



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:30 AM GMT

PDB ID : 2QEX
Title : Negamycin Binds to the Wall of the Nascent Chain Exit Tunnel of the 50S Ribosomal Subunit
Authors : Schroeder, S.J.; Blaha, G.
Deposited on : 2007-06-26
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

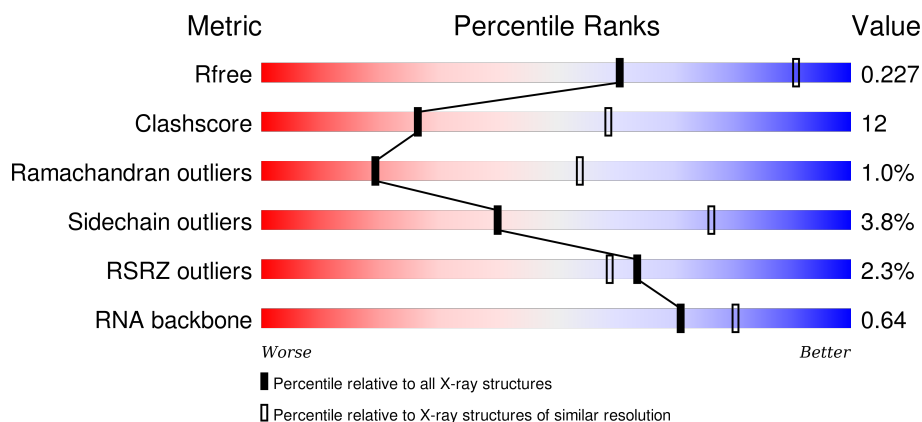
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)
RNA backbone	2183	1093 (3.30-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	2772	 61% 32% 6% .
2	9	122	 38% 50% 11% .
3	A	240	 71% 25% . .
4	B	338	 66% 31% .



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Mol	Chain	Length	Quality of chain
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	174	
11	J	145	
12	K	132	
13	L	165	
14	M	196	
15	N	187	
16	O	116	
17	P	149	
18	Q	96	
19	R	155	
20	S	85	
21	T	120	
22	U	67	
23	V	71	
24	W	154	
25	X	92	
26	Y	241	
27	Z	73	
28	1	57	
29	2	50	

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Mol	Chain	Length	Quality of chain
30	3	92	
31	I	162	

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
32	MG	0	8018	-	-	-	X
32	MG	0	8052	-	-	-	X
32	MG	0	8060	-	-	-	X
32	MG	0	8062	-	-	-	X
32	MG	0	8080	-	-	-	X
32	MG	0	8096	-	-	-	X
33	K	0	8401	-	-	-	X
34	NA	0	8503	-	-	-	X
34	NA	0	8510	-	-	-	X
34	NA	0	8514	-	-	-	X
34	NA	0	8520	-	-	-	X
34	NA	0	8521	-	-	-	X
34	NA	0	8523	-	-	-	X
34	NA	0	8526	-	-	-	X
34	NA	0	8527	-	-	-	X
34	NA	0	8535	-	-	-	X
34	NA	0	8559	-	-	-	X
34	NA	0	8561	-	-	-	X
34	NA	0	8562	-	-	-	X
34	NA	0	8564	-	-	-	X
34	NA	0	8565	-	-	-	X
34	NA	0	8566	-	-	-	X
34	NA	0	8568	-	-	-	X
34	NA	0	8571	-	-	-	X
34	NA	0	8572	-	-	-	X
34	NA	0	8573	-	-	-	X
34	NA	0	8576	-	-	-	X
34	NA	0	8577	-	-	-	X
34	NA	0	8578	-	-	-	X
34	NA	0	8582	-	-	-	X
34	NA	L	8580	-	-	-	X
34	NA	R	8586	-	-	-	X
36	NEG	0	8823	-	-	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99020 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59021	26350	10878	19048	2745			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
9	3073	G	A	CONFLICT	GB 6468293
9	3106	C	U	CONFLICT	GB 6468293

- Molecule 3 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	237	Total	C	N	O	S	0	0	0
			1753	1072	352	324	5			

- Molecule 4 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	337	Total	C	N	O	S	0	0	0
			2625	1616	493	511	5			

- Molecule 5 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	246	Total	C	N	O	S	0	0	0
			1859	1131	344	383	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	73	LEU	GLN	CONFLICT	UNP P12735

- Molecule 6 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	140	Total	C	N	O	S	0	0	0
			1094	685	195	210	4			

- Molecule 7 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	172	Total	C	N	O	S	0	0	0
			1357	840	224	289	4			

- Molecule 8 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	119	Total	C	N	O	S	0	0	0
			890	551	141	197	1			

- Molecule 9 is a protein called Acidic ribosomal protein P0 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	29	Total	C	N	O	S	0	0	0
			240	149	39	51	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	248	ASP	ALA	CONFLICT	UNP P15825

- Molecule 10 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	160	Total	C	N	O	S	0	0	0
			1266	785	237	238	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	164	ASP	-	INSERTION	UNP P60617
H	165	SER	LYS	CONFLICT	UNP P60617
H	166	SER	VAL	CONFLICT	UNP P60617
H	167	PRO	GLU	CONFLICT	UNP P60617
H	168	ALA	ARG	CONFLICT	UNP P60617
H	?	-	GLU	DELETION	UNP P60617
H	?	-	GLU	DELETION	UNP P60617
H	?	-	LEU	DELETION	UNP P60617
H	?	-	LEU	DELETION	UNP P60617
H	170	ASN	ILE	CONFLICT	UNP P60617

- Molecule 11 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 12 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	132	Total	C	N	O	S	0	0	0
			992	609	187	192	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	HIS	CONFLICT	UNP P22450

- Molecule 13 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	145	Total	C	N	O		0	0	0
			1118	670	222	226				

- Molecule 14 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	M	194	Total	C	N	O	S	0	0	0
			1559	943	332	283	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	CONFLICT	UNP P60618
M	194	ALA	GLY	CONFLICT	UNP P60618

- Molecule 15 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 16 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	115	Total	C	N	O		0	0	0
			865	529	161	175				

- Molecule 17 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	143	Total	C	N	O		0	0	0
			1136	683	229	224				

- Molecule 18 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	95	Total	C	N	O		0	0	0
			735	450	141	144				

- Molecule 19 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	150	Total	C	N	O	S	0	0	0
			1149	713	209	223	4			

- Molecule 20 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	81	Total	C	N	O	S	0	0	0
			641	389	111	138	3			

- Molecule 21 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	T	119	Total	C	N	O			
			950	568	180	202	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	U	53	Total	C	N	O	S			
			410	244	75	86	5	0	0	0

- Molecule 23 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	V	65	Total	C	N	O	S			
			499	304	94	100	1	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	W	154	Total	C	N	O	S			
			1196	737	209	244	6	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	X	82	Total	C	N	O	S			
			654	402	129	122	1	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	Y	142	Total	C	N	O			
			1130	686	228	216	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Z	73	Total	C	N	O	S			
			579	346	116	112	5	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	SER	CONFLICT	UNP P60619

- Molecule 28 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 29 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 30 is a protein called 50S ribosomal protein L44e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	1			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	108	Total	Mg	0	0
			108	108		
32	Y	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	A	2	Total	Mg	0	0
			2	2		
32	T	1	Total	Mg	0	0
			1	1		
32	9	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	3	1	Total	Mg	0	0
			1	1		

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	2	Total	K	0	0
			2	2		

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	72	Total	Na	0	0
			72	72		
34	J	1	Total	Na	0	0
			1	1		
34	Q	1	Total	Na	0	0
			1	1		
34	H	1	Total	Na	0	0
			1	1		
34	C	1	Total	Na	0	0
			1	1		
34	A	1	Total	Na	0	0
			1	1		
34	R	3	Total	Na	0	0
			3	3		
34	9	3	Total	Na	0	0
			3	3		
34	L	1	Total	Na	0	0
			1	1		
34	S	1	Total	Na	0	0
			1	1		
34	M	1	Total	Na	0	0
			1	1		

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

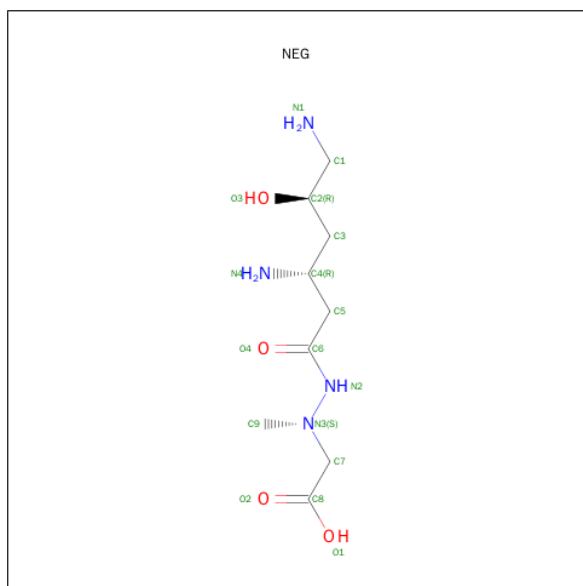
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	10	Total	Cl	0	0
			10	10		
35	J	3	Total	Cl	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	Q	1	Total	Cl	0	0
			1	1		
35	B	1	Total	Cl	0	0
			1	1		
35	A	1	Total	Cl	0	0
			1	1		
35	N	1	Total	Cl	0	0
			1	1		
35	O	1	Total	Cl	0	0
			1	1		
35	R	1	Total	Cl	0	0
			1	1		
35	L	1	Total	Cl	0	0
			1	1		
35	3	1	Total	Cl	0	0
			1	1		
35	M	1	Total	Cl	0	0
			1	1		

- Molecule 36 is NEGAMYCIN (three-letter code: NEG) (formula: $C_9H_{20}N_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	0	1	Total	C	N	O	0	0
			17	9	4	4		

- Molecule 37 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	O	1	Total Cd 1 1	0	0
37	Z	1	Total Cd 1 1	0	0
37	1	1	Total Cd 1 1	0	0
37	3	1	Total Cd 1 1	0	0
37	U	1	Total Cd 1 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	0	5923	Total O 5923 5923	0	0
38	9	142	Total O 142 142	0	0
38	A	112	Total O 112 112	0	0
38	B	137	Total O 137 137	0	0
38	C	167	Total O 167 167	0	0
38	D	44	Total O 44 44	0	0
38	E	45	Total O 45 45	0	0
38	F	27	Total O 27 27	0	0
38	G	16	Total O 16 16	0	0
38	H	70	Total O 70 70	0	0
38	J	51	Total O 51 51	0	0
38	K	57	Total O 57 57	0	0
38	L	85	Total O 85 85	0	0
38	M	122	Total O 122 122	0	0
38	N	61	Total O 61 61	0	0

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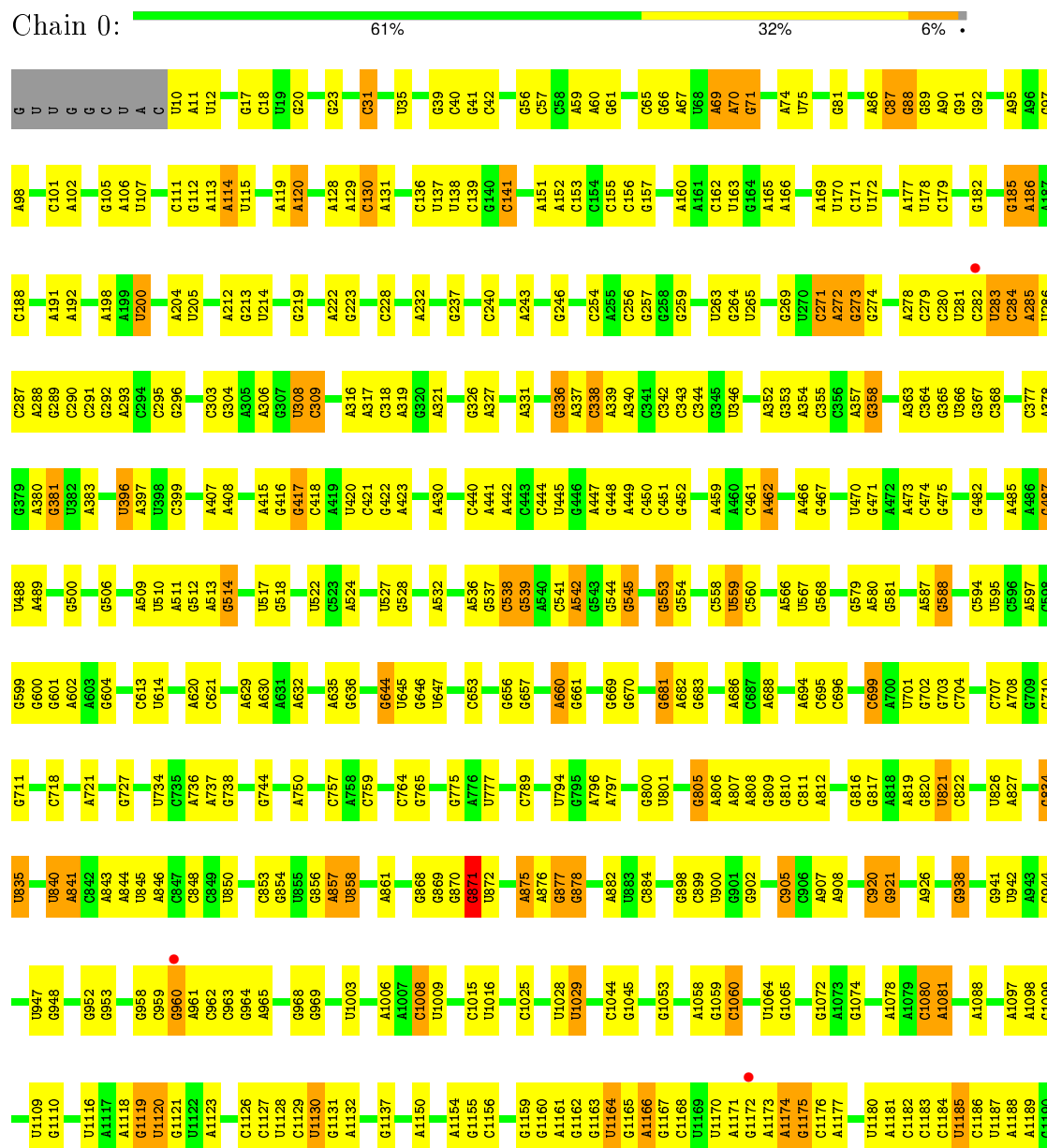
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	O	38	Total 38	O 38	0	0
38	P	63	Total 63	O 63	0	0
38	Q	50	Total 50	O 50	0	0
38	R	85	Total 85	O 85	0	0
38	S	39	Total 39	O 39	0	0
38	T	30	Total 30	O 30	0	0
38	U	28	Total 28	O 28	0	0
38	V	11	Total 11	O 11	0	0
38	W	69	Total 69	O 69	0	0
38	X	24	Total 24	O 24	0	0
38	Y	87	Total 87	O 87	0	0
38	Z	30	Total 30	O 30	0	0
38	1	60	Total 60	O 60	0	0
38	2	36	Total 36	O 36	0	0
38	3	74	Total 74	O 74	0	0
38	I	5	Total 5	O 5	0	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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

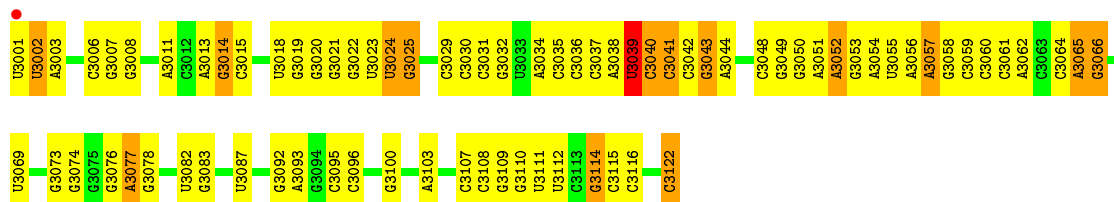
• Molecule 1: 23S ribosomal RNA



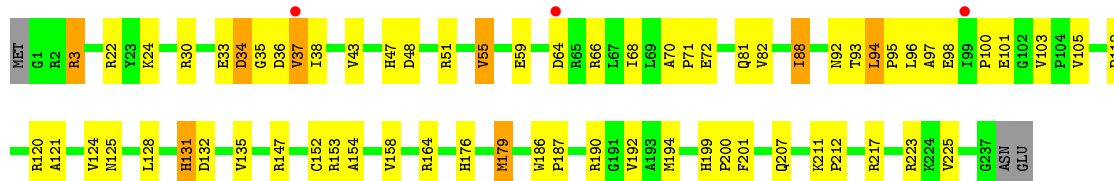




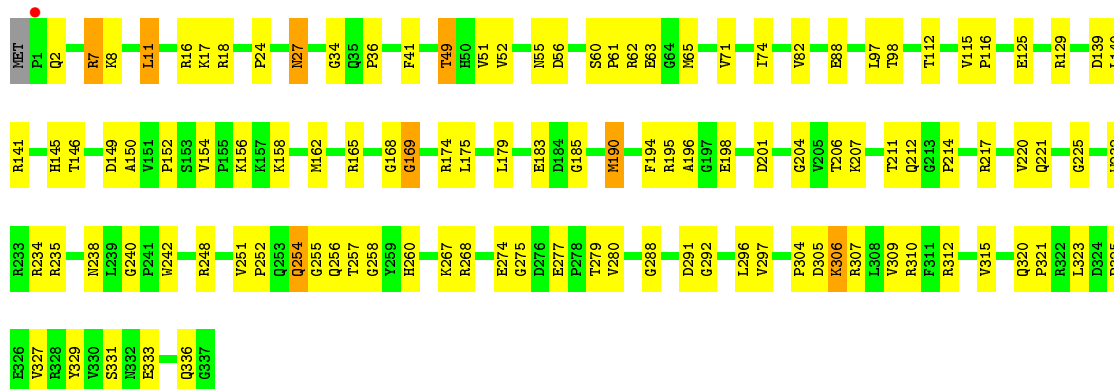
- Molecule 2: 5S ribosomal RNA



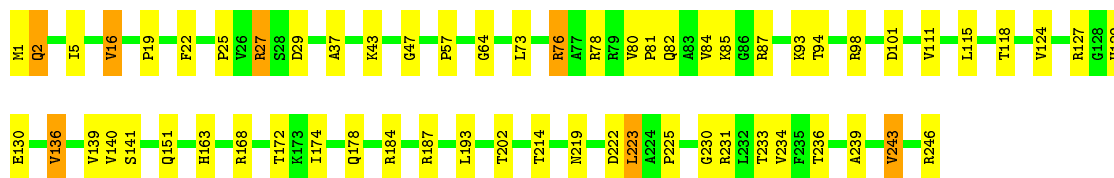
- Molecule 3: 50S ribosomal protein L2P



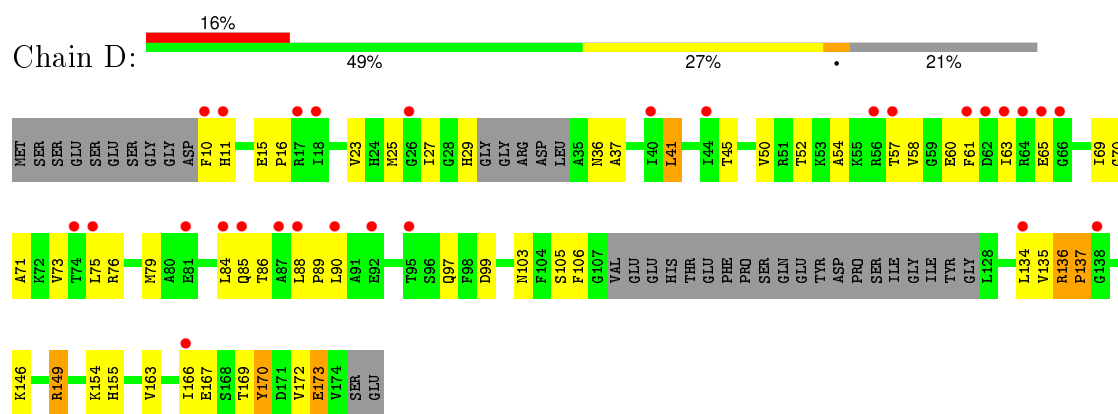
- Molecule 4: 50S ribosomal protein L3P



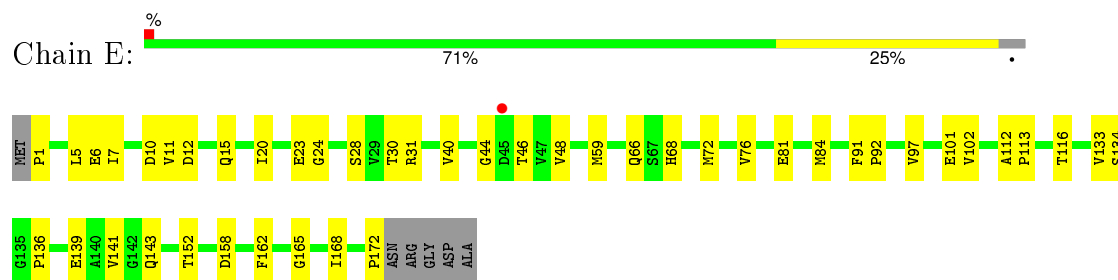
- Molecule 5: 50S ribosomal protein L4P



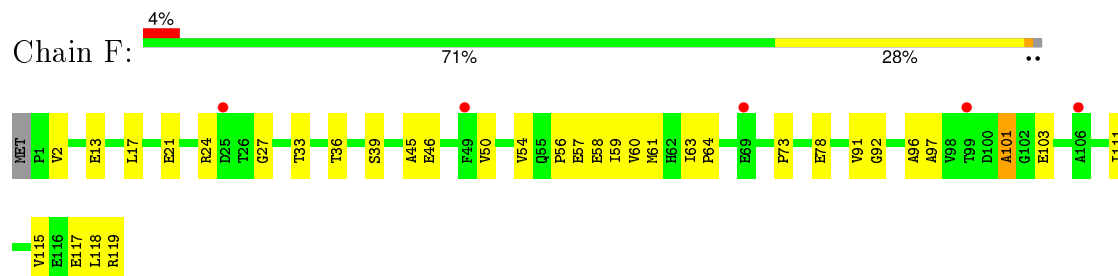
- Molecule 6: 50S ribosomal protein L5P



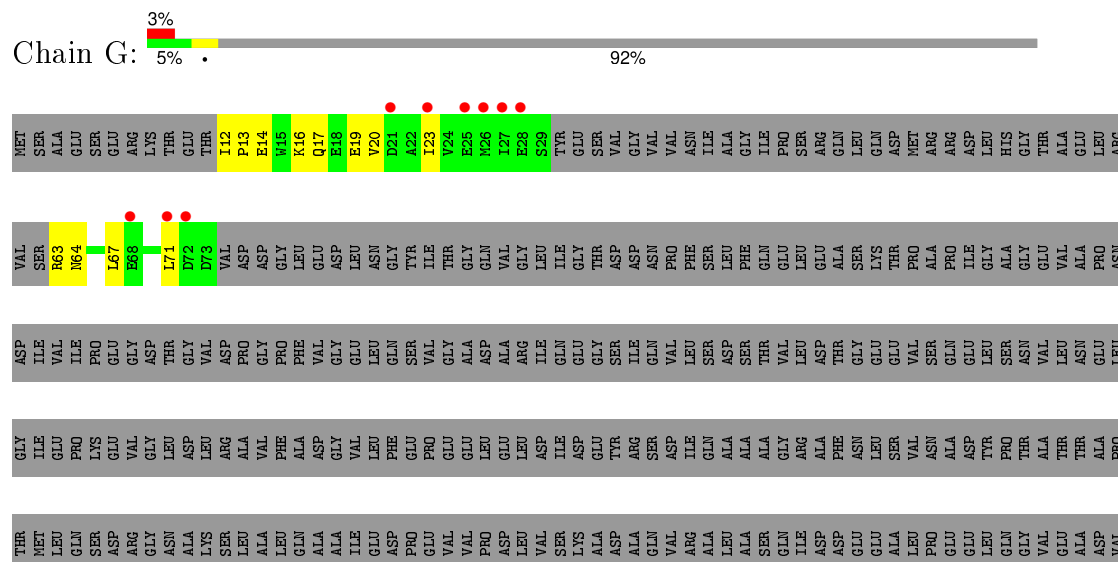
- Molecule 7: 50S ribosomal protein L6P



- Molecule 8: 50S ribosomal protein L7Ae



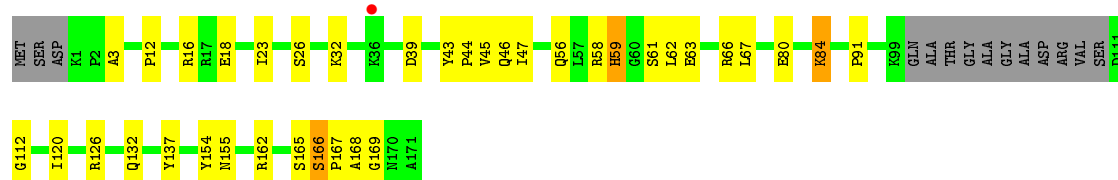
- Molecule 9: Acidic ribosomal protein P0 homolog



ALA THR GLU GLU PRO THR ASP ASP GLN ASP ASP ASP THR ALA SER GLU ASP ASP ALA ASP ALA ASP ASP ALA GLU GLU ALA ASP ASP ASP ASP ASP GLU ALA GLY ALA LEU GLY ALA MET PHE

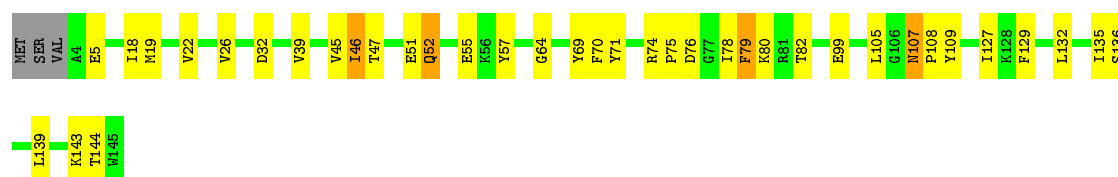
• Molecule 10: 50S ribosomal protein L10e

Chain H:  71% 20% 8%




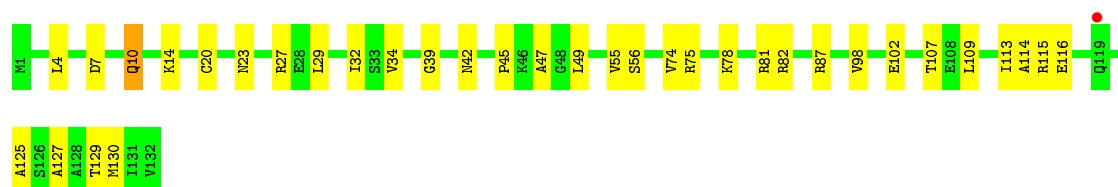
• Molecule 11: 50S ribosomal protein L13P

Chain J:  72% 23% 5%



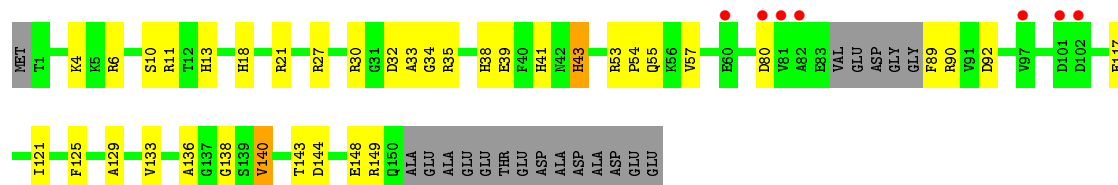
• Molecule 12: 50S ribosomal protein L14P

Chain K:  73% 26% 1%




• Molecule 13: 50S ribosomal protein L15P

Chain L:  65% 21% 12% 4%



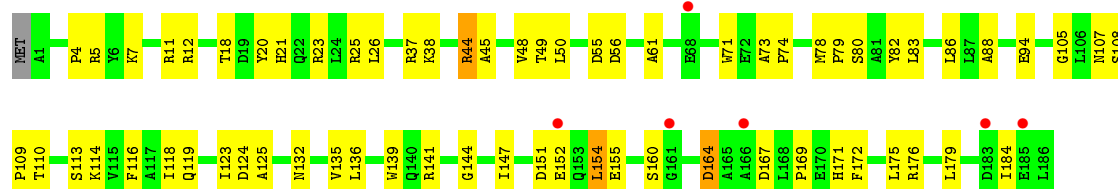
• Molecule 14: 50S ribosomal protein L15e

Chain M:  72% 25% 3%

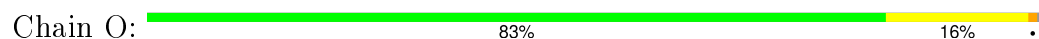




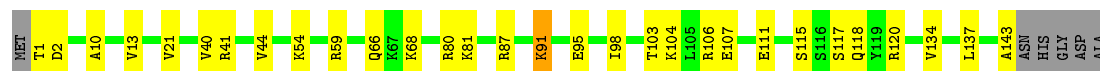
- Molecule 15: 50S ribosomal protein L18P



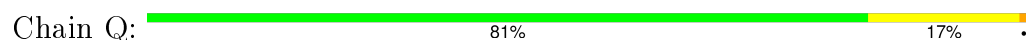
- Molecule 16: 50S ribosomal protein L18e



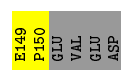
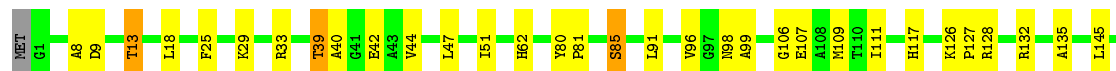
- Molecule 17: 50S ribosomal protein L19e



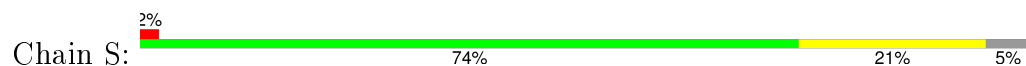
- Molecule 18: 50S ribosomal protein L21e



- Molecule 19: 50S ribosomal protein L22P

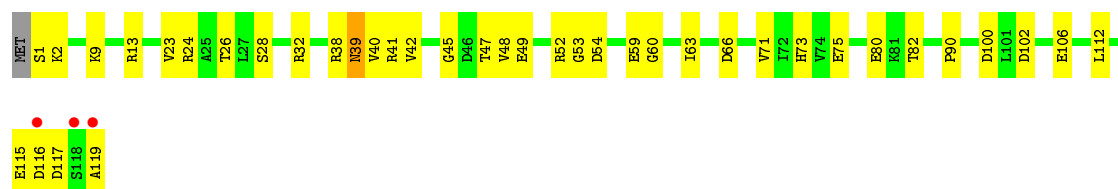


- Molecule 20: 50S ribosomal protein L23P

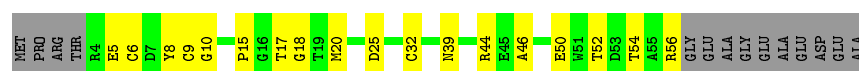




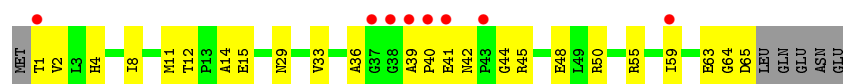
- Molecule 21: 50S ribosomal protein L24P



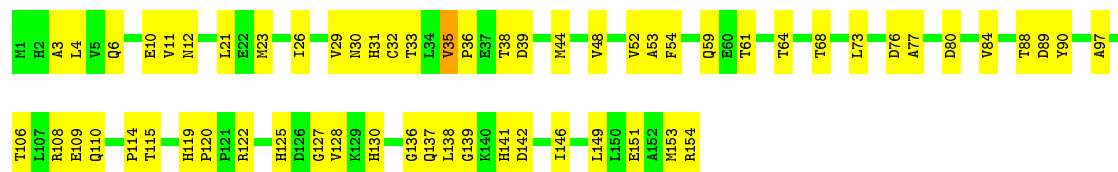
- Molecule 22: 50S ribosomal protein L24e



- Molecule 23: 50S ribosomal protein L29P



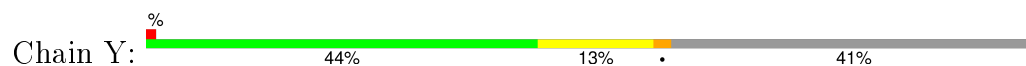
- Molecule 24: 50S ribosomal protein L30P

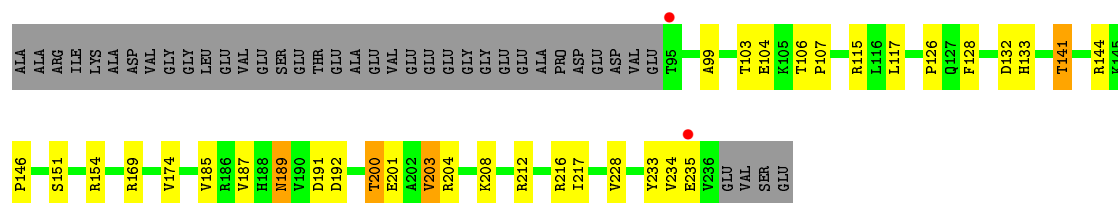


- Molecule 25: 50S ribosomal protein L31e



- Molecule 26: 50S ribosomal protein L32e





- Molecule 27: 50S ribosomal protein L37Ae

Chain Z: 75% 21% .



- Molecule 28: 50S ribosomal protein L37e

Chain 1: 74% 25% .



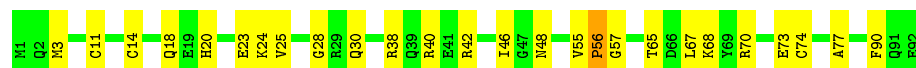
- Molecule 29: 50S ribosomal protein L39e

Chain 2: 6% 56% 36% 8%



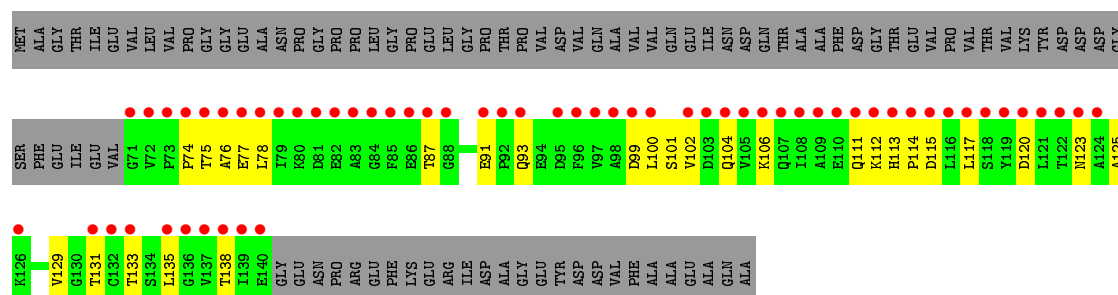
- Molecule 30: 50S ribosomal protein L44e

Chain 3: 72% 27% .



- Molecule 31: 50S ribosomal protein L11P

Chain I: 37% 26% 17% 57%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	214.62Å 304.05Å 578.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.92 – 2.90 86.68 – 2.43	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.92-2.90) 90.6 (86.68-2.43)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.77Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.204 , 0.241 0.194 , 0.227	Depositor DCC
R_{free} test set	4062 reflections (1.06%)	DCC
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 68.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 453193 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	99020	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, NEG, K, UR3, CD, OMU, NA, 1MA, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.38	0/65959	0.69	10/102870 (0.0%)
2	9	0.35	0/2905	0.71	1/4528 (0.0%)
3	A	0.34	0/1786	0.64	0/2408
4	B	0.32	0/2690	0.64	0/3652
5	C	0.36	0/1884	0.63	0/2551
6	D	0.33	0/1111	0.57	0/1498
7	E	0.33	0/1382	0.57	0/1880
8	F	0.35	0/901	0.58	0/1224
9	G	0.35	0/241	0.52	0/324
10	H	0.34	0/1287	0.65	1/1725 (0.1%)
11	J	0.35	0/1136	0.60	0/1530
12	K	0.35	0/1001	0.65	0/1347
13	L	0.33	0/1130	0.65	0/1509
14	M	0.35	0/1583	0.61	0/2119
15	N	0.30	0/1474	0.65	0/1999
16	O	0.34	0/874	0.62	1/1181 (0.1%)
17	P	0.35	0/1147	0.53	0/1528
18	Q	0.37	0/749	0.67	0/1005
19	R	0.40	0/1172	0.65	0/1578
20	S	0.34	0/648	0.57	0/875
21	T	0.32	0/958	0.62	0/1289
22	U	0.36	0/417	0.53	0/562
23	V	0.31	0/502	0.55	0/675
24	W	0.34	0/1219	0.63	0/1655
25	X	0.35	0/664	0.60	0/895
26	Y	0.35	0/1146	0.62	0/1536
27	Z	0.35	0/590	0.63	0/787
28	1	0.41	0/438	0.66	0/578
29	2	0.36	0/401	0.57	0/529
30	3	0.37	0/771	0.57	0/1024
31	I	0.34	0/526	0.53	0/716
All	All	0.37	0/98692	0.67	13/147577 (0.0%)

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
1	0	1	37
2	9	0	2
All	All	1	39

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	805	G	C2'-C3'-O3'	7.33	125.62	109.50
1	0	1942	A	C5'-C4'-C3'	6.85	126.95	116.00
1	0	871	G	C5'-C4'-O4'	-5.95	101.95	109.10
2	9	3039	U	N1-C1'-C2'	5.83	121.57	114.00
1	0	1942	A	C5'-C4'-O4'	5.80	116.06	109.10
1	0	1504	A	C1'-O4'-C4'	-5.67	105.36	109.90
1	0	1120	U	C5'-C4'-C3'	-5.56	107.11	116.00
10	H	112	GLY	N-CA-C	-5.55	99.22	113.10
1	0	1504	A	N9-C1'-C2'	5.47	121.11	114.00
1	0	841	A	C1'-O4'-C4'	-5.46	105.53	109.90
1	0	2726	U	N1-C1'-C2'	5.21	120.78	114.00
1	0	2291	A	N9-C1'-C2'	5.13	120.67	114.00
16	O	66	GLY	N-CA-C	5.07	125.78	113.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	805	G	C3'

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1078	A	Sidechain
1	0	1237	U	Sidechain
1	0	1304	U	Sidechain
1	0	1309	U	Sidechain
1	0	1340	G	Sidechain
1	0	1359	U	Sidechain
1	0	1368	U	Sidechain
1	0	1376	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	1430	G	Sidechain
1	0	1684	A	Sidechain
1	0	1777	G	Sidechain
1	0	1829	A	Sidechain
1	0	1839	A	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1972	U	Sidechain
1	0	1993	C	Sidechain
1	0	2115	U	Sidechain
1	0	23	G	Sidechain
1	0	2313	C	Sidechain
1	0	246	G	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2538	A	Sidechain
1	0	2552	C	Sidechain
1	0	2564	G	Sidechain
1	0	2842	G	Sidechain
1	0	396	U	Sidechain
1	0	462	A	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	858	U	Sidechain
1	0	900	U	Sidechain
2	9	3039	U	Sidechain
2	9	3087	U	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29810	1019	0
2	9	2600	0	1326	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1753	0	1766	61	0
4	B	2625	0	2533	85	0
5	C	1859	0	1816	53	0
6	D	1094	0	1085	39	0
7	E	1357	0	1266	32	0
8	F	890	0	843	24	0
9	G	240	0	231	12	0
10	H	1266	0	1268	31	0
11	J	1120	0	1098	36	0
12	K	992	0	1031	36	0
13	L	1118	0	1076	33	0
14	M	1559	0	1568	38	0
15	N	1445	0	1401	63	0
16	O	865	0	873	21	0
17	P	1136	0	1123	24	0
18	Q	735	0	729	12	0
19	R	1149	0	1122	29	0
20	S	641	0	605	15	0
21	T	950	0	923	27	0
22	U	410	0	364	19	0
23	V	499	0	511	17	0
24	W	1196	0	1137	54	0
25	X	654	0	653	22	0
26	Y	1130	0	1133	35	0
27	Z	579	0	539	19	0
28	1	431	0	426	19	0
29	2	396	0	413	18	0
30	3	755	0	730	19	0
31	I	519	0	500	30	0
32	0	108	0	0	0	0
32	3	1	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	2	0	0	0	0
34	0	72	0	0	1	0
34	9	3	0	0	0	0
34	A	1	0	0	0	0
34	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	H	1	0	0	0	0
34	J	1	0	0	0	0
34	L	1	0	0	1	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	3	0	0	0	0
34	S	1	0	0	0	0
35	0	10	0	0	1	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	2	0
35	L	1	0	0	0	0
35	M	1	0	0	1	0
35	N	1	0	0	1	0
35	O	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
36	0	17	0	19	5	0
37	1	1	0	0	0	0
37	3	1	0	0	1	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5923	0	0	177	0
38	1	60	0	0	2	0
38	2	36	0	0	3	0
38	3	74	0	0	6	0
38	9	142	0	0	14	0
38	A	112	0	0	7	0
38	B	137	0	0	14	0
38	C	167	0	0	10	0
38	D	44	0	0	5	0
38	E	45	0	0	3	0
38	F	27	0	0	2	0
38	G	16	0	0	1	0
38	H	70	0	0	5	0
38	I	5	0	0	2	0
38	J	51	0	0	3	0
38	K	57	0	0	6	0
38	L	85	0	0	11	0
38	M	122	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	N	61	0	0	7	0
38	O	38	0	0	5	0
38	P	63	0	0	1	0
38	Q	50	0	0	1	0
38	R	85	0	0	5	0
38	S	39	0	0	4	0
38	T	30	0	0	1	0
38	U	28	0	0	1	0
38	V	11	0	0	1	0
38	W	69	0	0	3	0
38	X	24	0	0	2	0
38	Y	87	0	0	7	0
38	Z	30	0	0	2	0
All	All	99020	0	59918	1837	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 12.

All (1837) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1160:G:C5'	1:0:1161:A:H5'	1.70	1.22
1:0:871:G:C8	1:0:871:G:H5'	1.81	1.14
2:9:3006:C:H5''	15:N:37:ARG:NH1	1.63	1.12
1:0:871:G:H8	1:0:871:G:H5'	1.10	1.11
1:0:656:G:H5'	16:O:3:THR:HG22	1.18	1.10
1:0:541:C:H2'	1:0:542:A:H5''	1.32	1.09
2:9:3006:C:H5''	15:N:37:ARG:HH12	0.94	1.09
1:0:1160:G:H5'	1:0:1161:A:C5'	1.82	1.07
1:0:1242:A:H5'	11:J:82:THR:HG23	1.33	1.05
10:H:46:GLN:HB3	10:H:167:PRO:HD2	1.38	1.05
2:9:3056:A:H2'	2:9:3057:A:H5''	1.40	1.03
1:0:1559:A:H1'	38:O:5694:HOH:O	1.58	1.02
1:0:2717:C:H2'	1:0:2718:C:H5''	1.41	1.02
1:0:2812:A:H2	1:0:2814:A:H62	1.05	1.02
2:9:3076:G:H3'	2:9:3077:A:H5''	1.41	1.01
2:9:3029:C:H2'	2:9:3030:C:H5'	1.43	1.00
1:0:2533:C:H5'	1:0:2533:C:H6	1.26	0.99
1:0:1474:C:H6	1:0:1474:C:H5'	1.21	0.98
12:K:10:GLN:H	12:K:10:GLN:HE21	1.07	0.98
1:0:282:C:H1'	1:0:368:C:N4	1.78	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:541:C:C2'	1:0:542:A:H5''	1.94	0.98
1:0:2672:C:H1'	38:B:8925:HOH:O	1.62	0.98
10:H:166:SER:HB2	10:H:167:PRO:HD3	1.45	0.97
1:0:2533:C:C6	1:0:2533:C:H5'	1.98	0.97
1:0:271:C:H41	1:0:378:A:H2	1.07	0.97
1:0:871:G:H8	1:0:871:G:C5'	1.79	0.96
1:0:2717:C:C2'	1:0:2718:C:H5''	1.95	0.96
1:0:1372:A:H3'	38:0:7013:HOH:O	1.64	0.95
1:0:1160:G:H5'	1:0:1161:A:H5'	0.96	0.95
1:0:1751:G:H2'	1:0:1752:G:H5''	1.45	0.95
25:X:43:VAL:HG13	25:X:76:ARG:HH12	1.31	0.95
1:0:542:A:H5'	1:0:542:A:H8	1.30	0.95
1:0:1189:A:H1'	1:0:1209:C:O4'	1.66	0.94
21:T:71:VAL:HG11	21:T:90:PRO:HB3	1.46	0.94
1:0:558:C:C2'	1:0:559:U:H5''	1.98	0.94
1:0:559:U:H5'	1:0:559:U:H6	1.31	0.94
1:0:656:G:H5'	16:O:3:THR:CG2	1.98	0.94
1:0:558:C:H2'	1:0:559:U:H5''	1.50	0.93
26:Y:187:VAL:HG23	26:Y:192:ASP:HB2	1.49	0.93
1:0:282:C:O2'	1:0:283:U:H5'	1.68	0.93
10:H:3:ALA:HA	10:H:58:ARG:HH12	1.33	0.93
1:0:1667:A:H8	1:0:1667:A:H5'	1.31	0.92
1:0:2489:G:H1'	38:0:7099:HOH:O	1.67	0.92
1:0:2291:A:C8	1:0:2309:C:H5'	2.05	0.91
1:0:2559:C:H4'	38:0:7080:HOH:O	1.71	0.91
1:0:156:C:H5''	14:M:171:ARG:HD3	1.51	0.91
1:0:1474:C:C6	1:0:1474:C:H5'	2.06	0.90
19:R:8:ALA:HB1	19:R:13:THR:HG21	1.53	0.90
1:0:2506:A:HO2'	1:0:2507:G:H8	0.92	0.90
30:3:74:CYS:HG	37:3:8704:CD:CD	0.92	0.89
1:0:962:C:H1'	15:N:5:ARG:NH1	1.87	0.89
1:0:2783:A:H3'	38:0:5060:HOH:O	1.73	0.89
24:W:137:GLN:HE21	24:W:141:HIS:HE1	1.18	0.89
4:B:162:MET:SD	4:B:310:ARG:HD3	2.13	0.89
1:0:545:G:H8	1:0:545:G:H5'	1.37	0.88
1:0:1441:G:H1'	38:0:7584:HOH:O	1.72	0.88
24:W:21:LEU:HD22	24:W:26:ILE:HD11	1.56	0.87
1:0:1329:A:H2	38:0:4515:HOH:O	1.58	0.87
1:0:69:A:H5'	1:0:69:A:H8	1.39	0.87
1:0:1666:C:O2'	1:0:1667:A:H5''	1.74	0.86
1:0:2694:A:H4'	7:E:91:PHE:CE1	2.10	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:29:LEU:HB3	12:K:55:VAL:HG11	1.57	0.86
1:0:182:G:H5'	38:0:4986:HOH:O	1.74	0.85
1:0:214:U:H5'	38:0:5968:HOH:O	1.76	0.85
1:0:2004:U:H4'	38:0:5134:HOH:O	1.77	0.85
1:0:1701:A:H4'	1:0:1702:U:H5''	1.57	0.84
1:0:1835:U:H5	1:0:1840:A:N7	1.74	0.84
1:0:2769:C:C2'	1:0:2770:G:H5'	2.08	0.84
1:0:1118:A:C8	1:0:1118:A:H3'	2.13	0.83
1:0:1919:A:H4'	38:0:4681:HOH:O	1.75	0.83
1:0:2908:A:H2'	1:0:2909:G:O4'	1.77	0.83
2:9:3056:A:C2'	2:9:3057:A:H5''	2.09	0.83
1:0:544:G:H2'	1:0:545:G:H5''	1.60	0.83
1:0:1450:C:H4'	1:0:1451:C:OP2	1.76	0.83
1:0:272:A:H5'	1:0:273:G:OP2	1.77	0.83
1:0:2533:C:H6	1:0:2533:C:C5'	1.90	0.83
1:0:1165:G:H4'	1:0:1174:A:O2'	1.79	0.83
6:D:134:LEU:HD11	6:D:166:ILE:HD11	1.61	0.83
1:0:1979:G:H2'	38:0:3110:HOH:O	1.78	0.83
23:V:12:THR:HG22	23:V:15:GLU:HG3	1.60	0.82
1:0:69:A:H5'	1:0:69:A:C8	2.14	0.82
1:0:1206:U:H5'	1:0:1206:U:H6	1.42	0.82
1:0:1118:A:H3'	1:0:1118:A:H8	1.43	0.82
1:0:1116:U:O2'	1:0:1118:A:H2	1.62	0.82
1:0:656:G:H3'	16:O:37:ARG:HH12	1.45	0.81
1:0:380:A:H2'	38:0:7050:HOH:O	1.79	0.81
2:9:3049:G:H5''	38:9:4707:HOH:O	1.80	0.81
1:0:1205:U:H2'	1:0:1206:U:C5'	2.11	0.81
1:0:2756:U:H3	1:0:2896:A:H2	1.28	0.80
17:P:115:SER:H	17:P:118:GLN:NE2	1.80	0.80
1:0:558:C:H2'	1:0:559:U:C5'	2.12	0.80
1:0:962:C:H1'	15:N:5:ARG:HH12	1.47	0.80
1:0:1180:U:H1'	38:0:3053:HOH:O	1.81	0.80
1:0:506:G:H22	1:0:509:A:H5'	1.47	0.80
1:0:711:G:H1'	38:0:6919:HOH:O	1.81	0.80
4:B:55:ASN:HB3	4:B:63:GLU:HA	1.63	0.80
1:0:1205:U:H2'	1:0:1206:U:H5''	1.62	0.80
11:J:107:ASN:HD22	11:J:109:TYR:H	1.27	0.80
3:A:211:LYS:HB3	3:A:212:PRO:HD2	1.64	0.80
1:0:1189:A:H3'	38:0:7501:HOH:O	1.82	0.79
1:0:2851:G:O2'	1:0:2852:A:H5'	1.82	0.79
1:0:2896:A:H5''	38:0:5925:HOH:O	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3006:C:C5'	15:N:37:ARG:NH1	2.43	0.79
1:0:870:G:H2'	1:0:871:G:H5''	1.63	0.79
2:9:3092:G:H2'	2:9:3093:A:C8	2.17	0.79
1:0:656:G:C5'	16:O:3:THR:HG22	2.09	0.78
1:0:2526:C:O2'	1:0:2527:U:H5'	1.83	0.78
15:N:71:TRP:CE3	15:N:175:LEU:HD22	2.18	0.78
2:9:3029:C:C2'	2:9:3030:C:H5'	2.14	0.78
1:0:2508:C:H2'	38:0:6580:HOH:O	1.83	0.78
7:E:20:ILE:HD11	7:E:40:VAL:HG11	1.64	0.78
5:C:139:VAL:HG13	38:C:8641:HOH:O	1.82	0.78
1:0:681:G:N3	1:0:681:G:H5'	1.98	0.78
1:0:871:G:C8	1:0:871:G:C5'	2.57	0.78
1:0:542:A:H5'	1:0:542:A:C8	2.17	0.78
1:0:2769:C:O2'	1:0:2770:G:H5'	1.83	0.78
17:P:59:ARG:HH22	17:P:66:GLN:HE22	1.31	0.77
1:0:926:A:H4'	13:L:39:GLU:HG2	1.65	0.77
1:0:1185:U:H5'	38:0:7289:HOH:O	1.84	0.77
1:0:1527:A:H1'	1:0:1528:A:C8	2.20	0.77
1:0:877:G:H5'	1:0:878:G:OP1	1.85	0.77
1:0:2426:G:H1'	38:0:5918:HOH:O	1.84	0.77
1:0:2502:C:C2'	1:0:2503:A:H5'	2.14	0.77
1:0:848:C:H5'	38:0:7096:HOH:O	1.84	0.77
4:B:212:GLN:HB2	4:B:257:THR:HG21	1.67	0.77
3:A:153:ARG:HH11	3:A:153:ARG:HB2	1.49	0.77
1:0:111:C:O2'	28:1:20:ARG:HG2	1.83	0.77
1:0:1603:A:H5'	1:0:1605:G:O4'	1.85	0.77
1:0:2506:A:O2'	1:0:2507:G:H8	1.68	0.76
24:W:137:GLN:HE21	24:W:141:HIS:CE1	2.01	0.76
1:0:1666:C:H2'	1:0:1667:A:H5'	1.68	0.76
1:0:1116:U:HO2'	1:0:1118:A:H2	0.81	0.76
1:0:130:C:H2'	38:0:9977:HOH:O	1.85	0.76
4:B:36:PRO:HA	4:B:168:GLY:HA3	1.67	0.76
1:0:1328:A:OP1	26:Y:169:ARG:HD2	1.86	0.76
24:W:4:LEU:HD22	24:W:52:VAL:HG21	1.68	0.75
30:3:25:VAL:HG22	30:3:68:LYS:HG3	1.67	0.75
3:A:88:ILE:HD13	3:A:100:PRO:HD3	1.68	0.75
5:C:127:ARG:NH2	5:C:225:PRO:HG2	2.01	0.75
1:0:541:C:H2'	1:0:542:A:C5'	2.15	0.75
26:Y:189:ASN:HD22	26:Y:191:ASP:H	1.34	0.75
1:0:1667:A:C8	1:0:1667:A:H5'	2.21	0.75
1:0:2851:G:C2'	1:0:2852:A:H5'	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:0:5050:HOH:O	12:K:39:GLY:HA2	1.86	0.75
1:0:2694:A:H4'	7:E:91:PHE:HE1	1.50	0.74
1:0:1377:C:H1'	38:0:3564:HOH:O	1.87	0.74
1:0:1166:A:H61	1:0:1180:U:H3	1.33	0.74
1:0:2780:C:H1'	7:E:143:GLN:HE21	1.50	0.74
1:0:2361:A:H5'	38:0:8824:HOH:O	1.87	0.73
1:0:1446:U:H2'	20:S:55:GLN:NE2	2.03	0.73
1:0:2799:A:H4'	38:0:7080:HOH:O	1.88	0.73
1:0:587:A:H5''	38:0:7109:HOH:O	1.88	0.73
1:0:2890:A:H1'	22:U:56:ARG:NH2	2.03	0.73
24:W:52:VAL:HG22	24:W:53:ALA:H	1.53	0.73
1:0:2507:G:H2'	1:0:2510:C:H42	1.53	0.73
1:0:1175:G:H1'	1:0:1193:A:H2'	1.69	0.73
26:Y:141:THR:HG23	38:Y:8167:HOH:O	1.88	0.73
11:J:107:ASN:HD21	11:J:109:TYR:HB2	1.53	0.73
2:9:3006:C:C5'	15:N:37:ARG:HH12	1.88	0.73
1:0:1119:G:N2	1:0:1246:A:C2	2.57	0.73
1:0:289:G:N2	1:0:363:A:C2	2.57	0.73
1:0:544:G:C2'	1:0:545:G:H5''	2.19	0.73
1:0:2004:U:H2'	1:0:2004:U:O2	1.87	0.72
1:0:1172:G:H5''	38:0:7084:HOH:O	1.89	0.72
1:0:1751:G:C2'	1:0:1752:G:H5''	2.19	0.72
4:B:238:ASN:HD22	4:B:240:GLY:H	1.38	0.72
9:G:67:LEU:O	9:G:71:LEU:HG	1.89	0.72
1:0:545:G:C8	1:0:545:G:H5'	2.22	0.72
38:0:3566:HOH:O	21:T:9:LYS:HD3	1.88	0.72
1:0:656:G:H3'	16:O:37:ARG:NH1	2.03	0.72
1:0:1183:C:H2'	38:0:6073:HOH:O	1.90	0.72
1:0:1701:A:H5'	38:0:6109:HOH:O	1.90	0.71
1:0:2716:G:H5''	4:B:206:THR:HG21	1.71	0.71
1:0:1973:A:H5'	1:0:1973:A:H8	1.54	0.71
1:0:1266:U:H4'	26:Y:115:ARG:HH21	1.53	0.71
1:0:2769:C:H2'	1:0:2770:G:H5'	1.70	0.71
1:0:1162:G:H1'	31:I:117:LEU:CD1	2.20	0.71
1:0:1184:C:H1'	38:0:7289:HOH:O	1.90	0.71
1:0:2748:G:H5'	38:0:7362:HOH:O	1.91	0.71
2:9:3014:G:H8	2:9:3014:G:H5'	1.56	0.71
1:0:952:G:H4'	38:0:6557:HOH:O	1.89	0.70
1:0:1615:A:H5'	38:0:4007:HOH:O	1.90	0.70
12:K:10:GLN:H	12:K:10:GLN:NE2	1.85	0.70
38:0:7249:HOH:O	23:V:42:ASN:HB3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3069:U:OP1	15:N:4:PRO:HG3	1.91	0.70
5:C:140:VAL:HB	38:C:8644:HOH:O	1.91	0.70
7:E:97:VAL:HG12	38:E:4191:HOH:O	1.91	0.70
6:D:154:LYS:HD2	6:D:154:LYS:H	1.57	0.70
38:0:4667:HOH:O	11:J:47:THR:HB	1.91	0.70
1:0:1641:A:H2'	1:0:1642:A:H5'	1.73	0.70
1:0:1441:G:O2'	1:0:1442:A:H5'	1.91	0.70
1:0:1116:U:H3	1:0:1246:A:H62	1.36	0.70
4:B:221:GLN:HE22	12:K:42:ASN:HD22	1.40	0.70
10:H:56:GLN:NE2	10:H:126:ARG:HE	1.89	0.70
2:9:3051:A:H5'	15:N:160:SER:HB3	1.73	0.69
1:0:2664:A:OP1	1:0:2664:A:H8	1.74	0.69
1:0:2135:A:O2'	1:0:2136:G:H5'	1.92	0.69
12:K:81:ARG:HB2	12:K:87:ARG:NH1	2.07	0.69
1:0:381:G:H5''	38:0:4148:HOH:O	1.91	0.69
1:0:1507:C:H4'	38:S:8524:HOH:O	1.92	0.69
1:0:2679:G:H2'	1:0:2681:A:OP2	1.92	0.69
3:A:48:ASP:HB3	38:A:8899:HOH:O	1.92	0.69
1:0:2505:G:O2'	1:0:2506:A:H5'	1.91	0.69
1:0:506:G:H22	1:0:509:A:C5'	2.06	0.69
1:0:513:A:N3	38:0:3468:HOH:O	2.24	0.69
1:0:1130:U:H5'	38:0:7493:HOH:O	1.93	0.69
10:H:3:ALA:HA	10:H:58:ARG:NH1	2.07	0.69
1:0:2878:U:H2'	1:0:2879:A:O4'	1.93	0.69
1:0:958:G:O2'	1:0:959:C:H5'	1.93	0.69
4:B:195:ARG:HG2	4:B:323:LEU:HD22	1.74	0.69
10:H:166:SER:CB	10:H:167:PRO:HD3	2.23	0.69
12:K:98:VAL:CG1	12:K:102:GLU:HA	2.23	0.69
1:0:870:G:OP2	3:A:3:ARG:HD3	1.92	0.69
11:J:107:ASN:ND2	11:J:109:TYR:H	1.90	0.69
1:0:1377:C:H6	1:0:1377:C:H5'	1.56	0.69
1:0:308:U:H5'	1:0:309:C:OP1	1.92	0.69
23:V:12:THR:HG23	23:V:14:ALA:H	1.57	0.68
1:0:1669:A:H2'	1:0:1670:G:C8	2.28	0.68
1:0:1120:U:H5'	1:0:1121:G:OP2	1.92	0.68
1:0:2578:G:H5'	1:0:2578:G:H8	1.57	0.68
4:B:8:LYS:HG3	4:B:220:VAL:HG12	1.73	0.68
1:0:271:C:N4	1:0:378:A:C2	2.58	0.68
1:0:2769:C:H2'	1:0:2770:G:C5'	2.23	0.68
1:0:2502:C:H2'	1:0:2503:A:H5'	1.76	0.68
1:0:2812:A:C2	1:0:2814:A:N6	2.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1163:G:H5'	31:I:115:ASP:O	1.92	0.68
1:0:74:A:H2'	1:0:75:U:H6	1.58	0.68
10:H:166:SER:HB2	10:H:167:PRO:CD	2.23	0.68
25:X:43:VAL:CG1	25:X:76:ARG:HH12	2.06	0.68
1:0:65:C:O2'	1:0:66:G:H5'	1.94	0.68
1:0:2054:A:N3	19:R:128:ARG:NH2	2.42	0.68
29:2:41:HIS:H	29:2:45:ASN:HD22	1.40	0.68
14:M:99:ARG:HD2	14:M:167:GLY:HA2	1.74	0.68
14:M:164:THR:HG23	14:M:167:GLY:H	1.57	0.68
14:M:24:GLN:HE21	14:M:27:ARG:HH11	1.41	0.68
1:0:2533:C:C6	1:0:2533:C:C5'	2.73	0.67
1:0:119:A:H2'	1:0:120:A:H5''	1.76	0.67
1:0:282:C:H1'	1:0:368:C:H42	1.60	0.67
13:L:143:THR:HG22	13:L:144:ASP:H	1.58	0.67
1:0:1537:C:H1'	38:0:6414:HOH:O	1.94	0.67
2:9:3031:C:H1'	38:9:1137:HOH:O	1.95	0.67
23:V:1:THR:HG23	23:V:2:VAL:H	1.57	0.67
4:B:267:LYS:HD3	38:B:8828:HOH:O	1.93	0.67
22:U:9:CYS:HA	22:U:52:THR:HG23	1.76	0.67
6:D:50:VAL:O	6:D:71:ALA:HA	1.95	0.67
1:0:699:C:H5'	38:0:3831:HOH:O	1.93	0.67
1:0:1118:A:H62	1:0:1244:U:H3	1.41	0.67
8:F:96:ALA:HA	38:F:3111:HOH:O	1.94	0.67
1:0:559:U:C5'	1:0:559:U:H6	2.07	0.67
12:K:81:ARG:HB2	12:K:87:ARG:HH11	1.59	0.67
8:F:21:GLU:O	8:F:24:ARG:HG2	1.95	0.67
2:9:3076:G:C3'	2:9:3077:A:H5''	2.23	0.67
1:0:1701:A:H5''	1:0:1702:U:H3'	1.76	0.67
1:0:1679:C:H5'	38:0:9137:HOH:O	1.95	0.67
1:0:1253:C:H4'	38:0:6300:HOH:O	1.94	0.67
1:0:1167:G:H4'	31:I:135:LEU:HD21	1.77	0.67
15:N:48:VAL:CG1	15:N:55:ASP:HB3	2.24	0.67
1:0:1878:G:H2'	38:0:3072:HOH:O	1.95	0.66
1:0:1508:C:H5'	20:S:21:GLN:NE2	2.10	0.66
19:R:99:ALA:HB1	19:R:109:MET:HE1	1.76	0.66
15:N:37:ARG:HH21	15:N:105:GLY:CA	2.08	0.66
2:9:3054:A:O2'	2:9:3055:U:H5'	1.95	0.66
31:I:78:LEU:HD12	31:I:112:LYS:NZ	2.09	0.66
12:K:74:VAL:HG11	12:K:113:ILE:HG12	1.76	0.66
1:0:2717:C:H2'	1:0:2718:C:C5'	2.22	0.66
1:0:1163:G:H5''	31:I:115:ASP:HB3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:31:C:H2'	38:0:7508:HOH:O	1.95	0.66
1:0:1921:A:O2'	1:0:1922:A:H5'	1.95	0.66
4:B:254:GLN:HG2	4:B:255:GLY:N	2.11	0.66
12:K:109:LEU:HD13	12:K:113:ILE:HD11	1.78	0.66
38:0:7279:HOH:O	4:B:211:THR:HG21	1.95	0.66
1:0:2507:G:H2'	1:0:2510:C:N4	2.11	0.65
1:0:74:A:H2'	1:0:75:U:C6	2.32	0.65
24:W:4:LEU:HD23	24:W:54:PHE:HB3	1.79	0.65
29:2:40:ARG:HA	29:2:45:ASN:HD22	1.61	0.65
1:0:1940:C:H4'	38:0:7170:HOH:O	1.96	0.65
11:J:75:PRO:HG2	11:J:105:LEU:HD21	1.77	0.65
15:N:144:GLY:O	15:N:147:ILE:HG22	1.95	0.65
1:0:1377:C:H5'	1:0:1377:C:C6	2.30	0.65
13:L:143:THR:HG22	13:L:144:ASP:N	2.11	0.65
1:0:2256:G:H2'	1:0:2257:G:H5'	1.78	0.65
7:E:6:GLU:HA	7:E:46:THR:HG22	1.79	0.65
4:B:248:ARG:O	4:B:251:VAL:HG22	1.97	0.65
24:W:125:HIS:HD2	24:W:127:GLY:H	1.43	0.65
1:0:794:U:H3	1:0:819:A:H61	1.44	0.65
1:0:2498:C:O2'	1:0:2499:U:H5'	1.97	0.65
1:0:200:U:H2'	38:0:3257:HOH:O	1.97	0.65
2:9:3058:G:H1'	38:9:3839:HOH:O	1.96	0.65
1:0:905:C:H4'	26:Y:144:ARG:NH1	2.12	0.65
1:0:1636:G:O2'	1:0:1637:A:H5'	1.97	0.65
1:0:1119:G:H8	11:J:52:GLN:HE22	1.45	0.65
2:9:3002:U:H4'	38:9:5321:HOH:O	1.95	0.65
7:E:24:GLY:HA3	7:E:76:VAL:HB	1.79	0.65
3:A:153:ARG:NH1	3:A:153:ARG:HB2	2.11	0.65
1:0:1393:A:H2'	1:0:1394:C:C6	2.32	0.65
4:B:232:TRP:HD1	4:B:235:ARG:HD2	1.60	0.65
5:C:5:ILE:HD11	5:C:16:VAL:HG22	1.78	0.65
14:M:80:GLY:O	14:M:81:ARG:HD3	1.97	0.65
1:0:1205:U:C2'	1:0:1206:U:H5''	2.27	0.64
24:W:6:GLN:HB2	24:W:26:ILE:HD12	1.79	0.64
30:3:38:ARG:HB3	30:3:42:ARG:HH12	1.62	0.64
1:0:1525:G:H5'	1:0:1526:A:OP2	1.97	0.64
1:0:2420:G:O2'	1:0:2421:G:H5'	1.95	0.64
3:A:199:HIS:HD2	3:A:201:PHE:H	1.45	0.64
1:0:2608:C:H3'	38:0:7627:HOH:O	1.96	0.64
5:C:236:THR:HG22	5:C:239:ALA:CB	2.27	0.64
1:0:1474:C:C5'	1:0:1474:C:H6	2.03	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:661:G:C5	1:0:686:A:C2	2.86	0.64
1:0:1189:A:O2'	1:0:1208:C:H2'	1.97	0.64
1:0:1162:G:H1'	31:I:117:LEU:HD12	1.79	0.64
2:9:3061:C:H2'	2:9:3062:A:H8	1.62	0.64
1:0:1364:G:H1'	38:0:4628:HOH:O	1.98	0.64
1:0:2256:G:C2'	1:0:2257:G:H5'	2.28	0.64
1:0:420:U:H2'	1:0:421:C:C6	2.33	0.64
3:A:55:VAL:HG22	3:A:68:ILE:O	1.98	0.63
2:9:3024:U:H3'	2:9:3025:G:C5'	2.28	0.63
1:0:2346:C:O5'	1:0:2346:C:H6	1.80	0.63
1:0:559:U:H5'	1:0:559:U:C6	2.24	0.63
24:W:21:LEU:HD22	24:W:26:ILE:CD1	2.28	0.63
1:0:1528:A:H2'	1:0:1529:G:O4'	1.98	0.63
20:S:37:VAL:O	20:S:41:VAL:HG23	1.98	0.63
1:0:2676:C:H4'	11:J:70:PHE:CE1	2.34	0.63
1:0:290:C:N3	1:0:363:A:C2	2.67	0.63
8:F:91:VAL:HG12	8:F:92:GLY:H	1.64	0.63
1:0:1834:C:H2'	1:0:1840:A:N6	2.13	0.63
26:Y:189:ASN:HD21	26:Y:191:ASP:HB2	1.63	0.63
8:F:91:VAL:HG12	8:F:92:GLY:N	2.13	0.63
24:W:64:THR:O	24:W:68:THR:HG22	1.99	0.63
19:R:39:THR:HG22	19:R:42:GLU:H	1.63	0.63
4:B:18:ARG:HE	4:B:256:GLN:NE2	1.97	0.63
1:0:450:C:OP1	5:C:184:ARG:NH2	2.31	0.63
1:0:1058:A:H2'	1:0:1060:C:H5''	1.81	0.63
1:0:2667:G:H1'	1:0:2914:A:N3	2.14	0.63
19:R:25:PHE:CE2	19:R:29:LYS:HE2	2.34	0.63
1:0:87:C:C2	29:2:30:ASP:OD2	2.52	0.62
1:0:960:G:H3'	1:0:960:G:N3	2.14	0.62
38:0:5288:HOH:O	9:G:12:ILE:HG23	1.99	0.62
28:1:37:CYS:SG	28:1:39:PHE:HB2	2.39	0.62
1:0:285:A:H2'	1:0:286:U:O4'	1.98	0.62
24:W:21:LEU:HD21	24:W:48:VAL:HG11	1.80	0.62
1:0:2768:A:O2'	1:0:2769:C:H5'	1.99	0.62
1:0:2256:G:H2'	1:0:2257:G:C5'	2.29	0.62
34:0:8503:NA:NA	38:0:9254:HOH:O	1.73	0.62
1:0:1174:A:C5	1:0:1201:C:H4'	2.34	0.62
3:A:199:HIS:CD2	3:A:201:PHE:H	2.16	0.62
1:0:407:A:H2'	1:0:408:A:C8	2.35	0.62
1:0:42:C:H3'	38:0:3992:HOH:O	1.99	0.62
14:M:24:GLN:NE2	14:M:27:ARG:HH11	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1666:C:H2'	1:0:1667:A:C5'	2.29	0.62
4:B:232:TRP:CD1	4:B:235:ARG:HD2	2.34	0.62
1:0:1634:G:H2'	1:0:1635:U:C6	2.34	0.62
6:D:65:GLU:HA	38:D:6752:HOH:O	1.99	0.62
1:0:380:A:OP2	14:M:9:ARG:HD2	1.98	0.62
21:T:9:LYS:HE3	21:T:13:ARG:NH1	2.13	0.62
1:0:1839:A:H3'	38:0:9460:HOH:O	1.99	0.62
1:0:155:C:OP2	14:M:188:ARG:HD3	2.00	0.62
1:0:1524:U:OP1	1:0:1524:U:H4'	2.00	0.62
1:0:1667:A:H2'	1:0:1668:U:C6	2.34	0.62
1:0:1835:U:C5	1:0:1840:A:N7	2.62	0.62
1:0:905:C:H4'	26:Y:144:ARG:HH11	1.64	0.62
1:0:1150:A:C2	9:G:20:VAL:HG21	2.35	0.62
1:0:1552:G:H2'	1:0:1553:C:C6	2.35	0.62
9:G:16:LYS:O	9:G:20:VAL:HG23	2.00	0.62
1:0:694:A:H1'	38:0:3628:HOH:O	1.98	0.62
1:0:1053:G:OP1	10:H:12:PRO:HG3	1.99	0.62
1:0:1209:C:H2'	1:0:1210:G:H8	1.65	0.62
6:D:99:ASP:HB3	6:D:103:ASN:H	1.64	0.62
1:0:1588:G:C6	1:0:1589:G:N1	2.67	0.62
1:0:2826:G:C6	1:0:2913:A:N6	2.68	0.62
1:0:558:C:O2'	1:0:559:U:H5''	2.00	0.61
26:Y:187:VAL:HG23	26:Y:192:ASP:CB	2.27	0.61
12:K:98:VAL:HG11	12:K:102:GLU:HA	1.81	0.61
29:2:40:ARG:HA	29:2:45:ASN:ND2	2.15	0.61
26:Y:200:THR:HG22	26:Y:201:GLU:HG3	1.81	0.61
1:0:2526:C:H5'	1:0:2526:C:C6	2.36	0.61
5:C:115:LEU:HD13	5:C:223:LEU:HD21	1.82	0.61
12:K:29:LEU:HB3	12:K:55:VAL:CG1	2.30	0.61
1:0:1165:G:H1'	1:0:1174:A:H1'	1.80	0.61
1:0:346:U:H4'	38:0:6669:HOH:O	2.00	0.61
13:L:92:ASP:HA	13:L:121:ILE:HB	1.80	0.61
1:0:2827:A:H2'	1:0:2828:G:O4'	1.99	0.61
1:0:902:G:N7	13:L:18:HIS:HD2	1.98	0.61
24:W:88:THR:HG23	24:W:110:GLN:HB3	1.82	0.61
1:0:59:A:H5'	38:0:4160:HOH:O	1.99	0.61
1:0:396:U:H1'	38:0:7448:HOH:O	2.01	0.61
1:0:653:C:H5''	38:0:7746:HOH:O	1.99	0.61
26:Y:126:PRO:HG2	26:Y:128:PHE:CE1	2.36	0.61
1:0:1666:C:C2'	1:0:1667:A:C5'	2.78	0.61
5:C:236:THR:HG22	5:C:239:ALA:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:39:THR:HG23	19:R:107:GLU:O	2.00	0.61
5:C:1:MET:HG2	5:C:2:GLN:H	1.65	0.61
1:0:2586:U:H3	1:0:2592:G:H22	1.47	0.61
1:0:396:U:O2'	1:0:418:C:H4'	2.00	0.61
17:P:13:VAL:HG21	17:P:41:ARG:HG2	1.82	0.61
1:0:2320:U:H4'	1:0:2321:A:O4'	2.00	0.61
3:A:125:ASN:HB3	3:A:158:VAL:HG12	1.82	0.61
1:0:399:C:H5'	14:M:179:GLY:O	2.01	0.61
1:0:1080:C:H4'	1:0:1081:A:OP1	1.99	0.61
25:X:43:VAL:HG13	25:X:76:ARG:NH1	2.11	0.61
1:0:1206:U:H2'	1:0:1207:A:O4'	2.00	0.60
1:0:1666:C:C2'	1:0:1667:A:H5''	2.29	0.60
2:9:3014:G:H5'	2:9:3014:G:C8	2.35	0.60
1:0:20:G:H21	19:R:117:HIS:HD2	1.48	0.60
6:D:146:LYS:NZ	15:N:107:ASN:HD21	1.99	0.60
12:K:32:ILE:HD11	12:K:56:SER:HB3	1.82	0.60
1:0:1701:A:H4'	1:0:1702:U:C5'	2.30	0.60
1:0:290:C:O2'	1:0:291:C:H5'	2.00	0.60
1:0:2373:U:H1'	38:0:4592:HOH:O	2.00	0.60
1:0:2421:G:H1'	38:0:4611:HOH:O	2.00	0.60
15:N:113:SER:HB2	38:N:8854:HOH:O	2.00	0.60
24:W:137:GLN:NE2	24:W:141:HIS:HE1	1.93	0.60
2:9:3122:C:H5	38:9:2536:HOH:O	1.82	0.60
1:0:2414:A:H2'	1:0:2415:A:C8	2.37	0.60
12:K:10:GLN:N	12:K:10:GLN:HE21	1.90	0.60
1:0:962:C:C1'	15:N:5:ARG:NH1	2.64	0.60
16:O:105:ASN:HD21	16:O:109:SER:H	1.49	0.60
1:0:475:G:OP1	5:C:73:LEU:HD22	2.00	0.60
30:3:70:ARG:HG2	30:3:77:ALA:HB2	1.83	0.60
15:N:114:LYS:O	15:N:118:ILE:HG13	2.01	0.60
1:0:130:C:H5'	38:0:5042:HOH:O	2.01	0.60
2:9:3064:C:H2'	2:9:3065:A:H5'	1.84	0.60
26:Y:133:HIS:HD2	38:Y:8161:HOH:O	1.84	0.60
1:0:1926:G:H2'	1:0:1927:A:C8	2.37	0.60
4:B:74:ILE:HD13	4:B:309:VAL:HG21	1.82	0.60
1:0:2329:C:O2'	1:0:2330:U:H5'	2.01	0.60
12:K:14:LYS:HB2	12:K:45:PRO:HG2	1.84	0.60
8:F:39:SER:HB3	8:F:45:ALA:HB2	1.84	0.60
15:N:37:ARG:HD3	35:N:8807:CL:CL	2.38	0.60
1:0:2908:A:C2'	1:0:2909:G:H5'	2.31	0.60
1:0:1167:G:H4'	31:I:135:LEU:CD2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:542:A:C5'	1:0:542:A:H8	2.08	0.60
2:9:3092:G:H2'	2:9:3093:A:H8	1.64	0.60
1:0:1377:C:H6	1:0:1377:C:C5'	2.15	0.60
4:B:125:GLU:O	4:B:129:ARG:HG3	2.00	0.60
1:0:1624:A:H5'	1:0:1626:A:O4'	2.02	0.60
1:0:2252:A:C5	1:0:2253:G:H1'	2.37	0.60
1:0:278:A:H2'	1:0:279:C:O4'	2.02	0.60
1:0:1819:G:H5'	38:0:4544:HOH:O	2.02	0.60
1:0:1279:U:O2	1:0:1279:U:H2'	2.02	0.60
15:N:37:ARG:HH21	15:N:105:GLY:HA3	1.67	0.59
31:I:113:HIS:N	31:I:114:PRO:HD2	2.17	0.59
34:L:8580:NA:NA	38:L:8831:HOH:O	1.73	0.59
26:Y:189:ASN:HD22	26:Y:191:ASP:N	1.99	0.59
29:2:35:ARG:HB2	38:2:2691:HOH:O	2.01	0.59
1:0:1562:C:H3'	1:0:1563:G:C8	2.38	0.59
23:V:39:ALA:N	23:V:40:PRO:HD2	2.17	0.59
1:0:1299:G:H5'	38:0:3895:HOH:O	2.02	0.59
2:9:3024:U:H3'	2:9:3025:G:H5'	1.82	0.59
10:H:84:LYS:HB2	10:H:84:LYS:NZ	2.18	0.59
1:0:282:C:O2'	1:0:283:U:C5'	2.48	0.59
22:U:46:ALA:HB1	22:U:52:THR:HG21	1.85	0.59
8:F:63:ILE:HB	8:F:64:PRO:HD3	1.84	0.59
13:L:138:GLY:HA3	38:L:8854:HOH:O	2.01	0.59
20:S:81:ILE:HG12	38:S:8541:HOH:O	2.03	0.59
1:0:2346:C:O2'	6:D:52:THR:HG21	2.03	0.59
29:2:19:SER:HB3	38:2:4479:HOH:O	2.03	0.59
4:B:320:GLN:HE21	4:B:321:PRO:HD3	1.67	0.59
4:B:312:ARG:HD3	4:B:315:VAL:HG13	1.83	0.59
1:0:510:U:O3'	36:0:8823:NEG:H31	2.03	0.59
2:9:3029:C:H5	38:N:8842:HOH:O	1.84	0.59
1:0:2316:G:H4'	38:0:5918:HOH:O	2.03	0.59
15:N:80:SER:HB2	38:N:8833:HOH:O	2.02	0.59
1:0:797:A:C4'	27:Z:10:ARG:N	2.65	0.59
2:9:3055:U:H4'	2:9:3056:A:C8	2.38	0.58
1:0:1181:A:H2'	1:0:1182:C:H5'	1.85	0.58
1:0:1523:G:C5	1:0:1524:U:C4	2.91	0.58
20:S:77:VAL:O	20:S:80:ARG:HG2	2.02	0.58
6:D:75:LEU:HD22	6:D:79:MET:HB3	1.85	0.58
22:U:44:ARG:HB3	38:U:3805:HOH:O	2.01	0.58
2:9:3048:C:H4'	15:N:141:ARG:HH21	1.69	0.58
18:Q:34:ASP:O	18:Q:37:GLU:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:96:VAL:HG13	19:R:106:GLY:HA3	1.85	0.58
11:J:76:ASP:HA	38:J:5907:HOH:O	2.03	0.58
21:T:112:LEU:HD23	21:T:119:ALA:HB3	1.85	0.58
7:E:133:VAL:HG12	7:E:141:VAL:HG13	1.85	0.58
3:A:200:PRO:HG2	3:A:225:VAL:HG21	1.85	0.58
2:9:3029:C:H2'	2:9:3030:C:C5'	2.26	0.58
4:B:217:ARG:HG3	4:B:257:THR:HG22	1.85	0.58
13:L:148:GLU:HA	38:L:8871:HOH:O	2.02	0.58
1:0:2635:A:O2'	1:0:2636:C:H5'	2.03	0.58
38:0:5484:HOH:O	3:A:192:VAL:HB	2.03	0.58
1:0:420:U:H2'	1:0:421:C:H6	1.69	0.58
3:A:97:ALA:HA	3:A:131:HIS:NE2	2.19	0.58
1:0:364:C:H2'	1:0:365:G:O4'	2.04	0.58
1:0:960:G:N3	1:0:960:G:C2'	2.66	0.58
24:W:80:ASP:O	24:W:84:VAL:HG23	2.02	0.58
1:0:1165:G:O2'	1:0:1174:A:H4'	2.02	0.58
17:P:59:ARG:NH2	17:P:66:GLN:HE22	2.00	0.58
1:0:2825:C:H4'	1:0:2826:G:O5'	2.04	0.58
26:Y:146:PRO:O	26:Y:154:ARG:HG3	2.04	0.58
1:0:2291:A:N9	1:0:2309:C:H5'	2.19	0.58
1:0:1587:U:H2'	1:0:1588:G:O4'	2.04	0.58
30:3:65:THR:HG22	30:3:67:LEU:HG	1.85	0.58
1:0:2908:A:O5'	1:0:2908:A:H8	1.87	0.58
31:I:78:LEU:HD12	31:I:112:LYS:HZ2	1.69	0.58
24:W:38:THR:HG22	24:W:39:ASP:N	2.19	0.58
1:0:621:C:H5'	26:Y:132:ASP:OD2	2.04	0.58
1:0:1174:A:C6	1:0:1201:C:H4'	2.39	0.57
1:0:1528:A:H62	1:0:1663:G:H21	1.52	0.57
24:W:88:THR:HG22	24:W:90:TYR:HD1	1.68	0.57
1:0:1603:A:H5''	1:0:1605:G:H5'	1.86	0.57
24:W:52:VAL:HG22	24:W:53:ALA:N	2.19	0.57
14:M:99:ARG:CD	14:M:167:GLY:HA2	2.33	0.57
1:0:1396:C:H4'	17:P:2:ASP:OD1	2.05	0.57
1:0:1778:A:H2'	1:0:1779:A:H5'	1.86	0.57
1:0:271:C:N4	1:0:378:A:H2	1.89	0.57
1:0:1130:U:H2'	1:0:1131:G:O4'	2.05	0.57
1:0:2815:G:N7	11:J:80:LYS:NZ	2.52	0.57
1:0:447:A:OP1	21:T:2:LYS:HG2	2.04	0.57
1:0:500:G:H21	19:R:98:ASN:HD21	1.53	0.57
1:0:2908:A:H2'	1:0:2909:G:C4'	2.33	0.57
1:0:2890:A:C4	22:U:56:ARG:CZ	2.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:0:6598:HOH:O	15:N:4:PRO:HD2	2.04	0.57
1:0:2256:G:O2'	1:0:2257:G:H5'	2.04	0.57
1:0:2415:A:C2	15:N:25:ARG:HB3	2.39	0.57
19:R:18:LEU:HG	19:R:91:LEU:HD13	1.87	0.57
8:F:36:THR:HG23	8:F:97:ALA:HB2	1.87	0.57
1:0:2005:G:H3'	1:0:2005:G:OP2	2.04	0.57
15:N:169:PRO:O	15:N:172:PHE:HB3	2.05	0.57
1:0:1205:U:H2'	1:0:1206:U:H5'	1.84	0.57
1:0:1181:A:C2'	1:0:1182:C:H5'	2.35	0.57
1:0:1249:U:H5	38:0:7333:HOH:O	1.87	0.57
1:0:1187:U:H2'	38:0:6725:HOH:O	2.03	0.57
1:0:870:G:C2'	1:0:871:G:H5''	2.33	0.57
1:0:1242:A:H5'	11:J:82:THR:CG2	2.20	0.57
14:M:66:SER:HB3	14:M:128:TRP:CD1	2.40	0.57
1:0:812:A:H1'	38:0:3773:HOH:O	2.03	0.57
1:0:1731:C:H1'	38:0:6270:HOH:O	2.05	0.57
1:0:1559:A:OP2	1:0:1559:A:H8	1.87	0.57
1:0:1162:G:H1'	31:I:117:LEU:HD11	1.85	0.57
1:0:517:U:OP2	36:0:8823:NEG:O4	2.23	0.57
1:0:2064:U:H5'	1:0:2652:U:O3'	2.05	0.57
8:F:58:GLU:HA	8:F:61:MET:HE2	1.87	0.57
1:0:470:U:O2'	28:1:16:HIS:HD2	1.88	0.57
3:A:105:VAL:CG1	3:A:154:ALA:HB1	2.35	0.57
7:E:101:GLU:HB2	7:E:116:THR:O	2.04	0.57
1:0:1878:G:H5''	38:0:9612:HOH:O	2.05	0.56
27:Z:46:ARG:HD3	27:Z:59:TYR:HB2	1.86	0.56
1:0:2874:G:H3'	38:0:9391:HOH:O	2.03	0.56
1:0:2717:C:O2'	1:0:2718:C:H5''	2.04	0.56
1:0:1181:A:N1	1:0:1192:A:O2'	2.37	0.56
15:N:175:LEU:HD11	38:N:8835:HOH:O	2.05	0.56
2:9:3002:U:OP2	2:9:3003:A:H5'	2.05	0.56
28:1:25:LYS:HD2	29:2:49:GLU:H	1.69	0.56
1:0:2846:C:H4'	38:0:4908:HOH:O	2.04	0.56
1:0:1687:C:O2	28:1:9:GLY:HA2	2.05	0.56
1:0:1170:U:H1'	1:0:1172:G:N7	2.20	0.56
1:0:1669:A:H2'	1:0:1670:G:H8	1.68	0.56
24:W:88:THR:HG22	24:W:89:ASP:H	1.70	0.56
1:0:797:A:H4'	27:Z:10:ARG:N	2.21	0.56
1:0:1699:C:H4'	38:0:6264:HOH:O	2.03	0.56
1:0:630:A:H1'	38:0:5640:HOH:O	2.04	0.56
2:9:3078:G:N2	2:9:3103:A:OP2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:120:ILE:HD12	10:H:120:ILE:H	1.69	0.56
1:0:1189:A:H1'	1:0:1209:C:C1'	2.35	0.56
4:B:212:GLN:HB2	4:B:257:THR:CG2	2.36	0.56
12:K:20:CYS:HB2	12:K:29:LEU:HG	1.88	0.56
10:H:56:GLN:HE21	10:H:126:ARG:HE	1.54	0.56
1:0:2374:A:H2'	1:0:2375:G:C8	2.40	0.56
3:A:153:ARG:CB	3:A:153:ARG:HH11	2.18	0.56
23:V:55:ARG:O	23:V:59:ILE:HG12	2.05	0.56
4:B:179:LEU:O	4:B:183:GLU:HG2	2.05	0.56
1:0:2787:C:H5	38:0:4466:HOH:O	1.88	0.56
1:0:1119:G:H2'	11:J:52:GLN:NE2	2.20	0.56
1:0:960:G:H2'	1:0:960:G:N3	2.20	0.56
1:0:2769:C:C2'	1:0:2770:G:C5'	2.83	0.56
7:E:11:VAL:HG12	7:E:12:ASP:N	2.20	0.56
1:0:1819:G:H2'	1:0:1820:G:H4'	1.85	0.56
27:Z:37:HIS:HB2	27:Z:47:VAL:HB	1.88	0.56
1:0:281:U:H2'	1:0:282:C:O4'	2.05	0.56
12:K:74:VAL:HG13	12:K:113:ILE:HG23	1.88	0.56
1:0:1741:U:O2'	1:0:2723:G:H4'	2.06	0.56
24:W:115:THR:HG23	38:W:5420:HOH:O	2.05	0.56
15:N:132:ASN:O	15:N:135:VAL:HG12	2.05	0.56
18:Q:66:LYS:HB2	18:Q:70:ALA:O	2.06	0.56
1:0:1641:A:C2'	1:0:1642:A:H5'	2.36	0.56
1:0:1552:G:H2'	1:0:1553:C:H6	1.70	0.56
1:0:1500:U:P	17:P:41:ARG:HH22	2.29	0.56
19:R:40:ALA:O	19:R:44:VAL:HG23	2.06	0.56
1:0:1654:U:H2'	3:A:47:HIS:HD2	1.70	0.56
13:L:136:ALA:HB3	38:L:8872:HOH:O	2.05	0.56
2:9:3001:U:O3'	2:9:3003:A:H5''	2.06	0.55
1:0:447:A:P	21:T:1:SER:HB2	2.47	0.55
2:9:3107:C:H5	38:9:3167:HOH:O	1.89	0.55
36:0:8823:NEG:O3	36:0:8823:NEG:N4	2.39	0.55
6:D:23:VAL:HG21	6:D:45:THR:HG21	1.88	0.55
1:0:2563:U:H2'	1:0:2565:C:O5'	2.06	0.55
20:S:33:SER:O	20:S:37:VAL:HG23	2.06	0.55
2:9:3064:C:C2'	2:9:3065:A:H5'	2.37	0.55
1:0:560:C:H42	1:0:597:A:H61	1.53	0.55
1:0:264:G:H1'	1:0:265:U:H5	1.71	0.55
9:G:12:ILE:HG22	9:G:17:GLN:NE2	2.22	0.55
1:0:2453:G:H5''	38:L:8842:HOH:O	2.07	0.55
8:F:33:THR:HG21	8:F:59:ILE:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:451:C:O2'	1:0:452:G:H5'	2.06	0.55
3:A:95:PRO:HG2	3:A:98:GLU:HG2	1.88	0.55
1:0:1319:G:H1'	38:0:4524:HOH:O	2.07	0.55
20:S:57:THR:HG23	38:S:8534:HOH:O	2.05	0.55
1:0:1787:C:H4'	1:0:2883:A:O4'	2.06	0.55
1:0:1126:C:O5'	1:0:1126:C:H6	1.89	0.55
1:0:280:C:H2'	1:0:281:U:O4'	2.06	0.55
1:0:2851:G:H2'	1:0:2852:A:H5'	1.87	0.55
7:E:11:VAL:HG12	7:E:12:ASP:H	1.71	0.55
1:0:1551:C:O2	1:0:1634:G:N2	2.37	0.55
4:B:307:ARG:HH11	4:B:307:ARG:HG3	1.71	0.55
25:X:21:PRO:HG2	25:X:24:LYS:HD3	1.87	0.55
1:0:10:U:H3'	38:0:3147:HOH:O	2.07	0.55
11:J:107:ASN:HD22	11:J:107:ASN:C	2.10	0.55
1:0:288:A:H61	1:0:364:C:H42	1.54	0.55
10:H:56:GLN:HE21	10:H:126:ARG:HG2	1.72	0.55
2:9:3061:C:H2'	2:9:3062:A:C8	2.41	0.55
3:A:72:GLU:HG3	27:Z:66:GLY:HA2	1.88	0.55
1:0:1192:A:H3'	1:0:1193:A:H5'	1.88	0.55
1:0:1172:G:H1'	38:0:4805:HOH:O	2.06	0.55
1:0:1167:G:H2'	1:0:1168:C:O4'	2.07	0.55
15:N:73:ALA:HB1	15:N:74:PRO:HD2	1.88	0.55
14:M:147:LEU:O	14:M:150:ILE:HG22	2.07	0.55
11:J:19:MET:HE2	11:J:79:PHE:HA	1.89	0.55
1:0:2649:A:H5'	1:0:2649:A:H8	1.72	0.55
9:G:63:ARG:O	9:G:67:LEU:HG	2.06	0.55
1:0:512:G:O3'	1:0:513:A:H8	1.90	0.55
14:M:102:GLU:OE1	14:M:164:THR:HG21	2.06	0.55
2:9:3039:U:H1'	2:9:3044:A:H61	1.71	0.55
1:0:90:A:H2'	1:0:91:G:O4'	2.07	0.54
1:0:1291:A:H2	38:0:5120:HOH:O	1.90	0.54
4:B:150:ALA:O	4:B:152:PRO:HD3	2.07	0.54
5:C:25:PRO:HG2	38:C:8522:HOH:O	2.07	0.54
1:0:644:G:N3	1:0:644:G:H5'	2.21	0.54
22:U:39:ASN:ND2	22:U:44:ARG:HH11	2.04	0.54
1:0:204:A:H2'	1:0:205:U:H5'	1.88	0.54
30:3:3:MET:O	30:3:90:PHE:HA	2.08	0.54
10:H:66:ARG:HD3	38:H:8582:HOH:O	2.06	0.54
18:Q:26:PRO:O	18:Q:30:VAL:HG23	2.08	0.54
1:0:737:A:H2'	1:0:738:G:O4'	2.07	0.54
23:V:29:ASN:O	23:V:33:VAL:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1902:G:O2'	1:0:1903:U:H5'	2.08	0.54
3:A:95:PRO:HA	3:A:153:ARG:HA	1.90	0.54
1:0:524:A:H5''	19:R:29:LYS:HD3	1.90	0.54
1:0:941:G:C5	1:0:942:U:C4	2.96	0.54
1:0:1684:A:H1'	29:2:43:ARG:HH22	1.71	0.54
38:0:4562:HOH:O	15:N:21:HIS:HD2	1.91	0.54
1:0:2001:G:O2'	1:0:2002:C:H5'	2.08	0.54
10:H:46:GLN:HB3	10:H:167:PRO:CD	2.26	0.54
1:0:363:A:O2'	1:0:364:C:H5'	2.08	0.54
1:0:1925:G:O2'	1:0:1926:G:H5'	2.08	0.54
3:A:82:VAL:HG13	3:A:93:THR:HB	1.90	0.54
1:0:711:G:C2	1:0:718:C:C2	2.96	0.54
1:0:1183:C:N4	1:0:1184:C:H41	2.06	0.54
23:V:1:THR:HG23	23:V:2:VAL:N	2.23	0.54
1:0:61:G:H1'	38:0:5570:HOH:O	2.07	0.54
1:0:1562:C:O2	1:0:1562:C:H2'	2.08	0.54
1:0:1973:A:H5'	1:0:1973:A:C8	2.40	0.54
1:0:1819:G:H2'	1:0:1820:G:C5'	2.38	0.54
1:0:105:G:O2'	1:0:106:A:H5'	2.08	0.54
15:N:154:LEU:O	15:N:155:GLU:HB3	2.08	0.54
1:0:657:G:OP1	5:C:27:ARG:NH2	2.37	0.54
24:W:21:LEU:HD21	24:W:48:VAL:CG1	2.38	0.54
19:R:99:ALA:HB1	19:R:109:MET:CE	2.38	0.54
1:0:1515:A:H2'	1:0:1516:C:C6	2.43	0.54
1:0:2300:A:H4'	1:0:2301:A:O5'	2.08	0.54
1:0:1118:A:C8	1:0:1118:A:C3'	2.76	0.53
5:C:236:THR:HA	38:C:8644:HOH:O	2.08	0.53
1:0:1766:U:O2	1:0:1778:A:H5'	2.08	0.53
1:0:2270:G:H4'	3:A:223:ARG:NH1	2.22	0.53
1:0:2401:A:H2'	1:0:2402:A:C8	2.43	0.53
1:0:2781:U:H2'	1:0:2782:G:H5'	1.90	0.53
10:H:46:GLN:HG3	10:H:137:TYR:CE2	2.42	0.53
1:0:1177:A:H8	1:0:1177:A:O5'	1.90	0.53
28:1:21:ARG:HD2	28:1:37:CYS:SG	2.48	0.53
5:C:101:ASP:HA	38:C:8642:HOH:O	2.08	0.53
5:C:233:THR:HG22	5:C:234:VAL:N	2.23	0.53
1:0:2718:C:H6	1:0:2718:C:H5'	1.73	0.53
1:0:1165:G:O2'	1:0:1174:A:C4'	2.57	0.53
1:0:2721:U:H4'	12:K:87:ARG:HG3	1.89	0.53
1:0:750:A:O3'	5:C:101:ASP:HB2	2.08	0.53
1:0:1321:A:H2'	1:0:1322:G:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:143:ALA:HA	38:P:5521:HOH:O	2.07	0.53
25:X:41:PHE:CZ	25:X:74:ALA:HB3	2.42	0.53
26:Y:106:THR:HG23	26:Y:107:PRO:HD2	1.90	0.53
1:0:797:A:H5'	27:Z:10:ARG:N	2.22	0.53
1:0:2649:A:H5'	1:0:2649:A:C8	2.44	0.53
1:0:635:A:H2'	1:0:636:G:H5''	1.89	0.53
1:0:321:A:H1'	38:0:6859:HOH:O	2.07	0.53
1:0:2870:C:H2'	1:0:2871:G:H8	1.73	0.53
1:0:1667:A:H2'	1:0:1668:U:H6	1.73	0.53
11:J:75:PRO:HD3	11:J:136:SER:OG	2.08	0.53
1:0:2699:A:H2'	1:0:2700:G:O4'	2.08	0.53
15:N:86:LEU:HD12	15:N:125:ALA:HB2	1.91	0.53
1:0:2435:U:H1'	38:0:5260:HOH:O	2.09	0.53
1:0:613:C:H2'	1:0:614:U:H6	1.72	0.53
9:G:19:GLU:O	9:G:23:ILE:HG13	2.08	0.53
16:O:73:ASP:HA	16:O:92:VAL:O	2.08	0.53
29:2:5:LYS:O	29:2:9:LYS:HG3	2.08	0.53
6:D:58:VAL:CG1	6:D:60:GLU:HG2	2.38	0.53
1:0:259:G:H21	14:M:58:GLN:NE2	2.07	0.53
28:1:10:LYS:HG3	38:1:2979:HOH:O	2.08	0.53
1:0:1562:C:N4	38:0:5694:HOH:O	2.40	0.53
9:G:23:ILE:HD13	9:G:67:LEU:HD23	1.90	0.53
1:0:1634:G:H2'	1:0:1635:U:H6	1.73	0.53
1:0:947:U:H2'	1:0:948:G:C8	2.44	0.53
4:B:214:PRO:HD2	38:B:8822:HOH:O	2.08	0.53
1:0:1596:U:H2'	1:0:1598:A:OP2	2.09	0.53
4:B:154:VAL:CG1	4:B:156:LYS:HG2	2.37	0.53
6:D:86:THR:O	6:D:90:LEU:HG	2.08	0.53
18:Q:94:GLN:HG2	18:Q:95:GLU:N	2.23	0.53
1:0:1736:A:H1'	38:0:7406:HOH:O	2.08	0.53
1:0:1739:G:O2'	1:0:1740:U:H5'	2.07	0.53
1:0:282:C:H1'	1:0:368:C:H41	1.67	0.53
1:0:2004:U:O2	1:0:2004:U:C2'	2.57	0.53
7:E:15:GLN:HG3	7:E:20:ILE:HG12	1.91	0.53
2:9:3020:G:O2'	2:9:3021:G:H5'	2.08	0.53
24:W:108:ARG:HG3	24:W:114:PRO:HG3	1.91	0.53
16:O:37:ARG:HG3	38:O:3002:HOH:O	2.09	0.53
1:0:119:A:H2'	1:0:120:A:C5'	2.38	0.53
1:0:841:A:OP2	19:R:128:ARG:HD2	2.08	0.53
14:M:164:THR:CG2	14:M:167:GLY:H	2.22	0.53
26:Y:235:GLU:H	26:Y:235:GLU:CD	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1677:U:OP2	29:2:8:LYS:NZ	2.42	0.53
1:0:2073:G:OP2	1:0:2490:A:H5'	2.09	0.53
1:0:545:G:H8	1:0:545:G:C5'	2.17	0.53
21:T:63:ILE:HD11	21:T:75:GLU:HB2	1.90	0.53
1:0:256:C:H2'	1:0:257:G:O4'	2.09	0.53
1:0:462:A:H2'	38:0:4714:HOH:O	2.09	0.53
1:0:2526:C:H5'	1:0:2526:C:H6	1.73	0.52
1:0:292:G:H2'	1:0:358:G:N2	2.24	0.52
1:0:447:A:OP2	21:T:1:SER:HB2	2.09	0.52
1:0:1594:C:OP2	17:P:120:ARG:HD2	2.09	0.52
3:A:51:ARG:HB2	38:A:8899:HOH:O	2.09	0.52
1:0:1768:C:H2'	1:0:1769:C:O4'	2.09	0.52
23:V:4:HIS:HB3	38:V:6622:HOH:O	2.09	0.52
1:0:2866:U:C5	22:U:50:GLU:HB2	2.44	0.52
1:0:645:U:OP2	13:L:4:LYS:HE3	2.09	0.52
24:W:88:THR:HB	38:W:6679:HOH:O	2.08	0.52
25:X:37:LEU:HD13	25:X:85:VAL:HG21	1.92	0.52
1:0:1226:G:H5'	38:0:4363:HOH:O	2.10	0.52
1:0:2364:A:H5''	18:Q:15:LYS:HD3	1.91	0.52
1:0:1717:A:H5''	17:P:54:LYS:HB2	1.90	0.52
1:0:1625:U:H3'	1:0:1625:U:H6	1.73	0.52
1:0:1244:U:OP1	11:J:18:ILE:HD13	2.09	0.52
15:N:48:VAL:HG11	15:N:55:ASP:HB3	1.90	0.52
1:0:1074:G:H4'	1:0:1260:G:C6	2.43	0.52
1:0:1171:A:H2'	1:0:1172:G:H5'	1.91	0.52
27:Z:10:ARG:HA	38:Z:8715:HOH:O	2.09	0.52
5:C:236:THR:CG2	5:C:239:ALA:H	2.23	0.52
1:0:1218:U:H2'	1:0:1219:U:C6	2.45	0.52
31:I:125:ALA:O	31:I:129:VAL:HG23	2.10	0.52
8:F:46:GLU:O	8:F:73:PRO:HD2	2.09	0.52
1:0:1370:G:O5'	19:R:62:HIS:HB3	2.09	0.52
26:Y:126:PRO:HG2	26:Y:128:PHE:CZ	2.44	0.52
1:0:2900:G:H2'	1:0:2901:C:O4'	2.10	0.52
25:X:78:GLU:HG2	25:X:79:GLU:H	1.74	0.52
1:0:1548:U:O2'	1:0:1549:C:H5'	2.09	0.52
1:0:2133:U:H5'	38:0:4024:HOH:O	2.09	0.52
1:0:1163:G:N1	1:0:1184:C:N4	2.58	0.52
1:0:1167:G:C4'	31:I:135:LEU:HD21	2.39	0.52
1:0:303:C:H2'	1:0:304:G:O4'	2.10	0.52
1:0:1044:C:H5''	38:0:8844:HOH:O	2.09	0.52
4:B:274:GLU:HA	4:B:292:GLY:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3100:G:H3'	38:9:7426:HOH:O	2.10	0.52
1:0:308:U:C4	1:0:342:C:H1'	2.45	0.52
1:0:845:U:H2'	38:0:9017:HOH:O	2.08	0.52
1:0:2134:G:C6	1:0:2258:A:C8	2.98	0.52
1:0:2756:U:N3	1:0:2896:A:H2	2.01	0.52
3:A:81:GLN:HB2	3:A:92:ASN:ND2	2.25	0.52
30:3:11:CYS:HB2	30:3:20:HIS:CE1	2.45	0.52
1:0:1477:C:H5'	1:0:1868:G:C5'	2.40	0.52
1:0:39:G:N2	1:0:444:C:C2	2.78	0.52
1:0:926:A:O2'	13:L:41:HIS:HD2	1.93	0.51
1:0:1266:U:H4'	26:Y:115:ARG:NH2	2.23	0.51
15:N:49:THR:HG22	15:N:56:ASP:HB2	1.92	0.51
7:E:84:MET:HG2	7:E:168:ILE:HA	1.92	0.51
1:0:1702:U:H5'	38:0:3239:HOH:O	2.11	0.51
26:Y:189:ASN:HA	26:Y:217:ILE:HD11	1.91	0.51
23:V:59:ILE:O	23:V:63:GLU:HG2	2.10	0.51
1:0:2862:G:H4'	4:B:336:GLN:O	2.09	0.51
1:0:1805:G:H2'	1:0:1806:G:H8	1.73	0.51
3:A:105:VAL:HG11	3:A:154:ALA:HB1	1.92	0.51
6:D:25:MET:HE2	6:D:41:LEU:HG	1.93	0.51
1:0:968:G:O2'	1:0:969:G:H5'	2.10	0.51
1:0:2520:G:H5'	10:H:61:SER:OG	2.10	0.51
3:A:36:ASP:O	3:A:38:ILE:N	2.43	0.51
1:0:1205:U:C2'	1:0:1206:U:C5'	2.84	0.51
1:0:1202:A:H2'	1:0:1203:G:C5'	2.41	0.51
27:Z:46:ARG:CD	27:Z:59:TYR:HB2	2.40	0.51
1:0:1741:U:H5'	1:0:1742:A:OP1	2.11	0.51
13:L:133:VAL:HA	38:L:8872:HOH:O	2.10	0.51
1:0:2326:U:H2'	1:0:2327:A:C8	2.46	0.51
21:T:24:ARG:HH21	21:T:39:ASN:HD22	1.57	0.51
11:J:64:GLY:HA3	35:J:8821:CL:CL	2.48	0.51
1:0:2717:C:OP1	4:B:207:LYS:HG3	2.11	0.51
1:0:1201:C:H2'	1:0:1202:A:H5'	1.92	0.51
24:W:4:LEU:HB2	24:W:33:THR:HG22	1.93	0.51
25:X:72:VAL:HG22	25:X:85:VAL:HG12	1.91	0.51
1:0:11:A:H5'	1:0:12:U:OP2	2.10	0.51
1:0:2387:U:H2'	1:0:2388:C:C6	2.45	0.51
1:0:1118:A:H8	1:0:1119:G:H5''	1.76	0.51
1:0:317:A:OP1	21:T:52:ARG:O	2.29	0.51
2:9:3039:U:H3'	2:9:3040:C:H5''	1.93	0.51
10:H:162:ARG:HD2	38:H:8583:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:13:GLU:OE2	8:F:78:GLU:HG2	2.10	0.51
9:G:12:ILE:N	9:G:13:PRO:HD3	2.26	0.51
4:B:201:ASP:HB2	4:B:312:ARG:HD2	1.93	0.51
28:1:8:GLN:HE22	28:1:11:LYS:NZ	2.09	0.51
6:D:88:LEU:HB2	6:D:89:PRO:HD3	1.92	0.51
1:0:1484:G:H2'	38:0:8919:HOH:O	2.09	0.51
1:0:136:C:H2'	1:0:137:U:O4'	2.11	0.51
16:O:37:ARG:NH1	38:O:5650:HOH:O	2.44	0.51
1:0:1181:A:H2'	1:0:1182:C:C5'	2.41	0.51
1:0:1200:A:H3'	38:0:5585:HOH:O	2.10	0.51
1:0:2270:G:H4'	3:A:223:ARG:HH12	1.75	0.51
4:B:16:ARG:NE	38:B:8854:HOH:O	2.39	0.51
1:0:820:G:O2'	1:0:856:G:H4'	2.11	0.51
1:0:544:G:C3'	1:0:545:G:H5''	2.41	0.51
6:D:103:ASN:ND2	6:D:134:LEU:H	2.09	0.51
9:G:12:ILE:HG22	9:G:17:GLN:HE21	1.76	0.51
1:0:106:A:H2'	1:0:107:U:O4'	2.11	0.51
20:S:17:ASP:HB3	20:S:23:LYS:HB2	1.92	0.51
1:0:1520:G:H2'	1:0:1521:C:C6	2.46	0.51
1:0:1992:U:H2'	1:0:1994:A:OP2	2.11	0.51
1:0:2019:A:H5'	38:0:4370:HOH:O	2.10	0.51
4:B:280:VAL:HG13	4:B:333:GLU:O	2.11	0.51
1:0:1159:G:H1	1:0:1208:C:H42	1.58	0.51
1:0:2135:A:C2'	1:0:2136:G:H5'	2.40	0.51
1:0:1576:G:H2'	1:0:1577:U:O4'	2.11	0.51
18:Q:11:ARG:HD3	38:Q:5620:HOH:O	2.10	0.51
1:0:1965:C:H6	1:0:1965:C:O5'	1.94	0.51
3:A:192:VAL:CG1	3:A:207:GLN:HB3	2.41	0.50
1:0:204:A:C2'	1:0:205:U:H5'	2.41	0.50
4:B:305:ASP:O	4:B:306:LYS:HB2	2.11	0.50
4:B:329:TYR:CE2	22:U:15:PRO:HG2	2.46	0.50
1:0:2505:G:C2'	1:0:2506:A:H5'	2.40	0.50
1:0:1175:G:C5	1:0:1193:A:C2	2.99	0.50
1:0:2502:C:H4'	10:H:155:ASN:ND2	2.26	0.50
5:C:5:ILE:HD11	5:C:16:VAL:CG2	2.41	0.50
1:0:2419:U:H5''	1:0:2420:G:H5'	1.93	0.50
11:J:19:MET:HE1	11:J:132:LEU:HD21	1.93	0.50
1:0:2338:G:H1'	6:D:105:SER:OG	2.11	0.50
20:S:10:VAL:HG11	23:V:36:ALA:HA	1.92	0.50
1:0:1064:U:H2'	1:0:1065:G:C8	2.47	0.50
3:A:96:LEU:HD22	3:A:128:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:4:LEU:O	24:W:32:CYS:HA	2.11	0.50
1:0:960:G:C3'	1:0:960:G:N3	2.74	0.50
2:9:3039:U:C2'	2:9:3040:C:OP1	2.59	0.50
1:0:850:U:H3'	38:0:6635:HOH:O	2.10	0.50
13:L:149:ARG:HB2	38:L:8840:HOH:O	2.11	0.50
1:0:1025:C:H5'	24:W:23:MET:O	2.11	0.50
1:0:2515:C:H2'	1:0:2516:G:O4'	2.11	0.50
1:0:682:A:H2'	1:0:683:G:O4'	2.11	0.50
4:B:88:GLU:HB3	4:B:97:LEU:HD12	1.92	0.50
1:0:2350:G:H2'	1:0:2351:C:H6	1.76	0.50
1:0:2010:A:H2'	38:0:5787:HOH:O	2.11	0.50
1:0:2526:C:HO2'	1:0:2527:U:H5'	1.75	0.50
1:0:2676:C:H4'	11:J:70:PHE:HE1	1.75	0.50
24:W:31:HIS:HB3	38:W:5420:HOH:O	2.11	0.50
31:I:102:VAL:HG12	31:I:106:LYS:HE3	1.94	0.50
2:9:3038:A:H2	2:9:3043:G:H5''	1.76	0.50
1:0:522:U:O2'	1:0:1366:C:H5'	2.10	0.50
16:O:105:ASN:HD21	16:O:109:SER:N	2.10	0.50
1:0:1625:U:H3'	1:0:1625:U:C6	2.47	0.50
1:0:1180:U:H4'	31:I:91:GLU:HG2	1.93	0.50
1:0:2429:A:H2'	1:0:2430:A:C8	2.47	0.50
1:0:1845:A:OP2	3:A:190:ARG:NH1	2.45	0.50
25:X:76:ARG:HH11	25:X:76:ARG:HG3	1.75	0.50
1:0:1198:U:C6	1:0:1200:A:OP2	2.64	0.50
1:0:289:G:N2	1:0:364:C:C2	2.79	0.50
22:U:52:THR:HG22	22:U:54:THR:N	2.26	0.50
1:0:960:G:H8	38:0:5800:HOH:O	1.94	0.50
1:0:820:G:H5'	1:0:821:U:H5'	1.93	0.50
1:0:2886:C:O2'	1:0:2887:G:H5'	2.12	0.50
1:0:721:A:H5''	16:O:51:TYR:CE2	2.47	0.50
1:0:156:C:H5''	14:M:171:ARG:CD	2.32	0.50
1:0:661:G:C6	1:0:686:A:C2	2.99	0.50
1:0:106:A:H1'	38:0:9311:HOH:O	2.12	0.50
23:V:64:GLY:O	23:V:65:ASP:HB2	2.12	0.50
1:0:920:C:H5''	1:0:921:G:O5'	2.12	0.50
14:M:30:GLU:O	14:M:34:GLU:HG3	2.10	0.50
1:0:88:G:H2'	1:0:89:G:C8	2.46	0.50
8:F:118:LEU:O	8:F:119:ARG:HB3	2.12	0.50
1:0:1557:G:O2'	1:0:1558:C:H5'	2.12	0.50
1:0:1209:C:H2'	1:0:1210:G:C8	2.46	0.49
1:0:2908:A:H2'	1:0:2909:G:C5'	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1588:G:C6	1:0:1589:G:C6	3.00	0.49
1:0:2591:C:H2'	1:0:2592:G:O4'	2.12	0.49
1:0:2416:G:O2'	15:N:25:ARG:HG2	2.12	0.49
1:0:1568:G:O2'	1:0:1569:U:H5'	2.12	0.49
17:P:134:VAL:O	17:P:137:LEU:HB3	2.12	0.49
27:Z:42:CYS:SG	27:Z:43:GLY:N	2.84	0.49
1:0:1289:C:O2'	1:0:1290:G:H5'	2.11	0.49
2:9:3003:A:H2	2:9:3021:G:N3	2.10	0.49
1:0:960:G:H4'	38:0:7254:HOH:O	2.11	0.49
28:1:1:THR:HA	38:1:435:HOH:O	2.11	0.49
22:U:6:CYS:HB2	22:U:32:CYS:HB3	1.95	0.49
24:W:125:HIS:CD2	24:W:127:GLY:H	2.26	0.49
24:W:125:HIS:NE2	24:W:128:VAL:HG13	2.27	0.49
1:0:2781:U:C2'	1:0:2782:G:H5'	2.42	0.49
1:0:1304:U:H2'	1:0:1305:C:C6	2.47	0.49
1:0:95:A:H5''	1:0:97:G:O4'	2.13	0.49
7:E:81:GLU:HG2	7:E:134:SER:HB3	1.94	0.49
1:0:1931:A:H2'	1:0:1932:G:H5'	1.94	0.49
11:J:18:ILE:O	11:J:22:VAL:HG23	2.12	0.49
1:0:475:G:H5'	5:C:73:LEU:CD2	2.42	0.49
25:X:7:GLU:HG3	25:X:74:ALA:O	2.12	0.49
1:0:920:C:H4'	1:0:921:G:C2	2.46	0.49
1:0:1764:C:H2'	1:0:1765:G:O4'	2.12	0.49
1:0:944:G:H21	24:W:44:MET:CE	2.26	0.49
2:9:3073:G:H2'	2:9:3074:G:C8	2.48	0.49
1:0:282:C:HO2'	1:0:368:C:N4	2.11	0.49
1:0:120:A:H2'	1:0:120:A:N3	2.27	0.49
5:C:57:PRO:HG2	5:C:73:LEU:HD13	1.94	0.49
1:0:517:U:P	36:0:8823:NEG:HN41	2.35	0.49
1:0:1342:C:C2'	1:0:1343:C:H5'	2.42	0.49
1:0:2100:A:H4'	5:C:64:GLY:O	2.12	0.49
1:0:1174:A:H3'	1:0:1176:C:OP2	2.12	0.49
4:B:304:PRO:HD2	4:B:307:ARG:NE	2.28	0.49
31:I:93:GLN:HE21	31:I:133:THR:CG2	2.26	0.49
1:0:1545:C:H2'	1:0:1546:G:O4'	2.13	0.49
1:0:1166:A:C6	1:0:1181:A:C2	3.01	0.49
1:0:308:U:C2	21:T:52:ARG:NH2	2.81	0.49
1:0:1097:A:H5''	24:W:125:HIS:CE1	2.47	0.49
1:0:2781:U:H1'	7:E:139:GLU:OE2	2.12	0.49
19:R:33:ARG:NH1	38:R:8842:HOH:O	2.41	0.49
4:B:145:HIS:HD2	4:B:146:THR:O	1.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2263:G:H1'	38:0:6449:HOH:O	2.12	0.49
17:P:80:ARG:HG2	17:P:87:ARG:CZ	2.43	0.49
10:H:169:GLY:HA3	38:H:8590:HOH:O	2.12	0.49
12:K:4:LEU:HD22	12:K:116:GLU:HB3	1.95	0.49
38:9:5071:HOH:O	15:N:20:TYR:HE2	1.95	0.49
1:0:1166:A:N3	1:0:1166:A:H2'	2.28	0.49
6:D:166:ILE:HB	38:D:6326:HOH:O	2.13	0.49
2:9:3049:G:O2'	2:9:3050:G:H5'	2.12	0.49
1:0:1520:G:C6	1:0:1521:C:N4	2.81	0.49
8:F:101:ALA:HA	38:F:5413:HOH:O	2.11	0.49
15:N:83:LEU:HD13	15:N:175:LEU:HD23	1.94	0.49
1:0:263:U:O4'	8:F:59:ILE:HD13	2.13	0.49
1:0:1594:C:O2'	1:0:1607:A:H4'	2.13	0.49
14:M:59:GLY:HA3	14:M:141:ILE:HD11	1.95	0.49
38:0:9642:HOH:O	4:B:252:PRO:HD3	2.12	0.49
2:9:3110:G:C5	2:9:3111:U:C5	3.01	0.49
4:B:140:LEU:HD12	4:B:174:ARG:HG3	1.94	0.49
25:X:10:VAL:HG12	25:X:11:THR:N	2.28	0.49
1:0:1165:G:O2'	1:0:1166:A:OP1	2.28	0.49
1:0:694:A:H2'	1:0:695:C:H5'	1.94	0.49
11:J:74:ARG:NH1	11:J:144:THR:HG21	2.28	0.49
20:S:76:GLU:HB3	38:S:8549:HOH:O	2.13	0.49
1:0:254:C:O2	1:0:254:C:H2'	2.11	0.49
31:I:120:ASP:HB2	31:I:123:ASN:HD22	1.78	0.48
1:0:1528:A:H62	1:0:1663:G:N2	2.10	0.48
26:Y:99:ALA:HB2	26:Y:233:TYR:CE2	2.48	0.48
1:0:415:A:O2'	1:0:416:G:H5'	2.13	0.48
11:J:99:GLU:HA	38:J:7377:HOH:O	2.13	0.48
24:W:149:LEU:HG	24:W:153:MET:HE2	1.95	0.48
1:0:1453:G:H2'	1:0:1454:U:O4'	2.12	0.48
26:Y:212:ARG:HD2	38:Y:8180:HOH:O	2.12	0.48
4:B:51:VAL:HG23	4:B:329:TYR:O	2.13	0.48
5:C:93:LYS:O	5:C:98:ARG:NH2	2.46	0.48
24:W:130:HIS:O	24:W:136:GLY:HA3	2.13	0.48
2:9:3092:G:C6	2:9:3093:A:N6	2.81	0.48
1:0:2372:A:H2'	1:0:2373:U:C6	2.48	0.48
1:0:875:A:C2	3:A:194:MET:HG2	2.48	0.48
38:K:7438:HOH:O	22:U:20:MET:HE1	2.13	0.48
10:H:165:SER:OG	10:H:168:ALA:HB3	2.13	0.48
1:0:1508:C:H5'	20:S:21:GLN:HE22	1.77	0.48
20:S:57:THR:HG22	20:S:58:MET:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:36:ASP:C	3:A:38:ILE:H	2.17	0.48
1:0:1497:G:H4'	1:0:1627:G:O2'	2.13	0.48
1:0:1238:C:H5''	1:0:1239:G:OP2	2.14	0.48
1:0:440:C:H2'	1:0:441:A:C8	2.47	0.48
1:0:1217:G:H2'	1:0:1218:U:C6	2.48	0.48
1:0:2385:G:H2'	1:0:2386:U:C6	2.48	0.48
1:0:178:U:H2'	1:0:179:C:H6	1.78	0.48
26:Y:189:ASN:ND2	26:Y:191:ASP:H	2.06	0.48
31:I:78:LEU:HD12	31:I:112:LYS:HZ1	1.78	0.48
15:N:73:ALA:HB1	15:N:74:PRO:CD	2.43	0.48
15:N:139:TRP:HA	15:N:139:TRP:CE3	2.49	0.48
1:0:1202:A:H2'	1:0:1203:G:O4'	2.14	0.48
1:0:1185:U:H5''	31:I:123:ASN:HB3	1.96	0.48
1:0:1641:A:H2'	1:0:1642:A:C5'	2.42	0.48
28:1:8:GLN:HE22	28:1:11:LYS:HZ2	1.62	0.48
1:0:2870:C:H2'	1:0:2871:G:C8	2.48	0.48
1:0:843:A:C2	1:0:846:A:C8	3.02	0.48
12:K:34:VAL:HG22	12:K:47:ALA:HB2	1.95	0.48
1:0:1657:A:H2'	1:0:1658:A:C8	2.48	0.48
11:J:57:TYR:HE2	11:J:71:TYR:HH	1.60	0.48
5:C:37:ALA:HB2	38:C:8572:HOH:O	2.12	0.48
29:2:41:HIS:N	29:2:45:ASN:HD22	2.09	0.48
1:0:699:C:C2	1:0:744:G:C2	3.02	0.48
1:0:2372:A:H2'	1:0:2373:U:H6	1.79	0.48
2:9:3065:A:N6	2:9:3112:U:C6	2.81	0.48
8:F:58:GLU:HB3	14:M:8:ILE:HG23	1.96	0.48
1:0:1218:U:H2'	1:0:1219:U:H6	1.78	0.48
24:W:149:LEU:HG	24:W:153:MET:CE	2.44	0.48
1:0:316:A:N3	1:0:336:G:O2'	2.45	0.48
2:9:3114:G:O6	15:N:11:ARG:HD3	2.14	0.48
8:F:2:VAL:HG22	8:F:57:GLU:OE1	2.14	0.48
5:C:118:THR:O	5:C:136:VAL:HG13	2.14	0.48
1:0:566:A:H2'	1:0:567:U:O4'	2.14	0.48
1:0:352:A:H2'	1:0:353:G:C8	2.48	0.48
1:0:128:A:H3'	1:0:128:A:C8	2.49	0.48
1:0:1299:G:O6	13:L:6:ARG:HD3	2.13	0.48
1:0:2010:A:C2'	38:0:5787:HOH:O	2.61	0.48
17:P:107:GLU:O	17:P:111:GLU:HG3	2.13	0.48
29:2:20:ARG:HB3	38:2:5444:HOH:O	2.12	0.48
1:0:1398:G:H2'	1:0:1399:A:C8	2.48	0.47
1:0:489:A:C8	21:T:82:THR:HG22	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1759:A:N3	1:0:1818:C:H2'	2.29	0.47
1:0:240:C:O2	1:0:240:C:H2'	2.14	0.47
1:0:1192:A:H3'	1:0:1193:A:C5'	2.44	0.47
1:0:1202:A:C2'	1:0:1203:G:H5'	2.44	0.47
1:0:407:A:H8	38:0:4289:HOH:O	1.97	0.47
5:C:27:ARG:HG3	5:C:29:ASP:OD1	2.15	0.47
6:D:25:MET:HE1	6:D:37:ALA:HB1	1.95	0.47
25:X:14:LEU:HD12	25:X:67:PRO:O	2.14	0.47
38:0:9771:HOH:O	5:C:78:ARG:HD3	2.13	0.47
6:D:106:PHE:HB2	38:D:5198:HOH:O	2.14	0.47
1:0:354:A:H2'	1:0:355:C:H6	1.79	0.47
1:0:366:U:O2'	1:0:367:G:H5'	2.14	0.47
4:B:221:GLN:HE22	12:K:42:ASN:ND2	2.09	0.47
4:B:154:VAL:HG12	4:B:156:LYS:HG2	1.95	0.47
13:L:13:HIS:HB3	38:L:8895:HOH:O	2.14	0.47
1:0:326:G:O2'	1:0:327:A:H5'	2.14	0.47
11:J:45:VAL:HG21	11:J:129:PHE:CD1	2.49	0.47
3:A:186:TRP:CG	3:A:187:PRO:HA	2.50	0.47
7:E:31:ARG:HH12	7:E:68:HIS:CD2	2.31	0.47
1:0:2570:G:H5''	38:0:4744:HOH:O	2.15	0.47
15:N:44:ARG:HG3	15:N:45:ALA:N	2.29	0.47
1:0:1201:C:H5''	38:0:6062:HOH:O	2.13	0.47
3:A:100:PRO:HG2	3:A:103:VAL:HG21	1.96	0.47
26:Y:189:ASN:ND2	26:Y:191:ASP:HB2	2.29	0.47
1:0:92:G:H5'	38:0:7249:HOH:O	2.13	0.47
1:0:2578:G:C8	1:0:2578:G:H5'	2.43	0.47
1:0:2251:G:H2'	1:0:2252:A:C8	2.49	0.47
1:0:1871:U:O4'	1:0:1873:G:C8	2.67	0.47
1:0:232:A:H4'	38:0:5909:HOH:O	2.12	0.47
1:0:1450:C:C4'	1:0:1451:C:OP2	2.56	0.47
1:0:1202:A:H2'	1:0:1203:G:H5'	1.97	0.47
29:2:41:HIS:HD2	29:2:44:ARG:H	1.62	0.47
1:0:775:G:OP1	28:1:16:HIS:HE1	1.97	0.47
4:B:51:VAL:CG2	4:B:327:VAL:HG13	2.43	0.47
30:3:18:GLN:HB3	38:3:8816:HOH:O	2.13	0.47
14:M:155:GLN:O	14:M:158:ARG:HG2	2.13	0.47
15:N:61:ALA:HB3	15:N:88:ALA:HB2	1.94	0.47
1:0:2524:G:H21	1:0:2526:C:N4	2.13	0.47
2:9:3014:G:H2'	2:9:3015:C:H5'	1.97	0.47
28:1:25:LYS:HD2	29:2:49:GLU:N	2.29	0.47
13:L:129:ALA:O	13:L:133:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:I:93:GLN:HE21	31:I:133:THR:HG21	1.80	0.47
38:9:5071:HOH:O	15:N:23:ARG:HD3	2.13	0.47
4:B:268:ARG:HH21	4:B:325:PRO:HG3	1.80	0.47
1:0:422:G:O2'	1:0:423:A:H5'	2.14	0.47
1:0:2382:A:H5'	38:3:8835:HOH:O	2.14	0.47
4:B:275:GLY:O	4:B:291:ASP:HA	2.14	0.47
1:0:1160:G:H5''	1:0:1161:A:H5'	1.81	0.47
17:P:115:SER:H	17:P:118:GLN:HE21	1.56	0.47
1:0:2716:G:C5'	4:B:206:THR:HG21	2.44	0.47
2:9:3003:A:OP2	2:9:3025:G:N2	2.47	0.47
1:0:2252:A:H2'	1:0:2253:G:O4'	2.15	0.47
2:9:3034:A:H2'	2:9:3035:C:O4'	2.14	0.47
1:0:1187:U:HO2'	1:0:1188:A:H8	1.60	0.47
28:1:25:LYS:O	28:1:25:LYS:HG2	2.15	0.47
6:D:23:VAL:CG2	6:D:73:VAL:HB	2.44	0.47
1:0:968:G:H1'	10:H:32:LYS:HD2	1.97	0.47
10:H:80:GLU:HA	38:H:8585:HOH:O	2.14	0.47
11:J:51:GLU:O	11:J:55:GLU:HG3	2.15	0.47
6:D:136:ARG:HD2	6:D:155:HIS:O	2.15	0.47
9:G:64:ASN:N	9:G:64:ASN:HD22	2.13	0.47
1:0:56:G:H5''	23:V:50:ARG:NH1	2.30	0.47
7:E:10:ASP:HA	38:E:3707:HOH:O	2.14	0.47
21:T:73:HIS:HB3	38:T:6320:HOH:O	2.15	0.47
1:0:1206:U:C5'	1:0:1206:U:H6	2.19	0.47
1:0:2502:C:O2'	1:0:2503:A:H5'	2.13	0.47
1:0:2415:A:H2'	1:0:2416:G:H5'	1.95	0.47
23:V:44:GLY:O	23:V:48:GLU:HG2	2.14	0.47
1:0:2247:C:H2'	1:0:2248:C:H6	1.79	0.47
27:Z:22:SER:O	27:Z:26:VAL:HG23	2.15	0.47
8:F:56:PRO:HG2	14:M:43:PRO:O	2.15	0.47
1:0:282:C:C2'	1:0:283:U:H5'	2.44	0.47
1:0:2768:A:H2'	1:0:2769:C:O4'	2.15	0.47
1:0:2908:A:O2'	1:0:2909:G:H5'	2.14	0.47
1:0:2890:A:C1'	22:U:56:ARG:NH2	2.76	0.47
1:0:1972:U:H2'	1:0:1973:A:C5'	2.45	0.47
1:0:1878:G:O2'	1:0:1879:U:P	2.72	0.47
1:0:1060:C:H6	1:0:1060:C:H5'	1.80	0.47
1:0:579:G:H2'	1:0:580:A:C8	2.50	0.47
1:0:1423:C:O2'	1:0:1424:A:H5'	2.15	0.47
1:0:2832:C:H5	38:0:7037:HOH:O	1.97	0.47
1:0:2016:U:H2'	1:0:2017:U:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:542:A:C5'	1:0:542:A:C8	2.91	0.47
38:9:4707:HOH:O	15:N:147:ILE:HB	2.15	0.47
38:0:6557:HOH:O	18:Q:13:LYS:HE2	2.15	0.47
1:0:2866:U:H4'	1:0:2867:G:H5'	1.97	0.47
2:9:3110:G:C5	2:9:3111:U:C6	3.03	0.47
15:N:78:MET:HB2	15:N:79:PRO:HD3	1.97	0.47
5:C:124:VAL:HA	5:C:230:GLY:O	2.15	0.47
5:C:129:HIS:CE1	5:C:231:ARG:HA	2.51	0.47
26:Y:103:THR:HG22	26:Y:104:GLU:OE2	2.15	0.47
1:0:319:A:H4'	1:0:338:C:C5	2.50	0.47
1:0:1181:A:C2	1:0:1192:A:C8	3.03	0.46
1:0:1197:G:H1'	1:0:1203:G:N2	2.29	0.46
1:0:1878:G:O2'	1:0:1879:U:C6	2.65	0.46
1:0:383:A:C2	1:0:407:A:C4	3.03	0.46
1:0:1249:U:H2'	1:0:1250:C:C6	2.50	0.46
26:Y:117:LEU:N	26:Y:174:VAL:HG21	2.30	0.46
1:0:2467:A:O2'	1:0:2468:A:H2'	2.16	0.46
1:0:2403:C:H2'	1:0:2404:G:O5'	2.15	0.46
1:0:273:G:H2'	1:0:274:G:O4'	2.15	0.46
1:0:1165:G:O2'	1:0:1174:A:C1'	2.63	0.46
1:0:130:C:O2'	1:0:131:A:N7	2.49	0.46
1:0:1878:G:H1'	38:0:5948:HOH:O	2.15	0.46
24:W:88:THR:HG22	24:W:90:TYR:CD1	2.50	0.46
1:0:138:U:OP2	1:0:139:C:H5	1.99	0.46
1:0:1714:C:O2'	1:0:1715:C:H5'	2.15	0.46
15:N:7:LYS:HE3	18:Q:21:ARG:O	2.16	0.46
10:H:47:ILE:HG12	10:H:165:SER:HA	1.96	0.46
1:0:1191:A:H2'	1:0:1193:A:H5'	1.96	0.46
1:0:958:G:H2'	1:0:959:C:H6	1.81	0.46
2:9:3003:A:C2	2:9:3021:G:N3	2.83	0.46
1:0:2064:U:H5'	1:0:2652:U:H4'	1.96	0.46
1:0:488:U:H2'	38:0:3825:HOH:O	2.15	0.46
1:0:1761:U:H2'	1:0:1762:C:C6	2.50	0.46
31:I:75:THR:HG21	38:I:5331:HOH:O	2.15	0.46
15:N:164:ASP:CG	15:N:167:ASP:HA	2.36	0.46
17:P:91:LYS:O	17:P:95:GLU:HG3	2.14	0.46
22:U:17:THR:HG22	22:U:18:GLY:N	2.29	0.46
38:0:6511:HOH:O	21:T:38:ARG:NH1	2.48	0.46
19:R:9:ASP:O	19:R:13:THR:HB	2.14	0.46
1:0:840:U:H2'	19:R:128:ARG:NH1	2.31	0.46
1:0:517:U:OP1	36:0:8823:NEG:N4	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:192:VAL:HG13	38:A:8852:HOH:O	2.15	0.46
1:0:113:A:OP2	1:0:114:A:H2'	2.15	0.46
1:0:417:G:P	38:0:7241:HOH:O	2.74	0.46
38:0:7244:HOH:O	3:A:22:ARG:HD3	2.15	0.46
1:0:807:A:H2'	1:0:808:A:O4'	2.16	0.46
1:0:1119:G:H2'	11:J:52:GLN:HE22	1.79	0.46
1:0:1174:A:H5'	38:0:4245:HOH:O	2.15	0.46
24:W:88:THR:HG23	24:W:110:GLN:HE21	1.80	0.46
5:C:76:ARG:HG2	5:C:78:ARG:NH1	2.30	0.46
1:0:568:G:OP2	24:W:122:ARG:HD3	2.14	0.46
1:0:1029:U:O2'	1:0:1273:C:OP1	2.33	0.46
4:B:190:MET:HE2	4:B:194:PHE:CD1	2.50	0.46
1:0:1665:G:O2'	1:0:1666:C:H5'	2.16	0.46
1:0:2488:A:H61	1:0:2534:C:H42	1.64	0.46
30:3:14:CYS:SG	30:3:74:CYS:SG	3.13	0.46
15:N:71:TRP:HE3	15:N:175:LEU:HD22	1.78	0.46
5:C:239:ALA:O	5:C:243:VAL:HB	2.16	0.46
24:W:88:THR:CG2	24:W:90:TYR:HD1	2.28	0.46
30:3:70:ARG:HB3	38:3:8875:HOH:O	2.14	0.46
23:V:39:ALA:N	23:V:40:PRO:CD	2.78	0.46
4:B:51:VAL:HG22	4:B:52:VAL:N	2.30	0.46
1:0:1592:G:O2'	1:0:1593:C:O5'	2.31	0.46
1:0:222:A:H2'	1:0:223:G:O4'	2.14	0.46
27:Z:23:ARG:NH1	38:Z:8704:HOH:O	2.48	0.46
1:0:816:G:C6	1:0:817:G:N1	2.83	0.46
6:D:163:VAL:HA	38:D:6326:HOH:O	2.15	0.46
31:I:113:HIS:H	31:I:114:PRO:HD2	1.79	0.46
1:0:287:C:H6	1:0:287:C:O5'	1.99	0.46
15:N:37:ARG:HH11	15:N:37:ARG:HG3	1.81	0.46
1:0:283:U:H5	1:0:284:C:N4	2.13	0.46
31:I:78:LEU:HD13	31:I:111:GLN:OE1	2.16	0.46
1:0:669:G:O2'	1:0:670:G:H5'	2.15	0.46
30:3:55:VAL:HB	30:3:56:PRO:HD2	1.98	0.46
1:0:2107:U:O2'	1:0:2108:A:H5'	2.15	0.46
1:0:1173:A:C2	1:0:1177:A:C8	3.04	0.46
12:K:74:VAL:CG1	12:K:113:ILE:HG12	2.42	0.46
1:0:2421:G:H3'	1:0:2422:U:H5''	1.98	0.46
11:J:46:ILE:HA	38:J:1123:HOH:O	2.16	0.46
1:0:789:C:H1'	1:0:827:A:C2	2.51	0.46
1:0:1447:U:H3'	1:0:1506:U:O2	2.16	0.46
1:0:1790:C:H2'	1:0:1791:U:H6	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:I:99:ASP:OD1	31:I:138:THR:HB	2.16	0.46
2:9:3056:A:C3'	2:9:3057:A:H5''	2.46	0.46
24:W:125:HIS:HD2	24:W:127:GLY:N	2.13	0.46
3:A:132:ASP:HB3	3:A:135:VAL:H	1.81	0.46
1:0:157:G:H4'	14:M:95:LYS:HE3	1.98	0.46
11:J:127:ILE:HG22	35:J:8801:CL:CL	2.52	0.46
19:R:132:ARG:NH1	38:R:8885:HOH:O	2.48	0.46
1:0:1003:U:H5''	38:0:9447:HOH:O	2.16	0.46
10:H:45:VAL:HG13	10:H:168:ALA:HB2	1.99	0.45
1:0:1193:A:C2	1:0:1194:A:N6	2.83	0.45
3:A:212:PRO:HB2	38:A:8855:HOH:O	2.15	0.45
2:9:3013:A:H3'	2:9:3014:G:H5'	1.98	0.45
13:L:143:THR:CG2	13:L:144:ASP:N	2.79	0.45
13:L:90:ARG:NH2	13:L:121:ILE:HD11	2.31	0.45
2:9:3065:A:C2'	2:9:3066:G:OP2	2.63	0.45
1:0:57:C:H5''	38:0:6585:HOH:O	2.15	0.45
1:0:1495:C:H1'	1:0:1573:A:H1'	1.99	0.45
3:A:121:ALA:O	3:A:124:VAL:HG22	2.15	0.45
1:0:553:G:H5'	38:0:3311:HOH:O	2.15	0.45
1:0:1371:U:H4'	38:0:7664:HOH:O	2.16	0.45
1:0:1118:A:C8	1:0:1119:G:H5''	2.51	0.45
1:0:1819:G:H2'	1:0:1820:G:C4'	2.47	0.45
2:9:3040:C:H2'	2:9:3041:C:OP1	2.17	0.45
1:0:1902:G:H2'	1:0:1903:U:O4'	2.15	0.45
1:0:1568:G:H2'	1:0:1569:U:O4'	2.16	0.45
1:0:834:G:H4'	1:0:835:U:OP2	2.16	0.45
1:0:1313:A:H5'	26:Y:208:LYS:O	2.16	0.45
1:0:2081:A:H4'	11:J:69:TYR:CE1	2.50	0.45
7:E:5:LEU:HD21	7:E:66:GLN:HG3	1.97	0.45
1:0:1200:A:H4'	38:0:7164:HOH:O	2.15	0.45
1:0:1625:U:C3'	1:0:1625:U:C6	2.99	0.45
38:0:9767:HOH:O	25:X:23:HIS:HD2	1.98	0.45
1:0:1330:A:H5''	38:Y:8192:HOH:O	2.15	0.45
1:0:1456:C:H2'	1:0:1457:U:C6	2.51	0.45
1:0:1177:A:C8	1:0:1177:A:O5'	2.68	0.45
1:0:120:A:H5'	28:1:20:ARG:HH21	1.82	0.45
1:0:2676:C:H4'	11:J:70:PHE:CD1	2.52	0.45
27:Z:57:CYS:SG	27:Z:59:TYR:HB3	2.56	0.45
3:A:35:GLY:O	3:A:36:ASP:HB3	2.15	0.45
4:B:112:THR:OG1	4:B:158:LYS:HG3	2.16	0.45
1:0:1947:G:N2	1:0:1966:U:C2	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2598:U:O2	1:0:2600:A:H8	2.00	0.45
14:M:184:ARG:HG3	14:M:185:PRO:HA	1.98	0.45
1:0:796:A:HO2'	27:Z:10:ARG:N	2.15	0.45
6:D:84:LEU:C	6:D:86:THR:H	2.19	0.45
1:0:462:A:H3'	38:0:4714:HOH:O	2.17	0.45
1:0:1342:C:O2'	1:0:1343:C:H5'	2.16	0.45
1:0:857:A:H4'	3:A:176:HIS:CD2	2.52	0.45
13:L:43:HIS:HD2	38:L:8830:HOH:O	1.99	0.45
26:Y:203:VAL:HG12	26:Y:228:VAL:HG22	1.99	0.45
1:0:2050:G:H5''	19:R:80:TYR:O	2.17	0.45
1:0:1462:C:H2'	1:0:1463:A:C8	2.52	0.45
21:T:45:GLY:HA3	21:T:102:ASP:HB2	1.98	0.45
10:H:26:SER:HA	10:H:59:HIS:HD2	1.82	0.45
1:0:2506:A:O2'	1:0:2507:G:O5'	2.34	0.45
1:0:1183:C:O2	1:0:1183:C:H2'	2.17	0.45
3:A:105:VAL:HG11	3:A:154:ALA:CB	2.46	0.45
28:1:8:GLN:NE2	28:1:11:LYS:HZ2	2.13	0.45
1:0:920:C:H5'	1:0:921:G:C4	2.52	0.45
1:0:1931:A:C2'	1:0:1932:G:H5'	2.47	0.45
1:0:1735:C:OP2	4:B:234:ARG:HG3	2.16	0.45
6:D:149:ARG:NH1	38:D:3066:HOH:O	2.48	0.45
21:T:48:VAL:O	21:T:59:GLU:HG3	2.16	0.45
1:0:2587:OMU:H2'	1:0:2589:U:OP2	2.16	0.45
1:0:340:A:O5'	1:0:340:A:C8	2.69	0.45
1:0:1165:G:O2'	1:0:1174:A:H1'	2.16	0.45
7:E:20:ILE:O	7:E:30:THR:HA	2.17	0.45
1:0:926:A:O2'	13:L:41:HIS:CD2	2.70	0.45
5:C:127:ARG:CZ	5:C:225:PRO:HG2	2.46	0.45
1:0:821:U:H4'	27:Z:17:ARG:HH12	1.80	0.45
1:0:1211:G:H2'	1:0:1212:C:H6	1.81	0.45
4:B:17:LYS:O	4:B:260:HIS:HD2	1.98	0.45
1:0:377:C:H5	38:0:3123:HOH:O	1.99	0.45
26:Y:216:ARG:HD2	38:Y:8151:HOH:O	2.17	0.45
2:9:3108:C:O2'	2:9:3109:G:H5'	2.17	0.45
2:9:3018:U:H2'	2:9:3019:G:H8	1.82	0.45
1:0:2502:C:H2'	1:0:2503:A:C5'	2.44	0.45
1:0:2664:A:OP1	1:0:2664:A:C8	2.63	0.45
1:0:2060:A:H4'	38:Y:8159:HOH:O	2.16	0.45
1:0:601:G:O2'	1:0:602:A:H5'	2.17	0.45
11:J:135:ILE:O	11:J:139:LEU:HG	2.16	0.45
1:0:1160:G:H5'	1:0:1161:A:C4'	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:871:G:H4'	38:0:4242:HOH:O	2.16	0.45
1:0:877:G:C5'	1:0:878:G:OP1	2.61	0.45
1:0:131:A:OP2	1:0:141:C:H5	2.00	0.45
38:0:5092:HOH:O	4:B:254:GLN:NE2	2.50	0.45
1:0:1573:A:N7	1:0:1574:C:C2	2.85	0.45
1:0:1213:C:O2'	1:0:1214:G:H5'	2.16	0.45
4:B:141:ARG:HG2	4:B:165:ARG:HA	1.99	0.45
1:0:1706:G:C6	1:0:1707:G:N1	2.84	0.45
1:0:710:G:OP1	16:O:24:ALA:HB3	2.17	0.45
1:0:1420:C:O2	1:0:1420:C:H2'	2.16	0.45
1:0:660:A:H4'	1:0:661:G:O5'	2.17	0.45
1:0:1514:C:O2'	1:0:1515:A:H5'	2.17	0.45
25:X:7:GLU:HA	25:X:74:ALA:O	2.17	0.45
1:0:2438:G:H2'	1:0:2439:C:C6	2.51	0.45
13:L:125:PHE:CE1	13:L:140:VAL:HG13	2.52	0.45
14:M:72:ALA:HB2	14:M:93:ARG:HG2	1.99	0.45
7:E:20:ILE:CD1	7:E:40:VAL:HG11	2.40	0.44
1:0:2720:C:O2	12:K:87:ARG:NH2	2.50	0.44
15:N:82:TYR:OH	15:N:176:ARG:NH1	2.50	0.44
6:D:57:THR:HG23	6:D:63:ILE:HG22	1.98	0.44
13:L:34:GLY:HA3	13:L:38:HIS:CE1	2.52	0.44
10:H:43:TYR:HA	10:H:44:PRO:HD3	1.79	0.44
16:O:39:THR:O	16:O:115:ARG:NH2	2.50	0.44
3:A:103:VAL:O	3:A:105:VAL:HG23	2.17	0.44
5:C:236:THR:HG21	38:C:8567:HOH:O	2.17	0.44
3:A:81:GLN:HB2	3:A:92:ASN:HD22	1.81	0.44
1:0:1481:G:H2'	1:0:1482:A:O4'	2.16	0.44
26:Y:185:VAL:HG12	38:Y:8152:HOH:O	2.17	0.44
1:0:1008:C:H5''	10:H:16:ARG:HH12	1.82	0.44
13:L:54:PRO:HG2	13:L:57:VAL:CG2	2.47	0.44
21:T:47:THR:HB	21:T:100:ASP:HB3	1.99	0.44
1:0:272:A:H3'	38:0:7352:HOH:O	2.17	0.44
3:A:94:LEU:HD12	3:A:98:GLU:HB2	1.99	0.44
1:0:2421:G:H3'	1:0:2422:U:C5'	2.48	0.44
1:0:2252:A:H2'	1:0:2253:G:H5'	1.98	0.44
4:B:304:PRO:HD2	4:B:307:ARG:HE	1.82	0.44
11:J:74:ARG:O	11:J:78:ILE:HG12	2.17	0.44
1:0:319:A:H4'	1:0:338:C:C4	2.53	0.44
1:0:1613:C:H2'	1:0:1614:G:O4'	2.16	0.44
22:U:5:GLU:HG3	22:U:10:GLY:O	2.17	0.44
4:B:27:ASN:H	4:B:27:ASN:HD22	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2842:G:H2'	1:0:2843:A:H5'	2.00	0.44
6:D:10:PHE:CG	6:D:11:HIS:N	2.85	0.44
1:0:1805:G:H2'	1:0:1806:G:C8	2.52	0.44
2:9:3052:A:H2'	2:9:3053:G:O4'	2.17	0.44
1:0:963:C:H2'	1:0:964:G:C8	2.53	0.44
1:0:2424:U:H1'	18:Q:7:LEU:HD12	1.99	0.44
1:0:2446:G:H2'	1:0:2447:A:C8	2.52	0.44
1:0:907:A:H2'	1:0:908:A:H8	1.82	0.44
1:0:2801:A:H2'	1:0:2801:A:N3	2.32	0.44
1:0:101:C:H2'	1:0:102:A:H8	1.83	0.44
1:0:2769:C:H2'	1:0:2770:G:O4'	2.18	0.44
22:U:52:THR:HG22	22:U:54:THR:H	1.83	0.44
19:R:29:LYS:HD2	38:R:8839:HOH:O	2.17	0.44
1:0:10:U:O4	1:0:532:A:OP2	2.36	0.44
24:W:29:VAL:O	24:W:30:ASN:HB2	2.17	0.44
1:0:899:C:H5'	38:0:3019:HOH:O	2.16	0.44
1:0:702:G:N2	1:0:727:G:H1'	2.31	0.44
1:0:703:G:O2'	1:0:704:C:H5'	2.18	0.44
1:0:343:C:O2'	1:0:344:C:H5'	2.17	0.44
12:K:125:ALA:C	12:K:127:ALA:H	2.20	0.44
1:0:281:U:O2'	1:0:282:C:H5'	2.18	0.44
1:0:1183:C:H42	1:0:1184:C:H41	1.65	0.44
3:A:88:ILE:HG22	3:A:88:ILE:O	2.17	0.44
5:C:236:THR:HG22	5:C:239:ALA:H	1.81	0.44
1:0:840:U:C2	1:0:2648:U:O4	2.70	0.44
1:0:1586:G:O2'	1:0:1587:U:H5'	2.17	0.44
31:I:113:HIS:N	31:I:114:PRO:CD	2.80	0.44
1:0:2472:C:O2'	1:0:2634:G:H4'	2.17	0.44
1:0:1154:A:H2'	1:0:1155:G:H8	1.81	0.44
21:T:41:ARG:NH1	21:T:42:VAL:O	2.50	0.44
1:0:558:C:C2'	1:0:559:U:C5'	2.78	0.44
1:0:545:G:C8	1:0:545:G:C5'	2.98	0.44
28:1:8:GLN:NE2	28:1:11:LYS:NZ	2.66	0.44
25:X:78:GLU:HG2	25:X:79:GLU:N	2.32	0.44
14:M:48:LYS:HE3	14:M:52:GLN:NE2	2.33	0.44
19:R:81:PRO:O	19:R:85:SER:HB2	2.18	0.44
1:0:2818:A:H2	38:B:8925:HOH:O	2.00	0.44
1:0:1589:G:H4'	38:0:6684:HOH:O	2.18	0.44
10:H:23:ILE:HA	10:H:120:ILE:HG21	1.99	0.44
15:N:49:THR:CG2	15:N:56:ASP:HB2	2.47	0.44
21:T:26:THR:HA	21:T:39:ASN:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:57:C:H42	1:0:89:G:H1	1.65	0.44
8:F:117:GLU:C	8:F:119:ARG:H	2.21	0.44
38:0:4993:HOH:O	4:B:260:HIS:HE1	2.01	0.44
1:0:81:G:N3	1:0:98:A:C2	2.86	0.44
1:0:1874:U:H2'	3:A:120:ARG:HG3	1.99	0.44
1:0:169:A:H5''	38:0:9502:HOH:O	2.17	0.44
1:0:2722:G:H4'	38:K:5029:HOH:O	2.18	0.44
19:R:47:LEU:O	19:R:51:ILE:HG13	2.18	0.44
1:0:172:U:H5'	38:0:3982:HOH:O	2.16	0.44
8:F:111:ILE:O	8:F:115:VAL:HG23	2.18	0.44
24:W:61:THR:HG23	24:W:151:GLU:HG3	2.00	0.44
1:0:2511:A:H5'	1:0:2511:A:H8	1.82	0.44
1:0:430:A:O5'	1:0:430:A:H8	2.01	0.44
7:E:91:PHE:HA	7:E:92:PRO:HD3	1.85	0.44
7:E:11:VAL:HG13	7:E:76:VAL:HG21	2.00	0.44
1:0:1217:G:C2	1:0:1218:U:C2	3.06	0.44
1:0:11:A:N3	1:0:11:A:H2'	2.33	0.44
1:0:707:C:C2	1:0:708:A:C8	3.05	0.44
12:K:23:ASN:HD21	12:K:107:THR:HB	1.82	0.44
1:0:70:A:H4'	1:0:71:G:O5'	2.18	0.44
4:B:24:PRO:CG	4:B:204:GLY:HA2	2.48	0.44
14:M:64:ARG:HD2	38:M:8879:HOH:O	2.17	0.44
1:0:1559:A:OP2	1:0:1559:A:C8	2.69	0.43
13:L:143:THR:CG2	13:L:144:ASP:H	2.27	0.43
30:3:70:ARG:HD3	38:3:8875:HOH:O	2.18	0.43
1:0:2330:U:H4'	1:0:2331:C:OP1	2.18	0.43
38:9:4350:HOH:O	18:Q:25:PRO:HB2	2.17	0.43
1:0:1761:U:H5'	17:P:81:LYS:O	2.18	0.43
15:N:12:ARG:HD3	15:N:18:THR:OG1	2.18	0.43
30:3:73:GLU:HB3	38:3:8863:HOH:O	2.18	0.43
12:K:55:VAL:HG12	12:K:56:SER:N	2.32	0.43
1:0:2896:A:N3	1:0:2896:A:H2'	2.33	0.43
1:0:711:G:N2	1:0:718:C:C2	2.86	0.43
4:B:195:ARG:HG3	4:B:196:ALA:N	2.33	0.43
5:C:1:MET:HG2	5:C:2:GLN:NE2	2.33	0.43
6:D:146:LYS:NZ	15:N:107:ASN:ND2	2.65	0.43
1:0:941:G:C6	1:0:942:U:C4	3.07	0.43
1:0:1515:A:H2'	1:0:1516:C:H6	1.83	0.43
6:D:135:VAL:HG22	6:D:136:ARG:H	1.83	0.43
2:9:3037:C:H4'	15:N:110:THR:HG23	1.99	0.43
2:9:3059:C:O5'	2:9:3059:C:H6	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:59:GLN:HE22	24:W:97:ALA:CB	2.30	0.43
15:N:108:SER:HA	15:N:109:PRO:HD3	1.73	0.43
1:0:1472:C:H6	1:0:1472:C:O5'	2.00	0.43
9:G:63:ARG:N	38:G:2569:HOH:O	2.50	0.43
5:C:140:VAL:HG12	5:C:141:SER:N	2.33	0.43
1:0:407:A:H5'	38:0:5854:HOH:O	2.18	0.43
1:0:2253:G:N2	1:0:2254:G:C4	2.86	0.43
1:0:757:C:OP1	13:L:27:ARG:HD2	2.18	0.43
1:0:2323:G:H5'	38:0:6847:HOH:O	2.17	0.43
1:0:1310:U:OP2	5:C:168:ARG:NH1	2.50	0.43
1:0:2456:A:H2'	1:0:2457:U:C6	2.54	0.43
1:0:86:A:C2	29:2:25:VAL:HG13	2.53	0.43
24:W:3:ALA:O	24:W:54:PHE:HA	2.19	0.43
14:M:66:SER:HB3	14:M:128:TRP:NE1	2.32	0.43
1:0:2842:G:C2'	1:0:2843:A:H5'	2.49	0.43
1:0:1132:A:N6	1:0:1229:C:H2'	2.34	0.43
1:0:2546:U:H4'	38:0:4855:HOH:O	2.19	0.43
2:9:3095:C:O2'	2:9:3096:C:H5'	2.18	0.43
1:0:2478:U:O2'	1:0:2479:A:H5'	2.18	0.43
1:0:1268:C:H2'	1:0:1269:G:H8	1.83	0.43
1:0:111:C:H2'	1:0:112:G:C5'	2.49	0.43
1:0:1328:A:C8	26:Y:169:ARG:HD3	2.53	0.43
22:U:52:THR:CG2	22:U:54:THR:HB	2.49	0.43
4:B:16:ARG:NH1	38:B:8911:HOH:O	2.51	0.43
1:0:2243:C:HO2'	1:0:2244:A:H8	1.65	0.43
1:0:514:G:H5'	38:0:6921:HOH:O	2.17	0.43
25:X:75:ALA:O	25:X:83:ALA:HA	2.19	0.43
1:0:1474:C:C5'	1:0:1474:C:C6	2.88	0.43
11:J:107:ASN:HA	11:J:108:PRO:HD2	1.94	0.43
1:0:926:A:C4'	13:L:39:GLU:HG2	2.42	0.43
1:0:1550:A:C2	1:0:1636:G:C2	3.06	0.43
1:0:1370:G:H5''	38:R:8851:HOH:O	2.18	0.43
13:L:54:PRO:HG2	13:L:57:VAL:HG21	1.99	0.43
23:V:8:ILE:HA	23:V:11:MET:CE	2.48	0.43
1:0:2613:G:O2'	1:0:2614:C:H5'	2.19	0.43
38:0:5239:HOH:O	3:A:164:ARG:NE	2.52	0.43
38:0:9363:HOH:O	30:3:46:ILE:HB	2.18	0.43
25:X:82:GLU:HB3	38:X:5564:HOH:O	2.17	0.43
2:9:3006:C:OP1	15:N:37:ARG:NH1	2.51	0.43
2:9:3013:A:H3'	2:9:3014:G:C5'	2.48	0.43
2:9:3014:G:C2'	2:9:3015:C:H5'	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:81:ARG:HG3	14:M:85:ARG:HB2	2.01	0.43
4:B:307:ARG:HD2	38:B:8943:HOH:O	2.19	0.43
26:Y:234:VAL:HG12	26:Y:235:GLU:N	2.32	0.43
1:0:338:C:H4'	5:C:174:ILE:CD1	2.49	0.43
13:L:125:PHE:CZ	13:L:140:VAL:HG13	2.54	0.43
16:O:49:GLU:HG2	38:O:5191:HOH:O	2.18	0.43
17:P:103:THR:HA	17:P:106:ARG:NH1	2.34	0.43
5:C:219:ASN:HB2	38:C:8590:HOH:O	2.18	0.43
1:0:2271:G:H4'	1:0:2272:G:OP1	2.18	0.43
1:0:1333:U:H2'	1:0:1334:C:C6	2.54	0.43
1:0:293:A:H5''	1:0:357:A:N1	2.34	0.43
1:0:1119:G:N2	1:0:1246:A:H2	2.11	0.43
1:0:290:C:H1'	38:0:5931:HOH:O	2.18	0.43
2:9:3014:G:H2'	2:9:3015:C:C5'	2.49	0.43
1:0:958:G:H2'	1:0:959:C:C6	2.54	0.43
4:B:267:LYS:HA	38:B:8828:HOH:O	2.17	0.43
1:0:475:G:H5'	5:C:73:LEU:HD23	2.00	0.43
1:0:2786:G:H5'	38:0:4466:HOH:O	2.19	0.43
1:0:2269:C:C2'	1:0:2270:G:H5'	2.48	0.43
1:0:1506:U:H6	1:0:1506:U:H5'	1.84	0.43
31:I:101:SER:OG	31:I:104:GLN:HG3	2.19	0.43
1:0:599:G:O2'	1:0:600:G:H5'	2.19	0.43
1:0:2274:A:O2'	1:0:2275:G:H5'	2.18	0.43
16:O:10:LEU:HD13	16:O:99:GLU:HG3	1.99	0.43
1:0:2577:A:H5'	38:0:7569:HOH:O	2.18	0.43
1:0:35:U:H5'	5:C:47:GLY:O	2.19	0.43
1:0:734:U:H2'	1:0:736:A:OP2	2.18	0.43
1:0:2879:A:H2'	1:0:2880:A:O4'	2.19	0.43
2:9:3031:C:H2'	2:9:3032:G:O4'	2.19	0.43
3:A:101:GLU:HG2	38:A:8871:HOH:O	2.19	0.43
31:I:75:THR:C	31:I:77:GLU:H	2.22	0.43
2:9:3052:A:O2'	2:9:3053:G:H5'	2.19	0.43
1:0:938:G:H4'	38:0:5242:HOH:O	2.18	0.43
1:0:2607:U:C4	4:B:242:TRP:CZ2	3.07	0.43
30:3:23:GLU:HG2	30:3:24:LYS:N	2.34	0.43
1:0:1803:C:H2'	1:0:1804:A:C8	2.54	0.43
1:0:2694:A:C4'	7:E:91:PHE:CE1	2.94	0.43
1:0:1972:U:H2'	1:0:1973:A:H5''	2.01	0.43
1:0:1878:G:H4'	38:0:3939:HOH:O	2.19	0.43
1:0:1588:G:C5	1:0:1589:G:C6	3.07	0.43
2:9:3039:U:H1'	2:9:3044:A:N6	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3039:U:HO2'	2:9:3042:C:H5	1.63	0.43
1:0:1289:C:H3'	38:0:6233:HOH:O	2.18	0.43
1:0:316:A:H5'	21:T:54:ASP:OD2	2.19	0.43
29:2:22:PRO:HG2	29:2:25:VAL:HG23	2.01	0.43
1:0:1773:G:N2	1:0:1774:G:C8	2.86	0.43
1:0:165:A:H5''	13:L:33:ALA:HB2	2.00	0.43
4:B:7:ARG:NH1	4:B:11:LEU:HD21	2.33	0.43
13:L:55:GLN:HG3	38:L:8882:HOH:O	2.18	0.43
35:0:8812:CL:CL	38:0:4953:HOH:O	2.59	0.43
1:0:185:G:H4'	1:0:186:A:OP1	2.19	0.43
1:0:1887:U:O5'	1:0:1887:U:H6	2.02	0.43
1:0:1160:G:H2'	38:0:5461:HOH:O	2.18	0.42
1:0:1299:G:N2	38:0:4515:HOH:O	2.51	0.42
1:0:2768:A:H2'	1:0:2769:C:C6	2.54	0.42
1:0:1878:G:O2'	1:0:1879:U:OP2	2.37	0.42
1:0:2781:U:H2'	1:0:2782:G:C5'	2.49	0.42
16:O:50:ARG:HD2	16:O:51:TYR:CE1	2.54	0.42
1:0:178:U:H2'	1:0:179:C:C6	2.54	0.42
1:0:964:G:H2'	1:0:965:A:O4'	2.19	0.42
1:0:2795:C:O2'	1:0:2796:U:H5'	2.18	0.42
1:0:764:C:H2'	1:0:765:G:O4'	2.19	0.42
5:C:193:LEU:HD22	5:C:222:ASP:O	2.19	0.42
1:0:1795:G:H2'	1:0:1796:A:O4'	2.18	0.42
1:0:2011:A:H5'	1:0:2013:G:H1'	1.99	0.42
7:E:158:ASP:O	7:E:162:PHE:HD1	2.01	0.42
6:D:170:TYR:CD1	6:D:170:TYR:N	2.87	0.42
24:W:137:GLN:NE2	24:W:141:HIS:CE1	2.78	0.42
1:0:2316:G:O2'	1:0:2462:G:O6	2.36	0.42
1:0:111:C:C2'	1:0:112:G:H5'	2.49	0.42
1:0:291:C:H2'	1:0:292:G:O4'	2.19	0.42
1:0:2748:G:H1'	38:0:7722:HOH:O	2.19	0.42
27:Z:10:ARG:HG3	27:Z:11:SER:H	1.83	0.42
3:A:101:GLU:OE2	3:A:131:HIS:HB2	2.20	0.42
1:0:1516:C:H2'	1:0:1517:U:C6	2.54	0.42
1:0:636:G:H1'	1:0:2058:G:C4	2.54	0.42
1:0:947:U:H2'	1:0:948:G:H8	1.82	0.42
12:K:34:VAL:CG2	12:K:47:ALA:HB2	2.48	0.42
8:F:54:VAL:HG12	8:F:56:PRO:O	2.19	0.42
27:Z:19:GLY:O	27:Z:23:ARG:HG2	2.18	0.42
1:0:1211:G:H2'	1:0:1212:C:C6	2.53	0.42
4:B:24:PRO:HG2	4:B:204:GLY:HA2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:172:VAL:HG12	6:D:173:GLU:N	2.34	0.42
1:0:1127:C:C5	1:0:1128:U:C4	3.07	0.42
1:0:844:A:C6	1:0:882:A:C6	3.07	0.42
12:K:75:ARG:NH1	38:K:4172:HOH:O	2.51	0.42
1:0:188:C:H5''	14:M:163:LEU:HD21	2.00	0.42
2:9:3013:A:O2'	2:9:3014:G:H5''	2.19	0.42
12:K:87:ARG:NH1	38:K:4066:HOH:O	2.52	0.42
1:0:1730:G:H4'	1:0:1731:C:H6	1.83	0.42
1:0:1519:U:H2'	1:0:1520:G:C8	2.55	0.42
1:0:441:A:H1'	1:0:442:A:N7	2.34	0.42
1:0:352:A:H2'	1:0:353:G:H8	1.83	0.42
1:0:354:A:H2'	1:0:355:C:C6	2.54	0.42
1:0:807:A:H2'	1:0:808:A:C8	2.54	0.42
1:0:1573:A:H2'	1:0:1574:C:O4'	2.19	0.42
1:0:553:G:P	26:Y:204:ARG:HH22	2.43	0.42
14:M:61:ILE:HG22	14:M:62:VAL:N	2.34	0.42
1:0:466:A:H2'	1:0:467:G:O4'	2.19	0.42
3:A:207:GLN:HA	38:A:8852:HOH:O	2.19	0.42
1:0:1187:U:O2'	1:0:1188:A:C8	2.71	0.42
6:D:58:VAL:HG12	6:D:60:GLU:HG2	2.01	0.42
12:K:115:ARG:HG3	12:K:116:GLU:N	2.33	0.42
1:0:1706:G:C6	1:0:1707:G:C6	3.07	0.42
1:0:1661:A:C8	38:0:5036:HOH:O	2.57	0.42
7:E:172:PRO:HB3	38:E:6931:HOH:O	2.18	0.42
24:W:11:VAL:O	24:W:12:ASN:HB2	2.19	0.42
14:M:159:VAL:HG12	35:M:8818:CL:CL	2.57	0.42
1:0:318:C:H5'	1:0:339:A:C2	2.53	0.42
25:X:30:MET:HE1	25:X:58:ALA:HB3	2.02	0.42
1:0:449:A:N7	5:C:43:LYS:HG2	2.35	0.42
4:B:62:ARG:HA	4:B:65:MET:CE	2.49	0.42
1:0:2487:C:H5	38:0:4719:HOH:O	2.03	0.42
1:0:459:A:H4'	38:0:9264:HOH:O	2.19	0.42
1:0:646:G:H2'	1:0:647:U:C6	2.54	0.42
7:E:152:THR:HG21	7:E:165:GLY:HA2	2.01	0.42
1:0:796:A:C2	1:0:797:A:C4	3.08	0.42
2:9:3035:C:H5''	38:9:4078:HOH:O	2.19	0.42
1:0:1789:G:H2'	1:0:1790:C:O5'	2.19	0.42
1:0:1156:C:O5'	1:0:1156:C:H6	2.03	0.42
1:0:1755:A:H2'	1:0:1756:G:O4'	2.19	0.42
1:0:2863:G:C2	1:0:2894:C:O2	2.73	0.42
1:0:2807:U:H2'	1:0:2808:U:H6	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:130:MET:SD	22:U:25:ASP:O	2.78	0.42
1:0:1098:A:H2'	1:0:1099:G:O4'	2.19	0.42
1:0:541:C:C3'	1:0:542:A:H5''	2.47	0.42
24:W:4:LEU:HD22	24:W:52:VAL:CG2	2.45	0.42
1:0:1523:G:H2'	1:0:1524:U:C6	2.55	0.42
1:0:2786:G:H3'	1:0:2787:C:H6	1.83	0.42
2:9:3044:A:O4'	6:D:76:ARG:NE	2.52	0.42
24:W:122:ARG:HH21	24:W:154:ARG:N	2.17	0.42
15:N:119:GLN:O	15:N:123:ILE:HG13	2.20	0.42
12:K:27:ARG:HD2	38:K:4747:HOH:O	2.20	0.42
5:C:111:VAL:HB	38:C:8521:HOH:O	2.19	0.42
24:W:106:THR:OG1	24:W:109:GLU:HG3	2.20	0.42
1:0:2090:G:H2'	1:0:2091:G:C8	2.54	0.42
10:H:63:GLU:O	10:H:67:LEU:HB2	2.20	0.42
2:9:3115:C:C4	2:9:3116:C:C5	3.07	0.42
1:0:213:G:H2'	38:0:6305:HOH:O	2.20	0.42
1:0:111:C:O2'	1:0:112:G:H5'	2.19	0.42
1:0:2054:A:H4'	19:R:135:ALA:O	2.19	0.42
1:0:1730:G:H4'	1:0:1731:C:C6	2.55	0.42
1:0:820:G:OP1	27:Z:17:ARG:NH2	2.53	0.42
3:A:179:MET:HG2	3:A:186:TRP:CG	2.55	0.42
38:0:4909:HOH:O	3:A:22:ARG:HG2	2.20	0.42
4:B:41:PHE:HB3	4:B:190:MET:HE1	2.00	0.42
13:L:53:ARG:NH2	13:L:57:VAL:HG12	2.35	0.42
1:0:101:C:H2'	1:0:102:A:C8	2.54	0.42
1:0:1307:A:H2'	1:0:1308:A:C8	2.55	0.42
4:B:139:ASP:HB3	38:B:8849:HOH:O	2.20	0.42
15:N:151:ASP:HB3	38:N:8824:HOH:O	2.20	0.42
1:0:1503:U:H2'	1:0:1504:A:O4'	2.19	0.42
25:X:8:ARG:NH1	38:X:2479:HOH:O	2.52	0.42
16:O:26:TRP:HB2	38:O:3062:HOH:O	2.20	0.42
1:0:1377:C:C5'	1:0:1377:C:C6	2.98	0.42
1:0:1170:U:H5	38:0:6824:HOH:O	2.03	0.42
24:W:128:VAL:O	24:W:138:LEU:HD11	2.20	0.42
1:0:1976:G:O2'	1:0:1977:U:H5'	2.20	0.42
1:0:1787:C:OP1	17:P:68:LYS:HE2	2.20	0.42
5:C:233:THR:HG22	5:C:234:VAL:H	1.83	0.42
26:Y:235:GLU:CD	26:Y:235:GLU:N	2.73	0.42
1:0:1343:C:H2'	1:0:1344:G:O5'	2.20	0.42
6:D:54:ALA:HB2	6:D:69:ILE:CD1	2.50	0.42
1:0:1164:U:OP1	31:I:74:PRO:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:112:PRO:HD3	3:A:152:CYS:SG	2.60	0.42
1:0:2265:U:H2'	1:0:2266:A:C8	2.54	0.42
16:O:98:LEU:O	16:O:102:ILE:HG13	2.20	0.42
1:0:2093:G:H5''	38:0:9291:HOH:O	2.19	0.42
1:0:243:A:H61	1:0:269:G:H1'	1.85	0.42
1:0:1889:C:H2'	1:0:1890:U:O4'	2.20	0.42
5:C:19:PRO:HG2	5:C:22:PHE:CE1	2.55	0.42
1:0:91:G:N2	1:0:92:G:H1'	2.34	0.42
7:E:68:HIS:O	7:E:72:MET:HG3	2.20	0.42
1:0:588:G:O6	24:W:154:ARG:NH1	2.53	0.42
14:M:162:GLY:HA2	38:M:8819:HOH:O	2.20	0.42
38:0:5186:HOH:O	17:P:117:SER:HB2	2.19	0.42
24:W:119:HIS:CD2	24:W:120:PRO:HD2	2.54	0.42
5:C:246:ARG:NE	38:C:8617:HOH:O	2.52	0.42
1:0:162:C:H2'	1:0:163:U:H5'	2.02	0.42
1:0:448:G:H5''	38:0:4017:HOH:O	2.18	0.42
19:R:149:GLU:HA	19:R:150:PRO:HD3	1.86	0.42
31:I:131:THR:HG22	31:I:131:THR:O	2.19	0.42
1:0:1209:C:O2'	1:0:1210:G:H5'	2.19	0.42
30:3:14:CYS:SG	38:3:8863:HOH:O	2.62	0.42
24:W:139:GLY:O	24:W:141:HIS:HD2	2.03	0.42
1:0:2748:G:N2	38:0:4977:HOH:O	2.52	0.42
1:0:420:U:O4'	1:0:1920:C:C4	2.73	0.42
1:0:1523:G:C6	1:0:1524:U:O4	2.73	0.42
29:2:20:ARG:HG3	29:2:39:ARG:HH21	1.85	0.42
1:0:1790:C:H2'	1:0:1791:U:C6	2.55	0.42
1:0:1155:G:H2'	1:0:1156:C:C6	2.54	0.42
7:E:162:PHE:CD1	7:E:162:PHE:N	2.87	0.42
1:0:1584:C:O2'	1:0:1585:C:H5'	2.20	0.42
15:N:171:HIS:CE1	38:N:8861:HOH:O	2.73	0.42
3:A:37:VAL:HG22	38:A:8891:HOH:O	2.20	0.42
1:0:2288:G:H2'	1:0:2289:G:O4'	2.19	0.42
8:F:50:VAL:HG13	8:F:60:VAL:HG11	2.02	0.42
1:0:1198:U:H1'	1:0:1201:C:H5	1.85	0.41
5:C:1:MET:HG2	5:C:2:GLN:N	2.34	0.41
1:0:2590:U:H2'	1:0:2591:C:H5'	2.00	0.41
17:P:10:ALA:O	17:P:13:VAL:HG12	2.20	0.41
1:0:1186:C:C4	1:0:1187:U:C4	3.08	0.41
19:R:33:ARG:NH2	38:R:8832:HOH:O	2.53	0.41
1:0:177:A:H2'	1:0:178:U:O4'	2.20	0.41
1:0:306:A:P	21:T:38:ARG:HH21	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:130:GLU:HG2	5:C:168:ARG:HD3	2.01	0.41
3:A:70:ALA:HA	3:A:71:PRO:HD3	1.80	0.41
4:B:115:VAL:HA	4:B:116:PRO:HD3	1.83	0.41
7:E:23:GLU:HG2	7:E:28:SER:CB	2.49	0.41
28:1:28:HIS:CD2	28:1:30:LYS:HB2	2.55	0.41
1:0:527:U:H2'	1:0:528:G:C8	2.54	0.41
21:T:28:SER:O	21:T:32:ARG:HG3	2.19	0.41
1:0:445:U:C1'	38:0:7159:HOH:O	2.66	0.41
4:B:198:GLU:HA	38:B:8947:HOH:O	2.19	0.41
6:D:167:GLU:C	6:D:169:THR:H	2.24	0.41
4:B:297:VAL:HB	38:B:8900:HOH:O	2.19	0.41
27:Z:60:CYS:O	27:Z:61:ASP:HB2	2.20	0.41
1:0:2553:A:H2'	1:0:2553:A:N3	2.35	0.41
1:0:1165:G:C4'	1:0:1174:A:O2'	2.59	0.41
4:B:36:PRO:HG3	4:B:169:GLY:H	1.84	0.41
22:U:6:CYS:C	22:U:8:TYR:H	2.24	0.41
1:0:1574:C:H2'	1:0:1575:C:C6	2.55	0.41
1:0:1154:A:H2'	1:0:1155:G:C8	2.55	0.41
1:0:1015:C:H2'	1:0:1016:U:C6	2.55	0.41
1:0:1409:G:C2	1:0:1410:G:C8	3.08	0.41
1:0:69:A:H8	1:0:69:A:C5'	2.22	0.41
38:0:7193:HOH:O	12:K:45:PRO:HB2	2.20	0.41
29:2:48:ASP:O	29:2:49:GLU:HB2	2.20	0.41
1:0:2871:G:H2'	1:0:2872:U:C6	2.55	0.41
38:0:9350:HOH:O	17:P:81:LYS:HG2	2.19	0.41
1:0:1028:U:H1'	38:0:3455:HOH:O	2.20	0.41
4:B:225:GLY:HA3	38:B:8864:HOH:O	2.19	0.41
1:0:1236:A:H2'	1:0:1237:U:O4'	2.19	0.41
1:0:1379:A:H1'	38:0:9505:HOH:O	2.20	0.41
1:0:2047:C:H2'	1:0:2048:C:H6	1.85	0.41
1:0:1603:A:C5'	1:0:1605:G:H5'	2.50	0.41
1:0:1500:U:OP2	17:P:41:ARG:NH2	2.52	0.41
26:Y:151:SER:HB3	26:Y:154:ARG:HB2	2.01	0.41
1:0:137:U:C5	1:0:139:C:N4	2.88	0.41
1:0:128:A:C8	1:0:128:A:C3'	3.03	0.41
2:9:3036:C:C5	2:9:3037:C:C5	3.09	0.41
4:B:139:ASP:HB2	38:B:8830:HOH:O	2.20	0.41
1:0:2898:G:H4'	4:B:288:GLY:HA2	2.03	0.41
1:0:1123:A:C2	1:0:1129:C:H4'	2.55	0.41
20:S:11:THR:H	20:S:14:ALA:HB3	1.86	0.41
21:T:115:GLU:HG3	21:T:116:ASP:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:295:C:C2'	1:0:296:G:H5'	2.51	0.41
12:K:82:ARG:HH11	12:K:82:ARG:HG3	1.86	0.41
1:0:826:U:O5'	1:0:826:U:H6	2.03	0.41
1:0:1189:A:C3'	38:0:7501:HOH:O	2.56	0.41
1:0:2533:C:C6	1:0:2533:C:C4'	3.03	0.41
1:0:1119:G:C6	1:0:1244:U:C5	3.08	0.41
11:J:22:VAL:O	11:J:26:VAL:HG23	2.21	0.41
1:0:365:G:C6	1:0:366:U:C4	3.09	0.41
1:0:474:C:O3'	5:C:73:LEU:HD21	2.19	0.41
1:0:2329:C:H2'	1:0:2330:U:C6	2.55	0.41
31:I:99:ASP:O	31:I:100:LEU:HD23	2.21	0.41
1:0:1504:A:H5'	38:0:4246:HOH:O	2.19	0.41
1:0:800:G:H2'	1:0:801:U:C6	2.56	0.41
3:A:43:VAL:HG21	3:A:59:GLU:HG3	2.01	0.41
4:B:82:VAL:HG12	4:B:82:VAL:O	2.20	0.41
10:H:45:VAL:HA	10:H:167:PRO:O	2.19	0.41
15:N:175:LEU:HD21	38:N:8835:HOH:O	2.20	0.41
3:A:94:LEU:N	3:A:94:LEU:HD23	2.35	0.41
1:0:2435:U:OP1	30:3:28:GLY:HA3	2.21	0.41
1:0:821:U:H2'	1:0:822:C:H6	1.86	0.41
1:0:489:A:C8	21:T:82:THR:CG2	3.04	0.41
1:0:169:A:H1'	30:3:48:ASN:ND2	2.36	0.41
1:0:853:C:H2'	1:0:854:G:O4'	2.20	0.41
1:0:1950:G:H2'	1:0:1951:G:C8	2.56	0.41
1:0:2543:G:H2'	1:0:2544:G:O4'	2.21	0.41
1:0:1261:A:H3'	1:0:1262:C:C6	2.55	0.41
19:R:126:LYS:HA	19:R:127:PRO:HD3	1.92	0.41
1:0:40:C:O2'	1:0:41:G:H5'	2.20	0.41
3:A:33:GLU:CD	3:A:33:GLU:H	2.23	0.41
1:0:1168:C:H5	38:0:7319:HOH:O	2.04	0.41
14:M:134:ILE:HG23	14:M:141:ILE:HD13	2.02	0.41
2:9:3110:G:C2'	2:9:3111:U:H5'	2.51	0.41
25:X:10:VAL:O	25:X:71:ARG:HA	2.21	0.41
38:0:3886:HOH:O	4:B:27:ASN:HB2	2.19	0.41
12:K:78:LYS:NZ	38:K:5029:HOH:O	2.53	0.41
1:0:243:A:H61	1:0:269:G:C1'	2.33	0.41
1:0:629:A:C2	1:0:2074:A:C2	3.09	0.41
4:B:49:THR:HG21	4:B:331:SER:O	2.21	0.41
1:0:876:A:N3	1:0:876:A:H2'	2.35	0.41
1:0:1159:G:C2	1:0:1160:G:H1'	2.55	0.41
1:0:1159:G:H2'	1:0:1160:G:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2748:G:H2'	38:0:7362:HOH:O	2.19	0.41
1:0:2663:U:C4	1:0:2664:A:C6	3.08	0.41
1:0:1819:G:C2'	1:0:1820:G:H5'	2.50	0.41
1:0:1396:C:H1'	17:P:1:THR:O	2.21	0.41
1:0:1976:G:H1'	1:0:2005:G:N2	2.34	0.41
2:9:3110:G:C6	2:9:3111:U:C5	3.09	0.41
1:0:2598:U:O2	1:0:2600:A:C8	2.74	0.41
21:T:59:GLU:HG2	21:T:60:GLY:N	2.35	0.41
16:O:26:TRP:HA	16:O:26:TRP:CE3	2.55	0.41
1:0:2697:A:H2'	1:0:2698:G:O4'	2.20	0.41
1:0:485:A:O2'	1:0:487:G:H5'	2.21	0.41
17:P:40:VAL:O	17:P:44:VAL:HG23	2.20	0.41
1:0:1512:G:H4'	38:0:4479:HOH:O	2.19	0.41
1:0:2362:A:H2'	1:0:2363:G:C8	2.56	0.41
1:0:810:G:H2'	1:0:811:C:C6	2.55	0.41
1:0:2488:A:H2	38:0:7099:HOH:O	2.03	0.41
1:0:1119:G:H8	11:J:52:GLN:NE2	2.14	0.41
7:E:40:VAL:HA	7:E:48:VAL:O	2.20	0.41
14:M:99:ARG:O	14:M:103:GLU:HG3	2.21	0.41
8:F:17:LEU:O	8:F:21:GLU:HG3	2.20	0.41
8:F:91:VAL:CG1	8:F:92:GLY:N	2.82	0.41
6:D:146:LYS:HZ1	15:N:107:ASN:HD21	1.67	0.41
1:0:797:A:C5'	27:Z:10:ARG:N	2.84	0.41
1:0:1687:C:H1'	28:1:8:GLN:O	2.21	0.41
6:D:58:VAL:HG11	6:D:60:GLU:HG2	2.02	0.41
25:X:78:GLU:CG	25:X:79:GLU:H	2.33	0.41
1:0:138:U:H5''	1:0:139:C:OP2	2.20	0.41
4:B:305:ASP:O	4:B:306:LYS:CB	2.69	0.41
1:0:160:A:C4	1:0:177:A:C2	3.09	0.41
3:A:135:VAL:HG21	3:A:147:ARG:HB3	2.03	0.41
4:B:234:ARG:NH1	38:B:8913:HOH:O	2.52	0.41
2:9:3059:C:H2'	2:9:3060:C:C6	2.55	0.41
2:9:3059:C:H2'	2:9:3060:C:H6	1.86	0.41
5:C:80:VAL:HA	5:C:81:PRO:HD3	1.99	0.41
14:M:36:ALA:O	14:M:65:VAL:HA	2.21	0.41
2:9:3011:A:P	18:Q:19:ARG:HH21	2.44	0.41
5:C:82:GLN:N	5:C:82:GLN:OE1	2.44	0.41
1:0:2285:G:O2'	1:0:2286:G:H5'	2.21	0.41
1:0:1826:C:O2'	1:0:1827:G:H5'	2.21	0.41
5:C:243:VAL:O	5:C:243:VAL:HG13	2.20	0.41
6:D:52:THR:HB	6:D:70:GLY:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3078:G:H5'	38:9:4932:HOH:O	2.20	0.41
11:J:45:VAL:HG22	11:J:46:ILE:N	2.35	0.41
15:N:164:ASP:OD1	15:N:167:ASP:HA	2.21	0.41
1:0:2600:A:H2'	1:0:2601:A:O4'	2.21	0.41
4:B:258:GLY:H	4:B:260:HIS:CE1	2.38	0.41
1:0:1008:C:H2'	1:0:1009:U:C6	2.55	0.41
1:0:1268:C:H2'	1:0:1269:G:C8	2.55	0.41
16:O:26:TRP:HA	16:O:26:TRP:HE3	1.86	0.41
5:C:84:VAL:HG12	5:C:85:LYS:HG2	2.03	0.41
1:0:2821:C:H2'	1:0:2822:C:C6	2.55	0.41
1:0:1339:G:C6	1:0:1340:G:N1	2.89	0.41
1:0:17:G:H2'	1:0:18:C:H6	1.86	0.41
16:O:16:SER:HB3	38:O:6661:HOH:O	2.21	0.41
1:0:538:C:H5'	1:0:539:G:C8	2.56	0.41
6:D:15:GLU:HA	6:D:16:PRO:HD3	1.71	0.41
4:B:71:VAL:HG11	4:B:296:LEU:HD22	2.03	0.41
1:0:1207:A:C8	1:0:1208:C:C5	3.09	0.40
2:9:3030:C:OP1	6:D:137:PRO:O	2.39	0.40
1:0:69:A:C8	1:0:69:A:C5'	2.97	0.40
1:0:1173:A:H4'	1:0:1174:A:C8	2.56	0.40
1:0:1202:A:O2'	1:0:1203:G:H5'	2.21	0.40
25:X:37:LEU:O	25:X:41:PHE:HB2	2.21	0.40
1:0:2012:U:C2'	1:0:2013:G:OP1	2.69	0.40
1:0:861:A:H4'	1:0:1697:G:H4'	2.03	0.40
1:0:152:A:O2'	1:0:153:C:H5'	2.21	0.40
7:E:112:ALA:HA	7:E:113:PRO:HD3	1.88	0.40
2:9:3082:U:H2'	2:9:3083:G:C8	2.56	0.40
1:0:536:A:H3'	38:0:4877:HOH:O	2.20	0.40
1:0:1822:A:O2'	1:0:1823:G:H5'	2.21	0.40
1:0:213:G:O2'	1:0:214:U:OP2	2.40	0.40
15:N:175:LEU:O	15:N:179:LEU:HG	2.20	0.40
3:A:105:VAL:HG12	3:A:154:ALA:HB1	2.02	0.40
1:0:1446:U:C2'	20:S:55:GLN:NE2	2.80	0.40
1:0:1914:C:C2	1:0:1926:G:N2	2.89	0.40
2:9:3035:C:H2'	15:N:141:ARG:HH12	1.86	0.40
1:0:2374:A:H2'	1:0:2375:G:H8	1.86	0.40
4:B:140:LEU:HD13	4:B:175:LEU:HA	2.02	0.40
1:0:2456:A:H2'	1:0:2457:U:H6	1.87	0.40
31:I:87:THR:HG22	38:I:5128:HOH:O	2.20	0.40
1:0:1419:U:H2'	1:0:1685:A:C2	2.56	0.40
3:A:30:ARG:HG3	3:A:66:ARG:NH1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:O:7301:HOH:O	14:M:55:LYS:HE2	2.20	0.40
1:O:2114:C:O2'	1:O:2115:U:H5'	2.21	0.40
13:L:89:PHE:N	38:L:8870:HOH:O	2.55	0.40
15:N:37:ARG:HH11	15:N:37:ARG:CG	2.34	0.40
1:O:1193:A:H2	1:O:1194:A:N6	2.18	0.40
1:O:1603:A:C5'	1:O:1605:G:O4'	2.64	0.40
1:O:2890:A:H1'	22:U:56:ARG:HH21	1.83	0.40
24:W:38:THR:HG22	24:W:39:ASP:H	1.86	0.40
14:M:42:ARG:HA	14:M:43:PRO:HD3	1.88	0.40
1:O:2092:G:H2'	1:O:2613:G:OP1	2.22	0.40
1:O:1883:U:H5'	1:O:2012:U:OP2	2.21	0.40
19:R:111:ILE:HG23	19:R:145:LEU:CD1	2.51	0.40
19:R:111:ILE:HG23	19:R:145:LEU:HD11	2.02	0.40
13:L:10:SER:O	13:L:11:ARG:HB3	2.21	0.40
7:E:1:PRO:HG2	7:E:59:MET:SD	2.61	0.40
15:N:116:PHE:HB3	15:N:136:LEU:HD23	2.03	0.40
1:O:170:U:H2'	1:O:171:C:H5'	2.01	0.40
4:B:60:SER:HA	4:B:61:PRO:HD3	1.81	0.40
17:P:104:LYS:HA	17:P:104:LYS:HD2	1.92	0.40
1:O:212:A:O4'	1:O:214:U:C6	2.75	0.40
1:O:1246:A:C4	1:O:1248:A:C8	3.09	0.40
1:O:74:A:O2'	1:O:75:U:H5'	2.21	0.40
1:O:699:C:C6	1:O:744:G:O4'	2.74	0.40
1:O:695:C:H2'	1:O:696:C:C6	2.56	0.40
6:D:86:THR:C	6:D:89:PRO:HD2	2.42	0.40
1:O:2326:U:H4'	1:O:2412:G:C4'	2.52	0.40
8:F:27:GLY:HA3	8:F:101:ALA:O	2.21	0.40
21:T:48:VAL:CG1	21:T:49:GLU:N	2.85	0.40
24:W:35:VAL:HA	24:W:36:PRO:HD3	1.83	0.40
1:O:1659:A:H2'	1:O:1660:G:O4'	2.21	0.40
1:O:594:C:C4	1:O:595:U:C4	3.10	0.40
1:O:2433:A:H4'	30:3:30:GLN:NE2	2.36	0.40
1:O:228:C:H5'	38:O:5233:HOH:O	2.20	0.40
20:S:25:GLN:HG2	20:S:65:VAL:HG22	2.04	0.40
1:O:2461:U:O2	1:O:2466:G:H1'	2.21	0.40
1:O:1808:C:O2'	1:O:1809:G:H5'	2.21	0.40
1:O:2750:G:H2'	1:O:2751:C:C6	2.57	0.40
1:O:1555:G:O2'	1:O:1556:G:H5'	2.22	0.40
13:L:117:GLU:O	13:L:117:GLU:HG3	2.21	0.40
1:O:120:A:OP1	28:1:32:LYS:NZ	2.47	0.40
4:B:36:PRO:CA	4:B:168:GLY:HA3	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1131:G:C6	1:0:1230:A:C4	3.09	0.40
12:K:113:ILE:HG22	12:K:114:ALA:N	2.36	0.40
1:0:2256:G:C6	1:0:2257:G:C4	3.09	0.40
23:V:39:ALA:C	23:V:41:GLU:H	2.24	0.40
18:Q:25:PRO:HA	18:Q:26:PRO:HD3	1.83	0.40
2:9:3008:G:P	38:9:5071:HOH:O	2.79	0.40
24:W:122:ARG:NH2	24:W:154:ARG:HB3	2.37	0.40
1:0:553:G:H2'	1:0:554:G:H5'	2.04	0.40
21:T:40:VAL:HG22	21:T:41:ARG:N	2.36	0.40
14:M:159:VAL:HG13	14:M:160:PHE:N	2.37	0.40
1:0:1204:C:H1'	38:0:4575:HOH:O	2.20	0.40
10:H:91:PRO:HG2	38:H:8570:HOH:O	2.20	0.40
1:0:2650:U:O2'	1:0:2651:C:H5'	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	
3	A	235/240 (98%)	215 (92%)	16 (7%)	4 (2%)	11	38
4	B	335/338 (99%)	307 (92%)	23 (7%)	5 (2%)	13	42
5	C	244/246 (99%)	220 (90%)	22 (9%)	2 (1%)	24	60
6	D	134/177 (76%)	108 (81%)	22 (16%)	4 (3%)	5	22
7	E	170/178 (96%)	161 (95%)	7 (4%)	2 (1%)	16	48
8	F	117/120 (98%)	105 (90%)	11 (9%)	1 (1%)	21	57
9	G	25/348 (7%)	25 (100%)	0	0	100	100
10	H	156/174 (90%)	144 (92%)	11 (7%)	1 (1%)	30	67
11	J	140/145 (97%)	132 (94%)	6 (4%)	2 (1%)	14	44
12	K	130/132 (98%)	125 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	L	141/165 (86%)	120 (85%)	19 (14%)	2 (1%)	14	44
14	M	192/196 (98%)	184 (96%)	8 (4%)	0	100	100
15	N	184/187 (98%)	163 (89%)	18 (10%)	3 (2%)	12	40
16	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
17	P	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
18	Q	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
19	R	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
20	S	79/85 (93%)	71 (90%)	8 (10%)	0	100	100
21	T	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	21	57
22	U	51/67 (76%)	48 (94%)	3 (6%)	0	100	100
23	V	63/71 (89%)	59 (94%)	4 (6%)	0	100	100
24	W	152/154 (99%)	147 (97%)	3 (2%)	2 (1%)	15	46
25	X	80/92 (87%)	71 (89%)	7 (9%)	2 (2%)	7	27
26	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100
27	Z	71/73 (97%)	61 (86%)	7 (10%)	3 (4%)	3	13
28	1	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
29	2	42/50 (84%)	42 (100%)	0	0	100	100
30	3	90/92 (98%)	85 (94%)	4 (4%)	1 (1%)	17	51
31	I	68/162 (42%)	50 (74%)	17 (25%)	1 (2%)	13	42
All	All	3705/4426 (84%)	3419 (92%)	250 (7%)	36 (1%)	19	54

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	37	VAL
8	F	101	ALA
15	N	154	LEU
15	N	184	ILE
24	W	77	ALA
27	Z	42	CYS
4	B	34	GLY
6	D	173	GLU
11	J	5	GLU
15	N	164	ASP
21	T	53	GLY

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Mol	Chain	Res	Type
30	3	57	GLY
3	A	34	ASP
6	D	97	GLN
10	H	166	SER
11	J	143	LYS
24	W	76	ASP
31	I	76	ALA
3	A	24	LYS
4	B	169	GLY
4	B	185	GLY
5	C	178	GLN
13	L	21	ARG
13	L	80	ASP
4	B	2	GLN
4	B	306	LYS
5	C	163	HIS
6	D	85	GLN
27	Z	41	ASN
25	X	68	SER
3	A	88	ILE
6	D	27	ILE
7	E	44	GLY
25	X	52	PRO
7	E	136	PRO
27	Z	43	GLY

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 X-ray entries followed by that with respect to entries of similar resolution.

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	
3	A	179/182 (98%)	171 (96%)	8 (4%)	34	70
4	B	282/283 (100%)	271 (96%)	11 (4%)	39	75
5	C	193/193 (100%)	179 (93%)	14 (7%)	17	45
6	D	117/148 (79%)	109 (93%)	8 (7%)	20	49
7	E	152/156 (97%)	150 (99%)	2 (1%)	76	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	F	93/94 (99%)	92 (99%)	1 (1%)	80	95
9	G	27/283 (10%)	26 (96%)	1 (4%)	41	77
10	H	132/141 (94%)	125 (95%)	7 (5%)	28	63
11	J	118/121 (98%)	112 (95%)	6 (5%)	29	65
12	K	106/106 (100%)	102 (96%)	4 (4%)	40	76
13	L	113/127 (89%)	108 (96%)	5 (4%)	35	70
14	M	158/160 (99%)	149 (94%)	9 (6%)	25	59
15	N	149/150 (99%)	142 (95%)	7 (5%)	32	68
16	O	93/94 (99%)	92 (99%)	1 (1%)	80	95
17	P	113/117 (97%)	110 (97%)	3 (3%)	52	84
18	Q	79/80 (99%)	76 (96%)	3 (4%)	40	76
19	R	117/122 (96%)	114 (97%)	3 (3%)	54	85
20	S	71/74 (96%)	71 (100%)	0	100	100
21	T	105/106 (99%)	99 (94%)	6 (6%)	25	59
22	U	44/53 (83%)	44 (100%)	0	100	100
23	V	51/57 (90%)	50 (98%)	1 (2%)	63	88
24	W	130/130 (100%)	125 (96%)	5 (4%)	40	76
25	X	66/74 (89%)	61 (92%)	5 (8%)	16	43
26	Y	120/196 (61%)	116 (97%)	4 (3%)	45	80
27	Z	60/60 (100%)	59 (98%)	1 (2%)	68	91
28	1	46/47 (98%)	46 (100%)	0	100	100
29	2	42/46 (91%)	41 (98%)	1 (2%)	57	86
30	3	79/79 (100%)	77 (98%)	2 (2%)	55	85
31	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3609 (86%)	2975 (96%)	118 (4%)	40	76

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	3	ARG
3	A	34	ASP
3	A	55	VAL
3	A	64	ASP
3	A	94	LEU

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Mol	Chain	Res	Type
3	A	131	HIS
3	A	179	MET
3	A	217	ARG
4	B	7	ARG
4	B	11	LEU
4	B	27	ASN
4	B	49	THR
4	B	56	ASP
4	B	98	THR
4	B	149	ASP
4	B	190	MET
4	B	254	GLN
4	B	277	GLU
4	B	279	THR
5	C	2	GLN
5	C	16	VAL
5	C	27	ARG
5	C	76	ARG
5	C	87	ARG
5	C	94	THR
5	C	136	VAL
5	C	151	GLN
5	C	172	THR
5	C	187	ARG
5	C	202	THR
5	C	214	THR
5	C	223	LEU
5	C	243	VAL
6	D	29	HIS
6	D	36	ASN
6	D	41	LEU
6	D	61	PHE
6	D	136	ARG
6	D	137	PRO
6	D	149	ARG
6	D	170	TYR
7	E	7	ILE
7	E	102	VAL
8	F	103	GLU
9	G	14	GLU
10	H	18	GLU
10	H	39	ASP

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Mol	Chain	Res	Type
10	H	59	HIS
10	H	62	LEU
10	H	84	LYS
10	H	132	GLN
10	H	154	TYR
11	J	32	ASP
11	J	39	VAL
11	J	46	ILE
11	J	52	GLN
11	J	79	PHE
11	J	107	ASN
12	K	7	ASP
12	K	10	GLN
12	K	49	LEU
12	K	129	THR
13	L	30	ARG
13	L	32	ASP
13	L	35	ARG
13	L	43	HIS
13	L	140	VAL
14	M	10	ASP
14	M	23	LEU
14	M	46	LEU
14	M	68	ARG
14	M	81	ARG
14	M	93	ARG
14	M	116	ASN
14	M	125	ARG
14	M	158	ARG
15	N	26	LEU
15	N	38	LYS
15	N	44	ARG
15	N	50	LEU
15	N	94	GLU
15	N	124	ASP
15	N	152	GLU
16	O	3	THR
17	P	21	VAL
17	P	91	LYS
17	P	98	ILE
18	Q	16	ASN
18	Q	57	ASP

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Mol	Chain	Res	Type
18	Q	95	GLU
19	R	13	THR
19	R	39	THR
19	R	85	SER
21	T	23	VAL
21	T	39	ASN
21	T	66	ASP
21	T	80	GLU
21	T	106	GLU
21	T	117	ASP
23	V	45	ARG
24	W	10	GLU
24	W	35	VAL
24	W	73	LEU
24	W	142	ASP
24	W	146	ILE
25	X	15	ARG
25	X	27	ASP
25	X	43	VAL
25	X	66	THR
25	X	79	GLU
26	Y	141	THR
26	Y	189	ASN
26	Y	200	THR
26	Y	203	VAL
27	Z	41	ASN
29	2	18	ASN
30	3	40	ARG
30	3	56	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	47	HIS
3	A	92	ASN
3	A	199	HIS
4	B	27	ASN
4	B	145	HIS
4	B	221	GLN
4	B	238	ASN
4	B	256	GLN
4	B	260	HIS

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Mol	Chain	Res	Type
4	B	320	GLN
4	B	332	ASN
5	C	2	GLN
5	C	129	HIS
6	D	103	ASN
6	D	133	ASN
7	E	106	ASN
7	E	119	HIS
7	E	143	GLN
9	G	17	GLN
9	G	64	ASN
10	H	31	HIS
10	H	46	GLN
10	H	56	GLN
10	H	59	HIS
10	H	155	ASN
11	J	52	GLN
11	J	107	ASN
11	J	142	ASN
12	K	10	GLN
13	L	18	HIS
13	L	41	HIS
13	L	42	ASN
13	L	55	GLN
13	L	116	HIS
14	M	24	GLN
14	M	58	GLN
14	M	137	ASN
15	N	107	ASN
17	P	50	GLN
17	P	66	GLN
17	P	118	GLN
18	Q	16	ASN
18	Q	40	HIS
19	R	94	ASN
19	R	98	ASN
19	R	113	HIS
19	R	117	HIS
19	R	123	GLN
20	S	9	HIS
20	S	21	GLN
20	S	53	ASN

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Mol	Chain	Res	Type
20	S	55	GLN
21	T	37	GLN
21	T	39	ASN
21	T	64	ASN
21	T	73	HIS
22	U	39	ASN
22	U	48	ASN
23	V	60	GLN
24	W	59	GLN
24	W	110	GLN
24	W	119	HIS
24	W	125	HIS
24	W	141	HIS
25	X	23	HIS
26	Y	133	HIS
26	Y	134	HIS
26	Y	189	ASN
28	1	8	GLN
28	1	16	HIS
28	1	28	HIS
29	2	18	ASN
29	2	41	HIS
29	2	45	ASN
30	3	30	GLN
30	3	48	ASN
31	I	93	GLN
31	I	104	GLN
31	I	123	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2772 (99%)	234 (8%)	28 (1%)
2	9	121/122 (99%)	17 (14%)	1 (0%)
All	All	2866/2894 (99%)	251 (8%)	29 (1%)

All (251) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	60	A

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Mol	Chain	Res	Type
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	185	G
1	0	186	A
1	0	191	A
1	0	192	A
1	0	198	A
1	0	200	U
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	285	A
1	0	308	U
1	0	309	C
1	0	331	A
1	0	336	G
1	0	337	A
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	461	C
1	0	473	A
1	0	487	G
1	0	511	A
1	0	514	G
1	0	537	G

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Mol	Chain	Res	Type
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	581	G
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	701	U
1	0	759	C
1	0	777	U
1	0	805	G
1	0	806	A
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	884	C
1	0	898	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	938	G
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C

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Mol	Chain	Res	Type
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1137	G
1	0	1164	U
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1208	C
1	0	1216	G
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1407	A
1	0	1451	C
1	0	1474	C
1	0	1488	U
1	0	1492	A
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1559	A
1	0	1580	A

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Mol	Chain	Res	Type
1	0	1592	G
1	0	1603	A
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1730	G
1	0	1731	C
1	0	1752	G
1	0	1778	A
1	0	1779	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1873	G
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1965	C
1	0	1971	G
1	0	1973	A
1	0	1974	G
1	0	1978	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	2004	U
1	0	2006	C
1	0	2008	U
1	0	2011	A

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Mol	Chain	Res	Type
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2063	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2110	G
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2317	C
1	0	2321	A
1	0	2354	A
1	0	2369	A
1	0	2422	U
1	0	2462	G
1	0	2465	A
1	0	2467	A
1	0	2476	C
1	0	2483	A
1	0	2507	G
1	0	2511	A
1	0	2526	C
1	0	2527	U
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2634	G
1	0	2645	U

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Mol	Chain	Res	Type
1	0	2649	A
1	0	2650	U
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2786	G
1	0	2800	A
1	0	2811	A
1	0	2812	A
1	0	2850	C
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	3002	U
2	9	3007	G
2	9	3014	G
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3025	G
2	9	3039	U
2	9	3040	C
2	9	3041	C
2	9	3043	G
2	9	3052	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C

All (29) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	69	A
1	0	129	A
1	0	338	C
1	0	681	G
1	0	699	C
1	0	805	G
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	1080	C
1	0	1237	U
1	0	1352	A
1	0	1377	C
1	0	1450	C
1	0	1474	C
1	0	1506	U
1	0	1684	A
1	0	1685	A
1	0	1942	A
1	0	2011	A
1	0	2467	A
1	0	2526	C
1	0	2536	C
1	0	2649	A
1	0	2718	C
1	0	2726	U
1	0	2761	A
2	9	3065	A

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMU	0	2587	1	12,22,23	1.06	1 (8%)	19,31,34	3.13	2 (10%)
1	OMG	0	2588	1	17,26,27	1.07	1 (5%)	21,38,41	2.53	3 (14%)
1	UR3	0	2619	1	12,22,23	0.80	0	16,32,35	0.82	0
1	PSU	0	2621	1	13,21,22	1.54	2 (15%)	18,30,33	6.08	3 (16%)
1	1MA	0	628	1	14,25,26	1.03	1 (7%)	15,37,40	1.08	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	0	2587	1	-	0/5/27/28	0/2/2/2
1	OMG	0	2588	1	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/3/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1	-	0/3/25/26	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-4.56	1.48	1.52
1	0	2621	PSU	C4-N3	2.51	1.37	1.33
1	0	2587	OMU	C4-N3	2.64	1.38	1.33
1	0	628	1MA	C6-N6	2.66	1.34	1.29
1	0	2588	OMG	C6-N1	3.22	1.39	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-21.37	114.70	128.33
1	0	2588	OMG	C5-C6-N1	-8.79	111.57	123.59
1	0	628	1MA	C2-N3-C4	-3.68	110.70	116.40
1	0	2587	OMU	C5-C4-N3	-3.36	114.51	123.12
1	0	2588	OMG	N3-C2-N1	-2.12	124.21	127.44
1	0	2621	PSU	C6-N1-C2	2.65	119.73	115.47
1	0	2588	OMG	C6-N1-C2	6.55	125.04	115.94
1	0	2587	OMU	C4-N3-C2	12.98	126.99	114.14
1	0	2621	PSU	C4-N3-C2	13.87	127.23	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 232 ligands modelled in this entry, 231 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	$\# Z > 2$
36	NEG	0	8823	32	11,16,16	1.49	1 (9%)	12,20,20	1.05	1 (8%)

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
36	NEG	0	8823	32	-	0/15/18/18	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	0	8823	NEG	N2-N3	-4.60	1.36	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
36	0	8823	NEG	C9-N3-C7	-3.30	110.28	121.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	0	8823	NEG	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2749/2772 (99%)	-0.70	8 (0%) 94 94	19, 42, 86, 144	0
2	9	122/122 (100%)	-0.75	1 (0%) 87 86	35, 59, 83, 147	0
3	A	237/240 (98%)	-0.47	3 (1%) 79 78	25, 46, 78, 99	0
4	B	337/338 (99%)	-0.69	1 (0%) 94 94	26, 50, 75, 85	0
5	C	246/246 (100%)	-0.63	0 100 100	23, 44, 66, 75	0
6	D	140/177 (79%)	1.04	28 (20%) 1 1	54, 94, 118, 126	0
7	E	172/178 (96%)	-0.52	1 (0%) 90 89	40, 63, 83, 88	0
8	F	119/120 (99%)	0.17	5 (4%) 40 33	42, 67, 89, 100	0
9	G	29/348 (8%)	1.11	9 (31%) 1 0	73, 89, 96, 98	0
10	H	160/174 (91%)	-0.15	1 (0%) 90 89	36, 56, 86, 95	0
11	J	142/145 (97%)	-0.69	0 100 100	32, 47, 68, 89	0
12	K	132/132 (100%)	-0.78	1 (0%) 87 86	29, 45, 67, 78	0
13	L	145/165 (87%)	-0.06	7 (4%) 34 28	23, 62, 102, 114	0
14	M	194/196 (98%)	-0.76	1 (0%) 91 90	30, 40, 55, 63	0
15	N	186/187 (99%)	-0.20	6 (3%) 51 43	37, 59, 103, 114	0
16	O	115/116 (99%)	-0.65	0 100 100	35, 51, 67, 76	0
17	P	143/149 (95%)	-0.60	0 100 100	36, 51, 63, 72	0
18	Q	95/96 (98%)	-0.64	0 100 100	33, 44, 56, 70	0
19	R	150/155 (96%)	-0.69	0 100 100	30, 43, 64, 79	0
20	S	81/85 (95%)	-0.10	2 (2%) 61 55	43, 58, 78, 80	0
21	T	119/120 (99%)	-0.33	3 (2%) 61 55	41, 54, 77, 95	0
22	U	53/67 (79%)	-0.59	0 100 100	37, 50, 70, 77	0
23	V	65/71 (91%)	0.78	8 (12%) 5 3	51, 72, 106, 114	0
24	W	154/154 (100%)	-0.56	0 100 100	33, 47, 63, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	X	82/92 (89%)	-0.26	4 (4%) 33 27	43, 56, 81, 96	0
26	Y	142/241 (58%)	-0.71	2 (1%) 78 76	25, 42, 64, 84	0
27	Z	73/73 (100%)	-0.44	0 100 100	45, 57, 74, 93	0
28	1	56/57 (98%)	-0.79	0 100 100	28, 32, 39, 48	0
29	2	46/50 (92%)	-0.25	3 (6%) 22 16	34, 60, 93, 102	0
30	3	92/92 (100%)	-0.62	0 100 100	32, 51, 64, 75	0
31	I	70/162 (43%)	3.82	60 (85%) 0 0	101, 115, 127, 129	0
All	All	6646/7320 (90%)	-0.49	154 (2%) 64 59	19, 48, 93, 147	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	V	1	THR	12.3
31	I	79	ILE	9.8
31	I	71	GLY	9.3
6	D	63	ILE	8.9
31	I	75	THR	7.8
25	X	88	GLU	7.0
31	I	109	ALA	7.0
6	D	57	THR	6.8
31	I	113	HIS	6.7
31	I	105	VAL	6.6
31	I	137	VAL	6.6
31	I	104	GLN	6.4
31	I	111	GLN	6.4
31	I	116	LEU	6.4
23	V	40	PRO	6.3
23	V	39	ALA	6.2
31	I	133	THR	6.1
31	I	88	GLY	6.1
31	I	114	PRO	5.9
15	N	161	GLY	5.8
6	D	88	LEU	5.7
31	I	107	GLN	5.4
31	I	85	PHE	5.4
31	I	83	ALA	5.4
31	I	93	GLN	5.2
31	I	84	GLY	5.2
31	I	120	ASP	5.1
6	D	66	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
31	I	118	SER	5.0
26	Y	95	THR	4.9
20	S	81	ILE	4.9
31	I	77	GLU	4.9
6	D	87	ALA	4.8
6	D	64	ARG	4.7
31	I	76	ALA	4.7
4	B	1	PRO	4.7
23	V	43	PRO	4.7
23	V	41	GLU	4.6
31	I	103	ASP	4.5
31	I	117	LEU	4.3
3	A	37	VAL	4.3
31	I	102	VAL	4.3
6	D	92	GLU	4.2
31	I	115	ASP	4.2
31	I	108	ILE	4.1
26	Y	235	GLU	4.1
23	V	37	GLY	4.0
25	X	80	GLU	4.0
31	I	72	VAL	4.0
31	I	122	THR	4.0
31	I	87	THR	3.9
31	I	119	TYR	3.8
31	I	106	LYS	3.8
15	N	183	ASP	3.7
31	I	81	ASP	3.7
31	I	98	ALA	3.7
13	L	80	ASP	3.6
31	I	121	LEU	3.5
31	I	91	GLU	3.5
21	T	119	ALA	3.5
31	I	138	THR	3.5
21	T	118	SER	3.5
12	K	119	GLN	3.4
15	N	166	ALA	3.4
8	F	99	THR	3.4
6	D	44	ILE	3.4
31	I	99	ASP	3.4
31	I	96	PHE	3.3
2	9	3001	U	3.3
14	M	194	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
6	D	90	LEU	3.2
6	D	18	ILE	3.2
1	0	1172	G	3.1
31	I	86	GLU	3.1
31	I	123	ASN	3.1
15	N	185	GLU	3.0
31	I	78	LEU	3.0
29	2	49	GLU	3.0
31	I	97	VAL	3.0
31	I	74	PRO	2.9
6	D	56	ARG	2.9
13	L	60	GLU	2.9
25	X	71	ARG	2.9
7	E	45	ASP	2.8
1	0	282	C	2.8
6	D	81	GLU	2.8
31	I	110	GLU	2.8
6	D	85	GLN	2.8
6	D	134	LEU	2.8
9	G	23	ILE	2.8
25	X	7	GLU	2.8
6	D	61	PHE	2.7
21	T	116	ASP	2.7
6	D	10	PHE	2.7
29	2	39	ARG	2.7
31	I	95	ASP	2.7
6	D	166	ILE	2.7
9	G	21	ASP	2.7
1	0	1199	A	2.7
13	L	81	VAL	2.7
31	I	124	ALA	2.6
6	D	62	ASP	2.6
6	D	65	GLU	2.6
9	G	25	GLU	2.6
6	D	84	LEU	2.6
9	G	72	ASP	2.5
1	0	2237	G	2.5
31	I	112	LYS	2.5
31	I	82	GLU	2.5
9	G	27	ILE	2.5
31	I	140	GLU	2.4
6	D	26	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
6	D	95	THR	2.4
13	L	101	ASP	2.4
31	I	92	PRO	2.4
31	I	136	GLY	2.4
31	I	126	LYS	2.4
6	D	11	HIS	2.3
31	I	131	THR	2.3
1	0	1951	G	2.3
1	0	1196	C	2.3
1	0	1197	G	2.3
23	V	38	GLY	2.3
15	N	152	GLU	2.3
31	I	73	PRO	2.2
13	L	82	ALA	2.2
10	H	36	LYS	2.2
8	F	69	GLU	2.2
13	L	102	ASP	2.2
31	I	139	ILE	2.2
8	F	25	ASP	2.2
3	A	64	ASP	2.2
6	D	138	GLY	2.2
8	F	106	ALA	2.2
23	V	59	ILE	2.2
1	0	960	G	2.2
9	G	71	LEU	2.2
9	G	26	MET	2.2
6	D	75	LEU	2.1
8	F	49	PHE	2.1
6	D	17	ARG	2.1
9	G	28	GLU	2.1
29	2	35	ARG	2.1
6	D	40	ILE	2.1
9	G	68	GLU	2.1
13	L	97	VAL	2.1
31	I	100	LEU	2.0
31	I	135	LEU	2.0
6	D	74	THR	2.0
31	I	132	CYS	2.0
31	I	80	LYS	2.0
3	A	99	ILE	2.0
20	S	78	ALA	2.0
15	N	68	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	OMU	0	2587	21/22	0.99	0.09	-	29,31,33,36	0
1	UR3	0	2619	21/22	0.97	0.12	-	32,34,35,37	0
1	1MA	0	628	23/24	0.98	0.14	-	26,29,30,31	0
1	OMG	0	2588	24/25	0.97	0.12	-	26,32,34,36	0
1	PSU	0	2621	20/21	0.98	0.11	-	23,27,32,33	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
34	NA	0	8577	1/1	0.57	0.53	29.60	70,70,70,70	0
34	NA	0	8520	1/1	0.96	0.34	24.90	35,35,35,35	0
34	NA	0	8571	1/1	0.81	0.28	24.19	46,46,46,46	0
34	NA	0	8573	1/1	0.90	0.32	22.85	56,56,56,56	0
33	K	0	8401	1/1	0.89	0.35	17.24	78,78,78,78	0
34	NA	0	8562	1/1	0.88	0.33	14.12	65,65,65,65	0
34	NA	0	8503	1/1	0.98	0.26	13.18	1,1,1,1	0
34	NA	0	8523	1/1	0.93	0.28	13.07	56,56,56,56	0
32	MG	0	8062	1/1	0.92	0.21	12.76	5,5,5,5	0
34	NA	0	8559	1/1	0.88	0.30	11.80	48,48,48,48	0
34	NA	0	8582	1/1	0.57	0.26	10.72	88,88,88,88	0
34	NA	0	8578	1/1	0.89	0.37	9.19	49,49,49,49	0
36	NEG	0	8823	17/17	0.90	0.18	8.38	68,72,82,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	NA	0	8565	1/1	0.96	1.02	7.40	52,52,52,52	0
34	NA	0	8576	1/1	0.98	0.20	7.18	24,24,24,24	0
34	NA	0	8514	1/1	0.98	0.26	5.98	37,37,37,37	0
34	NA	0	8561	1/1	0.93	0.34	5.85	61,61,61,61	0
34	NA	R	8586	1/1	0.91	0.28	5.85	29,29,29,29	0
34	NA	0	8535	1/1	0.86	0.19	5.83	39,39,39,39	0
34	NA	L	8580	1/1	0.96	0.27	5.18	1,1,1,1	0
34	NA	0	8572	1/1	0.91	0.20	5.17	68,68,68,68	0
34	NA	0	8526	1/1	0.93	0.16	5.07	63,63,63,63	0
34	NA	0	8564	1/1	0.85	0.21	4.62	50,50,50,50	0
32	MG	0	8060	1/1	0.87	0.21	4.53	43,43,43,43	0
32	MG	0	8096	1/1	0.89	0.12	3.19	52,52,52,52	0
32	MG	0	8080	1/1	0.68	0.18	3.05	48,48,48,48	0
32	MG	0	8018	1/1	0.98	0.17	2.94	26,26,26,26	0
34	NA	0	8568	1/1	0.82	0.12	2.79	61,61,61,61	0
34	NA	0	8527	1/1	0.94	0.15	2.21	46,46,46,46	0
34	NA	0	8566	1/1	0.93	0.11	2.09	74,74,74,74	0
34	NA	0	8521	1/1	0.99	0.21	2.07	43,43,43,43	0
34	NA	0	8510	1/1	0.99	0.13	2.05	22,22,22,22	0
32	MG	0	8052	1/1	0.95	0.14	2.03	77,77,77,77	0
32	MG	0	8006	1/1	0.97	0.14	1.87	32,32,32,32	0
34	NA	Q	8548	1/1	0.78	0.19	1.82	43,43,43,43	0
32	MG	0	8010	1/1	0.99	0.16	1.77	13,13,13,13	0
34	NA	0	8550	1/1	0.93	0.17	1.75	40,40,40,40	0
34	NA	0	8553	1/1	0.97	0.16	1.53	32,32,32,32	0
32	MG	3	8078	1/1	0.99	0.15	1.35	11,11,11,11	0
32	MG	0	8004	1/1	0.92	0.15	1.11	23,23,23,23	0
32	MG	0	8002	1/1	0.99	0.14	0.91	27,27,27,27	0
32	MG	0	8057	1/1	0.91	0.10	0.82	29,29,29,29	0
32	MG	0	8038	1/1	0.98	0.14	0.80	21,21,21,21	0
32	MG	0	8091	1/1	0.96	0.12	0.45	53,53,53,53	0
32	MG	0	8054	1/1	0.94	0.14	0.20	24,24,24,24	0
34	NA	0	8525	1/1	0.98	0.14	0.19	71,71,71,71	0
32	MG	0	8110	1/1	0.91	0.13	-0.03	54,54,54,54	0
34	NA	A	8545	1/1	0.80	0.12	-0.29	57,57,57,57	0
34	NA	R	8538	1/1	0.54	0.10	-0.39	55,55,55,55	0
32	MG	0	8033	1/1	1.00	0.09	-0.72	21,21,21,21	0
32	MG	A	8065	1/1	0.95	0.12	-0.75	37,37,37,37	0
37	CD	Z	8703	1/1	1.00	0.09	-0.78	63,63,63,63	0
35	CL	J	8821	1/1	0.89	0.11	-0.81	60,60,60,60	0
32	MG	0	8067	1/1	0.98	0.11	-0.81	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	Y	8109	1/1	0.91	0.10	-0.81	36,36,36,36	0
34	NA	0	8543	1/1	0.94	0.09	-0.91	32,32,32,32	0
32	MG	0	8107	1/1	0.98	0.08	-1.14	36,36,36,36	0
32	MG	0	8013	1/1	0.97	0.10	-1.15	26,26,26,26	0
34	NA	0	8532	1/1	0.92	0.09	-1.16	34,34,34,34	0
35	CL	O	8808	1/1	0.88	0.09	-1.30	66,66,66,66	0
32	MG	0	8020	1/1	0.97	0.10	-1.32	26,26,26,26	0
37	CD	3	8704	1/1	0.99	0.05	-1.51	53,53,53,53	0
37	CD	U	8701	1/1	0.99	0.06	-1.59	63,63,63,63	0
32	MG	0	8017	1/1	0.94	0.12	-1.69	25,25,25,25	0
32	MG	0	8077	1/1	0.99	0.12	-1.79	30,30,30,30	0
37	CD	1	8702	1/1	0.99	0.09	-1.82	55,55,55,55	0
32	MG	0	8056	1/1	0.98	0.06	-1.89	42,42,42,42	0
34	NA	0	8531	1/1	0.98	0.12	-1.92	35,35,35,35	0
32	MG	0	8014	1/1	1.00	0.10	-1.99	34,34,34,34	0
35	CL	0	8805	1/1	0.84	0.07	-2.00	58,58,58,58	0
32	MG	T	8073	1/1	0.91	0.04	-2.00	63,63,63,63	0
34	NA	0	8509	1/1	0.96	0.08	-2.04	23,23,23,23	0
32	MG	0	8074	1/1	0.99	0.04	-2.05	28,28,28,28	0
34	NA	J	8546	1/1	0.94	0.05	-2.06	27,27,27,27	0
35	CL	M	8818	1/1	0.99	0.09	-2.12	36,36,36,36	0
32	MG	0	8003	1/1	0.98	0.08	-2.21	29,29,29,29	0
35	CL	0	8812	1/1	0.97	0.06	-2.37	40,40,40,40	0
34	NA	0	8517	1/1	0.93	0.08	-2.42	24,24,24,24	0
32	MG	0	8112	1/1	0.94	0.07	-2.82	38,38,38,38	0
32	MG	0	8015	1/1	0.86	0.12	-2.90	34,34,34,34	0
32	MG	0	8012	1/1	0.95	0.08	-2.95	30,30,30,30	0
32	MG	0	8058	1/1	0.98	0.07	-3.09	32,32,32,32	0
32	MG	0	8001	1/1	0.97	0.09	-3.30	25,25,25,25	0
32	MG	0	8021	1/1	0.93	0.07	-3.32	37,37,37,37	0
34	NA	0	8539	1/1	0.89	0.11	-3.51	30,30,30,30	0
32	MG	0	8064	1/1	0.96	0.06	-3.54	28,28,28,28	0
32	MG	0	8032	1/1	0.85	0.06	-3.62	29,29,29,29	0
34	NA	0	8544	1/1	0.84	0.04	-3.65	14,14,14,14	0
32	MG	0	8044	1/1	0.95	0.06	-3.81	33,33,33,33	0
32	MG	0	8028	1/1	0.90	0.07	-4.12	39,39,39,39	0
34	NA	0	8533	1/1	0.96	0.06	-4.16	22,22,22,22	0
34	NA	M	8547	1/1	0.99	0.04	-4.20	35,35,35,35	0
35	CL	B	8819	1/1	0.93	0.06	-4.32	39,39,39,39	0
33	K	0	8402	1/1	0.95	0.10	-4.33	49,49,49,49	0
35	CL	3	8804	1/1	1.00	0.04	-4.49	42,42,42,42	0
32	MG	0	8108	1/1	0.91	0.04	-4.98	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8035	1/1	0.90	0.06	-5.21	36,36,36,36	0
32	MG	0	8019	1/1	0.92	0.04	-5.40	26,26,26,26	0
32	MG	0	8008	1/1	0.95	0.08	-5.50	27,27,27,27	0
32	MG	0	8084	1/1	0.99	0.03	-6.13	42,42,42,42	0
32	MG	0	8088	1/1	0.88	0.07	-6.56	22,22,22,22	0
34	NA	0	8556	1/1	0.96	0.08	-7.51	54,54,54,54	0
32	MG	0	8053	1/1	0.99	0.03	-8.23	50,50,50,50	0
32	MG	0	8104	1/1	0.96	0.16	-	67,67,67,67	0
32	MG	0	8040	1/1	0.85	0.12	-	46,46,46,46	0
34	NA	9	8552	1/1	0.85	0.15	-	47,47,47,47	0
32	MG	0	8029	1/1	0.98	0.06	-	36,36,36,36	0
32	MG	0	8116	1/1	0.94	0.10	-	47,47,47,47	0
32	MG	0	8072	1/1	0.90	0.09	-	55,55,55,55	0
34	NA	0	8513	1/1	0.85	0.09	-	46,46,46,46	0
32	MG	0	8102	1/1	0.85	0.14	-	70,70,70,70	0
34	NA	0	8511	1/1	0.93	0.09	-	46,46,46,46	0
34	NA	0	8560	1/1	0.96	0.08	-	44,44,44,44	0
34	NA	0	8541	1/1	0.98	0.11	-	47,47,47,47	0
32	MG	0	8063	1/1	0.89	0.30	-	89,89,89,89	0
34	NA	0	8536	1/1	0.95	0.06	-	38,38,38,38	0
32	MG	0	8016	1/1	0.99	0.13	-	19,19,19,19	0
32	MG	K	8069	1/1	0.98	0.07	-	54,54,54,54	0
32	MG	0	8009	1/1	0.94	0.15	-	31,31,31,31	0
32	MG	0	8039	1/1	0.99	0.11	-	43,43,43,43	0
32	MG	0	8087	1/1	0.86	0.11	-	61,61,61,61	0
32	MG	0	8049	1/1	0.99	0.12	-	30,30,30,30	0
32	MG	0	8037	1/1	0.98	0.09	-	38,38,38,38	0
32	MG	0	8100	1/1	0.94	0.21	-	37,37,37,37	0
32	MG	0	8024	1/1	0.72	0.65	-	80,80,80,80	0
32	MG	0	8007	1/1	1.00	0.14	-	9,9,9,9	0
34	NA	0	8557	1/1	0.94	0.05	-	49,49,49,49	0
32	MG	0	8081	1/1	0.97	0.11	-	34,34,34,34	0
32	MG	0	8027	1/1	0.99	0.06	-	39,39,39,39	0
34	NA	0	8528	1/1	0.94	0.18	-	39,39,39,39	0
35	CL	0	8803	1/1	0.94	0.07	-	52,52,52,52	0
35	CL	Q	8811	1/1	0.97	0.08	-	58,58,58,58	0
34	NA	0	8581	1/1	0.95	0.05	-	38,38,38,38	0
32	MG	0	8071	1/1	0.76	0.12	-	62,62,62,62	0
34	NA	0	8516	1/1	0.96	0.26	-	45,45,45,45	0
32	MG	0	8031	1/1	0.97	0.13	-	33,33,33,33	0
32	MG	0	8061	1/1	0.96	0.10	-	30,30,30,30	0
34	NA	0	8524	1/1	0.94	0.11	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8101	1/1	0.98	0.21	-	71,71,71,71	0
32	MG	0	8075	1/1	0.93	0.10	-	57,57,57,57	0
32	MG	0	8103	1/1	0.96	0.21	-	77,77,77,77	0
34	NA	0	8505	1/1	0.91	0.13	-	36,36,36,36	0
34	NA	0	8554	1/1	0.92	0.23	-	39,39,39,39	0
32	MG	B	8055	1/1	0.78	0.08	-	43,43,43,43	0
32	MG	0	8023	1/1	0.98	0.15	-	39,39,39,39	0
32	MG	0	8098	1/1	0.95	0.17	-	31,31,31,31	0
34	NA	9	8551	1/1	0.72	0.22	-	95,95,95,95	0
35	CL	0	8816	1/1	0.98	0.12	-	57,57,57,57	0
35	CL	0	8814	1/1	0.97	0.06	-	46,46,46,46	0
32	MG	0	8094	1/1	0.80	0.10	-	66,66,66,66	0
32	MG	0	8042	1/1	0.94	0.05	-	35,35,35,35	0
32	MG	0	8111	1/1	0.94	0.13	-	50,50,50,50	0
32	MG	9	8095	1/1	0.92	0.05	-	55,55,55,55	0
32	MG	0	8041	1/1	0.86	0.07	-	54,54,54,54	0
32	MG	0	8079	1/1	0.99	0.14	-	27,27,27,27	0
34	NA	0	8575	1/1	0.96	0.28	-	52,52,52,52	0
35	CL	J	8801	1/1	0.94	0.08	-	54,54,54,54	0
32	MG	0	8093	1/1	0.97	0.05	-	43,43,43,43	0
32	MG	0	8051	1/1	0.97	0.07	-	40,40,40,40	0
34	NA	0	8508	1/1	0.78	0.22	-	36,36,36,36	0
32	MG	0	8047	1/1	0.91	0.06	-	72,72,72,72	0
35	CL	0	8815	1/1	0.89	0.13	-	61,61,61,61	0
34	NA	0	8563	1/1	0.98	0.19	-	52,52,52,52	0
32	MG	0	8034	1/1	0.97	0.07	-	15,15,15,15	0
32	MG	0	8050	1/1	0.66	0.15	-	66,66,66,66	0
34	NA	0	8569	1/1	0.84	0.31	-	63,63,63,63	0
37	CD	O	8705	1/1	0.49	0.42	-	187,187,187,187	0
34	NA	0	8567	1/1	0.75	0.28	-	51,51,51,51	0
34	NA	C	8504	1/1	0.94	0.18	-	41,41,41,41	0
34	NA	0	8555	1/1	0.86	0.90	-	81,81,81,81	0
32	MG	0	8097	1/1	0.96	0.07	-	35,35,35,35	0
32	MG	0	8099	1/1	0.89	0.15	-	42,42,42,42	0
34	NA	9	8583	1/1	0.90	0.21	-	63,63,63,63	0
32	MG	0	8059	1/1	0.85	0.09	-	38,38,38,38	0
32	MG	0	8090	1/1	0.95	0.24	-	72,72,72,72	0
32	MG	0	8026	1/1	0.97	0.15	-	32,32,32,32	0
32	MG	0	8083	1/1	0.83	0.06	-	40,40,40,40	0
34	NA	0	8530	1/1	0.94	0.08	-	33,33,33,33	0
32	MG	0	8045	1/1	0.86	0.09	-	51,51,51,51	0
32	MG	0	8089	1/1	0.99	0.12	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	NA	0	8502	1/1	0.91	0.11	-	51,51,51,51	0
34	NA	0	8542	1/1	0.99	0.28	-	1,1,1,1	0
34	NA	0	8540	1/1	0.96	0.11	-	43,43,43,43	0
34	NA	S	8512	1/1	0.91	0.70	-	62,62,62,62	0
35	CL	L	8810	1/1	0.83	0.09	-	54,54,54,54	0
35	CL	0	8817	1/1	0.96	0.12	-	59,59,59,59	0
32	MG	0	8046	1/1	0.88	0.06	-	45,45,45,45	0
34	NA	0	8558	1/1	0.70	0.41	-	68,68,68,68	0
32	MG	0	8022	1/1	0.97	0.05	-	40,40,40,40	0
34	NA	0	8534	1/1	0.96	0.06	-	41,41,41,41	0
32	MG	0	8082	1/1	0.86	0.22	-	65,65,65,65	0
32	MG	0	8106	1/1	0.51	0.17	-	63,63,63,63	0
32	MG	0	8086	1/1	0.81	0.04	-	46,46,46,46	0
32	MG	0	8115	1/1	0.98	0.03	-	41,41,41,41	0
34	NA	0	8585	1/1	0.81	0.32	-	59,59,59,59	0
32	MG	0	8092	1/1	0.82	0.11	-	66,66,66,66	0
32	MG	0	8048	1/1	0.95	0.10	-	48,48,48,48	0
32	MG	0	8005	1/1	1.00	0.14	-	32,32,32,32	0
34	NA	0	8570	1/1	0.96	0.36	-	64,64,64,64	0
34	NA	0	8584	1/1	0.64	0.35	-	68,68,68,68	0
32	MG	0	8085	1/1	0.80	0.14	-	48,48,48,48	0
32	MG	0	8068	1/1	0.96	0.06	-	54,54,54,54	0
32	MG	0	8070	1/1	0.88	0.10	-	34,34,34,34	0
34	NA	0	8506	1/1	0.84	0.37	-	52,52,52,52	0
32	MG	0	8030	1/1	0.98	0.06	-	20,20,20,20	0
32	MG	0	8011	1/1	0.94	0.08	-	23,23,23,23	0
35	CL	R	8806	1/1	0.92	0.07	-	52,52,52,52	0
35	CL	N	8807	1/1	0.92	0.12	-	57,57,57,57	0
34	NA	H	8522	1/1	0.89	0.35	-	71,71,71,71	0
32	MG	0	8117	1/1	0.94	0.09	-	45,45,45,45	0
35	CL	J	8802	1/1	0.91	0.12	-	58,58,58,58	0
34	NA	0	8501	1/1	0.94	0.04	-	51,51,51,51	0
34	NA	0	8519	1/1	0.99	0.12	-	21,21,21,21	0
32	MG	0	8076	1/1	0.56	0.12	-	44,44,44,44	0
35	CL	0	8822	1/1	0.95	0.30	-	71,71,71,71	0
32	MG	A	8066	1/1	0.96	0.14	-	47,47,47,47	0
35	CL	A	8809	1/1	0.97	0.13	-	71,71,71,71	0
34	NA	0	8549	1/1	0.87	0.19	-	45,45,45,45	0
34	NA	0	8515	1/1	0.96	0.14	-	33,33,33,33	0
32	MG	0	8036	1/1	0.98	0.04	-	29,29,29,29	0
34	NA	0	8529	1/1	0.91	0.15	-	56,56,56,56	0
32	MG	0	8025	1/1	0.99	0.10	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8043	1/1	0.84	0.19	-	61,61,61,61	0
34	NA	0	8518	1/1	0.98	0.12	-	40,40,40,40	0
34	NA	0	8507	1/1	0.81	0.12	-	54,54,54,54	0
34	NA	0	8574	1/1	0.03	0.83	-	73,73,73,73	0
35	CL	0	8813	1/1	0.98	0.06	-	55,55,55,55	0
34	NA	R	8537	1/1	0.88	0.05	-	35,35,35,35	0
35	CL	0	8820	1/1	0.95	0.06	-	36,36,36,36	0
32	MG	0	8113	1/1	0.77	0.13	-	49,49,49,49	0
34	NA	0	8579	1/1	0.95	0.08	-	46,46,46,46	0
32	MG	0	8114	1/1	0.89	0.23	-	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.