.49
33:o:507:UNK:HG1	33:o:541:UNK:CB	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:p:217:ARG:HA	34:p:224:LEU:HD13	1.95	0.49
1:A:4:C:N4	4:E:427:ARG:HD3	2.28	0.49
1:A:357:G:H5'	9:K:98:GLN:HE21	1.78	0.49
1:A:761:U:OP1	28:i:32:LYS:NZ	2.39	0.49
1:A:824:G:N2	1:A:827:A:H61	2.10	0.49
13:P:100:HIS:CD2	13:P:102:MET:H	2.30	0.49
20:a:314:UNK:O	20:a:318:UNK:CG	2.35	0.49
24:e:394:UNK:CG	24:e:395:UNK:N	2.75	0.49
26:g:273:LEU:HB2	26:g:281:ILE:HD11	1.95	0.49
30:k:88:ARG:HB3	30:k:98:PRO:HB2	1.95	0.49
30:k:115:HIS:CD2	30:k:116:LEU:HG	2.48	0.49
33:o:116:ALA:O	33:o:120:ILE:HG12	2.12	0.49
33:o:127:TYR:CD1	33:o:127:TYR:N	2.81	0.49
33:o:280:UNK:CA	33:o:283:UNK:HG3	2.43	0.49
33:o:356:UNK:HA	33:o:359:UNK:HG3	1.95	0.49
33:o:459:UNK:HA	33:o:462:UNK:CG	2.43	0.49
1:A:228:G:H2'	1:A:229:U:C6	2.48	0.48
5:F:92:ASN:HD22	5:F:93:ILE:H	1.60	0.48
6:G:66:ARG:HB3	6:G:70:LYS:NZ	2.28	0.48
18:Y:56:Y5P:O2'	18:Y:57:Y5P:O4'	2.31	0.48
22:c:137:ARG:HH12	22:c:143:VAL:CG2	2.25	0.48
24:e:92:UNK:O	24:e:95:UNK:HG3	2.12	0.48
24:e:359:UNK:O	24:e:363:UNK:HG3	2.13	0.48
26:g:52:UNK:CG	26:g:66:UNK:N	2.76	0.48
26:g:54:UNK:CG	26:g:66:UNK:O	2.61	0.48
29:j:54:ALA:HB1	29:j:136:TYR:OH	2.13	0.48
29:j:120:PHE:HZ	29:j:202:ASP:HB2	1.79	0.48
18:V:23:Y5P:C4	18:V:24:Y5P:H4	2.39	0.48
18:Y:61:Y5P:H4A	18:Y:62:Y5P:H4	1.95	0.48
33:o:344:UNK:CG	33:o:345:UNK:N	2.75	0.48
33:o:443:UNK:O	33:o:447:UNK:HB1	2.13	0.48
3:C:37:ASN:H	3:C:37:ASN:ND2	2.12	0.48
8:J:68:GLU:HB2	33:o:62:LYS:HE2	1.94	0.48
23:d:68:ARG:O	23:d:72:LEU:HG	2.13	0.48
26:g:65:UNK:O	26:g:99:MET:HA	2.13	0.48
26:g:205:GLU:H	26:g:217:LYS:HB3	1.79	0.48
33:o:482:UNK:O	33:o:486:UNK:HB1	2.13	0.48
33:o:515:UNK:HA	33:o:518:UNK:HG3	1.93	0.48
1:A:195:G:C4	1:A:208:A:C2	3.00	0.48
1:A:624:U:H4'	1:A:625:U:H4'	1.95	0.48
1:A:928:A:H5'	1:A:930:G:N7	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:85:ARG:CZ	30:k:163:PRO:HD2	2.43	0.48
7:I:123:PRO:HA	30:k:89:MET:HG3	1.94	0.48
24:e:395:UNK:CA	24:e:398:UNK:HG3	2.40	0.48
31:m:85:LYS:O	31:m:88:SER:OG	2.20	0.48
33:o:336:UNK:HA	33:o:339:UNK:HB1	1.95	0.48
33:o:363:UNK:HG2	33:o:364:UNK:N	2.26	0.48
33:o:485:UNK:HA	33:o:488:UNK:HG3	1.95	0.48
1:A:386:U:H2'	1:A:387:C:C6	2.48	0.48
1:A:671:U:H2'	1:A:672:A:H8	1.77	0.48
7:I:323:ARG:HB3	7:I:327:HIS:CD2	2.48	0.48
13:P:73:ILE:O	13:P:77:ILE:HG13	2.12	0.48
18:Y:25:Y5P:H2'	18:Y:26:Y5P:C6	2.40	0.48
33:o:652:UNK:HB2	33:o:674:UNK:O	2.14	0.48
1:A:917:C:H5'	1:A:918:A:OP2	2.13	0.48
8:J:170:MET:HB3	30:k:159:VAL:CG1	2.43	0.48
18:V:12:Y5P:H4A	18:V:13:Y5P:C4	2.40	0.48
20:a:352:UNK:HG2	20:a:353:UNK:N	2.29	0.48
24:e:233:UNK:O	24:e:236:UNK:HG2	2.13	0.48
26:g:52:UNK:HG1	26:g:65:UNK:HA	1.95	0.48
29:j:150:PHE:O	29:j:153:UNK:HG2	2.14	0.48
31:m:68:LYS:HA	31:m:68:LYS:HD2	1.64	0.48
2:B:238:ASN:HD21	2:B:241:SER:HB3	1.79	0.48
6:G:68:PHE:HB3	7:I:367:GLN:NE2	2.22	0.48
20:a:166:HIS:O	20:a:188:ARG:NH2	2.46	0.48
24:e:93:UNK:O	24:e:97:UNK:HG3	2.13	0.48
24:e:105:UNK:HA	24:e:108:UNK:HG3	1.95	0.48
24:e:106:UNK:HG2	24:e:107:UNK:N	2.28	0.48
24:e:181:UNK:CG	24:e:210:UNK:HG3	2.04	0.48
26:g:68:UNK:HG3	26:g:69:UNK:N	2.28	0.48
29:j:129:ARG:CZ	29:j:206:LYS:HB3	2.44	0.48
31:m:53:MET:HE2	31:m:53:MET:HA	1.96	0.48
33:o:116:ALA:O	33:o:119:PHE:HB3	2.13	0.48
33:o:285:UNK:HA	33:o:288:UNK:HG3	1.94	0.48
33:o:359:UNK:HA	33:o:362:UNK:HG3	1.94	0.48
33:o:538:UNK:C	33:o:550:UNK:HG1	2.40	0.48
1:A:124:A:H4'	1:A:125:U:O5'	2.14	0.48
1:A:959:U:H4'	1:A:960:A:O5'	2.11	0.48
14:Q:57:GLN:O	14:Q:57:GLN:NE2	2.46	0.48
24:e:211:UNK:HA	24:e:216:UNK:HG1	1.95	0.48
31:m:64:GLU:HA	31:m:67:ARG:CZ	2.44	0.48
33:o:177:UNK:HA	33:o:180:UNK:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:o:204:UNK:HA	33:o:207:UNK:CG	2.41	0.48
33:o:550:UNK:C	33:o:553:UNK:HG3	2.43	0.48
33:o:602:UNK:HA	33:o:605:UNK:HG3	1.96	0.48
34:p:187:THR:O	34:p:189:PRO:HD3	2.14	0.48
34:p:210:GLU:OE2	34:p:217:ARG:NH2	2.47	0.48
1:A:96:U:O2'	13:P:38:HIS:ND1	2.43	0.48
2:B:140:ILE:HB	2:B:189:PRO:HA	1.96	0.48
3:C:80:ASP:HB3	3:C:81:HIS:CD2	2.49	0.48
3:C:92:LEU:HD21	3:C:147:TYR:HE2	1.79	0.48
5:F:71:PRO:HB3	12:O:97:GLU:O	2.13	0.48
7:I:358:THR:HG23	7:I:361:GLU:H	1.78	0.48
15:R:120:PHE:N	15:R:120:PHE:CD1	2.81	0.48
18:Y:55:Y5P:C6	18:Y:58:Y5P:H5	2.44	0.48
29:j:165:PRO:HG2	34:p:200:TYR:CE1	2.49	0.48
33:o:439:UNK:C	33:o:442:UNK:HG3	2.43	0.48
33:o:479:UNK:HA	33:o:482:UNK:HG3	1.95	0.48
1:A:37:A:OP1	22:c:162:LYS:NZ	2.31	0.48
1:A:202:A:N1	29:j:53:ARG:NH2	2.62	0.48
4:E:191:ARG:HH21	34:p:78:ARG:HG2	1.79	0.48
12:O:210:LEU:HB2	32:n:189:TRP:CZ2	2.49	0.48
20:a:326:UNK:HA	20:a:329:UNK:HG3	1.96	0.48
20:a:344:UNK:CA	20:a:347:UNK:HG3	2.44	0.48
26:g:325:GLN:HB3	30:k:306:ASP:OD2	2.14	0.48
33:o:656:UNK:HA	33:o:659:UNK:HG3	1.95	0.48
1:A:831:A:H2'	1:A:832:G:C8	2.49	0.47
2:B:140:ILE:HD12	2:B:140:ILE:H	1.79	0.47
3:C:105:ALA:HB3	3:C:122:LEU:HB3	1.96	0.47
12:O:129:ARG:HB2	12:O:167:MET:CE	2.40	0.47
18:V:36:P5P:H6	18:V:37:Y5P:H4	1.94	0.47
24:e:81:UNK:O	24:e:82:UNK:CG	2.53	0.47
26:g:203:VAL:HG13	26:g:245:GLU:HG2	1.96	0.47
33:o:601:UNK:HG1	33:o:655:UNK:HB1	1.95	0.47
1:A:159:C:H2'	1:A:160:C:H5'	1.95	0.47
1:A:276:U:H2'	1:A:277:A:H8	1.79	0.47
1:A:419:A:H2'	1:A:420:A:O4'	2.15	0.47
1:A:842:A:H5'	1:A:845:G:H4'	1.96	0.47
7:I:104:ILE:O	7:I:108:ILE:HG13	2.14	0.47
7:I:274:GLU:HG2	7:I:283:GLU:HG2	1.96	0.47
20:a:309:UNK:O	20:a:309:UNK:CG	2.61	0.47
25:f:145:LEU:HD21	25:f:148:LEU:HD13	1.96	0.47
26:g:140:ILE:HD13	26:g:306:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:j:98:THR:HG22	29:j:99:ARG:HG3	1.96	0.47
30:k:204:THR:HB	30:k:206:VAL:HG23	1.95	0.47
33:o:267:UNK:HA	33:o:270:UNK:CG	2.42	0.47
35:s:2361:UNK:C	35:s:2364:UNK:HG3	2.43	0.47
2:B:235:VAL:HG21	2:B:248:PHE:CE1	2.49	0.47
4:E:332:LEU:HD12	4:E:333:TYR:N	2.29	0.47
7:I:271:SER:OG	7:I:352:ALA:O	2.31	0.47
20:a:348:UNK:C	20:a:351:UNK:HG3	2.44	0.47
27:h:323:HIS:CD2	27:h:361:LYS:HZ1	2.15	0.47
29:j:6:VAL:C	29:j:7:ARG:HG2	2.40	0.47
30:k:264:ILE:HD11	30:k:294:TYR:CG	2.48	0.47
33:o:227:UNK:O	33:o:230:UNK:HG3	2.13	0.47
33:o:239:UNK:O	33:o:242:UNK:HG3	2.15	0.47
33:o:338:UNK:CA	33:o:341:UNK:HG3	2.42	0.47
33:o:437:UNK:HA	33:o:440:UNK:HG3	1.95	0.47
1:A:174:C:H2'	1:A:175:A:O4'	2.14	0.47
4:E:294:ILE:HB	4:E:305:MET:HG3	1.95	0.47
6:G:190:GLU:O	6:G:194:LYS:HG2	2.14	0.47
7:I:123:PRO:CA	30:k:89:MET:HG3	2.44	0.47
7:I:290:GLY:CA	7:I:328:ASP:HB2	2.45	0.47
7:I:318:LEU:HD23	7:I:353:LEU:HD11	1.95	0.47
26:g:145:ALA:HB2	26:g:151:ILE:HG13	1.96	0.47
1:A:358:U:H2'	1:A:359:U:H6	1.77	0.47
7:I:275:GLY:N	7:I:348:ALA:HB2	2.30	0.47
9:K:128:ILE:O	9:K:132:THR:OG1	2.29	0.47
12:O:126:LEU:HB3	12:O:171:LEU:HD21	1.96	0.47
18:V:8:Y5P:N3	18:V:14:Y5P:C5	2.69	0.47
20:a:285:ILE:HD11	20:a:340:UNK:HG1	1.97	0.47
24:e:82:UNK:O	24:e:82:UNK:HG2	2.15	0.47
26:g:56:UNK:HB2	26:g:146:LYS:NZ	2.30	0.47
26:g:184:SER:OG	26:g:232:VAL:HG13	2.15	0.47
33:o:174:UNK:HA	33:o:177:UNK:CG	2.41	0.47
33:o:231:UNK:O	33:o:235:UNK:CG	2.62	0.47
33:o:241:UNK:HA	33:o:244:UNK:CG	2.42	0.47
33:o:303:UNK:CG	33:o:340:UNK:HG2	2.44	0.47
33:o:478:UNK:HA	33:o:481:UNK:HG3	1.96	0.47
33:o:481:UNK:O	33:o:485:UNK:HG3	2.14	0.47
33:o:548:UNK:HA	33:o:551:UNK:HG3	1.95	0.47
1:A:87:U:H2'	1:A:88:C:C6	2.49	0.47
1:A:423:U:H2'	1:A:424:G:C8	2.49	0.47
1:A:637:A:N7	21:b:48:ARG:HD2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:858:C:H42	1:A:912:A:H61	1.62	0.47
2:B:232:THR:HA	21:b:44:PRO:HB3	1.95	0.47
4:E:126:LEU:HD21	28:i:81:GLU:OE1	2.14	0.47
8:J:180:LEU:HD23	8:J:181:PRO:HD2	1.95	0.47
15:R:104:LYS:HD3	15:R:104:LYS:HA	1.62	0.47
18:V:32:Y5P:H4A	18:V:33:Y5P:H4	1.97	0.47
18:V:36:P5P:C6	18:V:37:Y5P:H4	2.44	0.47
26:g:59:UNK:HG1	26:g:62:UNK:HG1	1.97	0.47
26:g:66:UNK:O	26:g:66:UNK:HG2	2.14	0.47
26:g:107:LEU:HD22	26:g:342:ILE:HD12	1.95	0.47
26:g:275:ARG:NH2	26:g:285:GLU:OE2	2.47	0.47
28:i:17:ARG:NH1	36:z:697:UNK:HA	2.28	0.47
29:j:52:MET:HA	29:j:55:TRP:CD1	2.49	0.47
29:j:95:TRP:HE1	29:j:131:ILE:HG12	1.80	0.47
29:j:114:ALA:C	29:j:115:TRP:CD1	2.92	0.47
33:o:411:UNK:HA	33:o:414:UNK:CG	2.45	0.47
33:o:464:UNK:HA	33:o:467:UNK:HG3	1.96	0.47
35:s:2370:UNK:HA	35:s:2373:UNK:CG	2.45	0.47
1:A:405:G:N1	1:A:452:C:O2'	2.44	0.47
1:A:546:U:O2'	1:A:547:A:H5'	2.15	0.47
1:A:604:U:C2	28:i:95:ARG:HD3	2.50	0.47
1:A:653:A:H2'	1:A:654:A:N7	2.30	0.47
1:A:787:A:H2'	1:A:788:G:C8	2.49	0.47
3:C:72:HIS:CD2	3:C:74:GLY:H	2.30	0.47
4:E:426:LYS:HB3	34:p:136:HIS:CD2	2.50	0.47
6:G:71:THR:HG23	7:I:253:UNK:CG	2.45	0.47
6:G:147:GLN:HG3	6:G:151:ASN:HD21	1.80	0.47
8:J:102:LEU:HB3	8:J:104:ILE:HG13	1.96	0.47
8:J:179:GLN:O	30:k:150:PRO:HD2	2.15	0.47
9:K:138:ALA:HB1	9:K:172:LEU:HB2	1.95	0.47
13:P:105:THR:OG1	23:d:56:LEU:HD21	2.14	0.47
18:V:12:Y5P:C4	18:V:13:Y5P:H4	2.39	0.47
18:Y:34:P5P:H8	18:Y:34:P5P:O5'	2.14	0.47
20:a:167:ARG:HH12	20:a:237:ASP:CG	2.22	0.47
20:a:300:VAL:HG11	20:a:330:UNK:HG1	1.95	0.47
24:e:53:UNK:O	24:e:57:UNK:HG3	2.14	0.47
24:e:68:UNK:HB2	24:e:70:UNK:HG3	1.97	0.47
24:e:86:UNK:O	24:e:89:UNK:HG3	2.13	0.47
24:e:109:UNK:HA	24:e:112:UNK:CG	2.42	0.47
30:k:268:LEU:HD23	30:k:271:ILE:HD12	1.97	0.47
33:o:157:UNK:HG3	33:o:177:UNK:HG1	1.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:o:282:UNK:HA	33:o:285:UNK:HG3	1.97	0.47
33:o:373:UNK:O	33:o:377:UNK:HG3	2.15	0.47
33:o:377:UNK:HG2	33:o:378:UNK:N	2.30	0.47
33:o:418:UNK:C	33:o:421:UNK:HG3	2.45	0.47
33:o:531:UNK:CA	33:o:534:UNK:HG3	2.43	0.47
33:o:653:UNK:HA	33:o:656:UNK:HG3	1.96	0.47
34:p:54:GLU:HA	34:p:55:PRO:HD3	1.45	0.47
1:A:672:A:C2	11:N:127:MET:HE3	2.45	0.47
3:C:125:ARG:HH11	33:o:94:TYR:HD2	1.62	0.47
7:I:296:VAL:HG13	7:I:331:CYS:SG	2.54	0.47
7:I:390:ARG:HD2	7:I:391:LYS:N	2.29	0.47
12:O:143:HIS:CE1	12:O:147:HIS:CD2	3.03	0.47
13:P:21:LEU:HB3	13:P:32:TYR:CD2	2.49	0.47
17:U:35:LEU:O	17:U:39:ILE:HG12	2.15	0.47
20:a:168:GLU:HG3	34:p:181:HIS:CD2	2.50	0.47
24:e:249:UNK:HG2	24:e:250:UNK:N	2.30	0.47
24:e:297:UNK:HG2	24:e:298:UNK:N	2.30	0.47
30:k:154:ASP:HB2	30:k:174:THR:HB	1.96	0.47
30:k:268:LEU:HA	30:k:271:ILE:HB	1.95	0.47
33:o:346:UNK:CG	33:o:379:UNK:HB2	2.37	0.47
1:A:357:G:N2	9:K:100:GLN:HE22	2.12	0.47
1:A:689:G:H5'	4:E:91:THR:HG22	1.95	0.47
7:I:94:GLU:HB2	7:I:99:PHE:CE2	2.50	0.47
7:I:119:LYS:HA	7:I:122:ARG:HD2	1.97	0.47
13:P:100:HIS:HB3	13:P:103:MET:HG3	1.96	0.47
14:Q:55:LEU:HB2	14:Q:57:GLN:HB2	1.96	0.47
18:V:63:Y5P:H2'	18:V:64:Y5P:H6	1.97	0.47
24:e:60:UNK:O	24:e:63:UNK:HG3	2.15	0.47
24:e:170:UNK:HG1	29:j:78:ARG:CZ	2.44	0.47
24:e:213:UNK:O	24:e:216:UNK:HG2	2.11	0.47
31:m:49:MET:O	31:m:53:MET:HG2	2.15	0.47
33:o:222:UNK:CA	33:o:225:UNK:HG3	2.43	0.47
33:o:434:UNK:HA	33:o:437:UNK:HG3	1.97	0.47
33:o:480:UNK:HB1	33:o:513:UNK:HB1	1.97	0.47
1:A:317:A:H2	1:A:318:C:H5	1.62	0.47
1:A:956:G:H2'	1:A:957:A:O4'	2.15	0.47
4:E:148:LEU:HD11	33:o:109:ALA:HB2	1.97	0.47
4:E:162:LYS:O	4:E:166:GLU:HG2	2.15	0.47
6:G:195:LYS:N	6:G:204:LYS:HZ1	2.13	0.47
7:I:206:LEU:HD23	7:I:206:LEU:HA	1.77	0.47
11:N:80:ARG:HD2	11:N:86:ARG:HH12	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:92:VAL:HG12	11:N:93:MET:HE3	1.96	0.47
24:e:279:UNK:CG	24:e:280:UNK:N	2.77	0.47
26:g:150:LEU:HD22	26:g:150:LEU:HA	1.61	0.47
30:k:214:CYS:HB3	30:k:219:GLN:OE1	2.15	0.47
32:n:189:TRP:HE1	32:n:191:THR:HG23	1.79	0.47
33:o:244:UNK:HA	33:o:247:UNK:HG3	1.97	0.47
1:A:158:C:H2'	1:A:159:C:C6	2.50	0.46
2:B:149:GLN:HG2	17:U:84:TRP:CE2	2.50	0.46
7:I:145:ARG:HA	7:I:146:PRO:HD3	1.69	0.46
7:I:323:ARG:HB3	7:I:327:HIS:HD2	1.80	0.46
7:I:373:ALA:O	7:I:375:PRO:HD3	2.15	0.46
20:a:340:UNK:C	20:a:343:UNK:HG3	2.35	0.46
20:a:347:UNK:CG	20:a:348:UNK:N	2.78	0.46
24:e:284:UNK:HA	24:e:287:UNK:CG	2.44	0.46
25:f:123:CYS:SG	25:f:168:ALA:HB3	2.55	0.46
27:h:296:TRP:HZ3	27:h:301:LYS:HD2	1.81	0.46
33:o:324:UNK:HA	33:o:327:UNK:HG3	1.97	0.46
4:E:95:ALA:HB2	28:i:74:GLU:HB3	1.97	0.46
11:N:70:VAL:O	11:N:74:GLU:HG2	2.15	0.46
12:O:100:ASN:OD1	12:O:101:GLN:N	2.47	0.46
15:R:87:PRO:HG2	15:R:88:PHE:CD2	2.51	0.46
20:a:235:GLU:CD	34:p:173:ARG:HH12	2.23	0.46
33:o:241:UNK:HG1	33:o:270:UNK:HB2	1.95	0.46
34:p:80:ASN:ND2	34:p:80:ASN:H	2.13	0.46
1:A:409:G:H4'	1:A:939:A:H4'	1.96	0.46
7:I:127:HIS:HD2	7:I:129:GLU:H	1.63	0.46
14:Q:27:LYS:HG3	14:Q:50:PHE:CE1	2.50	0.46
14:Q:98:LYS:NZ	14:Q:109:PRO:HG3	2.31	0.46
22:c:13:LEU:HA	22:c:13:LEU:HD23	1.81	0.46
24:e:216:UNK:HG2	24:e:217:UNK:N	2.30	0.46
24:e:406:UNK:C	24:e:407:UNK:HG3	2.45	0.46
25:f:142:ARG:HD2	25:f:175:GLU:HG3	1.96	0.46
30:k:78:PHE:HB2	30:k:112:ASN:ND2	2.31	0.46
33:o:192:UNK:O	33:o:195:UNK:HG3	2.15	0.46
1:A:815:U:H2'	1:A:816:U:C6	2.50	0.46
40:A:7154:HOH:O	18:V:29:Y5P:C4	2.59	0.46
7:I:252:UNK:HG2	7:I:252:UNK:O	2.16	0.46
15:R:89:THR:HG21	15:R:91:CYS:SG	2.55	0.46
21:b:125:LEU:O	21:b:130:VAL:HG22	2.15	0.46
24:e:124:UNK:HA	24:e:127:UNK:CG	2.45	0.46
25:f:123:CYS:HB2	25:f:166:ALA:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:o:497:UNK:HA	33:o:500:UNK:HG3	1.97	0.46
1:A:127:A:H4'	1:A:128:C:OP1	2.15	0.46
1:A:498:U:H5'	1:A:499:C:OP2	2.15	0.46
2:B:176:THR:HA	2:B:214:MET:HE1	1.98	0.46
3:C:129:PRO:HB2	33:o:106:PHE:HE1	1.81	0.46
12:O:178:VAL:O	12:O:182:ILE:HG12	2.15	0.46
22:c:94:SER:HB2	22:c:97:GLU:HG3	1.98	0.46
24:e:59:UNK:HA	24:e:62:UNK:CG	2.46	0.46
29:j:65:LEU:HD21	29:j:102:PRO:HB3	1.97	0.46
29:j:76:LEU:O	29:j:97:LEU:HB2	2.15	0.46
29:j:95:TRP:HZ3	29:j:118:LEU:HD22	1.80	0.46
34:p:150:LEU:HD23	34:p:150:LEU:HA	1.70	0.46
34:p:213:LEU:O	34:p:217:ARG:HG3	2.15	0.46
1:A:52:C:O2'	1:A:207:G:N7	2.43	0.46
1:A:344:G:H1	9:K:121:ASN:HB2	1.80	0.46
1:A:391:U:H4'	12:O:156:PHE:CE1	2.50	0.46
1:A:454:A:H2'	1:A:456:A:H5''	1.97	0.46
1:A:899:C:C3'	1:A:900:A:H4'	2.46	0.46
2:B:117:LEU:HD23	2:B:117:LEU:HA	1.78	0.46
2:B:230:LEU:HA	2:B:230:LEU:HD23	1.74	0.46
4:E:380:LEU:HD12	4:E:381:PRO:HD2	1.98	0.46
6:G:104:LYS:HD3	6:G:104:LYS:HA	1.70	0.46
24:e:74:UNK:HA	24:e:77:UNK:CG	2.44	0.46
24:e:91:UNK:O	24:e:94:UNK:CG	2.55	0.46
24:e:112:UNK:CA	24:e:115:UNK:HG3	2.40	0.46
24:e:127:UNK:O	24:e:131:UNK:CG	2.59	0.46
24:e:280:UNK:CA	24:e:283:UNK:HG3	2.46	0.46
33:o:264:UNK:HB2	33:o:289:UNK:HG2	1.98	0.46
1:A:42:A:HO2'	1:A:43:U:P	2.37	0.46
1:A:316:C:H2'	1:A:318:C:C5	2.50	0.46
2:B:161:CYS:SG	2:B:253:GLN:HA	2.56	0.46
7:I:94:GLU:HB2	7:I:99:PHE:HE2	1.81	0.46
16:T:63:UNK:CG	24:e:54:UNK:HG1	2.46	0.46
24:e:94:UNK:HG2	24:e:95:UNK:N	2.30	0.46
24:e:190:UNK:HG2	24:e:191:UNK:N	2.30	0.46
24:e:280:UNK:HA	24:e:283:UNK:CG	2.45	0.46
24:e:365:UNK:HG2	24:e:368:UNK:CG	2.45	0.46
29:j:83:LYS:O	29:j:86:LEU:HB2	2.16	0.46
30:k:86:PRO:HA	30:k:101:LYS:HD3	1.97	0.46
30:k:165:ILE:HG13	33:o:135:PRO:HD3	1.97	0.46
30:k:226:TYR:HD2	36:z:706:UNK:HG1	1.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:o:442:UNK:O	33:o:446:UNK:HG3	2.15	0.46
1:A:503:A:H2'	1:A:503:A:N3	2.31	0.46
1:A:899:C:C2'	1:A:900:A:H4'	2.46	0.46
14:Q:36:ASP:HA	14:Q:37:PRO:HD3	1.60	0.46
24:e:232:UNK:HG2	24:e:232:UNK:O	2.15	0.46
24:e:296:UNK:C	24:e:299:UNK:HG3	2.46	0.46
25:f:84:MET:HE2	25:f:84:MET:HB3	1.83	0.46
29:j:171:ARG:NH1	34:p:190:ALA:HA	2.31	0.46
31:m:17:ARG:HD3	31:m:18:ARG:N	2.29	0.46
34:p:105:CYS:HB3	34:p:106:PRO:HD2	1.97	0.46
1:A:649:U:H3'	1:A:650:A:H5''	1.96	0.46
9:K:131:GLN:HB2	9:K:169:MET:HE1	1.98	0.46
12:O:73:LEU:HD11	12:O:83:ILE:HG21	1.98	0.46
15:R:84:PHE:HE2	15:R:100:LEU:HD21	1.81	0.46
26:g:54:UNK:HG1	26:g:66:UNK:O	2.15	0.46
26:g:347:TYR:CD1	26:g:351:GLU:HB3	2.51	0.46
33:o:265:UNK:CA	33:o:268:UNK:HG3	2.46	0.46
34:p:79:ARG:NH2	34:p:90:THR:HA	2.30	0.46
1:A:93:A:O2'	23:d:79:ARG:NH1	2.49	0.46
1:A:896:A:H3'	1:A:897:C:H4'	1.97	0.46
4:E:289:THR:HG23	4:E:331:ASP:O	2.16	0.46
6:G:238:HIS:CE1	9:K:126:THR:HB	2.50	0.46
18:V:42:Y5P:H4A	18:V:43:Y5P:H4	1.98	0.46
18:Y:44:Y5P:O5'	18:Y:44:Y5P:H6	2.16	0.46
20:a:204:LEU:N	22:c:144:GLU:OE1	2.40	0.46
26:g:158:HIS:CD2	26:g:314:SER:HA	2.50	0.46
34:p:207:GLN:HA	34:p:208:PRO:HD3	1.71	0.46
1:A:59:C:N3	29:j:133:GLN:HB3	2.31	0.45
2:B:173:GLY:O	2:B:177:ASN:N	2.46	0.45
7:I:87:HIS:O	7:I:91:MET:HG2	2.17	0.45
12:O:80:VAL:HG23	12:O:83:ILE:HD11	1.98	0.45
18:Y:3:Y5P:O5'	18:Y:3:Y5P:H6	2.16	0.45
20:a:205:THR:HA	20:a:206:PRO:HD3	1.81	0.45
20:a:217:MET:HG2	20:a:226:VAL:HG22	1.98	0.45
24:e:109:UNK:O	24:e:113:UNK:HB1	2.16	0.45
26:g:101:ARG:HB3	26:g:103:PRO:HD2	1.98	0.45
33:o:355:UNK:C	33:o:358:UNK:HG3	2.46	0.45
33:o:367:UNK:HG2	33:o:368:UNK:N	2.31	0.45
33:o:373:UNK:O	33:o:376:UNK:HG3	2.15	0.45
1:A:303:U:OP2	1:A:398:G:N1	2.44	0.45
1:A:375:A:H2'	1:A:376:C:H6	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:U:O4	8:J:131:ARG:NH1	2.50	0.45
4:E:332:LEU:HD12	4:E:333:TYR:H	1.82	0.45
6:G:94:PHE:CD2	6:G:111:MET:HE1	2.52	0.45
8:J:183:HIS:CE1	36:z:708:UNK:HG2	2.51	0.45
9:K:176:SER:HB2	17:U:13:MET:HG2	1.99	0.45
18:Y:25:Y5P:C4	18:Y:26:Y5P:C5	2.94	0.45
24:e:28:UNK:HB1	24:e:369:UNK:CG	2.46	0.45
24:e:300:UNK:HA	24:e:303:UNK:HG3	1.97	0.45
30:k:165:ILE:HD11	33:o:135:PRO:HG3	1.97	0.45
30:k:226:TYR:CD2	36:z:706:UNK:CG	2.89	0.45
31:m:44:THR:O	31:m:45:CYS:HB2	2.15	0.45
33:o:210:UNK:HA	33:o:213:UNK:HG3	1.98	0.45
33:o:360:UNK:O	33:o:363:UNK:CG	2.38	0.45
1:A:442:A:H2'	1:A:443:U:H5'	1.97	0.45
1:A:487:C:H5'	1:A:488:A:OP2	2.16	0.45
6:G:190:GLU:HB3	6:G:194:LYS:HE2	1.99	0.45
7:I:203:LYS:HA	7:I:219:TYR:CD2	2.51	0.45
15:R:117:ILE:HA	15:R:117:ILE:HD13	1.59	0.45
17:U:78:LYS:HD2	17:U:80:ARG:HH21	1.82	0.45
21:b:103:TYR:CE2	21:b:117:LEU:HB3	2.51	0.45
24:e:121:UNK:HG2	24:e:122:UNK:N	2.30	0.45
29:j:58:VAL:HG13	29:j:137:HIS:CE1	2.51	0.45
30:k:264:ILE:HD11	30:k:294:TYR:CD2	2.51	0.45
33:o:192:UNK:CA	33:o:195:UNK:HG3	2.46	0.45
33:o:514:UNK:CB	33:o:537:UNK:HG3	2.41	0.45
1:A:739:A:H2'	1:A:739:A:N3	2.31	0.45
1:A:752:A:H3'	1:A:753:A:C5'	2.47	0.45
6:G:140:ASN:HB3	6:G:143:THR:HG22	1.99	0.45
11:N:57:LEU:HD21	27:h:368:PHE:HE1	1.82	0.45
12:O:164:ARG:HD2	12:O:188:ILE:HD13	1.99	0.45
18:Y:68:Y5P:H4A	18:Y:69:Y5P:C5	2.47	0.45
20:a:319:UNK:CG	20:a:320:UNK:H	2.21	0.45
20:a:328:UNK:C	20:a:331:UNK:HG3	2.46	0.45
24:e:301:UNK:HA	24:e:304:UNK:CG	2.47	0.45
26:g:349:PRO:HG3	26:g:385:ARG:HH12	1.80	0.45
27:h:354:PRO:O	30:k:215:PRO:HG3	2.15	0.45
33:o:231:UNK:O	33:o:235:UNK:HG3	2.16	0.45
33:o:340:UNK:CA	33:o:343:UNK:HG3	2.46	0.45
33:o:355:UNK:O	33:o:358:UNK:HG3	2.16	0.45
1:A:548:G:C2	1:A:549:A:C8	3.05	0.45
1:A:875:A:H62	29:j:17:ARG:NH1	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:85:LYS:HE2	7:I:99:PHE:HB3	1.98	0.45
9:K:102:VAL:HG12	9:K:106:HIS:HA	1.98	0.45
11:N:83:CYS:SG	11:N:86:ARG:HB2	2.56	0.45
20:a:225:ASP:HB3	34:p:167:ILE:HD12	1.98	0.45
22:c:141:CYS:HB3	22:c:149:CYS:HB2	1.98	0.45
24:e:213:UNK:HA	24:e:216:UNK:HG3	1.99	0.45
24:e:257:UNK:HA	24:e:260:UNK:HG3	1.98	0.45
24:e:402:UNK:O	24:e:406:UNK:CG	2.63	0.45
26:g:134:THR:O	26:g:137:LEU:HB3	2.15	0.45
26:g:160:TRP:N	26:g:160:TRP:CD1	2.83	0.45
26:g:314:SER:O	26:g:315:LEU:HD23	2.16	0.45
30:k:72:TYR:OH	30:k:79:LYS:HD2	2.16	0.45
33:o:476:UNK:HG1	33:o:510:UNK:H2	1.81	0.45
1:A:262:C:H2'	1:A:263:G:C8	2.51	0.45
1:A:954:U:O2	1:A:956:G:H5''	2.16	0.45
1:A:961:C:C2'	1:A:962:C:H5'	2.47	0.45
2:B:170:PHE:CE1	2:B:174:LEU:HD23	2.52	0.45
3:C:129:PRO:HB2	33:o:106:PHE:CE1	2.51	0.45
4:E:200:GLY:N	4:E:222:ILE:O	2.41	0.45
7:I:266:UNK:HG2	7:I:268:MET:HB3	1.98	0.45
10:L:32:THR:O	10:L:36:MET:HG3	2.16	0.45
14:Q:35:LEU:HB2	14:Q:42:TYR:CE1	2.51	0.45
18:V:51:Y5P:H2'	18:V:52:Y5P:C6	2.47	0.45
22:c:50:PHE:O	22:c:53:PRO:HD2	2.16	0.45
24:e:51:UNK:C	24:e:54:UNK:HG3	2.46	0.45
33:o:324:UNK:HA	33:o:327:UNK:CG	2.46	0.45
33:o:411:UNK:CB	35:s:2360:UNK:HG1	2.47	0.45
1:A:597:U:C5'	28:i:96:LYS:HZ1	2.29	0.45
1:A:926:A:H4'	32:n:134:ARG:NH2	2.31	0.45
2:B:105:LEU:HD23	2:B:105:LEU:HA	1.84	0.45
4:E:128:ARG:HD3	4:E:179:TRP:CE2	2.52	0.45
6:G:123:PHE:CE1	6:G:139:ARG:HG2	2.52	0.45
12:O:133:LEU:HD23	12:O:133:LEU:HA	1.72	0.45
15:R:79:GLN:NE2	23:d:190:ALA:HB2	2.32	0.45
18:V:43:Y5P:C2	18:V:44:Y5P:C5	2.95	0.45
18:Y:70:Y5P:H4A	18:Y:71:Y5P:H4	1.98	0.45
20:a:128:PRO:HD3	20:a:265:ARG:HG3	1.97	0.45
23:d:169:THR:HG22	23:d:170:ARG:H	1.82	0.45
24:e:284:UNK:C	24:e:287:UNK:HG3	2.47	0.45
26:g:122:ARG:NH1	26:g:336:LEU:HA	2.32	0.45
29:j:165:PRO:HG2	34:p:200:TYR:HE1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:o:230:UNK:O	33:o:234:UNK:HG3	2.16	0.45
33:o:322:UNK:HA	33:o:325:UNK:CG	2.45	0.45
33:o:373:UNK:HG2	33:o:374:UNK:N	2.31	0.45
1:A:228:G:H2'	1:A:229:U:O4'	2.17	0.45
1:A:301:U:H2'	1:A:302:U:C6	2.51	0.45
1:A:704:U:H2'	1:A:705:G:C8	2.52	0.45
3:C:73:THR:HG23	8:J:169:ALA:HB2	1.99	0.45
15:R:120:PHE:N	15:R:120:PHE:HD1	2.14	0.45
18:V:26:Y5P:H4A	18:V:27:Y5P:C4	2.41	0.45
19:X:20:Y5P:N3	19:X:21:Y5P:H4	2.32	0.45
24:e:214:UNK:O	24:e:217:UNK:HG3	2.16	0.45
24:e:278:UNK:HA	24:e:281:UNK:CG	2.47	0.45
26:g:242:VAL:O	26:g:246:LEU:HB2	2.16	0.45
26:g:338:PRO:HB3	30:k:294:TYR:HE2	1.82	0.45
28:i:89:ARG:HD2	28:i:91:LYS:HE3	1.98	0.45
1:A:60:C:H4'	29:j:34:TYR:CE2	2.49	0.45
1:A:202:A:C2	23:d:46:PRO:HG2	2.52	0.45
1:A:444:G:H5'	1:A:445:C:OP2	2.17	0.45
1:A:471:U:H5	1:A:638:A:OP1	1.99	0.45
1:A:516:C:O2'	1:A:517:A:H5'	2.16	0.45
2:B:81:ARG:NH1	25:f:84:MET:HE3	2.32	0.45
7:I:158:TYR:CZ	7:I:162:MET:HE3	2.52	0.45
9:K:150:ARG:HB3	9:K:175:ILE:HD11	1.99	0.45
14:Q:106:LEU:HD23	14:Q:106:LEU:HA	1.80	0.45
18:Y:62:Y5P:H2'	18:Y:63:Y5P:C6	2.47	0.45
24:e:113:UNK:HA	24:e:116:UNK:HG3	1.99	0.45
29:j:143:PRO:HB2	29:j:145:HIS:CE1	2.52	0.45
30:k:165:ILE:H	33:o:134:GLU:HB2	1.82	0.45
33:o:206:UNK:HA	33:o:209:UNK:CG	2.43	0.45
33:o:240:UNK:O	33:o:244:UNK:HG3	2.17	0.45
33:o:268:UNK:HA	33:o:271:UNK:HG3	1.99	0.45
33:o:378:UNK:C	33:o:381:UNK:HG3	2.47	0.45
33:o:500:UNK:HA	33:o:503:UNK:HG3	1.97	0.45
1:A:53:A:OP1	23:d:38:LYS:HE3	2.17	0.45
1:A:612:U:H5'	1:A:613:A:OP2	2.16	0.45
1:A:647:A:H3'	1:A:648:A:H5'	1.98	0.45
4:E:305:MET:HB2	4:E:332:LEU:HD11	1.98	0.45
18:Y:55:Y5P:H6	18:Y:57:Y5P:H5	1.97	0.45
20:a:300:VAL:CG1	20:a:330:UNK:HG1	2.47	0.45
20:a:349:UNK:CG	20:a:350:UNK:N	2.80	0.45
24:e:49:UNK:CG	24:e:52:UNK:CG	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:e:215:UNK:HA	24:e:218:UNK:CG	2.47	0.45
24:e:239:UNK:HG2	24:e:241:UNK:HG3	1.99	0.45
24:e:300:UNK:HA	24:e:303:UNK:CG	2.46	0.45
26:g:264:VAL:HG12	26:g:268:TRP:HZ3	1.82	0.45
31:m:56:TRP:HB3	31:m:61:PHE:CD1	2.52	0.45
33:o:339:UNK:CG	33:o:372:UNK:HB2	2.47	0.45
33:o:479:UNK:HG1	33:o:503:UNK:HB1	1.99	0.45
1:A:50:U:H2'	1:A:51:G:H8	1.82	0.44
1:A:538:C:H1'	1:A:540:U:C5	2.51	0.44
1:A:746:A:H2'	1:A:747:C:O4'	2.17	0.44
1:A:792:U:H4'	7:I:389:ARG:HG3	2.00	0.44
1:A:891:C:H4'	1:A:891:C:OP1	2.15	0.44
2:B:107:GLY:HA2	21:b:60:VAL:HG22	1.99	0.44
4:E:317:HIS:HD2	4:E:319:ALA:HB3	1.81	0.44
4:E:363:ALA:O	4:E:367:SER:N	2.51	0.44
5:F:121:LYS:HD3	5:F:123:ARG:NH2	2.31	0.44
6:G:118:VAL:HG23	6:G:206:SER:HB2	1.98	0.44
18:V:43:Y5P:C4	18:V:44:Y5P:H4	2.47	0.44
20:a:74:VAL:CG1	20:a:272:TRP:HE1	2.30	0.44
24:e:125:UNK:HG2	24:e:126:UNK:N	2.31	0.44
24:e:175:UNK:CB	24:e:368:UNK:HG3	2.47	0.44
24:e:218:UNK:HG1	24:e:296:UNK:CG	2.39	0.44
24:e:222:UNK:HA	24:e:225:UNK:HG3	1.98	0.44
24:e:223:UNK:HA	24:e:226:UNK:HG3	1.98	0.44
25:f:148:LEU:HD12	25:f:148:LEU:HA	1.85	0.44
26:g:376:LYS:O	26:g:380:LEU:HB2	2.17	0.44
33:o:550:UNK:HA	33:o:553:UNK:CG	2.47	0.44
34:p:52:LYS:HG2	34:p:53:ASP:H	1.82	0.44
35:s:2365:UNK:C	35:s:2368:UNK:HG3	2.47	0.44
1:A:660:A:H2'	1:A:661:U:O4'	2.18	0.44
4:E:136:ARG:HD3	28:i:67:PHE:CE1	2.52	0.44
4:E:425:LEU:HD23	4:E:425:LEU:HA	1.67	0.44
11:N:80:ARG:HD2	11:N:86:ARG:NH1	2.32	0.44
15:R:103:LYS:H	15:R:103:LYS:HG2	1.49	0.44
20:a:322:UNK:HG3	20:a:325:UNK:HG1	1.95	0.44
24:e:223:UNK:O	24:e:226:UNK:CG	2.65	0.44
24:e:254:UNK:O	24:e:257:UNK:HG3	2.17	0.44
24:e:268:UNK:HG2	34:p:214:SER:OG	2.15	0.44
24:e:281:UNK:HA	24:e:284:UNK:HG3	2.00	0.44
26:g:221:LEU:HD11	26:g:242:VAL:HG22	1.99	0.44
30:k:89:MET:HE1	30:k:106:GLU:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:s:2361:UNK:O	35:s:2364:UNK:CG	2.56	0.44
1:A:899:C:OP1	1:A:899:C:H4'	2.18	0.44
3:C:59:PRO:HB3	11:N:116:ASP:OD1	2.18	0.44
4:E:308:GLN:HG3	4:E:312:TYR:CD1	2.52	0.44
15:R:87:PRO:HG2	15:R:88:PHE:CE2	2.52	0.44
20:a:338:UNK:O	20:a:341:UNK:CG	2.64	0.44
22:c:44:ALA:O	22:c:47:PHE:HB3	2.17	0.44
27:h:289:GLY:O	27:h:292:GLU:HB3	2.18	0.44
29:j:29:ARG:HG3	29:j:31:SER:H	1.82	0.44
33:o:239:UNK:C	33:o:242:UNK:HG3	2.48	0.44
1:A:637:A:H4'	1:A:637:A:OP2	2.16	0.44
1:A:883:C:OP1	24:e:69:UNK:HB1	2.17	0.44
1:A:959:U:H3	31:m:25:LYS:HD2	1.81	0.44
4:E:151:ASN:N	4:E:151:ASN:OD1	2.51	0.44
5:F:79:MET:HE1	5:F:92:ASN:HA	1.99	0.44
5:F:117:LEU:HD23	5:F:117:LEU:HA	1.87	0.44
7:I:309:GLN:O	7:I:313:GLN:HG3	2.16	0.44
8:J:125:HIS:CD2	8:J:126:ILE:HG12	2.52	0.44
9:K:161:LEU:HA	9:K:161:LEU:HD23	1.73	0.44
11:N:79:PRO:O	11:N:82:SER:OG	2.15	0.44
14:Q:27:LYS:HG3	14:Q:50:PHE:HE1	1.83	0.44
14:Q:65:LEU:HB2	14:Q:85:ILE:HD11	2.00	0.44
18:Y:68:Y5P:C4	18:Y:69:Y5P:C5	2.96	0.44
20:a:150:THR:HG22	20:a:152:THR:HG23	1.99	0.44
24:e:91:UNK:O	24:e:95:UNK:HG3	2.18	0.44
28:i:18:LEU:HD23	30:k:231:LEU:HD23	1.99	0.44
29:j:79:LEU:O	29:j:142:VAL:HG22	2.17	0.44
30:k:142:ASP:HA	30:k:145:CYS:SG	2.57	0.44
1:A:200:A:H8	1:A:200:A:OP1	2.00	0.44
1:A:404:C:OP1	12:O:151:LYS:NZ	2.40	0.44
2:B:222:VAL:HG22	2:B:236:PRO:HA	1.99	0.44
2:B:235:VAL:HG21	2:B:248:PHE:HE1	1.82	0.44
4:E:428:ALA:HA	34:p:138:PRO:O	2.17	0.44
14:Q:13:VAL:CG2	14:Q:66:LEU:HB2	2.48	0.44
24:e:232:UNK:HG1	24:e:235:UNK:CG	2.37	0.44
29:j:154:UNK:O	29:j:154:UNK:HG2	2.17	0.44
30:k:112:ASN:HB2	30:k:114:LEU:HG	1.98	0.44
31:m:108:LEU:HA	31:m:108:LEU:HD23	1.81	0.44
33:o:126:LYS:HB2	33:o:127:TYR:CD1	2.53	0.44
34:p:93:MET:HE2	34:p:145:LYS:HD3	2.00	0.44
36:z:693:UNK:O	36:z:693:UNK:CG	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:48:LYS:NZ	7:I:319:HIS:O	2.46	0.44
7:I:214:LEU:HD23	7:I:214:LEU:HA	1.85	0.44
9:K:112:ALA:CB	9:K:137:ALA:HB2	2.48	0.44
18:Y:6:Y5P:C4	18:Y:7:Y5P:H4	2.45	0.44
20:a:154:LYS:HE2	20:a:173:VAL:HG11	2.00	0.44
20:a:341:UNK:CG	20:a:342:UNK:N	2.75	0.44
23:d:70:LEU:O	23:d:73:GLU:HB2	2.18	0.44
24:e:71:UNK:CA	24:e:74:UNK:HG3	2.44	0.44
24:e:218:UNK:HG2	24:e:219:UNK:N	2.32	0.44
24:e:399:UNK:O	24:e:402:UNK:HG2	2.18	0.44
25:f:140:ARG:C	25:f:174:GLN:HB2	2.43	0.44
26:g:165:ARG:HB2	26:g:181:LEU:HD11	2.00	0.44
29:j:65:LEU:HD22	29:j:111:HIS:O	2.17	0.44
29:j:95:TRP:HE1	29:j:131:ILE:CG1	2.31	0.44
32:n:193:LYS:HD2	32:n:196:LEU:HB2	1.99	0.44
1:A:471:U:OP2	21:b:50:ARG:NH2	2.50	0.44
1:A:602:A:O2'	4:E:136:ARG:NH2	2.51	0.44
1:A:804:A:N7	11:N:85:VAL:HB	2.33	0.44
1:A:902:C:H4'	1:A:903:C:H5'	1.99	0.44
8:J:120:LEU:HD23	8:J:120:LEU:HA	1.78	0.44
11:N:58:ARG:HB3	11:N:58:ARG:HH11	1.83	0.44
27:h:288:ASN:OD1	27:h:289:GLY:N	2.50	0.44
27:h:353:ASN:ND2	28:i:37:PHE:O	2.36	0.44
33:o:378:UNK:O	33:o:381:UNK:HG3	2.17	0.44
33:o:500:UNK:HG1	33:o:534:UNK:HB1	2.00	0.44
6:G:187:MET:HE2	6:G:187:MET:HB3	1.88	0.44
10:L:33:LEU:HA	10:L:33:LEU:HD23	1.65	0.44
12:O:96:LEU:HD13	12:O:104:LYS:HG2	2.00	0.44
12:O:202:ARG:HB3	32:n:194:ILE:HG21	1.99	0.44
22:c:36:THR:HG22	22:c:37:HIS:CD2	2.52	0.44
24:e:224:UNK:O	24:e:227:UNK:CG	2.62	0.44
24:e:227:UNK:O	24:e:230:UNK:HG3	2.18	0.44
24:e:379:UNK:O	24:e:383:UNK:CG	2.63	0.44
25:f:95:PRO:O	25:f:99:LYS:HE3	2.18	0.44
33:o:230:UNK:HG2	33:o:231:UNK:N	2.32	0.44
33:o:269:UNK:C	33:o:272:UNK:HG3	2.48	0.44
33:o:318:UNK:CA	33:o:321:UNK:HG3	2.42	0.44
33:o:413:UNK:C	33:o:416:UNK:HG3	2.48	0.44
33:o:444:UNK:O	33:o:447:UNK:HG3	2.17	0.44
33:o:496:UNK:O	33:o:499:UNK:HG3	2.18	0.44
34:p:103:ASN:HA	34:p:104:PRO:HD3	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:z:699:UNK:CG	36:z:700:UNK:N	2.81	0.44
1:A:566:U:H3	1:A:686:A:H62	1.66	0.44
1:A:635:C:H5''	2:B:213:LYS:HZ2	1.82	0.44
1:A:711:A:H2'	1:A:712:A:O4'	2.18	0.44
2:B:79:SER:OG	2:B:81:ARG:N	2.45	0.44
3:C:128:PRO:HA	3:C:129:PRO:HD3	1.89	0.44
4:E:164:ASP:O	4:E:168:VAL:HG23	2.18	0.44
9:K:166:GLY:HA2	9:K:169:MET:HE2	2.00	0.44
20:a:280:ILE:HG22	20:a:284:LEU:HG	2.00	0.44
24:e:93:UNK:HG2	24:e:94:UNK:N	2.32	0.44
24:e:135:UNK:HG1	29:j:74:PHE:HE2	1.83	0.44
24:e:256:UNK:HA	24:e:259:UNK:HG3	1.99	0.44
24:e:303:UNK:HA	24:e:306:UNK:HG3	2.00	0.44
34:p:134:ILE:H	34:p:134:ILE:HG13	1.60	0.44
1:A:298:G:C2	1:A:299:U:C6	3.06	0.43
1:A:370:A:O2'	15:R:109:THR:OG1	2.23	0.43
1:A:453:U:H2'	1:A:454:A:H5''	1.99	0.43
1:A:621:A:OP2	3:C:36:LYS:N	2.51	0.43
2:B:70:ASP:O	2:B:72:PHE:N	2.50	0.43
2:B:81:ARG:HH11	25:f:84:MET:HE3	1.83	0.43
6:G:73:LEU:O	6:G:74:ILE:HD13	2.18	0.43
7:I:390:ARG:HD2	7:I:391:LYS:H	1.83	0.43
9:K:151:VAL:HG12	9:K:177:ILE:HG23	1.99	0.43
18:Y:70:Y5P:C5	18:Y:71:Y5P:H5	2.48	0.43
23:d:74:PHE:O	23:d:77:GLU:HB2	2.18	0.43
23:d:79:ARG:HD3	23:d:79:ARG:HA	1.77	0.43
24:e:51:UNK:CA	24:e:54:UNK:HG3	2.47	0.43
24:e:390:UNK:HA	24:e:393:UNK:CG	2.47	0.43
26:g:257:LEU:HG	26:g:259:VAL:HG23	1.99	0.43
31:m:62:ARG:HG3	31:m:65:ALA:HB2	2.00	0.43
33:o:340:UNK:HA	33:o:343:UNK:CG	2.48	0.43
33:o:554:UNK:O	33:o:558:UNK:HG3	2.18	0.43
1:A:182:A:C6	1:A:183:A:C6	3.06	0.43
1:A:476:A:C8	31:m:12:ARG:HA	2.53	0.43
1:A:484:C:P	10:L:34:ASN:HD22	2.41	0.43
1:A:844:C:H5'	19:X:18:Y5P:H4A	2.00	0.43
2:B:201:VAL:HG12	31:m:112:PRO:HG3	2.00	0.43
4:E:141:TRP:H	4:E:145:ASN:ND2	2.14	0.43
4:E:369:HIS:CE1	4:E:391:LEU:HD22	2.54	0.43
5:F:2:PRO:HB2	5:F:96:HIS:CD2	2.53	0.43
6:G:182:LEU:HD23	6:G:182:LEU:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:123:SER:OG	8:J:124:VAL:N	2.51	0.43
8:J:147:HIS:HB3	30:k:135:TRP:CE2	2.53	0.43
20:a:352:UNK:O	20:a:356:UNK:HG3	2.19	0.43
21:b:94:SER:OG	21:b:95:THR:N	2.51	0.43
24:e:354:UNK:O	24:e:357:UNK:HG3	2.18	0.43
27:h:288:ASN:O	27:h:291:GLU:HB3	2.18	0.43
29:j:63:ARG:NE	29:j:66:GLN:HE21	2.16	0.43
33:o:227:UNK:C	33:o:230:UNK:HG3	2.49	0.43
33:o:323:UNK:HA	33:o:326:UNK:HG3	2.00	0.43
1:A:641:A:C2	1:A:642:G:C4	3.07	0.43
1:A:730:C:OP1	26:g:316:PHE:HA	2.17	0.43
1:A:757:U:H2'	1:A:758:U:O4'	2.18	0.43
2:B:164:TYR:CD2	7:I:149:PHE:HA	2.53	0.43
3:C:129:PRO:HG3	33:o:94:TYR:CE1	2.53	0.43
4:E:88:SER:HA	4:E:91:THR:OG1	2.18	0.43
4:E:323:ILE:HD13	4:E:350:PHE:HE1	1.83	0.43
6:G:163:LYS:HE3	19:X:12:Y5P:HA1	2.00	0.43
13:P:54:TYR:CD2	13:P:66:VAL:HG22	2.54	0.43
16:T:63:UNK:HG1	24:e:54:UNK:HG1	2.00	0.43
23:d:177:VAL:O	23:d:181:LEU:HG	2.17	0.43
24:e:124:UNK:CA	24:e:127:UNK:HG3	2.48	0.43
24:e:243:UNK:C	24:e:244:UNK:CG	2.95	0.43
24:e:356:UNK:O	24:e:360:UNK:HG3	2.17	0.43
26:g:350:LYS:HG3	26:g:351:GLU:H	1.82	0.43
30:k:128:LEU:HD21	33:o:74:LEU:HD21	2.01	0.43
33:o:341:UNK:HA	33:o:344:UNK:HG3	2.00	0.43
35:s:2367:UNK:HA	35:s:2370:UNK:HG3	2.00	0.43
1:A:267:A:H2'	1:A:268:A:O4'	2.17	0.43
1:A:505:U:C5	32:n:148:LYS:HG2	2.53	0.43
1:A:635:C:H5''	2:B:213:LYS:NZ	2.32	0.43
3:C:125:ARG:HD3	33:o:94:TYR:CD2	2.52	0.43
3:C:135:LEU:HA	3:C:135:LEU:HD23	1.73	0.43
4:E:203:LEU:HD11	4:E:268:PHE:HB3	1.99	0.43
4:E:370:VAL:HG13	4:E:385:ALA:HB3	2.00	0.43
6:G:37:TYR:CE1	7:I:375:PRO:HG2	2.53	0.43
12:O:127:GLU:O	12:O:131:VAL:HG23	2.18	0.43
13:P:104:ILE:O	13:P:107:ALA:HB3	2.19	0.43
18:Y:8:Y5P:C4	18:Y:14:Y5P:H5	2.46	0.43
20:a:315:UNK:O	20:a:319:UNK:CG	2.47	0.43
24:e:28:UNK:HB1	24:e:369:UNK:HG3	2.00	0.43
24:e:28:UNK:CB	24:e:369:UNK:HG3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:e:72:UNK:CA	24:e:75:UNK:HG3	2.47	0.43
24:e:114:UNK:CA	24:e:117:UNK:HG3	2.46	0.43
24:e:258:UNK:HA	24:e:261:UNK:HG3	2.00	0.43
26:g:350:LYS:HG3	26:g:351:GLU:N	2.33	0.43
30:k:78:PHE:HB2	30:k:112:ASN:HD22	1.83	0.43
30:k:91:TYR:CG	30:k:92:PRO:HD2	2.53	0.43
1:A:76:U:H4'	29:j:5:LYS:HE3	2.00	0.43
1:A:204:U:H2'	1:A:205:U:C6	2.54	0.43
1:A:563:U:H5'	1:A:564:A:OP2	2.19	0.43
1:A:901:A:H4'	1:A:902:C:OP2	2.18	0.43
2:B:163:GLU:OE1	2:B:163:GLU:HA	2.19	0.43
5:F:37:ARG:HG3	23:d:167:PHE:CE1	2.53	0.43
6:G:41:TYR:HA	6:G:73:LEU:O	2.18	0.43
6:G:140:ASN:ND2	6:G:143:THR:H	2.17	0.43
9:K:88:ALA:HB3	9:K:151:VAL:HG23	2.00	0.43
12:O:225:LYS:O	12:O:229:ARG:HG3	2.18	0.43
13:P:99:LEU:HD21	20:a:147:LEU:HD13	2.01	0.43
13:P:107:ALA:O	13:P:111:ARG:HG3	2.17	0.43
15:R:57:ASN:HA	15:R:58:PRO:HD3	1.71	0.43
15:R:133:ASP:HB3	15:R:134:PRO:CD	2.48	0.43
18:Y:30:Y5P:C4	18:Y:31:Y5P:H4	2.41	0.43
18:Y:39:Y5P:H4A	18:Y:40:Y5P:H4	2.00	0.43
20:a:334:UNK:O	20:a:334:UNK:CG	2.65	0.43
24:e:175:UNK:HB2	24:e:368:UNK:HG3	2.00	0.43
24:e:188:UNK:O	24:e:192:UNK:CG	2.49	0.43
24:e:190:UNK:CG	24:e:191:UNK:N	2.81	0.43
24:e:295:UNK:HA	24:e:298:UNK:HG3	2.00	0.43
24:e:392:UNK:CG	24:e:393:UNK:N	2.80	0.43
29:j:64:LEU:HB3	29:j:134:VAL:HG13	2.00	0.43
33:o:192:UNK:HA	33:o:195:UNK:CG	2.47	0.43
33:o:284:UNK:O	33:o:288:UNK:HG3	2.19	0.43
33:o:481:UNK:HA	33:o:484:UNK:HG3	2.00	0.43
1:A:338:U:H2'	1:A:339:A:H8	1.83	0.43
10:L:102:LEU:HA	10:L:102:LEU:HD23	1.85	0.43
18:Y:37:Y5P:HB	18:Y:38:Y5P:H6	2.01	0.43
20:a:341:UNK:O	20:a:345:UNK:HG3	2.17	0.43
22:c:137:ARG:H	22:c:137:ARG:HG2	1.40	0.43
24:e:75:UNK:HA	24:e:78:UNK:CG	2.48	0.43
24:e:105:UNK:HA	24:e:108:UNK:CG	2.48	0.43
26:g:170:SER:OG	26:g:172:TYR:HD2	2.02	0.43
31:m:84:ARG:HG2	31:m:87:ARG:CZ	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:o:187:UNK:O	33:o:191:UNK:HG3	2.18	0.43
33:o:381:UNK:HA	33:o:384:UNK:CG	2.49	0.43
1:A:11:G:H4'	4:E:237:ARG:CZ	2.48	0.43
1:A:197:A:H2'	1:A:198:C:O4'	2.19	0.43
1:A:229:U:O2'	1:A:236:A:N1	2.36	0.43
1:A:389:A:H2'	1:A:390:A:H5'	2.01	0.43
1:A:670:A:H1'	6:G:36:ARG:HD2	2.00	0.43
1:A:736:A:O2'	26:g:165:ARG:NH2	2.48	0.43
1:A:817:G:H5''	6:G:104:LYS:HG2	2.00	0.43
1:A:849:G:H5'	32:n:138:MET:HE3	2.01	0.43
1:A:959:U:H3	31:m:25:LYS:CD	2.30	0.43
2:B:168:ARG:HA	2:B:168:ARG:HD3	1.60	0.43
2:B:190:ASP:O	2:B:217:PRO:HD2	2.19	0.43
7:I:168:LYS:O	7:I:172:VAL:HG23	2.18	0.43
11:N:57:LEU:H	11:N:57:LEU:HG	1.55	0.43
15:R:56:GLU:CD	15:R:56:GLU:H	2.26	0.43
18:Y:68:Y5P:C5	18:Y:69:Y5P:H5	2.48	0.43
20:a:277:LYS:HG3	20:a:279:LYS:HE3	1.99	0.43
30:k:240:GLU:HG3	30:k:241:TRP:H	1.84	0.43
33:o:65:TRP:HD1	33:o:66:ASP:O	2.01	0.43
33:o:224:UNK:C	33:o:227:UNK:HG3	2.48	0.43
33:o:343:UNK:CA	33:o:379:UNK:HG1	2.45	0.43
33:o:442:UNK:HG2	33:o:443:UNK:N	2.34	0.43
1:A:285:C:C5	10:L:42:PRO:HB2	2.53	0.43
1:A:432:A:H4'	1:A:433:U:C5'	2.48	0.43
1:A:677:C:H2'	1:A:678:G:O4'	2.19	0.43
1:A:881:A:H3'	1:A:882:A:C8	2.53	0.43
2:B:57:LEU:HA	2:B:60:ARG:HD2	2.01	0.43
4:E:173:VAL:O	4:E:177:GLU:HG2	2.19	0.43
6:G:199:VAL:HG13	6:G:203:GLU:CD	2.43	0.43
14:Q:93:ASP:HA	14:Q:94:PRO:HD2	1.84	0.43
22:c:105:ILE:HG22	22:c:106:LEU:HD23	2.01	0.43
23:d:133:ARG:O	23:d:137:GLU:HG3	2.18	0.43
25:f:88:SER:O	25:f:92:GLN:HG3	2.19	0.43
32:n:165:LYS:HD3	32:n:195:TYR:CD1	2.53	0.43
33:o:235:UNK:CG	33:o:237:UNK:CG	2.97	0.43
33:o:284:UNK:HA	33:o:287:UNK:CG	2.46	0.43
33:o:659:UNK:HB2	33:o:670:UNK:HG1	1.99	0.43
35:s:2370:UNK:CA	35:s:2373:UNK:HG3	2.46	0.43
1:A:69:G:H2'	1:A:70:U:C6	2.54	0.43
1:A:491:G:OP1	32:n:135:ARG:NH2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:U:H2'	1:A:693:A:O4'	2.19	0.43
7:I:113:PRO:HD2	30:k:111:PRO:O	2.18	0.43
7:I:148:HIS:HB3	7:I:156:GLN:NE2	2.34	0.43
7:I:387:GLY:O	7:I:388:ALA:HB3	2.18	0.43
7:I:397:ARG:NH2	18:V:33:Y5P:OP2	2.52	0.43
8:J:151:SER:O	8:J:155:VAL:HG23	2.19	0.43
14:Q:71:VAL:HA	14:Q:72:PRO:HD3	1.93	0.43
22:c:24:LYS:HD2	22:c:106:LEU:HA	2.00	0.43
22:c:47:PHE:CD1	22:c:51:ASN:HB2	2.54	0.43
24:e:204:UNK:HA	24:e:223:UNK:HG1	2.01	0.43
24:e:374:UNK:CG	24:e:375:UNK:N	2.82	0.43
26:g:77:VAL:C	26:g:79:PRO:HD3	2.44	0.43
30:k:89:MET:HB3	30:k:89:MET:HE2	1.59	0.43
33:o:186:UNK:O	33:o:190:UNK:HG3	2.19	0.43
33:o:600:UNK:HA	33:o:603:UNK:HG3	2.00	0.43
1:A:217:U:H2'	1:A:218:A:H8	1.83	0.43
1:A:520:G:C2	1:A:521:G:N7	2.87	0.43
2:B:168:ARG:HG3	7:I:159:TYR:CE2	2.54	0.43
2:B:222:VAL:HG11	2:B:228:PRO:HB3	2.00	0.43
3:C:123:VAL:HG21	3:C:155:LEU:HG	2.01	0.43
3:C:138:TYR:OH	28:i:65:LEU:HD22	2.18	0.43
4:E:223:LEU:HD23	4:E:223:LEU:HA	1.81	0.43
7:I:314:LEU:HD12	7:I:314:LEU:HA	1.57	0.43
11:N:74:GLU:O	11:N:77:SER:HB2	2.19	0.43
11:N:111:PHE:CD1	11:N:111:PHE:C	2.97	0.43
13:P:55:ASP:HA	13:P:56:PRO:HD3	1.82	0.43
24:e:179:UNK:HG3	24:e:362:UNK:HB2	2.01	0.43
24:e:354:UNK:HG2	24:e:357:UNK:CG	2.48	0.43
26:g:205:GLU:CD	26:g:248:ARG:HH12	2.27	0.43
30:k:307:ASN:OD1	30:k:308:GLU:N	2.52	0.43
31:m:17:ARG:NH1	31:m:20:ILE:HD11	2.34	0.43
33:o:460:UNK:HA	33:o:463:UNK:CG	2.48	0.43
33:o:475:UNK:HG2	33:o:506:UNK:HB2	2.00	0.43
1:A:508:C:O5'	1:A:508:C:H6	2.02	0.42
1:A:622:U:H2'	1:A:623:C:C6	2.54	0.42
1:A:761:U:H2'	1:A:762:G:O4'	2.19	0.42
1:A:806:A:H5'	1:A:807:G:P	2.59	0.42
1:A:905:U:H2'	1:A:906:G:C8	2.54	0.42
5:F:58:HIS:CD2	5:F:89:ILE:HD11	2.54	0.42
7:I:91:MET:HE3	30:k:68:TRP:CD1	2.53	0.42
7:I:123:PRO:N	30:k:89:MET:HG3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:341:GLN:O	7:I:345:VAL:HG23	2.19	0.42
13:P:116:ARG:O	13:P:120:LEU:HG	2.19	0.42
24:e:92:UNK:HA	24:e:95:UNK:CG	2.49	0.42
24:e:358:UNK:CG	24:e:359:UNK:N	2.82	0.42
26:g:216:GLU:O	26:g:219:ARG:HG2	2.19	0.42
26:g:265:ASN:HD21	26:g:310:SER:N	2.17	0.42
30:k:158:TYR:HB2	30:k:167:ASN:HD22	1.84	0.42
33:o:245:UNK:HA	33:o:248:UNK:CG	2.47	0.42
33:o:266:UNK:HG3	33:o:267:UNK:N	2.31	0.42
33:o:303:UNK:HG1	33:o:340:UNK:HG2	2.01	0.42
1:A:87:U:H2'	1:A:88:C:H6	1.82	0.42
1:A:91:A:C6	29:j:195:ARG:NH1	2.87	0.42
1:A:304:A:H2'	1:A:305:A:O4'	2.18	0.42
1:A:861:A:C6	1:A:908:A:C6	3.07	0.42
1:A:947:G:H2'	1:A:948:U:H6	1.83	0.42
2:B:101:MET:HE3	2:B:228:PRO:HD3	2.00	0.42
2:B:166:HIS:CE1	7:I:153:THR:HA	2.54	0.42
8:J:157:LEU:HD23	8:J:157:LEU:HA	1.82	0.42
12:O:176:TYR:N	14:Q:89:GLY:O	2.46	0.42
21:b:75:TYR:CE1	25:f:99:LYS:NZ	2.88	0.42
24:e:128:UNK:HG2	24:e:129:UNK:N	2.34	0.42
24:e:221:UNK:CA	24:e:224:UNK:HG3	2.49	0.42
32:n:142:LYS:HD3	32:n:142:LYS:HA	1.63	0.42
33:o:172:UNK:HA	33:o:175:UNK:HG3	2.01	0.42
33:o:511:UNK:HA	33:o:514:UNK:HG3	2.00	0.42
1:A:76:U:H3'	1:A:77:G:O4'	2.18	0.42
1:A:327:U:O2'	1:A:328:A:N7	2.46	0.42
1:A:588:A:H1'	1:A:609:C:O2	2.19	0.42
7:I:371:LEU:H	7:I:371:LEU:HG	1.58	0.42
13:P:54:TYR:HD2	13:P:66:VAL:HG22	1.85	0.42
13:P:100:HIS:CG	13:P:101:PRO:HD2	2.55	0.42
15:R:66:CYS:SG	15:R:104:LYS:HG3	2.59	0.42
20:a:204:LEU:HD12	20:a:205:THR:H	1.83	0.42
24:e:213:UNK:CA	24:e:216:UNK:HG3	2.49	0.42
24:e:224:UNK:CA	24:e:227:UNK:HG3	2.48	0.42
24:e:243:UNK:O	24:e:244:UNK:HG3	2.19	0.42
24:e:251:UNK:HA	24:e:254:UNK:HG3	2.01	0.42
29:j:164:VAL:HG12	29:j:191:LEU:HB3	2.00	0.42
31:m:84:ARG:HG2	31:m:87:ARG:NH1	2.34	0.42
32:n:144:ARG:HA	32:n:144:ARG:HD2	1.34	0.42
33:o:127:TYR:N	33:o:127:TYR:HD1	2.15	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:A:N1	34:p:82:LYS:HE2	2.34	0.42
1:A:381:G:C6	1:A:382:U:C4	3.07	0.42
1:A:685:C:C4'	1:A:686:A:H5'	2.49	0.42
1:A:735:G:H1'	26:g:162:LYS:HD2	2.00	0.42
1:A:749:C:N4	1:A:750:G:C6	2.88	0.42
2:B:57:LEU:HB2	2:B:270:TYR:HE2	1.85	0.42
4:E:291:TYR:HE2	4:E:359:HIS:H	1.67	0.42
14:Q:31:THR:HG21	14:Q:44:ASN:HB3	2.02	0.42
15:R:77:ASN:OD1	15:R:77:ASN:N	2.50	0.42
18:Y:23:Y5P:C4	18:Y:24:Y5P:H4	2.34	0.42
24:e:45:UNK:O	24:e:45:UNK:HG2	2.18	0.42
26:g:85:ARG:HD2	26:g:391:GLU:OE2	2.19	0.42
26:g:264:VAL:HG11	26:g:307:LEU:HD13	2.00	0.42
26:g:265:ASN:OD1	26:g:309:VAL:HA	2.19	0.42
30:k:166:ARG:HB2	33:o:134:GLU:HG3	2.02	0.42
33:o:400:UNK:O	33:o:403:UNK:HG3	2.19	0.42
33:o:494:UNK:O	33:o:498:UNK:HG3	2.19	0.42
34:p:201:PRO:O	34:p:204:SER:OG	2.37	0.42
1:A:69:G:H2'	1:A:70:U:H6	1.85	0.42
4:E:365:LYS:HG3	4:E:366:LYS:HG2	2.02	0.42
5:F:6:LEU:HD12	5:F:92:ASN:O	2.19	0.42
6:G:52:ARG:HD3	6:G:52:ARG:HA	1.89	0.42
7:I:223:ILE:O	7:I:227:GLU:HG2	2.19	0.42
11:N:70:VAL:HG21	27:h:378:ILE:HD13	2.00	0.42
18:Y:24:Y5P:H4A	18:Y:25:Y5P:H4	2.01	0.42
20:a:275:VAL:HA	20:a:280:ILE:HD11	2.00	0.42
22:c:149:CYS:HA	22:c:150:PRO:HD3	1.85	0.42
33:o:117:ALA:O	33:o:121:ILE:HG13	2.19	0.42
33:o:229:UNK:CB	33:o:266:UNK:HG2	2.48	0.42
33:o:235:UNK:CG	33:o:237:UNK:HG1	2.49	0.42
33:o:237:UNK:HA	33:o:240:UNK:HG3	2.02	0.42
33:o:535:UNK:HA	33:o:538:UNK:CG	2.47	0.42
33:o:655:UNK:HG2	33:o:674:UNK:HB2	2.01	0.42
36:z:702:UNK:O	36:z:706:UNK:HG3	2.20	0.42
1:A:703:U:H2'	1:A:704:U:H6	1.84	0.42
4:E:395:PRO:HB3	20:a:109:GLN:HE21	1.84	0.42
5:F:96:HIS:HA	5:F:97:PRO:HD2	1.79	0.42
7:I:88:LEU:HD11	7:I:107:ALA:HB1	2.02	0.42
9:K:189:ARG:HA	9:K:190:PRO:HD3	1.85	0.42
10:L:107:VAL:O	10:L:131:ASP:HB2	2.20	0.42
13:P:64:LYS:HD2	20:a:155:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:a:340:UNK:O	20:a:344:UNK:HG2	2.19	0.42
22:c:158:GLU:HA	22:c:163:TYR:CD2	2.55	0.42
24:e:178:UNK:C	24:e:181:UNK:HG3	2.49	0.42
24:e:203:UNK:C	24:e:206:UNK:HG3	2.50	0.42
24:e:235:UNK:CA	24:e:238:UNK:HG3	2.49	0.42
26:g:205:GLU:CD	26:g:248:ARG:NH1	2.76	0.42
29:j:170:LEU:HD23	29:j:170:LEU:HA	1.87	0.42
32:n:194:ILE:H	32:n:194:ILE:HG12	1.62	0.42
33:o:92:ASP:OD1	33:o:92:ASP:N	2.40	0.42
33:o:239:UNK:CA	33:o:242:UNK:HG3	2.46	0.42
33:o:338:UNK:C	33:o:341:UNK:HG3	2.50	0.42
33:o:377:UNK:HA	33:o:380:UNK:HG3	2.01	0.42
33:o:392:UNK:HG2	33:o:393:UNK:N	2.33	0.42
35:s:2372:UNK:O	35:s:2375:UNK:HG3	2.20	0.42
1:A:255:G:O6	10:L:74:ASN:HB2	2.20	0.42
1:A:578:G:OP1	8:J:128:LYS:NZ	2.38	0.42
2:B:252:PHE:O	2:B:256:ILE:HG12	2.20	0.42
3:C:133:TYR:OH	33:o:90:GLN:N	2.52	0.42
4:E:401:VAL:HG11	22:c:50:PHE:CE1	2.55	0.42
4:E:401:VAL:HG21	22:c:50:PHE:CD1	2.55	0.42
5:F:86:ILE:H	5:F:86:ILE:HG13	1.70	0.42
6:G:88:ASP:HA	6:G:89:PRO:HD2	1.80	0.42
8:J:96:VAL:HA	8:J:106:ILE:HD11	2.02	0.42
13:P:94:SER:HB3	20:a:157:PHE:CD2	2.54	0.42
14:Q:103:THR:O	22:c:72:PRO:HB3	2.19	0.42
15:R:80:LEU:HD22	23:d:189:TRP:CZ3	2.54	0.42
18:V:13:Y5P:OP2	18:V:13:Y5P:H6	2.20	0.42
20:a:96:GLU:H	20:a:96:GLU:HG3	1.54	0.42
20:a:340:UNK:O	20:a:344:UNK:CG	2.67	0.42
22:c:3:MET:HE2	22:c:3:MET:HB3	1.93	0.42
24:e:116:UNK:CG	24:e:117:UNK:N	2.82	0.42
24:e:218:UNK:HG2	24:e:296:UNK:CB	2.50	0.42
33:o:225:UNK:HB1	33:o:248:UNK:CG	2.45	0.42
33:o:424:UNK:HA	33:o:427:UNK:HG3	2.01	0.42
33:o:657:UNK:HA	33:o:660:UNK:HG3	2.02	0.42
1:A:159:C:C2'	1:A:160:C:H5'	2.49	0.42
1:A:883:C:OP2	24:e:70:UNK:HG3	2.20	0.42
2:B:161:CYS:HB3	2:B:256:ILE:HG21	2.01	0.42
5:F:94:VAL:HG12	5:F:95:LYS:O	2.20	0.42
7:I:100:THR:HG22	7:I:101:GLN:H	1.84	0.42
7:I:119:LYS:HG2	7:I:122:ARG:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:161:LEU:HG	17:U:23:TYR:CE1	2.54	0.42
10:L:58:LEU:HB2	10:L:110:VAL:HG23	2.02	0.42
11:N:36:ARG:HB3	11:N:40:ARG:NH2	2.35	0.42
17:U:26:LEU:O	17:U:29:ILE:HB	2.20	0.42
17:U:72:ILE:HD13	17:U:72:ILE:HA	1.82	0.42
18:V:9:Y5P:H5	18:V:23:Y5P:H4A	2.01	0.42
19:X:16:Y5P:H2'	19:X:17:Y5P:O4'	2.20	0.42
20:a:344:UNK:HA	20:a:347:UNK:CG	2.50	0.42
24:e:243:UNK:HG1	24:e:245:UNK:CG	2.49	0.42
24:e:280:UNK:O	24:e:284:UNK:HG3	2.19	0.42
29:j:85:TRP:CD1	29:j:85:TRP:N	2.88	0.42
31:m:52:MET:SD	31:m:70:ILE:HD13	2.60	0.42
33:o:222:UNK:O	33:o:225:UNK:HG3	2.19	0.42
33:o:287:UNK:HA	33:o:290:UNK:CG	2.49	0.42
33:o:656:UNK:O	33:o:659:UNK:HG3	2.20	0.42
1:A:546:U:H2'	1:A:547:A:C8	2.55	0.42
1:A:617:C:H2'	1:A:618:G:O4'	2.20	0.42
1:A:896:A:C5	1:A:897:C:H1'	2.55	0.42
2:B:202:PHE:N	2:B:202:PHE:CD1	2.88	0.42
3:C:88:GLU:HG3	3:C:147:TYR:CZ	2.54	0.42
4:E:140:LEU:HD11	4:E:160:ARG:HG3	2.02	0.42
14:Q:24:LYS:HB3	14:Q:53:ASP:O	2.19	0.42
14:Q:109:PRO:HG2	23:d:124:LEU:HD12	2.01	0.42
18:V:48:Y5P:H6	18:V:48:Y5P:OP1	2.19	0.42
18:Y:42:Y5P:HB	18:Y:43:Y5P:HB2	2.02	0.42
24:e:96:UNK:HG2	24:e:97:UNK:N	2.34	0.42
24:e:105:UNK:CA	24:e:108:UNK:HG3	2.49	0.42
24:e:181:UNK:HG2	24:e:182:UNK:N	2.34	0.42
25:f:128:PRO:HD3	25:f:170:LEU:HD23	2.02	0.42
26:g:108:LEU:HD12	26:g:108:LEU:HA	1.78	0.42
29:j:104:TYR:HA	29:j:109:LEU:HD13	2.02	0.42
29:j:120:PHE:HE2	29:j:200:PRO:HG2	1.85	0.42
33:o:413:UNK:HA	33:o:416:UNK:CG	2.49	0.42
1:A:151:A:H1'	22:c:131:PRO:HG2	2.01	0.42
1:A:199:G:H5'	1:A:200:A:OP2	2.19	0.42
1:A:557:G:C6	1:A:715:G:C6	3.08	0.42
1:A:882:A:H2'	1:A:883:C:O4'	2.19	0.42
2:B:262:LYS:O	2:B:266:VAL:HG23	2.19	0.42
3:C:58:ALA:O	3:C:61:TYR:HB2	2.20	0.42
3:C:94:LYS:NZ	4:E:92:LYS:HB2	2.35	0.42
4:E:358:THR:HG22	4:E:360:GLN:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:229:LEU:HD23	7:I:229:LEU:HA	1.85	0.42
7:I:266:UNK:HG2	7:I:268:MET:CB	2.50	0.42
8:J:102:LEU:HD12	8:J:102:LEU:HA	1.93	0.42
9:K:67:PRO:HD3	17:U:13:MET:SD	2.60	0.42
12:O:74:LEU:HD12	12:O:77:TYR:CD2	2.55	0.42
12:O:86:VAL:HG13	23:d:161:GLN:CD	2.45	0.42
12:O:110:MET:HE3	12:O:111:GLN:HG2	2.02	0.42
18:Y:29:Y5P:H2'	18:Y:30:Y5P:O4'	2.20	0.42
20:a:158:THR:HG23	20:a:171:ILE:HD12	2.02	0.42
20:a:188:ARG:O	20:a:192:ILE:HG13	2.20	0.42
20:a:216:THR:O	20:a:220:GLN:HG2	2.20	0.42
20:a:290:ARG:HD3	20:a:290:ARG:HA	1.87	0.42
20:a:342:UNK:CA	20:a:345:UNK:HG3	2.49	0.42
23:d:147:GLN:O	23:d:151:GLN:HG3	2.20	0.42
24:e:283:UNK:HA	24:e:286:UNK:HG3	2.02	0.42
24:e:285:UNK:CA	24:e:288:UNK:HG3	2.49	0.42
26:g:85:ARG:O	26:g:88:MET:HB2	2.20	0.42
26:g:194:ASN:OD1	26:g:194:ASN:N	2.52	0.42
27:h:343:MET:HE1	27:h:368:PHE:CG	2.55	0.42
29:j:52:MET:HA	29:j:55:TRP:NE1	2.35	0.42
33:o:158:UNK:HA	33:o:161:UNK:CG	2.49	0.42
33:o:296:UNK:HA	33:o:299:UNK:HG3	2.02	0.42
33:o:415:UNK:HA	33:o:418:UNK:HG3	2.01	0.42
33:o:531:UNK:HA	33:o:534:UNK:CG	2.50	0.42
34:p:230:PRO:HA	34:p:231:PRO:HD3	1.51	0.42
1:A:55:G:H2'	1:A:56:U:O4'	2.20	0.41
1:A:276:U:H2'	1:A:277:A:C8	2.55	0.41
1:A:385:C:H2'	1:A:386:U:H6	1.84	0.41
2:B:219:VAL:HA	2:B:233:TYR:O	2.20	0.41
5:F:28:ALA:O	5:F:32:ARG:HG2	2.20	0.41
6:G:70:LYS:HB3	6:G:72:GLN:HG3	2.02	0.41
12:O:90:VAL:HG13	23:d:160:LEU:HD23	2.01	0.41
14:Q:40:LEU:HD12	14:Q:40:LEU:HA	1.84	0.41
15:R:141:TYR:HA	17:U:32:MET:HE3	2.02	0.41
19:X:23:Y5P:H2'	19:X:24:Y5P:H5	2.02	0.41
20:a:259:ASP:HA	20:a:262:ARG:HG2	2.02	0.41
22:c:95:ASN:O	22:c:99:VAL:HG23	2.19	0.41
24:e:282:UNK:CA	24:e:285:UNK:HG3	2.50	0.41
33:o:244:UNK:HA	33:o:247:UNK:CG	2.49	0.41
33:o:304:UNK:C	33:o:307:UNK:HG3	2.49	0.41
35:s:2365:UNK:HA	35:s:2368:UNK:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:U:O4	1:A:132:A:N6	2.53	0.41
1:A:654:A:OP1	7:I:213:LYS:NZ	2.53	0.41
1:A:903:C:H2'	1:A:904:A:C8	2.56	0.41
2:B:97:ARG:HA	2:B:224:THR:HG22	2.02	0.41
4:E:291:TYR:CD2	4:E:358:THR:HA	2.55	0.41
9:K:154:LYS:HG3	9:K:180:ASN:O	2.20	0.41
10:L:39:LEU:HD22	10:L:39:LEU:HA	1.62	0.41
12:O:80:VAL:HG11	23:d:153:LYS:HB3	2.02	0.41
15:R:50:ASP:HA	25:f:86:ARG:NH1	2.35	0.41
24:e:88:UNK:O	24:e:91:UNK:HG3	2.19	0.41
24:e:105:UNK:CG	24:e:106:UNK:N	2.81	0.41
25:f:85:LEU:HD23	25:f:85:LEU:HA	1.87	0.41
26:g:80:HIS:CE1	26:g:189:ASN:HB2	2.55	0.41
30:k:117:THR:HG23	30:k:118:PRO:HD2	2.03	0.41
33:o:550:UNK:CA	33:o:553:UNK:HG3	2.48	0.41
34:p:126:PHE:CE1	34:p:140:THR:HG21	2.49	0.41
1:A:114:A:N1	1:A:136:C:O2'	2.47	0.41
2:B:71:PHE:CE1	2:B:262:LYS:HG2	2.55	0.41
7:I:136:ARG:HH21	7:I:212:GLU:HA	1.84	0.41
9:K:175:ILE:O	17:U:14:VAL:HG13	2.20	0.41
11:N:91:CYS:HB3	11:N:94:THR:HG22	2.02	0.41
15:R:68:LEU:O	15:R:71:LYS:HB2	2.20	0.41
15:R:71:LYS:HD3	15:R:71:LYS:HA	1.81	0.41
21:b:14:SER:OG	21:b:15:ARG:N	2.53	0.41
24:e:243:UNK:O	24:e:244:UNK:HG2	2.20	0.41
24:e:284:UNK:CA	24:e:287:UNK:HG3	2.50	0.41
24:e:286:UNK:C	24:e:289:UNK:HG3	2.50	0.41
29:j:180:LYS:CG	34:p:181:HIS:HD2	2.33	0.41
30:k:165:ILE:CG1	33:o:135:PRO:HD3	2.51	0.41
31:m:13:LEU:HD23	31:m:13:LEU:HA	1.78	0.41
33:o:186:UNK:HG1	33:o:220:UNK:CB	2.50	0.41
33:o:193:UNK:HG1	33:o:210:UNK:HG1	2.01	0.41
33:o:299:UNK:HA	33:o:302:UNK:HG3	2.01	0.41
33:o:413:UNK:CA	33:o:416:UNK:HG3	2.50	0.41
33:o:651:UNK:HA	33:o:654:UNK:HG3	2.01	0.41
1:A:349:A:H2'	1:A:350:A:C8	2.55	0.41
1:A:460:A:H4'	1:A:461:A:OP2	2.20	0.41
2:B:57:LEU:HB2	2:B:270:TYR:CE2	2.55	0.41
4:E:264:ARG:HD2	4:E:268:PHE:CE2	2.56	0.41
22:c:22:VAL:HA	22:c:59:ASN:HD21	1.84	0.41
22:c:76:LEU:HB2	22:c:88:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:e:174:UNK:CG	24:e:177:UNK:HG3	2.49	0.41
26:g:349:PRO:HG3	26:g:385:ARG:NH1	2.35	0.41
27:h:361:LYS:O	27:h:365:ILE:HG12	2.20	0.41
32:n:130:ILE:HG23	32:n:130:ILE:HD12	1.84	0.41
33:o:300:UNK:HA	33:o:303:UNK:CG	2.46	0.41
1:A:358:U:H5''	9:K:89:HIS:ND1	2.35	0.41
1:A:533:C:H5''	31:m:37:ARG:CZ	2.50	0.41
1:A:555:C:C4	1:A:556:U:C4	3.09	0.41
2:B:148:ARG:O	2:B:149:GLN:C	2.63	0.41
3:C:69:LEU:HA	3:C:69:LEU:HD23	1.71	0.41
4:E:155:GLN:H	4:E:155:GLN:HG3	1.71	0.41
4:E:187:VAL:O	4:E:188:LYS:HG3	2.21	0.41
7:I:329:MET:SD	7:I:349:MET:HE2	2.60	0.41
8:J:149:THR:HG21	30:k:133:THR:HG23	2.02	0.41
14:Q:98:LYS:HE3	14:Q:109:PRO:HD3	2.03	0.41
18:V:9:Y5P:H4	18:V:23:Y5P:H5	2.03	0.41
20:a:326:UNK:O	20:a:330:UNK:CG	2.48	0.41
26:g:123:TYR:CE2	26:g:340:ILE:HD12	2.56	0.41
30:k:110:ILE:HA	30:k:110:ILE:HD13	1.79	0.41
30:k:200:TYR:CE2	30:k:202:LYS:HG2	2.56	0.41
31:m:48:GLU:H	31:m:48:GLU:HG2	1.62	0.41
33:o:436:UNK:HA	33:o:439:UNK:CG	2.49	0.41
33:o:600:UNK:O	33:o:604:UNK:HG3	2.20	0.41
33:o:671:UNK:HA	33:o:674:UNK:CG	2.48	0.41
1:A:19:C:H6	1:A:19:C:O5'	2.03	0.41
1:A:209:C:H2'	1:A:210:U:C6	2.56	0.41
1:A:250:A:H2'	1:A:251:C:H6	1.85	0.41
1:A:520:G:C2	1:A:521:G:C8	3.09	0.41
2:B:217:PRO:HG3	21:b:31:TRP:CB	2.51	0.41
4:E:305:MET:HE3	4:E:305:MET:HB3	1.82	0.41
6:G:95:THR:HA	6:G:111:MET:HE3	2.02	0.41
8:J:102:LEU:HD13	30:k:125:CYS:SG	2.61	0.41
21:b:62:ASP:OD1	21:b:62:ASP:N	2.54	0.41
23:d:131:GLN:O	23:d:135:GLN:HG2	2.21	0.41
24:e:67:UNK:C	24:e:100:UNK:HG1	2.51	0.41
24:e:78:UNK:CG	24:e:79:UNK:N	2.84	0.41
24:e:120:UNK:CG	24:e:123:UNK:HG3	2.51	0.41
24:e:277:UNK:O	24:e:281:UNK:CG	2.47	0.41
26:g:272:THR:OG1	26:g:315:LEU:HD13	2.21	0.41
29:j:41:MET:HE3	29:j:55:TRP:CD2	2.56	0.41
30:k:291:VAL:O	30:k:295:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:o:194:UNK:C	33:o:197:UNK:HG3	2.51	0.41
33:o:224:UNK:CA	33:o:227:UNK:HG3	2.48	0.41
33:o:320:UNK:CA	33:o:323:UNK:HG3	2.49	0.41
33:o:671:UNK:CA	33:o:674:UNK:HG3	2.49	0.41
1:A:26:A:H2'	1:A:27:U:C6	2.55	0.41
1:A:904:A:H2'	1:A:905:U:H6	1.84	0.41
2:B:188:LEU:HD23	2:B:188:LEU:HA	1.83	0.41
10:L:59:LYS:HB3	10:L:59:LYS:HE2	1.91	0.41
11:N:93:MET:H	11:N:93:MET:HG2	1.48	0.41
13:P:63:GLU:HB3	20:a:156:VAL:HG23	2.02	0.41
13:P:91:LEU:HD23	13:P:91:LEU:HA	1.84	0.41
20:a:198:ARG:HH11	20:a:201:ARG:HE	1.68	0.41
22:c:23:PHE:HD1	22:c:23:PHE:HA	1.71	0.41
24:e:203:UNK:CA	24:e:206:UNK:HG3	2.49	0.41
24:e:215:UNK:CA	24:e:218:UNK:HG3	2.49	0.41
24:e:250:UNK:O	24:e:254:UNK:HG3	2.20	0.41
24:e:283:UNK:HG2	24:e:284:UNK:N	2.35	0.41
24:e:389:UNK:O	24:e:393:UNK:N	2.54	0.41
30:k:74:VAL:HG12	30:k:75:ALA:H	1.86	0.41
33:o:243:UNK:HA	33:o:246:UNK:CG	2.46	0.41
33:o:287:UNK:CA	33:o:290:UNK:HG3	2.49	0.41
33:o:360:UNK:O	33:o:364:UNK:HG3	2.21	0.41
33:o:423:UNK:O	33:o:426:UNK:HG3	2.21	0.41
33:o:671:UNK:C	33:o:674:UNK:HG3	2.51	0.41
1:A:128:C:H2'	1:A:129:G:O4'	2.20	0.41
1:A:285:C:N4	10:L:43:LYS:O	2.53	0.41
1:A:488:A:H5''	1:A:488:A:H8	1.84	0.41
1:A:939:A:H2'	1:A:940:C:H6	1.83	0.41
2:B:126:LEU:HD13	21:b:40:PRO:HA	2.02	0.41
4:E:140:LEU:CD2	4:E:160:ARG:HE	2.30	0.41
4:E:293:ASP:OD1	4:E:306:LYS:HA	2.21	0.41
14:Q:95:VAL:HG11	23:d:120:ARG:CZ	2.51	0.41
20:a:350:UNK:HG2	20:a:351:UNK:N	2.36	0.41
20:a:352:UNK:CG	20:a:353:UNK:N	2.84	0.41
22:c:15:TYR:OH	22:c:50:PHE:HB3	2.20	0.41
24:e:178:UNK:HG2	24:e:210:UNK:HB1	2.03	0.41
24:e:304:UNK:C	24:e:307:UNK:HG3	2.51	0.41
28:i:61:LEU:HB2	33:o:127:TYR:CD2	2.45	0.41
33:o:97:PRO:HA	33:o:106:PHE:HE2	1.85	0.41
33:o:204:UNK:CA	33:o:207:UNK:HG3	2.45	0.41
33:o:238:UNK:HG2	33:o:239:UNK:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:o:400:UNK:HG2	33:o:401:UNK:N	2.34	0.41
36:z:703:UNK:O	36:z:707:UNK:CG	2.62	0.41
1:A:85:G:H2'	1:A:86:A:C8	2.56	0.41
1:A:393:A:OP1	12:O:136:LYS:NZ	2.36	0.41
1:A:582:G:H5'	1:A:806:A:N1	2.36	0.41
1:A:670:A:N7	40:A:7124:HOH:O	2.37	0.41
1:A:686:A:OP2	1:A:686:A:H4'	2.20	0.41
2:B:142:LEU:HD23	2:B:192:ILE:HD13	2.02	0.41
3:C:113:ARG:O	3:C:116:GLN:HG2	2.21	0.41
4:E:352:GLY:O	4:E:355:ARG:HB2	2.21	0.41
4:E:377:CYS:O	20:a:90:PHE:HB3	2.21	0.41
5:F:39:LEU:CD2	5:F:66:VAL:HG22	2.51	0.41
6:G:138:GLU:HG3	6:G:213:PHE:CZ	2.55	0.41
7:I:169:LEU:HD12	7:I:229:LEU:HD23	2.03	0.41
7:I:276:LYS:H	7:I:347:LEU:HD23	1.85	0.41
7:I:358:THR:HG22	7:I:361:GLU:OE1	2.21	0.41
12:O:112:LEU:HD12	12:O:112:LEU:HA	1.81	0.41
12:O:126:LEU:HD13	12:O:171:LEU:HD23	2.03	0.41
17:U:28:ARG:O	17:U:32:MET:HB2	2.21	0.41
17:U:51:ARG:HG3	17:U:54:ARG:NH1	2.35	0.41
20:a:227:LEU:O	20:a:231:VAL:HG23	2.21	0.41
20:a:253:ASP:HA	20:a:258:TYR:CZ	2.56	0.41
20:a:256:GLY:HA2	20:a:258:TYR:CE1	2.56	0.41
20:a:260:LEU:HD23	20:a:260:LEU:HA	1.93	0.41
23:d:48:VAL:HG11	34:p:220:TYR:CE2	2.56	0.41
24:e:248:UNK:C	24:e:251:UNK:HG3	2.51	0.41
24:e:257:UNK:O	24:e:260:UNK:HG3	2.20	0.41
26:g:85:ARG:HD3	26:g:85:ARG:HA	1.64	0.41
28:i:62:MET:HE2	28:i:62:MET:HA	2.02	0.41
30:k:68:TRP:N	30:k:69:PRO:HD2	2.36	0.41
30:k:133:THR:HB	33:o:63:LYS:HE3	2.03	0.41
30:k:199:ARG:HB3	30:k:208:THR:O	2.20	0.41
30:k:218:ARG:HG3	30:k:219:GLN:N	2.36	0.41
33:o:158:UNK:CA	33:o:161:UNK:HG3	2.50	0.41
33:o:302:UNK:HA	33:o:305:UNK:HG3	2.02	0.41
33:o:316:UNK:C	33:o:319:UNK:HG3	2.51	0.41
33:o:423:UNK:HB2	33:o:440:UNK:HG2	2.03	0.41
33:o:504:UNK:CB	33:o:537:UNK:HG2	2.51	0.41
33:o:521:UNK:HB1	33:o:534:UNK:HG1	1.99	0.41
33:o:535:UNK:HG2	33:o:554:UNK:HB2	2.03	0.41
36:z:706:UNK:CG	36:z:707:UNK:N	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:C:H6	1:A:65:C:H2'	1.74	0.41
1:A:836:G:H2'	1:A:837:C:C6	2.56	0.41
2:B:92:HIS:HE1	2:B:223:ASP:OD2	2.04	0.41
3:C:98:GLY:HA3	28:i:71:TYR:CE1	2.56	0.41
4:E:132:ILE:H	4:E:132:ILE:HG12	1.62	0.41
7:I:228:ARG:NH1	17:U:85:GLN:HG2	2.36	0.41
10:L:69:LYS:NZ	10:L:77:ASN:HB3	2.36	0.41
11:N:80:ARG:O	11:N:86:ARG:HD2	2.21	0.41
12:O:168:LEU:HD23	12:O:168:LEU:HA	1.79	0.41
13:P:104:ILE:HG23	20:a:146:ILE:HD12	2.03	0.41
20:a:80:LYS:HB3	20:a:80:LYS:HE3	1.83	0.41
22:c:9:ILE:HD13	22:c:9:ILE:HA	1.92	0.41
24:e:237:UNK:O	24:e:237:UNK:HG2	2.21	0.41
25:f:103:GLY:HA2	25:f:117:PHE:HA	2.03	0.41
26:g:115:ASN:HD22	26:g:118:HIS:CD2	2.39	0.41
32:n:149:ARG:H	32:n:149:ARG:HG3	1.75	0.41
33:o:238:UNK:C	33:o:241:UNK:HG3	2.51	0.41
33:o:514:UNK:HA	33:o:517:UNK:CG	2.51	0.41
33:o:669:UNK:HA	33:o:672:UNK:HG3	2.03	0.41
34:p:158:ARG:HB3	34:p:165:TYR:CE1	2.56	0.41
1:A:238:C:H2'	1:A:239:U:C6	2.56	0.40
1:A:317:A:C2	1:A:318:C:H5	2.39	0.40
1:A:502:A:H5'	1:A:503:A:N7	2.36	0.40
1:A:577:C:O3'	8:J:128:LYS:HD2	2.21	0.40
1:A:724:U:O4	6:G:98:MET:HG2	2.20	0.40
2:B:88:VAL:HG11	2:B:120:THR:HG21	2.03	0.40
5:F:89:ILE:O	5:F:90:ARG:HB2	2.20	0.40
7:I:143:ASP:OD1	7:I:143:ASP:N	2.45	0.40
8:J:104:ILE:O	8:J:105:SER:OG	2.39	0.40
12:O:96:LEU:HD23	12:O:96:LEU:HA	1.77	0.40
13:P:13:ARG:HH12	23:d:30:ARG:NH2	2.19	0.40
14:Q:63:ILE:HD13	14:Q:63:ILE:HA	1.86	0.40
17:U:50:ARG:HD2	17:U:50:ARG:HA	1.73	0.40
18:Y:25:Y5P:N3	18:Y:26:Y5P:H4	2.34	0.40
20:a:155:TYR:HB3	20:a:157:PHE:CE1	2.55	0.40
20:a:175:GLU:HG3	20:a:179:THR:HG22	2.03	0.40
20:a:204:LEU:HD12	20:a:205:THR:N	2.35	0.40
24:e:274:UNK:CG	24:e:275:UNK:N	2.83	0.40
30:k:148:HIS:O	30:k:150:PRO:HD3	2.21	0.40
33:o:174:UNK:CA	33:o:177:UNK:HG3	2.45	0.40
33:o:237:UNK:HA	33:o:240:UNK:CG	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:o:579:UNK:O	33:o:582:UNK:HG3	2.20	0.40
1:A:458:C:H6	1:A:458:C:H2'	1.70	0.40
1:A:521:G:C2	1:A:522:A:C4	3.09	0.40
6:G:122:GLN:HE21	6:G:210:LEU:HD13	1.86	0.40
6:G:199:VAL:HG13	6:G:203:GLU:OE1	2.20	0.40
7:I:170:LEU:HA	7:I:173:GLU:CD	2.46	0.40
22:c:76:LEU:CD1	22:c:102:ILE:HD11	2.50	0.40
26:g:338:PRO:HA	30:k:314:TYR:OH	2.21	0.40
29:j:63:ARG:HG2	29:j:66:GLN:HG3	2.03	0.40
30:k:139:LEU:HD23	30:k:139:LEU:HA	1.95	0.40
30:k:292:GLU:HA	30:k:295:ARG:HD2	2.03	0.40
1:A:886:A:H3'	29:j:101:ARG:NH2	2.37	0.40
5:F:10:LEU:HD12	5:F:64:PHE:CD1	2.56	0.40
8:J:158:GLU:HG2	33:o:70:ILE:HG21	2.03	0.40
15:R:125:TYR:CE2	17:U:4:HIS:HB3	2.51	0.40
17:U:41:ARG:NH2	17:U:58:GLU:OE2	2.51	0.40
17:U:78:LYS:HE2	31:m:111:PHE:HZ	1.87	0.40
24:e:92:UNK:O	24:e:95:UNK:HG2	2.21	0.40
26:g:325:GLN:HB3	30:k:306:ASP:CG	2.46	0.40
29:j:142:VAL:HA	29:j:143:PRO:HD3	1.91	0.40
30:k:151:ILE:HG23	30:k:177:VAL:HG22	2.03	0.40
33:o:206:UNK:CA	33:o:209:UNK:HG3	2.45	0.40
33:o:496:UNK:C	33:o:499:UNK:HG3	2.52	0.40
33:o:512:UNK:HG2	33:o:513:UNK:N	2.36	0.40
34:p:200:TYR:HB2	34:p:203:TYR:CE2	2.56	0.40
35:s:2362:UNK:CA	35:s:2365:UNK:HG3	2.48	0.40
1:A:646:C:C2	1:A:648:A:C6	3.10	0.40
6:G:52:ARG:NH1	7:I:364:TRP:HZ3	2.20	0.40
6:G:155:VAL:HG13	31:m:74:PHE:CZ	2.56	0.40
7:I:228:ARG:CD	17:U:85:GLN:HE21	2.16	0.40
19:X:14:Y5P:H2'	19:X:15:Y5P:O4'	2.21	0.40
24:e:112:UNK:C	24:e:115:UNK:HG3	2.51	0.40
24:e:122:UNK:O	24:e:125:UNK:HG3	2.21	0.40
24:e:140:UNK:HG1	24:e:174:UNK:HG1	2.02	0.40
25:f:140:ARG:HB2	25:f:174:GLN:HG2	2.02	0.40
25:f:155:LEU:CD1	31:m:27:LEU:HB3	2.51	0.40
26:g:154:ILE:HG13	26:g:186:TRP:NE1	2.37	0.40
30:k:87:VAL:O	30:k:101:LYS:HB3	2.22	0.40
30:k:200:TYR:HE1	30:k:205:ASP:HA	1.87	0.40
30:k:265:LEU:HD13	30:k:282:LYS:HE2	2.03	0.40
30:k:266:GLU:O	30:k:269:LEU:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:o:131:ASP:OD1	33:o:132:ILE:N	2.55	0.40
33:o:394:UNK:C	33:o:397:UNK:HG3	2.52	0.40
1:A:109:G:C6	1:A:110:U:N3	2.89	0.40
1:A:643:G:O2'	1:A:651:G:OP2	2.26	0.40
1:A:664:U:OP1	8:J:113:ARG:NH2	2.44	0.40
1:A:752:A:H8	1:A:753:A:C5'	2.35	0.40
2:B:92:HIS:CE1	2:B:223:ASP:OD2	2.75	0.40
4:E:245:VAL:HB	4:E:271:ALA:HB1	2.04	0.40
5:F:8:LEU:HD11	5:F:25:THR:HG21	2.03	0.40
7:I:119:LYS:HA	7:I:122:ARG:HG3	2.03	0.40
10:L:62:VAL:HG23	10:L:106:HIS:O	2.21	0.40
20:a:283:LEU:HD12	20:a:283:LEU:HA	1.87	0.40
21:b:19:LEU:HG	21:b:24:VAL:HB	2.02	0.40
24:e:243:UNK:HG2	24:e:245:UNK:CG	2.47	0.40
25:f:155:LEU:HD11	31:m:27:LEU:HB3	2.03	0.40
33:o:186:UNK:HG1	33:o:220:UNK:HA	2.02	0.40
33:o:243:UNK:C	33:o:246:UNK:HG3	2.52	0.40
33:o:362:UNK:C	33:o:365:UNK:HG3	2.51	0.40
33:o:668:UNK:HA	33:o:671:UNK:HG3	2.03	0.40
34:p:55:PRO:HD2	34:p:56:TRP:CD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	218/289 (75%)	209 (96%)	9 (4%)	0	100	100
3	C	130/167 (78%)	123 (95%)	7 (5%)	0	100	100
4	E	324/430 (75%)	308 (95%)	16 (5%)	0	100	100
5	F	121/124 (98%)	118 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	G	206/242 (85%)	204 (99%)	2 (1%)	0	100	100
7	I	291/397 (73%)	280 (96%)	11 (4%)	0	100	100
8	J	127/201 (63%)	117 (92%)	7 (6%)	3 (2%)	4	29
9	K	134/196 (68%)	128 (96%)	6 (4%)	0	100	100
10	L	107/139 (77%)	101 (94%)	6 (6%)	0	100	100
11	N	99/128 (77%)	97 (98%)	2 (2%)	0	100	100
12	O	173/239 (72%)	165 (95%)	8 (5%)	0	100	100
13	P	115/135 (85%)	112 (97%)	3 (3%)	0	100	100
14	Q	107/130 (82%)	102 (95%)	4 (4%)	1 (1%)	14	46
15	R	95/143 (66%)	93 (98%)	2 (2%)	0	100	100
17	U	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
20	a	243/360 (68%)	236 (97%)	7 (3%)	0	100	100
21	b	133/190 (70%)	128 (96%)	5 (4%)	0	100	100
22	c	167/173 (96%)	158 (95%)	9 (5%)	0	100	100
23	d	175/205 (85%)	173 (99%)	2 (1%)	0	100	100
25	f	97/188 (52%)	90 (93%)	7 (7%)	0	100	100
26	g	327/397 (82%)	319 (98%)	7 (2%)	1 (0%)	36	65
27	h	101/387 (26%)	97 (96%)	4 (4%)	0	100	100
28	i	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
29	j	204/218 (94%)	191 (94%)	13 (6%)	0	100	100
30	k	273/325 (84%)	266 (97%)	7 (3%)	0	100	100
31	m	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
32	n	70/199 (35%)	66 (94%)	4 (6%)	0	100	100
33	o	87/692 (13%)	83 (95%)	4 (5%)	0	100	100
34	p	186/258 (72%)	175 (94%)	11 (6%)	0	100	100
All	All	4605/6863 (67%)	4422 (96%)	178 (4%)	5 (0%)	49	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	J	179	GLN
8	J	185	ARG
14	Q	95	VAL

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Mol	Chain	Res	Type
8	J	160	ILE
26	g	337	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	187/233 (80%)	163 (87%)	24 (13%)	4	22
3	C	115/142 (81%)	102 (89%)	13 (11%)	5	26
4	E	273/351 (78%)	241 (88%)	32 (12%)	5	25
5	F	108/109 (99%)	99 (92%)	9 (8%)	10	35
6	G	181/205 (88%)	165 (91%)	16 (9%)	9	33
7	I	250/317 (79%)	225 (90%)	25 (10%)	7	30
8	J	119/181 (66%)	106 (89%)	13 (11%)	6	27
9	K	102/151 (68%)	90 (88%)	12 (12%)	5	24
10	L	92/116 (79%)	79 (86%)	13 (14%)	3	19
11	N	92/114 (81%)	68 (74%)	24 (26%)	0	4
12	O	159/205 (78%)	144 (91%)	15 (9%)	8	32
13	P	97/113 (86%)	89 (92%)	8 (8%)	10	36
14	Q	94/114 (82%)	78 (83%)	16 (17%)	2	13
15	R	89/127 (70%)	74 (83%)	15 (17%)	2	13
17	U	77/78 (99%)	65 (84%)	12 (16%)	2	16
20	a	222/272 (82%)	203 (91%)	19 (9%)	10	34
21	b	113/162 (70%)	104 (92%)	9 (8%)	11	37
22	c	152/155 (98%)	132 (87%)	20 (13%)	4	21
23	d	149/168 (89%)	136 (91%)	13 (9%)	9	34
25	f	86/160 (54%)	73 (85%)	13 (15%)	3	17
26	g	290/334 (87%)	267 (92%)	23 (8%)	11	37
27	h	95/345 (28%)	89 (94%)	6 (6%)	16	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	i	86/93 (92%)	79 (92%)	7 (8%)	11	36
29	j	182/184 (99%)	170 (93%)	12 (7%)	15	43
30	k	249/289 (86%)	226 (91%)	23 (9%)	8	33
31	m	100/102 (98%)	91 (91%)	9 (9%)	9	33
32	n	66/174 (38%)	57 (86%)	9 (14%)	3	20
33	o	79/141 (56%)	72 (91%)	7 (9%)	9	33
34	p	168/225 (75%)	149 (89%)	19 (11%)	5	26
All	All	4072/5360 (76%)	3636 (89%)	436 (11%)	8	28

All (436) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	57	LEU
2	B	79	SER
2	B	97	ARG
2	B	108	SER
2	B	115	ILE
2	B	126	LEU
2	B	141	ILE
2	B	144	VAL
2	B	152	HIS
2	B	153	LEU
2	B	157	THR
2	B	159	ARG
2	B	168	ARG
2	B	176	THR
2	B	181	LEU
2	B	190	ASP
2	B	192	ILE
2	B	201	VAL
2	B	206	VAL
2	B	209	ARG
2	B	230	LEU
2	B	235	VAL
2	B	249	CYS
2	B	251	LEU
3	C	37	ASN
3	C	38	ARG
3	C	41	ARG
3	C	44	VAL

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Mol	Chain	Res	Type
3	C	54	GLU
3	C	71	LEU
3	C	104	LEU
3	C	112	ARG
3	C	115	ASN
3	C	122	LEU
3	C	125	ARG
3	C	152	HIS
3	C	167	ILE
4	E	91	THR
4	E	100	LYS
4	E	105	GLU
4	E	131	ILE
4	E	132	ILE
4	E	136	ARG
4	E	146	ILE
4	E	156	THR
4	E	165	GLN
4	E	215	TYR
4	E	220	THR
4	E	225	VAL
4	E	226	ARG
4	E	228	VAL
4	E	234	LYS
4	E	239	ARG
4	E	245	VAL
4	E	247	VAL
4	E	258	ILE
4	E	289	THR
4	E	293	ASP
4	E	303	ILE
4	E	305	MET
4	E	314	LEU
4	E	323	ILE
4	E	336	VAL
4	E	340	VAL
4	E	346	THR
4	E	367	SER
4	E	370	VAL
4	E	404	ILE
4	E	420	SER
5	F	9	ILE

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Mol	Chain	Res	Type
5	F	13	MET
5	F	65	LEU
5	F	67	ASP
5	F	83	SER
5	F	86	ILE
5	F	89	ILE
5	F	92	ASN
5	F	120	THR
6	G	85	VAL
6	G	103	ASN
6	G	104	LYS
6	G	109	SER
6	G	114	THR
6	G	118	VAL
6	G	139	ARG
6	G	156	ILE
6	G	159	VAL
6	G	172	VAL
6	G	187	MET
6	G	197	ARG
6	G	200	LEU
6	G	205	LEU
6	G	219	VAL
6	G	224	HIS
7	I	90	ASN
7	I	98	THR
7	I	99	PHE
7	I	130	GLU
7	I	153	THR
7	I	161	LEU
7	I	202	ILE
7	I	206	LEU
7	I	209	MET
7	I	215	SER
7	I	217	GLN
7	I	226	LEU
7	I	234	CYS
7	I	237	THR
7	I	293	ARG
7	I	294	ILE
7	I	303	LEU
7	I	331	CYS

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Mol	Chain	Res	Type
7	I	338	ARG
7	I	353	LEU
7	I	357	VAL
7	I	371	LEU
7	I	372	THR
7	I	377	VAL
7	I	393	THR
8	J	72	LEU
8	J	84	ASP
8	J	92	GLU
8	J	116	GLU
8	J	126	ILE
8	J	136	MET
8	J	143	LEU
8	J	145	LEU
8	J	148	LEU
8	J	149	THR
8	J	158	GLU
8	J	166	GLU
8	J	184	ILE
9	K	65	TYR
9	K	75	LEU
9	K	87	ILE
9	K	98	GLN
9	K	109	LEU
9	K	116	THR
9	K	128	ILE
9	K	142	THR
9	K	151	VAL
9	K	152	VAL
9	K	153	VAL
9	K	178	THR
10	L	32	THR
10	L	39	LEU
10	L	52	THR
10	L	55	ARG
10	L	59	LYS
10	L	61	VAL
10	L	75	SER
10	L	77	ASN
10	L	95	ILE
10	L	110	VAL

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Mol	Chain	Res	Type
10	L	118	LEU
10	L	127	ARG
10	L	135	VAL
11	N	34	MET
11	N	37	ASP
11	N	56	SER
11	N	57	LEU
11	N	58	ARG
11	N	75	ILE
11	N	80	ARG
11	N	81	ASP
11	N	83	CYS
11	N	85	VAL
11	N	92	VAL
11	N	93	MET
11	N	94	THR
11	N	95	SER
11	N	100	VAL
11	N	106	LEU
11	N	107	SER
11	N	108	ARG
11	N	109	ILE
11	N	114	LEU
11	N	120	LEU
11	N	123	VAL
11	N	124	GLN
11	N	125	ARG
12	O	71	SER
12	O	72	MET
12	O	74	LEU
12	O	76	ASP
12	O	125	SER
12	O	130	ILE
12	O	135	VAL
12	O	144	MET
12	O	159	MET
12	O	161	ILE
12	O	162	ASP
12	O	198	ARG
12	O	205	VAL
12	O	212	THR
12	O	214	VAL

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Mol	Chain	Res	Type
13	P	10	ARG
13	P	16	HIS
13	P	31	PHE
13	P	35	VAL
13	P	65	LEU
13	P	90	LEU
13	P	97	TYR
13	P	110	LEU
14	Q	9	HIS
14	Q	18	ILE
14	Q	22	MET
14	Q	35	LEU
14	Q	40	LEU
14	Q	57	GLN
14	Q	59	THR
14	Q	64	VAL
14	Q	71	VAL
14	Q	74	THR
14	Q	77	VAL
14	Q	80	GLU
14	Q	81	LEU
14	Q	90	GLN
14	Q	96	THR
14	Q	108	SER
15	R	50	ASP
15	R	51	LEU
15	R	53	VAL
15	R	69	CYS
15	R	73	VAL
15	R	76	LYS
15	R	77	ASN
15	R	85	ILE
15	R	91	CYS
15	R	108	ILE
15	R	109	THR
15	R	117	ILE
15	R	120	PHE
15	R	136	VAL
15	R	139	ILE
17	U	14	VAL
17	U	46	GLU
17	U	47	LYS

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Mol	Chain	Res	Type
17	U	49	CYS
17	U	52	ARG
17	U	60	CYS
17	U	70	ARG
17	U	72	ILE
17	U	80	ARG
17	U	82	ASP
17	U	85	GLN
17	U	87	CYS
20	a	96	GLU
20	a	106	THR
20	a	127	MET
20	a	160	ILE
20	a	171	ILE
20	a	172	VAL
20	a	174	ARG
20	a	175	GLU
20	a	181	ARG
20	a	186	GLU
20	a	199	GLU
20	a	203	ILE
20	a	204	LEU
20	a	205	THR
20	a	227	LEU
20	a	228	ASN
20	a	238	SER
20	a	252	ILE
20	a	294	SER
21	b	6	LEU
21	b	12	ILE
21	b	15	ARG
21	b	17	ARG
21	b	20	ILE
21	b	30	LEU
21	b	45	VAL
21	b	60	VAL
21	b	135	VAL
22	c	3	MET
22	c	4	LYS
22	c	9	ILE
22	c	12	THR
22	c	18	GLN

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Mol	Chain	Res	Type
22	c	25	ASP
22	c	27	VAL
22	c	30	MET
22	c	31	THR
22	c	33	ASN
22	c	48	VAL
22	c	59	ASN
22	c	70	MET
22	c	82	SER
22	c	95	ASN
22	c	102	ILE
22	c	106	LEU
22	c	137	ARG
22	c	143	VAL
22	c	152	LEU
23	d	27	ARG
23	d	29	THR
23	d	30	ARG
23	d	92	GLU
23	d	115	ARG
23	d	160	LEU
23	d	166	THR
23	d	169	THR
23	d	186	SER
23	d	191	ILE
23	d	196	LEU
23	d	197	VAL
23	d	198	VAL
25	f	101	VAL
25	f	113	LEU
25	f	123	CYS
25	f	124	VAL
25	f	131	ASP
25	f	141	VAL
25	f	145	LEU
25	f	153	ARG
25	f	155	LEU
25	f	160	ASP
25	f	161	THR
25	f	162	THR
25	f	169	VAL
26	g	74	LEU

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Mol	Chain	Res	Type
26	g	98	LEU
26	g	107	LEU
26	g	134	THR
26	g	138	CYS
26	g	139	HIS
26	g	141	LEU
26	g	150	LEU
26	g	170	SER
26	g	178	ASP
26	g	196	HIS
26	g	215	THR
26	g	246	LEU
26	g	265	ASN
26	g	296	VAL
26	g	310	SER
26	g	311	GLN
26	g	337	ASP
26	g	357	GLN
26	g	365	LEU
26	g	372	THR
26	g	380	LEU
26	g	397	LEU
27	h	302	LEU
27	h	308	ASN
27	h	331	GLN
27	h	332	ASP
27	h	348	CYS
27	h	387	ASN
28	i	11	MET
28	i	18	LEU
28	i	30	SER
28	i	55	HIS
28	i	62	MET
28	i	89	ARG
28	i	91	LYS
29	j	29	ARG
29	j	50	LEU
29	j	57	ASP
29	j	65	LEU
29	j	80	VAL
29	j	136	TYR
29	j	150	PHE

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Mol	Chain	Res	Type
29	j	164	VAL
29	j	178	ARG
29	j	184	THR
29	j	186	THR
29	j	199	ASP
30	k	72	TYR
30	k	74	VAL
30	k	79	LYS
30	k	85	LEU
30	k	89	MET
30	k	93	VAL
30	k	125	CYS
30	k	134	GLU
30	k	152	GLU
30	k	157	ASP
30	k	159	VAL
30	k	165	ILE
30	k	166	ARG
30	k	180	SER
30	k	192	LEU
30	k	204	THR
30	k	247	GLU
30	k	251	GLU
30	k	279	GLU
30	k	298	VAL
30	k	306	ASP
30	k	309	ASN
30	k	317	SER
31	m	13	LEU
31	m	17	ARG
31	m	18	ARG
31	m	28	ILE
31	m	29	LEU
31	m	33	VAL
31	m	46	ILE
31	m	48	GLU
31	m	99	LEU
32	n	135	ARG
32	n	144	ARG
32	n	145	LYS
32	n	147	VAL
32	n	161	ARG

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Mol	Chain	Res	Type
32	n	173	LEU
32	n	175	ARG
32	n	191	THR
32	n	194	ILE
33	o	67	LYS
33	o	68	VAL
33	o	77	THR
33	o	96	ILE
33	o	107	LEU
33	o	120	ILE
33	o	134	GLU
34	p	53	ASP
34	p	80	ASN
34	p	90	THR
34	p	96	ARG
34	p	103	ASN
34	p	108	CYS
34	p	113	LEU
34	p	119	ASN
34	p	123	LEU
34	p	134	ILE
34	p	163	LEU
34	p	167	ILE
34	p	173	ARG
34	p	177	PHE
34	p	179	THR
34	p	193	LEU
34	p	195	SER
34	p	199	TRP
34	p	202	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	68	HIS
2	B	92	HIS
2	B	133	HIS
2	B	152	HIS
2	B	177	ASN
2	B	200	ASN
3	C	72	HIS
3	C	81	HIS

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Mol	Chain	Res	Type
3	C	115	ASN
3	C	126	GLN
3	C	145	HIS
3	C	154	HIS
3	C	156	GLN
4	E	145	ASN
4	E	165	GLN
4	E	175	GLN
4	E	196	ASN
4	E	288	HIS
4	E	308	GLN
4	E	317	HIS
4	E	356	GLN
4	E	369	HIS
5	F	58	HIS
5	F	92	ASN
6	G	122	GLN
6	G	147	GLN
6	G	151	ASN
6	G	227	HIS
6	G	233	ASN
7	I	101	GLN
7	I	127	HIS
7	I	156	GLN
7	I	221	GLN
7	I	319	HIS
7	I	327	HIS
7	I	367	GLN
8	J	83	HIS
8	J	125	HIS
9	K	98	GLN
9	K	100	GLN
10	L	34	ASN
10	L	35	GLN
10	L	77	ASN
11	N	124	GLN
12	O	147	HIS
12	O	153	HIS
12	O	201	HIS
12	O	219	GLN
13	P	28	ASN
13	P	50	GLN

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Mol	Chain	Res	Type
13	P	61	HIS
13	P	75	HIS
13	P	100	HIS
14	Q	44	ASN
14	Q	57	GLN
15	R	79	GLN
15	R	96	HIS
17	U	3	ASN
17	U	18	ASN
17	U	79	ASN
17	U	85	GLN
20	a	75	GLN
20	a	76	ASN
20	a	107	GLN
20	a	109	GLN
20	a	215	GLN
20	a	222	GLN
20	a	223	HIS
20	a	228	ASN
20	a	233	GLN
20	a	245	HIS
20	a	246	HIS
20	a	247	HIS
20	a	276	ASN
20	a	287	GLN
20	a	307	HIS
22	c	51	ASN
22	c	59	ASN
22	c	63	GLN
22	c	69	ASN
22	c	95	ASN
22	c	101	HIS
22	c	125	HIS
22	c	128	HIS
22	c	146	GLN
23	d	31	HIS
23	d	109	ASN
23	d	126	GLN
25	f	98	ASN
26	g	80	HIS
26	g	113	ASN
26	g	115	ASN

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Mol	Chain	Res	Type
26	g	118	HIS
26	g	173	ASN
26	g	196	HIS
26	g	290	HIS
26	g	366	GLN
26	g	386	ASN
27	h	323	HIS
27	h	364	HIS
28	i	55	HIS
28	i	75	HIS
29	j	66	GLN
29	j	111	HIS
30	k	124	HIS
30	k	233	HIS
30	k	263	ASN
30	k	303	ASN
31	m	109	HIS
31	m	113	ASN
32	n	140	HIS
32	n	178	GLN
32	n	198	ASN
34	p	80	ASN
34	p	169	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	959/962 (99%)	329 (34%)	10 (1%)
18	V	61/64 (95%)	12 (19%)	0
18	Y	60/64 (93%)	13 (21%)	0
19	X	12/13 (92%)	5 (41%)	0
All	All	1092/1103 (99%)	359 (32%)	10 (0%)

All (359) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	A
1	A	10	U
1	A	11	G
1	A	14	C
1	A	18	G

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Mol	Chain	Res	Type
1	A	28	U
1	A	34	U
1	A	36	A
1	A	39	A
1	A	42	A
1	A	45	A
1	A	49	A
1	A	51	G
1	A	54	A
1	A	55	G
1	A	58	U
1	A	60	C
1	A	61	G
1	A	63	G
1	A	65	C
1	A	66	C
1	A	67	C
1	A	71	G
1	A	75	A
1	A	77	G
1	A	78	C
1	A	92	A
1	A	97	C
1	A	98	A
1	A	101	A
1	A	102	G
1	A	103	G
1	A	104	A
1	A	111	A
1	A	115	A
1	A	118	A
1	A	119	C
1	A	120	A
1	A	121	C
1	A	124	A
1	A	125	U
1	A	126	A
1	A	127	A
1	A	128	C
1	A	129	G
1	A	138	U
1	A	142	G

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Mol	Chain	Res	Type
1	A	147	G
1	A	151	A
1	A	152	A
1	A	160	C
1	A	161	C
1	A	162	C
1	A	163	A
1	A	164	C
1	A	166	G
1	A	168	A
1	A	169	A
1	A	170	A
1	A	171	C
1	A	173	G
1	A	176	G
1	A	184	A
1	A	185	A
1	A	186	U
1	A	191	C
1	A	192	C
1	A	198	C
1	A	199	G
1	A	201	A
1	A	203	G
1	A	216	A
1	A	217	U
1	A	219	U
1	A	222	A
1	A	223	U
1	A	224	U
1	A	225	A
1	A	231	G
1	A	237	U
1	A	238	C
1	A	243	G
1	A	244	C
1	A	245	C
1	A	246	A
1	A	247	G
1	A	251	C
1	A	253	G
1	A	257	U

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Mol	Chain	Res	Type
1	A	258	C
1	A	259	A
1	A	265	U
1	A	267	A
1	A	273	A
1	A	280	A
1	A	281	G
1	A	285	C
1	A	286	A
1	A	287	C
1	A	288	G
1	A	294	A
1	A	295	A
1	A	297	A
1	A	298	G
1	A	310	A
1	A	311	A
1	A	313	A
1	A	316	C
1	A	317	A
1	A	318	C
1	A	319	A
1	A	320	A
1	A	322	A
1	A	334	U
1	A	337	C
1	A	340	A
1	A	341	G
1	A	345	U
1	A	354	C
1	A	355	U
1	A	361	A
1	A	362	A
1	A	367	A
1	A	368	A
1	A	369	U
1	A	377	G
1	A	378	A
1	A	381	G
1	A	385	C
1	A	391	U
1	A	394	U

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Mol	Chain	Res	Type
1	A	395	C
1	A	396	C
1	A	399	A
1	A	400	C
1	A	414	G
1	A	417	C
1	A	421	A
1	A	425	G
1	A	432	A
1	A	433	U
1	A	434	A
1	A	450	C
1	A	454	A
1	A	456	A
1	A	457	C
1	A	458	C
1	A	459	C
1	A	461	A
1	A	471	U
1	A	472	A
1	A	477	A
1	A	478	A
1	A	487	C
1	A	488	A
1	A	489	G
1	A	498	U
1	A	501	C
1	A	502	A
1	A	504	C
1	A	505	U
1	A	506	G
1	A	518	A
1	A	525	U
1	A	526	G
1	A	531	U
1	A	532	G
1	A	536	C
1	A	538	C
1	A	539	A
1	A	540	U
1	A	541	C
1	A	542	C

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Mol	Chain	Res	Type
1	A	547	A
1	A	559	U
1	A	561	U
1	A	562	A
1	A	564	A
1	A	566	U
1	A	571	A
1	A	574	C
1	A	576	C
1	A	577	C
1	A	579	A
1	A	588	A
1	A	589	C
1	A	592	A
1	A	593	C
1	A	594	C
1	A	597	U
1	A	598	G
1	A	603	U
1	A	604	U
1	A	606	A
1	A	607	G
1	A	609	C
1	A	610	U
1	A	612	U
1	A	619	C
1	A	620	C
1	A	625	U
1	A	627	A
1	A	628	G
1	A	631	A
1	A	637	A
1	A	638	A
1	A	639	A
1	A	640	A
1	A	641	A
1	A	644	A
1	A	645	A
1	A	646	C
1	A	647	A
1	A	648	A
1	A	649	U

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Mol	Chain	Res	Type
1	A	650	A
1	A	654	A
1	A	662	C
1	A	665	A
1	A	666	G
1	A	667	C
1	A	681	A
1	A	682	G
1	A	686	A
1	A	690	U
1	A	693	A
1	A	694	G
1	A	695	C
1	A	697	U
1	A	698	A
1	A	699	U
1	A	705	G
1	A	707	A
1	A	708	A
1	A	709	A
1	A	710	G
1	A	711	A
1	A	720	A
1	A	722	A
1	A	723	U
1	A	731	A
1	A	732	U
1	A	733	A
1	A	734	A
1	A	736	A
1	A	739	A
1	A	740	U
1	A	742	C
1	A	744	C
1	A	745	C
1	A	746	A
1	A	747	C
1	A	748	A
1	A	753	A
1	A	765	A
1	A	766	C
1	A	771	A

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Mol	Chain	Res	Type
1	A	775	A
1	A	780	A
1	A	783	A
1	A	786	U
1	A	789	C
1	A	790	A
1	A	791	G
1	A	802	A
1	A	803	U
1	A	807	G
1	A	808	U
1	A	821	A
1	A	822	A
1	A	823	G
1	A	824	G
1	A	825	C
1	A	826	C
1	A	841	C
1	A	842	A
1	A	846	C
1	A	854	C
1	A	863	G
1	A	867	G
1	A	868	U
1	A	869	A
1	A	870	G
1	A	871	U
1	A	872	A
1	A	874	U
1	A	876	A
1	A	877	A
1	A	878	A
1	A	880	U
1	A	881	A
1	A	882	A
1	A	884	C
1	A	885	U
1	A	886	A
1	A	890	U
1	A	891	C
1	A	894	U
1	A	895	U

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Mol	Chain	Res	Type
1	A	896	A
1	A	897	C
1	A	898	A
1	A	899	C
1	A	900	A
1	A	901	A
1	A	902	C
1	A	903	C
1	A	910	G
1	A	917	C
1	A	918	A
1	A	920	G
1	A	921	U
1	A	923	G
1	A	925	A
1	A	928	A
1	A	929	A
1	A	930	G
1	A	932	U
1	A	933	A
1	A	937	A
1	A	943	G
1	A	945	A
1	A	946	A
1	A	955	G
1	A	956	G
1	A	957	A
1	A	958	U
1	A	959	U
1	A	962	C
18	V	6	Y5P
18	V	8	Y5P
18	V	9	Y5P
18	V	14	Y5P
18	V	22	Y5P
18	V	23	Y5P
18	V	32	Y5P
18	V	37	Y5P
18	V	42	Y5P
18	V	52	Y5P
18	V	59	Y5P
18	V	70	Y5P

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Mol	Chain	Res	Type
19	X	13	Y5P
19	X	15	Y5P
19	X	22	Y5P
19	X	23	Y5P
19	X	24	Y5P
18	Y	2	Y5P
18	Y	9	Y5P
18	Y	15	Y5P
18	Y	23	Y5P
18	Y	34	P5P
18	Y	42	Y5P
18	Y	43	Y5P
18	Y	52	Y5P
18	Y	53	Y5P
18	Y	57	Y5P
18	Y	68	Y5P
18	Y	70	Y5P
18	Y	71	Y5P

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	124	A
1	A	127	A
1	A	316	C
1	A	317	A
1	A	390	A
1	A	395	C
1	A	825	C
1	A	899	C
1	A	900	A
1	A	901	A

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

141 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	$\# Z > 2$
18	Y5P	Y	45	18	14,19,20	4.20	2 (14%)	18,26,29	1.07	1 (5%)
18	Y5P	Y	42	18	14,19,20	4.68	2 (14%)	18,26,29	1.31	2 (11%)
18	Y5P	Y	37	18	14,19,20	4.76	3 (21%)	18,26,29	1.15	1 (5%)
18	Y5P	V	13	18	14,19,20	4.58	2 (14%)	18,26,29	1.32	2 (11%)
18	Y5P	V	1	18	14,16,20	4.66	3 (21%)	19,22,29	1.02	1 (5%)
18	Y5P	Y	44	18	14,19,20	4.65	3 (21%)	18,26,29	1.06	1 (5%)
18	Y5P	Y	12	18	14,19,20	4.29	2 (14%)	18,26,29	1.01	1 (5%)
18	Y5P	V	42	18	14,19,20	4.78	2 (14%)	18,26,29	1.25	1 (5%)
18	Y5P	Y	9	18	14,19,20	4.67	3 (21%)	18,26,29	1.09	1 (5%)
18	Y5P	V	43	18	14,19,20	4.67	2 (14%)	18,26,29	1.30	2 (11%)
18	Y5P	Y	52	18	14,19,20	4.63	3 (21%)	18,26,29	1.13	1 (5%)
18	Y5P	Y	7	18	14,19,20	4.65	3 (21%)	18,26,29	1.03	1 (5%)
18	Y5P	Y	23	18	14,19,20	4.66	3 (21%)	18,26,29	1.04	1 (5%)
18	Y5P	V	58	18	14,19,20	4.63	3 (21%)	18,26,29	1.09	1 (5%)
18	Y5P	V	14	18	14,19,20	4.66	3 (21%)	18,26,29	1.17	2 (11%)
18	Y5P	V	32	18	14,19,20	4.32	2 (14%)	18,26,29	1.00	1 (5%)
18	Y5P	V	37	18	14,19,20	4.66	3 (21%)	18,26,29	1.11	1 (5%)
19	Y5P	X	17	19	14,19,20	4.16	2 (14%)	18,26,29	1.00	1 (5%)
19	Y5P	X	19	19,37	14,19,20	4.23	2 (14%)	18,26,29	1.01	1 (5%)
18	Y5P	V	2	18	14,19,20	4.60	2 (14%)	18,26,29	1.34	2 (11%)
18	Y5P	Y	2	18	14,19,20	4.57	2 (14%)	18,26,29	1.35	2 (11%)
18	Y5P	Y	26	18	14,19,20	4.69	3 (21%)	18,26,29	1.06	1 (5%)
19	Y5P	X	20	19	14,19,20	4.22	2 (14%)	18,26,29	1.01	1 (5%)
18	Y5P	Y	14	18	14,19,20	4.68	3 (21%)	18,26,29	1.03	1 (5%)
18	Y5P	Y	63	18	14,19,20	4.64	3 (21%)	18,26,29	1.10	1 (5%)
18	Y5P	V	11	18	14,19,20	4.56	2 (14%)	18,26,29	1.40	2 (11%)
18	Y5P	V	54	18	14,19,20	4.34	2 (14%)	18,26,29	1.04	1 (5%)
18	Y5P	V	68	18	14,19,20	4.65	2 (14%)	18,26,29	1.31	1 (5%)
18	Y5P	Y	32	18	14,19,20	4.22	2 (14%)	18,26,29	0.99	1 (5%)
18	Y5P	V	24	18	14,19,20	4.65	3 (21%)	18,26,29	1.06	1 (5%)
18	Y5P	V	33	18	14,19,20	4.19	2 (14%)	18,26,29	0.84	1 (5%)
18	Y5P	V	40	18	14,19,20	4.72	2 (14%)	18,26,29	1.19	1 (5%)
18	Y5P	Y	15	18	14,19,20	4.64	3 (21%)	18,26,29	1.12	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	Y5P	V	45	18	14,19,20	4.33	2 (14%)	18,26,29	0.98	1 (5%)
19	Y5P	X	22	19	14,19,20	4.39	2 (14%)	18,26,29	1.10	1 (5%)
18	Y5P	V	21	18	14,19,20	4.74	3 (21%)	18,26,29	1.21	2 (11%)
18	Y5P	Y	69	18	14,19,20	4.69	3 (21%)	18,26,29	1.12	1 (5%)
18	Y5P	Y	67	18	14,19,20	4.63	2 (14%)	18,26,29	1.31	2 (11%)
18	Y5P	Y	66	18	14,19,20	4.32	2 (14%)	18,26,29	1.02	1 (5%)
18	Y5P	V	38	18	14,19,20	4.64	3 (21%)	18,26,29	1.13	1 (5%)
18	Y5P	V	69	18	14,19,20	4.66	3 (21%)	18,26,29	1.03	1 (5%)
18	Y5P	Y	59	18	14,19,20	4.36	2 (14%)	18,26,29	0.96	1 (5%)
18	Y5P	Y	55	18	14,19,20	4.35	2 (14%)	18,26,29	1.05	1 (5%)
18	Y5P	Y	29	18	14,19,20	4.68	3 (21%)	18,26,29	1.08	1 (5%)
18	Y5P	Y	54	18	14,19,20	4.32	2 (14%)	18,26,29	1.03	1 (5%)
18	Y5P	Y	68	18	14,19,20	4.58	2 (14%)	18,26,29	1.36	2 (11%)
18	Y5P	Y	33	18	14,19,20	4.34	2 (14%)	18,26,29	0.98	1 (5%)
18	Y5P	V	49	18	14,19,20	4.59	2 (14%)	18,26,29	1.35	2 (11%)
18	Y5P	Y	28	18	14,19,20	4.69	3 (21%)	18,26,29	1.10	1 (5%)
18	Y5P	Y	57	18	14,19,20	4.65	3 (21%)	18,26,29	1.03	1 (5%)
18	Y5P	V	30	18	14,19,20	4.64	3 (21%)	18,26,29	1.14	1 (5%)
18	Y5P	Y	25	18	14,19,20	4.61	2 (14%)	18,26,29	1.31	2 (11%)
19	Y5P	X	14	19	14,19,20	4.41	2 (14%)	18,26,29	0.98	1 (5%)
18	Y5P	V	3	18	14,19,20	4.54	2 (14%)	18,26,29	1.36	2 (11%)
18	Y5P	Y	41	18	14,19,20	4.57	2 (14%)	18,26,29	1.32	2 (11%)
18	Y5P	Y	22	18	14,19,20	4.65	3 (21%)	18,26,29	1.05	1 (5%)
18	Y5P	V	50	18	14,19,20	4.35	2 (14%)	18,26,29	1.01	1 (5%)
18	Y5P	V	64	18	14,19,20	4.67	3 (21%)	18,26,29	1.07	1 (5%)
18	Y5P	Y	60	18	14,19,20	4.36	2 (14%)	18,26,29	1.01	1 (5%)
18	Y5P	Y	30	18	14,19,20	4.63	3 (21%)	18,26,29	1.12	1 (5%)
18	Y5P	Y	1	18	14,16,20	4.64	3 (21%)	19,22,29	1.04	1 (5%)
18	Y5P	V	70	18	14,19,20	4.66	3 (21%)	18,26,29	1.05	1 (5%)
18	Y5P	Y	39	18	14,19,20	4.10	2 (14%)	18,26,29	1.09	1 (5%)
18	Y5P	Y	53	18	14,19,20	4.65	3 (21%)	18,26,29	1.11	1 (5%)
18	Y5P	V	56	18	14,19,20	4.61	2 (14%)	18,26,29	1.32	2 (11%)
18	Y5P	Y	64	18	14,19,20	4.64	3 (21%)	18,26,29	1.12	1 (5%)
19	Y5P	X	23	19	14,19,20	4.36	2 (14%)	18,26,29	1.02	1 (5%)
18	P5P	Y	35	18	20,23,24	0.54	0	27,33,36	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	Y5P	Y	50	18	14,19,20	4.34	2 (14%)	18,26,29	1.06	1 (5%)
18	Y5P	V	57	18	14,19,20	4.64	3 (21%)	18,26,29	1.07	1 (5%)
18	Y5P	V	39	18	14,19,20	4.23	2 (14%)	18,26,29	1.09	1 (5%)
18	Y5P	V	23	18	14,19,20	4.65	3 (21%)	18,26,29	1.06	1 (5%)
19	Y5P	X	21	19	14,19,20	4.55	2 (14%)	18,26,29	1.32	1 (5%)
18	P5P	Y	34	18	20,23,24	1.03	2 (10%)	27,33,36	2.05	4 (14%)
18	Y5P	V	48	18	14,19,20	4.65	2 (14%)	18,26,29	1.34	2 (11%)
18	Y5P	V	4	18	14,19,20	4.66	2 (14%)	18,26,29	1.25	2 (11%)
19	Y5P	X	18	19	14,19,20	4.52	2 (14%)	18,26,29	1.35	2 (11%)
18	Y5P	Y	65	18	14,19,20	4.67	3 (21%)	18,26,29	1.07	1 (5%)
18	Y5P	Y	40	37,18	14,19,20	4.57	2 (14%)	18,26,29	1.36	2 (11%)
18	Y5P	V	6	18	14,19,20	4.64	3 (21%)	18,26,29	1.08	1 (5%)
18	Y5P	V	53	18	14,19,20	4.70	3 (21%)	18,26,29	1.05	1 (5%)
18	Y5P	Y	6	18	14,19,20	4.70	3 (21%)	18,26,29	1.05	1 (5%)
18	Y5P	V	8	18	14,19,20	4.17	2 (14%)	18,26,29	1.00	1 (5%)
18	Y5P	Y	61	18	14,19,20	4.55	2 (14%)	18,26,29	1.31	2 (11%)
19	Y5P	X	16	19	14,19,20	3.99	2 (14%)	18,26,29	1.19	1 (5%)
18	Y5P	Y	24	18	14,19,20	4.64	3 (21%)	18,26,29	1.06	1 (5%)
18	Y5P	V	63	18	14,19,20	4.67	3 (21%)	18,26,29	1.12	1 (5%)
18	Y5P	V	51	18	14,19,20	4.42	2 (14%)	18,26,29	0.96	1 (5%)
18	Y5P	Y	58	18	14,19,20	4.65	3 (21%)	18,26,29	1.09	1 (5%)
18	Y5P	V	71	18	14,19,20	4.64	3 (21%)	18,26,29	1.03	1 (5%)
18	Y5P	V	61	18	14,19,20	4.58	2 (14%)	18,26,29	1.28	2 (11%)
18	Y5P	Y	70	18	14,19,20	4.65	3 (21%)	18,26,29	1.04	1 (5%)
18	Y5P	Y	38	18	14,19,20	4.70	3 (21%)	18,26,29	1.14	1 (5%)
18	Y5P	Y	43	18	14,19,20	4.68	2 (14%)	18,26,29	1.27	2 (11%)
19	Y5P	X	13	19	14,19,20	4.38	2 (14%)	18,26,29	1.00	1 (5%)
18	Y5P	Y	10	18	14,19,20	4.66	3 (21%)	18,26,29	1.08	1 (5%)
18	Y5P	V	66	18	14,19,20	4.34	2 (14%)	18,26,29	1.13	1 (5%)
18	Y5P	Y	49	18	14,19,20	4.54	2 (14%)	18,26,29	1.37	2 (11%)
18	Y5P	V	22	18	14,19,20	4.68	3 (21%)	18,26,29	1.08	1 (5%)
18	Y5P	V	26	18	14,19,20	4.69	3 (21%)	18,26,29	1.09	1 (5%)
18	Y5P	Y	62	18	14,19,20	4.69	2 (14%)	18,26,29	1.35	2 (11%)
18	Y5P	V	9	18	14,19,20	4.65	3 (21%)	18,26,29	1.08	1 (5%)
18	Y5P	V	65	18	14,19,20	4.66	3 (21%)	18,26,29	1.11	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	Y5P	Y	8	18	14,19,20	4.25	2 (14%)	18,26,29	1.02	1 (5%)
18	Y5P	V	10	18	14,19,20	4.65	3 (21%)	18,26,29	1.09	1 (5%)
18	Y5P	V	55	18	14,19,20	4.34	2 (14%)	18,26,29	1.06	1 (5%)
18	Y5P	V	7	18	14,19,20	4.63	3 (21%)	18,26,29	1.03	1 (5%)
18	Y5P	V	44	18	14,19,20	4.67	3 (21%)	18,26,29	1.09	1 (5%)
18	Y5P	Y	31	18	14,19,20	4.69	3 (21%)	18,26,29	1.07	1 (5%)
18	Y5P	V	31	18	14,19,20	4.62	3 (21%)	18,26,29	1.03	1 (5%)
18	Y5P	V	29	18	14,19,20	4.59	3 (21%)	18,26,29	1.17	1 (5%)
18	Y5P	Y	4	18	14,19,20	4.58	2 (14%)	18,26,29	1.31	2 (11%)
18	Y5P	V	27	18	14,19,20	4.63	3 (21%)	18,26,29	1.08	1 (5%)
18	Y5P	V	28	18	14,19,20	4.66	3 (21%)	18,26,29	1.08	1 (5%)
18	P5P	V	36	18	20,23,24	0.46	0	27,33,36	0.86	0
18	Y5P	Y	11	18	14,19,20	4.61	2 (14%)	18,26,29	1.34	2 (11%)
18	Y5P	V	62	18	14,19,20	4.59	2 (14%)	18,26,29	1.35	2 (11%)
18	Y5P	Y	71	18	14,19,20	4.66	3 (21%)	18,26,29	1.14	2 (11%)
18	Y5P	V	60	18	14,19,20	4.37	2 (14%)	18,26,29	1.08	1 (5%)
18	Y5P	Y	56	18	14,19,20	4.57	2 (14%)	18,26,29	1.36	2 (11%)
18	Y5P	V	5	18	14,19,20	4.65	3 (21%)	18,26,29	1.05	1 (5%)
18	Y5P	Y	48	18	14,19,20	4.59	2 (14%)	18,26,29	1.29	2 (11%)
18	Y5P	V	67	18	14,19,20	4.63	2 (14%)	18,26,29	1.32	2 (11%)
18	Y5P	Y	3	18	14,19,20	4.66	2 (14%)	18,26,29	1.26	2 (11%)
18	Y5P	V	25	18	14,19,20	4.53	2 (14%)	18,26,29	1.34	2 (11%)
18	Y5P	Y	27	18	14,19,20	4.68	3 (21%)	18,26,29	1.31	2 (11%)
18	Y5P	Y	21	18	14,19,20	4.70	3 (21%)	18,26,29	1.06	1 (5%)
18	P5P	Y	36	18	20,23,24	0.53	0	27,33,36	0.75	1 (3%)
19	Y5P	X	12	19	14,16,20	4.23	2 (14%)	19,22,29	1.11	1 (5%)
18	Y5P	Y	13	18	14,19,20	4.58	2 (14%)	18,26,29	1.36	2 (11%)
18	Y5P	V	41	18	14,19,20	4.73	2 (14%)	18,26,29	1.24	1 (5%)
18	P5P	V	34	18	20,23,24	1.12	3 (15%)	27,33,36	2.11	3 (11%)
18	Y5P	Y	5	18	14,19,20	4.69	3 (21%)	18,26,29	1.04	1 (5%)
19	Y5P	X	24	19	14,19,20	4.49	2 (14%)	18,26,29	1.00	1 (5%)
19	Y5P	X	15	19	14,19,20	4.44	2 (14%)	18,26,29	1.06	1 (5%)
18	Y5P	V	59	18	14,19,20	4.49	2 (14%)	18,26,29	0.98	1 (5%)
18	Y5P	V	52	18	14,19,20	4.66	3 (21%)	18,26,29	1.11	1 (5%)
18	P5P	V	35	18	20,23,24	0.52	0	27,33,36	0.83	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	Y5P	Y	51	18	14,19,20	4.25	2 (14%)	18,26,29	1.10	1 (5%)
18	Y5P	V	12	18	14,19,20	4.19	2 (14%)	18,26,29	1.05	1 (5%)
18	Y5P	V	15	18	14,19,20	4.61	3 (21%)	18,26,29	1.04	1 (5%)

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
18	Y5P	Y	45	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	42	18	-	3/7/33/34	0/2/2/2
18	Y5P	Y	37	18	-	3/7/33/34	0/2/2/2
18	Y5P	V	13	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	1	18	-	1/6/30/34	0/2/2/2
18	Y5P	Y	44	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	12	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	42	18	-	3/7/33/34	0/2/2/2
18	Y5P	Y	9	18	-	3/7/33/34	0/2/2/2
18	Y5P	V	43	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	52	18	-	3/7/33/34	0/2/2/2
18	Y5P	Y	7	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	23	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	58	18	-	4/7/33/34	0/2/2/2
18	Y5P	V	14	18	-	6/7/33/34	0/2/2/2
18	Y5P	V	32	18	-	3/7/33/34	0/2/2/2
18	Y5P	V	37	18	-	3/7/33/34	0/2/2/2
19	Y5P	X	17	19	-	1/7/33/34	0/2/2/2
19	Y5P	X	19	19,37	-	2/7/33/34	0/2/2/2
18	Y5P	V	2	18	-	3/7/33/34	0/2/2/2
18	Y5P	Y	2	18	-	2/7/33/34	0/2/2/2
18	Y5P	Y	26	18	-	1/7/33/34	0/2/2/2
19	Y5P	X	20	19	-	1/7/33/34	0/2/2/2
18	Y5P	Y	14	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	63	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	11	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	54	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	68	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	32	18	-	1/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	Y5P	V	24	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	33	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	40	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	15	18	-	3/7/33/34	0/2/2/2
18	Y5P	V	45	18	-	1/7/33/34	0/2/2/2
19	Y5P	X	22	19	-	3/7/33/34	0/2/2/2
18	Y5P	V	21	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	69	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	67	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	66	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	38	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	69	18	-	3/7/33/34	0/2/2/2
18	Y5P	Y	59	18	-	3/7/33/34	0/2/2/2
18	Y5P	Y	55	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	29	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	54	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	68	18	-	3/7/33/34	0/2/2/2
18	Y5P	Y	33	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	49	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	28	18	-	2/7/33/34	0/2/2/2
18	Y5P	Y	57	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	30	18	-	2/7/33/34	0/2/2/2
18	Y5P	Y	25	18	-	1/7/33/34	0/2/2/2
19	Y5P	X	14	19	-	1/7/33/34	0/2/2/2
18	Y5P	V	3	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	41	18	-	3/7/33/34	0/2/2/2
18	Y5P	Y	22	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	50	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	64	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	60	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	30	18	-	4/7/33/34	0/2/2/2
18	Y5P	Y	1	18	-	1/6/30/34	0/2/2/2
18	Y5P	V	70	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	39	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	53	18	-	3/7/33/34	0/2/2/2
18	Y5P	V	56	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	64	18	-	1/7/33/34	0/2/2/2
19	Y5P	X	23	19	-	3/7/33/34	0/2/2/2
18	P5P	Y	35	18	-	0/7/25/26	0/3/3/3
18	Y5P	Y	50	18	-	1/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	Y5P	V	57	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	39	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	23	18	-	3/7/33/34	0/2/2/2
19	Y5P	X	21	19	-	1/7/33/34	0/2/2/2
18	P5P	Y	34	18	-	2/7/25/26	0/3/3/3
18	Y5P	V	48	18	-	3/7/33/34	0/2/2/2
18	Y5P	V	4	18	-	3/7/33/34	0/2/2/2
19	Y5P	X	18	19	-	1/7/33/34	0/2/2/2
18	Y5P	Y	65	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	40	37,18	-	1/7/33/34	0/2/2/2
18	Y5P	V	6	18	-	4/7/33/34	0/2/2/2
18	Y5P	V	53	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	6	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	8	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	61	18	-	3/7/33/34	0/2/2/2
19	Y5P	X	16	19	-	1/7/33/34	0/2/2/2
18	Y5P	Y	24	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	63	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	51	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	58	18	-	4/7/33/34	0/2/2/2
18	Y5P	V	71	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	61	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	70	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	38	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	43	18	-	4/7/33/34	0/2/2/2
19	Y5P	X	13	19	-	3/7/33/34	0/2/2/2
18	Y5P	Y	10	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	66	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	49	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	22	18	-	3/7/33/34	0/2/2/2
18	Y5P	V	26	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	62	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	9	18	-	5/7/33/34	0/2/2/2
18	Y5P	V	65	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	8	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	10	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	55	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	7	18	-	3/7/33/34	0/2/2/2
18	Y5P	V	44	18	-	1/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	Y5P	Y	31	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	31	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	29	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	4	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	27	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	28	18	-	1/7/33/34	0/2/2/2
18	P5P	V	36	18	-	0/7/25/26	0/3/3/3
18	Y5P	Y	11	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	62	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	71	18	-	4/7/33/34	0/2/2/2
18	Y5P	V	60	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	56	18	-	2/7/33/34	0/2/2/2
18	Y5P	V	5	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	48	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	67	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	3	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	25	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	27	18	-	1/7/33/34	0/2/2/2
18	Y5P	Y	21	18	-	2/7/33/34	0/2/2/2
18	P5P	Y	36	18	-	0/7/25/26	0/3/3/3
19	Y5P	X	12	19	-	3/6/30/34	0/2/2/2
18	Y5P	Y	13	18	-	3/7/33/34	0/2/2/2
18	Y5P	V	41	18	-	1/7/33/34	0/2/2/2
18	P5P	V	34	18	-	0/7/25/26	0/3/3/3
18	Y5P	Y	5	18	-	1/7/33/34	0/2/2/2
19	Y5P	X	24	19	-	1/7/33/34	0/2/2/2
19	Y5P	X	15	19	-	4/7/33/34	0/2/2/2
18	Y5P	V	59	18	-	3/7/33/34	0/2/2/2
18	Y5P	V	52	18	-	2/7/33/34	0/2/2/2
18	P5P	V	35	18	-	0/7/25/26	0/3/3/3
18	Y5P	Y	51	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	12	18	-	1/7/33/34	0/2/2/2
18	Y5P	V	15	18	-	1/7/33/34	0/2/2/2

All (337) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	V	59	Y5P	C2-N3	14.85	1.38	1.27
19	X	24	Y5P	C2-N3	14.82	1.38	1.27
18	V	41	Y5P	C4-N3	-14.72	1.32	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	X	15	Y5P	C2-N3	14.66	1.38	1.27
19	X	14	Y5P	C2-N3	14.54	1.38	1.27
18	Y	31	Y5P	C2-N3	14.50	1.38	1.27
18	Y	5	Y5P	C2-N3	14.49	1.38	1.27
18	V	63	Y5P	C2-N3	14.48	1.38	1.27
18	Y	27	Y5P	C2-N3	14.47	1.38	1.27
18	Y	28	Y5P	C2-N3	14.45	1.38	1.27
18	V	7	Y5P	C2-N3	14.45	1.38	1.27
18	Y	24	Y5P	C2-N3	14.45	1.38	1.27
18	V	64	Y5P	C2-N3	14.45	1.38	1.27
18	Y	7	Y5P	C2-N3	14.45	1.38	1.27
18	Y	6	Y5P	C2-N3	14.44	1.38	1.27
18	Y	69	Y5P	C2-N3	14.44	1.38	1.27
18	V	1	Y5P	C2-N3	14.44	1.38	1.27
18	V	53	Y5P	C2-N3	14.43	1.38	1.27
18	Y	26	Y5P	C2-N3	14.43	1.38	1.27
18	Y	37	Y5P	C2-N3	14.42	1.38	1.27
18	Y	21	Y5P	C2-N3	14.42	1.38	1.27
18	V	9	Y5P	C2-N3	14.42	1.38	1.27
18	V	50	Y5P	C2-N3	14.42	1.38	1.27
18	Y	65	Y5P	C2-N3	14.42	1.38	1.27
18	Y	14	Y5P	C2-N3	14.42	1.38	1.27
18	V	24	Y5P	C2-N3	14.42	1.38	1.27
18	V	26	Y5P	C2-N3	14.41	1.38	1.27
18	Y	10	Y5P	C2-N3	14.41	1.38	1.27
18	V	69	Y5P	C2-N3	14.41	1.38	1.27
19	X	22	Y5P	C2-N3	14.41	1.38	1.27
18	Y	15	Y5P	C2-N3	14.40	1.38	1.27
18	V	52	Y5P	C2-N3	14.40	1.38	1.27
18	V	70	Y5P	C2-N3	14.40	1.38	1.27
18	Y	22	Y5P	C2-N3	14.40	1.38	1.27
18	V	28	Y5P	C2-N3	14.40	1.38	1.27
18	V	37	Y5P	C2-N3	14.40	1.38	1.27
18	Y	57	Y5P	C2-N3	14.39	1.38	1.27
18	Y	9	Y5P	C2-N3	14.39	1.38	1.27
18	Y	70	Y5P	C2-N3	14.38	1.38	1.27
18	V	6	Y5P	C2-N3	14.38	1.38	1.27
18	V	29	Y5P	C2-N3	14.38	1.38	1.27
18	Y	58	Y5P	C2-N3	14.38	1.38	1.27
18	Y	64	Y5P	C2-N3	14.38	1.38	1.27
18	V	65	Y5P	C2-N3	14.38	1.38	1.27
18	Y	29	Y5P	C2-N3	14.38	1.38	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Y	44	Y5P	C2-N3	14.37	1.38	1.27
18	V	23	Y5P	C2-N3	14.37	1.38	1.27
18	Y	71	Y5P	C2-N3	14.37	1.38	1.27
18	V	22	Y5P	C2-N3	14.37	1.38	1.27
18	V	30	Y5P	C2-N3	14.37	1.38	1.27
18	V	10	Y5P	C2-N3	14.36	1.38	1.27
18	V	14	Y5P	C2-N3	14.36	1.38	1.27
18	Y	63	Y5P	C2-N3	14.36	1.38	1.27
18	V	31	Y5P	C2-N3	14.35	1.38	1.27
18	Y	38	Y5P	C2-N3	14.35	1.38	1.27
18	V	38	Y5P	C2-N3	14.34	1.38	1.27
18	Y	1	Y5P	C2-N3	14.34	1.38	1.27
18	V	21	Y5P	C2-N3	14.34	1.38	1.27
18	V	27	Y5P	C2-N3	14.34	1.38	1.27
18	V	58	Y5P	C2-N3	14.34	1.38	1.27
18	V	5	Y5P	C2-N3	14.34	1.38	1.27
18	Y	30	Y5P	C2-N3	14.34	1.38	1.27
18	Y	52	Y5P	C2-N3	14.34	1.38	1.27
18	Y	23	Y5P	C2-N3	14.33	1.38	1.27
18	V	42	Y5P	C4-N3	-14.33	1.32	1.46
18	V	57	Y5P	C2-N3	14.32	1.38	1.27
18	Y	53	Y5P	C2-N3	14.30	1.38	1.27
18	Y	50	Y5P	C2-N3	14.30	1.38	1.27
18	V	15	Y5P	C2-N3	14.29	1.38	1.27
18	V	51	Y5P	C2-N3	14.29	1.38	1.27
18	V	44	Y5P	C2-N3	14.28	1.38	1.27
19	X	23	Y5P	C2-N3	14.28	1.38	1.27
18	V	60	Y5P	C2-N3	14.28	1.38	1.27
18	V	71	Y5P	C2-N3	14.28	1.38	1.27
19	X	13	Y5P	C2-N3	14.26	1.38	1.27
18	V	66	Y5P	C2-N3	14.25	1.38	1.27
18	V	54	Y5P	C2-N3	14.21	1.38	1.27
18	Y	60	Y5P	C2-N3	14.16	1.38	1.27
18	Y	54	Y5P	C2-N3	14.05	1.38	1.27
18	V	55	Y5P	C2-N3	14.03	1.38	1.27
18	Y	59	Y5P	C2-N3	14.00	1.38	1.27
18	Y	66	Y5P	C2-N3	13.97	1.38	1.27
18	V	32	Y5P	C2-N3	13.96	1.38	1.27
18	V	45	Y5P	C2-N3	13.94	1.38	1.27
19	X	12	Y5P	C2-N3	13.91	1.38	1.27
18	Y	51	Y5P	C2-N3	13.89	1.38	1.27
19	X	21	Y5P	C4-N3	-13.88	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	V	40	Y5P	C4-N3	-13.87	1.33	1.46
18	Y	12	Y5P	C2-N3	13.83	1.38	1.27
18	Y	55	Y5P	C2-N3	13.76	1.38	1.27
18	Y	40	Y5P	C4-N3	-13.64	1.33	1.46
18	V	12	Y5P	C2-N3	13.53	1.37	1.27
18	Y	33	Y5P	C2-N3	13.51	1.37	1.27
18	Y	8	Y5P	C2-N3	13.49	1.37	1.27
18	Y	48	Y5P	C4-N3	-13.40	1.33	1.46
18	Y	32	Y5P	C2-N3	13.34	1.37	1.27
19	X	18	Y5P	C4-N3	-13.30	1.33	1.46
18	V	8	Y5P	C2-N3	13.19	1.37	1.27
18	Y	25	Y5P	C4-N3	-13.18	1.33	1.46
18	V	2	Y5P	C4-N3	-13.17	1.33	1.46
19	X	20	Y5P	C2-N3	13.16	1.37	1.27
18	Y	62	Y5P	C4-N3	-13.15	1.33	1.46
18	Y	67	Y5P	C4-N3	-13.13	1.33	1.46
18	Y	41	Y5P	C4-N3	-13.11	1.33	1.46
18	V	39	Y5P	C2-N3	13.09	1.37	1.27
18	V	48	Y5P	C4-N3	-13.08	1.33	1.46
18	Y	42	Y5P	C4-N3	-13.06	1.34	1.46
18	Y	43	Y5P	C4-N3	-13.05	1.34	1.46
18	Y	11	Y5P	C4-N3	-13.04	1.34	1.46
18	V	68	Y5P	C4-N3	-13.03	1.34	1.46
18	V	61	Y5P	C4-N3	-13.02	1.34	1.46
18	Y	56	Y5P	C4-N3	-12.97	1.34	1.46
18	Y	45	Y5P	C2-N3	12.93	1.37	1.27
18	V	4	Y5P	C4-N3	-12.93	1.34	1.46
18	Y	3	Y5P	C4-N3	-12.93	1.34	1.46
18	Y	68	Y5P	C4-N3	-12.92	1.34	1.46
18	V	43	Y5P	C4-N3	-12.91	1.34	1.46
18	Y	2	Y5P	C4-N3	-12.86	1.34	1.46
18	Y	39	Y5P	C2-N3	12.85	1.37	1.27
18	V	3	Y5P	C4-N3	-12.85	1.34	1.46
18	Y	61	Y5P	C4-N3	-12.85	1.34	1.46
18	Y	13	Y5P	C4-N3	-12.82	1.34	1.46
18	V	56	Y5P	C4-N3	-12.80	1.34	1.46
18	Y	4	Y5P	C4-N3	-12.79	1.34	1.46
18	V	25	Y5P	C4-N3	-12.75	1.34	1.46
19	X	19	Y5P	C2-N3	12.75	1.37	1.27
18	V	11	Y5P	C4-N3	-12.68	1.34	1.46
18	Y	49	Y5P	C4-N3	-12.61	1.34	1.46
18	V	67	Y5P	C4-N3	-12.57	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	V	62	Y5P	C4-N3	-12.53	1.34	1.46
18	V	49	Y5P	C4-N3	-12.51	1.34	1.46
18	V	13	Y5P	C4-N3	-12.37	1.34	1.46
19	X	17	Y5P	C2-N3	12.36	1.37	1.27
18	V	67	Y5P	C2-N3	11.83	1.36	1.27
18	V	13	Y5P	C2-N3	11.79	1.36	1.27
18	V	49	Y5P	C2-N3	11.69	1.36	1.27
18	V	43	Y5P	C2-N3	11.65	1.36	1.27
18	V	62	Y5P	C2-N3	11.65	1.36	1.27
18	Y	43	Y5P	C2-N3	11.63	1.36	1.27
18	V	4	Y5P	C2-N3	11.61	1.36	1.27
18	Y	3	Y5P	C2-N3	11.59	1.36	1.27
19	X	16	Y5P	C2-N3	11.58	1.36	1.27
18	Y	42	Y5P	C2-N3	11.58	1.36	1.27
18	Y	62	Y5P	C2-N3	11.51	1.36	1.27
18	V	56	Y5P	C2-N3	11.47	1.36	1.27
18	V	68	Y5P	C2-N3	11.44	1.36	1.27
18	V	48	Y5P	C2-N3	11.41	1.36	1.27
18	V	33	Y5P	C2-N3	11.38	1.36	1.27
18	V	11	Y5P	C2-N3	11.36	1.36	1.27
18	Y	4	Y5P	C2-N3	11.33	1.36	1.27
18	Y	49	Y5P	C2-N3	11.31	1.36	1.27
18	Y	13	Y5P	C2-N3	11.30	1.36	1.27
18	Y	2	Y5P	C2-N3	11.23	1.36	1.27
18	Y	67	Y5P	C2-N3	11.19	1.36	1.27
18	Y	11	Y5P	C2-N3	11.19	1.36	1.27
18	Y	68	Y5P	C2-N3	11.16	1.36	1.27
18	Y	56	Y5P	C2-N3	11.11	1.36	1.27
18	V	25	Y5P	C2-N3	11.10	1.36	1.27
18	Y	61	Y5P	C2-N3	11.08	1.36	1.27
18	V	61	Y5P	C2-N3	11.06	1.36	1.27
18	V	3	Y5P	C2-N3	11.06	1.36	1.27
18	Y	25	Y5P	C2-N3	11.03	1.36	1.27
18	V	2	Y5P	C2-N3	11.00	1.36	1.27
18	Y	41	Y5P	C2-N3	10.89	1.35	1.27
18	V	40	Y5P	C2-N3	10.82	1.35	1.27
18	V	33	Y5P	C4-N3	-10.71	1.36	1.46
18	Y	48	Y5P	C2-N3	10.67	1.35	1.27
18	V	42	Y5P	C2-N3	10.64	1.35	1.27
19	X	18	Y5P	C2-N3	10.38	1.35	1.27
18	Y	40	Y5P	C2-N3	10.23	1.35	1.27
19	X	21	Y5P	C2-N3	9.80	1.35	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	V	41	Y5P	C2-N3	9.75	1.35	1.27
19	X	17	Y5P	C4-N3	-9.33	1.37	1.46
19	X	16	Y5P	C4-N3	-9.31	1.37	1.46
19	X	19	Y5P	C4-N3	-9.29	1.37	1.46
18	Y	33	Y5P	C4-N3	-8.94	1.37	1.46
18	V	22	Y5P	C4-N3	-8.88	1.37	1.46
18	V	53	Y5P	C4-N3	-8.87	1.37	1.46
18	Y	5	Y5P	C4-N3	-8.87	1.37	1.46
18	V	26	Y5P	C4-N3	-8.86	1.37	1.46
18	Y	69	Y5P	C4-N3	-8.86	1.37	1.46
18	Y	37	Y5P	C4-N3	-8.86	1.37	1.46
18	V	30	Y5P	C4-N3	-8.85	1.37	1.46
18	Y	26	Y5P	C4-N3	-8.84	1.38	1.46
18	Y	6	Y5P	C4-N3	-8.84	1.38	1.46
18	V	65	Y5P	C4-N3	-8.84	1.38	1.46
18	V	64	Y5P	C4-N3	-8.84	1.38	1.46
18	Y	45	Y5P	C4-N3	-8.83	1.38	1.46
18	Y	28	Y5P	C4-N3	-8.83	1.38	1.46
18	V	70	Y5P	C4-N3	-8.83	1.38	1.46
18	V	38	Y5P	C4-N3	-8.82	1.38	1.46
18	Y	29	Y5P	C4-N3	-8.82	1.38	1.46
18	V	29	Y5P	C4-N3	-8.82	1.38	1.46
18	Y	71	Y5P	C4-N3	-8.81	1.38	1.46
18	Y	22	Y5P	C4-N3	-8.81	1.38	1.46
18	Y	70	Y5P	C4-N3	-8.81	1.38	1.46
18	Y	27	Y5P	C4-N3	-8.80	1.38	1.46
18	Y	14	Y5P	C4-N3	-8.80	1.38	1.46
18	V	23	Y5P	C4-N3	-8.80	1.38	1.46
18	V	24	Y5P	C4-N3	-8.79	1.38	1.46
18	Y	9	Y5P	C4-N3	-8.79	1.38	1.46
18	V	10	Y5P	C4-N3	-8.79	1.38	1.46
18	V	21	Y5P	C4-N3	-8.79	1.38	1.46
18	V	27	Y5P	C4-N3	-8.79	1.38	1.46
18	Y	53	Y5P	C4-N3	-8.79	1.38	1.46
18	Y	57	Y5P	C4-N3	-8.79	1.38	1.46
18	V	71	Y5P	C4-N3	-8.79	1.38	1.46
18	Y	7	Y5P	C4-N3	-8.79	1.38	1.46
18	Y	65	Y5P	C4-N3	-8.78	1.38	1.46
18	V	9	Y5P	C4-N3	-8.78	1.38	1.46
18	V	15	Y5P	C4-N3	-8.78	1.38	1.46
18	Y	21	Y5P	C4-N3	-8.78	1.38	1.46
18	V	63	Y5P	C4-N3	-8.78	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Y	31	Y5P	C4-N3	-8.78	1.38	1.46
18	Y	64	Y5P	C4-N3	-8.78	1.38	1.46
18	V	28	Y5P	C4-N3	-8.77	1.38	1.46
18	V	37	Y5P	C4-N3	-8.77	1.38	1.46
18	V	58	Y5P	C4-N3	-8.77	1.38	1.46
18	Y	38	Y5P	C4-N3	-8.77	1.38	1.46
18	V	6	Y5P	C4-N3	-8.76	1.38	1.46
18	Y	10	Y5P	C4-N3	-8.75	1.38	1.46
18	V	39	Y5P	C4-N3	-8.75	1.38	1.46
18	Y	1	Y5P	C4-N3	-8.75	1.38	1.46
18	V	14	Y5P	C4-N3	-8.74	1.38	1.46
18	V	52	Y5P	C4-N3	-8.74	1.38	1.46
18	V	5	Y5P	C4-N3	-8.74	1.38	1.46
18	V	31	Y5P	C4-N3	-8.74	1.38	1.46
18	V	44	Y5P	C4-N3	-8.74	1.38	1.46
18	Y	23	Y5P	C4-N3	-8.73	1.38	1.46
18	Y	30	Y5P	C4-N3	-8.73	1.38	1.46
18	V	69	Y5P	C4-N3	-8.73	1.38	1.46
18	Y	24	Y5P	C4-N3	-8.73	1.38	1.46
18	V	1	Y5P	C4-N3	-8.72	1.38	1.46
18	Y	63	Y5P	C4-N3	-8.72	1.38	1.46
18	V	7	Y5P	C4-N3	-8.72	1.38	1.46
18	Y	44	Y5P	C4-N3	-8.72	1.38	1.46
18	Y	52	Y5P	C4-N3	-8.71	1.38	1.46
18	Y	58	Y5P	C4-N3	-8.69	1.38	1.46
18	Y	15	Y5P	C4-N3	-8.69	1.38	1.46
18	V	57	Y5P	C4-N3	-8.69	1.38	1.46
19	X	20	Y5P	C4-N3	-8.61	1.38	1.46
18	Y	55	Y5P	C4-N3	-8.57	1.38	1.46
18	Y	32	Y5P	C4-N3	-8.34	1.38	1.46
18	Y	8	Y5P	C4-N3	-8.34	1.38	1.46
18	Y	39	Y5P	C4-N3	-8.25	1.38	1.46
18	V	8	Y5P	C4-N3	-8.23	1.38	1.46
18	Y	59	Y5P	C4-N3	-8.23	1.38	1.46
18	V	51	Y5P	C4-N3	-8.15	1.38	1.46
18	V	45	Y5P	C4-N3	-8.09	1.38	1.46
18	Y	12	Y5P	C4-N3	-8.08	1.38	1.46
18	Y	66	Y5P	C4-N3	-8.01	1.38	1.46
18	V	55	Y5P	C4-N3	-8.01	1.38	1.46
18	Y	60	Y5P	C4-N3	-7.98	1.38	1.46
18	V	32	Y5P	C4-N3	-7.96	1.38	1.46
18	Y	54	Y5P	C4-N3	-7.89	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	X	13	Y5P	C4-N3	-7.88	1.38	1.46
18	V	60	Y5P	C4-N3	-7.86	1.38	1.46
18	V	12	Y5P	C4-N3	-7.84	1.38	1.46
19	X	23	Y5P	C4-N3	-7.75	1.39	1.46
18	V	54	Y5P	C4-N3	-7.72	1.39	1.46
19	X	22	Y5P	C4-N3	-7.69	1.39	1.46
19	X	24	Y5P	C4-N3	-7.68	1.39	1.46
18	V	59	Y5P	C4-N3	-7.65	1.39	1.46
18	V	66	Y5P	C4-N3	-7.64	1.39	1.46
19	X	14	Y5P	C4-N3	-7.63	1.39	1.46
18	Y	50	Y5P	C4-N3	-7.63	1.39	1.46
18	Y	51	Y5P	C4-N3	-7.63	1.39	1.46
19	X	15	Y5P	C4-N3	-7.60	1.39	1.46
19	X	12	Y5P	C4-N3	-7.45	1.39	1.46
18	V	50	Y5P	C4-N3	-7.44	1.39	1.46
18	V	21	Y5P	C1'-N1	5.49	1.61	1.46
18	Y	37	Y5P	C1'-N1	5.42	1.61	1.46
18	Y	38	Y5P	C1'-N1	5.01	1.60	1.46
18	V	44	Y5P	C1'-N1	4.86	1.59	1.46
18	Y	21	Y5P	C1'-N1	4.79	1.59	1.46
18	Y	6	Y5P	C1'-N1	4.63	1.59	1.46
18	Y	23	Y5P	C1'-N1	4.63	1.59	1.46
18	V	53	Y5P	C1'-N1	4.57	1.58	1.46
18	V	22	Y5P	C1'-N1	4.57	1.58	1.46
18	V	26	Y5P	C1'-N1	4.56	1.58	1.46
18	V	14	Y5P	C1'-N1	4.56	1.58	1.46
18	Y	29	Y5P	C1'-N1	4.56	1.58	1.46
18	Y	14	Y5P	C1'-N1	4.53	1.58	1.46
18	Y	26	Y5P	C1'-N1	4.53	1.58	1.46
18	Y	31	Y5P	C1'-N1	4.49	1.58	1.46
18	Y	28	Y5P	C1'-N1	4.48	1.58	1.46
18	Y	53	Y5P	C1'-N1	4.46	1.58	1.46
18	Y	9	Y5P	C1'-N1	4.43	1.58	1.46
18	V	5	Y5P	C1'-N1	4.42	1.58	1.46
18	Y	44	Y5P	C1'-N1	4.41	1.58	1.46
18	V	1	Y5P	C1'-N1	4.40	1.58	1.46
18	V	69	Y5P	C1'-N1	4.39	1.58	1.46
18	V	57	Y5P	C1'-N1	4.38	1.58	1.46
18	Y	69	Y5P	C1'-N1	4.37	1.58	1.46
18	Y	58	Y5P	C1'-N1	4.36	1.58	1.46
18	Y	1	Y5P	C1'-N1	4.36	1.58	1.46
18	Y	71	Y5P	C1'-N1	4.35	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	V	71	Y5P	C1'-N1	4.34	1.58	1.46
18	Y	27	Y5P	C1'-N1	4.34	1.58	1.46
18	V	52	Y5P	C1'-N1	4.31	1.58	1.46
18	Y	65	Y5P	C1'-N1	4.30	1.58	1.46
18	Y	63	Y5P	C1'-N1	4.30	1.58	1.46
18	Y	5	Y5P	C1'-N1	4.29	1.58	1.46
18	V	37	Y5P	C1'-N1	4.29	1.58	1.46
18	V	28	Y5P	C1'-N1	4.29	1.58	1.46
18	V	65	Y5P	C1'-N1	4.29	1.58	1.46
18	Y	10	Y5P	C1'-N1	4.25	1.58	1.46
18	V	64	Y5P	C1'-N1	4.24	1.58	1.46
18	Y	15	Y5P	C1'-N1	4.22	1.58	1.46
18	V	70	Y5P	C1'-N1	4.22	1.58	1.46
18	V	10	Y5P	C1'-N1	4.21	1.57	1.46
18	Y	57	Y5P	C1'-N1	4.19	1.57	1.46
18	V	63	Y5P	C1'-N1	4.18	1.57	1.46
18	V	23	Y5P	C1'-N1	4.15	1.57	1.46
18	Y	64	Y5P	C1'-N1	4.12	1.57	1.46
18	Y	52	Y5P	C1'-N1	4.11	1.57	1.46
18	Y	70	Y5P	C1'-N1	4.11	1.57	1.46
18	V	24	Y5P	C1'-N1	4.11	1.57	1.46
18	V	27	Y5P	C1'-N1	4.10	1.57	1.46
18	Y	30	Y5P	C1'-N1	4.08	1.57	1.46
18	V	58	Y5P	C1'-N1	4.04	1.57	1.46
18	V	6	Y5P	C1'-N1	4.03	1.57	1.46
18	Y	22	Y5P	C1'-N1	4.03	1.57	1.46
18	V	9	Y5P	C1'-N1	4.02	1.57	1.46
18	V	38	Y5P	C1'-N1	3.95	1.57	1.46
18	Y	7	Y5P	C1'-N1	3.93	1.57	1.46
18	V	15	Y5P	C1'-N1	3.89	1.57	1.46
18	V	31	Y5P	C1'-N1	3.87	1.57	1.46
18	Y	24	Y5P	C1'-N1	3.84	1.56	1.46
18	V	30	Y5P	C1'-N1	3.77	1.56	1.46
18	V	7	Y5P	C1'-N1	3.75	1.56	1.46
18	V	34	P5P	C6-N1	3.11	1.40	1.34
18	V	34	P5P	C2-N1	2.97	1.39	1.33
18	V	29	Y5P	C1'-N1	2.93	1.54	1.46
18	Y	34	P5P	C6-N1	2.86	1.40	1.34
18	Y	34	P5P	C2-N1	2.59	1.38	1.33
18	V	34	P5P	C6-C5	2.01	1.42	1.39

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	V	34	P5P	C6-N1-C2	8.61	125.96	115.80
18	Y	34	P5P	C6-N1-C2	8.48	125.81	115.80
18	Y	56	Y5P	C5-C4-N3	4.80	121.89	114.15
18	Y	40	Y5P	C5-C4-N3	4.79	121.88	114.15
19	X	18	Y5P	C5-C4-N3	4.78	121.86	114.15
18	Y	13	Y5P	C5-C4-N3	4.75	121.81	114.15
18	V	11	Y5P	C5-C4-N3	4.75	121.80	114.15
18	Y	2	Y5P	C5-C4-N3	4.74	121.80	114.15
18	V	3	Y5P	C5-C4-N3	4.72	121.76	114.15
18	Y	49	Y5P	C5-C4-N3	4.71	121.75	114.15
18	V	34	P5P	C5-C6-N1	-4.70	110.19	121.90
19	X	21	Y5P	C5-C4-N3	4.66	121.66	114.15
18	V	56	Y5P	C5-C4-N3	4.63	121.62	114.15
18	Y	48	Y5P	C5-C4-N3	4.62	121.59	114.15
18	Y	62	Y5P	C5-C4-N3	4.61	121.59	114.15
18	V	2	Y5P	C5-C4-N3	4.61	121.58	114.15
18	Y	68	Y5P	C5-C4-N3	4.61	121.58	114.15
18	V	25	Y5P	C5-C4-N3	4.59	121.55	114.15
18	V	41	Y5P	C5-C4-N3	4.58	121.53	114.15
18	V	62	Y5P	C5-C4-N3	4.58	121.53	114.15
18	Y	61	Y5P	C5-C4-N3	4.56	121.51	114.15
18	Y	41	Y5P	C5-C4-N3	4.55	121.49	114.15
18	Y	25	Y5P	C5-C4-N3	4.54	121.47	114.15
18	V	43	Y5P	C5-C4-N3	4.52	121.44	114.15
18	V	42	Y5P	C5-C4-N3	4.52	121.44	114.15
18	V	49	Y5P	C5-C4-N3	4.51	121.43	114.15
18	Y	4	Y5P	C5-C4-N3	4.51	121.42	114.15
18	Y	11	Y5P	C5-C4-N3	4.50	121.41	114.15
18	V	13	Y5P	C5-C4-N3	4.48	121.37	114.15
18	Y	42	Y5P	C5-C4-N3	4.46	121.35	114.15
18	Y	67	Y5P	C5-C4-N3	4.45	121.33	114.15
18	V	48	Y5P	C5-C4-N3	4.44	121.31	114.15
18	Y	43	Y5P	C5-C4-N3	4.43	121.29	114.15
18	V	61	Y5P	C5-C4-N3	4.43	121.29	114.15
18	V	67	Y5P	C5-C4-N3	4.35	121.17	114.15
18	Y	3	Y5P	C5-C4-N3	4.34	121.15	114.15
18	V	4	Y5P	C5-C4-N3	4.31	121.10	114.15
18	Y	34	P5P	C5-C6-N1	-4.26	111.29	121.90
18	V	68	Y5P	C5-C4-N3	4.26	121.01	114.15
18	Y	51	Y5P	N1-C2-N3	-4.10	114.03	125.39
19	X	12	Y5P	N1-C2-N3	-4.05	114.17	125.39
18	Y	50	Y5P	N1-C2-N3	-3.97	114.39	125.39
18	Y	39	Y5P	N1-C2-N3	-3.94	114.46	125.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	V	12	Y5P	N1-C2-N3	-3.91	114.53	125.39
19	X	22	Y5P	N1-C2-N3	-3.89	114.59	125.39
19	X	23	Y5P	N1-C2-N3	-3.85	114.72	125.39
18	Y	45	Y5P	N1-C2-N3	-3.84	114.75	125.39
18	V	40	Y5P	C5-C4-N3	3.82	120.31	114.15
18	V	54	Y5P	N1-C2-N3	-3.81	114.81	125.39
18	V	32	Y5P	N1-C2-N3	-3.81	114.82	125.39
18	Y	12	Y5P	N1-C2-N3	-3.81	114.83	125.39
18	Y	54	Y5P	N1-C2-N3	-3.80	114.84	125.39
18	V	66	Y5P	N1-C2-N3	-3.79	114.87	125.39
18	V	60	Y5P	N1-C2-N3	-3.76	114.95	125.39
18	Y	8	Y5P	N1-C2-N3	-3.76	114.97	125.39
18	V	8	Y5P	N1-C2-N3	-3.74	115.01	125.39
18	Y	66	Y5P	N1-C2-N3	-3.74	115.02	125.39
19	X	13	Y5P	N1-C2-N3	-3.74	115.03	125.39
18	Y	32	Y5P	N1-C2-N3	-3.74	115.03	125.39
18	V	39	Y5P	N1-C2-N3	-3.74	115.03	125.39
18	V	59	Y5P	N1-C2-N3	-3.73	115.04	125.39
19	X	14	Y5P	N1-C2-N3	-3.72	115.08	125.39
18	V	55	Y5P	N1-C2-N3	-3.70	115.13	125.39
18	Y	60	Y5P	N1-C2-N3	-3.69	115.15	125.39
19	X	20	Y5P	N1-C2-N3	-3.69	115.15	125.39
19	X	24	Y5P	N1-C2-N3	-3.69	115.16	125.39
18	V	65	Y5P	N1-C2-N3	-3.69	115.17	125.39
18	V	37	Y5P	N1-C2-N3	-3.68	115.18	125.39
18	V	64	Y5P	N1-C2-N3	-3.68	115.18	125.39
18	Y	6	Y5P	N1-C2-N3	-3.68	115.18	125.39
18	V	26	Y5P	N1-C2-N3	-3.68	115.18	125.39
18	V	70	Y5P	N1-C2-N3	-3.68	115.18	125.39
18	Y	28	Y5P	N1-C2-N3	-3.68	115.19	125.39
18	Y	31	Y5P	N1-C2-N3	-3.68	115.19	125.39
18	V	24	Y5P	N1-C2-N3	-3.68	115.19	125.39
18	Y	57	Y5P	N1-C2-N3	-3.68	115.19	125.39
18	Y	69	Y5P	N1-C2-N3	-3.68	115.19	125.39
18	Y	38	Y5P	N1-C2-N3	-3.68	115.20	125.39
19	X	16	Y5P	N1-C2-N3	-3.68	115.20	125.39
18	V	50	Y5P	N1-C2-N3	-3.68	115.20	125.39
18	Y	9	Y5P	N1-C2-N3	-3.68	115.20	125.39
18	Y	24	Y5P	N1-C2-N3	-3.67	115.20	125.39
18	Y	26	Y5P	N1-C2-N3	-3.67	115.20	125.39
18	Y	63	Y5P	N1-C2-N3	-3.67	115.20	125.39
18	Y	23	Y5P	N1-C2-N3	-3.67	115.20	125.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	V	63	Y5P	N1-C2-N3	-3.67	115.20	125.39
18	Y	7	Y5P	N1-C2-N3	-3.67	115.20	125.39
18	V	10	Y5P	N1-C2-N3	-3.67	115.20	125.39
19	X	17	Y5P	N1-C2-N3	-3.67	115.20	125.39
18	Y	5	Y5P	N1-C2-N3	-3.67	115.20	125.39
18	V	6	Y5P	N1-C2-N3	-3.67	115.20	125.39
18	Y	37	Y5P	N1-C2-N3	-3.67	115.20	125.39
18	Y	10	Y5P	N1-C2-N3	-3.67	115.20	125.39
18	Y	22	Y5P	N1-C2-N3	-3.67	115.20	125.39
18	V	30	Y5P	N1-C2-N3	-3.67	115.21	125.39
18	V	53	Y5P	N1-C2-N3	-3.67	115.21	125.39
18	Y	71	Y5P	N1-C2-N3	-3.67	115.21	125.39
18	Y	21	Y5P	N1-C2-N3	-3.67	115.22	125.39
18	Y	1	Y5P	N1-C2-N3	-3.67	115.22	125.39
18	V	14	Y5P	N1-C2-N3	-3.67	115.22	125.39
18	Y	27	Y5P	N1-C2-N3	-3.67	115.22	125.39
18	V	28	Y5P	N1-C2-N3	-3.67	115.23	125.39
18	V	7	Y5P	N1-C2-N3	-3.66	115.23	125.39
18	V	22	Y5P	N1-C2-N3	-3.66	115.23	125.39
18	Y	53	Y5P	N1-C2-N3	-3.66	115.23	125.39
18	Y	65	Y5P	N1-C2-N3	-3.66	115.23	125.39
18	V	9	Y5P	N1-C2-N3	-3.66	115.23	125.39
18	Y	14	Y5P	N1-C2-N3	-3.66	115.23	125.39
18	V	38	Y5P	N1-C2-N3	-3.66	115.23	125.39
18	V	29	Y5P	N1-C2-N3	-3.66	115.23	125.39
18	Y	29	Y5P	N1-C2-N3	-3.66	115.23	125.39
18	V	21	Y5P	N1-C2-N3	-3.66	115.23	125.39
18	V	57	Y5P	N1-C2-N3	-3.66	115.23	125.39
18	V	31	Y5P	N1-C2-N3	-3.66	115.24	125.39
18	V	69	Y5P	N1-C2-N3	-3.66	115.24	125.39
18	Y	70	Y5P	N1-C2-N3	-3.66	115.24	125.39
18	V	23	Y5P	N1-C2-N3	-3.66	115.24	125.39
18	V	58	Y5P	N1-C2-N3	-3.66	115.24	125.39
18	V	44	Y5P	N1-C2-N3	-3.66	115.24	125.39
18	Y	44	Y5P	N1-C2-N3	-3.66	115.24	125.39
18	Y	15	Y5P	N1-C2-N3	-3.66	115.24	125.39
18	V	52	Y5P	N1-C2-N3	-3.66	115.24	125.39
18	Y	30	Y5P	N1-C2-N3	-3.66	115.25	125.39
18	V	1	Y5P	N1-C2-N3	-3.66	115.25	125.39
18	V	5	Y5P	N1-C2-N3	-3.66	115.25	125.39
18	V	27	Y5P	N1-C2-N3	-3.66	115.25	125.39
18	V	15	Y5P	N1-C2-N3	-3.65	115.26	125.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Y	64	Y5P	N1-C2-N3	-3.65	115.27	125.39
18	V	71	Y5P	N1-C2-N3	-3.65	115.27	125.39
18	Y	58	Y5P	N1-C2-N3	-3.65	115.27	125.39
18	Y	52	Y5P	N1-C2-N3	-3.64	115.28	125.39
19	X	19	Y5P	N1-C2-N3	-3.63	115.32	125.39
18	Y	59	Y5P	N1-C2-N3	-3.63	115.32	125.39
18	V	45	Y5P	N1-C2-N3	-3.58	115.45	125.39
19	X	15	Y5P	N1-C2-N3	-3.57	115.48	125.39
18	Y	55	Y5P	N1-C2-N3	-3.57	115.49	125.39
18	V	51	Y5P	N1-C2-N3	-3.48	115.74	125.39
18	Y	27	Y5P	C1'-N1-C6	-3.36	113.68	120.77
18	Y	33	Y5P	N1-C2-N3	-3.24	116.41	125.39
18	V	33	Y5P	N1-C2-N3	-2.92	117.29	125.39
18	V	34	P5P	C6-C5-C4	2.81	119.31	116.24
18	V	67	Y5P	N1-C2-N3	-2.56	118.29	125.39
18	V	14	Y5P	C1'-N1-C6	-2.49	115.50	120.77
18	V	62	Y5P	N1-C2-N3	-2.45	118.61	125.39
18	V	25	Y5P	N1-C2-N3	-2.42	118.68	125.39
18	V	49	Y5P	N1-C2-N3	-2.40	118.74	125.39
18	Y	49	Y5P	N1-C2-N3	-2.39	118.77	125.39
18	V	13	Y5P	N1-C2-N3	-2.37	118.81	125.39
18	Y	62	Y5P	N1-C2-N3	-2.37	118.82	125.39
18	Y	34	P5P	N1-C2-N3	-2.37	123.31	127.33
18	Y	13	Y5P	N1-C2-N3	-2.33	118.93	125.39
18	V	2	Y5P	N1-C2-N3	-2.33	118.93	125.39
18	Y	41	Y5P	N1-C2-N3	-2.29	119.05	125.39
18	V	35	P5P	C6-N1-C2	2.28	118.50	115.80
18	V	3	Y5P	N1-C2-N3	-2.28	119.06	125.39
18	Y	2	Y5P	N1-C2-N3	-2.28	119.07	125.39
18	Y	36	P5P	C6-N1-C2	2.27	118.49	115.80
18	Y	42	Y5P	N1-C2-N3	-2.27	119.10	125.39
18	V	21	Y5P	O4'-C1'-N1	2.25	112.37	108.08
18	V	56	Y5P	N1-C2-N3	-2.23	119.19	125.39
18	Y	4	Y5P	N1-C2-N3	-2.22	119.22	125.39
18	V	11	Y5P	N1-C2-N3	-2.22	119.24	125.39
18	V	48	Y5P	N1-C2-N3	-2.21	119.25	125.39
18	Y	68	Y5P	N1-C2-N3	-2.21	119.25	125.39
18	Y	71	Y5P	C1'-N1-C6	-2.21	116.10	120.77
18	Y	56	Y5P	N1-C2-N3	-2.20	119.28	125.39
18	Y	61	Y5P	N1-C2-N3	-2.20	119.29	125.39
18	V	4	Y5P	N1-C2-N3	-2.18	119.33	125.39
18	V	61	Y5P	N1-C2-N3	-2.18	119.35	125.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Y	40	Y5P	N1-C2-N3	-2.15	119.43	125.39
18	Y	43	Y5P	N1-C2-N3	-2.12	119.50	125.39
18	Y	3	Y5P	N1-C2-N3	-2.12	119.51	125.39
18	Y	67	Y5P	N1-C2-N3	-2.11	119.52	125.39
18	Y	11	Y5P	N1-C2-N3	-2.11	119.54	125.39
18	Y	34	P5P	C5-C4-N3	2.09	130.06	127.18
18	Y	25	Y5P	N1-C2-N3	-2.08	119.61	125.39
18	Y	15	Y5P	C1'-N1-C6	-2.07	116.39	120.77
18	V	43	Y5P	N1-C2-N3	-2.05	119.69	125.39
19	X	18	Y5P	N1-C2-N3	-2.04	119.72	125.39
18	Y	48	Y5P	N1-C2-N3	-2.03	119.76	125.39

There are no chirality outliers.

All (226) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	Y	3	Y5P	O4'-C1'-N1-C2
18	V	6	Y5P	O4'-C4'-C5'-O5'
18	V	6	Y5P	C3'-C4'-C5'-O5'
18	Y	6	Y5P	O4'-C1'-N1-C2
18	V	8	Y5P	O4'-C1'-N1-C2
18	Y	8	Y5P	O4'-C1'-N1-C2
18	V	9	Y5P	C2'-C1'-N1-C6
18	Y	11	Y5P	O4'-C1'-N1-C2
18	V	12	Y5P	O4'-C1'-N1-C2
18	V	13	Y5P	O4'-C1'-N1-C2
18	V	14	Y5P	O4'-C4'-C5'-O5'
18	V	14	Y5P	O4'-C1'-N1-C2
18	Y	15	Y5P	O4'-C4'-C5'-O5'
18	Y	21	Y5P	O4'-C1'-N1-C2
18	V	22	Y5P	O4'-C4'-C5'-O5'
18	Y	22	Y5P	O4'-C1'-N1-C2
18	V	24	Y5P	O4'-C1'-N1-C2
18	Y	25	Y5P	O4'-C1'-N1-C2
18	Y	27	Y5P	O4'-C1'-N1-C2
18	V	28	Y5P	O4'-C1'-N1-C2
18	Y	28	Y5P	O4'-C1'-N1-C2
18	V	29	Y5P	O4'-C1'-N1-C2
18	V	31	Y5P	O4'-C1'-N1-C2
18	V	32	Y5P	O4'-C4'-C5'-O5'
18	V	32	Y5P	C3'-C4'-C5'-O5'
18	Y	32	Y5P	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
18	V	33	Y5P	O4'-C1'-N1-C2
18	V	37	Y5P	O4'-C4'-C5'-O5'
18	V	40	Y5P	O4'-C1'-N1-C2
18	V	42	Y5P	O4'-C4'-C5'-O5'
18	V	42	Y5P	C3'-C4'-C5'-O5'
18	Y	42	Y5P	O4'-C4'-C5'-O5'
18	Y	43	Y5P	C4'-C5'-O5'-P
18	Y	43	Y5P	O4'-C1'-N1-C2
18	V	48	Y5P	O4'-C4'-C5'-O5'
18	V	48	Y5P	C3'-C4'-C5'-O5'
18	Y	48	Y5P	O4'-C1'-N1-C2
18	V	49	Y5P	O4'-C1'-N1-C2
18	V	53	Y5P	O4'-C1'-N1-C2
18	V	54	Y5P	O4'-C1'-N1-C2
18	Y	54	Y5P	O4'-C1'-N1-C2
18	V	58	Y5P	C2'-C1'-N1-C6
18	V	59	Y5P	O4'-C4'-C5'-O5'
18	Y	59	Y5P	O4'-C1'-N1-C2
18	V	61	Y5P	O4'-C1'-N1-C2
18	Y	61	Y5P	O4'-C1'-N1-C2
18	V	63	Y5P	O4'-C1'-N1-C2
18	Y	64	Y5P	O4'-C1'-N1-C2
18	V	66	Y5P	O4'-C1'-N1-C2
18	Y	66	Y5P	O4'-C1'-N1-C2
18	V	67	Y5P	O4'-C1'-N1-C2
18	Y	68	Y5P	O4'-C1'-N1-C2
18	V	71	Y5P	O4'-C1'-N1-C2
19	X	13	Y5P	O4'-C4'-C5'-O5'
19	X	13	Y5P	C3'-C4'-C5'-O5'
19	X	14	Y5P	O4'-C1'-N1-C2
19	X	23	Y5P	O4'-C4'-C5'-O5'
19	X	23	Y5P	O4'-C1'-N1-C2
18	V	1	Y5P	O4'-C1'-N1-C2
18	Y	1	Y5P	O4'-C1'-N1-C2
18	V	2	Y5P	O4'-C1'-N1-C2
18	Y	2	Y5P	O4'-C1'-N1-C2
18	V	3	Y5P	O4'-C1'-N1-C2
18	V	4	Y5P	O4'-C1'-N1-C2
18	Y	4	Y5P	O4'-C1'-N1-C2
18	V	5	Y5P	O4'-C1'-N1-C2
18	Y	5	Y5P	O4'-C1'-N1-C2
18	V	6	Y5P	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
18	Y	9	Y5P	O4'-C1'-N1-C2
18	V	10	Y5P	O4'-C1'-N1-C2
18	Y	10	Y5P	O4'-C1'-N1-C2
18	V	11	Y5P	O4'-C1'-N1-C2
18	Y	12	Y5P	O4'-C1'-N1-C2
18	Y	13	Y5P	O4'-C1'-N1-C2
18	Y	14	Y5P	O4'-C1'-N1-C2
18	V	15	Y5P	O4'-C1'-N1-C2
18	Y	15	Y5P	O4'-C1'-N1-C2
18	V	21	Y5P	O4'-C1'-N1-C2
18	V	22	Y5P	O4'-C1'-N1-C2
18	V	23	Y5P	O4'-C1'-N1-C2
18	Y	23	Y5P	O4'-C1'-N1-C2
18	Y	24	Y5P	O4'-C1'-N1-C2
18	V	25	Y5P	O4'-C1'-N1-C2
18	V	26	Y5P	O4'-C1'-N1-C2
18	Y	26	Y5P	O4'-C1'-N1-C2
18	V	27	Y5P	O4'-C1'-N1-C2
18	Y	29	Y5P	O4'-C1'-N1-C2
18	V	30	Y5P	O4'-C1'-N1-C2
18	Y	30	Y5P	O4'-C1'-N1-C2
18	Y	31	Y5P	O4'-C1'-N1-C2
18	V	32	Y5P	O4'-C1'-N1-C2
18	Y	33	Y5P	O4'-C1'-N1-C2
18	V	37	Y5P	O4'-C1'-N1-C2
18	Y	37	Y5P	O4'-C1'-N1-C2
18	V	38	Y5P	O4'-C1'-N1-C2
18	Y	38	Y5P	O4'-C1'-N1-C2
18	V	39	Y5P	O4'-C1'-N1-C2
18	Y	39	Y5P	O4'-C1'-N1-C2
18	Y	40	Y5P	O4'-C1'-N1-C2
18	V	41	Y5P	O4'-C1'-N1-C2
18	Y	41	Y5P	O4'-C1'-N1-C2
18	V	42	Y5P	O4'-C1'-N1-C2
18	Y	42	Y5P	O4'-C1'-N1-C2
18	V	43	Y5P	O4'-C1'-N1-C2
18	V	44	Y5P	O4'-C1'-N1-C2
18	Y	44	Y5P	O4'-C1'-N1-C2
18	Y	45	Y5P	O4'-C1'-N1-C2
18	Y	49	Y5P	O4'-C1'-N1-C2
18	V	50	Y5P	O4'-C1'-N1-C2
18	Y	50	Y5P	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
18	V	51	Y5P	O4'-C1'-N1-C2
18	Y	51	Y5P	O4'-C1'-N1-C2
18	V	52	Y5P	O4'-C1'-N1-C2
18	Y	52	Y5P	O4'-C1'-N1-C2
18	Y	53	Y5P	O4'-C1'-N1-C2
18	V	56	Y5P	O4'-C1'-N1-C2
18	V	57	Y5P	O4'-C1'-N1-C2
18	V	59	Y5P	O4'-C1'-N1-C2
18	V	62	Y5P	O4'-C1'-N1-C2
18	Y	62	Y5P	O4'-C1'-N1-C2
18	Y	63	Y5P	O4'-C1'-N1-C2
18	V	64	Y5P	O4'-C1'-N1-C2
18	V	65	Y5P	O4'-C1'-N1-C2
18	Y	65	Y5P	O4'-C1'-N1-C2
18	Y	67	Y5P	O4'-C1'-N1-C2
18	V	69	Y5P	O4'-C1'-N1-C2
18	Y	69	Y5P	O4'-C1'-N1-C2
18	V	70	Y5P	O4'-C1'-N1-C2
18	Y	70	Y5P	O4'-C1'-N1-C2
18	Y	71	Y5P	O4'-C1'-N1-C2
19	X	12	Y5P	O4'-C1'-N1-C2
19	X	13	Y5P	O4'-C1'-N1-C2
19	X	15	Y5P	O4'-C1'-N1-C2
19	X	16	Y5P	O4'-C1'-N1-C2
19	X	17	Y5P	O4'-C1'-N1-C2
19	X	19	Y5P	O4'-C1'-N1-C2
19	X	20	Y5P	O4'-C1'-N1-C2
19	X	24	Y5P	O4'-C1'-N1-C2
19	X	12	Y5P	C3'-C4'-C5'-O5'
18	Y	34	P5P	O4'-C4'-C5'-O5'
18	V	9	Y5P	C3'-C4'-C5'-O5'
18	Y	13	Y5P	O4'-C4'-C5'-O5'
18	V	14	Y5P	C3'-C4'-C5'-O5'
18	Y	15	Y5P	C3'-C4'-C5'-O5'
18	V	22	Y5P	C3'-C4'-C5'-O5'
18	Y	30	Y5P	O4'-C4'-C5'-O5'
18	Y	30	Y5P	C3'-C4'-C5'-O5'
18	V	37	Y5P	C3'-C4'-C5'-O5'
18	Y	41	Y5P	C3'-C4'-C5'-O5'
18	Y	42	Y5P	C3'-C4'-C5'-O5'
18	Y	59	Y5P	O4'-C4'-C5'-O5'
18	Y	68	Y5P	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
18	Y	71	Y5P	O4'-C4'-C5'-O5'
18	Y	71	Y5P	C3'-C4'-C5'-O5'
19	X	15	Y5P	C3'-C4'-C5'-O5'
19	X	23	Y5P	C3'-C4'-C5'-O5'
18	V	9	Y5P	C2'-C1'-N1-C2
18	V	58	Y5P	C2'-C1'-N1-C2
18	V	9	Y5P	O4'-C4'-C5'-O5'
18	Y	9	Y5P	C3'-C4'-C5'-O5'
18	Y	13	Y5P	C3'-C4'-C5'-O5'
18	Y	41	Y5P	O4'-C4'-C5'-O5'
19	X	12	Y5P	O4'-C4'-C5'-O5'
19	X	21	Y5P	O4'-C1'-N1-C2
18	Y	9	Y5P	O4'-C4'-C5'-O5'
18	V	59	Y5P	C3'-C4'-C5'-O5'
18	V	45	Y5P	O4'-C1'-N1-C2
18	V	55	Y5P	O4'-C1'-N1-C2
18	V	68	Y5P	O4'-C1'-N1-C2
19	X	22	Y5P	O4'-C1'-N1-C2
18	V	23	Y5P	C3'-C4'-C5'-O5'
18	Y	59	Y5P	C3'-C4'-C5'-O5'
18	V	69	Y5P	C3'-C4'-C5'-O5'
19	X	15	Y5P	O4'-C4'-C5'-O5'
19	X	22	Y5P	C3'-C4'-C5'-O5'
18	V	7	Y5P	O4'-C1'-N1-C2
18	Y	34	P5P	C3'-C4'-C5'-O5'
18	V	2	Y5P	C3'-C4'-C5'-O5'
18	Y	68	Y5P	C3'-C4'-C5'-O5'
19	X	22	Y5P	O4'-C4'-C5'-O5'
18	V	9	Y5P	O4'-C1'-N1-C6
18	V	7	Y5P	O4'-C4'-C5'-O5'
18	V	48	Y5P	O4'-C1'-N1-C2
18	V	23	Y5P	O4'-C4'-C5'-O5'
18	Y	37	Y5P	C3'-C4'-C5'-O5'
18	Y	58	Y5P	C2'-C1'-N1-C2
18	Y	43	Y5P	O4'-C4'-C5'-O5'
18	V	2	Y5P	O4'-C4'-C5'-O5'
18	Y	58	Y5P	C2'-C1'-N1-C6
18	V	4	Y5P	C3'-C4'-C5'-O5'
18	Y	43	Y5P	C3'-C4'-C5'-O5'
18	Y	55	Y5P	O4'-C1'-N1-C6
18	Y	7	Y5P	O4'-C1'-N1-C2
18	Y	57	Y5P	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
19	X	18	Y5P	O4'-C1'-N1-C2
18	Y	58	Y5P	O4'-C1'-N1-C2
18	V	58	Y5P	O4'-C1'-N1-C6
18	Y	61	Y5P	O4'-C4'-C5'-O5'
18	Y	58	Y5P	O4'-C1'-N1-C6
18	Y	2	Y5P	C4'-C5'-O5'-P
18	V	30	Y5P	C3'-C4'-C5'-O5'
18	Y	52	Y5P	C3'-C4'-C5'-O5'
18	Y	61	Y5P	C3'-C4'-C5'-O5'
18	V	69	Y5P	O4'-C4'-C5'-O5'
18	V	60	Y5P	O4'-C1'-N1-C2
18	V	7	Y5P	C3'-C4'-C5'-O5'
18	Y	60	Y5P	O4'-C1'-N1-C2
19	X	15	Y5P	C4'-C5'-O5'-P
18	V	14	Y5P	C2'-C1'-N1-C6
18	Y	56	Y5P	O4'-C1'-N1-C2
18	V	58	Y5P	O4'-C1'-N1-C2
18	V	4	Y5P	O4'-C4'-C5'-O5'
18	Y	37	Y5P	O4'-C4'-C5'-O5'
18	Y	28	Y5P	C4'-C5'-O5'-P
18	V	52	Y5P	C4'-C5'-O5'-P
18	Y	53	Y5P	C4'-C5'-O5'-P
18	V	6	Y5P	C4'-C5'-O5'-P
18	Y	53	Y5P	C2'-C1'-N1-C6
18	Y	30	Y5P	C4'-C5'-O5'-P
18	Y	71	Y5P	C4'-C5'-O5'-P
19	X	19	Y5P	C2'-C1'-N1-C6
18	Y	56	Y5P	C2'-C1'-N1-C2
18	Y	21	Y5P	O4'-C4'-C5'-O5'
18	V	14	Y5P	C2'-C1'-N1-C2
18	V	14	Y5P	C4'-C5'-O5'-P
18	Y	52	Y5P	C4'-C5'-O5'-P

There are no ring outliers.

99 monomers are involved in 136 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	Y	42	Y5P	1	0
18	Y	37	Y5P	1	0
18	V	13	Y5P	4	0
18	Y	44	Y5P	1	0
18	V	42	Y5P	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	Y	9	Y5P	6	0
18	V	43	Y5P	7	0
18	Y	52	Y5P	4	0
18	Y	7	Y5P	2	0
18	Y	23	Y5P	3	0
18	V	58	Y5P	3	0
18	V	14	Y5P	3	0
18	V	32	Y5P	2	0
18	V	37	Y5P	2	0
19	X	17	Y5P	1	0
18	V	2	Y5P	1	0
18	Y	26	Y5P	9	0
19	X	20	Y5P	3	0
18	Y	14	Y5P	4	0
18	Y	63	Y5P	2	0
18	V	11	Y5P	1	0
18	V	54	Y5P	5	0
18	V	68	Y5P	1	0
18	Y	32	Y5P	4	0
18	V	24	Y5P	4	0
18	V	33	Y5P	2	0
18	Y	15	Y5P	1	0
18	Y	69	Y5P	6	0
18	Y	67	Y5P	2	0
18	Y	66	Y5P	1	0
18	Y	59	Y5P	1	0
18	Y	55	Y5P	4	0
18	Y	29	Y5P	2	0
18	Y	54	Y5P	4	0
18	Y	68	Y5P	7	0
18	Y	33	Y5P	1	0
18	V	49	Y5P	2	0
18	Y	28	Y5P	1	0
18	Y	57	Y5P	2	0
18	V	30	Y5P	3	0
18	Y	25	Y5P	10	0
19	X	14	Y5P	1	0
18	V	3	Y5P	1	0
18	Y	22	Y5P	6	0
18	V	50	Y5P	1	0
18	V	64	Y5P	1	0
18	Y	60	Y5P	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	Y	30	Y5P	3	0
18	Y	39	Y5P	1	0
18	Y	53	Y5P	1	0
19	X	23	Y5P	1	0
18	V	57	Y5P	4	0
18	V	23	Y5P	5	0
19	X	21	Y5P	2	0
18	Y	34	P5P	1	0
18	V	48	Y5P	1	0
19	X	18	Y5P	1	0
18	Y	40	Y5P	1	0
18	Y	6	Y5P	2	0
18	V	8	Y5P	4	0
18	Y	61	Y5P	1	0
19	X	16	Y5P	1	0
18	Y	24	Y5P	4	0
18	V	63	Y5P	2	0
18	V	51	Y5P	1	0
18	Y	58	Y5P	3	0
18	Y	70	Y5P	3	0
18	Y	38	Y5P	1	0
18	Y	43	Y5P	2	0
18	V	66	Y5P	1	0
18	V	26	Y5P	6	0
18	Y	62	Y5P	3	0
18	V	9	Y5P	4	0
18	Y	8	Y5P	3	0
18	V	10	Y5P	2	0
18	V	55	Y5P	6	0
18	V	44	Y5P	6	0
18	Y	31	Y5P	5	0
18	V	31	Y5P	2	0
18	V	29	Y5P	2	0
18	V	27	Y5P	2	0
18	V	36	P5P	2	0
18	V	62	Y5P	1	0
18	Y	71	Y5P	3	0
18	V	60	Y5P	1	0
18	Y	56	Y5P	1	0
18	V	67	Y5P	2	0
18	Y	3	Y5P	1	0
18	V	25	Y5P	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	Y	27	Y5P	1	0
18	Y	36	P5P	1	0
19	X	12	Y5P	1	0
18	V	41	Y5P	1	0
19	X	24	Y5P	1	0
19	X	15	Y5P	1	0
18	V	59	Y5P	1	0
18	V	52	Y5P	1	0
18	Y	51	Y5P	3	0
18	V	12	Y5P	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 148 ligands modelled in this entry, 147 are monoatomic - leaving 1 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	$\# Z > 2$
39	GDP	g	500	37	29,30,30	1.29	4 (13%)	45,47,47	1.71	8 (17%)

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
39	GDP	g	500	37	-	0/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	g	500	GDP	PA-O3A	3.39	1.63	1.59
39	g	500	GDP	C5-C4	3.26	1.47	1.38
39	g	500	GDP	C6-N1	-2.38	1.34	1.38
39	g	500	GDP	C5-N7	-2.16	1.34	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	g	500	GDP	C5-C4-N3	-5.59	119.50	128.39
39	g	500	GDP	C2-N3-C4	4.52	120.09	112.30
39	g	500	GDP	N9-C4-N3	3.97	133.90	125.95
39	g	500	GDP	C6-C5-N7	3.00	135.75	130.29
39	g	500	GDP	C3'-C2'-C1'	2.40	106.00	101.46
39	g	500	GDP	C4-C5-N7	-2.32	106.99	110.67
39	g	500	GDP	O6-C6-C5	-2.19	120.75	126.53
39	g	500	GDP	O3B-PB-O3A	2.17	111.92	104.64

There are no chirality outliers.

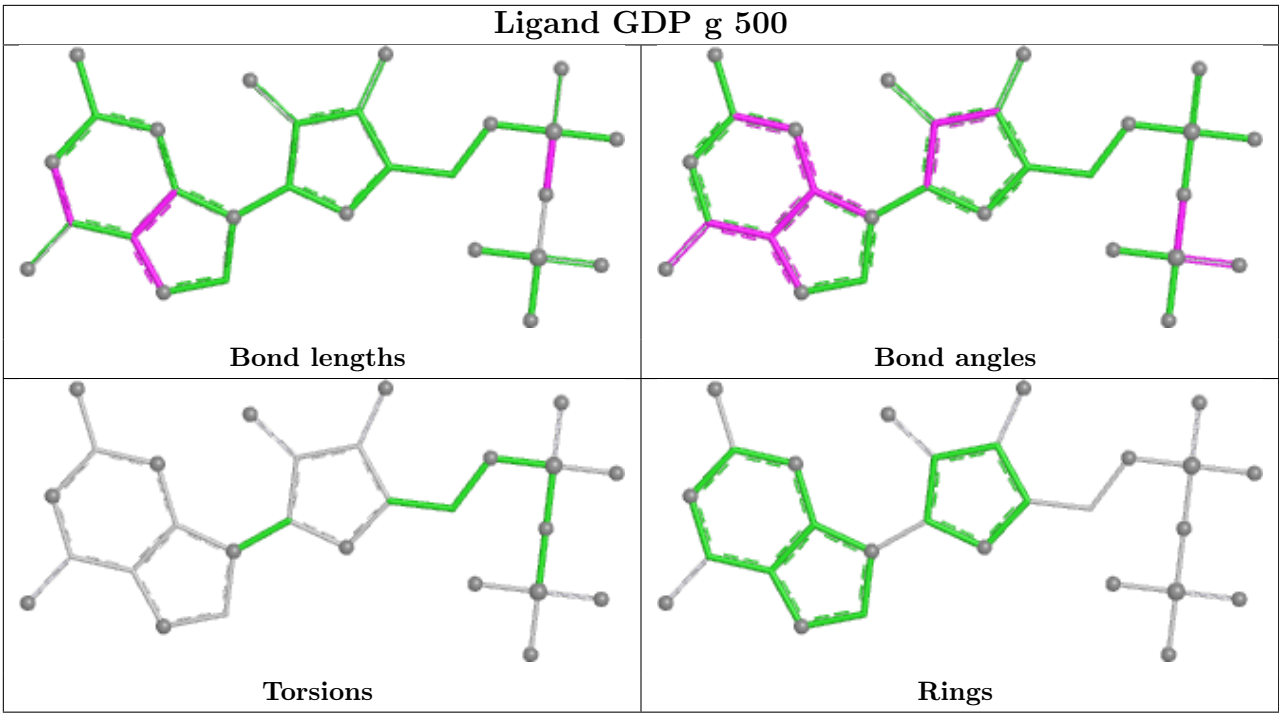
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	g	500	GDP	1	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
33	o	25
24	e	4
18	Y	3
18	V	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	e	262:UNK	C	263:UNK	N	41.49
1	e	309:UNK	C	354:UNK	N	30.03
1	o	405:UNK	C	410:UNK	N	21.38
1	o	368:UNK	C	371:UNK	N	15.76
1	Y	15:Y5P	O3'	21:Y5P	P	15.57
1	V	15:Y5P	O3'	21:Y5P	P	14.68
1	o	181:UNK	C	185:UNK	N	14.46
1	o	250:UNK	C	260:UNK	N	13.60

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	o	585:UNK	C	593:UNK	N	13.45
1	o	349:UNK	C	355:UNK	N	13.19
1	o	292:UNK	C	295:UNK	N	12.90
1	o	560:UNK	C	575:UNK	N	12.90
1	e	292:UNK	C	293:UNK	N	12.39
1	o	607:UNK	C	651:UNK	N	12.19
1	o	447:UNK	C	456:UNK	N	12.09
1	o	310:UNK	C	315:UNK	N	11.79
1	o	215:UNK	C	220:UNK	N	11.64
1	o	661:UNK	C	666:UNK	N	11.25
1	o	490:UNK	C	492:UNK	N	11.20
1	o	330:UNK	C	335:UNK	N	10.74
1	Y	45:Y5P	O3'	48:Y5P	P	10.45
1	o	275:UNK	C	277:UNK	N	10.14
1	o	525:UNK	C	531:UNK	N	10.11
1	o	198:UNK	C	200:UNK	N	9.81
1	V	45:Y5P	O3'	48:Y5P	P	9.72
1	e	211:UNK	C	212:UNK	N	9.06
1	o	165:UNK	C	167:UNK	N	7.92
1	o	470:UNK	C	475:UNK	N	7.88
1	o	385:UNK	C	390:UNK	N	7.52
1	o	507:UNK	C	510:UNK	N	7.46
1	o	235:UNK	C	237:UNK	N	7.25
1	o	430:UNK	C	433:UNK	N	6.61
1	o	542:UNK	C	546:UNK	N	5.36
1	Y	7:Y5P	O3'	8:Y5P	P	3.72

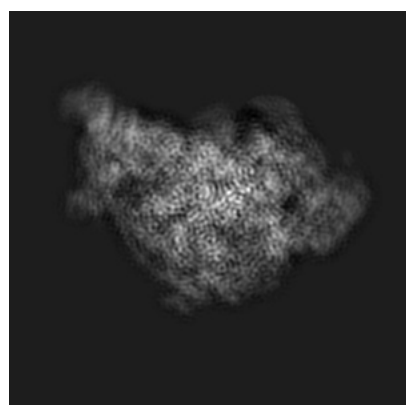
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2913. These allow visual inspection of the internal detail of the map and identification of artifacts.

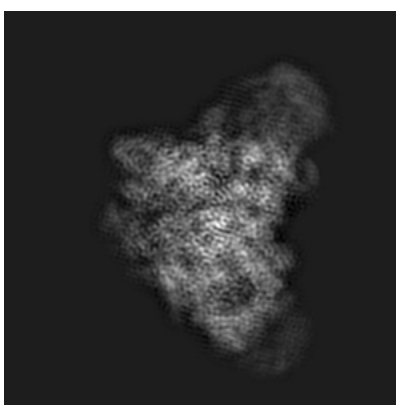
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

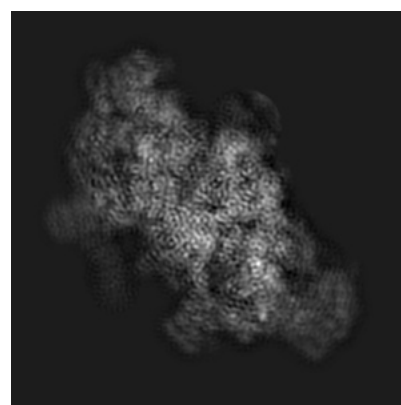
6.1.1 Primary map



X



Y

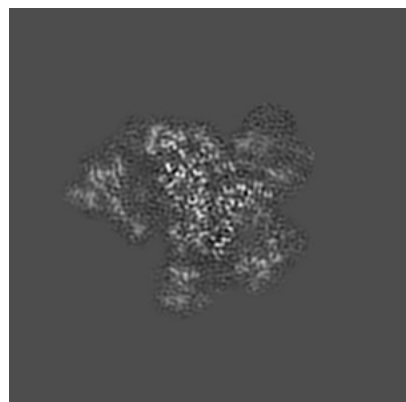


Z

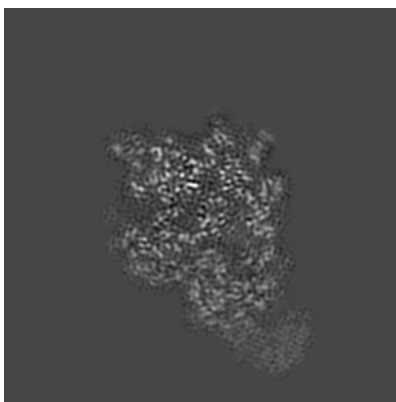
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

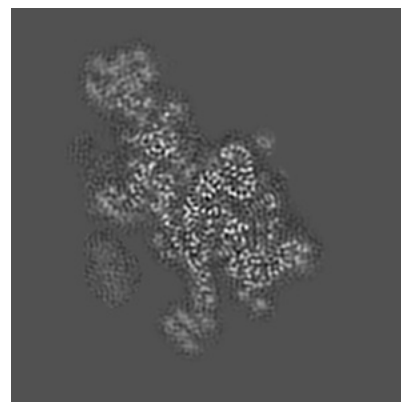
6.2.1 Primary map



X Index: 108



Y Index: 108

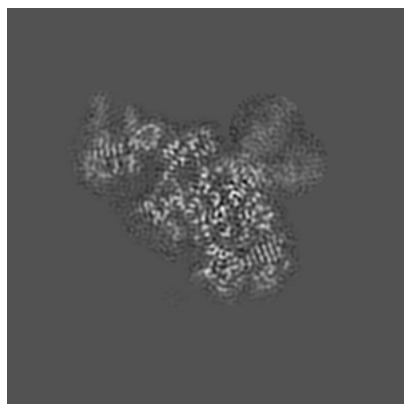


Z Index: 108

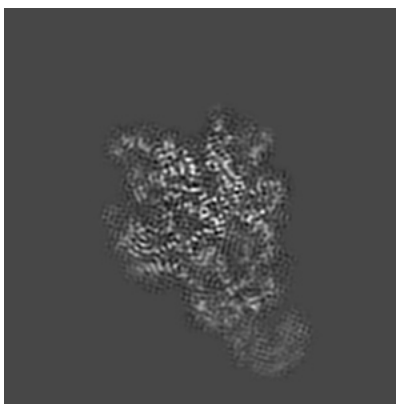
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

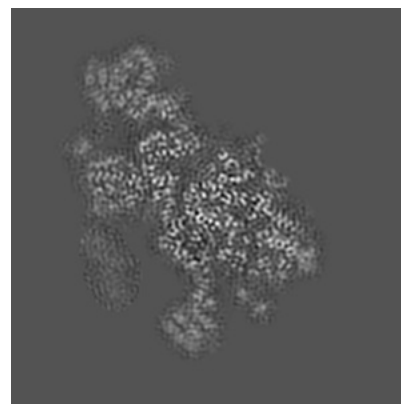
6.3.1 Primary map



X Index: 118



Y Index: 106

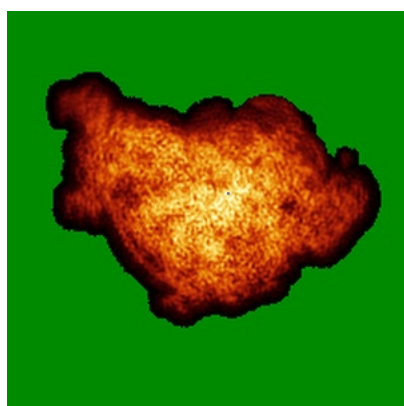


Z Index: 112

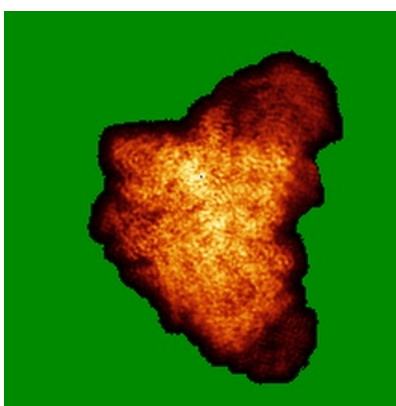
The images above show the largest variance slices of the map in three orthogonal directions.

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

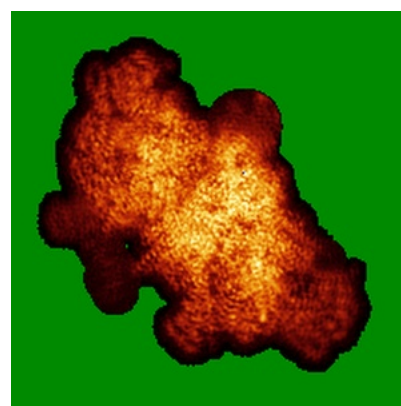
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

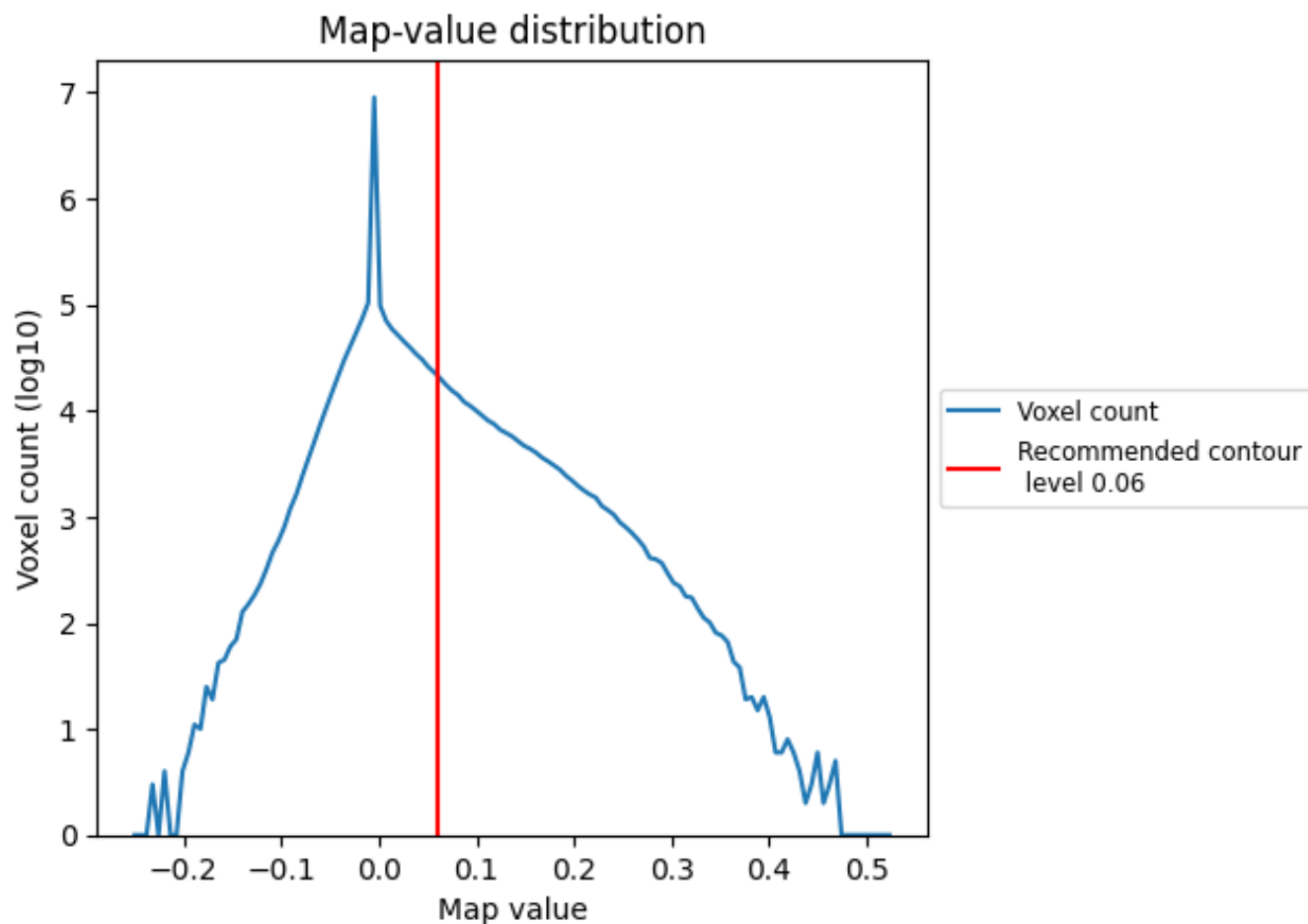
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

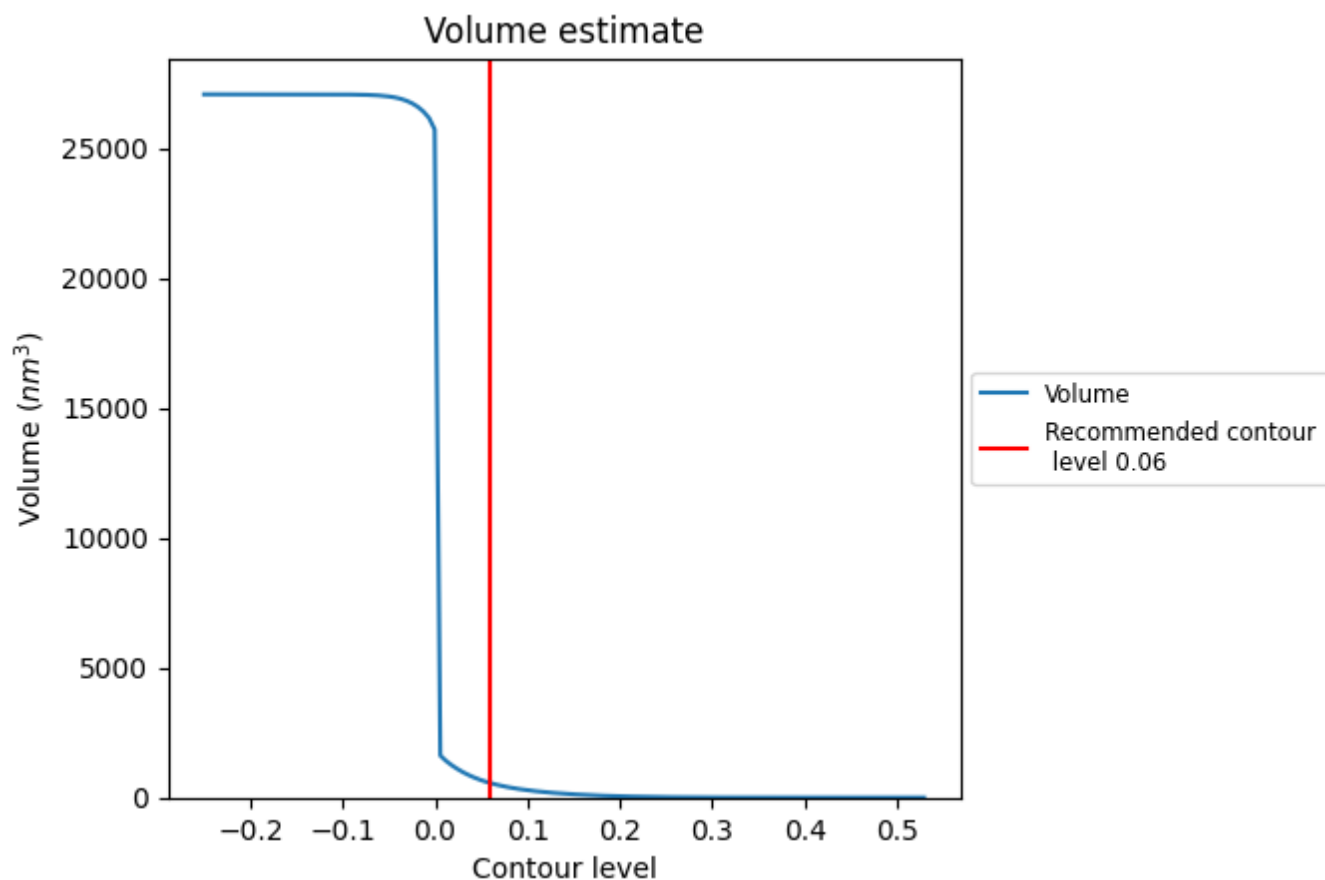
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

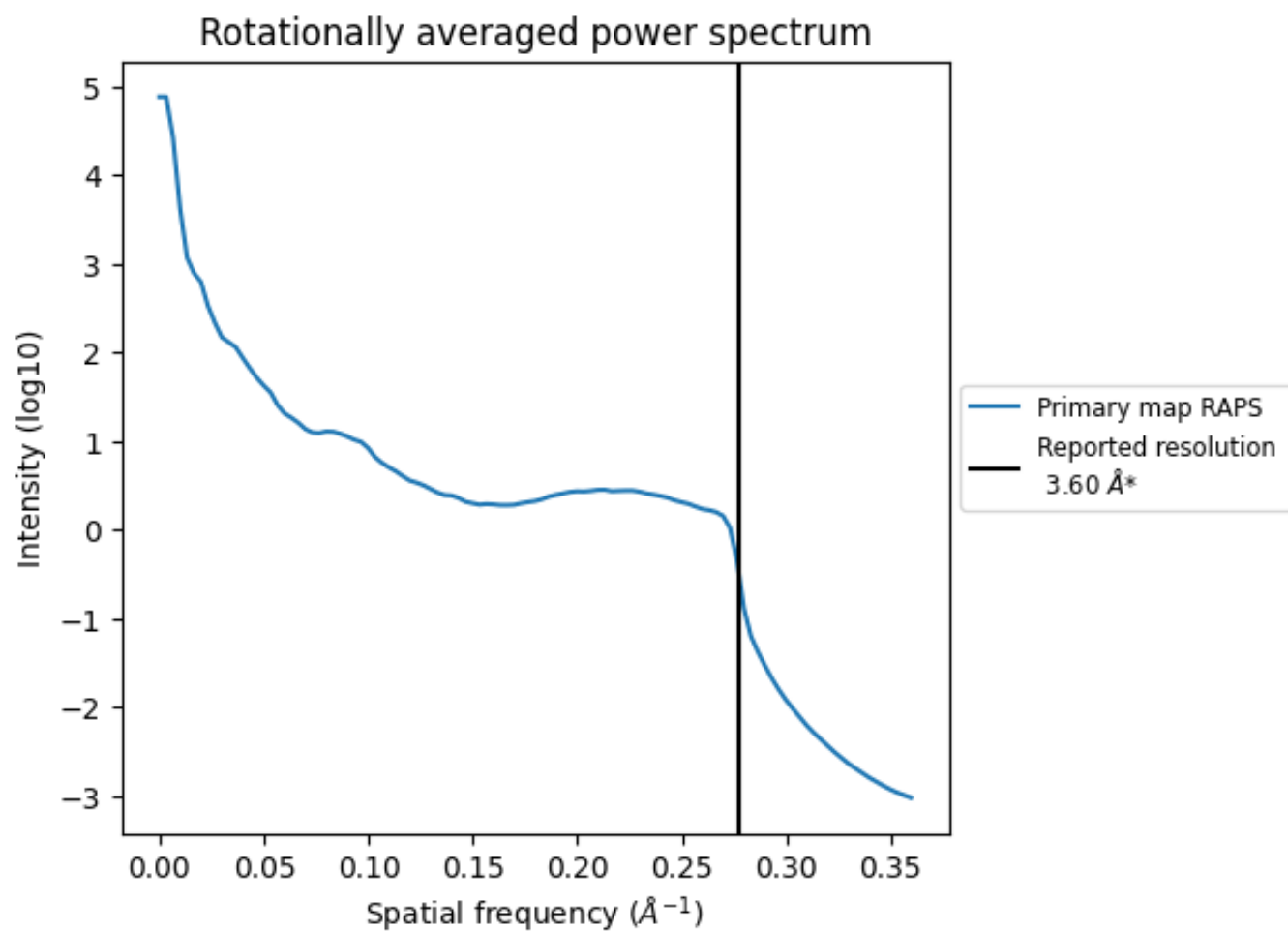
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 556 nm³; this corresponds to an approximate mass of 502 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 0.278 Å⁻¹

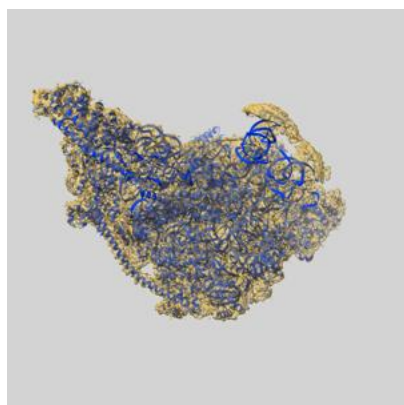
8 Fourier-Shell correlation

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

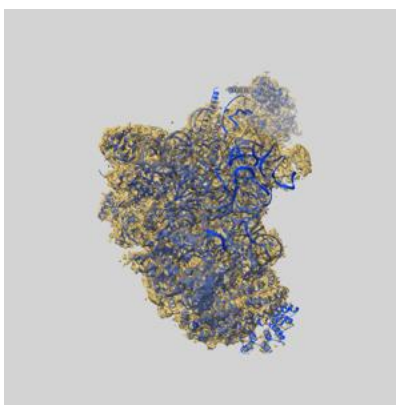
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2913 and PDB model 5AJ3. Per-residue inclusion information can be found in section 3 on page 24.

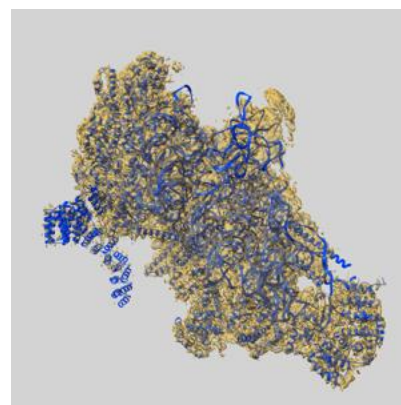
9.1 Map-model overlay [i](#)



X



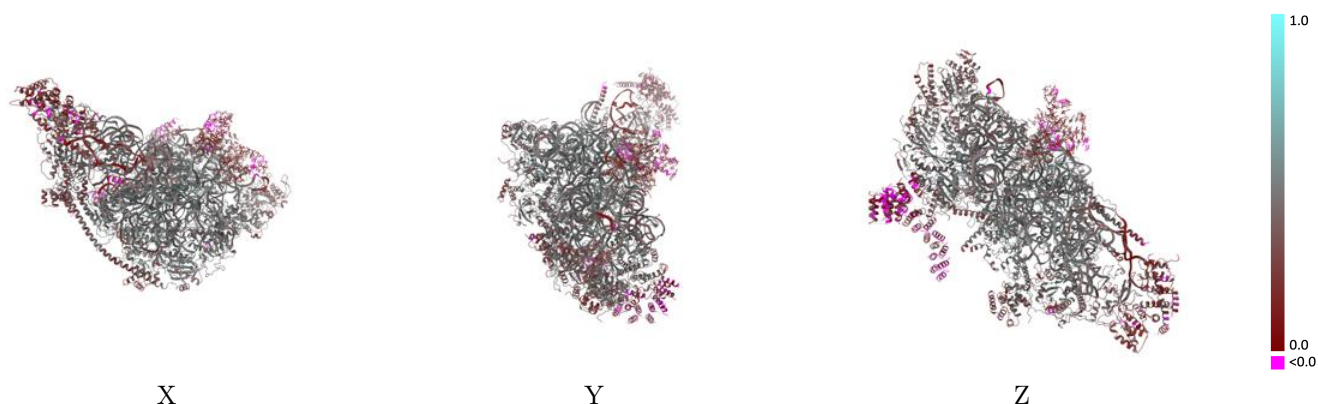
Y



Z

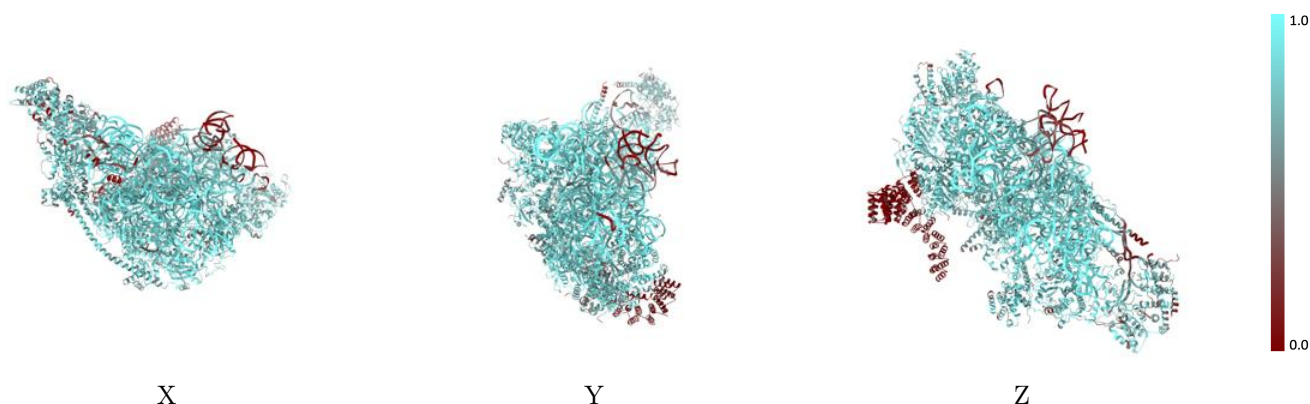
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



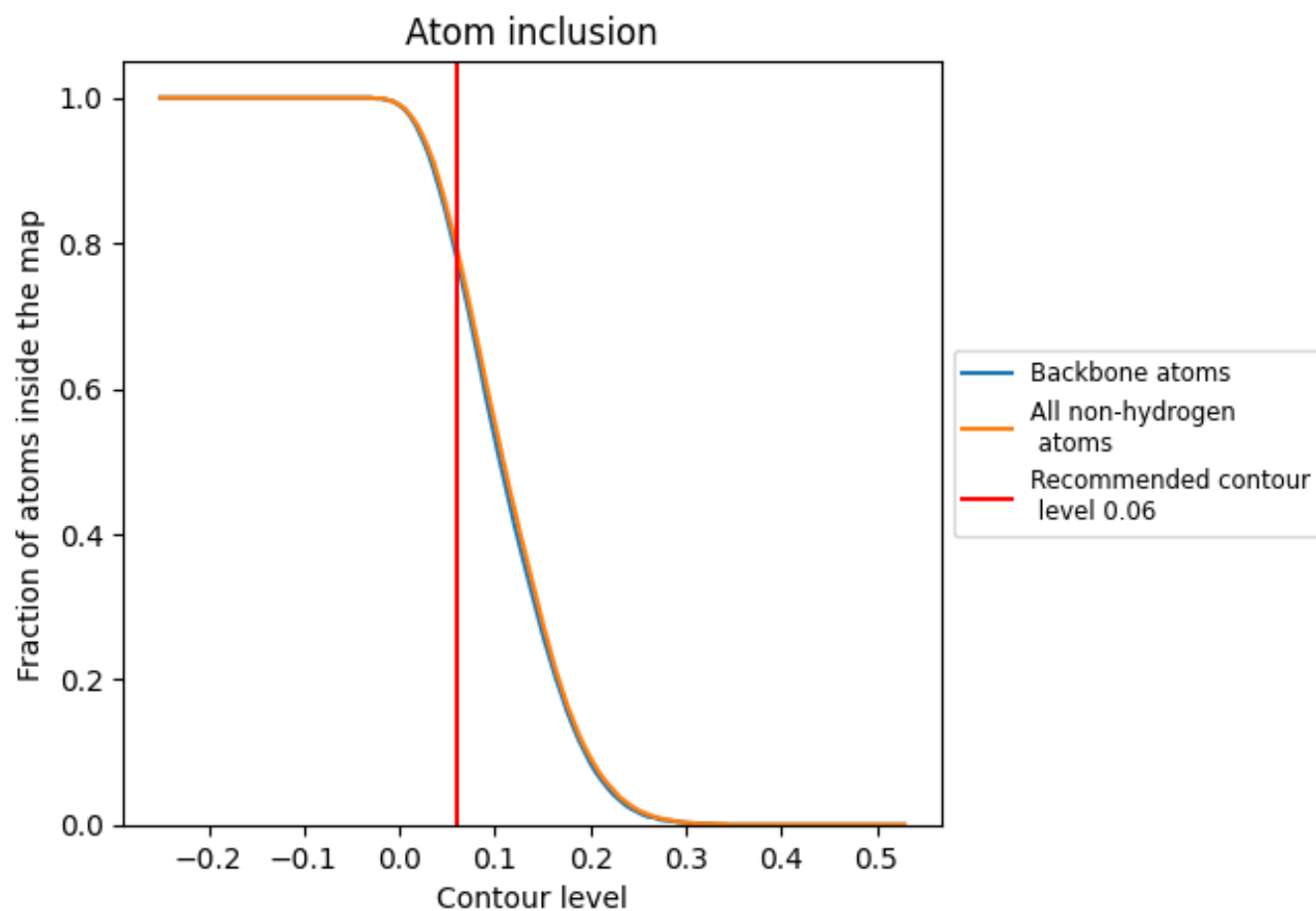
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion ⓘ



At the recommended contour level, 78% of all backbone atoms, 80% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7960	 0.4110
A	 0.9300	 0.4520
B	 0.8740	 0.4690
C	 0.8340	 0.4850
E	 0.8210	 0.4570
F	 0.8070	 0.4530
G	 0.7920	 0.4250
I	 0.8150	 0.4340
J	 0.8150	 0.4560
K	 0.8350	 0.4620
L	 0.8410	 0.4810
N	 0.8860	 0.4770
O	 0.7770	 0.4280
P	 0.8450	 0.4440
Q	 0.8380	 0.4570
R	 0.8670	 0.4870
T	 0.3810	 0.2350
U	 0.8610	 0.4760
V	 0.4430	 0.2670
X	 0.8230	 0.4690
Y	 0.4040	 0.1900
a	 0.8010	 0.3820
b	 0.7720	 0.3960
c	 0.8420	 0.4560
d	 0.7870	 0.3670
e	 0.6470	 0.2410
f	 0.8350	 0.4590
g	 0.8060	 0.3770
h	 0.8290	 0.4180
i	 0.8070	 0.4400
j	 0.6660	 0.3510
k	 0.7740	 0.3990
m	 0.7790	 0.4500
n	 0.7750	 0.4560
o	 0.2420	 0.1750



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Chain	Atom inclusion	Q-score
p	 0.8560	 0.4410
s	 0.0420	 0.0500
z	 0.6760	 0.2370