



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:53 PM BST

PDB ID : 5AJ3
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 wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

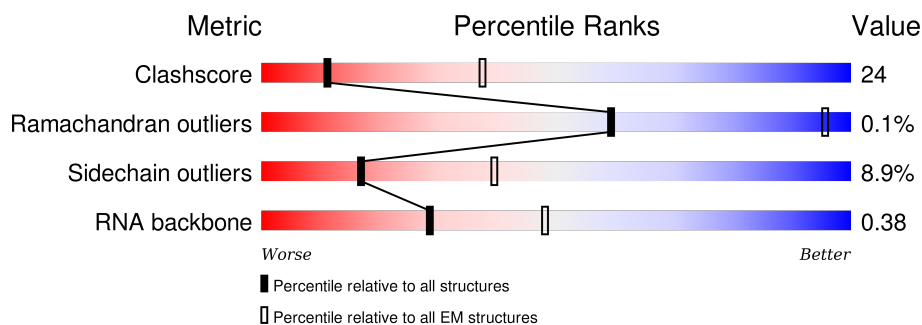
1 Overall quality at a glance

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)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	962	40% 43% 15% .
2	B	289	51% 22% . 24%
3	C	167	50% 26% . 21%
4	E	430	49% 23% . 24%
5	F	124	66% 30% . .
6	G	242	59% 26% . 14%
7	I	397	50% 26% . 22%
8	J	201	41% 20% . 36%



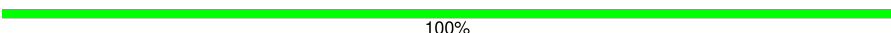
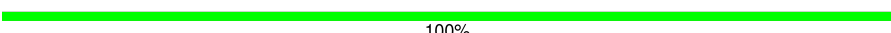
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Mol	Chain	Length	Quality of chain
9	K	196	
10	L	139	
11	N	128	
12	O	239	
13	P	135	
14	Q	130	
15	R	143	
16	T	14	
17	U	87	
18	V	64	
18	Y	64	
19	X	13	
20	a	360	
21	b	190	
22	c	173	
23	d	205	
24	e	336	
25	f	188	
26	g	397	
27	h	387	
28	i	106	
29	j	218	
30	k	325	
31	m	118	
32	n	199	

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Mol	Chain	Length	Quality of chain
33	o	692	 68% 31%
34	p	258	 66% 7% 27%
35	s	16	 100%
36	z	17	 100%

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		

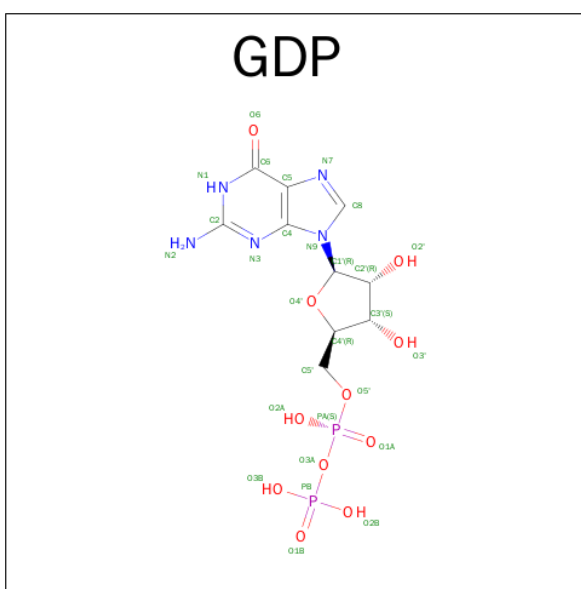
- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 39 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$).



Mol	Chain	Residues	Atoms					AltConf
39	g	1	Total	C	N	O	P	0
			28	10	5	11	2	

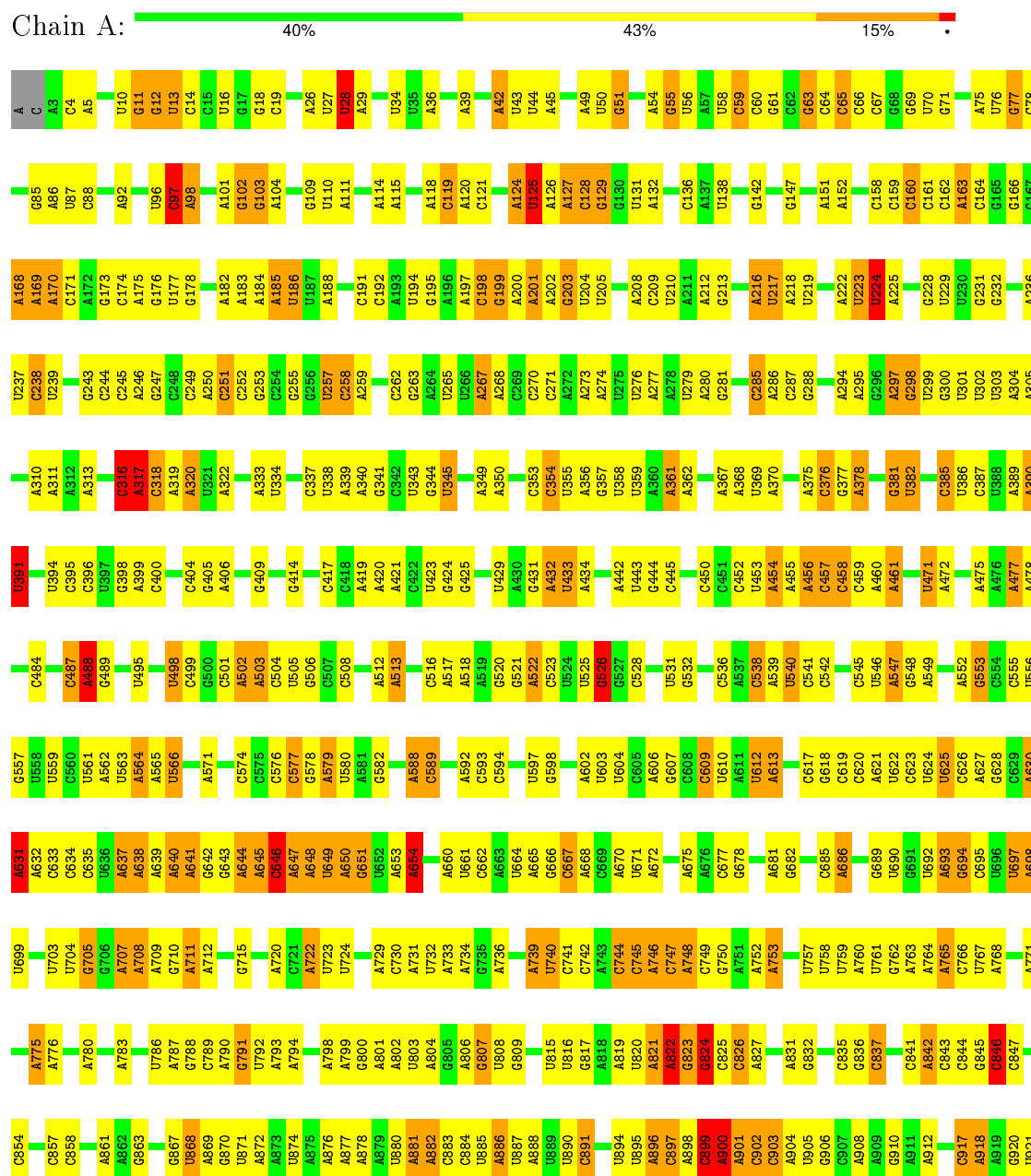
- Molecule 40 is water.

Mol	Chain	Residues	Atoms	AltConf
40	A	114	Total O 114 114	0
40	g	4	Total O 4 4	0

3 Residue-property plots

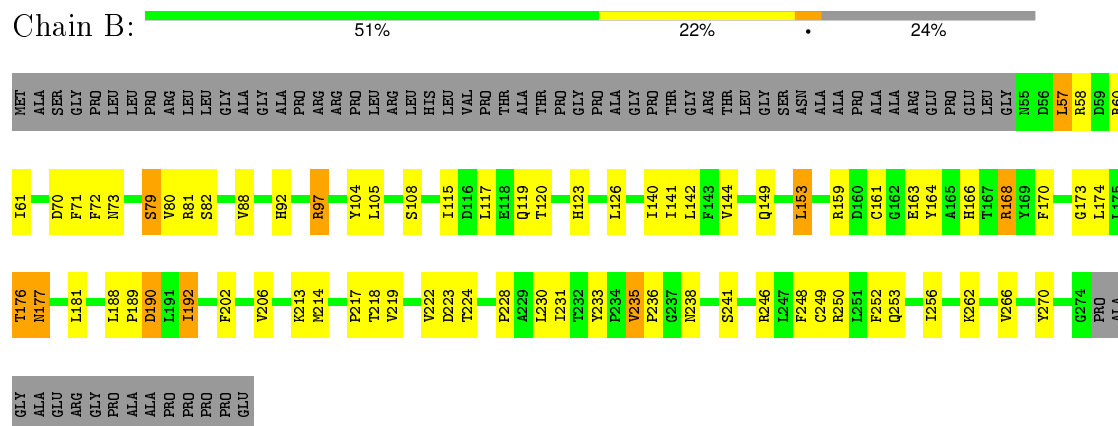
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. 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

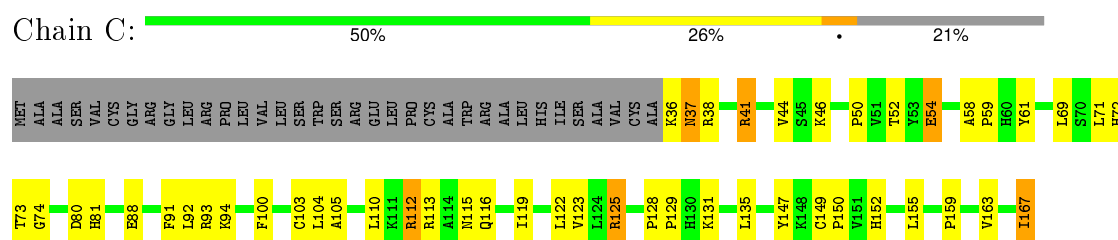




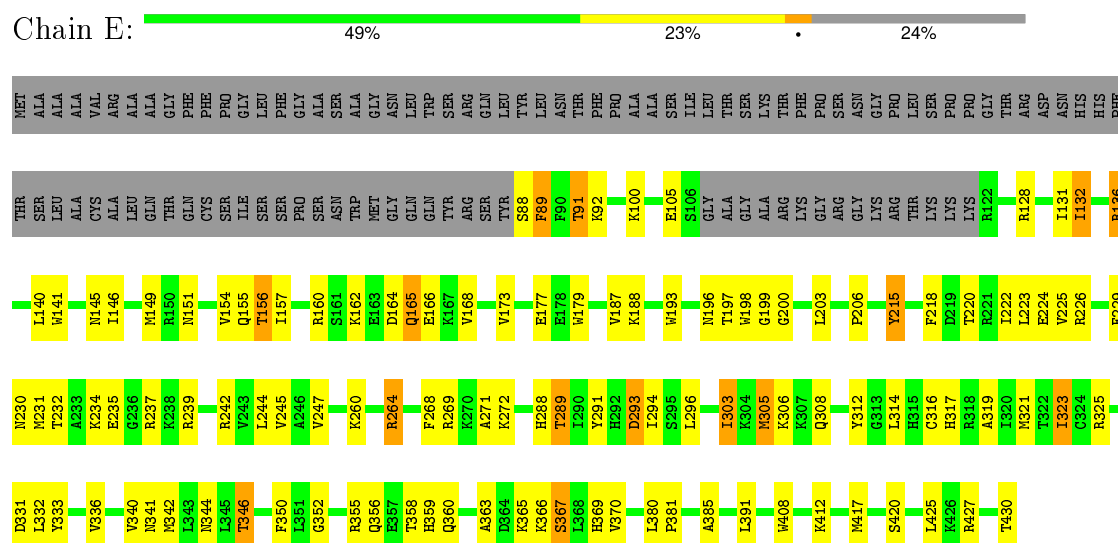
• Molecule 2: MITORIBOSOMAL PROTEIN US2M, MRPS2



• Molecule 3: MITORIBOSOMAL PROTEIN US3M, MRPS24

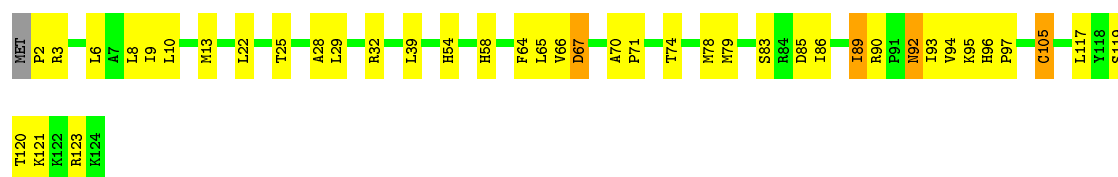


• Molecule 4: MITORIBOSOMAL PROTEIN US5M, MRPS5



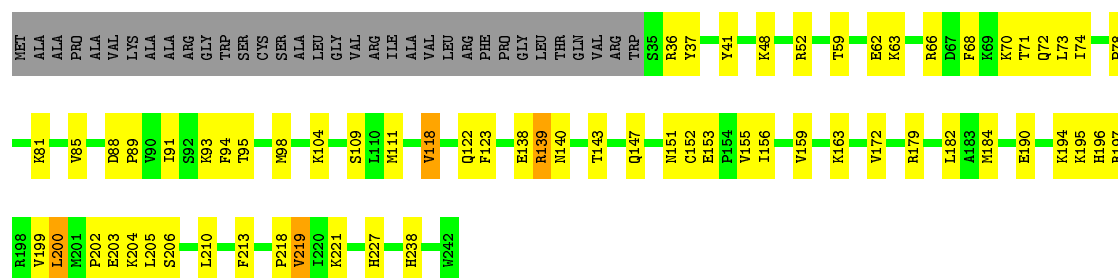
• Molecule 5: MITORIBOSOMAL PROTEIN BS6M, MRPS6





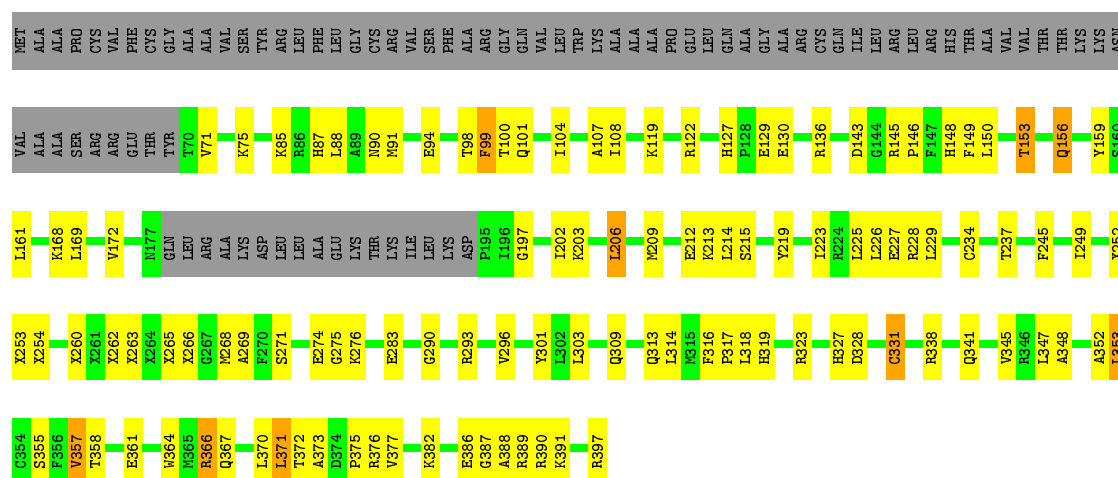
- Molecule 6: MITORIBOSOMAL PROTEIN US7M, MRPS7

Chain G: 59% 26% 14%



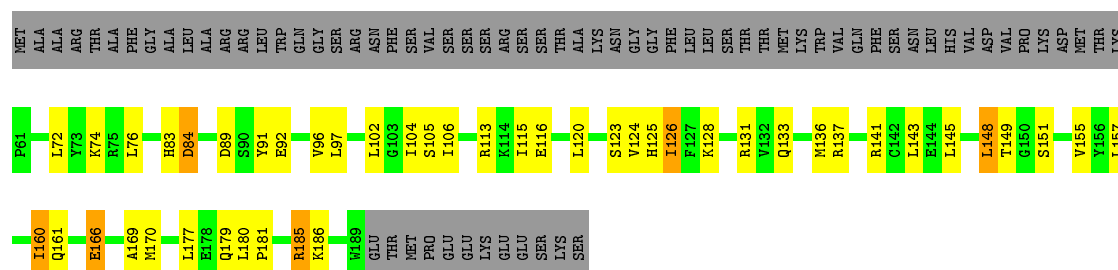
- Molecule 7: MITORIBOSOMAL PROTEIN US9M, MRPS9

Chain I: 50% 26% 22%



- Molecule 8: MITORIBOSOMAL PROTEIN US10M, MRPS10

Chain J: 41% 20% 36%



- Molecule 9: MITORIBOSOMAL PROTEIN US11M, MRPS11

MET	GLN	VAL	ARG	ASN	ALA	GLY	SER	ARG	LEU	LEU	GLN	SER	TRP	ALA	TRP	PRO	PRO	LYS	THR	ILE	ILE	VAL	ALA	GLY	LEU	PRO	ALA	SER	THR	ILE	HIS	ARG	SER	ALA	PRO	PRO	HIS	LEU	GLN	ASP	ASP	LYS	GLU	GLU	ALA	ARG	THR	PRO	SER	HIS	SER												
S61		I64	Y65	P66	P67	I68	P69	G70		L75	A88	H89		N96	T97	Q98	I99	Q100	V101	V102		H106		A112		N121		T126	G127	I128		T132		A137	A138		R150	V151	V152	V153	K154		R160	L161		L172		I175	S176	I177	T178	D179	N180		I183		R189	P190		R194	R195	L196	

- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
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| R78 | R84 | R95 | R96 | L102 | H106 | V107 | V110 | R114 | D117 | L118 | R127 | D131 | R139 | R78 | R79 | R80 | R81 | R82 | R83 | R84 | R85 | R86 | R87 | R88 | R89 | R90 | R91 | R92 | R93 | R94 | R95 | R96 | R97 | R98 | R99 | P00 | P01 | P02 | P03 | P04 | P05 | P06 | P07 | P08 | P09 | P10 | P11 | P12 | P13 | P14 | P15 | P16 | P17 | P18 | P19 | P20 | P21 | P22 | P23 | P24 | P25 | P26 | P27 | P28 | P29 | P30 | P31 | P32 | P33 | P34 | P35 | P36 | P37 | P38 | P39 | P40 | P41 | P42 | P43 | P44 | P45 | P46 | P47 | P48 | P49 | P50 | P51 | P52 | P53 | P54 | P55 | P56 | P57 | P58 | P59 | P60 | P61 | P62 | P63 | P64 | P65 | P66 | P67 | P68 | P69 | P70 | P71 | P72 | P73 | P74 | P75 | P76 | P77 | P78 | P79 | P80 | P81 | P82 | P83 | P84 | P85 | P86 | P87 | P88 | P89 | P90 | P91 | P92 | P93 | P94 | P95 | P96 | P97 | P98 | P99 | M00 | M01 | M02 | M03 | M04 | M05 | M06 | M07 | M08 | M09 | M10 | M11 | M12 | M13 | M14 | M15 | M16 | M17 | M18 | M19 | M20 | M21 | M22 | M23 | M24 | M25 | M26 | M27 | M28 | M29 | M30 | M31 | M32 | M33 | M34 | M35 | M36 | M37 | M38 | M39 | M40 | M41 | M42 | M43 | M44 | M45 | M46 | M47 | M48 | M49 | M50 | M51 | M52 | M53 | M54 | M55 | M56 | M57 | M58 | M59 | M60 | M61 | M62 | M63 | M64 | M65 | M66 | M67 | M68 | M69 | M70 | M71 | M72 | M73 | M74 | M75 | M76 | M77 | M78 | M79 | M80 | M81 | M82 | M83 | M84 | M85 | M86 | M87 | M88 | M89 | M90 | M91 | M92 | M93 | M94 | M95 | M96 | M97 | M98 | M99 |
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| D81 | R81 | MET |
| S82 | ALA | ALA |
| C83 | ALA | ALA |
| P84 | MET | SER |
| R85 | MET | MET |
| R86 | LEU | LEU |
| C91 | GLY | PHE |
| V92 | LEU | LEU |
| M93 | LEU | ARG |
| T94 | THR | THR |
| S95 | VAL | VAL |
| R98 | ARG | GLN |
| R103 | MET | MET |
| R104 | VAL | VAL |
| S107 | PRO | PRO |
| R108 | SER | SER |
| I109 | ALA | ALA |
| D116 | SER | SER |
| H117 | GLY | GLY |
| G118 | GLN | GLN |
| Q119 | VAL | VAL |
| L120 | ARG | ARG |
| S121 | SER | SER |
| G122 | GLY | GLY |
| V123 | GLN | GLN |
| Q124 | VAL | VAL |
| R125 | ARG | ARG |
| H128 | SER | SER |
| | Y28 | |
| | R33 | |
| | M34 | |
| | L35 | |
| | R36 | |
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| | S56 | |
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| | M59 | |
| | M60 | |
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| | L63 | |
| | P64 | |
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| | Q68 | |
| | E69 | |
| | V70 | |
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| | E74 | |
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| | L78 | |
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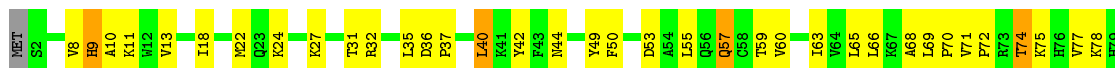
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| L188 | L171 | R172 | Y176 | A177 | V178 | F179 | I182 | L186 | G187 | I188 | R198 | V205 | T212 | R216 | R225 | R239 | G239 | VAL | GLN | PRO | ASN | Q65 | P69 | P70 | S71 | M72 | L73 | L74 | Y77 | V80 | I83 | R92 | L96 | E97 | N100 | Q101 | K104 | L112 | V116 | S125 | L126 | E127 | A128 | R129 | I130 | V131 | A132 | L133 | H143 | H147 | K151 | A152 | H153 | F156 | M159 | D162 | Q163 | R164 | M167 | GLN | PRO | ARG | LEU | ALA | ASP | THR | GLY | LEU | ILE | ARG | PRO | ALA | GLY | LEU | ILE | ARG | ALA | ALA | ARG | GLY | TYR | ALA | ALA | GLN | LYS | PRO | ASP | THR | GLY | LEU | ILE | ARG | PRO | ASN | Q65 | P69 | P70 | S71 | M72 | L73 | L74 | Y77 | V80 | I83 | R92 | L96 | E97 | N100 | Q101 | K104 | L112 | V116 | S125 | L126 | E127 | A128 | R129 | I130 | V131 | A132 | L133 | H143 | H147 | K151 | A152 | H153 | F156 | M159 | D162 | Q163 | R164 | M167 | GLN | PRO | ARG | LEU | ALA | ASP | THR | GLY | LEU | ILE | ARG | PRO | ALA | GLY | LEU | ILE | ARG | PRO | ASN | Q65 | P69 | P70 | S71 | M72 | L73 | L74 | Y77 | V80 | I83 | R92 | L96 | E97 | N100 | Q101 | K104 | L112 | V116 | S125 | L126 | E127 | A128 | R129 | I130 | V131 | A132 | L133 | H143 | H147 | K151 | A152 | H153 | F156 | M159 | D162 | Q163 | R164 | M167 | GLN | PRO | ARG | LEU | ALA | ASP | THR | GLY | LEU | ILE | ARG | PRO | ALA | GLY | LEU | ILE | ARG | PRO | ASN | Q65 | P69 | P70 | S71 | M72 | L73 | L74 | Y77 | V80 | I83 | R92 | L96 | E97 | N100 | Q101 | K104 | L112 | V116 | S125 | L126 | E127 | A128 | R129 | I130 | V131 | A132 | L133 | H143 | H147 | K151 | A152 | H153 | F156 | M159 | D162 | Q163 | R164 | M167 | GLN | PRO | ARG | LEU | ALA | ASP | THR | GLY | LEU | ILE | ARG | PRO | ALA | GLY | LEU | ILE | ARG | PRO | ASN | Q65 | P69 | P70 | S71 | M72 | L73 | L74 | Y77 | V80 | I83 | R92 | L96 | E97 | N100 | Q101 | K104 | L112 | V116 | S125 | L126 | E127 | A128 | R129 | I130 | V131 | A132 | L133 | H143 | H147 | K151 | A152 | H153 | F156 | M159 | D162 | Q163 | R164 | M167 | GLN | PRO | ARG | LEU | ALA | ASP | THR | GLY | LEU | ILE | ARG | PRO | ALA | GLY | LEU | ILE | ARG | PRO | ASN | Q65 | P69 | P70 | S71 | M72 | L73 | L74 | Y77 | V80 | I83 | R92 | L96 | E97 | N100 | Q101 | K104 | L112 | V116 | S125 | L126 | E127 | A128 | R129 | I130 | V131 | A132 | L133 | H143 | H147 | K151 | A152 | H153 | F156 | M159 | D162 | Q163 | R164 | M167 | GLN | PRO | ARG | LEU | ALA | ASP | THR | GLY | LEU | ILE | ARG | PRO | ALA | GLY | LEU | ILE | ARG | PRO | ASN | Q65 | P69 | P70 | S71 | M72 | L73 | L74 | Y77 | V80 | I83 | R92 | L96 | E97 | N100 | Q101 | K104 | L112 | V116 | S125 | L126 | E127 | A128 | R129 | I130 | V131 | A132 | L133 | H143 | H147 | K151 | A152 | H153 | F156 | M159 | D162 | Q163 | R164 | M167 | GLN | PRO | ARG | LEU | ALA | ASP | THR | GLY | LEU | ILE | ARG | PRO | ALA | GLY | LEU | ILE | ARG | PRO | ASN | Q65 | P69 | P70 | S71 | M72 | L73 | L74 | Y77 | V80 | I83 | R92 | L96 | E97 | N100 | Q101 | K104 | L112 | V116 | S125 | L126 | E127 | A128 | R129 | I130 | V131 | A132 | L133 | H143 | H147 | K151 | A152 | H153 | F156 | M159 | D162 | Q163 | R164 | M167 | GLN | PRO | ARG | LEU | ALA | ASP | THR | GLY | LEU | ILE | ARG | PRO | ALA | GLY | LEU | ILE | ARG | PRO | ASN | Q65 | P69 | P70 | S71 | M72 | L73 | L74 | Y77 | V80 | I83 | R92 | L96 | E97 | N100 | Q101 | K104 | L112 | V116 | S125 | L126 | E127 | A128 | R129 | I130 | V131 | A132 | L133 | H143 | H147 | K151 | A152 | H153 | F156 | M159 | D162 | Q163 | R164 | M167 | GLN | PRO | ARG | LEU | ALA | ASP | THR | GLY | LEU | ILE | ARG | PRO | ALA | GLY | LEU | ILE | ARG | PRO | ASN | Q65 | P69 | P70 | S71 | M72 | L73 | L74 | Y77 | V80 | I83 | R92 | L96 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|
| MET | VAL | GIN | LEU | THR | THR | VAL | LEU | CYS | R10 | L17 | L21 | F31 | Y32 | R33 | I34 | V35 | H38 | P42 | R43 | D44 | G45 | L51 | Y54 | D55 | P56 | V66 | I73 | I77 | A81 | F86 | L90 | L91 | Y97 | H100 | P101 | M102 | M103 | I104 | A107 | L110 | R111 | R113 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|



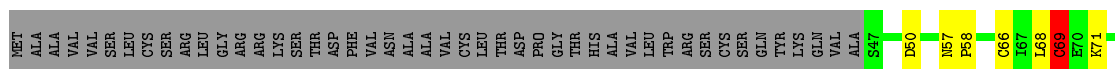
- Molecule 14: MITORIBOSOMAL PROTEIN US17M, MRPS17

Chain Q:



- Molecule 15: MITORIBOSOMAL PROTEIN BS18M, MRPS18C

Chain R:



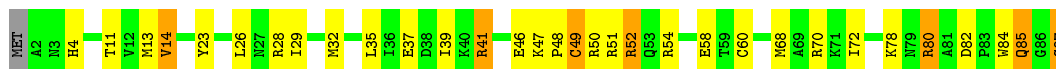
- Molecule 16: MITORIBOSOMAL PROTEIN BL19M, MRPL19

Chain T:



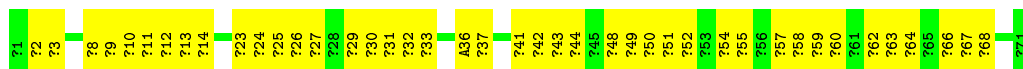
- Molecule 17: MITORIBOSOMAL PROTEIN BS21M, MRPS21

Chain U:



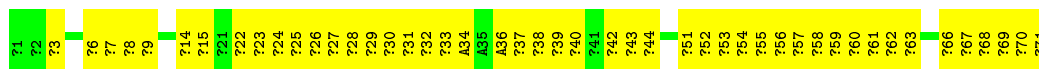
- Molecule 18: P-SITE AND A-SITE TRNA

Chain V:



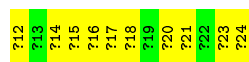
- Molecule 18: P-SITE AND A-SITE TRNA

Chain Y:




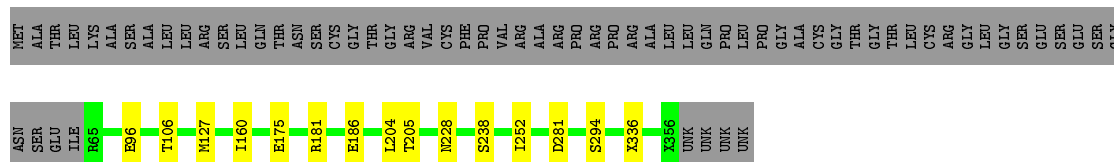
- Molecule 19: MRNA

Chain X:  23% 77%



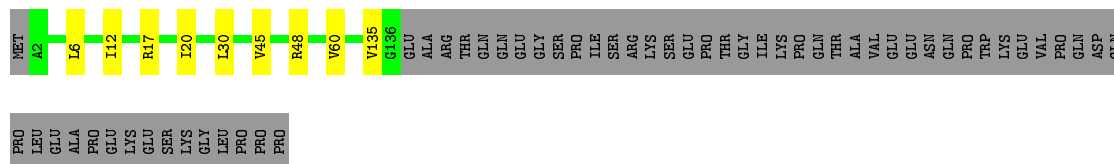
- Molecule 20: MITORIBOSOMAL PROTEIN MS22, MRPS22

Chain a:  77% 19%




- Molecule 21: MITORIBOSOMAL PROTEIN MS23, MRPS23

Chain b:  66% 5% 29%




- Molecule 22: MITORIBOSOMAL PROTEIN MS25, MRPS25

Chain c:  88% 9%



- Molecule 23: MITORIBOSOMAL PROTEIN MS26, MRPS26

Chain d:  80% 6% 14%



- Molecule 24: MITORIBOSOMAL PROTEIN MS27, MRPS27

Chain e:  100%

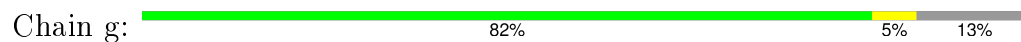


- Molecule 25: MITORIBOSOMAL PROTEIN MS28, MRPS28

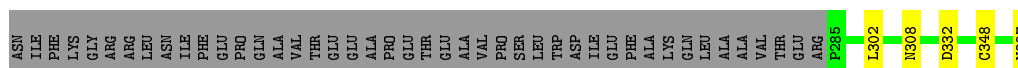
Chain f:  47% 5% 47%



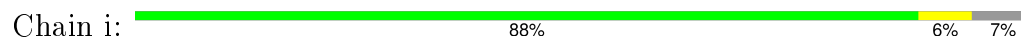
- Molecule 26: MITORIBOSOMAL PROTEIN MS29, MRPS29



- Molecule 27: MITORIBOSOMAL PROTEIN MS31, MRPS31



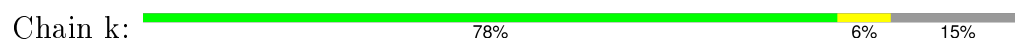
- Molecule 28: MITORIBOSOMAL PROTEIN MS33, MRPS33

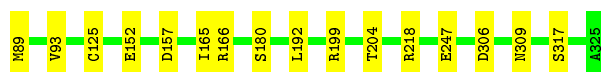


- Molecule 29: MITORIBOSOMAL PROTEIN MS34, MRPS34



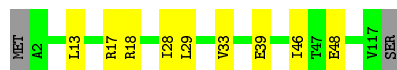
- Molecule 30: MITORIBOSOMAL PROTEIN MS35, MRPS35





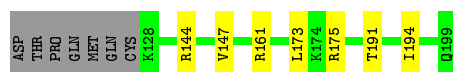
- Molecule 31: MITORIBOSOMAL PROTEIN MS37, MRPS37

Chain m: 91% 8%



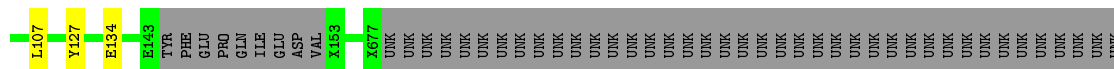
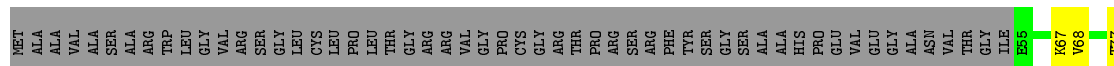
- Molecule 32: MITORIBOSOMAL PROTEIN MS38, MRPS38

Chain n: 33% 64%



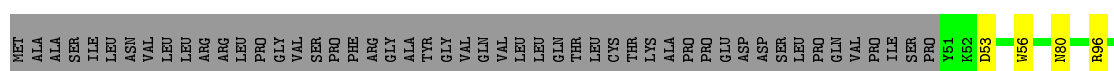
- Molecule 33: MITORIBOSOMAL PROTEIN MS39, MRPS39

Chain o: 68% 31%



- Molecule 34: MITORIBOSOMAL PROTEIN MS40, MRPS18B

Chain p: 66% 7% 27%



- Molecule 35: UNASSIGNED HELICES

Chain s: 100%

There are no outlier residues recorded for this chain.

- Molecule 36: UNASSIGNED HELICES

Chain z:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PER DETECTOR FRAME	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 2$	RMSZ	# $ Z > 2$
1	A	0.67	4/22852 (0.0%)	1.16	72/35580 (0.2%)
10	L	0.42	0/858	0.60	0/1152
11	N	0.45	0/874	0.60	0/1171
12	O	0.42	0/1473	0.58	0/1970
13	P	0.45	0/954	0.62	0/1284
14	Q	0.43	0/871	0.64	0/1181
15	R	0.55	1/802 (0.1%)	0.69	0/1079
17	U	0.46	0/745	0.59	0/993
2	B	0.48	0/1804	0.61	0/2445
20	a	0.35	0/2052	0.52	0/2774
21	b	0.39	0/1126	0.54	0/1514
22	c	0.45	0/1399	0.64	1/1881 (0.1%)
23	d	0.40	0/1490	0.51	0/2005
25	f	0.42	0/790	0.60	0/1064
26	g	0.34	0/2731	0.52	0/3696
27	h	0.35	0/903	0.52	0/1215
28	i	0.38	0/841	0.53	0/1121
29	j	0.34	0/1779	0.59	0/2404
3	C	0.41	0/1105	0.65	0/1496
30	k	0.35	0/2268	0.54	0/3069
31	m	0.42	0/947	0.56	0/1268
32	n	0.51	0/650	0.60	0/858
33	o	0.36	0/726	0.53	0/988
34	p	0.44	1/1602 (0.1%)	0.60	0/2175
4	E	0.46	0/2673	0.59	0/3591
5	F	0.42	0/1008	0.63	1/1358 (0.1%)
6	G	0.39	0/1763	0.54	0/2368
7	I	0.39	0/2455	0.52	0/3291
8	J	0.45	0/1091	0.63	0/1474
9	K	0.44	0/1021	0.65	0/1381
All	All	0.52	6/61653 (0.0%)	0.86	74/87846 (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
20	a	0	1
24	e	0	1
8	J	0	2
9	K	0	1
All	All	0	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	R	69	CYS	CB-SG	6.80	1.93	1.82
1	A	843	C	N1-C6	-6.07	1.33	1.37
1	A	822	A	N9-C4	5.59	1.41	1.37
1	A	406	A	N9-C4	-5.18	1.34	1.37
34	p	105	CYS	CB-SG	-5.15	1.73	1.81
1	A	457	C	N1-C6	-5.14	1.34	1.37

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	A	C8-N9-C4	7.75	108.90	105.80
1	A	488	A	N1-C2-N3	7.73	133.17	129.30
1	A	28	U	C5-C6-N1	-7.65	118.87	122.70
1	A	119	C	N1-C2-O2	7.53	123.42	118.90
22	c	141	CYS	CA-CB-SG	7.37	127.27	114.00
1	A	455	A	C8-N9-C4	7.17	108.67	105.80
1	A	59	C	C6-N1-C2	-6.78	117.59	120.30
1	A	945	A	C8-N9-C4	-6.75	103.10	105.80
1	A	488	A	C2-N3-C4	-6.56	107.32	110.60
1	A	940	C	C6-N1-C2	-6.50	117.70	120.30
1	A	376	C	C6-N1-C2	-6.41	117.74	120.30
5	F	105	CYS	CA-CB-SG	6.37	125.47	114.00
1	A	837	C	N3-C4-C5	6.34	124.44	121.90
1	A	224	U	C2-N1-C1'	6.28	125.24	117.70
1	A	522	A	C4-C5-N7	-6.18	107.61	110.70
1	A	59	C	C2-N1-C1'	6.14	125.55	118.80
1	A	553	G	C8-N9-C4	-6.14	103.94	106.40
1	A	944	A	C5-C6-N6	6.11	128.59	123.70
1	A	522	A	C5-N7-C8	6.06	106.93	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	U	C5-C6-N1	6.05	125.73	122.70
1	A	119	C	C2-N1-C1'	6.05	125.45	118.80
1	A	944	A	N9-C4-C5	6.03	108.21	105.80
1	A	947	G	N1-C6-O6	-6.03	116.28	119.90
1	A	900	A	O4'-C1'-N9	6.01	113.01	108.20
1	A	317	A	N1-C2-N3	5.99	132.29	129.30
1	A	654	A	N1-C6-N6	5.97	122.18	118.60
1	A	630	A	N1-C2-N3	5.95	132.28	129.30
1	A	631	A	N1-C6-N6	-5.93	115.04	118.60
1	A	125	U	C2-N1-C1'	5.89	124.76	117.70
1	A	477	A	C8-N9-C4	5.86	108.14	105.80
1	A	944	A	C8-N9-C4	-5.81	103.47	105.80
1	A	646	C	C4-C5-C6	5.80	120.30	117.40
1	A	899	C	C6-N1-C2	-5.71	118.01	120.30
1	A	824	G	C4-N9-C1'	5.71	133.92	126.50
1	A	613	A	C8-N9-C4	5.69	108.08	105.80
1	A	949	G	N3-C4-C5	-5.68	125.76	128.60
1	A	457	C	C5-C6-N1	-5.66	118.17	121.00
1	A	522	A	N1-C6-N6	-5.64	115.22	118.60
1	A	522	A	N7-C8-N9	-5.63	110.98	113.80
1	A	513	A	N1-C6-N6	-5.63	115.22	118.60
1	A	16	U	N1-C2-N3	5.62	118.27	114.90
1	A	252	C	C6-N1-C2	-5.60	118.06	120.30
1	A	97	C	C2-N1-C1'	5.59	124.95	118.80
1	A	846	C	C6-N1-C2	-5.55	118.08	120.30
1	A	944	A	N1-C2-N3	5.54	132.07	129.30
1	A	297	A	C4-C5-C6	-5.53	114.23	117.00
1	A	376	C	N3-C2-O2	-5.51	118.04	121.90
1	A	316	C	OP2-P-O3'	5.46	117.22	105.20
1	A	391	U	C5-C6-N1	-5.45	119.98	122.70
1	A	843	C	C6-N1-C2	5.44	122.47	120.30
1	A	937	A	N1-C2-N3	5.41	132.00	129.30
1	A	654	A	C5-C6-N6	-5.40	119.38	123.70
1	A	945	A	C4-C5-C6	5.38	119.69	117.00
1	A	13	U	C5-C6-N1	-5.38	120.01	122.70
1	A	947	G	C5-C6-N1	5.36	114.18	111.50
1	A	526	G	C4-N9-C1'	5.34	133.44	126.50
1	A	945	A	N7-C8-N9	5.27	116.43	113.80
1	A	252	C	N3-C4-C5	-5.26	119.80	121.90
1	A	953	U	N1-C2-N3	5.26	118.05	114.90
1	A	59	C	C5-C6-N1	5.23	123.61	121.00
1	A	694	G	C4-N9-C1'	5.21	133.28	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	406	A	C8-N9-C4	5.20	107.88	105.80
1	A	944	A	N1-C6-N6	-5.18	115.49	118.60
1	A	345	U	C2-N1-C1'	5.18	123.92	117.70
1	A	320	A	C2-N3-C4	-5.16	108.02	110.60
1	A	523	C	C4-C5-C6	5.13	119.97	117.40
1	A	382	U	N1-C2-N3	5.12	117.97	114.90
1	A	378	A	N1-C2-N3	5.11	131.86	129.30
1	A	651	G	C8-N9-C4	5.11	108.44	106.40
1	A	12	G	N3-C4-C5	-5.06	126.07	128.60
1	A	495	U	C5-C6-N1	-5.04	120.18	122.70
1	A	503	A	C2-N3-C4	5.04	113.12	110.60
1	A	523	C	N1-C2-N3	5.03	122.72	119.20
1	A	119	C	C6-N1-C1'	-5.01	114.79	120.80

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	317	0
2	B	1762	0	1774	56	0
3	C	1075	0	1087	33	0
4	E	2621	0	2640	82	0
5	F	990	0	1025	30	0
6	G	1721	0	1747	52	0
7	I	2498	0	2474	92	0
8	J	1067	0	1101	32	0
9	K	1001	0	1037	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	L	840	0	890	20	0
11	N	858	0	883	28	0
12	O	1448	0	1536	30	0
13	P	932	0	951	21	0
14	Q	853	0	913	30	0
15	R	784	0	813	27	0
16	T	84	0	86	6	0
17	U	734	0	745	28	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	0	0
21	b	1101	0	1118	0	0
22	c	1367	0	1385	0	0
23	d	1467	0	1466	0	0
24	e	2016	0	2028	0	0
25	f	778	0	791	0	0
26	g	2774	0	2810	0	0
27	h	876	0	832	0	0
28	i	824	0	842	0	0
29	j	1777	0	1789	0	0
30	k	2222	0	2270	0	0
31	m	930	0	959	0	0
32	n	639	0	709	0	0
33	o	3028	0	3081	0	0
34	p	1551	0	1519	0	0
35	s	96	0	98	0	0
36	z	102	0	104	0	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	0	0
40	A	114	0	0	8	0
40	g	4	0	0	0	0
All	All	66363	0	55866	939	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 (939) 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)
7:I:253:UNK:CG	7:I:366:ARG:HH22	1.39	1.33
18:V:55:Y5P:C2'	18:V:57:Y5P:H5	1.77	1.15
18:V:25:Y5P:H4A	18:V:26:Y5P:H4	1.26	1.13
18:Y:25:Y5P:H4A	18:Y:26:Y5P:H4	1.32	1.07
18:Y:9:Y5P:H4A	18:Y:22:Y5P:H4A	1.33	1.06
7:I:253:UNK:HG1	7:I:366:ARG:HH22	1.21	1.04
7:I:253:UNK:CG	7:I:366:ARG:NH2	2.20	1.04
18:V:55:Y5P:O2'	18:V:57:Y5P:H5	1.65	0.96
18:Y:68:Y5P:H4A	18:Y:69:Y5P:H4	1.49	0.94
7:I:228:ARG:HD2	17:U:85:GLN:HE21	1.31	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
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
10:L:78:ARG:HG3	10:L:118:LEU:HD21	1.54	0.89
18:Y:54:Y5P:H4A	18:Y:55:Y5P:H4A	1.55	0.88
18:Y:9:Y5P:H4	18:Y:22:Y5P:H5	1.58	0.85
12:O:171:LEU:HB3	12:O:179:PHE:HB2	1.58	0.84
17:U:49:CYS:SG	17:U:50:ARG:N	2.51	0.84
18:V:54:Y5P:N3	18:V:58:Y5P:H5	1.93	0.83
1:A:566:U:O2	1:A:686:A:N6	2.11	0.83
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
18:V:49:Y5P:H4A	18:V:50:Y5P:H4	1.63	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
6:G:68:PHE:HB3	7:I:367:GLN:HE21	1.44	0.81
1:A:103:G:H4'	14:Q:8:VAL:HG13	1.63	0.81
7:I:253:UNK:HG3	7:I:366:ARG:HH22	1.43	0.81
1:A:630:A:H2	1:A:654:A:H61	1.29	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
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
5:F:65:LEU:HD21	15:R:76:LYS:HD3	1.63	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
18:Y:9:Y5P:H4	18:Y:22:Y5P:C5	2.11	0.79
18:Y:25:Y5P:C4	18:Y:26:Y5P:H4	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:V:25:Y5P:C4	18:V:26:Y5P:H4	2.12	0.79
1:A:124:A:H1'	1:A:125:U:H5	1.47	0.78
7:I:253:UNK:HG3	7:I:366:ARG:NH2	1.96	0.78
1:A:300:G:N7	40:A:7098:HOH:O	2.14	0.78
18:V:26:Y5P:H4A	18:V:27:Y5P:H4	1.64	0.78
4:E:215:TYR:HB3	4:E:218:PHE:HD2	1.49	0.78
18:Y:8:Y5P:N3	18:Y:14:Y5P:H5	1.99	0.77
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
18:Y:9:Y5P:C4	18:Y:22:Y5P:C4	2.63	0.77
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
18:V:9:Y5P:O2'	18:V:10:Y5P:C5	2.34	0.76
18:Y:14:Y5P:H4A	18:Y:15:Y5P:H4	1.68	0.75
8:J:123:SER:O	11:N:108:ARG:NH2	2.19	0.75
4:E:160:ARG:HD2	4:E:165:GLN:HE22	1.49	0.75
40:A:7150:HOH:O	18:V:30:Y5P:H4A	1.86	0.75
18:V:23:Y5P:H4A	18:V:24:Y5P:H4	1.66	0.74
1:A:405:G:H1	1:A:452:C:HO2'	1.36	0.74
5:F:105:CYS:HB3	15:R:69:CYS:SG	2.28	0.73
1:A:249:C:N4	10:L:117:ASP:OD1	2.21	0.73
1:A:343:U:OP2	9:K:96:ASN:ND2	2.21	0.73
1:A:124:A:H1'	1:A:125:U:C5	2.24	0.73
18:Y:27:Y5P:O5'	18:Y:27:Y5P:H6	1.87	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
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
18:V:43:Y5P:H2'	18:V:44:Y5P:H6	1.71	0.72
4:E:203:LEU:HD13	4:E:222:ILE:HD11	1.72	0.71
4:E:206:PRO:HA	4:E:272:LYS:HD2	1.71	0.71
18:V:62:Y5P:H4A	18:V:63:Y5P:H4	1.71	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
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
4:E:412:LYS:HG2	4:E:417:MET:HB2	1.74	0.70
2:B:219:VAL:HG22	2:B:233:TYR:HB2	1.73	0.69
18:V:54:Y5P:N3	18:V:58:Y5P:C5	2.55	0.69
1:A:96:U:H4'	13:P:17:LEU:HD13	1.72	0.69
1:A:744:C:HO2'	1:A:746:A:HO2'	1.38	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:E:140:LEU:HD21	4:E:160:ARG:HE	1.58	0.69
1:A:697:U:H5''	1:A:698:A:C8	2.28	0.69
8:J:74:LYS:HB2	8:J:177:LEU:HD21	1.75	0.69
4:E:149:MET:HG2	4:E:154:VAL:H	1.57	0.69
1:A:954:U:H4'	1:A:955:G:H5'	1.73	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
18:V:59:Y5P:H4A	18:V:60:Y5P:H4	1.74	0.68
1:A:798:A:H2'	1:A:799:A:H8	1.58	0.68
5:F:67:ASP:N	5:F:67:ASP:OD1	2.26	0.68
18:V:54:Y5P:H4A	18:V:55:Y5P:H4	1.75	0.68
18:V:30:Y5P:H4A	18:V:31:Y5P:H4	1.75	0.68
1:A:223:U:O2'	1:A:224:U:OP1	2.10	0.68
16:T:66:UNK:HG3	16:T:66:UNK:O	1.93	0.67
1:A:707:A:H3'	1:A:708:A:H5''	1.77	0.67
1:A:257:U:H4'	1:A:258:C:H5'	1.76	0.67
2:B:153:LEU:HD11	2:B:246:ARG:HG2	1.75	0.67
1:A:646:C:H4'	1:A:647:A:H5'	1.77	0.67
4:E:197:THR:HG22	4:E:199:GLY:H	1.59	0.67
6:G:153:GLU:HG3	6:G:179:ARG:HB3	1.76	0.67
4:E:141:TRP:H	4:E:145:ASN:HD22	1.42	0.67
18:V:55:Y5P:O2'	18:V:57:Y5P:C5	2.41	0.66
18:Y:31:Y5P:H4A	18:Y:32:Y5P:C4	2.23	0.66
6:G:78:PRO:HG2	6:G:81:LYS:HB2	1.77	0.66
7:I:253:UNK:HG1	7:I:366:ARG:NH2	2.01	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
18:V:2:Y5P:H4A	18:V:3:Y5P:H4	1.77	0.66
9:K:64:ILE:HG22	9:K:66:PRO:HD2	1.76	0.66
3:C:128:PRO:HD2	3:C:131:LYS:HD2	1.78	0.66
1:A:647:A:H3'	1:A:648:A:C5'	2.26	0.66
8:J:115:ILE:HG12	8:J:137:ARG:HG2	1.78	0.65
1:A:826:C:H2'	1:A:827:A:H8	1.61	0.65
1:A:317:A:H2	1:A:318:C:C5	2.15	0.65
1:A:285:C:HO2'	1:A:488:A:H2	1.43	0.65
18:V:25:Y5P:H4A	18:V:26:Y5P:C4	2.16	0.65
18:V:8:Y5P:C4	18:V:14:Y5P:H5	2.27	0.65
2:B:70:ASP:O	2:B:73:ASN:N	2.22	0.65
7:I:290:GLY:HA2	7:I:328:ASP:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:P:17:LEU:HD23	13:P:81:ALA:HB2	1.79	0.65
1:A:316:C:H4'	1:A:317:A:OP2	1.95	0.64
8:J:104:ILE:HG23	8:J:148:LEU:HD21	1.79	0.64
6:G:155:VAL:H	6:G:227:HIS:HE1	1.42	0.64
18:Y:51:Y5P:H4A	18:Y:52:Y5P:C4	2.27	0.64
1:A:499:C:O2	40:A:7194:HOH:O	2.12	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
11:N:117:HIS:HB2	11:N:119:GLN:HG3	1.80	0.64
2:B:176:THR:HA	2:B:214:MET:HE1	1.78	0.64
2:B:228:PRO:HA	2:B:231:ILE:HD12	1.79	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
2:B:119:GLN:O	2:B:123:HIS:ND1	2.30	0.63
1:A:644:A:O2'	1:A:645:A:O5'	2.17	0.62
3:C:72:HIS:HD2	3:C:74:GLY:H	1.47	0.62
2:B:168:ARG:HG3	7:I:159:TYR:CZ	2.35	0.62
1:A:136:C:O2	12:O:198:ARG:NH2	2.32	0.62
16:T:55:UNK:HG2	16:T:55:UNK:O	1.99	0.62
18:V:25:Y5P:H2'	18:V:26:Y5P:H6	1.82	0.62
3:C:100:PHE:HB3	3:C:103:CYS:SG	2.39	0.62
1:A:4:C:C4	4:E:427:ARG:HD3	2.35	0.62
15:R:125:TYR:HE2	17:U:4:HIS:HB3	1.65	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
1:A:794:A:OP1	7:I:390:ARG:NH1	2.32	0.62
1:A:792:U:H2'	1:A:793:A:H8	1.65	0.62
1:A:747:C:N4	1:A:749:C:OP1	2.32	0.61
18:Y:68:Y5P:H4A	18:Y:69:Y5P:C4	2.26	0.61
1:A:633:C:OP1	4:E:269:ARG:NH1	2.32	0.61
16:T:60:UNK:O	16:T:60:UNK:HG2	1.99	0.61
17:U:48:PRO:O	17:U:52:ARG:HD2	1.99	0.61
12:O:172:ARG:NH1	14:Q:60:VAL:O	2.32	0.61
8:J:83:HIS:CE1	11:N:122:GLY:HA3	2.36	0.61
9:K:160:ARG:NH1	17:U:23:TYR:OH	2.34	0.61
13:P:42:PRO:HG2	13:P:45:GLY:HA3	1.82	0.61
1:A:767:U:H2'	1:A:768:A:H8	1.64	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
1:A:250:A:H2'	1:A:251:C:C6	2.36	0.60
7:I:275:GLY:H	7:I:348:ALA:HB2	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:V:23:Y5P:H6	18:V:23:Y5P:OP2	2.01	0.60
1:A:868:U:O2'	1:A:900:A:N6	2.35	0.60
9:K:65:TYR:HB3	17:U:13:MET:H	1.66	0.60
8:J:84:ASP:OD1	8:J:84:ASP:N	2.23	0.60
3:C:69:LEU:HD13	3:C:93:ARG:HH12	1.65	0.60
1:A:767:U:H2'	1:A:768:A:C8	2.37	0.60
1:A:747:C:H2'	1:A:748:A:H5''	1.83	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
1:A:177:U:H2'	1:A:178:G:C8	2.36	0.60
7:I:262:UNK:HA	7:I:269:ALA:HA	1.84	0.60
1:A:338:U:H2'	1:A:339:A:C8	2.37	0.60
5:F:71:PRO:HG2	5:F:74:THR:OG1	2.02	0.60
9:K:183:ILE:HG12	17:U:39:ILE:HD11	1.84	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
1:A:552:A:H2'	1:A:553:G:C8	2.37	0.59
1:A:59:C:H42	8:J:133:GLN:CG	149.89	0.59
1:A:708:A:H4'	1:A:708:A:OP2	2.02	0.59
1:A:201:A:H2'	1:A:202:A:C8	2.37	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
1:A:28:U:H2'	1:A:29:A:H8	1.67	0.59
12:O:69:PRO:HD2	12:O:72:MET:HG3	1.84	0.58
1:A:356:A:H2'	1:A:357:G:C8	2.38	0.58
6:G:218:PRO:HA	6:G:221:LYS:HE3	1.85	0.58
1:A:186:U:HO2'	1:A:188:A:H8	1.51	0.58
18:V:54:Y5P:C4	18:V:58:Y5P:H5	2.34	0.58
9:K:175:ILE:HG13	9:K:176:SER:H	1.69	0.58
9:K:65:TYR:OH	15:R:142:ARG:HD2	2.04	0.58
18:V:9:Y5P:O2'	18:V:10:Y5P:H5	2.02	0.58
2:B:79:SER:H	2:B:82:SER:HB3	1.68	0.58
1:A:882:A:N3	1:A:886:A:N6	2.51	0.58
7:I:263:UNK:N	7:I:268:MET:O	2.37	0.58
40:A:7150:HOH:O	18:V:30:Y5P:C4	2.48	0.58
6:G:203:GLU:O	6:G:206:SER:OG	2.17	0.57
18:Y:59:Y5P:H4A	18:Y:60:Y5P:H4	1.86	0.57
4:E:198:TRP:HB2	4:E:225:VAL:CG1	2.34	0.57
1:A:763:A:O3'	11:N:58:ARG:NH2	2.37	0.57
13:P:110:LEU:O	13:P:114:ARG:HG2	2.04	0.57
1:A:625:U:O2'	1:A:626:C:OP2	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:203:LEU:HD23	4:E:272:LYS:HG3	1.85	0.57
6:G:159:VAL:HB	6:G:172:VAL:HG21	1.86	0.57
1:A:285:C:O2'	1:A:488:A:H2	1.86	0.57
1:A:232:G:H5''	4:E:196:ASN:ND2	2.19	0.57
12:O:129:ARG:HB2	12:O:167:MET:HE3	1.87	0.57
1:A:168:A:H2'	1:A:169:A:C8	2.40	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
4:E:198:TRP:HB2	4:E:225:VAL:HG11	1.85	0.57
1:A:59:C:H42	8:J:133:GLN:HG2	149.82	0.57
1:A:741:C:N4	1:A:744:C:N3	2.52	0.57
1:A:77:G:H8	1:A:77:G:OP1	1.88	0.57
1:A:203:G:H2'	1:A:204:U:C6	2.39	0.57
18:V:43:Y5P:H4A	18:V:44:Y5P:H4	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
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
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
1:A:641:A:OP1	4:E:230:ASN:HB2	2.05	0.56
1:A:512:A:H2'	1:A:513:A:C8	2.40	0.56
6:G:94:PHE:HD1	6:G:184:MET:HG2	1.71	0.56
1:A:961:C:H2'	1:A:962:C:H5'	1.88	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
1:A:318:C:H3'	15:R:106:LYS:HE2	1.88	0.56
18:Y:32:Y5P:H4A	18:Y:33:Y5P:H4	1.87	0.55
2:B:104:TYR:HD2	2:B:236:PRO:HG3	1.71	0.55
18:Y:31:Y5P:C4	18:Y:32:Y5P:H4	2.33	0.55
1:A:358:U:H2'	1:A:359:U:C6	2.41	0.55
1:A:13:U:H1'	1:A:640:A:N3	2.21	0.55
10:L:61:VAL:HG23	10:L:84:ARG:HB2	1.88	0.55
5:F:8:LEU:HB2	5:F:64:PHE:HB2	1.89	0.55
1:A:160:C:H2'	1:A:163:A:H61	1.72	0.55
12:O:153:HIS:HA	12:O:156:PHE:HD2	1.72	0.55
2:B:58:ARG:O	2:B:61:ILE:HG22	2.07	0.55
14:Q:8:VAL:HG12	14:Q:10:ALA:H	1.71	0.55
1:A:887:U:H2'	1:A:888:A:C8	2.42	0.55
1:A:209:C:H4'	13:P:43:ARG:HH12	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:52:THR:HG22	3:C:54:GLU:H	1.72	0.55
1:A:526:G:H1'	4:E:231:MET:HB3	1.88	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
4:E:244:LEU:HD21	4:E:346:THR:HG21	1.89	0.55
7:I:316:PHE:HB3	7:I:317:PRO:HD3	1.89	0.54
1:A:429:U:O2'	1:A:431:G:N7	2.34	0.54
1:A:102:G:O3'	14:Q:78:LYS:NZ	2.40	0.54
17:U:37:GLU:O	17:U:41:ARG:HB2	2.07	0.54
4:E:224:GLU:HB2	4:E:342:MET:HG2	1.90	0.54
1:A:823:G:H5'	1:A:824:G:OP2	2.08	0.54
6:G:71:THR:HG23	7:I:253:UNK:HB2	1.88	0.54
1:A:333:A:N7	1:A:361:A:H2	2.05	0.54
9:K:112:ALA:HB3	9:K:137:ALA:HB2	1.88	0.54
7:I:129:GLU:HG3	7:I:130:GLU:HG3	1.89	0.54
18:Y:43:Y5P:HA	18:Y:43:Y5P:OP2	2.07	0.54
6:G:94:PHE:HD2	6:G:111:MET:HE1	1.72	0.54
6:G:94:PHE:CD2	6:G:111:MET:HE1	2.42	0.54
14:Q:11:LYS:HA	14:Q:68:ALA:HB2	1.89	0.54
1:A:821:A:H5'	1:A:822:A:OP1	2.08	0.54
3:C:91:PHE:HD1	4:E:89:PHE:CE2	2.26	0.54
13:P:110:LEU:O	13:P:113:LYS:HG2	2.07	0.54
1:A:739:A:H4'	1:A:740:U:C2	2.43	0.54
5:F:119:SER:HB3	5:F:121:LYS:HE3	1.90	0.54
4:E:288:HIS:HD2	4:E:289:THR:OG1	1.90	0.54
18:V:11:Y5P:H4A	18:V:12:Y5P:H4	1.90	0.54
13:P:34:ILE:HG22	13:P:51:LEU:HB2	1.89	0.54
1:A:56:U:OP1	1:A:204:U:O2'	2.22	0.53
11:N:125:ARG:HG2	11:N:125:ARG:HH11	1.73	0.53
1:A:762:G:N2	1:A:764:A:H3'	2.24	0.53
11:N:103:ARG:HB3	11:N:104:TRP:CE3	2.43	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
6:G:62:GLU:CD	6:G:66:ARG:HH21	2.11	0.53
1:A:545:C:H1'	1:A:820:U:H1'	1.89	0.53
8:J:166:GLU:N	8:J:166:GLU:OE1	2.32	0.53
1:A:344:G:H1	9:K:121:ASN:CB	2.21	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
5:F:105:CYS:CB	15:R:69:CYS:SG	2.94	0.53
11:N:63:LEU:HD22	11:N:64:PRO:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:939:A:H2'	1:A:940:C:C6	2.44	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
1:A:390:A:O2'	12:O:153:HIS:HE1	1.92	0.53
10:L:96:PRO:O	10:L:127:ARG:NH1	2.41	0.53
1:A:640:A:OP1	4:E:260:LYS:NZ	2.40	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
4:E:193:TRP:CE3	4:E:199:GLY:HA3	2.44	0.53
2:B:223:ASP:OD1	2:B:224:THR:N	2.39	0.53
4:E:341:ASN:OD1	4:E:344:ASN:HB2	2.09	0.53
1:A:931:G:H4'	1:A:932:U:H5''	1.90	0.53
18:V:67:Y5P:H4A	18:V:68:Y5P:H4	1.90	0.52
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
1:A:103:G:H1'	14:Q:9:HIS:HE1	1.73	0.52
1:A:791:G:C8	7:I:376:ARG:HB3	2.45	0.52
1:A:670:A:N3	6:G:36:ARG:NH1	2.57	0.52
14:Q:32:ARG:NH2	14:Q:49:TYR:OH	2.43	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
1:A:800:G:H2'	1:A:801:A:C8	2.44	0.52
14:Q:74:THR:HG22	14:Q:75:LYS:H	1.75	0.52
1:A:667:C:H3'	1:A:668:A:H8	1.73	0.52
18:V:31:Y5P:H4A	18:V:32:Y5P:H4	1.92	0.52
1:A:168:A:O2'	1:A:170:A:N1	2.39	0.52
1:A:43:U:H2'	1:A:44:U:O4'	2.10	0.52
6:G:196:HIS:H	6:G:196:HIS:CD2	5.02	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
1:A:826:C:H2'	1:A:827:A:C8	2.42	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
1:A:835:C:H2'	1:A:836:G:C8	2.44	0.52
1:A:947:G:H2'	1:A:948:U:C6	2.44	0.52
10:L:60:GLY:HA2	10:L:84:ARG:O	2.10	0.52
1:A:899:C:H2'	1:A:900:A:H4'	1.90	0.52
18:V:66:Y5P:H4A	18:V:67:Y5P:H4	1.92	0.52
7:I:260:UNK:HG3	7:I:355:SER:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:A:H5'	1:A:125:U:OP1	2.09	0.52
4:E:296:LEU:HB3	4:E:303:ILE:HG22	1.91	0.52
18:V:41:Y5P:H4A	18:V:42:Y5P:C5	2.40	0.52
1:A:667:C:H3'	1:A:668:A:C8	2.45	0.51
12:O:129:ARG:HB2	12:O:167:MET:CE	2.40	0.51
7:I:228:ARG:HD2	17:U:85:GLN:NE2	2.14	0.51
7:I:127:HIS:CD2	7:I:129:GLU:HG2	2.45	0.51
5:F:22:LEU:HD11	5:F:64:PHE:CE2	2.45	0.51
11:N:53:ARG:O	11:N:56:SER:OG	2.27	0.51
1:A:42:A:O2'	1:A:43:U:OP1	2.27	0.51
19:X:20:Y5P:H4A	19:X:21:Y5P:H4	1.92	0.51
6:G:59:THR:HG22	6:G:63:LYS:HE3	1.92	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
19:X:20:Y5P:H4	18:Y:36:P5P:N1	2.25	0.51
1:A:63:G:H5'	1:A:64:C:OP2	2.11	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
1:A:216:A:C6	1:A:274:A:N7	2.78	0.51
6:G:238:HIS:CE1	9:K:127:GLY:H	2.29	0.51
1:A:729:A:H2'	1:A:730:C:O4'	2.10	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
6:G:238:HIS:HE1	9:K:127:GLY:H	1.59	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
1:A:752:A:H3'	1:A:753:A:H5'	1.92	0.51
1:A:565:A:HO2'	1:A:589:C:HO2'	1.57	0.51
1:A:103:G:H1'	14:Q:9:HIS:CE1	2.46	0.51
11:N:120:LEU:HD23	11:N:123:VAL:HG21	1.92	0.50
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
4:E:291:TYR:H	4:E:356:GLN:HE21	1.59	0.50
11:N:58:ARG:HG3	11:N:75:ILE:HD11	1.92	0.50
1:A:317:A:C2	1:A:318:C:C5	2.98	0.50
7:I:382:LYS:HD2	7:I:388:ALA:HA	1.93	0.50
4:E:140:LEU:HB3	4:E:146:ILE:HD13	1.92	0.50
18:Y:52:Y5P:H4A	18:Y:53:Y5P:H4	1.93	0.50
18:Y:62:Y5P:N3	18:Y:63:Y5P:H4	2.26	0.50
1:A:675:A:OP1	3:C:41:ARG:NH1	2.45	0.50
1:A:12:G:H5'	4:E:229:PHE:HD2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:V:43:Y5P:N3	18:V:44:Y5P:H4	2.27	0.50
1:A:645:A:H5'	1:A:646:C:H5	1.77	0.50
18:Y:25:Y5P:C6	18:Y:26:Y5P:H5	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
1:A:475:A:OP2	5:F:123:ARG:NH2	2.45	0.50
18:Y:66:Y5P:H4A	18:Y:67:Y5P:H4	1.94	0.50
1:A:846:C:H2'	1:A:847:C:O4'	2.12	0.50
1:A:707:A:H3'	1:A:708:A:C5'	2.42	0.50
16:T:60:UNK:CG	16:T:60:UNK:O	2.59	0.50
1:A:775:A:HO2'	1:A:776:A:H8	1.60	0.50
4:E:156:THR:HG22	4:E:157:ILE:H	1.76	0.50
18:Y:68:Y5P:H2'	18:Y:69:Y5P:H6	1.94	0.50
1:A:577:C:OP2	8:J:128:LYS:HD3	2.12	0.50
16:T:56:UNK:O	16:T:56:UNK:HG2	2.11	0.50
18:V:8:Y5P:O5'	18:V:8:Y5P:H6	2.12	0.50
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
3:C:94:LYS:HZ1	4:E:92:LYS:HB2	1.77	0.49
18:Y:51:Y5P:H4A	18:Y:52:Y5P:C5	2.41	0.49
1:A:857:C:H2'	1:A:858:C:C6	2.47	0.49
7:I:253:UNK:O	7:I:254:UNK:HG2	2.13	0.49
1:A:807:G:C6	1:A:809:G:C2	3.00	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
2:B:168:ARG:HH22	17:U:87:CYS:C	2.15	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
18:V:49:Y5P:O5'	18:V:49:Y5P:H6	2.11	0.49
8:J:91:TYR:OH	8:J:160:ILE:HG23	2.13	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
1:A:97:C:H5'	1:A:98:A:OP2	2.13	0.49
3:C:110:LEU:HD22	3:C:119:ILE:HG12	1.94	0.49
3:C:37:ASN:HD22	3:C:37:ASN:H	1.60	0.49
1:A:765:A:HO2'	1:A:767:U:H5	1.59	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
1:A:28:U:H2'	1:A:29:A:C8	2.46	0.49
16:T:65:UNK:HG2	16:T:67:UNK:HB1	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:A:H8	1:A:579:A:OP1	1.95	0.49
18:V:54:Y5P:H4A	18:V:55:Y5P:C4	2.43	0.49
7:I:316:PHE:CE1	7:I:370:LEU:HD21	2.48	0.49
6:G:152:CYS:SG	6:G:219:VAL:HB	2.53	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
13:P:100:HIS:CD2	13:P:102:MET:H	2.30	0.49
1:A:357:G:H5'	9:K:98:GLN:HE21	1.78	0.49
1:A:824:G:N2	1:A:827:A:H61	2.10	0.49
1:A:4:C:N4	4:E:427:ARG:HD3	2.28	0.49
1:A:228:G:H2'	1:A:229:U:C6	2.48	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
5:F:92:ASN:HD22	5:F:93:ILE:H	1.60	0.48
18:Y:61:Y5P:H4A	18:Y:62:Y5P:H4	1.95	0.48
18:V:23:Y5P:C4	18:V:24:Y5P:H4	2.39	0.48
3:C:37:ASN:ND2	3:C:37:ASN:H	2.12	0.48
1:A:624:U:H4'	1:A:625:U:H4'	1.95	0.48
1:A:195:G:C4	1:A:208:A:C2	3.00	0.48
1:A:928:A:H5'	1:A:930:G:N7	2.28	0.48
13:P:73:ILE:O	13:P:77:ILE:HG13	2.12	0.48
7:I:323:ARG:HB3	7:I:327:HIS:CD2	2.48	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
18:Y:25:Y5P:H2'	18:Y:26:Y5P:C6	2.40	0.48
1:A:96:U:O2'	13:P:38:HIS:ND1	2.43	0.48
1:A:917:C:H5'	1:A:918:A:OP1	2.13	0.48
18:V:12:Y5P:H4A	18:V:13:Y5P:C4	2.40	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
8:J:161:GLN:HG2	8:J:170:MET:HE2	1.95	0.48
14:Q:57:GLN:NE2	14:Q:57:GLN:O	2.46	0.48
1:A:959:U:H4'	1:A:960:A:O5'	2.11	0.48
1:A:124:A:H4'	1:A:125:U:O5'	2.14	0.48
7:I:358:THR:HG23	7:I:361:GLU:H	1.78	0.48
2:B:140:ILE:HB	2:B:189:PRO:HA	1.96	0.48
3:C:92:LEU:HD21	3:C:147:TYR:HE2	1.79	0.48
15:R:120:PHE:CD1	15:R:120:PHE:N	2.81	0.48
18:Y:55:Y5P:C6	18:Y:58:Y5P:H5	2.44	0.48
5:F:71:PRO:HB3	12:O:97:GLU:O	2.13	0.48
3:C:80:ASP:HB3	3:C:81:HIS:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:105:ALA:HB3	3:C:122:LEU:HB3	1.96	0.47
2:B:140:ILE:HD12	2:B:140:ILE:H	1.79	0.47
18:V:36:P5P:H6	18:V:37:Y5P:H4	1.94	0.47
1:A:831:A:H2'	1:A:832:G:C8	2.49	0.47
1:A:276:U:H2'	1:A:277:A:H8	1.79	0.47
7:I:104:ILE:O	7:I:108:ILE:HG13	2.14	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:274:GLU:HG2	7:I:283:GLU:HG2	1.96	0.47
1:A:159:C:H2'	1:A:160:C:H5'	1.95	0.47
4:E:332:LEU:HD12	4:E:333:TYR:N	2.29	0.47
2:B:235:VAL:HG21	2:B:248:PHE:CE1	2.49	0.47
7:I:271:SER:OG	7:I:352:ALA:O	2.31	0.47
6:G:190:GLU:O	6:G:194:LYS:HG2	2.14	0.47
7:I:318:LEU:HD23	7:I:353:LEU:HD11	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
7:I:290:GLY:CA	7:I:328:ASP:HB2	2.45	0.47
1:A:358:U:H2'	1:A:359:U:H6	1.77	0.47
1:A:819:A:P	6:G:93:LYS:HZ3	2.38	0.47
9:K:128:ILE:O	9:K:132:THR:OG1	2.29	0.47
18:V:8:Y5P:N3	18:V:14:Y5P:C5	2.69	0.47
12:O:126:LEU:HB3	12:O:171:LEU:HD21	1.96	0.47
7:I:275:GLY:N	7:I:348:ALA:HB2	2.30	0.47
1:A:858:C:H42	1:A:912:A:H61	1.62	0.47
18:V:36:P5P:C6	18:V:37:Y5P:H4	2.44	0.47
1:A:423:U:H2'	1:A:424:G:C8	2.49	0.47
15:R:104:LYS:HD3	15:R:104:LYS:HA	1.62	0.47
1:A:87:U:H2'	1:A:88:C:C6	2.49	0.47
18:V:32:Y5P:H4A	18:V:33:Y5P:H4	1.97	0.47
8:J:180:LEU:HD23	8:J:181:PRO:HD2	1.95	0.47
6:G:71:THR:HG23	7:I:253:UNK:CG	2.45	0.47
1:A:787:A:H2'	1:A:788:G:C8	2.49	0.47
6:G:147:GLN:HG3	6:G:151:ASN:HD21	1.80	0.47
18:Y:34:P5P:H8	18:Y:34:P5P:O5'	2.14	0.47
1:A:546:U:O2'	1:A:547:A:H5'	2.15	0.47
9:K:138:ALA:HB1	9:K:172:LEU:HB2	1.95	0.47
8:J:102:LEU:HB3	8:J:104:ILE:HG13	1.96	0.47
1:A:653:A:H2'	1:A:654:A:N7	2.30	0.47
18:V:12:Y5P:C4	18:V:13:Y5P:H4	2.39	0.47
3:C:72:HIS:CD2	3:C:74:GLY:H	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:U:35:LEU:O	17:U:39:ILE:HG12	2.15	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
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
13:P:100:HIS:HB3	13:P:103:MET:HG3	1.96	0.47
1:A:357:G:N2	9:K:100:GLN:HE22	2.12	0.47
14:Q:55:LEU:HB2	14:Q:57:GLN:HB2	1.96	0.47
7:I:119:LYS:HA	7:I:122:ARG:HD2	1.97	0.47
7:I:94:GLU:HB2	7:I:99:PHE:CE2	2.50	0.47
1:A:689:G:H5'	4:E:91:THR:HG22	1.95	0.47
18:V:63:Y5P:H2'	18:V:64:Y5P:H6	1.97	0.47
1:A:317:A:H2	1:A:318:C:H5	1.62	0.47
11:N:80:ARG:HD2	11:N:86:ARG:HH12	1.80	0.47
4:E:325:ARG:HH21	4:E:430:THR:C	2.17	0.47
7:I:206:LEU:HA	7:I:206:LEU:HD23	1.77	0.47
1:A:956:G:H2'	1:A:957:A:O4'	2.15	0.47
4:E:162:LYS:O	4:E:166:GLU:HG2	2.15	0.47
7:I:323:ARG:HB3	7:I:327:HIS:HD2	1.80	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:373:ALA:O	7:I:375:PRO:HD3	2.15	0.46
1:A:158:C:H2'	1:A:159:C:C6	2.50	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
11:N:70:VAL:O	11:N:74:GLU:HG2	2.15	0.46
7:I:127:HIS:HD2	7:I:129:GLU:H	1.63	0.46
1:A:409:G:H4'	1:A:939:A:H4'	1.96	0.46
2:B:141:ILE:HB	2:B:163:GLU:CD	2.35	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
1:A:815:U:H2'	1:A:816:U:C6	2.50	0.46
15:R:89:THR:HG21	15:R:91:CYS:SG	2.55	0.46
7:I:252:UNK:HG2	7:I:252:UNK:O	2.16	0.46
40:A:7154:HOH:O	18:V:29:Y5P:C4	2.59	0.46
8:J:76:LEU:O	8:J:97:LEU:HB2	16.42	0.46
1:A:127:A:H4'	1:A:128:C:OP2	2.15	0.46
1:A:498:U:H5'	1:A:499:C:OP2	2.15	0.46
12:O:178:VAL:O	12:O:182:ILE:HG12	2.15	0.46
1:A:391:U:H4'	12:O:156:PHE:CE1	2.50	0.46
1:A:344:G:H1	9:K:121:ASN:HB2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:117:LEU:HA	2:B:117:LEU:HD23	1.78	0.46
4:E:380:LEU:HD12	4:E:381:PRO:HD2	1.98	0.46
1:A:454:A:H2'	1:A:456:A:H5''	1.97	0.46
6:G:104:LYS:HD3	6:G:104:LYS:HA	1.70	0.46
2:B:230:LEU:HA	2:B:230:LEU:HD23	1.74	0.46
1:A:899:C:C3'	1:A:900:A:H4'	2.46	0.46
1:A:42:A:HO2'	1:A:43:U:P	2.37	0.46
2:B:161:CYS:SG	2:B:253:GLN:HA	2.56	0.46
1:A:316:C:H2'	1:A:318:C:C5	2.50	0.46
7:I:94:GLU:HB2	7:I:99:PHE:HE2	1.81	0.46
1:A:503:A:H2'	1:A:503:A:N3	2.31	0.46
14:Q:36:ASP:HA	14:Q:37:PRO:HD3	1.60	0.46
1:A:899:C:C2'	1:A:900:A:H4'	2.46	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
1:A:649:U:H3'	1:A:650:A:H5''	1.96	0.46
6:G:238:HIS:CE1	9:K:126:THR:HB	2.50	0.46
1:A:896:A:H3'	1:A:897:C:H4'	1.97	0.46
18:Y:44:Y5P:H6	18:Y:44:Y5P:O5'	2.16	0.46
4:E:289:THR:HG23	4:E:331:ASP:O	2.16	0.46
18:V:42:Y5P:H4A	18:V:43:Y5P:H4	1.98	0.46
12:O:80:VAL:HG23	12:O:83:ILE:HD11	1.98	0.45
2:B:173:GLY:O	2:B:177:ASN:N	2.46	0.45
1:A:59:C:N3	8:J:133:GLN:HB3	150.95	0.45
18:Y:3:Y5P:O5'	18:Y:3:Y5P:H6	2.16	0.45
7:I:87:HIS:O	7:I:91:MET:HG2	2.17	0.45
1:A:303:U:OP2	1:A:398:G:N1	2.44	0.45
4:E:332:LEU:HD12	4:E:333:TYR:H	1.82	0.45
18:Y:25:Y5P:C4	18:Y:26:Y5P:C5	2.94	0.45
1:A:580:U:O4	8:J:131:ARG:NH1	2.50	0.45
1:A:375:A:H2'	1:A:376:C:H6	1.81	0.45
9:K:176:SER:HB2	17:U:13:MET:HG2	1.99	0.45
1:A:487:C:H5'	1:A:488:A:OP2	2.16	0.45
1:A:442:A:H2'	1:A:443:U:H5'	1.97	0.45
6:G:190:GLU:HB3	6:G:194:LYS:HE2	1.99	0.45
15:R:117:ILE:HA	15:R:117:ILE:HD13	1.59	0.45
7:I:203:LYS:HA	7:I:219:TYR:CD2	2.51	0.45
17:U:78:LYS:HD2	17:U:80:ARG:HH21	1.82	0.45
5:F:29:LEU:HG	5:F:78:MET:HE2	1.96	0.45
1:A:739:A:N3	1:A:739:A:H2'	2.31	0.45
1:A:752:A:H3'	1:A:753:A:C5'	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:140:ASN:HB3	6:G:143:THR:HG22	1.99	0.45
18:Y:68:Y5P:H4A	18:Y:69:Y5P:C5	2.47	0.45
12:O:164:ARG:HD2	12:O:188:ILE:HD13	1.99	0.45
9:K:102:VAL:HG12	9:K:106:HIS:HA	1.98	0.45
7:I:85:LYS:HE2	7:I:99:PHE:HB3	1.98	0.45
11:N:83:CYS:SG	11:N:86:ARG:HB2	2.56	0.45
1:A:548:G:C2	1:A:549:A:C8	3.05	0.45
1:A:961:C:C2'	1:A:962:C:H5'	2.47	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
10:L:32:THR:O	10:L:36:MET:HG3	2.16	0.45
1:A:262:C:H2'	1:A:263:G:C8	2.51	0.45
2:B:170:PHE:CE1	2:B:174:LEU:HD23	2.52	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
1:A:954:U:O2	1:A:956:G:H5''	2.16	0.45
18:Y:70:Y5P:H4A	18:Y:71:Y5P:H4	1.98	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
2:B:105:LEU:HA	2:B:105:LEU:HD23	1.84	0.45
12:O:133:LEU:HD23	12:O:133:LEU:HA	1.72	0.45
18:V:43:Y5P:C2	18:V:44:Y5P:C5	2.95	0.45
15:R:120:PHE:HD1	15:R:120:PHE:N	2.14	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
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
3:C:73:THR:HG23	8:J:169:ALA:HB2	1.99	0.45
18:Y:62:Y5P:H2'	18:Y:63:Y5P:C6	2.47	0.45
1:A:516:C:O2'	1:A:517:A:H5'	2.16	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
14:Q:106:LEU:HD23	14:Q:106:LEU:HA	1.80	0.45
9:K:150:ARG:HB3	9:K:175:ILE:HD11	1.99	0.45
1:A:612:U:H5'	1:A:613:A:OP1	2.16	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
1:A:647:A:H3'	1:A:648:A:H5'	1.98	0.45
6:G:118:VAL:HG23	6:G:206:SER:HB2	1.98	0.44
5:F:121:LYS:HD3	5:F:123:ARG:NH2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:891:C:H4'	1:A:891:C:OP1	2.15	0.44
1:A:538:C:H1'	1:A:540:U:C5	2.51	0.44
4:E:317:HIS:HD2	4:E:319:ALA:HB3	1.81	0.44
1:A:50:U:H2'	1:A:51:G:H8	1.82	0.44
4:E:363:ALA:O	4:E:367:SER:N	2.51	0.44
1:A:746:A:H2'	1:A:747:C:O4'	2.17	0.44
18:V:43:Y5P:C4	18:V:44:Y5P:H4	2.47	0.44
1:A:792:U:H4'	7:I:389:ARG:HG3	2.00	0.44
11:N:80:ARG:HD2	11:N:86:ARG:NH1	2.32	0.44
1:A:660:A:H2'	1:A:661:U:O4'	2.18	0.44
15:R:103:LYS:HG2	15:R:103:LYS:H	1.49	0.44
4:E:425:LEU:HD23	4:E:425:LEU:HA	1.67	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
1:A:899:C:H4'	1:A:899:C:OP1	2.18	0.44
5:F:117:LEU:HD23	5:F:117:LEU:HA	1.87	0.44
1:A:637:A:H4'	1:A:637:A:OP1	2.16	0.44
14:Q:27:LYS:HG3	14:Q:50:PHE:HE1	1.83	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
14:Q:65:LEU:HB2	14:Q:85:ILE:HD11	2.00	0.44
11:N:79:PRO:O	11:N:82:SER:OG	2.15	0.44
4:E:151:ASN:OD1	4:E:151:ASN:N	2.51	0.44
18:Y:68:Y5P:C4	18:Y:69:Y5P:C5	2.96	0.44
9:K:161:LEU:HD23	9:K:161:LEU:HA	1.73	0.44
2:B:235:VAL:HG21	2:B:248:PHE:HE1	1.82	0.44
14:Q:13:VAL:CG2	14:Q:66:LEU:HB2	2.48	0.44
1:A:200:A:OP1	1:A:200:A:H8	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
9:K:112:ALA:CB	9:K:137:ALA:HB2	2.48	0.44
6:G:48:LYS:NZ	7:I:319:HIS:O	2.46	0.44
7:I:214:LEU:HA	7:I:214:LEU:HD23	1.85	0.44
18:Y:6:Y5P:C4	18:Y:7:Y5P:H4	2.45	0.44
11:N:58:ARG:HH11	11:N:58:ARG:HB3	1.83	0.44
8:J:120:LEU:HA	8:J:120:LEU:HD23	1.78	0.44
1:A:804:A:N7	11:N:85:VAL:HB	2.33	0.44
1:A:602:A:O2'	4:E:136:ARG:NH2	2.51	0.44
1:A:902:C:H4'	1:A:903:C:H5'	1.99	0.44
12:O:96:LEU:HD13	12:O:104:LYS:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:33:LEU:HA	10:L:33:LEU:HD23	1.65	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
4:E:164:ASP:O	4:E:168:VAL:HG23	2.18	0.44
1:A:566:U:H3	1:A:686:A:H62	1.66	0.44
3:C:128:PRO:HA	3:C:129:PRO:HD3	1.89	0.44
2:B:79:SER:OG	2:B:81:ARG:N	2.45	0.44
18:Y:70:Y5P:C5	18:Y:71:Y5P:H5	2.48	0.43
9:K:151:VAL:HG12	9:K:177:ILE:HG23	1.99	0.43
1:A:453:U:H2'	1:A:454:A:H5"	1.99	0.43
1:A:370:A:O2'	15:R:109:THR:OG1	2.23	0.43
6:G:73:LEU:O	6:G:74:ILE:HD13	2.18	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
7:I:390:ARG:HD2	7:I:391:LYS:H	1.83	0.43
1:A:298:G:C2	1:A:299:U:C6	3.06	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
1:A:844:C:H5'	19:X:18:Y5P:H4A	2.00	0.43
1:A:484:C:P	10:L:34:ASN:HD22	2.41	0.43
1:A:182:A:C6	1:A:183:A:C6	3.06	0.43
6:G:182:LEU:HD23	6:G:182:LEU:HA	1.84	0.43
8:J:123:SER:OG	8:J:124:VAL:N	2.51	0.43
4:E:141:TRP:H	4:E:145:ASN:ND2	2.14	0.43
13:P:54:TYR:CD2	13:P:66:VAL:HG22	2.54	0.43
1:A:641:A:C2	1:A:642:G:C4	3.07	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
2:B:164:TYR:CD2	7:I:149:PHE:HA	2.53	0.43
1:A:757:U:H2'	1:A:758:U:O4'	2.18	0.43
4:E:88:SER:HA	4:E:91:THR:OG1	2.18	0.43
13:P:104:ILE:O	13:P:107:ALA:HB3	2.19	0.43
1:A:267:A:H2'	1:A:268:A:O4'	2.17	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
4:E:203:LEU:HD11	4:E:268:PHE:HB3	1.99	0.43
1:A:635:C:H5"	2:B:213:LYS:NZ	2.32	0.43
3:C:135:LEU:HD23	3:C:135:LEU:HA	1.73	0.43
12:O:127:GLU:O	12:O:131:VAL:HG23	2.18	0.43
18:Y:8:Y5P:C4	18:Y:14:Y5P:H5	2.46	0.43
13:P:107:ALA:O	13:P:111:ARG:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:GLU:HA	2:B:163:GLU:OE1	2.19	0.43
9:K:88:ALA:HB3	9:K:151:VAL:HG23	2.00	0.43
6:G:140:ASN:ND2	6:G:143:THR:H	2.17	0.43
18:Y:39:Y5P:H4A	18:Y:40:Y5P:H4	2.00	0.43
15:R:57:ASN:HA	15:R:58:PRO:HD3	1.71	0.43
1:A:563:U:H5'	1:A:564:A:OP2	2.19	0.43
12:O:225:LYS:O	12:O:229:ARG:HG3	2.18	0.43
18:Y:30:Y5P:C4	18:Y:31:Y5P:H4	2.41	0.43
15:R:133:ASP:HB3	15:R:134:PRO:CD	2.48	0.43
1:A:204:U:H2'	1:A:205:U:C6	2.54	0.43
6:G:41:TYR:HA	6:G:73:LEU:O	2.18	0.43
1:A:901:A:H4'	1:A:902:C:OP2	2.18	0.43
1:A:338:U:H2'	1:A:339:A:H8	1.83	0.43
18:Y:37:Y5P:HB	18:Y:38:Y5P:H6	2.01	0.43
10:L:102:LEU:HD23	10:L:102:LEU:HA	1.85	0.43
4:E:305:MET:HB3	4:E:305:MET:HE3	1.93	0.43
1:A:389:A:H2'	1:A:390:A:H5'	2.01	0.43
2:B:190:ASP:O	2:B:217:PRO:HD2	2.19	0.43
1:A:670:A:H1'	6:G:36:ARG:HD2	2.00	0.43
1:A:817:G:H5''	6:G:104:LYS:HG2	2.00	0.43
1:A:229:U:O2'	1:A:236:A:N1	2.36	0.43
11:N:57:LEU:HG	11:N:57:LEU:H	1.55	0.43
7:I:168:LYS:O	7:I:172:VAL:HG23	2.18	0.43
1:A:11:G:H4'	4:E:237:ARG:CZ	2.48	0.43
18:Y:68:Y5P:C5	18:Y:69:Y5P:H5	2.48	0.43
1:A:197:A:H2'	1:A:198:C:O4'	2.19	0.43
2:B:168:ARG:HA	2:B:168:ARG:HD3	1.60	0.43
8:J:161:GLN:HG2	8:J:170:MET:CE	2.48	0.43
1:A:881:A:H3'	1:A:882:A:C8	2.53	0.43
1:A:432:A:H4'	1:A:433:U:C5'	2.48	0.43
1:A:285:C:C5	10:L:42:PRO:HB2	2.53	0.43
1:A:677:C:H2'	1:A:678:G:O4'	2.19	0.43
4:E:173:VAL:O	4:E:177:GLU:HG2	2.19	0.43
2:B:57:LEU:HA	2:B:60:ARG:HD2	2.01	0.43
14:Q:93:ASP:HA	14:Q:94:PRO:HD2	1.84	0.43
1:A:69:G:H2'	1:A:70:U:C6	2.54	0.43
7:I:387:GLY:O	7:I:388:ALA:HB3	2.18	0.43
1:A:692:U:H2'	1:A:693:A:O4'	2.19	0.43
7:I:148:HIS:HB3	7:I:156:GLN:NE2	2.34	0.43
14:Q:71:VAL:HA	14:Q:72:PRO:HD3	1.93	0.43
7:I:397:ARG:NH2	18:V:33:Y5P:OP2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:151:SER:O	8:J:155:VAL:HG23	2.19	0.43
1:A:217:U:H2'	1:A:218:A:H8	1.83	0.43
13:P:55:ASP:HA	13:P:56:PRO:HD3	1.82	0.43
4:E:223:LEU:HD23	4:E:223:LEU:HA	1.81	0.43
3:C:123:VAL:HG21	3:C:155:LEU:HG	2.01	0.43
1:A:520:G:C2	1:A:521:G:N7	2.87	0.43
7:I:314:LEU:HA	7:I:314:LEU:HD12	1.57	0.43
2:B:222:VAL:HG11	2:B:228:PRO:HB3	2.00	0.43
2:B:168:ARG:HG3	7:I:159:TYR:CE2	2.54	0.43
11:N:74:GLU:O	11:N:77:SER:HB2	2.19	0.43
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
5:F:58:HIS:CD2	5:F:89:ILE:HD11	2.54	0.42
1:A:622:U:H2'	1:A:623:C:C6	2.54	0.42
7:I:341:GLN:O	7:I:345:VAL:HG23	2.19	0.42
1:A:508:C:O5'	1:A:508:C:H6	2.02	0.42
13:P:116:ARG:O	13:P:120:LEU:HG	2.19	0.42
1:A:905:U:H2'	1:A:906:G:C8	2.54	0.42
1:A:947:G:H2'	1:A:948:U:H6	1.83	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
8:J:157:LEU:HA	8:J:157:LEU:HD23	1.82	0.42
1:A:87:U:H2'	1:A:88:C:H6	1.82	0.42
12:O:176:TYR:N	14:Q:89:GLY:O	2.46	0.42
2:B:166:HIS:CE1	7:I:153:THR:HA	2.54	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
13:P:54:TYR:HD2	13:P:66:VAL:HG22	1.85	0.42
7:I:371:LEU:H	7:I:371:LEU:HG	1.58	0.42
1:A:588:A:H1'	1:A:609:C:O2	2.19	0.42
1:A:76:U:H3'	1:A:77:G:O4'	2.18	0.42
14:Q:31:THR:HG21	14:Q:44:ASN:HB3	2.02	0.42
1:A:381:G:C6	1:A:382:U:C4	3.07	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
1:A:685:C:C4'	1:A:686:A:H5'	2.49	0.42
1:A:749:C:N4	1:A:750:G:C6	2.88	0.42
4:E:291:TYR:HE2	4:E:359:HIS:H	1.67	0.42
2:B:57:LEU:HB2	2:B:270:TYR:HE2	1.85	0.42
1:A:69:G:H2'	1:A:70:U:H6	1.85	0.42
7:I:223:ILE:O	7:I:227:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:52:ARG:HD3	6:G:52:ARG:HA	1.89	0.42
18:Y:24:Y5P:H4A	18:Y:25:Y5P:H4	2.01	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
3:C:149:CYS:HA	3:C:150:PRO:HD3	2.40	0.42
9:K:189:ARG:HA	9:K:190:PRO:HD3	1.85	0.42
1:A:634:C:O2'	1:A:650:A:N1	2.41	0.42
1:A:703:U:H2'	1:A:704:U:H6	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
10:L:107:VAL:O	10:L:131:ASP:HB2	2.20	0.42
6:G:195:LYS:N	6:G:204:LYS:HZ1	2.17	0.42
2:B:252:PHE:O	2:B:256:ILE:HG12	2.20	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
1:A:255:G:O6	10:L:74:ASN:HB2	2.20	0.42
5:F:86:ILE:H	5:F:86:ILE:HG13	1.70	0.42
18:V:13:Y5P:OP2	18:V:13:Y5P:H6	2.20	0.42
1:A:578:G:OP1	8:J:128:LYS:NZ	2.38	0.42
17:U:72:ILE:HA	17:U:72:ILE:HD13	1.82	0.42
2:B:161:CYS:HB3	2:B:256:ILE:HG21	2.01	0.42
7:I:119:LYS:HG2	7:I:122:ARG:HD2	2.01	0.42
7:I:100:THR:HG22	7:I:101:GLN:H	1.84	0.42
19:X:16:Y5P:H2'	19:X:17:Y5P:O4'	2.20	0.42
10:L:58:LEU:HB2	10:L:110:VAL:HG23	2.02	0.42
17:U:26:LEU:O	17:U:29:ILE:HB	2.20	0.42
11:N:36:ARG:HB3	11:N:40:ARG:NH2	2.35	0.42
18:V:9:Y5P:H5	18:V:23:Y5P:H4A	2.01	0.42
5:F:94:VAL:HG12	5:F:95:LYS:O	2.20	0.42
1:A:159:C:C2'	1:A:160:C:H5'	2.49	0.42
9:K:161:LEU:HG	17:U:23:TYR:CE1	2.54	0.42
18:Y:42:Y5P:HB	18:Y:43:Y5P:HB2	2.02	0.42
3:C:88:GLU:HG3	3:C:147:TYR:CZ	2.54	0.42
1:A:546:U:H2'	1:A:547:A:C8	2.55	0.42
1:A:896:A:C5	1:A:897:C:H1'	2.55	0.42
1:A:617:C:H2'	1:A:618:G:O4'	2.20	0.42
14:Q:24:LYS:HB3	14:Q:53:ASP:O	2.19	0.42
2:B:202:PHE:CD1	2:B:202:PHE:N	2.88	0.42
18:V:48:Y5P:OP1	18:V:48:Y5P:H6	2.19	0.42
4:E:140:LEU:HD11	4:E:160:ARG:HG3	2.02	0.42
1:A:882:A:H2'	1:A:883:C:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:358:THR:HG22	4:E:360:GLN:H	1.84	0.42
12:O:74:LEU:HD12	12:O:77:TYR:CD2	2.55	0.42
1:A:199:G:H5'	1:A:200:A:OP2	2.19	0.42
3:C:58:ALA:O	3:C:61:TYR:HB2	2.20	0.42
2:B:262:LYS:O	2:B:266:VAL:HG23	2.19	0.42
1:A:557:G:C6	1:A:715:G:C6	3.08	0.42
7:I:229:LEU:HA	7:I:229:LEU:HD23	1.85	0.42
3:C:94:LYS:NZ	4:E:92:LYS:HB2	2.35	0.42
18:Y:29:Y5P:H2'	18:Y:30:Y5P:O4'	2.20	0.42
8:J:102:LEU:HA	8:J:102:LEU:HD12	1.93	0.42
7:I:266:UNK:HG2	7:I:268:MET:CB	2.50	0.42
9:K:67:PRO:HD3	17:U:13:MET:SD	2.60	0.42
1:A:276:U:H2'	1:A:277:A:C8	2.55	0.41
14:Q:40:LEU:HD12	14:Q:40:LEU:HA	1.84	0.41
1:A:385:C:H2'	1:A:386:U:H6	1.84	0.41
19:X:23:Y5P:H2'	19:X:24:Y5P:H5	2.02	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
2:B:219:VAL:HA	2:B:233:TYR:O	2.20	0.41
1:A:55:G:H2'	1:A:56:U:O4'	2.20	0.41
9:K:154:LYS:HG3	9:K:180:ASN:O	2.20	0.41
10:L:39:LEU:HA	10:L:39:LEU:HD22	1.62	0.41
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
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
1:A:903:C:H2'	1:A:904:A:C8	2.56	0.41
2:B:71:PHE:CE1	2:B:262:LYS:HG2	2.55	0.41
11:N:91:CYS:HB3	11:N:94:THR:HG22	2.02	0.41
7:I:136:ARG:HH21	7:I:212:GLU:HA	1.84	0.41
15:R:68:LEU:O	15:R:71:LYS:HB2	2.20	0.41
15:R:71:LYS:HA	15:R:71:LYS:HD3	1.81	0.41
1:A:114:A:N1	1:A:136:C:O2'	2.47	0.41
9:K:175:ILE:O	17:U:14:VAL:HG13	2.20	0.41
1:A:349:A:H2'	1:A:350:A:C8	2.55	0.41
4:E:264:ARG:HD2	4:E:268:PHE:CE2	2.56	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
1:A:358:U:H5"	9:K:89:HIS:ND1	2.35	0.41
1:A:555:C:C4	1:A:556:U:C4	3.09	0.41
4:E:155:GLN:H	4:E:155:GLN:HG3	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:V:9:Y5P:H4	18:V:23:Y5P:H5	2.03	0.41
4:E:187:VAL:O	4:E:188:LYS:HG3	2.21	0.41
3:C:69:LEU:HA	3:C:69:LEU:HD23	1.71	0.41
14:Q:98:LYS:HE3	14:Q:109:PRO:HD3	2.03	0.41
1:A:209:C:H2'	1:A:210:U:C6	2.56	0.41
1:A:520:G:C2	1:A:521:G:C8	3.09	0.41
1:A:19:C:H6	1:A:19:C:O5'	2.03	0.41
1:A:250:A:H2'	1:A:251:C:H6	1.85	0.41
13:P:91:LEU:HA	13:P:91:LEU:HD23	1.84	0.41
1:A:26:A:H2'	1:A:27:U:C6	2.55	0.41
11:N:93:MET:HG2	11:N:93:MET:H	1.48	0.41
10:L:59:LYS:HB3	10:L:59:LYS:HE2	1.91	0.41
2:B:188:LEU:HD23	2:B:188:LEU:HA	1.83	0.41
1:A:904:A:H2'	1:A:905:U:H6	1.84	0.41
1:A:939:A:H2'	1:A:940:C:H6	1.83	0.41
1:A:488:A:H5"	1:A:488:A:H8	1.84	0.41
1:A:285:C:N4	10:L:43:LYS:O	2.53	0.41
1:A:643:G:O2'	1:A:651:G:OP2	2.26	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
1:A:128:C:H2'	1:A:129:G:O4'	2.20	0.41
7:I:358:THR:HG22	7:I:361:GLU:OE1	2.21	0.41
6:G:138:GLU:HG3	6:G:213:PHE:CZ	2.55	0.41
17:U:51:ARG:HG3	17:U:54:ARG:NH1	2.35	0.41
4:E:352:GLY:O	4:E:355:ARG:HB2	2.21	0.41
1:A:670:A:N7	40:A:7124:HOH:O	2.37	0.41
1:A:582:G:H5'	1:A:806:A:N1	2.36	0.41
7:I:169:LEU:HD12	7:I:229:LEU:HD23	2.03	0.41
17:U:28:ARG:O	17:U:32:MET:HB2	2.21	0.41
2:B:142:LEU:HD23	2:B:192:ILE:HD13	2.02	0.41
12:O:112:LEU:HD12	12:O:112:LEU:HA	1.81	0.41
3:C:113:ARG:O	3:C:116:GLN:HG2	2.21	0.41
1:A:85:G:H2'	1:A:86:A:C8	2.56	0.41
12:O:126:LEU:HD13	12:O:171:LEU:HD23	2.03	0.41
1:A:686:A:H4'	1:A:686:A:OP2	2.20	0.41
5:F:39:LEU:CD2	5:F:66:VAL:HG22	2.51	0.41
7:I:276:LYS:H	7:I:347:LEU:HD23	1.85	0.41
1:A:836:G:H2'	1:A:837:C:C6	2.56	0.41
10:L:69:LYS:NZ	10:L:77:ASN:HB3	2.36	0.41
4:E:132:ILE:HG12	4:E:132:ILE:H	1.62	0.41
1:A:65:C:H6	1:A:65:C:H2'	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:80:ARG:O	11:N:86:ARG:HD2	2.21	0.41
7:I:228:ARG:NH1	17:U:85:GLN:HG2	2.36	0.41
12:O:168:LEU:HD23	12:O:168:LEU:HA	1.79	0.41
2:B:92:HIS:HE1	2:B:223:ASP:OD2	2.04	0.41
5:F:89:ILE:O	5:F:90:ARG:HB2	2.20	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
2:B:88:VAL:HG11	2:B:120:THR:HG21	2.03	0.40
1:A:238:C:H2'	1:A:239:U:C6	2.56	0.40
14:Q:63:ILE:HA	14:Q:63:ILE:HD13	1.86	0.40
7:I:143:ASP:OD1	7:I:143:ASP:N	2.45	0.40
1:A:724:U:O4	6:G:98:MET:HG2	2.20	0.40
18:Y:25:Y5P:N3	18:Y:26:Y5P:H4	2.34	0.40
8:J:104:ILE:O	8:J:105:SER:OG	2.39	0.40
17:U:50:ARG:HD2	17:U:50:ARG:HA	1.73	0.40
12:O:96:LEU:HD23	12:O:96:LEU:HA	1.77	0.40
1:A:577:C:O3'	8:J:128:LYS:HD2	2.21	0.40
6:G:199:VAL:HG13	6:G:203:GLU:OE1	2.20	0.40
1:A:521:G:C2	1:A:522:A:C4	3.09	0.40
1:A:458:C:H2'	1:A:458:C:H6	1.70	0.40
6:G:122:GLN:HE21	6:G:210:LEU:HD13	1.86	0.40
5:F:10:LEU:HD12	5:F:64:PHE:CD1	2.56	0.40
17:U:41:ARG:NH2	17:U:58:GLU:OE2	2.51	0.40
15:R:125:TYR:CE2	17:U:4:HIS:HB3	2.51	0.40
19:X:14:Y5P:H2'	19:X:15:Y5P:O4'	2.21	0.40
6:G:52:ARG:NH1	7:I:364:TRP:HZ3	2.20	0.40
7:I:228:ARG:CD	17:U:85:GLN:HE21	2.16	0.40
1:A:646:C:C2	1:A:648:A:C6	3.10	0.40
5:F:8:LEU:HD11	5:F:25:THR:HG21	2.03	0.40
1:A:752:A:H8	1:A:753:A:C5'	2.35	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
1:A:664:U:OP1	8:J:113:ARG:NH2	2.44	0.40
4:E:245:VAL:HB	4:E:271:ALA:HB1	2.04	0.40
2:B:92:HIS:CE1	2:B:223:ASP:OD2	2.75	0.40
1:A:109:G:C6	1:A:110:U:N3	2.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	7	49
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%)	21	67
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%)	46	83
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	59	90

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	J	179	GLN
8	J	185	ARG
14	Q	95	VAL
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%)	168 (90%)	19 (10%)	9	42
3	C	115/142 (81%)	103 (90%)	12 (10%)	9	42
4	E	273/351 (78%)	245 (90%)	28 (10%)	9	42
5	F	108/109 (99%)	101 (94%)	7 (6%)	21	63
6	G	181/205 (88%)	172 (95%)	9 (5%)	30	70
7	I	250/317 (79%)	227 (91%)	23 (9%)	11	48
8	J	119/181 (66%)	108 (91%)	11 (9%)	11	48
9	K	102/151 (68%)	94 (92%)	8 (8%)	16	55
10	L	92/116 (79%)	81 (88%)	11 (12%)	6	33
11	N	92/114 (81%)	71 (77%)	21 (23%)	1	8
12	O	159/205 (78%)	148 (93%)	11 (7%)	19	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	P	97/113 (86%)	91 (94%)	6 (6%)	23	65
14	Q	94/114 (82%)	81 (86%)	13 (14%)	4	28
15	R	89/127 (70%)	79 (89%)	10 (11%)	7	38
17	U	77/78 (99%)	64 (83%)	13 (17%)	2	18
20	a	222/272 (82%)	208 (94%)	14 (6%)	22	64
21	b	113/162 (70%)	104 (92%)	9 (8%)	15	54
22	c	152/155 (98%)	137 (90%)	15 (10%)	10	44
23	d	149/168 (89%)	137 (92%)	12 (8%)	15	54
25	f	86/160 (54%)	76 (88%)	10 (12%)	7	36
26	g	290/334 (87%)	271 (93%)	19 (7%)	21	63
27	h	95/345 (28%)	90 (95%)	5 (5%)	28	69
28	i	86/93 (92%)	80 (93%)	6 (7%)	19	60
29	j	182/184 (99%)	172 (94%)	10 (6%)	27	68
30	k	249/289 (86%)	229 (92%)	20 (8%)	15	54
31	m	100/102 (98%)	91 (91%)	9 (9%)	12	49
32	n	66/174 (38%)	59 (89%)	7 (11%)	8	40
33	o	79/141 (56%)	73 (92%)	6 (8%)	16	56
34	p	168/225 (75%)	151 (90%)	17 (10%)	9	43
All	All	4072/5360 (76%)	3711 (91%)	361 (9%)	17	50

All (361) 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	144	VAL
2	B	153	LEU
2	B	159	ARG
2	B	168	ARG
2	B	176	THR
2	B	177	ASN
2	B	181	LEU

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Mol	Chain	Res	Type
2	B	190	ASP
2	B	192	ILE
2	B	206	VAL
2	B	235	VAL
2	B	249	CYS
2	B	250	ARG
3	C	37	ASN
3	C	38	ARG
3	C	41	ARG
3	C	44	VAL
3	C	54	GLU
3	C	71	LEU
3	C	104	LEU
3	C	112	ARG
3	C	115	ASN
3	C	125	ARG
3	C	152	HIS
3	C	167	ILE
4	E	89	PHE
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	156	THR
4	E	165	GLN
4	E	215	TYR
4	E	220	THR
4	E	226	ARG
4	E	234	LYS
4	E	239	ARG
4	E	242	ARG
4	E	247	VAL
4	E	264	ARG
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

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Mol	Chain	Res	Type
4	E	340	VAL
4	E	346	THR
4	E	367	SER
4	E	420	SER
5	F	13	MET
5	F	67	ASP
5	F	79	MET
5	F	83	SER
5	F	89	ILE
5	F	92	ASN
5	F	120	THR
6	G	85	VAL
6	G	109	SER
6	G	118	VAL
6	G	139	ARG
6	G	156	ILE
6	G	197	ARG
6	G	200	LEU
6	G	205	LEU
6	G	219	VAL
7	I	90	ASN
7	I	98	THR
7	I	99	PHE
7	I	153	THR
7	I	156	GLN
7	I	161	LEU
7	I	202	ILE
7	I	206	LEU
7	I	209	MET
7	I	215	SER
7	I	234	CYS
7	I	237	THR
7	I	293	ARG
7	I	301	TYR
7	I	303	LEU
7	I	331	CYS
7	I	338	ARG
7	I	353	LEU
7	I	357	VAL
7	I	366	ARG
7	I	371	LEU
7	I	372	THR

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Mol	Chain	Res	Type
7	I	377	VAL
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	166	GLU
9	K	65	TYR
9	K	75	LEU
9	K	98	GLN
9	K	128	ILE
9	K	151	VAL
9	K	153	VAL
9	K	176	SER
9	K	178	THR
10	L	39	LEU
10	L	52	THR
10	L	55	ARG
10	L	61	VAL
10	L	75	SER
10	L	77	ASN
10	L	95	ILE
10	L	110	VAL
10	L	114	ARG
10	L	118	LEU
10	L	127	ARG
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	92	VAL
11	N	93	MET

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Mol	Chain	Res	Type
11	N	94	THR
11	N	95	SER
11	N	98	ARG
11	N	107	SER
11	N	108	ARG
11	N	109	ILE
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	125	SER
12	O	130	ILE
12	O	159	MET
12	O	162	ASP
12	O	198	ARG
12	O	205	VAL
12	O	212	THR
12	O	216	ARG
13	P	10	ARG
13	P	31	PHE
13	P	35	VAL
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	40	LEU
14	Q	57	GLN
14	Q	59	THR
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	69	CYS

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Mol	Chain	Res	Type
15	R	76	LYS
15	R	77	ASN
15	R	91	CYS
15	R	108	ILE
15	R	117	ILE
15	R	120	PHE
15	R	126	LYS
15	R	139	ILE
17	U	14	VAL
17	U	41	ARG
17	U	46	GLU
17	U	47	LYS
17	U	49	CYS
17	U	52	ARG
17	U	60	CYS
17	U	68	MET
17	U	70	ARG
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	175	GLU
20	a	181	ARG
20	a	186	GLU
20	a	204	LEU
20	a	205	THR
20	a	228	ASN
20	a	238	SER
20	a	252	ILE
20	a	281	ASP
20	a	294	SER
21	b	6	LEU
21	b	12	ILE
21	b	17	ARG
21	b	20	ILE
21	b	30	LEU
21	b	45	VAL
21	b	48	ARG

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Mol	Chain	Res	Type
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	23	PHE
22	c	25	ASP
22	c	27	VAL
22	c	33	ASN
22	c	59	ASN
22	c	70	MET
22	c	82	SER
22	c	95	ASN
22	c	106	LEU
22	c	137	ARG
22	c	152	LEU
23	d	27	ARG
23	d	29	THR
23	d	30	ARG
23	d	41	ARG
23	d	92	GLU
23	d	115	ARG
23	d	166	THR
23	d	186	SER
23	d	191	ILE
23	d	196	LEU
23	d	197	VAL
23	d	198	VAL
25	f	113	LEU
25	f	123	CYS
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	98	LEU
26	g	107	LEU
26	g	138	CYS

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Mol	Chain	Res	Type
26	g	139	HIS
26	g	150	LEU
26	g	170	SER
26	g	178	ASP
26	g	196	HIS
26	g	231	ARG
26	g	246	LEU
26	g	265	ASN
26	g	300	TRP
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
27	h	302	LEU
27	h	308	ASN
27	h	332	ASP
27	h	348	CYS
27	h	387	ASN
28	i	11	MET
28	i	30	SER
28	i	50	ASP
28	i	55	HIS
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	136	TYR
29	j	150	PHE
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

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Mol	Chain	Res	Type
30	k	93	VAL
30	k	125	CYS
30	k	152	GLU
30	k	157	ASP
30	k	165	ILE
30	k	166	ARG
30	k	180	SER
30	k	192	LEU
30	k	199	ARG
30	k	204	THR
30	k	218	ARG
30	k	247	GLU
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	39	GLU
31	m	46	ILE
31	m	48	GLU
32	n	144	ARG
32	n	147	VAL
32	n	161	ARG
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	107	LEU
33	o	127	TYR
33	o	134	GLU
34	p	53	ASP
34	p	56	TRP
34	p	80	ASN
34	p	96	ARG
34	p	103	ASN

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Mol	Chain	Res	Type
34	p	108	CYS
34	p	113	LEU
34	p	123	LEU
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) 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
3	C	72	HIS
3	C	75	ASN
3	C	81	HIS
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	196	ASN
4	E	288	HIS
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

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Mol	Chain	Res	Type
6	G	238	HIS
7	I	87	HIS
7	I	127	HIS
7	I	156	GLN
7	I	221	GLN
7	I	319	HIS
7	I	367	GLN
8	J	83	HIS
9	K	98	GLN
10	L	34	ASN
10	L	35	GLN
10	L	37	HIS
10	L	77	ASN
12	O	147	HIS
12	O	153	HIS
12	O	201	HIS
13	P	28	ASN
13	P	50	GLN
13	P	61	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	85	GLN
20	a	75	GLN
20	a	76	ASN
20	a	107	GLN
20	a	109	GLN
20	a	213	ASN
20	a	222	GLN
20	a	223	HIS
20	a	228	ASN
20	a	247	HIS
20	a	276	ASN
20	a	307	HIS
22	c	35	ASN
22	c	51	ASN
22	c	59	ASN
22	c	63	GLN

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Mol	Chain	Res	Type
22	c	69	ASN
22	c	95	ASN
22	c	101	HIS
22	c	125	HIS
22	c	146	GLN
23	d	31	HIS
23	d	109	ASN
23	d	126	GLN
25	f	98	ASN
26	g	115	ASN
26	g	158	HIS
26	g	196	HIS
26	g	290	HIS
26	g	386	ASN
27	h	309	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	263	ASN
30	k	303	ASN
31	m	113	ASN
32	n	129	ASN
32	n	178	GLN
32	n	198	ASN
34	p	80	ASN
34	p	147	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	959/962 (99%)	329 (34%)	10 (1%)
18	V	0/64	-	-
18	Y	0/64	-	-
19	X	0/13	-	-
All	All	959/1103 (86%)	329 (34%)	10 (1%)

All (329) 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
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

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Mol	Chain	Res	Type
1	A	128	C
1	A	129	G
1	A	138	U
1	A	142	G
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

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Mol	Chain	Res	Type
1	A	247	G
1	A	251	C
1	A	253	G
1	A	257	U
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

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Mol	Chain	Res	Type
1	A	381	G
1	A	385	C
1	A	391	U
1	A	394	U
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

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Mol	Chain	Res	Type
1	A	539	A
1	A	540	U
1	A	541	C
1	A	542	C
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

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Mol	Chain	Res	Type
1	A	646	C
1	A	647	A
1	A	648	A
1	A	649	U
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

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Mol	Chain	Res	Type
1	A	753	A
1	A	765	A
1	A	766	C
1	A	771	A
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

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Mol	Chain	Res	Type
1	A	890	U
1	A	891	C
1	A	894	U
1	A	895	U
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

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

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Mol	Chain	Res	Type
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	V	1	18	15,16,20	3.48	3 (20%)	18,22,29	2.82	2 (11%)
18	Y5P	V	10	18	14,19,20	3.61	3 (21%)	18,26,29	2.85	2 (11%)
18	Y5P	V	11	18	14,19,20	4.79	3 (21%)	18,26,29	1.75	1 (5%)
18	Y5P	V	12	18	14,19,20	3.12	2 (14%)	18,26,29	2.99	2 (11%)
18	Y5P	V	13	18	14,19,20	4.67	3 (21%)	18,26,29	1.82	1 (5%)
18	Y5P	V	14	18	14,19,20	3.62	3 (21%)	18,26,29	2.88	3 (16%)
18	Y5P	V	15	18	14,19,20	3.58	3 (21%)	18,26,29	2.83	2 (11%)
18	Y5P	V	2	18	14,19,20	4.94	3 (21%)	18,26,29	1.79	1 (5%)
18	Y5P	V	21	18	14,19,20	3.71	3 (21%)	18,26,29	2.90	3 (16%)
18	Y5P	V	22	18	14,19,20	3.66	3 (21%)	18,26,29	2.84	2 (11%)
18	Y5P	V	23	18	14,19,20	3.60	3 (21%)	18,26,29	2.83	2 (11%)
18	Y5P	V	24	18	14,19,20	3.60	3 (21%)	18,26,29	2.84	2 (11%)
18	Y5P	V	25	18	14,19,20	4.80	3 (21%)	18,26,29	1.85	1 (5%)
18	Y5P	V	26	18	14,19,20	3.65	3 (21%)	18,26,29	2.86	2 (11%)
18	Y5P	V	27	18	14,19,20	3.60	3 (21%)	18,26,29	2.84	2 (11%)
18	Y5P	V	28	18	14,19,20	3.61	3 (21%)	18,26,29	2.84	2 (11%)
18	Y5P	V	29	18	14,19,20	3.54	3 (21%)	18,26,29	2.88	2 (11%)
18	Y5P	V	3	18	14,19,20	4.83	3 (21%)	18,26,29	1.76	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	Y5P	V	30	18	14,19,20	3.60	3 (21%)	18,26,29	2.87	2 (11%)
18	Y5P	V	31	18	14,19,20	3.57	3 (21%)	18,26,29	2.82	2 (11%)
18	Y5P	V	32	18	14,19,20	3.16	2 (14%)	18,26,29	2.94	2 (11%)
18	Y5P	V	33	18	14,19,20	4.05	2 (14%)	18,26,29	2.32	2 (11%)
18	P5P	V	34	18	16,23,24	1.53	2 (12%)	15,33,36	1.98	2 (13%)
18	P5P	V	35	18	16,23,24	0.86	0	15,33,36	0.83	0
18	P5P	V	36	18	16,23,24	0.91	1 (6%)	15,33,36	0.90	0
18	Y5P	V	37	18	14,19,20	3.61	3 (21%)	18,26,29	2.87	2 (11%)
18	Y5P	V	38	18	14,19,20	3.60	3 (21%)	18,26,29	2.86	2 (11%)
18	Y5P	V	39	18	14,19,20	3.46	3 (21%)	18,26,29	2.91	2 (11%)
18	Y5P	V	4	18	14,19,20	4.88	3 (21%)	18,26,29	1.69	1 (5%)
18	Y5P	V	40	18	14,19,20	5.17	2 (14%)	18,26,29	1.49	1 (5%)
18	Y5P	V	41	18	14,19,20	5.47	3 (21%)	18,26,29	1.32	1 (5%)
18	Y5P	V	42	18	14,19,20	5.36	3 (21%)	18,26,29	1.46	1 (5%)
18	Y5P	V	43	18	14,19,20	4.92	3 (21%)	18,26,29	1.61	1 (5%)
18	Y5P	V	44	18	14,19,20	3.64	3 (21%)	18,26,29	2.85	2 (11%)
18	Y5P	V	45	18	14,19,20	3.24	2 (14%)	18,26,29	2.79	2 (11%)
18	Y5P	V	48	18	14,19,20	4.94	3 (21%)	18,26,29	1.75	1 (5%)
18	Y5P	V	49	18	14,19,20	4.72	3 (21%)	18,26,29	1.85	1 (5%)
18	Y5P	V	5	18	14,19,20	3.60	3 (21%)	18,26,29	2.83	2 (11%)
18	Y5P	V	50	18	14,19,20	3.05	3 (21%)	18,26,29	2.84	2 (11%)
18	Y5P	V	51	18	14,19,20	3.28	2 (14%)	18,26,29	2.73	2 (11%)
18	Y5P	V	52	18	14,19,20	3.60	3 (21%)	18,26,29	2.85	2 (11%)
18	Y5P	V	53	18	14,19,20	3.66	3 (21%)	18,26,29	2.84	2 (11%)
18	Y5P	V	54	18	14,19,20	3.12	2 (14%)	18,26,29	2.95	2 (11%)
18	Y5P	V	55	18	14,19,20	3.20	2 (14%)	18,26,29	2.88	2 (11%)
18	Y5P	V	56	18	14,19,20	4.84	3 (21%)	18,26,29	1.72	1 (5%)
18	Y5P	V	57	18	14,19,20	3.58	3 (21%)	18,26,29	2.84	2 (11%)
18	Y5P	V	58	18	14,19,20	3.59	3 (21%)	18,26,29	2.85	2 (11%)
18	Y5P	V	59	18	14,19,20	3.14	3 (21%)	18,26,29	2.90	2 (11%)
18	Y5P	V	6	18	14,19,20	3.58	3 (21%)	18,26,29	2.85	2 (11%)
18	Y5P	V	60	18	14,19,20	3.18	2 (14%)	18,26,29	2.94	2 (11%)
18	Y5P	V	61	18	14,19,20	4.89	3 (21%)	18,26,29	1.70	1 (5%)
18	Y5P	V	62	18	14,19,20	4.75	3 (21%)	18,26,29	1.87	1 (5%)
18	Y5P	V	63	18	14,19,20	3.61	3 (21%)	18,26,29	2.86	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	Y5P	V	64	18	14,19,20	3.63	3 (21%)	18,26,29	2.86	2 (11%)
18	Y5P	V	65	18	14,19,20	3.63	3 (21%)	18,26,29	2.87	2 (11%)
18	Y5P	V	66	18	14,19,20	3.10	3 (21%)	18,26,29	2.97	2 (11%)
18	Y5P	V	67	18	14,19,20	4.76	3 (21%)	18,26,29	1.96	1 (5%)
18	Y5P	V	68	18	14,19,20	4.91	3 (21%)	18,26,29	1.63	1 (5%)
18	Y5P	V	69	18	14,19,20	3.60	3 (21%)	18,26,29	2.82	2 (11%)
18	Y5P	V	7	18	14,19,20	3.56	3 (21%)	18,26,29	2.83	2 (11%)
18	Y5P	V	70	18	14,19,20	3.62	3 (21%)	18,26,29	2.84	2 (11%)
18	Y5P	V	71	18	14,19,20	3.61	3 (21%)	18,26,29	2.82	2 (11%)
18	Y5P	V	8	18	14,19,20	3.24	2 (14%)	18,26,29	2.87	2 (11%)
18	Y5P	V	9	18	14,19,20	3.60	3 (21%)	18,26,29	2.84	2 (11%)
19	Y5P	X	12	19	15,16,20	2.91	2 (13%)	18,22,29	3.10	2 (11%)
19	Y5P	X	13	19	14,19,20	3.20	3 (21%)	18,26,29	2.88	2 (11%)
19	Y5P	X	14	19	14,19,20	3.15	3 (21%)	18,26,29	2.87	2 (11%)
19	Y5P	X	15	19	14,19,20	3.13	3 (21%)	18,26,29	2.83	2 (11%)
19	Y5P	X	16	19	14,19,20	3.58	3 (21%)	18,26,29	2.83	2 (11%)
19	Y5P	X	17	19	14,19,20	3.59	2 (14%)	18,26,29	2.83	2 (11%)
19	Y5P	X	18	19	14,19,20	5.00	3 (21%)	18,26,29	1.61	1 (5%)
19	Y5P	X	19	19,37	14,19,20	3.62	3 (21%)	18,26,29	2.82	2 (11%)
19	Y5P	X	20	19	14,19,20	3.37	2 (14%)	18,26,29	2.85	2 (11%)
19	Y5P	X	21	19	14,19,20	5.17	3 (21%)	18,26,29	1.58	1 (5%)
19	Y5P	X	22	19	14,19,20	3.12	2 (14%)	18,26,29	3.02	2 (11%)
19	Y5P	X	23	19	14,19,20	3.13	2 (14%)	18,26,29	2.95	2 (11%)
19	Y5P	X	24	19	14,19,20	3.16	3 (21%)	18,26,29	2.87	2 (11%)
18	Y5P	Y	1	18	15,16,20	3.48	3 (20%)	18,22,29	2.84	2 (11%)
18	Y5P	Y	10	18	14,19,20	3.60	3 (21%)	18,26,29	2.85	2 (11%)
18	Y5P	Y	11	18	14,19,20	4.90	3 (21%)	18,26,29	1.67	1 (5%)
18	Y5P	Y	12	18	14,19,20	3.21	2 (14%)	18,26,29	2.92	2 (11%)
18	Y5P	Y	13	18	14,19,20	4.82	3 (21%)	18,26,29	1.78	1 (5%)
18	Y5P	Y	14	18	14,19,20	3.64	3 (21%)	18,26,29	2.82	2 (11%)
18	Y5P	Y	15	18	14,19,20	3.58	3 (21%)	18,26,29	2.86	2 (11%)
18	Y5P	Y	2	18	14,19,20	4.84	3 (21%)	18,26,29	1.74	1 (5%)
18	Y5P	Y	21	18	14,19,20	3.65	3 (21%)	18,26,29	2.84	2 (11%)
18	Y5P	Y	22	18	14,19,20	3.60	3 (21%)	18,26,29	2.84	2 (11%)
18	Y5P	Y	23	18	14,19,20	3.62	3 (21%)	18,26,29	2.84	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	Y5P	Y	24	18	14,19,20	3.56	3 (21%)	18,26,29	2.84	2 (11%)
18	Y5P	Y	25	18	14,19,20	4.94	3 (21%)	18,26,29	1.63	1 (5%)
18	Y5P	Y	26	18	14,19,20	3.65	3 (21%)	18,26,29	2.85	2 (11%)
18	Y5P	Y	27	18	14,19,20	3.62	3 (21%)	18,26,29	2.93	3 (16%)
18	Y5P	Y	28	18	14,19,20	3.65	3 (21%)	18,26,29	2.86	2 (11%)
18	Y5P	Y	29	18	14,19,20	3.64	3 (21%)	18,26,29	2.84	2 (11%)
18	Y5P	Y	3	18	14,19,20	4.87	3 (21%)	18,26,29	1.65	1 (5%)
18	Y5P	Y	30	18	14,19,20	3.58	3 (21%)	18,26,29	2.85	2 (11%)
18	Y5P	Y	31	18	14,19,20	3.63	3 (21%)	18,26,29	2.85	2 (11%)
18	Y5P	Y	32	18	14,19,20	3.28	2 (14%)	18,26,29	2.87	2 (11%)
18	Y5P	Y	33	18	14,19,20	3.48	2 (14%)	18,26,29	2.58	2 (11%)
18	P5P	Y	34	18	16,23,24	1.44	2 (12%)	15,33,36	2.05	2 (13%)
18	P5P	Y	35	18	16,23,24	0.77	0	15,33,36	1.05	1 (6%)
18	P5P	Y	36	18	16,23,24	0.75	0	15,33,36	0.87	0
18	Y5P	Y	37	18	14,19,20	3.73	3 (21%)	18,26,29	2.87	2 (11%)
18	Y5P	Y	38	18	14,19,20	3.66	3 (21%)	18,26,29	2.87	2 (11%)
18	Y5P	Y	39	18	14,19,20	3.25	2 (14%)	18,26,29	3.01	2 (11%)
18	Y5P	Y	4	18	14,19,20	4.83	3 (21%)	18,26,29	1.72	1 (5%)
18	Y5P	Y	40	18,37	14,19,20	5.08	3 (21%)	18,26,29	1.66	1 (5%)
18	Y5P	Y	41	18	14,19,20	4.92	3 (21%)	18,26,29	1.77	1 (5%)
18	Y5P	Y	42	18	14,19,20	4.93	3 (21%)	18,26,29	1.76	1 (5%)
18	Y5P	Y	43	18	14,19,20	4.92	3 (21%)	18,26,29	1.66	1 (5%)
18	Y5P	Y	44	18	14,19,20	3.60	3 (21%)	18,26,29	2.84	2 (11%)
18	Y5P	Y	45	18	14,19,20	3.43	2 (14%)	18,26,29	2.99	2 (11%)
18	Y5P	Y	48	18	14,19,20	5.01	3 (21%)	18,26,29	1.58	1 (5%)
18	Y5P	Y	49	18	14,19,20	4.75	3 (21%)	18,26,29	1.83	1 (5%)
18	Y5P	Y	5	18	14,19,20	3.64	3 (21%)	18,26,29	2.84	2 (11%)
18	Y5P	Y	50	18	14,19,20	3.08	2 (14%)	18,26,29	3.05	2 (11%)
18	Y5P	Y	51	18	14,19,20	3.06	2 (14%)	18,26,29	3.13	2 (11%)
18	Y5P	Y	52	18	14,19,20	3.58	3 (21%)	18,26,29	2.85	2 (11%)
18	Y5P	Y	53	18	14,19,20	3.62	3 (21%)	18,26,29	2.85	2 (11%)
18	Y5P	Y	54	18	14,19,20	3.16	2 (14%)	18,26,29	2.93	2 (11%)
18	Y5P	Y	55	18	14,19,20	3.40	3 (21%)	18,26,29	2.81	2 (11%)
18	Y5P	Y	56	18	14,19,20	4.88	3 (21%)	18,26,29	1.70	1 (5%)
18	Y5P	Y	57	18	14,19,20	3.61	3 (21%)	18,26,29	2.83	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	Y5P	Y	58	18	14,19,20	3.59	3 (21%)	18,26,29	2.84	2 (11%)
18	Y5P	Y	59	18	14,19,20	3.28	2 (14%)	18,26,29	2.80	2 (11%)
18	Y5P	Y	6	18	14,19,20	3.65	3 (21%)	18,26,29	2.84	2 (11%)
18	Y5P	Y	60	18	14,19,20	3.20	2 (14%)	18,26,29	2.86	2 (11%)
18	Y5P	Y	61	18	14,19,20	4.83	3 (21%)	18,26,29	1.69	1 (5%)
18	Y5P	Y	62	18	14,19,20	4.96	3 (21%)	18,26,29	1.82	1 (5%)
18	Y5P	Y	63	18	14,19,20	3.59	3 (21%)	18,26,29	2.86	2 (11%)
18	Y5P	Y	64	18	14,19,20	3.60	3 (21%)	18,26,29	2.85	2 (11%)
18	Y5P	Y	65	18	14,19,20	3.61	3 (21%)	18,26,29	2.84	2 (11%)
18	Y5P	Y	66	18	14,19,20	3.20	2 (14%)	18,26,29	2.89	2 (11%)
18	Y5P	Y	67	18	14,19,20	4.94	3 (21%)	18,26,29	1.67	1 (5%)
18	Y5P	Y	68	18	14,19,20	4.86	3 (21%)	18,26,29	1.73	1 (5%)
18	Y5P	Y	69	18	14,19,20	3.64	3 (21%)	18,26,29	2.87	2 (11%)
18	Y5P	Y	7	18	14,19,20	3.59	3 (21%)	18,26,29	2.83	2 (11%)
18	Y5P	Y	70	18	14,19,20	3.61	3 (21%)	18,26,29	2.83	2 (11%)
18	Y5P	Y	71	18	14,19,20	3.63	3 (21%)	18,26,29	2.87	3 (16%)
18	Y5P	Y	8	18	14,19,20	3.29	2 (14%)	18,26,29	2.89	2 (11%)
18	Y5P	Y	9	18	14,19,20	3.63	3 (21%)	18,26,29	2.85	2 (11%)

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	V	1	18	-	0/6/30/34	0/2/2/2
18	Y5P	V	10	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	11	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	12	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	13	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	14	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	15	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	2	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	21	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	22	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	23	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	24	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	25	18	-	0/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	Y5P	V	26	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	27	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	28	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	29	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	3	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	30	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	31	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	32	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	33	18	-	0/7/33/34	0/2/2/2
18	P5P	V	34	18	-	0/3/25/26	0/3/3/3
18	P5P	V	35	18	-	0/3/25/26	0/3/3/3
18	P5P	V	36	18	-	0/3/25/26	0/3/3/3
18	Y5P	V	37	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	38	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	39	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	4	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	40	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	41	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	42	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	43	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	44	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	45	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	48	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	49	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	5	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	50	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	51	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	52	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	53	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	54	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	55	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	56	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	57	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	58	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	59	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	6	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	60	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	61	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	62	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	63	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	64	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	65	18	-	0/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	Y5P	V	66	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	67	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	68	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	69	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	7	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	70	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	71	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	8	18	-	0/7/33/34	0/2/2/2
18	Y5P	V	9	18	-	0/7/33/34	0/2/2/2
19	Y5P	X	12	19	-	0/6/30/34	0/2/2/2
19	Y5P	X	13	19	-	0/7/33/34	0/2/2/2
19	Y5P	X	14	19	-	0/7/33/34	0/2/2/2
19	Y5P	X	15	19	-	0/7/33/34	0/2/2/2
19	Y5P	X	16	19	-	0/7/33/34	0/2/2/2
19	Y5P	X	17	19	-	0/7/33/34	0/2/2/2
19	Y5P	X	18	19	-	0/7/33/34	0/2/2/2
19	Y5P	X	19	19,37	-	0/7/33/34	0/2/2/2
19	Y5P	X	20	19	-	0/7/33/34	0/2/2/2
19	Y5P	X	21	19	-	0/7/33/34	0/2/2/2
19	Y5P	X	22	19	-	0/7/33/34	0/2/2/2
19	Y5P	X	23	19	-	0/7/33/34	0/2/2/2
19	Y5P	X	24	19	-	0/7/33/34	0/2/2/2
18	Y5P	Y	1	18	-	0/6/30/34	0/2/2/2
18	Y5P	Y	10	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	11	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	12	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	13	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	14	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	15	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	2	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	21	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	22	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	23	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	24	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	25	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	26	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	27	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	28	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	29	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	3	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	30	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	31	18	-	0/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	Y5P	Y	32	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	33	18	-	0/7/33/34	0/2/2/2
18	P5P	Y	34	18	-	0/3/25/26	0/3/3/3
18	P5P	Y	35	18	-	0/3/25/26	0/3/3/3
18	P5P	Y	36	18	-	0/3/25/26	0/3/3/3
18	Y5P	Y	37	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	38	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	39	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	4	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	40	18,37	-	0/7/33/34	0/2/2/2
18	Y5P	Y	41	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	42	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	43	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	44	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	45	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	48	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	49	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	5	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	50	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	51	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	52	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	53	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	54	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	55	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	56	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	57	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	58	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	59	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	6	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	60	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	61	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	62	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	63	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	64	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	65	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	66	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	67	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	68	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	69	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	7	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	70	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	71	18	-	0/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	Y5P	Y	8	18	-	0/7/33/34	0/2/2/2
18	Y5P	Y	9	18	-	0/7/33/34	0/2/2/2

All (383) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	V	41	Y5P	C4-N3	-20.12	1.32	1.46
18	V	42	Y5P	C4-N3	-19.59	1.32	1.46
19	X	21	Y5P	C4-N3	-18.99	1.33	1.46
18	V	40	Y5P	C4-N3	-18.96	1.33	1.46
18	Y	40	Y5P	C4-N3	-18.65	1.33	1.46
18	Y	48	Y5P	C4-N3	-18.33	1.33	1.46
19	X	18	Y5P	C4-N3	-18.20	1.33	1.46
18	Y	25	Y5P	C4-N3	-18.03	1.33	1.46
18	V	2	Y5P	C4-N3	-18.01	1.33	1.46
18	Y	62	Y5P	C4-N3	-17.99	1.33	1.46
18	Y	67	Y5P	C4-N3	-17.96	1.33	1.46
18	Y	41	Y5P	C4-N3	-17.93	1.33	1.46
18	V	48	Y5P	C4-N3	-17.89	1.33	1.46
18	Y	42	Y5P	C4-N3	-17.86	1.34	1.46
18	Y	43	Y5P	C4-N3	-17.85	1.34	1.46
18	Y	11	Y5P	C4-N3	-17.84	1.34	1.46
18	V	68	Y5P	C4-N3	-17.83	1.34	1.46
18	V	61	Y5P	C4-N3	-17.81	1.34	1.46
18	Y	56	Y5P	C4-N3	-17.74	1.34	1.46
18	V	4	Y5P	C4-N3	-17.69	1.34	1.46
18	Y	3	Y5P	C4-N3	-17.69	1.34	1.46
18	Y	68	Y5P	C4-N3	-17.67	1.34	1.46
18	V	43	Y5P	C4-N3	-17.67	1.34	1.46
18	Y	2	Y5P	C4-N3	-17.60	1.34	1.46
18	Y	61	Y5P	C4-N3	-17.58	1.34	1.46
18	V	3	Y5P	C4-N3	-17.58	1.34	1.46
18	Y	13	Y5P	C4-N3	-17.55	1.34	1.46
18	V	56	Y5P	C4-N3	-17.52	1.34	1.46
18	Y	4	Y5P	C4-N3	-17.50	1.34	1.46
18	V	25	Y5P	C4-N3	-17.45	1.34	1.46
18	V	11	Y5P	C4-N3	-17.35	1.34	1.46
18	Y	49	Y5P	C4-N3	-17.26	1.34	1.46
18	V	67	Y5P	C4-N3	-17.20	1.34	1.46
18	V	62	Y5P	C4-N3	-17.15	1.34	1.46
18	V	49	Y5P	C4-N3	-17.13	1.34	1.46
18	V	13	Y5P	C4-N3	-16.93	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	V	33	Y5P	C4-N3	-14.68	1.36	1.46
19	X	17	Y5P	C4-N3	-12.81	1.37	1.46
19	X	16	Y5P	C4-N3	-12.77	1.37	1.46
19	X	19	Y5P	C4-N3	-12.74	1.37	1.46
18	Y	33	Y5P	C4-N3	-12.28	1.37	1.46
18	V	22	Y5P	C4-N3	-12.18	1.37	1.46
18	V	53	Y5P	C4-N3	-12.18	1.37	1.46
18	Y	5	Y5P	C4-N3	-12.17	1.37	1.46
18	V	26	Y5P	C4-N3	-12.16	1.37	1.46
18	Y	69	Y5P	C4-N3	-12.16	1.37	1.46
18	Y	37	Y5P	C4-N3	-12.16	1.37	1.46
18	V	30	Y5P	C4-N3	-12.15	1.37	1.46
18	Y	26	Y5P	C4-N3	-12.14	1.38	1.46
18	V	65	Y5P	C4-N3	-12.13	1.38	1.46
18	Y	6	Y5P	C4-N3	-12.13	1.38	1.46
18	V	64	Y5P	C4-N3	-12.13	1.38	1.46
18	Y	45	Y5P	C4-N3	-12.12	1.38	1.46
18	Y	28	Y5P	C4-N3	-12.12	1.38	1.46
18	V	70	Y5P	C4-N3	-12.12	1.38	1.46
18	V	38	Y5P	C4-N3	-12.11	1.38	1.46
18	Y	29	Y5P	C4-N3	-12.11	1.38	1.46
18	V	29	Y5P	C4-N3	-12.10	1.38	1.46
18	Y	71	Y5P	C4-N3	-12.10	1.38	1.46
18	Y	22	Y5P	C4-N3	-12.10	1.38	1.46
18	Y	70	Y5P	C4-N3	-12.09	1.38	1.46
18	Y	27	Y5P	C4-N3	-12.09	1.38	1.46
18	Y	14	Y5P	C4-N3	-12.09	1.38	1.46
18	V	23	Y5P	C4-N3	-12.08	1.38	1.46
18	V	24	Y5P	C4-N3	-12.07	1.38	1.46
18	V	27	Y5P	C4-N3	-12.07	1.38	1.46
18	V	10	Y5P	C4-N3	-12.07	1.38	1.46
18	V	21	Y5P	C4-N3	-12.07	1.38	1.46
18	Y	9	Y5P	C4-N3	-12.07	1.38	1.46
18	Y	57	Y5P	C4-N3	-12.07	1.38	1.46
18	Y	53	Y5P	C4-N3	-12.07	1.38	1.46
18	V	71	Y5P	C4-N3	-12.06	1.38	1.46
18	Y	7	Y5P	C4-N3	-12.06	1.38	1.46
18	Y	65	Y5P	C4-N3	-12.06	1.38	1.46
18	V	9	Y5P	C4-N3	-12.06	1.38	1.46
18	V	15	Y5P	C4-N3	-12.06	1.38	1.46
18	V	63	Y5P	C4-N3	-12.06	1.38	1.46
18	Y	21	Y5P	C4-N3	-12.06	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Y	31	Y5P	C4-N3	-12.05	1.38	1.46
18	Y	64	Y5P	C4-N3	-12.05	1.38	1.46
18	V	28	Y5P	C4-N3	-12.05	1.38	1.46
18	V	37	Y5P	C4-N3	-12.04	1.38	1.46
18	V	58	Y5P	C4-N3	-12.04	1.38	1.46
18	Y	38	Y5P	C4-N3	-12.04	1.38	1.46
18	V	6	Y5P	C4-N3	-12.03	1.38	1.46
18	Y	10	Y5P	C4-N3	-12.02	1.38	1.46
18	V	39	Y5P	C4-N3	-12.02	1.38	1.46
18	Y	1	Y5P	C4-N3	-12.01	1.38	1.46
18	V	14	Y5P	C4-N3	-12.01	1.38	1.46
18	V	52	Y5P	C4-N3	-12.00	1.38	1.46
18	V	5	Y5P	C4-N3	-12.00	1.38	1.46
18	V	31	Y5P	C4-N3	-11.99	1.38	1.46
18	V	44	Y5P	C4-N3	-11.99	1.38	1.46
18	Y	30	Y5P	C4-N3	-11.99	1.38	1.46
18	Y	23	Y5P	C4-N3	-11.99	1.38	1.46
18	V	69	Y5P	C4-N3	-11.99	1.38	1.46
18	Y	24	Y5P	C4-N3	-11.98	1.38	1.46
18	V	1	Y5P	C4-N3	-11.98	1.38	1.46
18	Y	63	Y5P	C4-N3	-11.97	1.38	1.46
18	V	7	Y5P	C4-N3	-11.97	1.38	1.46
18	Y	44	Y5P	C4-N3	-11.97	1.38	1.46
18	Y	52	Y5P	C4-N3	-11.96	1.38	1.46
18	Y	58	Y5P	C4-N3	-11.94	1.38	1.46
18	Y	15	Y5P	C4-N3	-11.93	1.38	1.46
18	V	57	Y5P	C4-N3	-11.93	1.38	1.46
19	X	20	Y5P	C4-N3	-11.82	1.38	1.46
18	Y	55	Y5P	C4-N3	-11.77	1.38	1.46
18	Y	32	Y5P	C4-N3	-11.46	1.38	1.46
18	Y	8	Y5P	C4-N3	-11.45	1.38	1.46
18	Y	39	Y5P	C4-N3	-11.34	1.38	1.46
18	Y	59	Y5P	C4-N3	-11.31	1.38	1.46
18	V	8	Y5P	C4-N3	-11.31	1.38	1.46
18	V	51	Y5P	C4-N3	-11.20	1.38	1.46
18	V	45	Y5P	C4-N3	-11.12	1.38	1.46
18	Y	12	Y5P	C4-N3	-11.10	1.38	1.46
18	Y	66	Y5P	C4-N3	-11.01	1.38	1.46
18	V	55	Y5P	C4-N3	-11.01	1.38	1.46
18	Y	60	Y5P	C4-N3	-10.97	1.38	1.46
18	V	32	Y5P	C4-N3	-10.94	1.38	1.46
18	Y	54	Y5P	C4-N3	-10.85	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	X	13	Y5P	C4-N3	-10.84	1.38	1.46
18	V	60	Y5P	C4-N3	-10.81	1.38	1.46
18	V	12	Y5P	C4-N3	-10.77	1.38	1.46
19	X	23	Y5P	C4-N3	-10.66	1.39	1.46
18	V	54	Y5P	C4-N3	-10.62	1.39	1.46
19	X	22	Y5P	C4-N3	-10.57	1.39	1.46
19	X	24	Y5P	C4-N3	-10.57	1.39	1.46
18	V	59	Y5P	C4-N3	-10.51	1.39	1.46
18	V	66	Y5P	C4-N3	-10.50	1.39	1.46
19	X	14	Y5P	C4-N3	-10.49	1.39	1.46
18	Y	51	Y5P	C4-N3	-10.49	1.39	1.46
18	Y	50	Y5P	C4-N3	-10.49	1.39	1.46
19	X	15	Y5P	C4-N3	-10.45	1.39	1.46
19	X	12	Y5P	C4-N3	-10.25	1.39	1.46
18	V	50	Y5P	C4-N3	-10.23	1.39	1.46
18	V	36	P5P	C6-N1	2.01	1.36	1.32
18	V	66	Y5P	C2-N1	2.01	1.39	1.36
19	X	15	Y5P	C2-N1	2.02	1.39	1.36
18	V	50	Y5P	C2-N1	2.06	1.39	1.36
19	X	16	Y5P	C2-N1	2.07	1.39	1.36
18	V	59	Y5P	C2-N1	2.08	1.39	1.36
18	Y	40	Y5P	C2-N1	2.08	1.39	1.36
19	X	24	Y5P	C2-N1	2.12	1.39	1.36
18	Y	55	Y5P	C2-N1	2.17	1.39	1.36
18	V	13	Y5P	C2-N1	2.18	1.39	1.36
19	X	13	Y5P	C2-N1	2.19	1.39	1.36
19	X	21	Y5P	C2-N1	2.20	1.40	1.36
18	V	41	Y5P	C2-N1	2.22	1.40	1.36
18	Y	48	Y5P	C2-N1	2.24	1.40	1.36
18	Y	25	Y5P	C2-N1	2.29	1.40	1.36
19	X	19	Y5P	C2-N1	2.35	1.40	1.36
18	Y	61	Y5P	C2-N1	2.40	1.40	1.36
18	Y	3	Y5P	C2-N1	2.42	1.40	1.36
18	V	61	Y5P	C2-N1	2.42	1.40	1.36
18	Y	13	Y5P	C2-N1	2.43	1.40	1.36
18	V	49	Y5P	C2-N1	2.46	1.40	1.36
18	Y	11	Y5P	C2-N1	2.48	1.40	1.36
19	X	14	Y5P	C2-N1	2.49	1.40	1.36
18	Y	41	Y5P	C2-N1	2.50	1.40	1.36
18	V	39	Y5P	C2-N1	2.50	1.40	1.36
18	V	2	Y5P	C2-N1	2.51	1.40	1.36
18	V	3	Y5P	C2-N1	2.52	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Y	49	Y5P	C2-N1	2.54	1.40	1.36
18	V	68	Y5P	C2-N1	2.55	1.40	1.36
18	Y	68	Y5P	C2-N1	2.55	1.40	1.36
18	Y	67	Y5P	C2-N1	2.58	1.40	1.36
18	V	25	Y5P	C2-N1	2.60	1.40	1.36
18	V	29	Y5P	C1'-N1	2.64	1.54	1.46
18	Y	2	Y5P	C2-N1	2.64	1.40	1.36
18	V	41	Y5P	C2-N3	2.67	1.35	1.29
18	Y	56	Y5P	C2-N1	2.67	1.40	1.36
19	X	21	Y5P	C2-N3	2.68	1.35	1.29
18	Y	34	P5P	C2-N1	2.69	1.38	1.33
18	V	67	Y5P	C2-N1	2.71	1.40	1.36
18	V	4	Y5P	C2-N1	2.71	1.40	1.36
18	Y	43	Y5P	C2-N1	2.73	1.40	1.36
18	V	42	Y5P	C2-N1	2.76	1.40	1.36
18	V	11	Y5P	C2-N1	2.78	1.41	1.36
18	Y	40	Y5P	C2-N3	2.84	1.35	1.29
18	Y	42	Y5P	C2-N1	2.86	1.41	1.36
18	Y	4	Y5P	C2-N1	2.86	1.41	1.36
18	V	56	Y5P	C2-N1	2.87	1.41	1.36
18	V	62	Y5P	C2-N1	2.89	1.41	1.36
19	X	18	Y5P	C2-N3	2.89	1.35	1.29
18	Y	62	Y5P	C2-N1	2.97	1.41	1.36
18	V	42	Y5P	C2-N3	2.99	1.35	1.29
18	Y	48	Y5P	C2-N3	3.00	1.35	1.29
19	X	18	Y5P	C2-N1	3.02	1.41	1.36
18	V	40	Y5P	C2-N3	3.05	1.35	1.29
18	V	34	P5P	C2-N1	3.06	1.39	1.33
18	Y	41	Y5P	C2-N3	3.07	1.35	1.29
18	V	2	Y5P	C2-N3	3.11	1.36	1.29
18	Y	25	Y5P	C2-N3	3.12	1.36	1.29
18	V	3	Y5P	C2-N3	3.13	1.36	1.29
18	V	61	Y5P	C2-N3	3.14	1.36	1.29
18	Y	61	Y5P	C2-N3	3.14	1.36	1.29
18	V	25	Y5P	C2-N3	3.15	1.36	1.29
18	Y	56	Y5P	C2-N3	3.15	1.36	1.29
18	Y	68	Y5P	C2-N3	3.17	1.36	1.29
18	Y	11	Y5P	C2-N3	3.18	1.36	1.29
18	Y	67	Y5P	C2-N3	3.18	1.36	1.29
18	Y	2	Y5P	C2-N3	3.20	1.36	1.29
18	V	48	Y5P	C2-N1	3.22	1.41	1.36
18	Y	13	Y5P	C2-N3	3.22	1.36	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Y	49	Y5P	C2-N3	3.23	1.36	1.29
18	Y	4	Y5P	C2-N3	3.23	1.36	1.29
18	V	11	Y5P	C2-N3	3.25	1.36	1.29
18	V	33	Y5P	C2-N3	3.25	1.36	1.29
18	V	48	Y5P	C2-N3	3.26	1.36	1.29
18	V	68	Y5P	C2-N3	3.27	1.36	1.29
18	V	56	Y5P	C2-N3	3.29	1.36	1.29
18	Y	62	Y5P	C2-N3	3.30	1.36	1.29
18	Y	42	Y5P	C2-N3	3.32	1.36	1.29
19	X	16	Y5P	C2-N3	3.32	1.36	1.29
18	Y	3	Y5P	C2-N3	3.33	1.36	1.29
18	V	4	Y5P	C2-N3	3.34	1.36	1.29
18	Y	43	Y5P	C2-N3	3.34	1.36	1.29
18	V	62	Y5P	C2-N3	3.35	1.36	1.29
18	V	43	Y5P	C2-N3	3.35	1.36	1.29
18	V	49	Y5P	C2-N3	3.36	1.36	1.29
18	V	7	Y5P	C1'-N1	3.39	1.56	1.46
18	V	13	Y5P	C2-N3	3.40	1.36	1.29
18	V	67	Y5P	C2-N3	3.41	1.36	1.29
18	V	30	Y5P	C1'-N1	3.42	1.56	1.46
18	Y	24	Y5P	C1'-N1	3.48	1.56	1.46
18	V	31	Y5P	C1'-N1	3.51	1.57	1.46
18	V	15	Y5P	C1'-N1	3.53	1.57	1.46
18	V	43	Y5P	C2-N1	3.54	1.42	1.36
18	Y	7	Y5P	C1'-N1	3.56	1.57	1.46
18	V	38	Y5P	C1'-N1	3.58	1.57	1.46
19	X	17	Y5P	C2-N3	3.60	1.37	1.29
18	V	9	Y5P	C1'-N1	3.64	1.57	1.46
18	Y	22	Y5P	C1'-N1	3.65	1.57	1.46
18	V	6	Y5P	C1'-N1	3.66	1.57	1.46
18	V	58	Y5P	C1'-N1	3.66	1.57	1.46
18	Y	30	Y5P	C1'-N1	3.70	1.57	1.46
18	V	27	Y5P	C1'-N1	3.72	1.57	1.46
18	V	24	Y5P	C1'-N1	3.72	1.57	1.46
18	Y	70	Y5P	C1'-N1	3.72	1.57	1.46
18	Y	52	Y5P	C1'-N1	3.73	1.57	1.46
18	Y	64	Y5P	C1'-N1	3.73	1.57	1.46
19	X	19	Y5P	C2-N3	3.74	1.37	1.29
18	V	23	Y5P	C1'-N1	3.76	1.57	1.46
18	Y	39	Y5P	C2-N3	3.78	1.37	1.29
18	V	63	Y5P	C1'-N1	3.79	1.57	1.46
18	Y	57	Y5P	C1'-N1	3.80	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Y	45	Y5P	C2-N3	3.81	1.37	1.29
18	V	10	Y5P	C1'-N1	3.82	1.57	1.46
18	V	70	Y5P	C1'-N1	3.83	1.58	1.46
18	Y	15	Y5P	C1'-N1	3.83	1.58	1.46
18	V	64	Y5P	C1'-N1	3.85	1.58	1.46
18	Y	10	Y5P	C1'-N1	3.85	1.58	1.46
18	V	39	Y5P	C2-N3	3.87	1.37	1.29
18	V	65	Y5P	C1'-N1	3.89	1.58	1.46
18	V	28	Y5P	C1'-N1	3.89	1.58	1.46
19	X	20	Y5P	C2-N3	3.89	1.37	1.29
18	V	37	Y5P	C1'-N1	3.90	1.58	1.46
18	Y	5	Y5P	C1'-N1	3.90	1.58	1.46
18	Y	63	Y5P	C1'-N1	3.90	1.58	1.46
18	Y	65	Y5P	C1'-N1	3.90	1.58	1.46
18	V	8	Y5P	C2-N3	3.90	1.37	1.29
18	V	52	Y5P	C1'-N1	3.91	1.58	1.46
18	Y	27	Y5P	C1'-N1	3.93	1.58	1.46
18	V	71	Y5P	C1'-N1	3.94	1.58	1.46
18	Y	71	Y5P	C1'-N1	3.95	1.58	1.46
18	Y	1	Y5P	C1'-N1	3.95	1.58	1.46
18	Y	32	Y5P	C2-N3	3.96	1.37	1.29
18	Y	58	Y5P	C1'-N1	3.96	1.58	1.46
18	Y	69	Y5P	C1'-N1	3.96	1.58	1.46
18	V	57	Y5P	C1'-N1	3.98	1.58	1.46
18	V	69	Y5P	C1'-N1	3.99	1.58	1.46
18	V	1	Y5P	C1'-N1	3.99	1.58	1.46
18	Y	44	Y5P	C1'-N1	4.00	1.58	1.46
18	Y	8	Y5P	C2-N3	4.01	1.37	1.29
18	V	5	Y5P	C1'-N1	4.01	1.58	1.46
18	Y	33	Y5P	C2-N3	4.02	1.37	1.29
18	Y	9	Y5P	C1'-N1	4.02	1.58	1.46
18	V	12	Y5P	C2-N3	4.03	1.37	1.29
18	Y	53	Y5P	C1'-N1	4.05	1.58	1.46
18	Y	28	Y5P	C1'-N1	4.07	1.58	1.46
18	Y	31	Y5P	C1'-N1	4.08	1.58	1.46
18	Y	55	Y5P	C2-N3	4.11	1.38	1.29
18	Y	26	Y5P	C1'-N1	4.11	1.58	1.46
18	Y	14	Y5P	C1'-N1	4.11	1.58	1.46
18	Y	12	Y5P	C2-N3	4.13	1.38	1.29
18	Y	29	Y5P	C1'-N1	4.14	1.58	1.46
18	V	14	Y5P	C1'-N1	4.14	1.58	1.46
18	V	26	Y5P	C1'-N1	4.14	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	V	22	Y5P	C1'-N1	4.15	1.58	1.46
18	V	53	Y5P	C1'-N1	4.15	1.58	1.46
18	Y	51	Y5P	C2-N3	4.15	1.38	1.29
19	X	12	Y5P	C2-N3	4.16	1.38	1.29
18	V	45	Y5P	C2-N3	4.17	1.38	1.29
18	V	32	Y5P	C2-N3	4.18	1.38	1.29
18	Y	66	Y5P	C2-N3	4.18	1.38	1.29
18	Y	59	Y5P	C2-N3	4.19	1.38	1.29
18	Y	23	Y5P	C1'-N1	4.20	1.59	1.46
18	Y	6	Y5P	C1'-N1	4.20	1.59	1.46
18	V	55	Y5P	C2-N3	4.21	1.38	1.29
18	Y	54	Y5P	C2-N3	4.21	1.38	1.29
18	Y	60	Y5P	C2-N3	4.25	1.38	1.29
18	V	54	Y5P	C2-N3	4.27	1.38	1.29
18	V	66	Y5P	C2-N3	4.28	1.38	1.29
19	X	13	Y5P	C2-N3	4.29	1.38	1.29
18	V	71	Y5P	C2-N3	4.29	1.38	1.29
18	V	60	Y5P	C2-N3	4.29	1.38	1.29
19	X	23	Y5P	C2-N3	4.29	1.38	1.29
18	V	44	Y5P	C2-N3	4.30	1.38	1.29
18	V	51	Y5P	C2-N3	4.30	1.38	1.29
18	V	15	Y5P	C2-N3	4.30	1.38	1.29
18	Y	50	Y5P	C2-N3	4.30	1.38	1.29
18	Y	53	Y5P	C2-N3	4.30	1.38	1.29
18	V	57	Y5P	C2-N3	4.31	1.38	1.29
18	Y	23	Y5P	C2-N3	4.31	1.38	1.29
18	V	5	Y5P	C2-N3	4.31	1.38	1.29
18	Y	30	Y5P	C2-N3	4.31	1.38	1.29
18	Y	52	Y5P	C2-N3	4.31	1.38	1.29
18	V	27	Y5P	C2-N3	4.32	1.38	1.29
18	V	58	Y5P	C2-N3	4.32	1.38	1.29
18	Y	1	Y5P	C2-N3	4.32	1.38	1.29
18	V	21	Y5P	C2-N3	4.32	1.38	1.29
18	V	38	Y5P	C2-N3	4.32	1.38	1.29
18	Y	38	Y5P	C2-N3	4.32	1.38	1.29
18	V	31	Y5P	C2-N3	4.32	1.38	1.29
18	V	14	Y5P	C2-N3	4.32	1.38	1.29
18	Y	63	Y5P	C2-N3	4.32	1.38	1.29
18	V	10	Y5P	C2-N3	4.33	1.38	1.29
18	V	30	Y5P	C2-N3	4.33	1.38	1.29
18	V	22	Y5P	C2-N3	4.33	1.38	1.29
18	Y	71	Y5P	C2-N3	4.33	1.38	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	V	23	Y5P	C2-N3	4.33	1.38	1.29
18	Y	44	Y5P	C2-N3	4.33	1.38	1.29
18	Y	29	Y5P	C2-N3	4.33	1.38	1.29
18	V	65	Y5P	C2-N3	4.33	1.38	1.29
18	Y	64	Y5P	C2-N3	4.33	1.38	1.29
18	Y	58	Y5P	C2-N3	4.33	1.38	1.29
18	V	6	Y5P	C2-N3	4.33	1.38	1.29
18	V	29	Y5P	C2-N3	4.33	1.38	1.29
18	Y	70	Y5P	C2-N3	4.33	1.38	1.29
18	Y	9	Y5P	C2-N3	4.33	1.38	1.29
18	Y	57	Y5P	C2-N3	4.34	1.38	1.29
18	V	28	Y5P	C2-N3	4.34	1.38	1.29
18	V	37	Y5P	C2-N3	4.34	1.38	1.29
18	Y	22	Y5P	C2-N3	4.34	1.38	1.29
18	V	52	Y5P	C2-N3	4.34	1.38	1.29
18	V	70	Y5P	C2-N3	4.34	1.38	1.29
18	Y	15	Y5P	C2-N3	4.34	1.38	1.29
19	X	22	Y5P	C2-N3	4.34	1.38	1.29
18	V	69	Y5P	C2-N3	4.34	1.38	1.29
18	Y	10	Y5P	C2-N3	4.34	1.38	1.29
18	V	26	Y5P	C2-N3	4.34	1.38	1.29
18	Y	14	Y5P	C2-N3	4.34	1.38	1.29
18	V	24	Y5P	C2-N3	4.34	1.38	1.29
18	Y	65	Y5P	C2-N3	4.34	1.38	1.29
18	V	50	Y5P	C2-N3	4.34	1.38	1.29
18	V	9	Y5P	C2-N3	4.35	1.38	1.29
18	Y	21	Y5P	C2-N3	4.35	1.38	1.29
18	Y	37	Y5P	C2-N3	4.35	1.38	1.29
18	Y	26	Y5P	C2-N3	4.35	1.38	1.29
18	V	53	Y5P	C2-N3	4.35	1.38	1.29
18	V	1	Y5P	C2-N3	4.35	1.38	1.29
18	Y	21	Y5P	C1'-N1	4.35	1.59	1.46
18	Y	69	Y5P	C2-N3	4.35	1.38	1.29
18	Y	6	Y5P	C2-N3	4.35	1.38	1.29
18	Y	7	Y5P	C2-N3	4.35	1.38	1.29
18	V	64	Y5P	C2-N3	4.36	1.38	1.29
18	Y	24	Y5P	C2-N3	4.36	1.38	1.29
18	V	7	Y5P	C2-N3	4.36	1.38	1.29
18	Y	28	Y5P	C2-N3	4.36	1.38	1.29
18	Y	27	Y5P	C2-N3	4.36	1.38	1.29
18	V	63	Y5P	C2-N3	4.37	1.38	1.29
18	Y	5	Y5P	C2-N3	4.37	1.38	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Y	31	Y5P	C2-N3	4.37	1.38	1.29
19	X	14	Y5P	C2-N3	4.39	1.38	1.29
18	V	44	Y5P	C1'-N1	4.41	1.59	1.46
19	X	15	Y5P	C2-N3	4.43	1.38	1.29
19	X	24	Y5P	C2-N3	4.49	1.38	1.29
18	V	59	Y5P	C2-N3	4.50	1.38	1.29
18	Y	38	Y5P	C1'-N1	4.55	1.60	1.46
18	Y	34	P5P	C6-N1	4.56	1.40	1.32
18	V	34	P5P	C6-N1	4.88	1.40	1.32
18	Y	37	Y5P	C1'-N1	4.93	1.61	1.46
18	V	21	Y5P	C1'-N1	4.99	1.61	1.46

All (243) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Y	51	Y5P	N1-C2-N3	-12.43	114.03	125.85
19	X	12	Y5P	N1-C2-N3	-12.28	114.17	125.85
18	Y	50	Y5P	N1-C2-N3	-12.05	114.39	125.85
18	Y	39	Y5P	N1-C2-N3	-11.97	114.46	125.85
18	V	12	Y5P	N1-C2-N3	-11.90	114.53	125.85
19	X	22	Y5P	N1-C2-N3	-11.84	114.59	125.85
19	X	23	Y5P	N1-C2-N3	-11.70	114.72	125.85
18	Y	45	Y5P	N1-C2-N3	-11.67	114.75	125.85
18	V	54	Y5P	N1-C2-N3	-11.61	114.81	125.85
18	V	32	Y5P	N1-C2-N3	-11.60	114.82	125.85
18	Y	12	Y5P	N1-C2-N3	-11.59	114.83	125.85
18	Y	54	Y5P	N1-C2-N3	-11.57	114.84	125.85
18	V	66	Y5P	N1-C2-N3	-11.54	114.87	125.85
18	V	60	Y5P	N1-C2-N3	-11.46	114.95	125.85
18	Y	8	Y5P	N1-C2-N3	-11.44	114.97	125.85
18	V	8	Y5P	N1-C2-N3	-11.40	115.01	125.85
18	Y	66	Y5P	N1-C2-N3	-11.38	115.02	125.85
19	X	13	Y5P	N1-C2-N3	-11.38	115.03	125.85
18	Y	32	Y5P	N1-C2-N3	-11.38	115.03	125.85
18	V	39	Y5P	N1-C2-N3	-11.38	115.03	125.85
18	V	59	Y5P	N1-C2-N3	-11.36	115.04	125.85
19	X	14	Y5P	N1-C2-N3	-11.32	115.08	125.85
18	V	55	Y5P	N1-C2-N3	-11.27	115.13	125.85
19	X	20	Y5P	N1-C2-N3	-11.25	115.15	125.85
18	Y	60	Y5P	N1-C2-N3	-11.25	115.15	125.85
19	X	24	Y5P	N1-C2-N3	-11.24	115.16	125.85
18	V	65	Y5P	N1-C2-N3	-11.23	115.17	125.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	V	37	Y5P	N1-C2-N3	-11.22	115.18	125.85
18	V	64	Y5P	N1-C2-N3	-11.22	115.18	125.85
18	V	26	Y5P	N1-C2-N3	-11.22	115.18	125.85
18	Y	6	Y5P	N1-C2-N3	-11.22	115.18	125.85
18	V	70	Y5P	N1-C2-N3	-11.21	115.18	125.85
18	Y	31	Y5P	N1-C2-N3	-11.21	115.19	125.85
18	Y	28	Y5P	N1-C2-N3	-11.21	115.19	125.85
18	V	24	Y5P	N1-C2-N3	-11.21	115.19	125.85
18	Y	57	Y5P	N1-C2-N3	-11.20	115.19	125.85
18	Y	69	Y5P	N1-C2-N3	-11.20	115.19	125.85
18	Y	38	Y5P	N1-C2-N3	-11.20	115.20	125.85
19	X	16	Y5P	N1-C2-N3	-11.20	115.20	125.85
18	V	50	Y5P	N1-C2-N3	-11.20	115.20	125.85
18	Y	9	Y5P	N1-C2-N3	-11.20	115.20	125.85
18	Y	24	Y5P	N1-C2-N3	-11.20	115.20	125.85
18	Y	26	Y5P	N1-C2-N3	-11.20	115.20	125.85
18	Y	63	Y5P	N1-C2-N3	-11.20	115.20	125.85
18	V	63	Y5P	N1-C2-N3	-11.20	115.20	125.85
18	Y	23	Y5P	N1-C2-N3	-11.20	115.20	125.85
18	Y	7	Y5P	N1-C2-N3	-11.19	115.20	125.85
18	V	10	Y5P	N1-C2-N3	-11.19	115.20	125.85
19	X	17	Y5P	N1-C2-N3	-11.19	115.20	125.85
18	V	6	Y5P	N1-C2-N3	-11.19	115.20	125.85
18	Y	5	Y5P	N1-C2-N3	-11.19	115.20	125.85
18	Y	37	Y5P	N1-C2-N3	-11.19	115.20	125.85
18	Y	22	Y5P	N1-C2-N3	-11.19	115.20	125.85
18	Y	10	Y5P	N1-C2-N3	-11.19	115.20	125.85
18	V	30	Y5P	N1-C2-N3	-11.19	115.21	125.85
18	V	53	Y5P	N1-C2-N3	-11.19	115.21	125.85
18	Y	71	Y5P	N1-C2-N3	-11.18	115.21	125.85
18	Y	21	Y5P	N1-C2-N3	-11.18	115.22	125.85
18	Y	1	Y5P	N1-C2-N3	-11.17	115.22	125.85
18	V	14	Y5P	N1-C2-N3	-11.17	115.22	125.85
18	Y	27	Y5P	N1-C2-N3	-11.17	115.22	125.85
18	V	28	Y5P	N1-C2-N3	-11.17	115.23	125.85
18	V	22	Y5P	N1-C2-N3	-11.17	115.23	125.85
18	V	7	Y5P	N1-C2-N3	-11.17	115.23	125.85
18	Y	65	Y5P	N1-C2-N3	-11.17	115.23	125.85
18	Y	53	Y5P	N1-C2-N3	-11.17	115.23	125.85
18	Y	14	Y5P	N1-C2-N3	-11.17	115.23	125.85
18	V	9	Y5P	N1-C2-N3	-11.17	115.23	125.85
18	V	38	Y5P	N1-C2-N3	-11.17	115.23	125.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Y	29	Y5P	N1-C2-N3	-11.16	115.23	125.85
18	V	29	Y5P	N1-C2-N3	-11.16	115.23	125.85
18	V	21	Y5P	N1-C2-N3	-11.16	115.23	125.85
18	V	57	Y5P	N1-C2-N3	-11.16	115.23	125.85
18	V	31	Y5P	N1-C2-N3	-11.16	115.24	125.85
18	V	69	Y5P	N1-C2-N3	-11.16	115.24	125.85
18	Y	70	Y5P	N1-C2-N3	-11.16	115.24	125.85
18	V	23	Y5P	N1-C2-N3	-11.16	115.24	125.85
18	V	58	Y5P	N1-C2-N3	-11.16	115.24	125.85
18	Y	44	Y5P	N1-C2-N3	-11.16	115.24	125.85
18	V	44	Y5P	N1-C2-N3	-11.16	115.24	125.85
18	Y	15	Y5P	N1-C2-N3	-11.15	115.24	125.85
18	V	52	Y5P	N1-C2-N3	-11.15	115.24	125.85
18	Y	30	Y5P	N1-C2-N3	-11.15	115.25	125.85
18	V	5	Y5P	N1-C2-N3	-11.15	115.25	125.85
18	V	1	Y5P	N1-C2-N3	-11.15	115.25	125.85
18	V	27	Y5P	N1-C2-N3	-11.14	115.25	125.85
18	V	15	Y5P	N1-C2-N3	-11.14	115.26	125.85
18	Y	64	Y5P	N1-C2-N3	-11.13	115.27	125.85
18	V	71	Y5P	N1-C2-N3	-11.12	115.27	125.85
18	Y	58	Y5P	N1-C2-N3	-11.12	115.27	125.85
18	Y	52	Y5P	N1-C2-N3	-11.11	115.28	125.85
19	X	19	Y5P	N1-C2-N3	-11.07	115.32	125.85
18	Y	59	Y5P	N1-C2-N3	-11.07	115.32	125.85
18	V	45	Y5P	N1-C2-N3	-10.93	115.45	125.85
19	X	15	Y5P	N1-C2-N3	-10.90	115.48	125.85
18	Y	55	Y5P	N1-C2-N3	-10.89	115.49	125.85
18	V	51	Y5P	N1-C2-N3	-10.62	115.74	125.85
18	Y	33	Y5P	N1-C2-N3	-9.92	116.41	125.85
18	V	33	Y5P	N1-C2-N3	-9.00	117.29	125.85
18	V	67	Y5P	N1-C2-N3	-7.94	118.29	125.85
18	V	62	Y5P	N1-C2-N3	-7.62	118.61	125.85
18	V	25	Y5P	N1-C2-N3	-7.54	118.68	125.85
18	V	49	Y5P	N1-C2-N3	-7.48	118.74	125.85
18	Y	49	Y5P	N1-C2-N3	-7.44	118.77	125.85
18	V	13	Y5P	N1-C2-N3	-7.40	118.81	125.85
18	Y	62	Y5P	N1-C2-N3	-7.39	118.82	125.85
18	Y	13	Y5P	N1-C2-N3	-7.28	118.93	125.85
18	V	2	Y5P	N1-C2-N3	-7.27	118.93	125.85
18	Y	41	Y5P	N1-C2-N3	-7.15	119.05	125.85
18	V	3	Y5P	N1-C2-N3	-7.14	119.06	125.85
18	Y	2	Y5P	N1-C2-N3	-7.13	119.07	125.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Y	42	Y5P	N1-C2-N3	-7.09	119.10	125.85
18	V	56	Y5P	N1-C2-N3	-7.00	119.19	125.85
18	Y	4	Y5P	N1-C2-N3	-6.97	119.22	125.85
18	V	11	Y5P	N1-C2-N3	-6.95	119.24	125.85
18	V	48	Y5P	N1-C2-N3	-6.93	119.25	125.85
18	Y	68	Y5P	N1-C2-N3	-6.93	119.25	125.85
18	Y	56	Y5P	N1-C2-N3	-6.91	119.28	125.85
18	Y	61	Y5P	N1-C2-N3	-6.89	119.29	125.85
18	V	4	Y5P	N1-C2-N3	-6.85	119.33	125.85
18	V	61	Y5P	N1-C2-N3	-6.83	119.35	125.85
18	Y	40	Y5P	N1-C2-N3	-6.74	119.43	125.85
18	Y	43	Y5P	N1-C2-N3	-6.67	119.50	125.85
18	Y	3	Y5P	N1-C2-N3	-6.67	119.51	125.85
18	Y	67	Y5P	N1-C2-N3	-6.65	119.52	125.85
18	Y	11	Y5P	N1-C2-N3	-6.63	119.54	125.85
18	Y	25	Y5P	N1-C2-N3	-6.56	119.61	125.85
18	V	43	Y5P	N1-C2-N3	-6.47	119.69	125.85
19	X	18	Y5P	N1-C2-N3	-6.44	119.72	125.85
18	Y	48	Y5P	N1-C2-N3	-6.40	119.76	125.85
18	V	68	Y5P	N1-C2-N3	-6.30	119.86	125.85
19	X	21	Y5P	N1-C2-N3	-6.27	119.88	125.85
18	V	42	Y5P	N1-C2-N3	-5.87	120.26	125.85
18	V	40	Y5P	N1-C2-N3	-5.74	120.39	125.85
18	V	41	Y5P	N1-C2-N3	-5.30	120.81	125.85
18	Y	34	P5P	N1-C2-N3	-3.32	123.31	127.66
18	Y	27	Y5P	C1'-N1-C6	-3.18	113.68	120.80
18	V	34	P5P	N1-C2-N3	-2.78	124.00	127.66
18	V	14	Y5P	C1'-N1-C6	-2.37	115.50	120.80
18	Y	71	Y5P	C1'-N1-C6	-2.10	116.10	120.80
18	V	21	Y5P	O4'-C1'-N1	2.24	112.37	108.09
18	Y	35	P5P	C1'-N9-C4	2.69	129.80	126.81
19	X	16	Y5P	C4-N3-C2	3.19	125.34	117.71
18	V	33	Y5P	C4-N3-C2	3.43	125.90	117.71
18	V	9	Y5P	C4-N3-C2	3.73	126.62	117.71
18	V	1	Y5P	C4-N3-C2	3.73	126.62	117.71
18	Y	52	Y5P	C4-N3-C2	3.73	126.62	117.71
18	Y	14	Y5P	C4-N3-C2	3.74	126.64	117.71
18	V	7	Y5P	C4-N3-C2	3.74	126.64	117.71
18	V	5	Y5P	C4-N3-C2	3.74	126.64	117.71
18	Y	15	Y5P	C4-N3-C2	3.74	126.64	117.71
18	Y	65	Y5P	C4-N3-C2	3.74	126.64	117.71
18	V	69	Y5P	C4-N3-C2	3.74	126.64	117.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	V	71	Y5P	C4-N3-C2	3.74	126.65	117.71
18	V	52	Y5P	C4-N3-C2	3.74	126.65	117.71
18	Y	38	Y5P	C4-N3-C2	3.74	126.66	117.71
18	Y	58	Y5P	C4-N3-C2	3.74	126.66	117.71
18	V	29	Y5P	C4-N3-C2	3.75	126.66	117.71
18	Y	64	Y5P	C4-N3-C2	3.75	126.66	117.71
18	V	38	Y5P	C4-N3-C2	3.75	126.66	117.71
18	Y	31	Y5P	C4-N3-C2	3.75	126.66	117.71
18	Y	24	Y5P	C4-N3-C2	3.75	126.66	117.71
18	Y	27	Y5P	C4-N3-C2	3.75	126.66	117.71
18	V	23	Y5P	C4-N3-C2	3.75	126.66	117.71
18	V	63	Y5P	C4-N3-C2	3.75	126.66	117.71
18	V	28	Y5P	C4-N3-C2	3.75	126.66	117.71
18	Y	30	Y5P	C4-N3-C2	3.75	126.67	117.71
18	Y	7	Y5P	C4-N3-C2	3.75	126.67	117.71
18	Y	53	Y5P	C4-N3-C2	3.75	126.67	117.71
18	V	27	Y5P	C4-N3-C2	3.75	126.67	117.71
18	Y	37	Y5P	C4-N3-C2	3.75	126.67	117.71
18	Y	71	Y5P	C4-N3-C2	3.75	126.67	117.71
18	V	58	Y5P	C4-N3-C2	3.75	126.67	117.71
18	Y	44	Y5P	C4-N3-C2	3.75	126.67	117.71
18	V	70	Y5P	C4-N3-C2	3.75	126.68	117.71
18	V	31	Y5P	C4-N3-C2	3.75	126.68	117.71
18	Y	10	Y5P	C4-N3-C2	3.75	126.68	117.71
18	V	14	Y5P	C4-N3-C2	3.76	126.68	117.71
18	Y	28	Y5P	C4-N3-C2	3.76	126.68	117.71
18	V	21	Y5P	C4-N3-C2	3.76	126.68	117.71
18	V	24	Y5P	C4-N3-C2	3.76	126.68	117.71
18	V	22	Y5P	C4-N3-C2	3.76	126.69	117.71
18	Y	6	Y5P	C4-N3-C2	3.76	126.69	117.71
18	V	57	Y5P	C4-N3-C2	3.76	126.69	117.71
18	Y	29	Y5P	C4-N3-C2	3.76	126.69	117.71
18	Y	22	Y5P	C4-N3-C2	3.76	126.69	117.71
18	V	26	Y5P	C4-N3-C2	3.76	126.69	117.71
18	Y	1	Y5P	C4-N3-C2	3.76	126.69	117.71
18	Y	70	Y5P	C4-N3-C2	3.76	126.69	117.71
18	Y	9	Y5P	C4-N3-C2	3.76	126.69	117.71
18	V	53	Y5P	C4-N3-C2	3.76	126.69	117.71
18	Y	5	Y5P	C4-N3-C2	3.76	126.69	117.71
18	V	64	Y5P	C4-N3-C2	3.76	126.69	117.71
18	Y	57	Y5P	C4-N3-C2	3.76	126.69	117.71
18	V	6	Y5P	C4-N3-C2	3.76	126.69	117.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	V	44	Y5P	C4-N3-C2	3.76	126.70	117.71
18	Y	26	Y5P	C4-N3-C2	3.76	126.70	117.71
18	Y	21	Y5P	C4-N3-C2	3.76	126.70	117.71
18	Y	63	Y5P	C4-N3-C2	3.76	126.70	117.71
18	V	15	Y5P	C4-N3-C2	3.77	126.71	117.71
18	V	10	Y5P	C4-N3-C2	3.77	126.71	117.71
18	V	65	Y5P	C4-N3-C2	3.77	126.71	117.71
18	V	30	Y5P	C4-N3-C2	3.77	126.71	117.71
18	Y	23	Y5P	C4-N3-C2	3.77	126.72	117.71
18	Y	69	Y5P	C4-N3-C2	3.77	126.73	117.71
18	V	37	Y5P	C4-N3-C2	3.78	126.73	117.71
18	Y	33	Y5P	C4-N3-C2	3.85	126.91	117.71
18	Y	39	Y5P	C4-N3-C2	3.91	127.04	117.71
18	V	50	Y5P	C4-N3-C2	3.92	127.07	117.71
19	X	20	Y5P	C4-N3-C2	3.94	127.11	117.71
18	Y	8	Y5P	C4-N3-C2	3.94	127.12	117.71
18	V	12	Y5P	C4-N3-C2	3.96	127.17	117.71
18	Y	32	Y5P	C4-N3-C2	3.97	127.18	117.71
19	X	17	Y5P	C4-N3-C2	3.98	127.21	117.71
18	V	8	Y5P	C4-N3-C2	4.00	127.27	117.71
18	Y	59	Y5P	C4-N3-C2	4.01	127.29	117.71
18	V	55	Y5P	C4-N3-C2	4.01	127.29	117.71
19	X	23	Y5P	C4-N3-C2	4.03	127.34	117.71
18	Y	12	Y5P	C4-N3-C2	4.03	127.35	117.71
18	Y	54	Y5P	C4-N3-C2	4.06	127.41	117.71
18	V	39	Y5P	C4-N3-C2	4.06	127.41	117.71
18	V	45	Y5P	C4-N3-C2	4.06	127.42	117.71
19	X	19	Y5P	C4-N3-C2	4.07	127.42	117.71
19	X	12	Y5P	C4-N3-C2	4.07	127.43	117.71
19	X	13	Y5P	C4-N3-C2	4.07	127.44	117.71
18	Y	60	Y5P	C4-N3-C2	4.08	127.45	117.71
18	Y	66	Y5P	C4-N3-C2	4.10	127.50	117.71
18	V	66	Y5P	C4-N3-C2	4.11	127.52	117.71
18	V	60	Y5P	C4-N3-C2	4.12	127.55	117.71
19	X	14	Y5P	C4-N3-C2	4.15	127.63	117.71
18	Y	55	Y5P	C4-N3-C2	4.17	127.67	117.71
18	V	51	Y5P	C4-N3-C2	4.18	127.69	117.71
18	Y	50	Y5P	C4-N3-C2	4.20	127.75	117.71
19	X	22	Y5P	C4-N3-C2	4.22	127.78	117.71
18	V	54	Y5P	C4-N3-C2	4.24	127.84	117.71
18	Y	51	Y5P	C4-N3-C2	4.25	127.86	117.71
18	V	32	Y5P	C4-N3-C2	4.28	127.94	117.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	X	24	Y5P	C4-N3-C2	4.28	127.94	117.71
19	X	15	Y5P	C4-N3-C2	4.29	127.97	117.71
18	V	59	Y5P	C4-N3-C2	4.43	128.30	117.71
18	Y	45	Y5P	C4-N3-C2	4.47	128.40	117.71
18	Y	34	P5P	C6-N1-C2	6.81	125.81	115.99
18	V	34	P5P	C6-N1-C2	6.91	125.96	115.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

99 monomers are involved in 136 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	V	10	Y5P	2	0
18	V	11	Y5P	1	0
18	V	12	Y5P	4	0
18	V	13	Y5P	4	0
18	V	14	Y5P	3	0
18	V	2	Y5P	1	0
18	V	23	Y5P	5	0
18	V	24	Y5P	4	0
18	V	25	Y5P	6	0
18	V	26	Y5P	6	0
18	V	27	Y5P	2	0
18	V	29	Y5P	2	0
18	V	3	Y5P	1	0
18	V	30	Y5P	3	0
18	V	31	Y5P	2	0
18	V	32	Y5P	2	0
18	V	33	Y5P	2	0
18	V	36	P5P	2	0
18	V	37	Y5P	2	0
18	V	41	Y5P	1	0
18	V	42	Y5P	2	0
18	V	43	Y5P	7	0
18	V	44	Y5P	6	0
18	V	48	Y5P	1	0
18	V	49	Y5P	2	0
18	V	50	Y5P	1	0
18	V	51	Y5P	1	0
18	V	52	Y5P	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	V	54	Y5P	5	0
18	V	55	Y5P	6	0
18	V	57	Y5P	4	0
18	V	58	Y5P	3	0
18	V	59	Y5P	1	0
18	V	60	Y5P	1	0
18	V	62	Y5P	1	0
18	V	63	Y5P	2	0
18	V	64	Y5P	1	0
18	V	66	Y5P	1	0
18	V	67	Y5P	2	0
18	V	68	Y5P	1	0
18	V	8	Y5P	4	0
18	V	9	Y5P	4	0
19	X	12	Y5P	1	0
19	X	14	Y5P	1	0
19	X	15	Y5P	1	0
19	X	16	Y5P	1	0
19	X	17	Y5P	1	0
19	X	18	Y5P	1	0
19	X	20	Y5P	3	0
19	X	21	Y5P	2	0
19	X	23	Y5P	1	0
19	X	24	Y5P	1	0
18	Y	14	Y5P	4	0
18	Y	15	Y5P	1	0
18	Y	22	Y5P	6	0
18	Y	23	Y5P	3	0
18	Y	24	Y5P	4	0
18	Y	25	Y5P	10	0
18	Y	26	Y5P	9	0
18	Y	27	Y5P	1	0
18	Y	28	Y5P	1	0
18	Y	29	Y5P	2	0
18	Y	3	Y5P	1	0
18	Y	30	Y5P	3	0
18	Y	31	Y5P	5	0
18	Y	32	Y5P	4	0
18	Y	33	Y5P	1	0
18	Y	34	P5P	1	0
18	Y	36	P5P	1	0
18	Y	37	Y5P	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	Y	38	Y5P	1	0
18	Y	39	Y5P	1	0
18	Y	40	Y5P	1	0
18	Y	42	Y5P	1	0
18	Y	43	Y5P	2	0
18	Y	44	Y5P	1	0
18	Y	51	Y5P	3	0
18	Y	52	Y5P	4	0
18	Y	53	Y5P	1	0
18	Y	54	Y5P	4	0
18	Y	55	Y5P	4	0
18	Y	56	Y5P	1	0
18	Y	57	Y5P	2	0
18	Y	58	Y5P	3	0
18	Y	59	Y5P	1	0
18	Y	6	Y5P	2	0
18	Y	60	Y5P	1	0
18	Y	61	Y5P	1	0
18	Y	62	Y5P	3	0
18	Y	63	Y5P	2	0
18	Y	66	Y5P	1	0
18	Y	67	Y5P	2	0
18	Y	68	Y5P	7	0
18	Y	69	Y5P	6	0
18	Y	7	Y5P	2	0
18	Y	70	Y5P	3	0
18	Y	71	Y5P	3	0
18	Y	8	Y5P	3	0
18	Y	9	Y5P	6	0

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	24,30,30	1.15	2 (8%)	26,47,47	1.92	4 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	GDP	g	500	37	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	g	500	GDP	C5-C4	3.20	1.47	1.40
39	g	500	GDP	C6-C5	3.29	1.48	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	g	500	GDP	C5-C6-N1	-4.72	117.36	123.52
39	g	500	GDP	N3-C2-N1	-3.19	123.22	127.56
39	g	500	GDP	C6-C5-C4	-3.15	117.26	120.86
39	g	500	GDP	C6-N1-C2	5.71	122.57	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.