



Full wwPDB X-ray Structure Validation Report i

May 8, 2014 – 03:42 AM EDT

PDB ID : 3CC2
Title : The Refined Crystal Structure of the Haloarcula Marismortui Large Ribosomal Subunit at 2.4 Angstrom Resolution with rrnA Sequence for the 23S rRNA and Genome-derived Sequences for r-Proteins
Authors : Gurel, G.; Blaha, G.
Deposited on : 2008-02-23
Resolution : 2.40 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

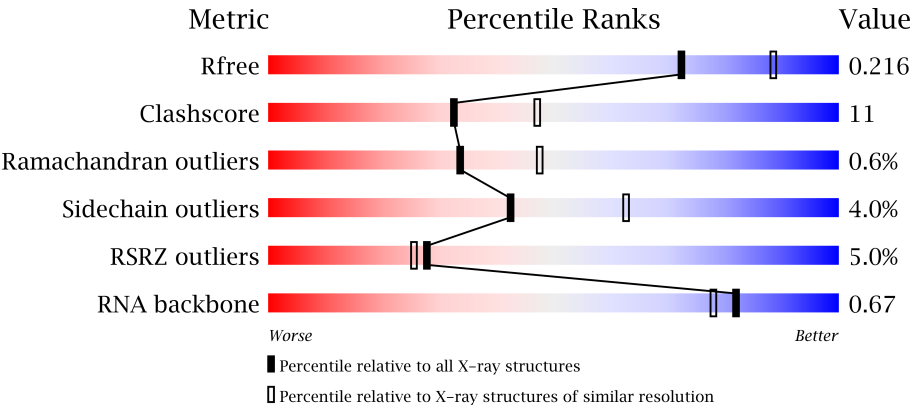
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable22978
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22978

1 Overall quality at a glance

The reported resolution of this entry is 2.40 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}	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)
RNA backbone	1838	1029 (3.00-1.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	240	
2	B	338	
3	C	246	
4	D	177	
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	

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Mol	Chain	Length	Quality of chain
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	
30	0	2923	
31	9	122	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
32	MG	0	8007	-	X
32	MG	0	8034	-	X
32	MG	0	8041	-	X
32	MG	0	8047	-	X
32	MG	0	8049	-	X
32	MG	0	8057	-	X
32	MG	0	8060	-	X
32	MG	0	8066	-	X
32	MG	0	8082	-	X
32	MG	0	8087	-	X
32	MG	0	8101	-	X
32	MG	0	8103	-	X
34	NA	0	8302	-	X
34	NA	0	8306	-	X
34	NA	0	8307	-	X
34	NA	0	8308	-	X
34	NA	0	8311	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
34	NA	0	8314	-	X
34	NA	0	8318	-	X
34	NA	0	8320	-	X
34	NA	0	8326	-	X
34	NA	0	8328	-	X
34	NA	0	8329	-	X
34	NA	0	8335	-	X
34	NA	0	8340	-	X
34	NA	0	8350	-	X
34	NA	0	8355	-	X
34	NA	0	8358	-	X
34	NA	0	8359	-	X
34	NA	0	8361	-	X
34	NA	0	8362	-	X
34	NA	0	8363	-	X
34	NA	0	8364	-	X
34	NA	0	8365	-	X
34	NA	0	8366	-	X
34	NA	0	8367	-	X
34	NA	0	8369	-	X
34	NA	0	8370	-	X
34	NA	0	8371	-	X
34	NA	0	8372	-	X
34	NA	0	8373	-	X
34	NA	0	8374	-	X
34	NA	0	8376	-	X
34	NA	0	8377	-	X
34	NA	0	8378	-	X
34	NA	0	8379	-	X
34	NA	0	8382	-	X
34	NA	0	8385	-	X
34	NA	9	8383	-	X
34	NA	L	8380	-	X
34	NA	R	8386	-	X
35	CL	0	8522	-	X

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 99049 atoms, of which 0 are hydrogen and 0 are deuterium.

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 protein called 50S ribosomal protein L2P.

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

- Molecule 2 is a protein called 50S ribosomal protein L3P.

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

- Molecule 3 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	246	Total	C	N	O	S	0	0	0
			1860	1130	345	384	1			

- Molecule 4 is a protein called 50S ribosomal protein L5P.

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

- Molecule 5 is a protein called 50S ribosomal protein L6P.

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

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 7 is a protein called 50S ribosomal protein L10E.

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

- Molecule 8 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 9 is a protein called 50S ribosomal protein L11P.

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

- Molecule 10 is a protein called 50S ribosomal protein L13P.

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

- Molecule 11 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 12 is a protein called 50S ribosomal protein L15P.

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

- Molecule 13 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	194	Total	C	N	O	S	0	0	0
			1558	943	333	281	1			

- Molecule 14 is a protein called 50S ribosomal protein L18P.

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

- Molecule 15 is a protein called 50S ribosomal protein L18e.

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

- Molecule 16 is a protein called 50S ribosomal protein L19e.

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

- Molecule 17 is a protein called 50S ribosomal protein L21e.

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

- Molecule 18 is a protein called 50S ribosomal protein L22P.

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

- Molecule 19 is a protein called 50S ribosomal protein L23P.

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

- Molecule 20 is a protein called 50S ribosomal protein L24P.

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

- Molecule 21 is a protein called 50S ribosomal protein L24e.

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

- Molecule 22 is a protein called 50S ribosomal protein L29P.

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

- Molecule 23 is a protein called 50S ribosomal protein L30P.

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

- Molecule 24 is a protein called 50S ribosomal protein L31e.

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

- Molecule 25 is a protein called 50S ribosomal protein L32e.

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

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			573	343	113	112	5			

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 28 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 30 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59021	26349	10873	19054	2745			

- Molecule 31 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	109	Total	Mg	0	0
			109	109		
32	9	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	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		
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 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	73	Total Na 73 73	0	0
34	J	1	Total Na 1 1	0	0
34	Q	1	Total Na 1 1	0	0
34	H	1	Total Na 1 1	0	0
34	C	1	Total Na 1 1	0	0
34	A	1	Total Na 1 1	0	0
34	R	2	Total Na 2 2	0	0
34	9	3	Total Na 3 3	0	0
34	L	1	Total Na 1 1	0	0
34	S	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	10	Total Cl 10 10	0	0
35	J	3	Total Cl 3 3	0	0
35	B	1	Total Cl 1 1	0	0
35	A	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0
35	O	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	R	1	Total 1	Cl 1	0	0
35	Y	1	Total 1	Cl 1	0	0
35	L	1	Total 1	Cl 1	0	0
35	3	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	0	0

- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	O	1	Total 1	Cd 1	0	0
36	Z	1	Total 1	Cd 1	0	0
36	1	1	Total 1	Cd 1	0	0
36	3	1	Total 1	Cd 1	0	0
36	U	1	Total 1	Cd 1	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	5949	Total 5949	O 5949	0	0
37	A	117	Total 117	O 117	0	0
37	B	146	Total 146	O 146	0	0
37	C	170	Total 170	O 170	0	0
37	D	47	Total 47	O 47	0	0
37	E	42	Total 42	O 42	0	0
37	F	24	Total 24	O 24	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	G	19	Total 19	O 19	0	0
37	H	72	Total 72	O 72	0	0
37	I	9	Total 9	O 9	0	0
37	J	51	Total 51	O 51	0	0
37	K	56	Total 56	O 56	0	0
37	L	72	Total 72	O 72	0	0
37	M	119	Total 119	O 119	0	0
37	N	65	Total 65	O 65	0	0
37	O	39	Total 39	O 39	0	0
37	P	63	Total 63	O 63	0	0
37	Q	52	Total 52	O 52	0	0
37	R	80	Total 80	O 80	0	0
37	S	33	Total 33	O 33	0	0
37	T	38	Total 38	O 38	0	0
37	U	27	Total 27	O 27	0	0
37	V	14	Total 14	O 14	0	0
37	W	66	Total 66	O 66	0	0
37	X	29	Total 29	O 29	0	0
37	Y	94	Total 94	O 94	0	0
37	Z	26	Total 26	O 26	0	0
37	1	53	Total 53	O 53	0	0

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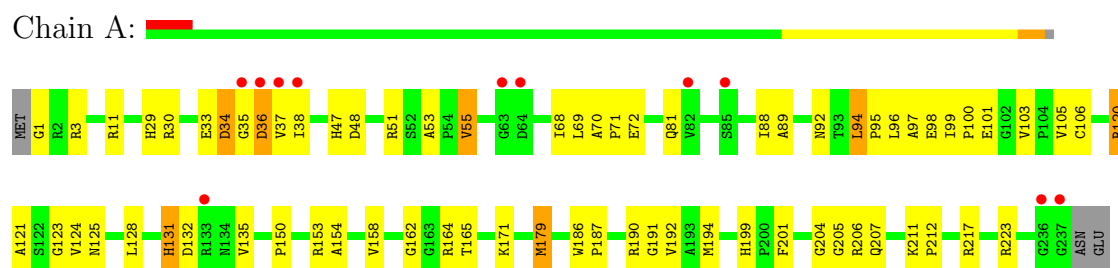
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	2	40	Total 40	O 40	0	0
37	3	72	Total 72	O 72	0	0
37	9	139	Total 139	O 139	0	0

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 ($RSRZ > 2$). 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.

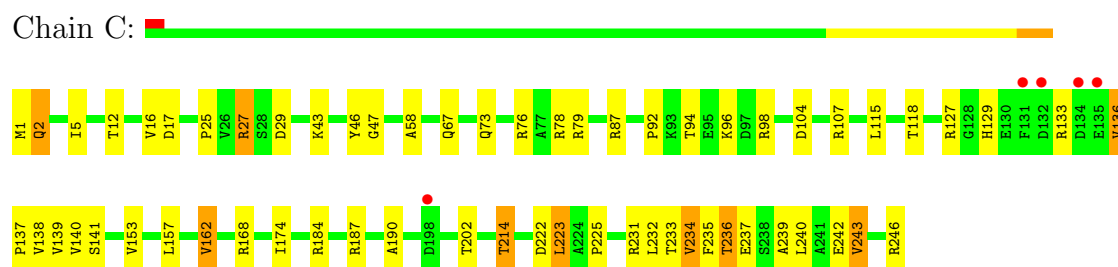
- Molecule 1: 50S ribosomal protein L2P



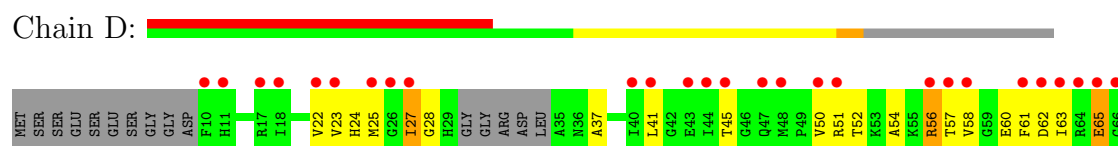
- Molecule 2: 50S ribosomal protein L3P

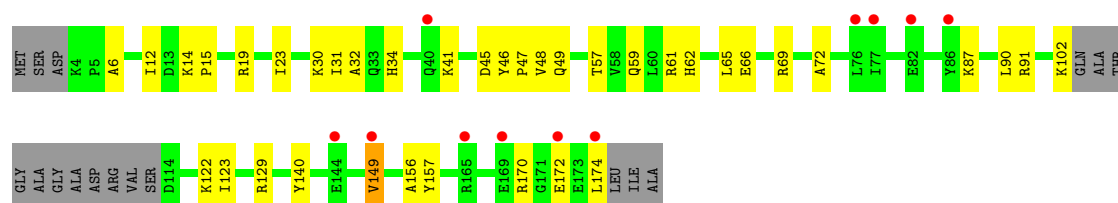


- Molecule 3: 50S ribosomal protein L4P



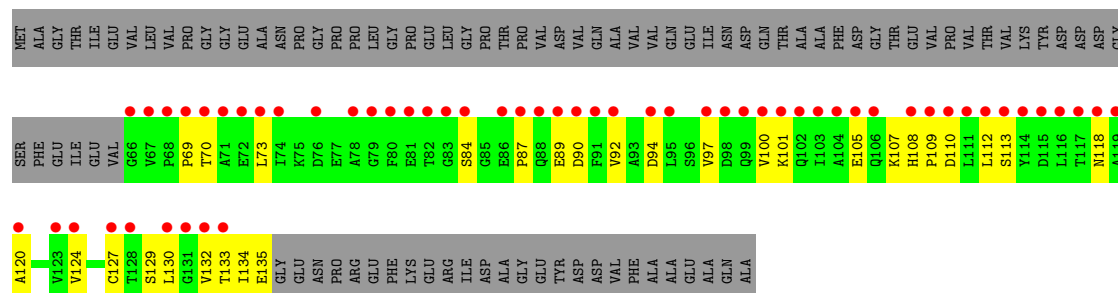
- Molecule 4: 50S ribosomal protein L5P





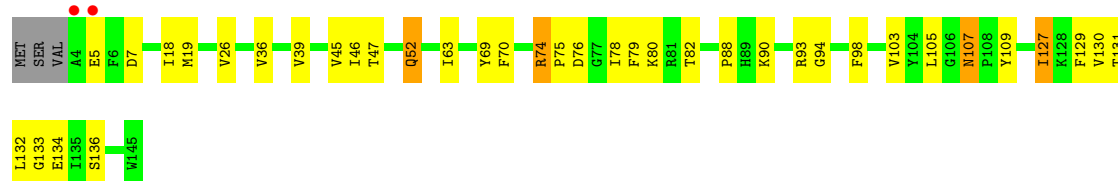
• Molecule 9: 50S ribosomal protein L11P

Chain I:



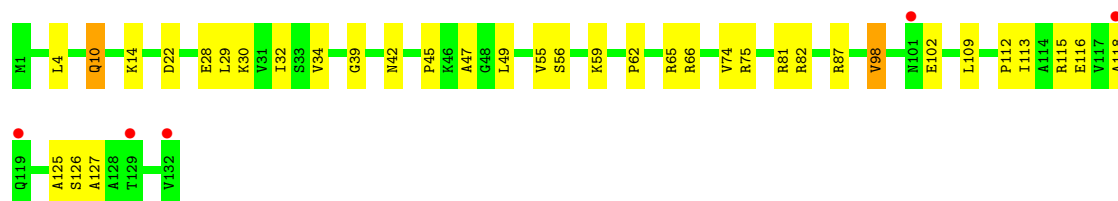
• Molecule 10: 50S ribosomal protein L13P

Chain J:



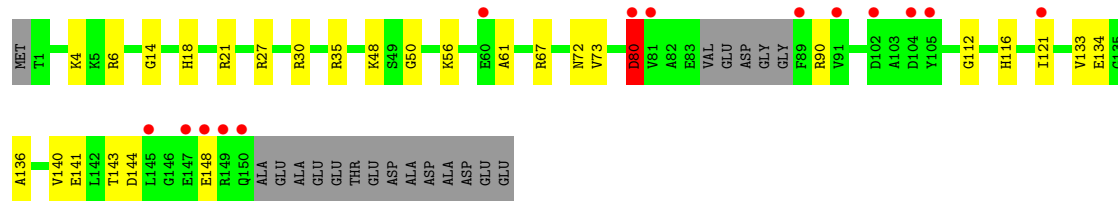
• Molecule 11: 50S ribosomal protein L14P

Chain K:



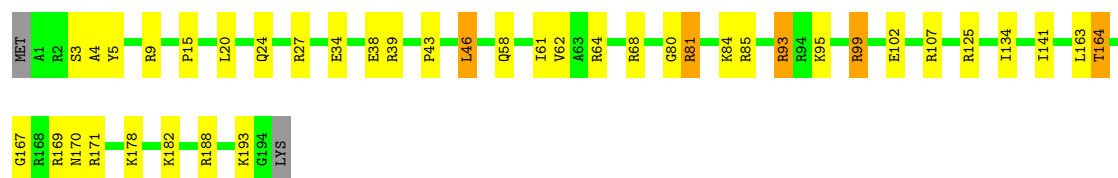
• Molecule 12: 50S ribosomal protein L15P

Chain L:



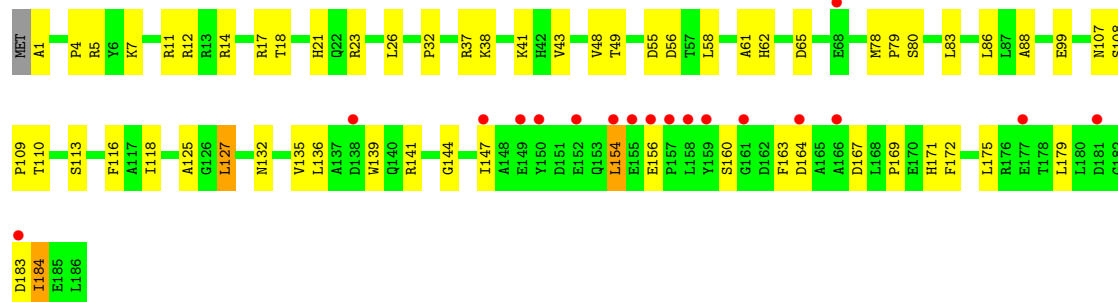
• Molecule 13: 50S ribosomal protein L15e

Chain M: 



- Molecule 14: 50S ribosomal protein L18P

Chain N: 



- Molecule 15: 50S ribosomal protein L18e

Chain O: 



- Molecule 16: 50S ribosomal protein L19e

Chain P: 



- Molecule 17: 50S ribosomal protein L21e

Chain Q: 



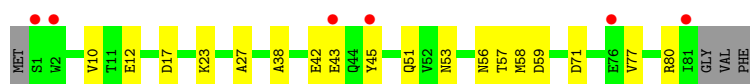
- Molecule 18: 50S ribosomal protein L22P

Chain R: 



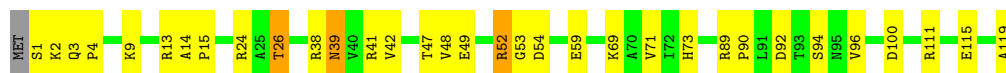
- Molecule 19: 50S ribosomal protein L23P

Chain S: 



- Molecule 20: 50S ribosomal protein L24P

Chain T:



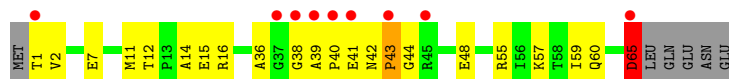
- Molecule 21: 50S ribosomal protein L24e

Chain U:



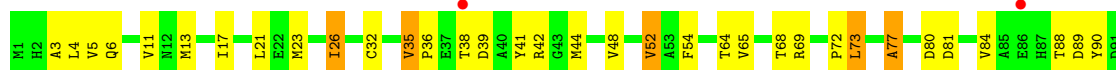
- Molecule 22: 50S ribosomal protein L29P

Chain V:



- Molecule 23: 50S ribosomal protein L30P

Chain W:



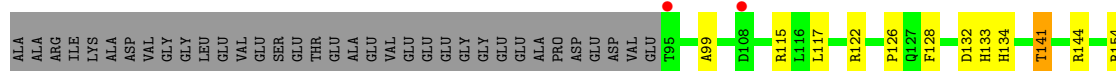
- Molecule 24: 50S ribosomal protein L31e

Chain X:

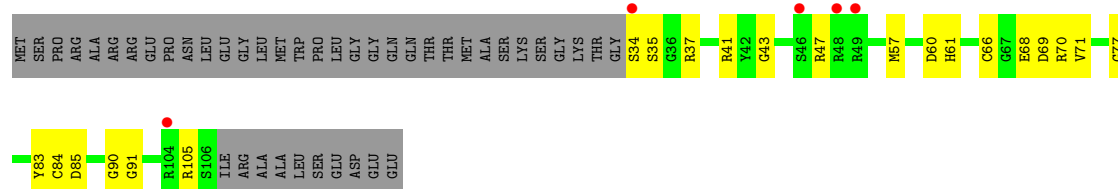


- Molecule 25: 50S ribosomal protein L32e

Chain Y:



- Molecule 26: 50S ribosomal protein L37Ae

Chain Z: 

- Molecule 27: 50S ribosomal protein L37e

Chain 1: 

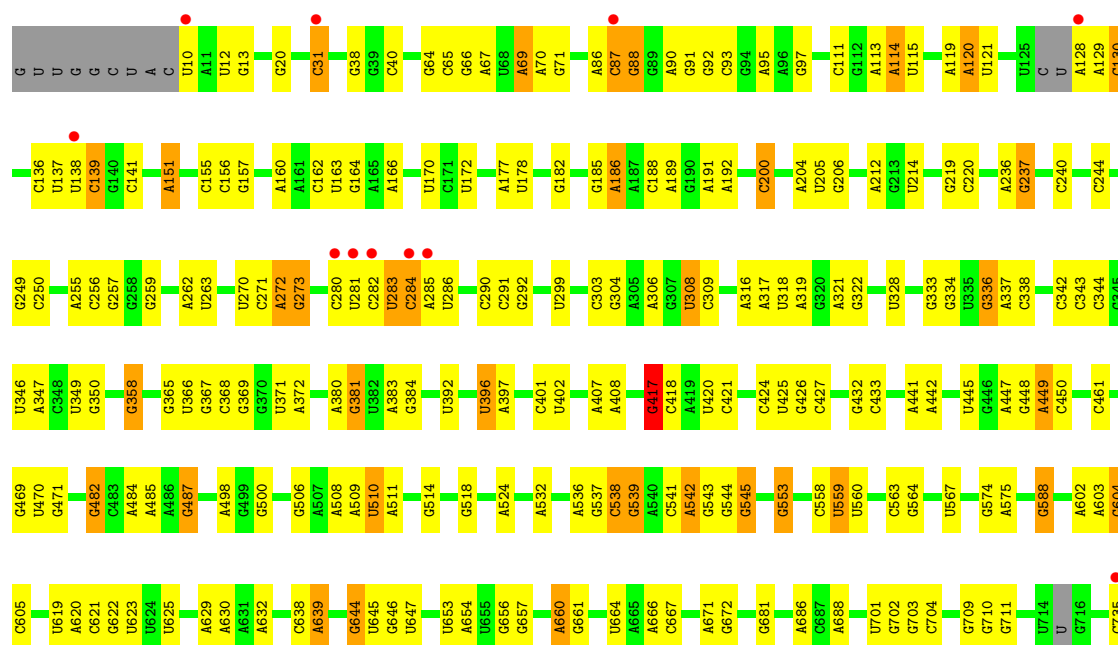
- Molecule 28: 50S ribosomal protein L39e

Chain 2: 

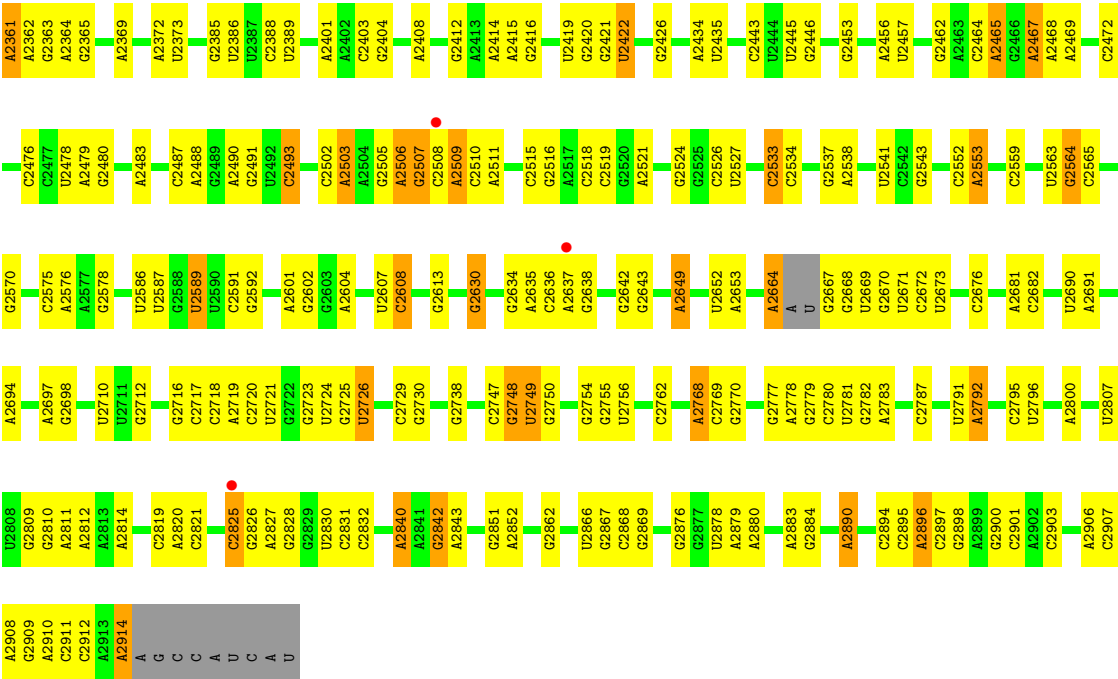
- Molecule 29: 50S ribosomal protein L44E

Chain 3: 

- Molecule 30: 23S RIBOSOMAL RNA

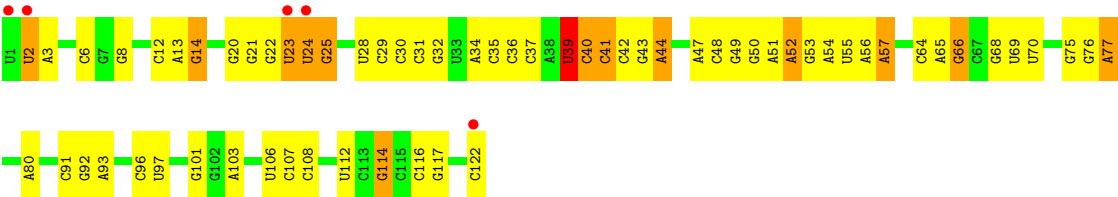
Chain 0: 





• Molecule 31: 5S RIBOSOMAL RNA

Chain 9:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.65Å 299.67Å 573.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.95 – 2.40 85.47 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.5 (49.95-2.40) 90.6 (85.47-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.199 , 0.231 0.183 , 0.216	Depositor DCC
R_{free} test set	6200 reflections (0.98%)	DCC
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 666819 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99049	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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, NA, K, CD, OMU, UR3, 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	A	0.33	0/1786	0.66	0/2408
2	B	0.32	0/2690	0.64	0/3652
3	C	0.36	0/1885	0.64	0/2552
4	D	0.32	0/1111	0.56	0/1498
5	E	0.31	0/1382	0.56	0/1880
6	F	0.32	0/901	0.54	0/1224
7	G	0.42	0/241	0.74	0/324
8	H	0.39	0/1302	0.68	0/1743
9	I	0.34	0/526	0.53	0/716
10	J	0.33	0/1136	0.58	0/1530
11	K	0.32	0/1004	0.65	0/1351
12	L	0.34	0/1130	0.65	0/1509
13	M	0.33	0/1582	0.62	0/2116
14	N	0.28	0/1474	0.61	0/1999
15	O	0.32	0/874	0.59	1/1181 (0.1%)
16	P	0.32	0/1147	0.52	0/1528
17	Q	0.33	0/749	0.67	0/1005
18	R	1.31	7/1172 (0.6%)	1.13	5/1578 (0.3%)
19	S	0.33	0/648	0.59	1/875 (0.1%)
20	T	0.31	0/958	0.62	1/1289 (0.1%)
21	U	0.36	0/417	0.60	0/562
22	V	0.36	0/502	0.68	1/675 (0.1%)
23	W	0.33	0/1219	0.65	1/1655 (0.1%)
24	X	0.36	0/664	0.59	0/895
25	Y	0.36	0/1146	0.62	0/1536
26	Z	0.34	0/584	0.66	0/781
27	1	0.42	0/438	0.65	0/578
28	2	0.33	0/401	0.56	0/529
29	3	0.36	0/771	0.59	0/1024
30	0	0.33	0/65958	0.69	21/102869 (0.0%)
31	9	0.29	0/2904	0.69	1/4526 (0.0%)
All	All	0.36	7/98702 (0.0%)	0.68	32/147588 (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
18	R	1	0
30	0	0	39
31	9	0	1
All	All	1	40

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CA-C	-29.63	0.93	1.52
18	R	150	PRO	CB-CG	16.19	2.31	1.50
18	R	150	PRO	N-CA	14.71	1.72	1.47
18	R	150	PRO	CA-CB	12.12	1.77	1.53
18	R	150	PRO	CG-CD	11.79	1.89	1.50
18	R	150	PRO	C-O	11.61	1.46	1.23
18	R	150	PRO	N-CD	9.24	1.60	1.47

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	N-CA-C	-24.01	49.68	112.10
18	R	150	PRO	CB-CA-C	-19.94	62.16	112.00
18	R	150	PRO	CA-C-O	-16.63	80.28	120.20
30	0	1942	A	C5'-C4'-C3'	8.15	129.05	116.00
18	R	150	PRO	CA-N-CD	7.93	122.80	111.70
22	V	65	ASP	CB-CG-OD1	7.92	125.43	118.30
30	0	871	G	C5'-C4'-O4'	-7.20	100.46	109.10
18	R	150	PRO	N-CA-CB	6.86	111.54	103.30
30	0	1819	G	C5'-C4'-C3'	6.74	126.79	116.00
30	0	1504	A	C1'-O4'-C4'	-6.54	104.67	109.90
31	9	39	U	N1-C1'-C2'	6.47	122.41	114.00
30	0	2316	G	C5'-C4'-C3'	-6.43	105.71	116.00
30	0	1979	G	C2'-C3'-O3'	6.36	123.87	113.70
30	0	1878	G	N9-C1'-C2'	-6.28	105.09	112.00
30	0	1942	A	C5'-C4'-O4'	6.20	116.54	109.10
30	0	2467	A	C1'-O4'-C4'	-6.18	104.95	109.90
30	0	206	G	C5'-C4'-C3'	-6.05	106.32	116.00
30	0	2291	A	N9-C1'-C2'	5.93	121.71	114.00
30	0	1829	A	N9-C1'-C2'	-5.85	105.56	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	1592	G	N9-C1'-C2'	5.66	121.36	114.00
30	0	1942	A	C4'-C3'-C2'	-5.44	97.16	102.60
30	0	1942	A	C1'-O4'-C4'	-5.30	105.66	109.90
23	W	122	ARG	NE-CZ-NH1	5.27	122.94	120.30
30	0	1504	A	N9-C1'-C2'	5.25	120.83	114.00
30	0	2313	C	C5'-C4'-O4'	5.25	115.40	109.10
30	0	841	A	C1'-O4'-C4'	-5.23	105.72	109.90
15	O	66	GLY	N-CA-C	5.16	126.01	113.10
30	0	777	U	O4'-C1'-N1	5.15	112.32	108.20
19	S	27	ALA	N-CA-C	-5.09	97.27	111.00
20	T	52	ARG	N-CA-C	5.06	124.66	111.00
30	0	1819	G	C4'-C3'-C2'	-5.05	97.55	102.60
30	0	1120	U	C5'-C4'-C3'	-5.02	107.97	116.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

All (40) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1039	G	Sidechain
30	0	1078	A	Sidechain
30	0	1237	U	Sidechain
30	0	1340	G	Sidechain
30	0	1342	C	Sidechain
30	0	1417	G	Sidechain
30	0	1450	C	Sidechain
30	0	1829	A	Sidechain
30	0	1845	A	Sidechain
30	0	1848	G	Sidechain
30	0	1863	G	Sidechain
30	0	1867	G	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	1972	U	Sidechain
30	0	2103	A	Sidechain
30	0	2316	G	Sidechain
30	0	2465	A	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain

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Mol	Chain	Res	Type	Group
30	0	2506	A	Sidechain
30	0	2543	G	Sidechain
30	0	2552	C	Sidechain
30	0	2564	G	Sidechain
30	0	2607	U	Sidechain
30	0	2630	G	Sidechain
30	0	270	U	Sidechain
30	0	2842	G	Sidechain
30	0	396	U	Sidechain
30	0	417	G	Sidechain
30	0	449	A	Sidechain
30	0	469	G	Sidechain
30	0	471	G	Sidechain
30	0	482	G	Sidechain
30	0	518	G	Sidechain
30	0	619	U	Sidechain
30	0	639	A	Sidechain
30	0	795	G	Sidechain
30	0	867	A	Sidechain
31	9	39	U	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	74	0
2	B	2625	0	2533	80	0
3	C	1860	0	1813	65	0
4	D	1094	0	1085	45	0
5	E	1357	0	1266	42	0
6	F	890	0	843	26	0
7	G	240	0	231	11	0
8	H	1282	0	1292	34	0
9	I	519	0	500	23	0
10	J	1120	0	1098	39	0
11	K	994	0	1027	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	1118	0	1076	26	0
13	M	1558	0	1572	44	0
14	N	1445	0	1401	55	0
15	O	865	0	873	19	0
16	P	1136	0	1123	20	0
17	Q	735	0	728	11	0
18	R	1149	0	1122	31	0
19	S	641	0	605	13	0
20	T	950	0	923	24	0
21	U	410	0	364	16	0
22	V	499	0	511	19	0
23	W	1196	0	1137	66	0
24	X	654	0	653	21	0
25	Y	1130	0	1133	30	0
26	Z	573	0	532	14	0
27	1	431	0	426	17	0
28	2	396	0	413	24	0
29	3	755	0	728	16	0
30	0	59021	0	29809	870	0
31	9	2599	0	1325	72	0
32	0	109	0	0	0	0
32	3	1	0	0	0	0
32	9	1	0	0	0	0
32	A	1	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	73	0	0	0	0
34	9	3	0	0	0	0
34	A	1	0	0	0	0
34	C	1	0	0	0	0
34	H	1	0	0	0	0
34	J	1	0	0	0	0
34	L	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	2	0	0	0	0
34	S	1	0	0	0	0
35	0	10	0	0	0	0
35	3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	1	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	N	1	0	0	0	0
35	O	1	0	0	0	0
35	R	1	0	0	0	0
35	Y	1	0	0	0	0
36	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	5949	0	0	149	0
37	1	53	0	0	2	0
37	2	40	0	0	4	0
37	3	72	0	0	6	0
37	9	139	0	0	7	0
37	A	117	0	0	14	0
37	B	146	0	0	13	0
37	C	170	0	0	18	0
37	D	47	0	0	5	0
37	E	42	0	0	4	0
37	F	24	0	0	2	0
37	G	19	0	0	1	0
37	H	72	0	0	5	0
37	I	9	0	0	3	0
37	J	51	0	0	2	0
37	K	56	0	0	5	0
37	L	72	0	0	9	0
37	M	119	0	0	9	0
37	N	65	0	0	10	0
37	O	39	0	0	3	0
37	P	63	0	0	1	0
37	Q	52	0	0	3	0
37	R	80	0	0	2	0
37	S	33	0	0	2	0
37	T	38	0	0	2	0
37	U	27	0	0	1	0
37	V	14	0	0	1	0
37	W	66	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	X	29	0	0	5	0
37	Y	94	0	0	10	0
37	Z	26	0	0	2	0
All	All	99049	0	59908	1694	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (1694) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:R:150:PRO:CG	18:R:150:PRO:CD	1.89	1.50
14:N:37:ARG:NH1	31:9:6:C:H5"	1.61	1.14
30:0:871:G:C8	30:0:871:G:H5'	1.86	1.10
30:0:960:G:H4'	37:0:6980:HOH:O	1.49	1.09
18:R:150:PRO:CG	18:R:150:PRO:CB	2.30	1.08
18:R:150:PRO:CG	18:R:150:PRO:C	2.21	1.08
30:0:1160:G:C5'	30:0:1161:A:H5'	1.85	1.06
15:O:3:THR:HG22	30:0:656:G:H5'	1.38	1.06
10:J:82:THR:HG23	30:0:1242:A:H5'	1.37	1.05
13:M:171:ARG:HD3	30:0:156:C:H5"	1.37	1.05
30:0:2812:A:H2	30:0:2814:A:H62	1.08	1.02
30:0:1160:G:H5'	30:0:1161:A:H5'	1.02	1.01
31:9:56:A:H2'	31:9:57:A:H5"	1.42	1.01
30:0:1372:A:H3'	37:0:6737:HOH:O	1.60	1.00
30:0:1160:G:H5'	30:0:1161:A:C5'	1.91	1.00
30:0:2717:C:H2'	30:0:2718:C:H5"	1.43	0.99
11:K:29:LEU:HB3	11:K:55:VAL:HG11	1.44	0.99
31:9:76:G:H3'	31:9:77:A:H5"	1.44	0.98
30:0:2710:U:H1'	37:0:7172:HOH:O	1.62	0.98
30:0:1474:C:H6	30:0:1474:C:H5'	1.30	0.97
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.46	0.96
30:0:542:A:H5'	30:0:542:A:H8	1.28	0.96
30:0:871:G:H8	30:0:871:G:H5'	1.25	0.95
30:0:2717:C:C2'	30:0:2718:C:H5"	1.96	0.95
28:2:41:HIS:H	28:2:45:ASN:HD22	1.11	0.95
4:D:134:LEU:HD11	4:D:166:ILE:HD11	1.49	0.94
30:0:214:U:H5'	37:0:5687:HOH:O	1.67	0.94
30:0:541:C:H2'	30:0:542:A:H5"	1.50	0.94
11:K:10:GLN:H	11:K:10:GLN:HE21	0.96	0.93
30:0:1835:U:H5	30:0:1840:A:N7	1.66	0.93
30:0:1625:U:H4'	37:0:4207:HOH:O	1.68	0.93
3:C:236:THR:HG22	3:C:239:ALA:H	1.30	0.93

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.17	0.92
30:0:381:G:H5"	37:0:3859:HOH:O	1.67	0.92
13:M:164:THR:HG22	13:M:167:GLY:H	1.33	0.92
30:0:282:C:H1'	30:0:368:C:N4	1.85	0.91
30:0:871:G:H8	30:0:871:G:C5'	1.83	0.91
20:T:71:VAL:HG11	20:T:90:PRO:HB3	1.53	0.90
30:0:1184:C:H1'	37:0:7015:HOH:O	1.70	0.90
30:0:870:G:H2'	30:0:871:G:H5"	1.51	0.90
30:0:2291:A:C8	30:0:2309:C:H5'	2.06	0.90
21:U:52:THR:HG22	21:U:54:THR:H	1.35	0.90
30:0:1116:U:O2'	30:0:1118:A:H2	1.55	0.89
30:0:1667:A:H8	30:0:1667:A:H5'	1.36	0.89
30:0:2748:G:H2'	37:0:7089:HOH:O	1.72	0.89
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.54	0.89
30:0:1666:C:O2'	30:0:1667:A:H5"	1.70	0.89
30:0:1701:A:H4'	30:0:1702:U:H5"	1.53	0.89
30:0:236:A:H4'	30:0:237:G:H5'	1.55	0.87
30:0:541:C:C2'	30:0:542:A:H5"	2.03	0.87
2:B:140:LEU:HA	37:B:8581:HOH:O	1.74	0.87
11:K:39:GLY:HA2	37:0:4763:HOH:O	1.73	0.87
30:0:871:G:C8	30:0:871:G:C5'	2.58	0.87
30:0:1116:U:H3	30:0:1246:A:H62	1.23	0.86
16:P:115:SER:H	16:P:118:GLN:HE21	1.19	0.86
30:0:69:A:H5'	30:0:69:A:C8	2.10	0.86
4:D:154:LYS:HD2	4:D:154:LYS:H	1.38	0.86
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.19	0.86
30:0:2506:A:O2'	30:0:2507:G:H8	1.59	0.86
23:W:6:GLN:HB2	23:W:26:ILE:HD12	1.55	0.85
30:0:1300:G:H1'	37:0:4223:HOH:O	1.77	0.85
14:N:37:ARG:HH12	31:9:6:C:H5"	1.39	0.85
1:A:223:ARG:HH12	30:0:2270:G:H4'	1.42	0.85
31:9:39:U:H1'	31:9:44:A:H61	1.42	0.85
30:0:282:C:O2'	30:0:283:U:H5'	1.77	0.84
26:Z:70:ARG:HD2	26:Z:83:TYR:HB2	1.58	0.84
30:0:545:G:H8	30:0:545:G:H5'	1.40	0.84
23:W:88:THR:HB	37:W:6679:HOH:O	1.77	0.84
30:0:506:G:H22	30:0:509:A:C5'	1.91	0.83
30:0:1119:G:N2	30:0:1246:A:C2	2.46	0.83
30:0:69:A:H5'	30:0:69:A:H8	1.42	0.83
31:9:14:G:H5'	31:9:14:G:H8	1.43	0.83
2:B:206:THR:HG21	30:0:2716:G:H5"	1.60	0.83
30:0:1730:G:H5'	30:0:1731:C:C5	2.14	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
26:Z:34:SER:HB2	37:Z:8414:HOH:O	1.77	0.82
30:0:1862:C:H1'	37:0:6768:HOH:O	1.80	0.82
30:0:2586:U:H3	30:0:2592:G:H22	1.28	0.82
30:0:1118:A:H3'	30:0:1118:A:H8	1.44	0.82
30:0:272:A:H3'	37:0:7079:HOH:O	1.79	0.81
30:0:2769:C:C2'	30:0:2770:G:H5'	2.10	0.81
37:I:5128:HOH:O	30:0:1168:C:H4'	1.81	0.81
25:Y:200:THR:HG22	25:Y:201:GLU:HG3	1.61	0.81
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.63	0.81
30:0:506:G:H22	30:0:509:A:H5''	1.45	0.81
30:0:564:G:H1'	37:0:5857:HOH:O	1.81	0.81
30:0:346:U:H4'	37:0:6392:HOH:O	1.80	0.81
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.26	0.81
30:0:2851:G:O2'	30:0:2852:A:H5'	1.81	0.81
11:K:10:GLN:N	11:K:10:GLN:HE21	1.79	0.81
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.63	0.81
8:H:170:ARG:HD2	37:H:8342:HOH:O	1.79	0.80
31:9:56:A:C2'	31:9:57:A:H5''	2.11	0.80
23:W:88:THR:HG23	23:W:110:GLN:HE21	1.46	0.80
21:U:46:ALA:HB1	21:U:52:THR:HG21	1.63	0.80
30:0:1474:C:C6	30:0:1474:C:H5'	2.17	0.80
30:0:1973:A:H5'	30:0:1973:A:H8	1.47	0.80
30:0:2908:A:H2'	30:0:2909:G:O4'	1.82	0.80
30:0:1118:A:H3'	30:0:1118:A:C8	2.16	0.80
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.63	0.80
30:0:2637:A:H5'	37:0:8794:HOH:O	1.80	0.79
1:A:199:HIS:HD2	1:A:201:PHE:H	1.27	0.79
2:B:238:ASN:HD22	2:B:240:GLY:H	1.26	0.79
3:C:127:ARG:NH2	3:C:225:PRO:HG2	1.98	0.79
2:B:307:ARG:HG3	2:B:307:ARG:HH11	1.47	0.79
30:0:544:G:H2'	30:0:545:G:H5''	1.65	0.78
31:9:29:C:H2'	31:9:30:C:H5'	1.66	0.78
30:0:1119:G:H22	30:0:1246:A:H2	1.32	0.78
30:0:541:C:H2'	30:0:542:A:C5'	2.14	0.78
15:O:3:THR:CG2	30:0:656:G:H5'	2.12	0.78
13:M:102:GLU:OE1	13:M:164:THR:HG21	1.83	0.78
11:K:81:ARG:HB2	11:K:87:ARG:HH11	1.49	0.78
23:W:122:ARG:NH2	23:W:154:ARG:HB3	1.99	0.78
30:0:182:G:H5'	37:0:4697:HOH:O	1.83	0.78
8:H:30:LYS:H	8:H:62:HIS:HD2	1.31	0.77
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.81	0.77
30:0:1919:A:H4'	37:0:4389:HOH:O	1.85	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2896:A:H5''	37:0:5645:HOH:O	1.84	0.77
3:C:1:MET:HG2	3:C:2:GLN:H	1.49	0.77
30:0:1206:U:H6	30:0:1206:U:H5'	1.50	0.76
30:0:1165:G:H4'	30:0:1174:A:O2'	1.86	0.76
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.67	0.76
30:0:1080:C:H4'	30:0:1081:A:OP1	1.84	0.76
22:V:1:THR:HG23	22:V:2:VAL:H	1.50	0.76
23:W:4:LEU:HD22	23:W:52:VAL:HG21	1.68	0.76
30:0:2004:U:H4'	37:0:4853:HOH:O	1.85	0.76
30:0:542:A:H5'	30:0:542:A:C8	2.18	0.76
14:N:144:GLY:O	14:N:147:ILE:HG22	1.85	0.76
30:0:603:A:H5''	30:0:604:G:OP1	1.86	0.75
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.66	0.75
30:0:2769:C:H2'	30:0:2770:G:H5'	1.68	0.75
30:0:2506:A:HO2'	30:0:2507:G:H8	0.81	0.75
30:0:1701:A:H4'	30:0:1702:U:C5'	2.16	0.75
10:J:19:MET:HE3	10:J:132:LEU:HD21	1.69	0.75
14:N:37:ARG:NH1	31:9:6:C:C5'	2.48	0.75
2:B:321:PRO:HA	37:B:8656:HOH:O	1.85	0.75
30:0:877:G:H5'	30:0:878:G:OP1	1.86	0.74
29:3:65:THR:HG22	29:3:67:LEU:HG	1.69	0.74
30:0:2635:A:O2'	30:0:2636:C:H5'	1.88	0.74
30:0:559:U:H5'	30:0:559:U:H6	1.53	0.74
30:0:870:G:C2'	30:0:871:G:H5''	2.18	0.74
4:D:99:ASP:HB3	4:D:103:ASN:H	1.53	0.74
31:9:39:U:H1'	31:9:44:A:N6	2.03	0.74
2:B:86:ALA:HA	37:B:8581:HOH:O	1.87	0.73
30:0:1603:A:H5'	30:0:1605:G:O4'	1.88	0.73
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.69	0.73
37:B:8634:HOH:O	30:0:2672:C:H1'	1.87	0.73
30:0:2323:G:H5''	37:0:4318:HOH:O	1.88	0.73
5:E:143:GLN:NE2	30:0:2779:G:H21	1.86	0.73
30:0:558:C:O2'	30:0:559:U:H5''	1.89	0.73
14:N:113:SER:HB2	37:N:8558:HOH:O	1.87	0.73
30:0:1497:G:H4'	30:0:1627:G:O2'	1.88	0.72
9:I:73:LEU:HD12	9:I:107:LYS:HZ2	1.53	0.72
30:0:1666:C:H2'	30:0:1667:A:H5'	1.70	0.72
1:A:35:GLY:O	1:A:36:ASP:HB3	1.90	0.72
30:0:1130:U:H5'	37:0:7223:HOH:O	1.89	0.72
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.71	0.72
30:0:2505:G:O2'	30:0:2506:A:H5'	1.89	0.72
3:C:174:ILE:CD1	30:0:338:C:H4'	2.19	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:O:3:THR:HG22	30:0:656:G:C5'	2.18	0.72
30:0:2507:G:H2'	30:0:2510:C:H42	1.55	0.72
30:0:1180:U:H1'	37:0:9766:HOH:O	1.90	0.71
4:D:25:MET:HE3	4:D:37:ALA:HB1	1.71	0.71
14:N:23:ARG:HD3	37:N:8546:HOH:O	1.90	0.71
9:I:127:CYS:HB3	9:I:132:VAL:HB	1.71	0.71
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.71	0.71
11:K:10:GLN:H	11:K:10:GLN:NE2	1.80	0.71
30:0:2756:U:H3	30:0:2896:A:H2	1.34	0.71
1:A:211:LYS:HB2	37:A:8612:HOH:O	1.91	0.71
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.71	0.71
21:U:9:CYS:HA	21:U:52:THR:HG23	1.73	0.71
26:Z:34:SER:OG	30:0:797:A:H4'	1.90	0.71
1:A:51:ARG:HB2	37:A:8599:HOH:O	1.91	0.71
30:0:1667:A:C8	30:0:1667:A:H5'	2.25	0.70
30:0:299:U:H5'	37:0:6885:HOH:O	1.91	0.70
28:2:41:HIS:N	28:2:45:ASN:HD22	1.88	0.70
30:0:1835:U:C5	30:0:1840:A:N7	2.56	0.70
30:0:1634:G:H3'	37:0:3430:HOH:O	1.90	0.70
30:0:1166:A:H61	30:0:1180:U:H3	1.38	0.70
30:0:1183:C:N4	30:0:1184:C:H41	1.90	0.70
30:0:558:C:C2'	30:0:559:U:H5''	2.21	0.70
31:9:14:G:H5'	31:9:14:G:C8	2.26	0.70
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.73	0.70
16:P:59:ARG:NH2	16:P:66:GLN:HE22	1.90	0.70
9:I:97:VAL:HG12	9:I:101:LYS:HE3	1.74	0.70
13:M:171:ARG:CD	30:0:156:C:H5''	2.19	0.69
30:0:2426:G:H1'	37:0:5638:HOH:O	1.92	0.69
30:0:2533:C:H5'	30:0:2533:C:H6	1.57	0.69
28:2:39:ARG:HG2	37:2:3143:HOH:O	1.92	0.69
13:M:178:LYS:HB2	37:0:6424:HOH:O	1.90	0.69
18:R:128:ARG:NH2	30:0:2054:A:N3	2.40	0.69
1:A:223:ARG:NH1	30:0:2270:G:H4'	2.07	0.69
2:B:41:PHE:CD1	2:B:79:MET:HE2	2.27	0.69
30:0:281:U:H2'	30:0:282:C:O4'	1.91	0.69
30:0:951:A:C2'	30:0:952:G:H5'	2.22	0.69
1:A:191:GLY:HA2	1:A:194:MET:CE	2.22	0.69
10:J:76:ASP:HA	37:J:5907:HOH:O	1.93	0.69
30:0:1603:A:H5''	30:0:1605:G:H5'	1.75	0.69
30:0:536:A:H3'	37:0:4588:HOH:O	1.92	0.69
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.74	0.69
30:0:558:C:H2'	30:0:559:U:C5'	2.23	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1058:A:H2'	30:0:1060:C:H5''	1.74	0.68
30:0:1632:A:H2'	30:0:1633:C:H5'	1.74	0.68
30:0:2812:A:C2	30:0:2814:A:N6	2.59	0.68
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.74	0.68
30:0:2756:U:N3	30:0:2896:A:C2	2.59	0.68
2:B:211:THR:HG21	37:0:7003:HOH:O	1.92	0.68
30:0:2769:C:H2'	30:0:2770:G:C5'	2.23	0.68
30:0:2787:C:H5	37:0:4174:HOH:O	1.76	0.68
30:0:1166:A:H1'	30:0:1192:A:C2	2.28	0.68
30:0:1730:G:C5'	30:0:1731:C:C6	2.77	0.68
28:2:41:HIS:H	28:2:45:ASN:ND2	1.89	0.68
3:C:76:ARG:HG2	3:C:78:ARG:NH1	2.08	0.68
1:A:191:GLY:HA2	1:A:194:MET:HE3	1.76	0.68
30:0:1766:U:O2	30:0:1778:A:H5'	1.94	0.68
30:0:1701:A:H5'	37:0:5830:HOH:O	1.93	0.67
30:0:1730:G:H5'	30:0:1731:C:H5	1.58	0.67
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.76	0.67
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.76	0.67
25:Y:169:ARG:HD2	30:0:1328:A:OP1	1.94	0.67
30:0:1189:A:H3'	37:0:7231:HOH:O	1.93	0.67
30:0:1878:G:H1'	37:0:5667:HOH:O	1.94	0.67
19:S:57:THR:HG22	19:S:59:ASP:H	1.58	0.67
30:0:1441:G:O2'	30:0:1442:A:H5'	1.94	0.67
30:0:272:A:H5'	30:0:273:G:OP2	1.94	0.67
18:R:98:ASN:HD21	30:0:500:G:H21	1.41	0.67
23:W:125:HIS:HD2	23:W:127:GLY:H	1.42	0.67
3:C:140:VAL:HB	37:C:8449:HOH:O	1.93	0.67
30:0:2064:U:H5'	30:0:2652:U:O3'	1.94	0.67
30:0:1377:C:H6	30:0:1377:C:H5'	1.60	0.67
30:0:1187:U:O2'	30:0:1189:A:H2	1.77	0.67
10:J:74:ARG:HB3	10:J:74:ARG:HH11	1.58	0.67
30:0:1819:G:H2'	30:0:1820:G:H4'	1.76	0.67
29:3:48:ASN:HD21	30:0:2468:A:H61	1.41	0.67
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.10	0.67
11:K:81:ARG:HB2	11:K:87:ARG:NH1	2.09	0.66
30:0:2827:A:H2'	30:0:2828:G:O4'	1.95	0.66
30:0:31:C:H4'	37:0:6974:HOH:O	1.94	0.66
30:0:856:G:H2'	37:0:4975:HOH:O	1.94	0.66
1:A:199:HIS:CD2	1:A:201:PHE:H	2.11	0.66
23:W:141:HIS:HB2	23:W:146:ILE:HG12	1.78	0.66
6:F:91:VAL:HG12	6:F:92:GLY:H	1.60	0.66
22:V:12:THR:HG22	22:V:15:GLU:HG3	1.78	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:U:56:ARG:NH2	30:0:2890:A:H1'	2.11	0.66
30:0:545:G:C8	30:0:545:G:H5'	2.27	0.66
23:W:21:LEU:HD22	23:W:26:ILE:HD11	1.77	0.66
10:J:52:GLN:HE22	30:0:1119:G:H8	1.42	0.66
30:0:711:G:H1'	37:0:6640:HOH:O	1.95	0.66
30:0:1205:U:H2'	30:0:1206:U:C5'	2.25	0.66
3:C:115:LEU:HD13	3:C:223:LEU:HD21	1.77	0.66
3:C:139:VAL:HG13	37:C:8446:HOH:O	1.95	0.66
30:0:1209:C:H2'	30:0:1210:G:H8	1.61	0.66
30:0:2783:A:H3'	37:0:4774:HOH:O	1.95	0.66
3:C:236:THR:HG21	37:C:8373:HOH:O	1.96	0.66
30:0:1185:U:H2'	30:0:1186:C:C6	2.31	0.66
30:0:544:G:C2'	30:0:545:G:H5''	2.24	0.66
3:C:236:THR:HG22	3:C:239:ALA:N	2.08	0.66
4:D:135:VAL:HG22	4:D:136:ARG:H	1.60	0.66
30:0:1205:U:H2'	30:0:1206:U:H5''	1.76	0.65
22:V:1:THR:HB	30:0:93:C:H5''	1.76	0.65
12:L:30:ARG:HD3	30:0:164:G:H4'	1.78	0.65
23:W:6:GLN:HB2	23:W:26:ILE:CD1	2.26	0.65
30:0:2414:A:H2'	30:0:2415:A:C8	2.31	0.65
30:0:856:G:C8	37:0:4975:HOH:O	2.48	0.65
14:N:49:THR:HG22	14:N:56:ASP:HB2	1.78	0.65
23:W:122:ARG:HH11	23:W:122:ARG:CG	2.08	0.65
23:W:21:LEU:HD22	23:W:26:ILE:CD1	2.26	0.65
31:9:64:C:H2'	31:9:65:A:H5'	1.79	0.65
30:0:1741:U:H5'	30:0:1742:A:OP1	1.96	0.65
14:N:5:ARG:NH1	30:0:962:C:H1'	2.10	0.65
31:9:54:A:O2'	31:9:55:U:H5'	1.96	0.65
3:C:5:ILE:HD11	3:C:16:VAL:HG23	1.78	0.65
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.78	0.65
18:R:29:LYS:HE2	30:0:524:A:C5'	2.26	0.65
3:C:5:ILE:HD11	3:C:16:VAL:CG2	2.27	0.65
6:F:96:ALA:HA	37:F:3111:HOH:O	1.97	0.65
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.42	0.65
23:W:88:THR:HG23	23:W:110:GLN:NE2	2.11	0.65
30:0:1878:G:O2'	30:0:1879:U:C6	2.48	0.65
2:B:185:GLY:HA2	37:B:8633:HOH:O	1.97	0.65
16:P:117:SER:HB3	30:0:1593:C:OP1	1.98	0.64
30:0:2608:C:H2'	37:0:3110:HOH:O	1.96	0.64
4:D:54:ALA:HB2	4:D:69:ILE:HD12	1.78	0.64
5:E:97:VAL:HG12	37:E:4191:HOH:O	1.97	0.64
12:L:133:VAL:HA	37:L:8562:HOH:O	1.95	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:L:18:HIS:HD2	30:0:902:G:N7	1.95	0.64
22:V:42:ASN:HB3	37:V:7247:HOH:O	1.97	0.64
30:0:1632:A:C2'	30:0:1633:C:H5'	2.28	0.64
27:1:16:HIS:HD2	30:0:470:U:O2'	1.81	0.64
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.09	0.64
30:0:31:C:H2'	37:0:7238:HOH:O	1.97	0.64
30:0:1666:C:C2'	30:0:1667:A:H5''	2.27	0.64
8:H:49:GLN:HE21	8:H:140:TYR:HE2	1.46	0.64
30:0:1666:C:H2'	30:0:1667:A:C5'	2.27	0.64
14:N:4:PRO:HG3	31:9:69:U:OP1	1.98	0.63
9:I:73:LEU:HD12	9:I:107:LYS:NZ	2.12	0.63
30:0:1641:A:H2'	30:0:1642:A:H5'	1.79	0.63
2:B:41:PHE:HB3	2:B:190:MET:HE3	1.80	0.63
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.34	0.63
19:S:51:GLN:HE21	19:S:53:ASN:HD21	1.45	0.63
30:0:2649:A:H5'	30:0:2649:A:H8	1.63	0.63
30:0:2717:C:H2'	30:0:2718:C:C5'	2.24	0.63
11:K:32:ILE:HD11	11:K:56:SER:HB3	1.78	0.63
13:M:99:ARG:HH21	13:M:170:ASN:HD22	1.45	0.63
30:0:1330:A:H2	37:0:4223:HOH:O	1.81	0.63
30:0:2769:C:O2'	30:0:2770:G:H5'	1.97	0.63
5:E:139:GLU:OE2	30:0:2781:U:H1'	1.99	0.63
25:Y:141:THR:HG23	37:Y:8586:HOH:O	1.99	0.63
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.81	0.63
25:Y:187:VAL:HG12	25:Y:205:ILE:HA	1.81	0.63
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.81	0.63
30:0:281:U:O2'	30:0:282:C:H5'	1.99	0.63
30:0:558:C:H2'	30:0:559:U:H5'	1.81	0.63
30:0:506:G:H22	30:0:509:A:H5'	1.64	0.62
18:R:39:THR:HG23	18:R:107:GLU:O	1.98	0.62
20:T:9:LYS:HB2	37:0:6974:HOH:O	1.98	0.62
27:1:20:ARG:HG2	30:0:111:C:O2'	1.99	0.62
27:1:25:LYS:HE2	37:2:7213:HOH:O	1.98	0.62
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.34	0.62
30:0:2832:C:H5	37:0:6762:HOH:O	1.82	0.62
25:Y:185:VAL:HG12	37:Y:8567:HOH:O	1.99	0.62
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.64	0.62
9:I:120:ALA:O	9:I:124:VAL:HG23	1.99	0.62
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.80	0.62
1:A:192:VAL:HB	37:A:8587:HOH:O	1.99	0.62
2:B:7:ARG:HG2	2:B:7:ARG:HH11	1.65	0.62
30:0:138:U:H5''	30:0:139:C:OP2	1.99	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1666:C:C2'	30:0:1667:A:C5'	2.78	0.62
30:0:2717:C:O2'	30:0:2718:C:H5''	1.99	0.62
30:0:2768:A:H2'	30:0:2769:C:O4'	1.99	0.62
2:B:195:ARG:HG2	2:B:323:LEU:HD22	1.81	0.62
4:D:57:THR:HG23	4:D:63:ILE:HA	1.82	0.62
5:E:3:VAL:HG22	5:E:49:ILE:HB	1.80	0.62
10:J:47:THR:HB	37:0:4375:HOH:O	2.00	0.62
30:0:1730:G:H5''	30:0:1731:C:H6	1.65	0.62
2:B:145:HIS:HD2	2:B:146:THR:O	1.83	0.62
4:D:99:ASP:HA	37:0:5842:HOH:O	2.00	0.62
30:0:1118:A:C8	30:0:1118:A:C3'	2.79	0.61
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.82	0.61
29:3:73:GLU:HB3	37:3:8559:HOH:O	2.00	0.61
31:9:29:C:C2'	31:9:30:C:H5'	2.30	0.61
31:9:2:U:OP2	31:9:3:A:H5'	2.00	0.61
30:0:1130:U:H2'	30:0:1131:G:O4'	2.00	0.61
30:0:396:U:O2'	30:0:418:C:H4'	2.00	0.61
2:B:179:LEU:O	2:B:183:GLU:HG2	1.99	0.61
2:B:211:THR:HG23	30:0:2840:A:OP1	2.00	0.61
6:F:91:VAL:HG12	6:F:92:GLY:N	2.14	0.61
12:L:136:ALA:HB3	37:L:8562:HOH:O	1.99	0.61
13:M:80:GLY:O	13:M:81:ARG:HD3	1.99	0.61
30:0:1778:A:H2'	30:0:1779:A:H5'	1.82	0.61
30:0:2346:C:O5'	30:0:2346:C:H6	1.83	0.61
30:0:2533:C:C6	30:0:2533:C:H5'	2.34	0.61
3:C:236:THR:H	3:C:239:ALA:HB3	1.65	0.61
18:R:39:THR:HG22	18:R:42:GLU:H	1.65	0.61
30:0:1189:A:H1'	30:0:1209:C:H1'	1.83	0.61
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.83	0.61
3:C:96:LYS:NZ	30:0:1351:G:OP1	2.33	0.61
2:B:16:ARG:NH1	37:B:8617:HOH:O	2.34	0.61
30:0:1201:C:H2'	30:0:1202:A:H5'	1.82	0.61
30:0:951:A:O2'	30:0:952:G:H5'	2.01	0.61
30:0:960:G:H2'	30:0:960:G:N3	2.16	0.61
30:0:1189:A:H1'	30:0:1209:C:C1'	2.30	0.61
30:0:2502:C:C2'	30:0:2503:A:H5'	2.30	0.61
15:O:42:GLU:HB2	37:O:2176:HOH:O	2.00	0.61
31:9:13:A:O2'	31:9:14:G:H5''	2.00	0.61
26:Z:35:SER:HB3	26:Z:47:ARG:HB2	1.81	0.61
10:J:82:THR:HG23	30:0:1242:A:C5'	2.24	0.60
2:B:238:ASN:HD22	2:B:240:GLY:N	1.98	0.60
12:L:143:THR:HG22	12:L:144:ASP:N	2.16	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:163:VAL:HA	37:D:6326:HOH:O	2.02	0.60
11:K:118:ALA:HA	11:K:125:ALA:HB2	1.81	0.60
23:W:21:LEU:HB3	23:W:26:ILE:HG12	1.82	0.60
8:H:6:ALA:HA	8:H:61:ARG:HH12	1.67	0.60
13:M:61:ILE:HG13	37:M:8617:HOH:O	1.99	0.60
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.46	0.60
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.65	0.60
30:0:2587:OMU:H2'	30:0:2589:U:H5''	1.83	0.60
12:L:4:LYS:HE2	30:0:645:U:OP2	2.01	0.60
1:A:105:VAL:CG1	1:A:154:ALA:HB1	2.31	0.60
1:A:48:ASP:HB3	37:A:8599:HOH:O	2.02	0.60
30:0:2415:A:H2'	30:0:2416:G:H5'	1.82	0.60
14:N:37:ARG:NH1	31:9:6:C:OP1	2.34	0.60
9:I:110:ASP:O	30:0:1163:G:H5'	2.02	0.60
30:0:2768:A:O2'	30:0:2769:C:H5'	2.01	0.60
30:0:1528:A:H2'	30:0:1529:G:O4'	2.01	0.60
30:0:1172:G:H5''	37:0:6809:HOH:O	2.01	0.60
30:0:1377:C:H5'	30:0:1377:C:C6	2.37	0.60
30:0:1559:A:H1'	37:0:5413:HOH:O	2.02	0.60
2:B:267:LYS:HD3	37:B:8526:HOH:O	2.01	0.60
18:R:117:HIS:HD2	30:0:20:G:H21	1.50	0.60
23:W:88:THR:HG22	23:W:89:ASP:N	2.17	0.60
25:Y:235:GLU:H	25:Y:235:GLU:CD	2.05	0.60
30:0:1205:U:C2'	30:0:1206:U:H5''	2.32	0.59
30:0:1350:U:H4'	37:0:4662:HOH:O	2.02	0.59
30:0:2670:G:O2'	30:0:2671:U:H5'	2.02	0.59
10:J:18:ILE:HD13	30:0:1244:U:OP1	2.02	0.59
30:0:2578:G:H5'	30:0:2578:G:H8	1.67	0.59
2:B:212:GLN:HB2	2:B:257:THR:CG2	2.29	0.59
25:Y:133:HIS:HD2	37:Y:8579:HOH:O	1.85	0.59
30:0:1175:G:H1'	30:0:1193:A:H2'	1.84	0.59
30:0:2488:A:H2	37:0:6826:HOH:O	1.84	0.59
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.32	0.59
31:9:49:G:O2'	31:9:50:G:H5'	2.01	0.59
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.35	0.59
23:W:4:LEU:O	23:W:32:CYS:HA	2.03	0.59
23:W:88:THR:HG22	23:W:89:ASP:H	1.67	0.59
30:0:2756:U:N3	30:0:2896:A:H2	1.98	0.59
31:9:23:U:O2'	31:9:24:U:H4'	2.02	0.59
23:W:84:VAL:HG12	37:W:6679:HOH:O	2.02	0.59
30:0:567:U:H5''	37:0:5949:HOH:O	2.01	0.59
30:0:2420:G:O2'	30:0:2421:G:H5'	2.02	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:27:ARG:NH2	30:0:657:G:OP1	2.31	0.59
10:J:107:ASN:HD21	10:J:109:TYR:HB2	1.68	0.59
23:W:139:GLY:O	23:W:141:HIS:HD2	1.85	0.59
30:0:1159:G:H1	30:0:1208:C:H42	1.50	0.59
30:0:204:A:C2'	30:0:205:U:H5'	2.32	0.59
30:0:2649:A:H5'	30:0:2649:A:C8	2.38	0.59
30:0:1120:U:H5''	30:0:1120:U:C6	2.37	0.58
9:I:112:LEU:HD11	30:0:1162:G:H1'	1.84	0.58
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.85	0.58
11:K:109:LEU:HD13	11:K:113:ILE:HD11	1.85	0.58
23:W:122:ARG:HH11	23:W:122:ARG:HG2	1.68	0.58
30:0:1182:C:H1'	30:0:1192:A:H8	1.68	0.58
30:0:1667:A:H2'	30:0:1668:U:C6	2.38	0.58
30:0:2316:G:H4'	37:0:5638:HOH:O	2.03	0.58
31:9:64:C:C2'	31:9:65:A:H5'	2.33	0.58
18:R:17:MET:SD	37:R:8542:HOH:O	2.57	0.58
31:9:75:G:H1	31:9:106:U:H3	1.51	0.58
8:H:48:VAL:HA	8:H:170:ARG:O	2.03	0.58
18:R:29:LYS:HE2	30:0:524:A:H5'	1.85	0.58
30:0:1730:G:C5'	30:0:1731:C:H6	2.16	0.58
30:0:2604:A:H5'	37:0:5339:HOH:O	2.04	0.58
20:T:52:ARG:HD2	30:0:317:A:H5''	1.84	0.58
3:C:236:THR:CG2	3:C:239:ALA:H	2.11	0.58
18:R:99:ALA:HB1	18:R:109:MET:CE	2.32	0.58
1:A:211:LYS:HB3	1:A:212:PRO:HD2	1.84	0.58
3:C:76:ARG:HD3	37:C:8366:HOH:O	2.04	0.58
5:E:100:ASP:HB2	37:E:2789:HOH:O	2.03	0.58
23:W:64:THR:O	23:W:68:THR:HG22	2.04	0.58
23:W:80:ASP:O	23:W:84:VAL:HG23	2.02	0.58
30:0:2320:U:H4'	30:0:2321:A:O4'	2.03	0.58
30:0:2718:C:H6	30:0:2718:C:H5'	1.69	0.58
4:D:146:LYS:NZ	14:N:107:ASN:HD21	2.01	0.58
25:Y:134:HIS:HE1	30:0:538:C:OP2	1.87	0.58
14:N:80:SER:HB2	37:N:8535:HOH:O	2.02	0.58
19:S:51:GLN:NE2	19:S:53:ASN:HD21	2.02	0.58
30:0:1118:A:H8	30:0:1119:G:H5''	1.67	0.58
31:9:92:G:H2'	31:9:93:A:C8	2.39	0.58
12:L:148:GLU:HA	37:L:8561:HOH:O	2.04	0.58
14:N:43:VAL:HG13	14:N:118:ILE:HD11	1.84	0.58
30:0:2064:U:H4'	30:0:2653:A:OP1	2.04	0.57
29:3:60:LYS:HG3	37:0:7104:HOH:O	2.04	0.57
31:9:20:G:O2'	31:9:21:G:H5'	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:107:ASN:ND2	10:J:109:TYR:H	2.01	0.57
30:0:2878:U:H2'	30:0:2879:A:O4'	2.04	0.57
31:9:35:C:H5''	37:9:8455:HOH:O	2.04	0.57
3:C:78:ARG:HG3	3:C:78:ARG:HH11	1.67	0.57
16:P:10:ALA:HA	16:P:13:VAL:HG12	1.86	0.57
18:R:29:LYS:HE2	30:0:524:A:H5''	1.87	0.57
3:C:76:ARG:HG2	3:C:78:ARG:HH12	1.68	0.57
4:D:103:ASN:ND2	4:D:134:LEU:H	2.02	0.57
30:0:1119:G:N2	30:0:1246:A:H2	1.95	0.57
31:9:28:U:H2'	31:9:29:C:C6	2.39	0.57
2:B:162:MET:HE2	2:B:310:ARG:HD3	1.87	0.57
19:S:57:THR:HG22	19:S:59:ASP:N	2.18	0.57
30:0:1819:G:H5'	37:0:4250:HOH:O	2.05	0.57
30:0:1972:U:H2'	30:0:1973:A:H5''	1.85	0.57
23:W:38:THR:HG22	37:W:3580:HOH:O	2.03	0.57
30:0:1679:C:H5'	37:0:8846:HOH:O	2.04	0.57
30:0:1701:A:H5''	30:0:1702:U:H3'	1.86	0.57
30:0:1834:C:H2'	30:0:1840:A:N6	2.18	0.57
30:0:432:G:O2'	30:0:433:C:H5'	2.05	0.57
30:0:1289:C:O2'	30:0:1290:G:H5'	2.05	0.57
12:L:6:ARG:HD3	30:0:1299:G:O6	2.04	0.57
30:0:2064:U:H5'	30:0:2652:U:H4'	1.85	0.57
30:0:1730:G:C5'	30:0:1731:C:C5	2.87	0.57
30:0:558:C:C2'	30:0:559:U:C5'	2.82	0.57
3:C:115:LEU:HD21	3:C:243:VAL:HG13	1.87	0.57
23:W:125:HIS:CD2	23:W:127:GLY:H	2.23	0.57
30:0:558:C:H2'	30:0:559:U:H5''	1.86	0.56
30:0:681:G:N3	30:0:681:G:H5'	2.20	0.56
1:A:121:ALA:O	1:A:124:VAL:HG22	2.04	0.56
6:F:50:VAL:CG1	6:F:60:VAL:HG11	2.35	0.56
13:M:182:LYS:HE2	30:0:392:U:O2'	2.05	0.56
13:M:24:GLN:NE2	13:M:27:ARG:HH11	2.03	0.56
25:Y:144:ARG:NH1	37:Y:8573:HOH:O	2.37	0.56
30:0:1181:A:C2'	30:0:1182:C:H5'	2.36	0.56
30:0:2467:A:H1'	37:0:4272:HOH:O	2.04	0.56
30:0:282:C:O2'	30:0:283:U:C5'	2.51	0.56
27:1:42:SER:HB2	37:1:8409:HOH:O	2.05	0.56
25:Y:204:ARG:HH22	30:0:553:G:P	2.28	0.56
30:0:703:G:O2'	30:0:704:C:H5'	2.06	0.56
13:M:24:GLN:HE21	13:M:27:ARG:HH11	1.53	0.56
14:N:7:LYS:HE3	17:Q:21:ARG:O	2.05	0.56
21:U:14:GLU:O	21:U:17:THR:HB	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1878:G:O2'	30:0:1879:U:H6	1.89	0.56
30:0:2435:U:H1'	37:0:4978:HOH:O	2.06	0.56
1:A:192:VAL:HG13	37:A:8553:HOH:O	2.05	0.56
10:J:103:VAL:HG12	37:J:5907:HOH:O	2.04	0.56
19:S:43:GLU:HB3	37:S:7106:HOH:O	2.05	0.56
30:0:2488:A:H61	30:0:2534:C:H42	1.53	0.56
30:0:2851:G:C2'	30:0:2852:A:H5'	2.35	0.56
3:C:1:MET:HG2	3:C:2:GLN:N	2.20	0.56
3:C:162:VAL:HG22	3:C:232:LEU:HD21	1.86	0.56
30:0:2300:A:H4'	30:0:2301:A:O5'	2.06	0.56
16:P:143:ALA:HA	37:P:184:HOH:O	2.03	0.56
30:0:1118:A:H62	30:0:1244:U:H3	1.54	0.56
6:F:38:LYS:HE3	30:0:244:C:OP2	2.06	0.56
30:0:282:C:H1'	30:0:368:C:H42	1.70	0.56
1:A:153:ARG:HH11	1:A:153:ARG:HB2	1.71	0.56
10:J:107:ASN:HD22	10:J:109:TYR:H	1.53	0.56
30:0:1278:A:H4'	30:0:1279:U:C4	2.41	0.56
2:B:139:ASP:HB2	2:B:165:ARG:HE	1.70	0.56
11:K:34:VAL:CG2	11:K:47:ALA:HB2	2.36	0.56
22:V:39:ALA:N	22:V:40:PRO:HD2	2.21	0.56
30:0:1477:C:H5'	30:0:1868:G:C5'	2.35	0.56
30:0:899:C:H5'	37:0:9733:HOH:O	2.05	0.56
13:M:95:LYS:HE2	30:0:157:G:H4'	1.88	0.56
30:0:2251:G:H2'	30:0:2252:A:C8	2.41	0.56
27:1:8:GLN:HE22	27:1:11:LYS:NZ	2.04	0.56
1:A:223:ARG:HG3	37:A:8595:HOH:O	2.05	0.56
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.71	0.56
11:K:55:VAL:HG12	11:K:56:SER:N	2.21	0.56
14:N:37:ARG:NE	37:N:8533:HOH:O	2.39	0.56
30:0:2502:C:H2'	30:0:2503:A:H5'	1.87	0.56
4:D:50:VAL:HG22	31:9:41:C:O4'	2.05	0.56
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.70	0.56
30:0:1120:U:H5'	30:0:1121:G:OP2	2.05	0.55
30:0:1250:C:O2'	30:0:1251:C:H5'	2.05	0.55
30:0:2825:C:H4'	30:0:2826:G:O5'	2.06	0.55
30:0:396:U:H1'	37:0:7180:HOH:O	2.06	0.55
31:9:91:C:H2'	31:9:92:G:O4'	2.05	0.55
20:T:53:GLY:HA3	37:T:6384:HOH:O	2.05	0.55
30:0:2361:A:H5''	37:0:8523:HOH:O	2.07	0.55
37:N:8545:HOH:O	31:9:49:G:H5''	2.05	0.55
1:A:96:LEU:HD22	1:A:128:LEU:HD13	1.87	0.55
5:E:68:HIS:O	5:E:72:MET:HG3	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:81:GLU:HG2	5:E:134:SER:HB3	1.86	0.55
11:K:98:VAL:CG1	11:K:102:GLU:HA	2.35	0.55
16:P:120:ARG:HD2	30:0:1594:C:OP2	2.07	0.55
21:U:37:GLU:HB3	37:U:408:HOH:O	2.06	0.55
4:D:25:MET:CE	4:D:37:ALA:HB1	2.36	0.55
14:N:110:THR:HB	14:N:113:SER:OG	2.06	0.55
14:N:141:ARG:HH21	31:9:48:C:H4'	1.71	0.55
30:0:1783:A:O2'	30:0:1784:U:H5'	2.06	0.55
30:0:88:G:H5'	30:0:88:G:H8	1.72	0.55
23:W:115:THR:HG23	37:W:5420:HOH:O	2.06	0.55
23:W:21:LEU:HD21	23:W:48:VAL:CG1	2.36	0.55
30:0:204:A:H2'	30:0:205:U:H5'	1.88	0.55
11:K:74:VAL:HG12	11:K:75:ARG:HG3	1.87	0.55
13:M:188:ARG:HD3	30:0:155:C:OP2	2.06	0.55
18:R:25:PHE:CE2	18:R:29:LYS:HE3	2.41	0.55
30:0:1636:G:O2'	30:0:1637:A:H5'	2.07	0.55
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.42	0.55
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.07	0.55
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.87	0.55
23:W:122:ARG:HG3	23:W:152:ALA:O	2.06	0.55
5:E:91:PHE:CE1	30:0:2694:A:H4'	2.41	0.55
22:V:39:ALA:C	22:V:41:GLU:H	2.09	0.55
30:0:1595:G:O2'	30:0:1596:U:H5'	2.07	0.55
27:1:16:HIS:HE1	30:0:775:G:OP1	1.90	0.55
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.88	0.55
2:B:17:LYS:O	2:B:260:HIS:HD2	1.90	0.55
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.36	0.55
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.89	0.55
30:0:1135:G:H5'	37:0:5475:HOH:O	2.05	0.54
30:0:1165:G:O2'	30:0:1174:A:H1'	2.07	0.54
30:0:661:G:C5	30:0:686:A:C2	2.95	0.54
13:M:84:LYS:HE2	37:M:8571:HOH:O	2.06	0.54
14:N:11:ARG:HG3	14:N:14:ARG:NH1	2.22	0.54
14:N:41:LYS:HD3	37:9:8439:HOH:O	2.08	0.54
30:0:1972:U:H2'	30:0:1973:A:C5'	2.37	0.54
30:0:2467:A:O2'	30:0:2468:A:H2'	2.06	0.54
10:J:70:PHE:HE1	30:0:2676:C:H4'	1.72	0.54
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.43	0.54
30:0:1181:A:H2'	30:0:1182:C:H5'	1.89	0.54
30:0:2419:U:H5''	30:0:2420:G:H5'	1.89	0.54
30:0:485:A:N3	30:0:487:G:H5''	2.22	0.54
2:B:125:GLU:O	2:B:129:ARG:HG3	2.07	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1158:G:O2'	30:0:1159:G:H5'	2.08	0.54
30:0:2712:G:H5'	37:0:4763:HOH:O	2.07	0.54
3:C:79:ARG:O	3:C:87:ARG:HG2	2.08	0.54
9:I:100:VAL:HG11	9:I:124:VAL:HG22	1.89	0.54
11:K:29:LEU:HB3	11:K:55:VAL:CG1	2.28	0.54
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.88	0.54
18:R:17:MET:HE1	37:0:3769:HOH:O	2.06	0.54
9:I:69:PRO:HA	30:0:1164:U:OP1	2.08	0.54
30:0:1299:G:H5'	37:0:3611:HOH:O	2.06	0.54
30:0:1926:G:H2'	30:0:1927:A:C8	2.43	0.54
30:0:2524:G:H21	30:0:2526:C:N4	2.05	0.54
30:0:343:C:O2'	30:0:344:C:H5'	2.06	0.54
31:9:76:G:C3'	31:9:77:A:H5''	2.28	0.54
2:B:18:ARG:HG3	2:B:256:GLN:HG3	1.89	0.54
2:B:254:GLN:HG3	37:0:9223:HOH:O	2.08	0.54
30:0:1615:A:H5'	37:0:3722:HOH:O	2.06	0.54
30:0:200:C:H2'	37:0:9976:HOH:O	2.08	0.54
3:C:115:LEU:O	3:C:118:THR:HB	2.08	0.54
4:D:159:PRO:O	4:D:163:VAL:HG23	2.07	0.54
25:Y:187:VAL:HG22	25:Y:192:ASP:HB2	1.89	0.54
30:0:1279:U:O2	30:0:1279:U:H2'	2.06	0.54
30:0:644:G:N3	30:0:644:G:H5'	2.22	0.54
4:D:23:VAL:HG21	4:D:45:THR:HG21	1.88	0.54
11:K:82:ARG:NH2	11:K:115:ARG:HG2	2.23	0.54
30:0:1268:C:O2'	30:0:1269:G:H5'	2.07	0.54
30:0:1973:A:H5'	30:0:1973:A:C8	2.35	0.54
30:0:2638:G:H5'	37:0:4469:HOH:O	2.08	0.54
24:X:43:VAL:HG12	24:X:44:ASP:N	2.23	0.54
30:0:1972:U:C2'	30:0:1973:A:H5''	2.37	0.54
30:0:280:C:H2'	30:0:281:U:O4'	2.08	0.54
2:B:51:VAL:CG2	2:B:327:VAL:HG13	2.38	0.54
4:D:54:ALA:CB	4:D:69:ILE:HD12	2.38	0.54
12:L:80:ASP:HB2	12:L:90:ARG:O	2.08	0.54
17:Q:95:GLU:HA	30:0:949:U:H4'	1.89	0.54
9:I:87:PRO:C	9:I:89:GLU:H	2.10	0.53
2:B:336:GLN:O	30:0:2862:G:H4'	2.07	0.53
24:X:25:ARG:HD2	37:X:3861:HOH:O	2.07	0.53
3:C:184:ARG:HD2	30:0:1306:U:OP1	2.08	0.53
14:N:160:SER:HB3	31:9:51:A:H5'	1.89	0.53
14:N:4:PRO:HD2	37:0:6319:HOH:O	2.08	0.53
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.89	0.53
9:I:113:SER:HB2	9:I:118:ASN:HB2	1.89	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:M:169:ARG:HD2	37:M:8587:HOH:O	2.08	0.53
30:0:1730:G:H5''	30:0:1731:C:C6	2.41	0.53
30:0:2001:G:O2'	30:0:2002:C:H5'	2.08	0.53
30:0:95:A:H5''	30:0:97:G:O4'	2.08	0.53
1:A:36:ASP:O	1:A:38:ILE:N	2.34	0.53
5:E:11:VAL:HG12	5:E:12:ASP:N	2.23	0.53
20:T:1:SER:HB2	30:0:447:A:OP2	2.08	0.53
2:B:329:TYR:CE2	21:U:15:PRO:HG2	2.44	0.53
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.89	0.53
30:0:814:G:H4'	37:0:9664:HOH:O	2.08	0.53
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.48	0.53
1:A:88:ILE:HD13	1:A:100:PRO:HD3	1.90	0.53
8:H:32:ALA:HB3	8:H:69:ARG:HH12	1.73	0.53
1:A:105:VAL:HG11	1:A:154:ALA:HB1	1.90	0.53
21:U:39:ASN:ND2	21:U:44:ARG:HH11	2.06	0.53
30:0:1116:U:O2'	30:0:1118:A:C2	2.40	0.53
30:0:172:U:H5'	37:0:3697:HOH:O	2.09	0.53
31:9:24:U:H3'	31:9:25:G:H5'	1.90	0.53
1:A:97:ALA:HB2	1:A:150:PRO:HB2	1.91	0.53
2:B:51:VAL:HG23	2:B:329:TYR:O	2.09	0.53
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.43	0.53
5:E:69:ILE:HA	5:E:72:MET:HE3	1.90	0.53
6:F:101:ALA:HA	37:F:5413:HOH:O	2.09	0.53
13:M:81:ARG:HG3	13:M:85:ARG:HB2	1.91	0.53
16:P:73:HIS:HE1	30:0:1789:G:O6	1.91	0.52
30:0:2563:U:H2'	30:0:2565:C:O5'	2.08	0.52
13:M:58:GLN:NE2	30:0:259:G:H21	2.08	0.52
31:9:107:C:H5	37:9:8435:HOH:O	1.91	0.52
30:0:1189:A:H1'	30:0:1209:C:O4'	2.09	0.52
30:0:1525:G:H5'	30:0:1526:A:OP2	2.09	0.52
29:3:17:HIS:O	29:3:18:GLN:HG3	2.10	0.52
2:B:307:ARG:HG3	2:B:307:ARG:NH1	2.20	0.52
6:F:58:GLU:HA	6:F:61:MET:HE2	1.90	0.52
14:N:163:PHE:HZ	14:N:171:HIS:HD1	1.55	0.52
22:V:57:LYS:HA	22:V:60:GLN:HE21	1.74	0.52
30:0:2866:U:H4'	30:0:2867:G:H5'	1.90	0.52
6:F:39:SER:HB3	6:F:45:ALA:HB2	1.91	0.52
7:G:64:ASN:N	7:G:64:ASN:HD22	2.06	0.52
14:N:12:ARG:HD3	14:N:18:THR:OG1	2.09	0.52
16:P:83:LYS:HG2	30:0:793:A:H5''	1.92	0.52
17:Q:40:HIS:HE1	30:0:949:U:O2'	1.92	0.52
16:P:41:ARG:HH22	30:0:1500:U:P	2.32	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2256:G:H2'	30:0:2257:G:C5'	2.39	0.52
1:A:81:GLN:HB2	1:A:92:ASN:ND2	2.23	0.52
6:F:53:ASP:OD1	6:F:80:GLN:HB2	2.09	0.52
18:R:18:LEU:HG	18:R:91:LEU:HD13	1.90	0.52
30:0:2241:C:O2'	30:0:2242:U:H5'	2.09	0.52
30:0:794:U:H3	30:0:819:A:H61	1.57	0.52
4:D:135:VAL:HG22	4:D:136:ARG:N	2.24	0.52
30:0:1211:G:O2'	30:0:1212:C:H5'	2.10	0.52
1:A:123:GLY:HA3	1:A:162:GLY:HA2	1.92	0.52
3:C:246:ARG:NH1	37:C:8369:HOH:O	2.42	0.52
13:M:163:LEU:HD21	30:0:188:C:H5''	1.91	0.52
17:Q:25:PRO:HB2	37:Q:4350:HOH:O	2.10	0.52
23:W:151:GLU:O	23:W:154:ARG:HB2	2.09	0.52
1:A:95:PRO:HG2	1:A:98:GLU:HG2	1.91	0.52
15:O:47:ARG:HG3	15:O:47:ARG:HH11	1.75	0.52
5:E:69:ILE:HA	5:E:72:MET:CE	2.40	0.52
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.92	0.52
23:W:130:HIS:O	23:W:136:GLY:HA3	2.10	0.52
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.10	0.52
30:0:319:A:H4'	30:0:338:C:C4	2.45	0.52
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.10	0.52
30:0:65:C:O2'	30:0:66:G:H5'	2.09	0.52
30:0:820:G:O2'	30:0:856:G:H4'	2.10	0.52
14:N:11:ARG:NH1	31:9:8:G:O6	2.42	0.52
20:T:1:SER:HB2	30:0:447:A:P	2.50	0.52
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.74	0.51
1:A:179:MET:HG2	1:A:186:TRP:CB	2.40	0.51
9:I:108:HIS:N	9:I:109:PRO:HD2	2.25	0.51
30:0:1118:A:C8	30:0:1119:G:H5''	2.45	0.51
30:0:1120:U:H6	30:0:1120:U:H5''	1.75	0.51
30:0:2329:C:O2'	30:0:2330:U:H5'	2.10	0.51
30:0:291:C:H2'	30:0:292:G:O4'	2.11	0.51
10:J:19:MET:HE2	10:J:132:LEU:HD11	1.92	0.51
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.91	0.51
30:0:1406:A:H4'	30:0:1407:A:H5''	1.92	0.51
30:0:2507:G:H2'	30:0:2510:C:N4	2.23	0.51
30:0:256:C:H2'	30:0:257:G:O4'	2.11	0.51
15:O:25:VAL:HG12	30:0:709:G:O2'	2.10	0.51
2:B:305:ASP:O	2:B:306:LYS:HB2	2.11	0.51
8:H:66:GLU:HA	37:H:8381:HOH:O	2.09	0.51
17:Q:11:ARG:HD3	37:Q:5620:HOH:O	2.09	0.51
19:S:51:GLN:HE21	19:S:53:ASN:ND2	2.08	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
24:X:71:ARG:HD3	37:X:2171:HOH:O	2.10	0.51
25:Y:187:VAL:HB	25:Y:203:VAL:HG22	1.91	0.51
30:0:1165:G:O2'	30:0:1174:A:C1'	2.59	0.51
30:0:1942:A:H3'	37:0:6896:HOH:O	2.11	0.51
30:0:1996:U:O2'	30:0:1997:A:H5'	2.11	0.51
30:0:2769:C:H2'	30:0:2770:G:O4'	2.11	0.51
30:0:951:A:H2'	30:0:952:G:H5'	1.92	0.51
28:2:31:ARG:NH2	37:2:7177:HOH:O	2.43	0.51
3:C:236:THR:HA	37:C:8449:HOH:O	2.10	0.51
9:I:124:VAL:O	9:I:124:VAL:HG12	2.11	0.51
30:0:2795:C:O2'	30:0:2796:U:H5'	2.09	0.51
30:0:920:C:H5'	30:0:921:G:C4	2.45	0.51
8:H:12:ILE:HG23	8:H:129:ARG:CZ	2.41	0.51
14:N:48:VAL:HG11	14:N:55:ASP:HB3	1.93	0.51
25:Y:169:ARG:HB2	30:0:1268:C:O2'	2.11	0.51
30:0:1527:A:H1'	30:0:1528:A:C8	2.45	0.51
30:0:2072:G:C6	30:0:2533:C:H1'	2.46	0.51
30:0:969:G:H1	30:0:999:C:H42	1.59	0.51
1:A:192:VAL:HG12	1:A:207:GLN:HB3	1.91	0.51
1:A:191:GLY:HA2	1:A:194:MET:HE2	1.93	0.51
19:S:10:VAL:HG11	22:V:36:ALA:HA	1.92	0.51
30:0:1342:C:O2'	30:0:1343:C:H5'	2.10	0.51
30:0:2830:U:H3'	37:0:4770:HOH:O	2.09	0.51
30:0:90:A:H2'	30:0:91:G:O4'	2.11	0.51
29:3:48:ASN:ND2	29:3:50:GLY:H	2.09	0.51
4:D:23:VAL:HG21	4:D:45:THR:CG2	2.41	0.51
30:0:2301:A:H5''	30:0:2302:A:H5'	1.91	0.51
30:0:2591:C:H2'	30:0:2592:G:O4'	2.11	0.51
30:0:848:C:H5'	37:0:6823:HOH:O	2.10	0.51
31:9:49:G:H2'	31:9:50:G:O4'	2.11	0.51
4:D:104:PHE:CE2	4:D:132:VAL:HB	2.46	0.51
4:D:84:LEU:HA	4:D:87:ALA:HB3	1.93	0.51
5:E:23:GLU:HG2	5:E:28:SER:HB3	1.93	0.51
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.41	0.51
12:L:30:ARG:HD2	37:0:8538:HOH:O	2.11	0.51
22:V:55:ARG:O	22:V:59:ILE:HG12	2.11	0.51
24:X:15:ARG:NH1	30:0:2896:A:OP1	2.44	0.51
1:A:53:ALA:HB3	37:A:8599:HOH:O	2.10	0.51
23:W:65:VAL:HA	23:W:68:THR:HG22	1.92	0.51
30:0:1180:U:H2'	30:0:1181:A:C8	2.46	0.51
30:0:2478:U:O2'	30:0:2479:A:H5'	2.10	0.51
11:K:30:LYS:O	11:K:55:VAL:HG13	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:U:33:SER:O	21:U:37:GLU:HG3	2.10	0.51
30:0:1333:U:H2'	30:0:1334:C:C6	2.46	0.50
30:0:1503:U:H2'	30:0:1504:A:O4'	2.12	0.50
30:0:2445:U:H2'	30:0:2446:G:C8	2.46	0.50
30:0:2756:U:C2	30:0:2896:A:H2	2.28	0.50
30:0:960:G:N3	30:0:960:G:C2'	2.74	0.50
31:9:56:A:C3'	31:9:57:A:H5''	2.40	0.50
3:C:214:THR:HG23	37:C:8435:HOH:O	2.10	0.50
4:D:25:MET:HE2	4:D:41:LEU:HG	1.93	0.50
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.46	0.50
30:0:2265:U:H2'	30:0:2266:A:C8	2.47	0.50
28:2:35:ARG:HB2	37:2:2691:HOH:O	2.11	0.50
2:B:264:GLU:HG2	2:B:267:LYS:CE	2.41	0.50
2:B:212:GLN:HA	30:0:1733:A:H4'	1.92	0.50
30:0:1741:U:O2'	30:0:2723:G:H4'	2.11	0.50
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.10	0.50
27:1:28:HIS:HE1	30:0:776:A:OP1	1.94	0.50
2:B:288:GLY:HA2	30:0:2898:G:H4'	1.93	0.50
7:G:16:LYS:O	7:G:20:VAL:HG23	2.12	0.50
8:H:41:LYS:HE2	8:H:45:ASP:HB3	1.93	0.50
16:P:54:LYS:HB2	30:0:1717:A:H5''	1.94	0.50
30:0:2415:A:C2'	30:0:2416:G:H5'	2.41	0.50
30:0:2472:C:O2'	30:0:2634:G:H4'	2.12	0.50
30:0:1603:A:C5'	30:0:1605:G:O4'	2.60	0.50
30:0:1921:A:C6	30:0:1922:A:C2	3.00	0.50
30:0:2842:G:H2'	30:0:2843:A:H5'	1.93	0.50
30:0:447:A:O2'	30:0:448:G:H5'	2.12	0.50
4:D:76:ARG:NE	31:9:44:A:O4'	2.45	0.50
2:B:214:PRO:HD2	37:B:8521:HOH:O	2.12	0.50
5:E:15:GLN:HG2	5:E:19:ASP:O	2.12	0.50
9:I:112:LEU:CD1	30:0:1162:G:H1'	2.41	0.50
14:N:86:LEU:HD12	14:N:125:ALA:HB2	1.94	0.50
23:W:122:ARG:NH2	37:0:4835:HOH:O	2.45	0.50
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.74	0.50
3:C:174:ILE:HD11	30:0:338:C:H4'	1.94	0.50
10:J:45:VAL:HG21	10:J:129:PHE:CD1	2.46	0.50
20:T:24:ARG:HH21	20:T:39:ASN:ND2	2.09	0.50
30:0:1342:C:C2'	30:0:1343:C:H5'	2.42	0.50
30:0:1419:U:H5'	30:0:1420:C:OP2	2.11	0.50
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.43	0.50
30:0:861:A:C8	37:0:5228:HOH:O	2.55	0.50
29:3:62:THR:HB	37:3:8549:HOH:O	2.10	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:T:38:ARG:NH1	37:T:6217:HOH:O	2.44	0.50
25:Y:187:VAL:HG23	37:Y:8567:HOH:O	2.11	0.50
30:0:2505:G:C2'	30:0:2506:A:H5'	2.41	0.50
30:0:308:U:C4	30:0:342:C:H1'	2.46	0.50
30:0:702:G:O2'	30:0:703:G:H5'	2.12	0.50
22:V:44:GLY:HA3	30:0:92:G:H4'	1.94	0.50
2:B:254:GLN:HG2	2:B:255:GLY:N	2.25	0.50
29:3:3:MET:O	29:3:90:PHE:HA	2.12	0.50
6:F:59:ILE:HD13	30:0:263:U:O4'	2.11	0.50
8:H:14:LYS:HE2	37:0:3382:HOH:O	2.11	0.50
8:H:49:GLN:HG3	8:H:140:TYR:CE2	2.47	0.50
11:K:62:PRO:HG3	11:K:65:ARG:NH2	2.26	0.50
26:Z:77:GLY:HA2	26:Z:91:GLY:O	2.12	0.50
10:J:52:GLN:NE2	30:0:1119:G:H8	2.06	0.49
1:A:3:ARG:HD3	30:0:870:G:OP2	2.11	0.49
1:A:179:MET:HA	1:A:179:MET:CE	2.42	0.49
17:Q:15:LYS:HD3	30:0:2364:A:H5''	1.93	0.49
37:R:8545:HOH:O	30:0:1370:G:H5''	2.12	0.49
30:0:2256:G:H2'	30:0:2257:G:H5'	1.95	0.49
2:B:102:THR:HG21	2:B:182:VAL:O	2.11	0.49
3:C:98:ARG:NH1	37:C:8355:HOH:O	2.44	0.49
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.94	0.49
14:N:179:LEU:HA	14:N:184:ILE:HD12	1.93	0.49
23:W:13:MET:CE	23:W:17:ILE:HG22	2.42	0.49
30:0:185:G:H4'	30:0:186:A:H4'	1.94	0.49
30:0:2061:C:C2'	30:0:2062:A:H5'	2.42	0.49
30:0:542:A:H2'	30:0:543:G:O4'	2.13	0.49
1:A:128:LEU:HG	37:A:8568:HOH:O	2.11	0.49
2:B:102:THR:HG23	2:B:182:VAL:HG12	1.95	0.49
7:G:20:VAL:O	7:G:24:VAL:HG23	2.12	0.49
13:M:164:THR:HG22	13:M:167:GLY:N	2.14	0.49
23:W:11:VAL:HG11	30:0:1086:A:C6	2.46	0.49
30:0:1127:C:C5	30:0:1128:U:C4	3.00	0.49
27:1:16:HIS:CD2	30:0:470:U:O2'	2.65	0.49
30:0:602:A:O2'	30:0:605:C:H4'	2.11	0.49
15:O:24:ALA:HB3	30:0:710:G:OP1	2.11	0.49
30:0:941:G:O2'	30:0:942:U:H5'	2.12	0.49
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.47	0.49
20:T:49:GLU:HB3	20:T:59:GLU:HG2	1.95	0.49
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.94	0.49
25:Y:115:ARG:HH21	30:0:1266:U:H4'	1.76	0.49
30:0:1137:G:H1'	37:0:3414:HOH:O	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1206:U:H2'	30:0:1207:A:O4'	2.13	0.49
3:C:43:LYS:HG2	30:0:449:A:N7	2.27	0.49
30:0:858:U:C6	37:0:4975:HOH:O	2.66	0.49
4:D:154:LYS:H	4:D:154:LYS:CD	2.18	0.49
22:V:16:ARG:NH1	22:V:65:ASP:O	2.46	0.49
30:0:1189:A:O2'	30:0:1208:C:H2'	2.11	0.49
30:0:1819:G:H2'	30:0:1820:G:C4'	2.43	0.49
30:0:2010:A:H2'	37:0:5505:HOH:O	2.11	0.49
30:0:1787:C:H4'	30:0:2883:A:O4'	2.12	0.49
3:C:233:THR:HG22	3:C:234:VAL:N	2.26	0.49
1:A:211:LYS:O	30:0:1943:C:H4'	2.13	0.49
30:0:407:A:H5'	37:0:5572:HOH:O	2.13	0.49
4:D:23:VAL:HG22	4:D:73:VAL:HB	1.95	0.49
26:Z:37:ARG:NH1	37:Z:8419:HOH:O	2.45	0.49
30:0:1205:U:H2'	30:0:1206:U:H5'	1.95	0.49
28:2:22:PRO:HG2	28:2:25:VAL:CG2	2.42	0.49
4:D:65:GLU:HG3	37:D:6752:HOH:O	2.12	0.49
30:0:1641:A:C2'	30:0:1642:A:H5'	2.43	0.49
28:2:5:LYS:HD2	30:0:1675:C:H5''	1.95	0.49
30:0:2289:G:N2	30:0:2291:A:C2	2.71	0.49
30:0:441:A:H1'	30:0:442:A:N7	2.28	0.49
31:9:20:G:H3'	37:9:8434:HOH:O	2.13	0.49
30:0:1167:G:H2'	30:0:1168:C:O4'	2.13	0.49
30:0:2089:A:O2'	30:0:2090:G:H5'	2.13	0.49
30:0:2896:A:N3	30:0:2896:A:H2'	2.28	0.49
30:0:482:G:H4'	30:0:508:A:N1	2.28	0.49
1:A:194:MET:SD	30:0:875:A:C2	3.06	0.49
22:V:1:THR:CB	30:0:93:C:H5''	2.43	0.49
2:B:221:GLN:HE22	11:K:42:ASN:ND2	2.03	0.49
3:C:78:ARG:HG3	3:C:78:ARG:NH1	2.27	0.49
8:H:49:GLN:NE2	8:H:140:TYR:HE2	2.11	0.49
10:J:88:PRO:O	10:J:94:GLY:HA3	2.13	0.49
30:0:1314:U:H5''	30:0:1316:G:O4'	2.13	0.48
30:0:559:U:H2'	30:0:560:U:O4'	2.13	0.48
30:0:871:G:H4'	37:0:3951:HOH:O	2.12	0.48
24:X:80:GLU:HB3	37:X:5564:HOH:O	2.12	0.48
30:0:1291:A:H2	37:0:4838:HOH:O	1.96	0.48
10:J:19:MET:CE	10:J:132:LEU:HD11	2.43	0.48
30:0:1730:G:H5'	30:0:1731:C:C6	2.43	0.48
30:0:737:A:H2'	30:0:738:G:O4'	2.13	0.48
2:B:154:VAL:HG12	2:B:156:LYS:HG2	1.96	0.48
30:0:1014:A:H2'	30:0:1015:C:H5'	1.95	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1506:U:H6	30:0:1506:U:H5'	1.79	0.48
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.29	0.48
2:B:62:ARG:HA	2:B:65:MET:CE	2.43	0.48
3:C:129:HIS:HE1	3:C:231:ARG:HA	1.79	0.48
7:G:12:ILE:N	7:G:13:PRO:HD3	2.28	0.48
12:L:18:HIS:CD2	30:0:902:G:N7	2.79	0.48
30:0:1339:G:C6	30:0:1340:G:N1	2.80	0.48
30:0:1667:A:H2'	30:0:1668:U:H6	1.77	0.48
5:E:91:PHE:HE1	30:0:2694:A:H4'	1.78	0.48
30:0:2911:C:H2'	30:0:2912:C:C6	2.49	0.48
2:B:264:GLU:HG2	2:B:267:LYS:HE2	1.95	0.48
2:B:297:VAL:HB	37:B:8606:HOH:O	2.12	0.48
13:M:107:ARG:NH1	37:M:8573:HOH:O	2.46	0.48
16:P:81:LYS:HG2	37:0:9060:HOH:O	2.14	0.48
30:0:1044:C:H3'	30:0:1045:G:H5''	1.95	0.48
30:0:1377:C:C5'	30:0:1377:C:H6	2.25	0.48
30:0:1588:G:C6	30:0:1589:G:N1	2.82	0.48
30:0:2314:G:C2'	30:0:2315:C:H5'	2.43	0.48
1:A:125:ASN:HB3	1:A:158:VAL:HG12	1.95	0.48
14:N:58:LEU:N	14:N:58:LEU:HD12	2.29	0.48
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.43	0.48
22:V:39:ALA:N	22:V:40:PRO:CD	2.77	0.48
30:0:1159:G:H21	30:0:1189:A:H8	1.62	0.48
30:0:1772:C:H5'	30:0:1773:G:C5	2.49	0.48
30:0:2421:G:H4'	37:0:4318:HOH:O	2.13	0.48
30:0:871:G:H8	30:0:871:G:H5''	1.74	0.48
31:9:2:U:OP2	31:9:2:U:H4'	2.14	0.48
2:B:82:VAL:HG12	2:B:82:VAL:O	2.12	0.48
2:B:85:ARG:NH1	37:B:8634:HOH:O	2.46	0.48
4:D:166:ILE:HD12	37:D:6326:HOH:O	2.13	0.48
13:M:99:ARG:HH21	13:M:170:ASN:ND2	2.11	0.48
24:X:23:HIS:HE1	30:0:2044:G:OP1	1.96	0.48
30:0:1409:G:H5'	37:0:3263:HOH:O	2.14	0.48
30:0:255:A:H2'	30:0:256:C:C6	2.49	0.48
30:0:2754:G:C2'	30:0:2755:G:H5'	2.44	0.48
31:9:55:U:H4'	31:9:56:A:C8	2.48	0.48
1:A:29:HIS:HB2	1:A:153:ARG:HH12	1.79	0.48
2:B:268:ARG:NH2	2:B:325:PRO:HG3	2.28	0.48
3:C:12:THR:HB	37:C:8439:HOH:O	2.13	0.48
4:D:137:PRO:O	31:9:30:C:OP1	2.32	0.48
10:J:74:ARG:NH1	10:J:76:ASP:HB2	2.28	0.48
12:L:67:ARG:HB2	12:L:112:GLY:HA3	1.95	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:M:15:PRO:HA	13:M:20:LEU:HD23	1.95	0.48
23:W:108:ARG:HE	23:W:114:PRO:HG3	1.78	0.48
24:X:25:ARG:HG2	37:X:5356:HOH:O	2.13	0.48
30:0:1202:A:C2'	30:0:1203:G:H5'	2.44	0.48
30:0:1419:U:H2'	30:0:1685:A:C2	2.49	0.48
30:0:2134:G:C6	30:0:2258:A:C8	3.01	0.48
30:0:236:A:C4'	30:0:237:G:H5'	2.38	0.48
30:0:2909:G:H2'	30:0:2910:A:H8	1.78	0.48
14:N:11:ARG:HD3	31:9:114:G:O6	2.13	0.48
3:C:27:ARG:HG3	3:C:29:ASP:OD1	2.14	0.48
18:R:29:LYS:HD3	37:0:4262:HOH:O	2.14	0.48
30:0:1484:G:H2'	37:0:8620:HOH:O	2.14	0.48
23:W:154:ARG:NH1	30:0:588:G:O6	2.46	0.48
11:K:87:ARG:NH2	30:0:2720:C:O2	2.47	0.48
13:M:125:ARG:HD3	37:0:4520:HOH:O	2.13	0.48
23:W:38:THR:HG22	23:W:39:ASP:N	2.29	0.48
26:Z:35:SER:CB	26:Z:47:ARG:HB2	2.44	0.48
30:0:2668:G:H2'	30:0:2669:U:C6	2.49	0.47
30:0:2768:A:H5''	37:0:3966:HOH:O	2.13	0.47
30:0:10:U:O4	30:0:532:A:OP2	2.31	0.47
3:C:87:ARG:NH2	30:0:894:A:C2	2.82	0.47
1:A:212:PRO:HB2	37:A:8556:HOH:O	2.14	0.47
14:N:4:PRO:HB2	30:0:1010:C:H4'	1.96	0.47
30:0:1202:A:H2'	30:0:1203:G:H5'	1.96	0.47
30:0:1735:C:O2'	30:0:1736:A:H5'	2.12	0.47
30:0:1883:U:O2'	30:0:1884:G:H5'	2.13	0.47
30:0:2487:C:H5	37:0:4427:HOH:O	1.97	0.47
30:0:764:C:H2'	30:0:765:G:O4'	2.14	0.47
5:E:111:LYS:HE3	30:0:2690:U:O2'	2.14	0.47
8:H:6:ALA:CA	8:H:61:ARG:HH12	2.26	0.47
14:N:132:ASN:O	14:N:135:VAL:HG12	2.13	0.47
16:P:115:SER:OG	16:P:118:GLN:HG3	2.15	0.47
23:W:149:LEU:HG	23:W:153:MET:CE	2.44	0.47
30:0:1474:C:C5'	30:0:1474:C:H6	2.15	0.47
30:0:1878:G:O2'	30:0:1879:U:P	2.73	0.47
30:0:285:A:H2'	30:0:286:U:O4'	2.14	0.47
30:0:920:C:H5''	30:0:921:G:O5'	2.14	0.47
9:I:84:SER:HB3	9:I:92:VAL:CG2	2.44	0.47
10:J:131:THR:HG22	10:J:134:GLU:H	1.79	0.47
10:J:45:VAL:HG23	10:J:130:VAL:O	2.14	0.47
17:Q:66:LYS:HB2	17:Q:70:ALA:O	2.14	0.47
23:W:38:THR:O	23:W:42:ARG:HB2	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:W:4:LEU:HD22	23:W:52:VAL:CG2	2.40	0.47
23:W:72:PRO:HG2	23:W:77:ALA:HB3	1.97	0.47
30:0:1450:C:H4'	30:0:1493:A:C5	2.49	0.47
30:0:407:A:H8	37:0:4000:HOH:O	1.96	0.47
30:0:816:G:C6	30:0:817:G:N1	2.82	0.47
1:A:164:ARG:NE	37:A:8580:HOH:O	2.47	0.47
23:W:38:THR:HG22	23:W:39:ASP:H	1.79	0.47
30:0:2724:U:H2'	30:0:2725:G:O4'	2.14	0.47
30:0:426:G:H2'	30:0:427:C:O4'	2.14	0.47
30:0:834:G:H4'	30:0:835:U:OP2	2.15	0.47
29:3:70:ARG:HD3	37:3:8571:HOH:O	2.14	0.47
18:R:14:ALA:HB3	18:R:147:LEU:HB2	1.97	0.47
21:U:17:THR:HG22	21:U:18:GLY:N	2.29	0.47
30:0:1006:A:N1	30:0:2311:A:H1'	2.29	0.47
30:0:1116:U:HO2'	30:0:1118:A:H2	0.72	0.47
30:0:1132:A:N6	30:0:1229:C:H2'	2.30	0.47
30:0:1187:U:HO2'	30:0:1188:A:H8	1.60	0.47
30:0:603:A:H4'	30:0:604:G:O5'	2.15	0.47
1:A:211:LYS:HD3	37:A:8604:HOH:O	2.14	0.47
11:K:87:ARG:NH1	37:K:4066:HOH:O	2.47	0.47
15:O:14:LEU:HD23	15:O:102:ILE:HD11	1.96	0.47
22:V:12:THR:HG23	22:V:14:ALA:H	1.80	0.47
25:Y:189:ASN:HA	25:Y:217:ILE:HD11	1.94	0.47
30:0:506:G:N2	30:0:509:A:H5''	2.22	0.47
5:E:84:MET:HE1	5:E:148:ILE:HD12	1.97	0.47
13:M:107:ARG:HH11	13:M:107:ARG:HG3	1.80	0.47
13:M:61:ILE:HA	37:M:8617:HOH:O	2.15	0.47
25:Y:144:ARG:NE	37:Y:8610:HOH:O	2.47	0.47
30:0:1056:U:H2'	30:0:1057:A:O4'	2.15	0.47
30:0:162:C:H2'	30:0:163:U:H5'	1.96	0.47
30:0:1681:G:H5''	30:0:1682:A:H5'	1.96	0.47
30:0:2900:G:H2'	30:0:2901:C:O4'	2.15	0.47
3:C:214:THR:HB	37:0:9200:HOH:O	2.13	0.47
4:D:94:ALA:HB3	4:D:97:GLN:HG3	1.96	0.47
25:Y:122:ARG:NH2	37:Y:8535:HOH:O	2.48	0.47
30:0:2291:A:N9	30:0:2309:C:H5'	2.29	0.47
30:0:2831:C:C2'	30:0:2832:C:H5'	2.45	0.47
5:E:132:THR:HB	37:E:2227:HOH:O	2.14	0.47
5:E:35:TYR:HA	10:J:127:ILE:HD12	1.96	0.47
14:N:1:ALA:HB2	31:9:14:G:O2'	2.15	0.47
20:T:71:VAL:HG11	20:T:90:PRO:CB	2.36	0.47
30:0:1181:A:H2'	30:0:1182:C:C5'	2.45	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2019:A:H5'	37:0:4079:HOH:O	2.15	0.47
30:0:2506:A:O2'	30:0:2507:G:O5'	2.33	0.47
10:J:75:PRO:HD3	10:J:136:SER:OG	2.15	0.47
30:0:1562:C:O2	30:0:1562:C:H2'	2.14	0.47
30:0:1657:A:H2'	30:0:1658:A:C8	2.50	0.47
30:0:417:G:P	37:0:6968:HOH:O	2.71	0.47
31:9:24:U:H3'	31:9:25:G:C5'	2.45	0.47
11:K:66:ARG:HD2	30:0:1992:U:OP2	2.15	0.47
30:0:1205:U:C2'	30:0:1206:U:C5'	2.93	0.46
30:0:1213:C:O2'	30:0:1214:G:H5'	2.15	0.46
30:0:1353:C:P	37:0:4219:HOH:O	2.73	0.46
30:0:2361:A:H2'	30:0:2362:A:C8	2.50	0.46
4:D:172:VAL:HG12	4:D:173:GLU:N	2.30	0.46
14:N:38:LYS:HE2	14:N:107:ASN:ND2	2.30	0.46
30:0:2256:G:C2'	30:0:2257:G:H5'	2.44	0.46
30:0:2419:U:H5''	30:0:2420:G:C5'	2.45	0.46
30:0:920:C:H4'	30:0:921:G:C2	2.49	0.46
31:9:31:C:H2'	31:9:32:G:O4'	2.16	0.46
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.76	0.46
2:B:27:ASN:HB2	37:0:3602:HOH:O	2.16	0.46
6:F:30:LYS:HE2	6:F:99:THR:HG21	1.97	0.46
20:T:54:ASP:OD2	30:0:316:A:H5'	2.16	0.46
20:T:92:ASP:OD1	20:T:94:SER:HB3	2.16	0.46
25:Y:189:ASN:ND2	25:Y:192:ASP:H	2.14	0.46
26:Z:41:ARG:NH1	30:0:821:U:H4'	2.31	0.46
30:0:1441:G:H1'	37:0:7314:HOH:O	2.15	0.46
12:L:73:VAL:HG21	12:L:116:HIS:CD2	2.50	0.46
14:N:147:ILE:HB	37:N:8545:HOH:O	2.14	0.46
21:U:14:GLU:OE1	21:U:15:PRO:HD2	2.16	0.46
30:0:1200:A:H4'	37:0:6890:HOH:O	2.14	0.46
30:0:2112:A:H2'	30:0:2113:G:C8	2.51	0.46
30:0:2456:A:H5'	37:0:5242:HOH:O	2.15	0.46
30:0:445:U:H1'	37:0:6885:HOH:O	2.14	0.46
4:D:27:ILE:HD11	4:D:37:ALA:HB3	1.98	0.46
7:G:19:GLU:O	7:G:23:ILE:HG13	2.15	0.46
15:O:87:THR:O	15:O:91:GLN:HG3	2.16	0.46
20:T:111:ARG:HB3	20:T:119:ALA:HB2	1.98	0.46
30:0:1044:C:H5	37:0:6150:HOH:O	1.96	0.46
30:0:1174:A:C5	30:0:1201:C:H4'	2.50	0.46
30:0:136:C:H2'	30:0:137:U:O4'	2.15	0.46
16:P:41:ARG:NH2	30:0:1500:U:OP2	2.48	0.46
30:0:1625:U:H5''	37:0:5568:HOH:O	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:69:A:H8	30:0:69:A:C5'	2.20	0.46
31:9:31:C:C2	31:9:50:G:N2	2.84	0.46
12:L:61:ALA:HA	37:L:8553:HOH:O	2.15	0.46
19:S:56:ASN:O	28:2:8:LYS:NZ	2.46	0.46
20:T:9:LYS:HE3	20:T:13:ARG:NH1	2.30	0.46
24:X:30:MET:HE1	24:X:58:ALA:HB3	1.97	0.46
30:0:2010:A:C2'	37:0:5505:HOH:O	2.62	0.46
30:0:2256:G:O2'	30:0:2257:G:H5'	2.16	0.46
30:0:284:C:H4'	30:0:285:A:H8	1.80	0.46
30:0:538:C:H5''	30:0:539:G:C8	2.50	0.46
27:1:8:GLN:HE22	27:1:11:LYS:HZ2	1.62	0.46
31:9:55:U:H4'	31:9:56:A:H8	1.78	0.46
7:G:23:ILE:O	7:G:27:ILE:HG13	2.15	0.46
30:0:1181:A:N1	30:0:1192:A:O2'	2.48	0.46
30:0:1252:A:H2'	30:0:1253:C:O4'	2.15	0.46
24:X:30:MET:HG2	30:0:1384:C:H5'	1.98	0.46
30:0:1947:G:H2'	30:0:1948:G:H8	1.81	0.46
30:0:821:U:H5''	37:0:9582:HOH:O	2.15	0.46
3:C:118:THR:O	3:C:136:VAL:HG13	2.16	0.46
30:0:1393:A:H2'	30:0:1394:C:C6	2.51	0.46
5:E:143:GLN:HE22	30:0:2779:G:H21	1.59	0.46
30:0:876:A:N3	30:0:876:A:H2'	2.31	0.46
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.15	0.46
20:T:69:LYS:O	20:T:71:VAL:HG23	2.16	0.46
25:Y:220:GLU:HG3	37:Y:8546:HOH:O	2.15	0.46
30:0:1592:G:O2'	30:0:1593:C:O5'	2.34	0.46
30:0:2570:G:H5''	37:0:4452:HOH:O	2.15	0.46
30:0:304:G:H1'	30:0:347:A:N6	2.31	0.46
31:9:36:C:C5	31:9:37:C:C5	3.04	0.46
1:A:88:ILE:HG22	1:A:88:ILE:O	2.16	0.46
3:C:104:ASP:HA	3:C:107:ARG:NH1	2.31	0.46
4:D:22:VAL:HG22	4:D:74:THR:HG22	1.96	0.46
8:H:102:LYS:HD3	8:H:122:LYS:HD3	1.97	0.46
5:E:36:PRO:HD3	10:J:127:ILE:HD12	1.97	0.46
11:K:81:ARG:HD3	11:K:87:ARG:NH1	2.31	0.46
23:W:3:ALA:O	23:W:54:PHE:HA	2.16	0.46
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.96	0.46
30:0:1249:U:H2'	30:0:1250:C:C6	2.51	0.46
30:0:2672:C:O2'	30:0:2673:U:H5'	2.16	0.46
30:0:2831:C:H2'	30:0:2832:C:H5'	1.97	0.46
30:0:1314:U:H2'	37:0:5422:HOH:O	2.15	0.45
30:0:2726:U:O2	30:0:2749:U:O5'	2.34	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:574:G:O2'	30:0:575:A:H5'	2.16	0.45
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.46	0.45
13:M:99:ARG:CD	13:M:167:GLY:HA2	2.46	0.45
14:N:164:ASP:OD1	14:N:167:ASP:HA	2.15	0.45
30:0:119:A:H2'	30:0:120:A:H5''	1.96	0.45
30:0:138:U:OP2	30:0:139:C:H5	1.98	0.45
30:0:2716:G:O2'	30:0:2717:C:H5'	2.17	0.45
2:B:98:THR:HG22	30:0:2820:A:OP1	2.16	0.45
30:0:69:A:C8	30:0:69:A:C5'	2.92	0.45
31:9:52:A:H2'	31:9:53:G:O4'	2.16	0.45
14:N:154:LEU:C	14:N:156:GLU:H	2.19	0.45
19:S:45:TYR:HD2	37:S:4527:HOH:O	1.99	0.45
20:T:3:GLN:HA	20:T:4:PRO:HD3	1.82	0.45
30:0:1119:G:C6	30:0:1244:U:C5	3.04	0.45
30:0:1559:A:C1'	37:0:5413:HOH:O	2.62	0.45
30:0:2061:C:H2'	30:0:2062:A:H5'	1.98	0.45
3:C:168:ARG:NH2	3:C:190:ALA:O	2.49	0.45
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.98	0.45
37:C:8357:HOH:O	15:O:3:THR:HG21	2.15	0.45
30:0:1183:C:H42	30:0:1184:C:H41	1.62	0.45
30:0:130:C:H5'	37:0:4755:HOH:O	2.16	0.45
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.81	0.45
5:E:31:ARG:NH1	37:E:5919:HOH:O	2.49	0.45
14:N:164:ASP:CG	14:N:167:ASP:HA	2.37	0.45
19:S:38:ALA:O	19:S:42:GLU:HG3	2.15	0.45
30:0:1878:G:O2'	30:0:1879:U:C5	2.67	0.45
20:T:2:LYS:HG2	30:0:447:A:OP1	2.17	0.45
30:0:844:A:C6	30:0:882:A:C5	3.04	0.45
28:2:41:HIS:HE1	30:0:1439:C:OP1	1.99	0.45
5:E:7:ILE:HG22	5:E:45:ASP:O	2.16	0.45
8:H:69:ARG:HD3	37:H:8381:HOH:O	2.16	0.45
14:N:108:SER:HA	14:N:109:PRO:HD3	1.76	0.45
15:O:35:LYS:HD3	37:0:4157:HOH:O	2.17	0.45
16:P:16:VAL:CG1	16:P:20:ARG:HB2	2.46	0.45
30:0:1505:U:H1'	37:0:7139:HOH:O	2.16	0.45
30:0:1925:G:O2'	30:0:1926:G:H5'	2.17	0.45
30:0:2289:G:N2	30:0:2291:A:H2	2.13	0.45
30:0:2326:C:H4'	30:0:2412:G:H4'	1.99	0.45
13:M:171:ARG:NH2	30:0:189:A:OP1	2.49	0.45
14:N:127:LEU:HD13	37:N:8556:HOH:O	2.16	0.45
16:P:115:SER:H	16:P:118:GLN:NE2	2.00	0.45
26:Z:84:CYS:O	26:Z:85:ASP:HB2	2.15	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1188:A:N7	30:0:1189:A:C2	2.85	0.45
30:0:1545:C:H2'	30:0:1546:G:O4'	2.17	0.45
30:0:2526:C:H5'	30:0:2526:C:C6	2.51	0.45
30:0:816:G:H5'	30:0:1598:A:H4'	1.98	0.45
3:C:104:ASP:HA	3:C:107:ARG:HH12	1.80	0.45
5:E:5:LEU:HD21	5:E:66:GLN:HG3	1.99	0.45
10:J:107:ASN:C	10:J:107:ASN:HD22	2.20	0.45
30:0:1060:C:H6	30:0:1060:C:H5'	1.82	0.45
30:0:1200:A:H3'	37:0:5302:HOH:O	2.16	0.45
30:0:1596:U:H2'	30:0:1598:A:OP2	2.16	0.45
18:R:80:TYR:O	30:0:2050:G:H5''	2.17	0.45
30:0:2667:G:H1'	30:0:2914:A:N3	2.31	0.45
1:A:100:PRO:HG2	1:A:103:VAL:CG2	2.44	0.45
2:B:72:THR:HB	37:B:8606:HOH:O	2.16	0.45
3:C:127:ARG:CZ	3:C:225:PRO:HG2	2.45	0.45
9:I:133:THR:HG22	9:I:134:ILE:N	2.32	0.45
15:O:96:VAL:HG13	15:O:100:GLN:HB2	1.98	0.45
16:P:13:VAL:HG21	16:P:41:ARG:HG2	1.99	0.45
30:0:1183:C:H2'	37:0:5790:HOH:O	2.17	0.45
1:A:1:GLY:HA2	30:0:2114:C:OP1	2.17	0.45
4:D:52:THR:HG21	30:0:2346:C:O2'	2.16	0.45
30:0:2361:A:H8	30:0:2361:A:H5'	1.82	0.45
30:0:2509:A:OP2	30:0:2510:C:H5	2.00	0.45
30:0:2515:C:H2'	30:0:2516:G:O4'	2.16	0.45
30:0:2781:U:C2'	30:0:2782:G:H5'	2.46	0.45
30:0:484:A:N1	30:0:506:G:H4'	2.32	0.45
30:0:541:C:C2'	30:0:542:A:C5'	2.82	0.45
1:A:33:GLU:CD	1:A:33:GLU:H	2.20	0.45
6:F:60:VAL:HG12	6:F:60:VAL:O	2.17	0.45
13:M:134:ILE:CG2	13:M:141:ILE:HD13	2.47	0.45
15:O:39:THR:O	15:O:115:ARG:NH2	2.49	0.45
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.99	0.45
30:0:1209:C:H2'	30:0:1210:G:C8	2.48	0.45
12:L:14:GLY:O	30:0:1295:G:H5''	2.17	0.45
30:0:2883:A:H2'	30:0:2884:G:O4'	2.17	0.45
30:0:999:C:O2'	30:0:1000:C:H5'	2.18	0.44
30:0:1979:G:O2'	30:0:1980:U:OP1	2.29	0.44
27:1:10:LYS:HG3	37:1:8431:HOH:O	2.17	0.44
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.16	0.44
4:D:51:ARG:HH11	4:D:68:PRO:HB3	1.81	0.44
6:F:16:ALA:HA	6:F:111:ILE:HD13	1.99	0.44
8:H:23:ILE:HG23	8:H:123:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:61:ARG:HH11	8:H:61:ARG:HG3	1.82	0.44
11:K:74:VAL:HG13	11:K:113:ILE:HG23	1.98	0.44
30:0:1044:C:H5''	37:0:8543:HOH:O	2.17	0.44
30:0:1058:A:H2'	30:0:1060:C:C5'	2.44	0.44
37:I:5128:HOH:O	30:0:1168:C:C5'	2.64	0.44
28:2:42:TRP:HB3	30:0:1418:U:OP1	2.18	0.44
30:0:1942:A:O2'	30:0:1943:C:H5'	2.18	0.44
30:0:2553:A:H2'	30:0:2553:A:N3	2.31	0.44
30:0:2781:U:H2'	30:0:2782:G:H5'	2.00	0.44
30:0:292:G:H2'	30:0:358:G:N2	2.33	0.44
30:0:316:A:N3	30:0:336:G:O2'	2.43	0.44
29:3:70:ARG:HG2	29:3:77:ALA:HB2	1.99	0.44
3:C:16:VAL:HG12	3:C:17:ASP:H	1.81	0.44
11:K:75:ARG:HD3	11:K:112:PRO:O	2.16	0.44
13:M:164:THR:HB	37:M:8519:HOH:O	2.17	0.44
13:M:167:GLY:O	13:M:171:ARG:HG3	2.17	0.44
15:O:37:ARG:HD2	30:0:656:G:OP2	2.17	0.44
30:0:1477:C:H5'	30:0:1868:G:H5''	1.98	0.44
30:0:2090:G:H2'	30:0:2091:G:C8	2.51	0.44
30:0:2135:A:O2'	30:0:2136:G:H5'	2.16	0.44
30:0:212:A:O4'	30:0:214:U:C6	2.71	0.44
30:0:2103:A:N7	30:0:2538:A:N6	2.65	0.44
30:0:2642:G:H2'	30:0:2643:G:O4'	2.17	0.44
30:0:2712:G:P	37:0:4763:HOH:O	2.75	0.44
30:0:2791:U:H1'	30:0:2792:A:H5''	1.99	0.44
30:0:958:G:H2'	30:0:959:C:C6	2.52	0.44
27:1:25:LYS:HD2	28:2:48:ASP:HA	1.98	0.44
31:9:57:A:N6	37:9:8441:HOH:O	2.47	0.44
3:C:25:PRO:HG2	37:C:8322:HOH:O	2.17	0.44
8:H:59:GLN:HE21	8:H:129:ARG:NE	2.00	0.44
18:R:128:ARG:HH22	30:0:2054:A:H2	1.61	0.44
30:0:2812:A:N7	37:0:7067:HOH:O	2.36	0.44
31:9:2:U:C4'	37:9:8480:HOH:O	2.66	0.44
3:C:236:THR:HG22	3:C:239:ALA:CB	2.47	0.44
4:D:88:LEU:HB2	4:D:89:PRO:HD3	1.98	0.44
5:E:3:VAL:CG2	5:E:49:ILE:HB	2.48	0.44
10:J:90:LYS:HB2	35:J:8502:CL:CL	2.54	0.44
10:J:93:ARG:HH11	10:J:93:ARG:HB3	1.81	0.44
12:L:21:ARG:N	37:L:8524:HOH:O	2.50	0.44
15:O:14:LEU:CD2	15:O:102:ILE:HD11	2.48	0.44
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.17	0.44
18:R:111:ILE:HG23	18:R:145:LEU:CD1	2.48	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:Y:144:ARG:NH2	37:Y:8610:HOH:O	2.49	0.44
30:0:2115:U:H2'	30:0:2116:U:C6	2.53	0.44
30:0:281:U:H3'	37:0:6755:HOH:O	2.17	0.44
2:B:244:PRO:HB3	30:0:1234:U:N3	2.32	0.44
3:C:2:GLN:HB3	37:C:8333:HOH:O	2.17	0.44
3:C:2:GLN:HB3	37:C:8384:HOH:O	2.18	0.44
4:D:50:VAL:O	4:D:71:ALA:HA	2.18	0.44
4:D:56:ARG:N	37:D:6752:HOH:O	2.50	0.44
8:H:62:HIS:HA	8:H:65:LEU:HD23	1.99	0.44
12:L:133:VAL:HB	37:L:8547:HOH:O	2.17	0.44
18:R:106:GLY:HA2	18:R:109:MET:CE	2.47	0.44
30:0:1940:C:H4'	37:0:6896:HOH:O	2.16	0.44
30:0:1948:G:H2'	30:0:1949:G:O4'	2.18	0.44
30:0:2004:U:H2'	30:0:2005:G:OP1	2.16	0.44
29:3:28:GLY:HA3	30:0:2434:A:O3'	2.17	0.44
13:M:193:LYS:HB3	30:0:392:U:C5'	2.48	0.44
30:0:559:U:H5'	30:0:559:U:C6	2.42	0.44
30:0:834:G:H3'	30:0:835:U:H4'	1.99	0.44
30:0:1014:A:H5"	31:9:101:G:O2'	2.18	0.44
2:B:57:GLU:HA	2:B:58:PRO:HD2	1.89	0.44
3:C:153:VAL:O	3:C:157:LEU:HG	2.18	0.44
5:E:116:THR:HG22	5:E:151:LEU:HD22	2.00	0.44
22:V:7:GLU:O	22:V:11:MET:HG3	2.18	0.44
30:0:1423:C:O2'	30:0:1424:A:H5'	2.18	0.44
30:0:2353:A:H4'	30:0:2354:A:O5'	2.17	0.44
30:0:737:A:H2	37:0:6249:HOH:O	1.98	0.44
27:1:28:HIS:CD2	27:1:30:LYS:HB2	2.52	0.44
2:B:71:VAL:HG11	2:B:296:LEU:HD22	1.99	0.44
3:C:140:VAL:HG12	3:C:141:SER:N	2.33	0.44
7:G:63:ARG:NH1	30:0:1151:G:OP1	2.50	0.44
11:K:45:PRO:HB2	37:0:6920:HOH:O	2.17	0.44
21:U:13:ILE:HG12	21:U:32:CYS:HB3	1.99	0.44
30:0:113:A:OP2	30:0:114:A:H2'	2.17	0.44
30:0:1299:G:N2	37:0:4223:HOH:O	2.49	0.44
3:C:184:ARG:NH2	30:0:450:C:OP1	2.35	0.44
30:0:660:A:H4'	30:0:661:G:O5'	2.18	0.44
14:N:160:SER:CB	31:9:51:A:H5'	2.48	0.44
3:C:237:GLU:HB2	37:C:8428:HOH:O	2.16	0.44
3:C:235:PHE:HE2	3:C:243:VAL:HG21	1.82	0.44
5:E:31:ARG:NH1	5:E:68:HIS:CG	2.86	0.44
8:H:172:GLU:HB3	37:H:8392:HOH:O	2.18	0.44
12:L:143:THR:HG22	12:L:144:ASP:H	1.78	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2403:C:H2'	30:0:2404:G:O5'	2.17	0.44
29:3:14:CYS:SG	37:3:8559:HOH:O	2.62	0.44
31:9:34:A:H2'	31:9:35:C:O4'	2.18	0.44
30:0:2031:C:H2'	30:0:2032:U:O4'	2.17	0.43
30:0:2401:A:H5'	37:0:9014:HOH:O	2.18	0.43
30:0:240:C:O2	30:0:240:C:H2'	2.18	0.43
30:0:2326:C:H4'	30:0:2412:G:C4'	2.48	0.43
31:9:49:G:C2'	31:9:50:G:H5'	2.48	0.43
1:A:171:LYS:HB2	30:0:820:G:C5	2.53	0.43
8:H:41:LYS:HE2	8:H:45:ASP:CB	2.47	0.43
14:N:139:TRP:HA	14:N:139:TRP:CE3	2.53	0.43
14:N:169:PRO:O	14:N:172:PHE:HB3	2.18	0.43
22:V:12:THR:HG22	22:V:15:GLU:CG	2.46	0.43
23:W:137:GLN:NE2	23:W:141:HIS:HE1	1.99	0.43
30:0:1592:G:O2'	30:0:1593:C:O4'	2.34	0.43
30:0:2820:A:H2'	30:0:2821:C:O4'	2.18	0.43
30:0:653:U:H2'	30:0:654:A:C8	2.53	0.43
12:L:27:ARG:HD2	30:0:757:C:OP1	2.18	0.43
28:2:20:ARG:HG2	28:2:21:VAL:N	2.33	0.43
2:B:41:PHE:CD2	2:B:190:MET:HE3	2.53	0.43
3:C:107:ARG:NH1	37:C:8429:HOH:O	2.51	0.43
5:E:20:ILE:CD1	5:E:40:VAL:HG11	2.44	0.43
22:V:44:GLY:O	22:V:48:GLU:HG2	2.18	0.43
23:W:125:HIS:HE1	37:W:3071:HOH:O	2.01	0.43
23:W:5:VAL:HG11	23:W:153:MET:HE3	1.98	0.43
24:X:74:ALA:HB2	24:X:85:VAL:HG13	2.00	0.43
30:0:1825:U:O2'	30:0:1826:C:H5'	2.18	0.43
30:0:2073:G:OP2	30:0:2490:A:H5'	2.19	0.43
30:0:2508:C:H2'	37:0:6301:HOH:O	2.17	0.43
30:0:2697:A:H2'	30:0:2698:G:O4'	2.18	0.43
30:0:333:G:O2'	30:0:334:G:H5'	2.19	0.43
30:0:510:U:H6	37:0:6987:HOH:O	2.01	0.43
2:B:14:GLY:HA3	37:B:8609:HOH:O	2.17	0.43
2:B:62:ARG:HA	2:B:65:MET:HE2	2.01	0.43
13:M:64:ARG:HD2	37:M:8581:HOH:O	2.17	0.43
14:N:116:PHE:HB3	14:N:136:LEU:HD23	2.00	0.43
30:0:1367:A:H2'	30:0:1368:U:O4'	2.18	0.43
30:0:1684:A:O2'	30:0:1685:A:H5''	2.18	0.43
30:0:2754:G:O2'	30:0:2755:G:H5'	2.17	0.43
30:0:2768:A:H3'	37:0:3966:HOH:O	2.17	0.43
28:2:48:ASP:O	28:2:49:GLU:HB2	2.18	0.43
31:9:65:A:N6	31:9:112:U:C6	2.86	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
31:9:80:A:C2	31:9:103:A:C4	3.07	0.43
2:B:30:PRO:HB2	2:B:39:GLN:NE2	2.33	0.43
3:C:242:GLU:HG3	37:C:8381:HOH:O	2.19	0.43
7:G:12:ILE:HA	37:O:5006:HOH:O	2.17	0.43
15:O:38:ARG:NH1	37:O:7674:HOH:O	2.50	0.43
21:U:9:CYS:CA	21:U:52:THR:HG23	2.47	0.43
23:W:88:THR:HG22	23:W:90:TYR:HD1	1.82	0.43
30:0:2464:C:H5'	30:0:2465:A:OP1	2.18	0.43
30:0:941:G:C5	30:0:942:U:C4	3.06	0.43
31:9:39:U:HO2'	31:9:42:C:H5	1.58	0.43
1:A:33:GLU:O	1:A:34:ASP:HB2	2.18	0.43
10:J:74:ARG:O	10:J:78:ILE:HG12	2.18	0.43
13:M:39:ARG:NH2	37:M:8617:HOH:O	2.51	0.43
18:R:111:ILE:HG23	18:R:145:LEU:HD11	2.01	0.43
20:T:41:ARG:NH1	20:T:42:VAL:O	2.51	0.43
30:0:1406:A:H4'	30:0:1407:A:C5'	2.49	0.43
30:0:2072:G:H3'	30:0:2073:G:C5'	2.49	0.43
30:0:2269:C:C2'	30:0:2270:G:H5'	2.49	0.43
1:A:206:ARG:NH2	30:0:2630:G:O6	2.48	0.43
30:0:380:A:H4'	30:0:381:G:OP1	2.19	0.43
13:M:9:ARG:HD2	30:0:380:A:OP2	2.18	0.43
30:0:876:A:N3	30:0:876:A:C2'	2.82	0.43
1:A:153:ARG:HD3	37:A:8528:HOH:O	2.18	0.43
2:B:314:ALA:HB3	2:B:317:PRO:HG3	2.00	0.43
5:E:137:ASP:O	5:E:141:VAL:HG23	2.19	0.43
14:N:11:ARG:NH2	37:N:8519:HOH:O	2.51	0.43
16:P:80:ARG:HG2	16:P:87:ARG:CZ	2.48	0.43
23:W:119:HIS:HD2	23:W:120:PRO:O	2.01	0.43
24:X:43:VAL:HG22	24:X:76:ARG:NH1	2.32	0.43
25:Y:117:LEU:HA	25:Y:174:VAL:HG11	2.01	0.43
26:Z:37:ARG:HD3	30:0:818:A:O2'	2.19	0.43
30:0:1535:G:H2'	30:0:1536:C:C6	2.54	0.43
30:0:249:G:O2'	30:0:250:C:H5'	2.18	0.43
6:F:59:ILE:CD1	30:0:263:U:C2	3.01	0.43
5:E:31:ARG:HH12	5:E:68:HIS:CG	2.36	0.43
9:I:84:SER:HB2	9:I:90:ASP:HB2	1.99	0.43
11:K:28:GLU:HB3	11:K:59:LYS:HB2	2.00	0.43
19:S:57:THR:CG2	19:S:58:MET:N	2.82	0.43
23:W:108:ARG:HE	23:W:114:PRO:CG	2.32	0.43
23:W:126:ASP:HB3	23:W:135:GLY:O	2.18	0.43
24:X:25:ARG:HD3	24:X:64:ALA:O	2.18	0.43
30:0:1556:G:O2'	30:0:1557:G:H5'	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1701:A:H1'	37:0:5924:HOH:O	2.18	0.43
30:0:2456:A:H2'	30:0:2457:U:C6	2.53	0.43
30:0:567:U:C5'	37:0:5949:HOH:O	2.65	0.43
1:A:105:VAL:HG12	1:A:106:CYS:N	2.33	0.43
6:F:36:THR:HG23	6:F:97:ALA:HB2	2.00	0.43
18:R:132:ARG:HG2	18:R:133:ALA:N	2.34	0.43
22:V:1:THR:HG23	22:V:2:VAL:N	2.28	0.43
30:0:1098:A:H2'	30:0:1099:G:O4'	2.19	0.43
30:0:1163:G:H2'	30:0:1164:U:C5	2.54	0.43
30:0:1771:U:O2'	30:0:1773:G:N7	2.51	0.43
30:0:2842:G:C2'	30:0:2843:A:H5'	2.48	0.43
30:0:2868:C:H2'	30:0:2869:G:O4'	2.19	0.43
30:0:303:C:H2'	30:0:304:G:O4'	2.19	0.43
5:E:11:VAL:HG13	5:E:23:GLU:O	2.19	0.43
20:T:14:ALA:HA	20:T:15:PRO:HD3	1.91	0.43
30:0:1883:U:C2'	30:0:1884:G:H5'	2.49	0.43
12:L:50:GLY:C	30:0:2453:G:H4'	2.39	0.43
30:0:407:A:H2'	30:0:408:A:C8	2.54	0.43
27:1:28:HIS:HD2	27:1:30:LYS:H	1.65	0.43
1:A:171:LYS:HB2	30:0:820:G:C6	2.54	0.43
1:A:186:TRP:CG	1:A:187:PRO:HA	2.54	0.43
2:B:36:PRO:HA	2:B:168:GLY:CA	2.46	0.43
4:D:58:VAL:CG1	4:D:60:GLU:HG2	2.48	0.43
6:F:50:VAL:CG2	6:F:63:ILE:HG21	2.49	0.43
8:H:149:VAL:HG22	37:H:8378:HOH:O	2.18	0.43
11:K:125:ALA:C	11:K:127:ALA:H	2.23	0.43
17:Q:45:PRO:O	30:0:2365:G:H4'	2.18	0.43
37:Q:5998:HOH:O	30:0:2296:C:H5	2.01	0.42
30:0:283:U:C5	30:0:284:C:N3	2.87	0.42
30:0:559:U:C5'	30:0:559:U:H6	2.28	0.42
30:0:818:A:H5''	37:0:6135:HOH:O	2.18	0.42
28:2:28:LYS:O	30:0:87:C:H2'	2.19	0.42
28:2:40:ARG:HG3	28:2:45:ASN:CB	2.49	0.42
1:A:55:VAL:HG22	1:A:68:ILE:O	2.19	0.42
2:B:190:MET:HE1	2:B:194:PHE:CD1	2.54	0.42
2:B:49:THR:HG21	2:B:331:SER:O	2.19	0.42
9:I:129:SER:O	9:I:130:LEU:HD23	2.19	0.42
12:L:143:THR:CG2	12:L:144:ASP:N	2.80	0.42
14:N:62:HIS:HB3	14:N:65:ASP:OD1	2.19	0.42
37:I:3512:HOH:O	30:0:1163:G:N2	2.52	0.42
30:0:1165:G:H1'	30:0:1174:A:H1'	2.01	0.42
30:0:1202:A:H2'	30:0:1203:G:C5'	2.50	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:128:A:O2'	30:0:129:A:H5'	2.19	0.42
30:0:1427:A:H61	30:0:1440:U:H1'	1.84	0.42
30:0:1562:C:H42	30:0:2738:G:H1	1.67	0.42
13:M:81:ARG:HD2	30:0:160:A:O3'	2.19	0.42
30:0:946:C:H2'	30:0:947:U:C6	2.54	0.42
27:1:28:HIS:CD2	27:1:31:LYS:HG3	2.53	0.42
29:3:3:MET:HG3	29:3:4:PRO:HD2	2.01	0.42
1:A:11:ARG:HD3	37:0:8736:HOH:O	2.19	0.42
12:L:72:ASN:HB2	37:L:8570:HOH:O	2.17	0.42
23:W:119:HIS:HE1	37:0:9078:HOH:O	2.02	0.42
24:X:74:ALA:CB	24:X:85:VAL:HG22	2.49	0.42
23:W:23:MET:O	30:0:1025:C:H5'	2.19	0.42
30:0:1641:A:H2'	30:0:1642:A:C5'	2.48	0.42
6:F:91:VAL:HG11	30:0:262:A:OP2	2.19	0.42
30:0:907:A:H4'	30:0:1328:A:C2	2.54	0.42
4:D:173:GLU:HG3	4:D:174:VAL:HG23	2.02	0.42
6:F:49:PHE:HE1	6:F:98:VAL:HG23	1.84	0.42
8:H:34:HIS:HD2	8:H:90:LEU:O	2.01	0.42
30:0:1183:C:N4	30:0:1184:C:N4	2.64	0.42
30:0:1980:U:O2	30:0:2008:U:H4'	2.19	0.42
30:0:2290:U:H2'	37:0:6681:HOH:O	2.18	0.42
30:0:2372:A:H2'	30:0:2373:U:C6	2.55	0.42
30:0:2493:C:O2	30:0:2493:C:H2'	2.17	0.42
30:0:2526:C:O2'	30:0:2527:U:H5'	2.19	0.42
4:D:76:ARG:NH1	31:9:42:C:O2	2.51	0.42
5:E:21:THR:HG23	5:E:30:THR:OG1	2.19	0.42
14:N:32:PRO:HD2	14:N:99:GLU:O	2.20	0.42
17:Q:33:PHE:HE2	17:Q:93:ARG:HG3	1.83	0.42
23:W:11:VAL:HG11	30:0:1086:A:N6	2.34	0.42
30:0:1462:C:O2'	30:0:1463:U:H5'	2.19	0.42
30:0:1701:A:H4'	30:0:1702:U:O5'	2.18	0.42
1:A:187:PRO:HB2	30:0:1845:A:O3'	2.20	0.42
5:E:6:GLU:HG2	5:E:46:THR:HG22	2.01	0.42
10:J:130:VAL:HG12	10:J:131:THR:N	2.35	0.42
23:W:41:TYR:HA	23:W:44:MET:HE3	2.01	0.42
23:W:73:LEU:HA	23:W:73:LEU:HD12	1.77	0.42
24:X:18:ARG:NH1	37:X:4132:HOH:O	2.52	0.42
30:0:1433:G:O2'	30:0:1434:A:H5'	2.20	0.42
30:0:2243:C:H5''	37:0:3288:HOH:O	2.19	0.42
30:0:2323:G:H5'	37:0:6566:HOH:O	2.19	0.42
37:3:8515:HOH:O	30:0:2408:A:H2	2.02	0.42
30:0:2421:G:H3'	30:0:2422:U:C5'	2.50	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2769:C:C2'	30:0:2770:G:C5'	2.86	0.42
30:0:349:U:O2'	30:0:350:G:H5'	2.20	0.42
30:0:366:U:H2'	30:0:367:G:O4'	2.19	0.42
30:0:912:A:C4	30:0:1294:A:C2	3.08	0.42
29:3:18:GLN:HG2	37:3:8514:HOH:O	2.19	0.42
31:9:116:C:O2'	31:9:117:G:H5'	2.20	0.42
31:9:39:U:C2'	31:9:40:C:OP1	2.68	0.42
4:D:166:ILE:HB	37:D:6326:HOH:O	2.18	0.42
13:M:43:PRO:HG3	13:M:62:VAL:HG21	2.00	0.42
24:X:43:VAL:HG12	24:X:44:ASP:H	1.84	0.42
24:X:72:VAL:HG22	24:X:85:VAL:HG12	2.01	0.42
30:0:1482:A:O2'	30:0:1483:C:H5'	2.20	0.42
30:0:1624:A:H4'	30:0:1625:U:H5'	2.02	0.42
30:0:177:A:H2'	30:0:178:U:O4'	2.19	0.42
30:0:1878:G:O2'	30:0:1879:U:OP2	2.37	0.42
30:0:2271:G:N3	30:0:2271:G:H2'	2.34	0.42
30:0:2831:C:H2'	30:0:2832:C:C5'	2.49	0.42
30:0:2894:C:O2'	30:0:2895:C:H5'	2.19	0.42
30:0:790:A:H2'	30:0:791:A:O4'	2.20	0.42
2:B:258:GLY:H	2:B:260:HIS:CE1	2.36	0.42
3:C:133:ARG:NH1	37:C:8406:HOH:O	2.51	0.42
3:C:202:THR:HG22	30:0:328:U:O4'	2.20	0.42
9:I:101:LYS:O	9:I:105:GLU:HG3	2.19	0.42
13:M:5:TYR:HE2	13:M:46:LEU:HD13	1.84	0.42
14:N:23:ARG:NH1	37:N:8546:HOH:O	2.52	0.42
18:R:18:LEU:HD12	18:R:143:VAL:CG1	2.49	0.42
25:Y:208:LYS:O	30:0:1313:A:H5'	2.19	0.42
30:0:1042:U:O2'	30:0:1043:C:H5'	2.20	0.42
30:0:1589:G:N2	30:0:1605:G:H1'	2.35	0.42
1:A:199:HIS:HE1	30:0:1881:A:OP1	2.02	0.42
30:0:1565:C:O4'	30:0:2738:G:H1'	2.20	0.42
30:0:282:C:O2'	30:0:283:U:C4'	2.68	0.42
30:0:420:U:H2'	30:0:421:C:C6	2.55	0.42
30:0:441:A:H8	30:0:441:A:O5'	2.03	0.42
1:A:132:ASP:HB3	1:A:135:VAL:H	1.85	0.42
5:E:84:MET:HB2	5:E:131:LEU:HB2	2.01	0.42
8:H:46:TYR:HA	8:H:47:PRO:HD3	1.76	0.42
8:H:30:LYS:N	8:H:62:HIS:HD2	2.07	0.42
10:J:131:THR:HG22	10:J:133:GLY:N	2.35	0.42
16:P:88:GLN:HE22	30:0:1799:G:H21	1.67	0.42
30:0:1119:G:N2	30:0:1246:A:N1	2.67	0.42
30:0:1304:U:H2'	30:0:1305:C:C6	2.55	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1453:G:N2	30:0:1675:C:C2	2.88	0.42
30:0:2909:G:O2'	30:0:2910:A:H5'	2.20	0.42
30:0:870:G:C3'	30:0:871:G:H5''	2.50	0.42
30:0:883:U:C2'	30:0:883:U:O2	2.68	0.42
31:9:65:A:O2'	31:9:66:G:P	2.78	0.42
2:B:115:VAL:HA	2:B:116:PRO:HD3	1.87	0.42
12:L:134:GLU:HG3	37:L:8547:HOH:O	2.18	0.42
18:R:84:ALA:O	18:R:88:PHE:HD1	2.02	0.42
30:0:1218:U:H2'	30:0:1219:U:C6	2.54	0.42
30:0:12:U:H2'	30:0:13:G:H5'	2.02	0.42
30:0:1634:G:H2'	30:0:1635:U:C6	2.54	0.42
30:0:2070:G:H5''	37:0:3318:HOH:O	2.20	0.42
30:0:2403:C:C2'	30:0:2404:G:O5'	2.68	0.42
37:L:8533:HOH:O	30:0:2453:G:H5''	2.19	0.42
30:0:2491:G:H1'	37:0:6418:HOH:O	2.19	0.42
30:0:2559:C:H4'	37:0:6805:HOH:O	2.19	0.42
30:0:2664:A:OP1	30:0:2664:A:H8	2.03	0.42
30:0:2879:A:H2'	30:0:2880:A:O4'	2.20	0.42
30:0:290:C:O2'	30:0:291:C:H5'	2.20	0.42
30:0:151:A:C2	30:0:442:A:C8	3.08	0.42
3:C:118:THR:CG2	3:C:137:PRO:HB3	2.50	0.42
20:T:26:THR:HA	20:T:39:ASN:HB3	2.01	0.42
21:U:31:PHE:CG	21:U:37:GLU:HG2	2.55	0.42
21:U:50:GLU:HB3	30:0:2866:U:C4	2.55	0.42
30:0:1131:G:C6	30:0:1230:A:C4	3.07	0.41
13:M:93:ARG:HD2	30:0:1470:A:OP1	2.20	0.41
30:0:1613:C:H2'	30:0:1614:G:O4'	2.19	0.41
30:0:1615:A:H4'	37:0:5434:HOH:O	2.20	0.41
30:0:1697:G:O2'	30:0:1698:U:H5'	2.20	0.41
30:0:1947:G:H2'	30:0:1948:G:C8	2.54	0.41
30:0:1993:C:C4	30:0:1994:A:C6	3.08	0.41
12:L:56:LYS:HE3	30:0:2443:C:O3'	2.20	0.41
30:0:2777:G:O2'	30:0:2778:A:H5'	2.19	0.41
30:0:383:A:H2'	30:0:384:G:O4'	2.20	0.41
30:0:638:C:H2'	30:0:639:A:C8	2.54	0.41
27:1:28:HIS:HD2	27:1:31:LYS:H	1.68	0.41
28:2:18:ASN:HD21	28:2:40:ARG:H	1.68	0.41
28:2:36:ASN:HB3	28:2:39:ARG:HG3	2.01	0.41
1:A:11:ARG:HA	37:0:6768:HOH:O	2.20	0.41
2:B:294:TYR:HE2	37:B:8649:HOH:O	2.02	0.41
3:C:133:ARG:NE	3:C:138:VAL:HG22	2.35	0.41
7:G:67:LEU:O	7:G:71:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1842:A:C4	30:0:1979:G:C6	3.09	0.41
30:0:1946:C:H2'	30:0:1971:G:C8	2.55	0.41
30:0:1985:U:C2	30:0:1996:U:O4'	2.73	0.41
30:0:1909:A:N1	30:0:2128:G:H1'	2.34	0.41
30:0:2356:A:H2'	30:0:2357:G:O4'	2.19	0.41
30:0:2385:G:H2'	30:0:2386:U:C6	2.56	0.41
30:0:2388:C:O2'	30:0:2389:U:H5'	2.21	0.41
30:0:284:C:N4	37:0:6734:HOH:O	2.52	0.41
31:9:47:A:C2	31:9:48:C:C2	3.08	0.41
11:K:4:LEU:HD22	11:K:116:GLU:HB3	2.02	0.41
30:0:1103:C:C2	30:0:1241:G:N2	2.88	0.41
30:0:2312:G:H2'	30:0:2313:C:H5'	2.02	0.41
5:E:143:GLN:NE2	30:0:2780:C:H1'	2.34	0.41
30:0:283:U:H5	30:0:284:C:N3	2.18	0.41
30:0:321:A:O2'	30:0:322:G:H5'	2.20	0.41
30:0:542:A:C5'	30:0:542:A:C8	2.99	0.41
30:0:629:A:H2'	30:0:630:A:O4'	2.21	0.41
30:0:827:A:H2'	30:0:828:G:O4'	2.20	0.41
30:0:932:U:H2'	30:0:933:C:C6	2.55	0.41
31:9:65:A:C2'	31:9:66:G:OP2	2.67	0.41
1:A:153:ARG:NH1	1:A:153:ARG:HB2	2.35	0.41
1:A:89:ALA:HB3	37:A:8616:HOH:O	2.19	0.41
23:W:21:LEU:HD13	23:W:26:ILE:HD11	2.02	0.41
30:0:1257:C:H2'	30:0:1258:G:O4'	2.20	0.41
30:0:1819:G:H2'	30:0:1820:G:C5'	2.51	0.41
30:0:2518:C:H2'	30:0:2519:C:O4'	2.20	0.41
30:0:2809:G:H2'	30:0:2810:G:O4'	2.21	0.41
18:R:98:ASN:ND2	30:0:500:G:H21	2.14	0.41
30:0:664:U:O4	30:0:681:G:H5'	2.20	0.41
28:2:18:ASN:ND2	28:2:40:ARG:H	2.17	0.41
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.50	0.41
5:E:108:LEU:HD11	5:E:164:ASP:HB2	2.02	0.41
7:G:65:THR:O	7:G:69:ARG:HB2	2.19	0.41
18:R:119:VAL:HG21	18:R:142:ASP:CG	2.40	0.41
30:0:1171:A:H2'	30:0:1172:G:H5'	2.02	0.41
30:0:1926:G:H2'	30:0:1927:A:H8	1.82	0.41
30:0:2003:U:H4'	30:0:2004:U:H5	1.84	0.41
27:1:2:GLY:O	27:1:6:PRO:HG2	2.20	0.41
7:G:63:ARG:N	37:G:2569:HOH:O	2.53	0.41
20:T:2:LYS:HE2	37:0:6955:HOH:O	2.20	0.41
23:W:81:ASP:OD1	23:W:92:ASP:HB2	2.19	0.41
30:0:1185:U:H2'	30:0:1186:C:H6	1.82	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1413:A:H2'	30:0:1414:A:O4'	2.20	0.41
1:A:204:GLY:N	30:0:2634:G:OP2	2.41	0.41
30:0:2729:C:O2'	30:0:2730:G:H5'	2.20	0.41
30:0:2897:C:H2'	30:0:2898:G:H8	1.85	0.41
30:0:371:U:H2'	30:0:372:A:H8	1.86	0.41
30:0:666:A:H2'	30:0:667:C:O4'	2.21	0.41
29:3:7:PHE:HE2	29:3:22:VAL:HG21	1.86	0.41
31:9:107:C:H2'	31:9:108:C:C6	2.55	0.41
31:9:68:G:C6	31:9:69:U:C4	3.08	0.41
1:A:101:GLU:OE2	1:A:131:HIS:HB2	2.20	0.41
2:B:217:ARG:HG3	2:B:257:THR:HG22	2.01	0.41
5:E:154:ILE:HD11	5:E:157:LYS:HE2	2.03	0.41
9:I:94:ASP:OD1	9:I:133:THR:HB	2.21	0.41
10:J:52:GLN:NE2	30:0:1119:G:C8	2.87	0.41
11:K:65:ARG:HD3	37:K:5358:HOH:O	2.20	0.41
12:L:48:LYS:HE2	30:0:220:C:C2	2.56	0.41
16:P:59:ARG:HH22	16:P:66:GLN:NE2	2.16	0.41
22:V:38:GLY:C	22:V:40:PRO:HD2	2.41	0.41
25:Y:186:ARG:HG2	25:Y:186:ARG:HH11	1.86	0.41
26:Z:43:GLY:O	26:Z:47:ARG:HG2	2.21	0.41
30:0:625:U:H5'	30:0:1044:C:N4	2.35	0.41
30:0:1172:G:H1'	37:0:4513:HOH:O	2.20	0.41
30:0:2015:A:H2'	30:0:2016:U:O4'	2.21	0.41
30:0:255:A:H2'	30:0:256:C:H6	1.84	0.41
30:0:401:C:H2'	30:0:402:U:C6	2.55	0.41
30:0:558:C:H5'	37:0:4803:HOH:O	2.20	0.41
30:0:940:G:C5	30:0:1027:G:C2	3.08	0.41
1:A:95:PRO:HA	1:A:153:ARG:HA	2.02	0.41
4:D:96:SER:C	4:D:98:PHE:H	2.23	0.41
5:E:47:VAL:HG11	5:E:69:ILE:HD13	2.03	0.41
15:O:25:VAL:HG23	15:O:26:TRP:N	2.36	0.41
30:0:1529:G:H5'	37:0:6937:HOH:O	2.20	0.41
30:0:1626:A:H2'	30:0:1627:G:O4'	2.20	0.41
30:0:1815:A:H2'	30:0:1816:C:O4'	2.21	0.41
30:0:368:C:H2'	30:0:369:G:H5'	2.02	0.41
30:0:646:G:H2'	30:0:647:U:C6	2.56	0.41
3:C:214:THR:HG21	37:C:8399:HOH:O	2.20	0.41
4:D:151:ILE:HA	4:D:152:PRO:HD3	1.95	0.41
12:L:121:ILE:HG12	12:L:141:GLU:HB2	2.01	0.41
30:0:1023:C:H2'	30:0:1024:G:O4'	2.20	0.41
30:0:2718:C:H5'	30:0:2718:C:C6	2.53	0.41
2:B:28:SER:HB2	30:0:2807:U:OP2	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2756:U:O2	30:0:2896:A:H2	2.03	0.41
30:0:2906:A:H5'	30:0:2907:C:O4'	2.21	0.41
30:0:38:G:N2	37:0:6885:HOH:O	2.54	0.41
30:0:424:C:H2'	30:0:425:U:C6	2.55	0.41
1:A:165:THR:HG22	37:A:8611:HOH:O	2.21	0.41
3:C:46:TYR:CE2	3:C:98:ARG:NH1	2.89	0.41
6:F:111:ILE:O	6:F:115:VAL:HG23	2.20	0.41
6:F:34:ASN:HA	13:M:4:ALA:HB2	2.03	0.41
9:I:133:THR:HG22	9:I:134:ILE:H	1.86	0.41
13:M:169:ARG:NH2	37:M:8548:HOH:O	2.51	0.41
20:T:47:THR:HB	20:T:100:ASP:HB3	2.01	0.41
37:K:7438:HOH:O	21:U:20:MET:HE1	2.21	0.41
30:0:1611:G:O2'	30:0:1612:A:H5'	2.21	0.41
30:0:1883:U:H5'	30:0:2012:U:OP2	2.20	0.41
30:0:282:C:C2'	30:0:283:U:H5'	2.51	0.41
30:0:290:C:H1'	37:0:5650:HOH:O	2.20	0.41
30:0:365:G:C6	30:0:366:U:C4	3.09	0.41
30:0:603:A:H1'	30:0:605:C:C2	2.56	0.41
1:A:205:GLY:HA3	37:0:5905:HOH:O	2.21	0.41
10:J:26:VAL:HG13	10:J:36:VAL:HG11	2.02	0.41
10:J:63:ILE:HD11	30:0:1236:A:C8	2.56	0.41
11:K:22:ASP:HB2	37:K:5264:HOH:O	2.21	0.41
14:N:171:HIS:CE1	37:N:8566:HOH:O	2.74	0.41
20:T:38:ARG:HH21	30:0:306:A:P	2.44	0.41
30:0:1139:U:H2'	30:0:1140:C:C6	2.56	0.41
30:0:1159:G:H1	30:0:1208:C:N4	2.18	0.41
30:0:1429:U:C2'	30:0:1430:G:H5'	2.51	0.41
30:0:2362:A:H2'	30:0:2363:G:C8	2.56	0.41
30:0:661:G:C6	30:0:686:A:C2	3.08	0.41
31:9:96:C:H2'	31:9:97:U:C6	2.56	0.41
8:H:31:ILE:HA	8:H:66:GLU:OE1	2.20	0.41
6:F:38:LYS:NZ	13:M:3:SER:HA	2.36	0.41
25:Y:99:ALA:HB2	25:Y:233:TYR:CZ	2.55	0.41
1:A:72:GLU:HG3	26:Z:90:GLY:HA2	2.03	0.41
30:0:1080:C:O5'	30:0:1080:C:H6	2.03	0.40
30:0:2237:G:H1'	37:0:4393:HOH:O	2.20	0.40
30:0:2691:A:OP1	30:0:2691:A:H8	2.04	0.40
30:0:812:A:H2'	30:0:813:C:O4'	2.20	0.40
30:0:999:C:H2'	30:0:1000:C:O4'	2.21	0.40
31:9:12:C:H5'	31:9:70:U:O4'	2.21	0.40
1:A:211:LYS:HB3	1:A:212:PRO:CD	2.50	0.40
2:B:116:PRO:HG3	30:0:2821:C:H4'	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:I:87:PRO:C	9:I:89:GLU:N	2.75	0.40
10:J:80:LYS:HE2	10:J:98:PHE:CE1	2.56	0.40
15:O:26:TRP:HB2	37:O:3062:HOH:O	2.19	0.40
23:W:149:LEU:HG	23:W:153:MET:HE1	2.03	0.40
25:Y:155:ARG:NH1	37:Y:8556:HOH:O	2.53	0.40
30:0:1076:G:C2	30:0:1084:C:C2	3.09	0.40
30:0:1191:A:H2'	30:0:1193:A:H5'	2.03	0.40
30:0:1976:G:O2'	30:0:1977:U:H5'	2.21	0.40
30:0:2103:A:O2'	30:0:2104:C:H5'	2.21	0.40
30:0:2819:C:H2'	30:0:2820:A:C8	2.56	0.40
30:0:40:C:H6	30:0:40:C:O5'	2.04	0.40
11:K:115:ARG:NH2	37:K:3160:HOH:O	2.53	0.40
11:K:62:PRO:HG3	11:K:65:ARG:HH21	1.85	0.40
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.77	0.40
23:W:125:HIS:CE1	30:0:1097:A:H5''	2.55	0.40
30:0:1181:A:O2'	30:0:1182:C:H5'	2.20	0.40
28:2:10:ARG:NH2	30:0:121:U:OP2	2.40	0.40
30:0:1632:A:H2'	30:0:1633:C:C5'	2.46	0.40
30:0:1714:C:O2'	30:0:1715:C:H5'	2.21	0.40
10:J:70:PHE:CD1	30:0:2676:C:H4'	2.56	0.40
30:0:383:A:C2	30:0:407:A:C4	3.09	0.40
30:0:64:G:H2'	30:0:65:C:O4'	2.22	0.40
30:0:858:U:H2'	30:0:859:C:C6	2.56	0.40
31:9:107:C:O2'	31:9:108:C:H5'	2.22	0.40
1:A:69:LEU:HD21	1:A:120:ARG:HB3	2.03	0.40
2:B:141:ARG:HG2	2:B:165:ARG:HA	2.03	0.40
2:B:56:ASP:OD1	2:B:322:ARG:HB3	2.21	0.40
4:D:58:VAL:HB	4:D:62:ASP:HB3	2.02	0.40
5:E:91:PHE:HA	5:E:92:PRO:HD3	1.92	0.40
8:H:12:ILE:HD12	8:H:57:THR:HG22	2.03	0.40
23:W:35:VAL:HA	23:W:36:PRO:HD3	1.78	0.40
23:W:5:VAL:HG11	23:W:153:MET:CE	2.51	0.40
24:X:78:GLU:HG2	24:X:79:GLU:H	1.86	0.40
25:Y:184:GLU:OE1	25:Y:204:ARG:NH1	2.55	0.40
30:0:1046:G:N3	30:0:1082:A:H2	2.19	0.40
30:0:1434:A:H2'	30:0:1436:C:C5	2.56	0.40
30:0:2314:G:H2'	30:0:2315:C:H5'	2.03	0.40
30:0:10:U:C4	30:0:532:A:N7	2.89	0.40
28:2:40:ARG:HG3	28:2:45:ASN:HB2	2.04	0.40
31:9:2:U:H4'	37:9:8480:HOH:O	2.20	0.40
1:A:153:ARG:CB	1:A:153:ARG:HH11	2.33	0.40
2:B:53:LEU:HD11	2:B:327:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:91:VAL:CG1	6:F:92:GLY:N	2.84	0.40
9:I:70:THR:OG1	9:I:107:LYS:HE2	2.22	0.40
14:N:37:ARG:HH12	31:9:6:C:C5'	2.23	0.40
14:N:78:MET:HB2	14:N:79:PRO:HD3	2.02	0.40
24:X:30:MET:CE	24:X:58:ALA:HB3	2.52	0.40
30:0:1333:U:H2'	30:0:1334:C:H6	1.86	0.40
30:0:1571:G:C2'	30:0:1626:A:H61	2.34	0.40
30:0:1656:A:H2'	30:0:1657:A:O4'	2.21	0.40
30:0:2002:C:H2'	30:0:2003:U:H5'	2.03	0.40
30:0:2575:C:H2'	30:0:2576:A:O4'	2.21	0.40
30:0:553:G:O4'	30:0:1325:G:H5'	2.20	0.40
30:0:563:C:H2'	30:0:564:G:O4'	2.22	0.40
30:0:622:G:O2'	30:0:623:U:H5'	2.21	0.40
15:O:38:ARG:HD3	30:0:654:A:OP2	2.22	0.40
30:0:671:A:O2'	30:0:672:G:H2'	2.22	0.40
2:B:36:PRO:HG3	2:B:169:GLY:H	1.86	0.40
2:B:275:GLY:O	2:B:291:ASP:HA	2.21	0.40
2:B:41:PHE:CZ	2:B:79:MET:HG3	2.56	0.40
3:C:138:VAL:O	3:C:234:VAL:HA	2.21	0.40
5:E:22:VAL:O	5:E:28:SER:HA	2.22	0.40
14:N:21:HIS:HD2	37:0:4268:HOH:O	2.05	0.40
14:N:38:LYS:HB2	14:N:38:LYS:HE3	1.81	0.40
19:S:77:VAL:O	19:S:80:ARG:HG2	2.22	0.40
23:W:88:THR:CG2	23:W:89:ASP:H	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
1	A	235/240 (98%)	220 (94%)	13 (6%)	2 (1%)	25	35
2	B	335/338 (99%)	315 (94%)	17 (5%)	3 (1%)	25	35
3	C	244/246 (99%)	231 (95%)	13 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	134/177 (76%)	115 (86%)	15 (11%)	4 (3%)	7	5
5	E	170/178 (96%)	165 (97%)	5 (3%)	0	100	100
6	F	117/120 (98%)	106 (91%)	9 (8%)	2 (2%)	14	17
7	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
8	H	156/177 (88%)	148 (95%)	8 (5%)	0	100	100
9	I	68/162 (42%)	57 (84%)	11 (16%)	0	100	100
10	J	140/145 (97%)	132 (94%)	7 (5%)	1 (1%)	30	43
11	K	130/132 (98%)	124 (95%)	5 (4%)	1 (1%)	27	39
12	L	141/165 (86%)	126 (89%)	14 (10%)	1 (1%)	30	43
13	M	192/196 (98%)	187 (97%)	5 (3%)	0	100	100
14	N	184/187 (98%)	170 (92%)	11 (6%)	3 (2%)	14	18
15	O	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
16	P	141/149 (95%)	140 (99%)	1 (1%)	0	100	100
17	Q	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
18	R	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
19	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
20	T	117/120 (98%)	112 (96%)	5 (4%)	0	100	100
21	U	51/67 (76%)	48 (94%)	2 (4%)	1 (2%)	11	13
22	V	63/71 (89%)	60 (95%)	2 (3%)	1 (2%)	14	18
23	W	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	30	43
24	X	80/92 (87%)	74 (92%)	5 (6%)	1 (1%)	18	24
25	Y	140/241 (58%)	140 (100%)	0	0	100	100
26	Z	71/116 (61%)	63 (89%)	6 (8%)	2 (3%)	8	6
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	42 (100%)	0	0	100	100
29	3	90/92 (98%)	87 (97%)	3 (3%)	0	100	100
All	All	3705/4472 (83%)	3505 (95%)	177 (5%)	23 (1%)	33	47

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
6	F	101	ALA

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Mol	Chain	Res	Type
10	J	5	GLU
12	L	80	ASP
14	N	154	LEU
14	N	184	ILE
4	D	27	ILE
14	N	183	ASP
22	V	43	PRO
23	W	77	ALA
26	Z	105	ARG
2	B	185	GLY
4	D	56	ARG
4	D	65	GLU
21	U	55	ALA
26	Z	66	CYS
1	A	34	ASP
4	D	171	ASP
2	B	169	GLY
11	K	126	SER
6	F	100	ASP
2	B	2	GLN
24	X	70	ILE

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	
1	A	179/182 (98%)	171 (96%)	8 (4%)	38	57
2	B	282/283 (100%)	268 (95%)	14 (5%)	34	51
3	C	193/193 (100%)	179 (93%)	14 (7%)	20	30
4	D	117/148 (79%)	112 (96%)	5 (4%)	40	59
5	E	152/156 (97%)	148 (97%)	4 (3%)	59	79
6	F	93/94 (99%)	92 (99%)	1 (1%)	84	94
7	G	27/282 (10%)	26 (96%)	1 (4%)	45	66
8	H	134/145 (92%)	129 (96%)	5 (4%)	45	66
9	I	58/130 (45%)	57 (98%)	1 (2%)	73	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	118/121 (98%)	110 (93%)	8 (7%)	22	34
11	K	106/106 (100%)	103 (97%)	3 (3%)	56	77
12	L	113/127 (89%)	110 (97%)	3 (3%)	57	78
13	M	158/160 (99%)	152 (96%)	6 (4%)	44	65
14	N	149/150 (99%)	146 (98%)	3 (2%)	68	86
15	O	93/94 (99%)	90 (97%)	3 (3%)	51	72
16	P	113/117 (97%)	111 (98%)	2 (2%)	71	88
17	Q	79/80 (99%)	75 (95%)	4 (5%)	33	50
18	R	117/122 (96%)	115 (98%)	2 (2%)	73	89
19	S	71/74 (96%)	69 (97%)	2 (3%)	56	77
20	T	105/106 (99%)	98 (93%)	7 (7%)	23	35
21	U	44/53 (83%)	44 (100%)	0	100	100
22	V	51/57 (90%)	49 (96%)	2 (4%)	43	64
23	W	130/130 (100%)	123 (95%)	7 (5%)	31	47
24	X	66/74 (89%)	60 (91%)	6 (9%)	14	20
25	Y	120/196 (61%)	112 (93%)	8 (7%)	23	35
26	Z	60/94 (64%)	58 (97%)	2 (3%)	50	71
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	61	81
29	3	79/79 (100%)	78 (99%)	1 (1%)	80	93
All	All	3095/3646 (85%)	2972 (96%)	123 (4%)	42	63

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	36	ASP
1	A	55	VAL
1	A	94	LEU
1	A	120	ARG
1	A	131	HIS
1	A	179	MET
1	A	217	ARG
2	B	7	ARG
2	B	11	LEU

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Mol	Chain	Res	Type
2	B	27	ASN
2	B	49	THR
2	B	53	LEU
2	B	56	ASP
2	B	97	LEU
2	B	98	THR
2	B	162	MET
2	B	174	ARG
2	B	190	MET
2	B	254	GLN
2	B	264	GLU
2	B	312	ARG
3	C	2	GLN
3	C	27	ARG
3	C	67	GLN
3	C	94	THR
3	C	136	VAL
3	C	162	VAL
3	C	187	ARG
3	C	214	THR
3	C	222	ASP
3	C	223	LEU
3	C	234	VAL
3	C	236	THR
3	C	240	LEU
3	C	243	VAL
4	D	24	HIS
4	D	61	PHE
4	D	133	ASN
4	D	136	ARG
4	D	137	PRO
5	E	16	ASP
5	E	86	VAL
5	E	102	VAL
5	E	164	ASP
6	F	12	LEU
7	G	73	ASP
8	H	87	LYS
8	H	91	ARG
8	H	149	VAL
8	H	157	TYR
8	H	174	LEU

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Mol	Chain	Res	Type
9	I	135	GLU
10	J	7	ASP
10	J	39	VAL
10	J	46	ILE
10	J	52	GLN
10	J	74	ARG
10	J	79	PHE
10	J	107	ASN
10	J	127	ILE
11	K	10	GLN
11	K	49	LEU
11	K	98	VAL
12	L	35	ARG
12	L	80	ASP
12	L	140	VAL
13	M	46	LEU
13	M	68	ARG
13	M	81	ARG
13	M	93	ARG
13	M	99	ARG
13	M	164	THR
14	N	17	ARG
14	N	26	LEU
14	N	127	LEU
15	O	3	THR
15	O	98	LEU
15	O	111	VAL
16	P	91	LYS
16	P	98	ILE
17	Q	11	ARG
17	Q	16	ASN
17	Q	57	ASP
17	Q	95	GLU
18	R	13	THR
18	R	39	THR
19	S	12	GLU
19	S	71	ASP
20	T	26	THR
20	T	39	ASN
20	T	48	VAL
20	T	73	HIS
20	T	89	ARG

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Mol	Chain	Res	Type
20	T	96	VAL
20	T	115	GLU
22	V	43	PRO
22	V	65	ASP
23	W	26	ILE
23	W	35	VAL
23	W	52	VAL
23	W	73	LEU
23	W	122	ARG
23	W	142	ASP
23	W	146	ILE
24	X	15	ARG
24	X	27	ASP
24	X	49	ARG
24	X	72	VAL
24	X	82	GLU
24	X	88	GLU
25	Y	141	THR
25	Y	154	ARG
25	Y	172	THR
25	Y	187	VAL
25	Y	189	ASN
25	Y	200	THR
25	Y	203	VAL
25	Y	220	GLU
26	Z	57	MET
26	Z	68	GLU
28	2	18	ASN
29	3	42	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	HIS
2	B	27	ASN
2	B	145	HIS
2	B	221	GLN
2	B	238	ASN
2	B	256	GLN
2	B	260	HIS
2	B	320	GLN
2	B	332	ASN

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Mol	Chain	Res	Type
3	C	39	GLN
3	C	73	GLN
3	C	129	HIS
3	C	151	GLN
3	C	163	HIS
4	D	103	ASN
4	D	133	ASN
5	E	106	ASN
5	E	119	HIS
5	E	143	GLN
7	G	17	GLN
7	G	64	ASN
8	H	34	HIS
8	H	59	GLN
8	H	62	HIS
8	H	73	ASN
10	J	52	GLN
10	J	107	ASN
10	J	126	ASN
11	K	10	GLN
11	K	44	HIS
12	L	18	HIS
12	L	41	HIS
13	M	24	GLN
13	M	58	GLN
13	M	137	ASN
13	M	170	ASN
14	N	21	HIS
14	N	107	ASN
16	P	50	GLN
16	P	66	GLN
16	P	73	HIS
16	P	88	GLN
16	P	118	GLN
17	Q	40	HIS
18	R	61	GLN
18	R	94	ASN
18	R	98	ASN
18	R	113	HIS
18	R	117	HIS
19	S	9	HIS
19	S	51	GLN

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Mol	Chain	Res	Type
20	T	39	ASN
21	U	39	ASN
21	U	48	ASN
22	V	60	GLN
23	W	110	GLN
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS
24	X	23	HIS
25	Y	133	HIS
25	Y	134	HIS
25	Y	149	GLN
25	Y	189	ASN
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	16	ASN
28	2	18	ASN
28	2	41	HIS
28	2	45	ASN
29	3	2	GLN
29	3	15	ASN
29	3	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	224 (8%)	0
31	9	121/122 (99%)	16 (13%)	0
All	All	2866/3045 (94%)	240 (8%)	0

All (240) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G
30	0	86	A
30	0	87	C

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Mol	Chain	Res	Type
30	0	88	G
30	0	114	A
30	0	115	U
30	0	120	A
30	0	130	C
30	0	139	C
30	0	141	C
30	0	151	A
30	0	166	A
30	0	170	U
30	0	186	A
30	0	191	A
30	0	192	A
30	0	200	C
30	0	219	G
30	0	237	G
30	0	271	C
30	0	272	A
30	0	273	G
30	0	283	U
30	0	284	C
30	0	308	U
30	0	309	C
30	0	318	U
30	0	336	G
30	0	337	A
30	0	358	G
30	0	381	G
30	0	397	A
30	0	417	G
30	0	461	C
30	0	487	G
30	0	498	A
30	0	510	U
30	0	511	A
30	0	514	G
30	0	537	G
30	0	538	C
30	0	539	G
30	0	542	A
30	0	545	G
30	0	553	G

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Mol	Chain	Res	Type
30	0	559	U
30	0	588	G
30	0	604	G
30	0	620	A
30	0	632	A
30	0	644	G
30	0	660	A
30	0	688	A
30	0	701	U
30	0	735	C
30	0	759	C
30	0	777	U
30	0	809	G
30	0	821	U
30	0	835	U
30	0	840	U
30	0	868	G
30	0	869	G
30	0	871	G
30	0	872	U
30	0	875	A
30	0	877	G
30	0	878	G
30	0	884	C
30	0	885	G
30	0	898	G
30	0	905	C
30	0	921	G
30	0	923	A
30	0	953	G
30	0	960	G
30	0	961	A
30	0	1006	A
30	0	1008	C
30	0	1029	U
30	0	1045	G
30	0	1059	G
30	0	1060	C
30	0	1072	G
30	0	1081	A
30	0	1087	G
30	0	1088	A

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Mol	Chain	Res	Type
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1130	U
30	0	1137	G
30	0	1164	U
30	0	1165	G
30	0	1166	A
30	0	1174	A
30	0	1175	G
30	0	1185	U
30	0	1192	A
30	0	1193	A
30	0	1206	U
30	0	1216	G
30	0	1238	C
30	0	1239	G
30	0	1279	U
30	0	1289	C
30	0	1342	C
30	0	1353	C
30	0	1360	C
30	0	1377	C
30	0	1407	A
30	0	1409	G
30	0	1474	C
30	0	1485	A
30	0	1505	U
30	0	1506	U
30	0	1524	U
30	0	1525	G
30	0	1526	A
30	0	1528	A
30	0	1592	G
30	0	1603	A
30	0	1625	U
30	0	1626	A
30	0	1634	G
30	0	1656	A
30	0	1667	A
30	0	1682	A
30	0	1684	A

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Mol	Chain	Res	Type
30	0	1685	A
30	0	1692	C
30	0	1701	A
30	0	1722	U
30	0	1723	G
30	0	1725	C
30	0	1731	C
30	0	1752	G
30	0	1778	A
30	0	1779	A
30	0	1798	C
30	0	1820	G
30	0	1829	A
30	0	1856	C
30	0	1879	U
30	0	1919	A
30	0	1942	A
30	0	1943	C
30	0	1971	G
30	0	1973	A
30	0	1978	A
30	0	1979	G
30	0	1980	U
30	0	1996	U
30	0	2008	U
30	0	2011	A
30	0	2012	U
30	0	2013	G
30	0	2033	G
30	0	2034	U
30	0	2064	U
30	0	2072	G
30	0	2073	G
30	0	2074	A
30	0	2096	A
30	0	2101	A
30	0	2102	G
30	0	2103	A
30	0	2104	C
30	0	2110	G
30	0	2243	C
30	0	2258	A

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Mol	Chain	Res	Type
30	0	2271	G
30	0	2272	G
30	0	2291	A
30	0	2317	C
30	0	2321	A
30	0	2354	A
30	0	2361	A
30	0	2369	A
30	0	2422	U
30	0	2462	G
30	0	2469	A
30	0	2476	C
30	0	2480	G
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2533	C
30	0	2537	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2589	U
30	0	2601	A
30	0	2602	G
30	0	2608	C
30	0	2613	G
30	0	2649	A
30	0	2664	A
30	0	2681	A
30	0	2682	C
30	0	2719	A
30	0	2726	U
30	0	2747	C
30	0	2748	G
30	0	2749	U
30	0	2750	G
30	0	2762	C
30	0	2768	A
30	0	2792	A
30	0	2800	A
30	0	2811	A

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Mol	Chain	Res	Type
30	0	2825	C
30	0	2840	A
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	0	2903	C
30	0	2914	A
31	9	2	U
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	40	C
31	9	41	C
31	9	43	G
31	9	44	A
31	9	52	A
31	9	57	A
31	9	66	G
31	9	77	A
31	9	114	G
31	9	122	C

There are no RNA pucker outliers to report.

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	$\# Z > 2$
30	OMU	0	2587	30	20,22,23	1.36	1 (5%)	24,31,34	0.73	0
30	OMG	0	2588	30	24,26,27	0.84	0	33,38,41	5.30	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	UR3	0	2619	30	20,22,23	1.41	1 (5%)	23,32,35	0.76	0
30	PSU	0	2621	30	19,21,22	1.39	1 (5%)	23,30,33	0.94	0
30	1MA	0	628	30,34	23,25,26	0.95	1 (4%)	32,37,40	0.96	1 (3%)

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
30	OMU	0	2587	30	-	0/8/27/28	0/2/2/2
30	OMG	0	2588	30	-	0/10/27/28	0/3/3/3
30	UR3	0	2619	30	-	0/6/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/8/25/26	0/2/2/2
30	1MA	0	628	30,34	-	1/8/25/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2619	UR3	C5-C4	5.48	1.43	1.37
30	0	2587	OMU	C5-C4	5.10	1.43	1.37
30	0	2621	PSU	C5-C1'	-4.69	1.48	1.52
30	0	628	1MA	C6-N6	2.30	1.33	1.29

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2588	OMG	C6-C5-N7	-28.58	130.29	134.14
30	0	2588	OMG	C6-N1-C2	8.95	125.25	120.20
30	0	628	1MA	C2-N3-C4	-3.43	110.65	116.23
30	0	2588	OMG	C2-N3-C4	-2.91	111.81	115.30
30	0	2588	OMG	C5-C4-N3	2.12	128.50	126.07

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	0	628	1MA	C2'-C1'-N9-C8

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 231 ligands modelled in this entry, 231 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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	A	237/240 (98%)	0.18	11 (4%) 31 29	19, 38, 77, 98	0
2	B	337/338 (99%)	0.20	10 (2%) 48 45	21, 46, 74, 84	0
3	C	246/246 (100%)	0.07	5 (2%) 62 59	15, 36, 60, 71	0
4	D	140/177 (79%)	2.21	68 (48%) 1 0	47, 90, 115, 123	0
5	E	172/178 (96%)	0.64	14 (8%) 12 10	39, 61, 81, 85	0
6	F	119/120 (99%)	0.65	12 (10%) 7 7	34, 61, 90, 104	0
7	G	29/348 (8%)	1.98	12 (41%) 1 0	69, 86, 95, 98	0
8	H	160/177 (90%)	0.54	11 (6%) 17 15	30, 48, 83, 90	0
9	I	70/162 (43%)	3.98	57 (81%) 0 0	122, 136, 154, 155	0
10	J	142/145 (97%)	0.20	2 (1%) 72 71	29, 43, 66, 89	0
11	K	132/132 (100%)	0.02	5 (3%) 38 36	27, 42, 65, 77	0
12	L	145/165 (87%)	0.51	14 (9%) 8 7	18, 55, 101, 117	0
13	M	194/196 (98%)	-0.33	0 100 100	20, 31, 47, 55	0
14	N	186/187 (99%)	0.52	18 (9%) 8 7	32, 53, 102, 112	0
15	O	115/116 (99%)	0.04	3 (2%) 53 51	29, 45, 62, 70	0
16	P	143/149 (95%)	0.10	1 (0%) 84 84	31, 45, 57, 68	0
17	Q	95/96 (98%)	0.04	1 (1%) 77 77	26, 35, 54, 66	0
18	R	150/155 (96%)	-0.13	1 (0%) 84 84	22, 37, 58, 71	0
19	S	81/85 (95%)	0.43	6 (7%) 14 13	31, 48, 72, 82	0
20	T	119/120 (99%)	0.27	0 100 100	29, 46, 78, 98	0
21	U	53/67 (79%)	0.09	1 (1%) 64 61	34, 48, 66, 76	0
22	V	65/71 (91%)	1.50	9 (13%) 4 3	40, 62, 106, 113	0
23	W	154/154 (100%)	0.26	4 (2%) 53 51	28, 42, 59, 71	0
24	X	82/92 (89%)	0.41	5 (6%) 21 18	36, 50, 78, 94	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	-0.09	5 (3%) 42 40	22, 36, 60, 80	0
26	Z	73/116 (62%)	0.19	5 (6%) 17 15	34, 48, 68, 87	0
27	1	56/57 (98%)	-0.26	0 100 100	19, 24, 31, 40	0
28	2	46/50 (92%)	0.41	3 (6%) 18 17	26, 50, 75, 89	0
29	3	92/92 (100%)	0.05	1 (1%) 77 77	22, 45, 62, 76	0
30	0	2754/2923 (94%)	-0.19	55 (1%) 62 59	16, 36, 81, 155	0
31	9	122/122 (100%)	-0.09	5 (4%) 35 33	31, 54, 77, 138	0
All	All	6651/7517 (88%)	0.13	344 (5%) 28 24	15, 42, 89, 155	0

All (344) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	V	1	THR	13.0
22	V	39	ALA	10.8
14	N	166	ALA	9.9
4	D	63	ILE	9.8
22	V	40	PRO	9.4
9	I	91	PHE	8.8
9	I	128	THR	8.6
1	A	237	GLY	8.4
9	I	97	VAL	8.0
9	I	80	PHE	7.6
4	D	57	THR	7.3
9	I	88	GLN	7.1
9	I	74	ILE	6.7
8	H	174	LEU	6.6
9	I	79	GLY	6.5
24	X	88	GLU	6.4
9	I	72	GLU	6.3
9	I	66	GLY	6.3
22	V	38	GLY	6.2
9	I	108	HIS	6.0
9	I	76	ASP	5.9
9	I	132	VAL	5.9
4	D	64	ARG	5.8
9	I	116	LEU	5.8
9	I	113	SER	5.6
4	D	10	PHE	5.6
1	A	37	VAL	5.5
9	I	111	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
9	I	99	GLN	5.4
9	I	70	THR	5.4
9	I	98	ASP	5.4
9	I	109	PRO	5.4
4	D	44	ILE	5.3
9	I	104	ALA	5.3
9	I	112	LEU	5.3
19	S	81	ILE	5.2
9	I	106	GLN	5.2
4	D	61	PHE	5.2
7	G	27	ILE	5.2
9	I	102	GLN	5.0
30	0	960	G	5.0
9	I	83	GLY	4.9
6	F	119	ARG	4.9
7	G	24	VAL	4.9
30	0	1172	G	4.9
9	I	114	TYR	4.9
30	0	1198	U	4.8
30	0	282	C	4.8
22	V	43	PRO	4.7
30	0	1199	A	4.7
9	I	84	SER	4.7
30	0	1171	A	4.7
9	I	71	ALA	4.6
30	0	1202	A	4.6
4	D	166	ILE	4.6
4	D	165	PHE	4.6
4	D	18	ILE	4.6
9	I	100	VAL	4.5
31	9	1	U	4.5
12	L	80	ASP	4.4
9	I	86	GLU	4.3
9	I	92	VAL	4.3
12	L	150	GLN	4.3
4	D	170	TYR	4.3
28	2	49	GLU	4.2
9	I	73	LEU	4.2
4	D	75	LEU	4.2
22	V	41	GLU	4.2
5	E	87	PHE	4.1
9	I	78	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
4	D	93	LEU	4.1
9	I	89	GLU	4.0
9	I	68	PRO	4.0
7	G	71	LEU	4.0
4	D	172	VAL	4.0
4	D	74	THR	3.9
8	H	169	GLU	3.9
4	D	58	VAL	3.9
30	0	1173	A	3.9
31	9	24	U	3.9
14	N	152	GLU	3.9
30	0	1203	G	3.9
4	D	66	GLY	3.8
4	D	85	GLN	3.8
4	D	68	PRO	3.8
25	Y	235	GLU	3.8
7	G	28	GLU	3.7
19	S	2	TRP	3.7
24	X	80	GLU	3.7
9	I	81	GLU	3.7
12	L	81	VAL	3.7
4	D	56	ARG	3.7
9	I	69	PRO	3.7
9	I	105	GLU	3.7
30	0	1279	U	3.7
4	D	104	PHE	3.7
4	D	40	ILE	3.7
6	F	117	GLU	3.7
30	0	284	C	3.6
25	Y	108	ASP	3.6
9	I	118	ASN	3.6
30	0	1200	A	3.6
7	G	26	MET	3.6
4	D	69	ILE	3.5
5	E	10	ASP	3.5
8	H	172	GLU	3.5
9	I	67	VAL	3.5
25	Y	95	THR	3.5
4	D	98	PHE	3.5
4	D	27	ILE	3.5
4	D	95	THR	3.5
19	S	1	SER	3.4

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Mol	Chain	Res	Type	RSRZ
4	D	106	PHE	3.4
30	0	1951	G	3.4
30	0	2637	A	3.4
12	L	149	ARG	3.4
3	C	132	ASP	3.4
1	A	35	GLY	3.4
9	I	115	ASP	3.4
30	0	2237	G	3.4
22	V	37	GLY	3.4
9	I	103	ILE	3.3
26	Z	34	SER	3.3
7	G	23	ILE	3.3
30	0	1196	C	3.3
2	B	1	PRO	3.3
4	D	157	LEU	3.2
4	D	17	ARG	3.2
4	D	11	HIS	3.2
4	D	92	GLU	3.2
4	D	134	LEU	3.2
5	E	45	ASP	3.2
30	0	10	U	3.2
4	D	65	GLU	3.2
23	W	86	GLU	3.2
31	9	23	U	3.2
12	L	105	TYR	3.1
8	H	76	LEU	3.1
9	I	130	LEU	3.1
14	N	154	LEU	3.1
11	K	119	GLN	3.1
4	D	45	THR	3.1
4	D	101	THR	3.1
5	E	170	ARG	3.1
30	0	1197	G	3.1
4	D	81	GLU	3.1
25	Y	236	VAL	3.1
4	D	84	LEU	3.1
8	H	40	GLN	3.0
21	U	47	ARG	3.0
12	L	148	GLU	3.0
30	0	1195	G	3.0
30	0	2238	A	3.0
4	D	22	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
9	I	119	ALA	3.0
4	D	48	MET	3.0
2	B	104	GLU	3.0
30	0	2103	A	3.0
4	D	94	ALA	3.0
30	0	1201	C	3.0
11	K	118	ALA	3.0
4	D	139	TYR	3.0
4	D	62	ASP	3.0
10	J	4	ALA	3.0
4	D	43	GLU	3.0
9	I	87	PRO	2.9
30	0	128	A	2.9
30	0	1177	A	2.9
24	X	71	ARG	2.9
4	D	174	VAL	2.9
1	A	64	ASP	2.9
4	D	26	GLY	2.9
14	N	138	ASP	2.9
19	S	76	GLU	2.9
14	N	161	GLY	2.9
30	0	1169	U	2.9
1	A	36	ASP	2.9
4	D	171	ASP	2.9
30	0	1204	C	2.9
30	0	2508	C	2.9
9	I	110	ASP	2.9
30	0	1180	U	2.8
18	R	150	PRO	2.8
5	E	11	VAL	2.8
24	X	85	VAL	2.8
4	D	167	GLU	2.8
4	D	173	GLU	2.8
30	0	1165	G	2.8
30	0	1950	G	2.8
9	I	131	GLY	2.8
4	D	23	VAL	2.8
7	G	73	ASP	2.8
9	I	82	THR	2.8
30	0	1163	G	2.8
30	0	1168	C	2.8
11	K	132	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	38	ILE	2.8
30	0	1181	A	2.8
5	E	100	ASP	2.8
5	E	127	ASP	2.8
5	E	126	ILE	2.8
14	N	158	LEU	2.8
9	I	120	ALA	2.7
30	0	1525	G	2.7
14	N	147	ILE	2.7
5	E	169	THR	2.7
31	9	122	C	2.7
6	F	44	SER	2.7
9	I	123	VAL	2.7
7	G	72	ASP	2.7
9	I	117	THR	2.6
12	L	104	ASP	2.6
14	N	183	ASP	2.6
4	D	47	GLN	2.6
8	H	165	ARG	2.6
30	0	1182	C	2.6
4	D	80	ALA	2.6
30	0	735	C	2.6
9	I	133	THR	2.6
30	0	970	U	2.6
4	D	73	VAL	2.6
31	9	2	U	2.6
4	D	99	ASP	2.5
14	N	155	GLU	2.5
6	F	98	VAL	2.5
8	H	77	ILE	2.5
9	I	95	LEU	2.5
4	D	67	ASP	2.5
7	G	12	ILE	2.5
9	I	94	ASP	2.5
30	0	138	U	2.5
15	O	23	GLY	2.5
30	0	2825	C	2.5
9	I	101	LYS	2.5
4	D	90	LEU	2.5
9	I	124	VAL	2.5
1	A	85	SER	2.5
26	Z	104	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
14	N	164	ASP	2.4
12	L	145	LEU	2.4
30	O	1948	G	2.4
30	O	2344	G	2.4
26	Z	48	ARG	2.4
4	D	77	ASP	2.4
2	B	117	GLU	2.4
12	L	147	GLU	2.4
4	D	86	THR	2.4
10	J	5	GLU	2.4
2	B	109	LEU	2.4
9	I	127	CYS	2.4
4	D	89	PRO	2.4
30	O	999	C	2.4
2	B	116	PRO	2.4
14	N	150	TYR	2.4
9	I	90	ASP	2.4
4	D	135	VAL	2.3
12	L	60	GLU	2.3
2	B	92	TYR	2.3
4	D	88	LEU	2.3
3	C	135	GLU	2.3
12	L	91	VAL	2.3
6	F	29	VAL	2.3
4	D	25	MET	2.3
26	Z	46	SER	2.3
6	F	118	LEU	2.3
2	B	181	ILE	2.3
4	D	71	ALA	2.3
5	E	154	ILE	2.3
30	O	1625	U	2.3
4	D	132	VAL	2.3
2	B	57	GLU	2.3
1	A	63	GLY	2.3
8	H	86	TYR	2.3
14	N	159	TYR	2.3
7	G	20	VAL	2.3
19	S	45	TYR	2.3
3	C	134	ASP	2.3
24	X	10	VAL	2.3
5	E	28	SER	2.3
26	Z	49	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
14	N	177	GLU	2.3
14	N	157	PRO	2.2
14	N	149	GLU	2.2
15	O	1	SER	2.2
28	2	35	ARG	2.2
30	0	1174	A	2.2
1	A	236	GLY	2.2
3	C	198	ASP	2.2
22	V	65	ASP	2.2
6	F	116	GLU	2.2
30	0	1170	U	2.2
17	Q	92	ARG	2.2
11	K	101	ASN	2.2
5	E	129	GLU	2.2
5	E	76	VAL	2.2
2	B	184	ASP	2.2
7	G	21	ASP	2.2
29	3	56	PRO	2.2
6	F	39	SER	2.2
5	E	88	TYR	2.2
6	F	17	LEU	2.2
4	D	156	ARG	2.2
11	K	129	THR	2.2
30	0	1192	A	2.2
15	O	104	ASN	2.1
1	A	82	VAL	2.1
4	D	130	VAL	2.1
14	N	68	GLU	2.1
7	G	25	GLU	2.1
14	N	156	GLU	2.1
19	S	43	GLU	2.1
30	0	2004	U	2.1
6	F	100	ASP	2.1
16	P	76	GLY	2.1
23	W	38	THR	2.1
2	B	119	HIS	2.1
8	H	82	GLU	2.1
12	L	121	ILE	2.1
4	D	164	ALA	2.1
30	0	280	C	2.1
23	W	96	LEU	2.1
25	Y	216	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	133	ARG	2.1
4	D	51	ARG	2.1
4	D	41	LEU	2.1
30	0	281	U	2.1
30	0	1205	U	2.1
22	V	45	ARG	2.1
30	0	285	A	2.1
12	L	102	ASP	2.1
8	H	144	GLU	2.0
6	F	18	GLU	2.0
4	D	50	VAL	2.0
8	H	149	VAL	2.0
30	0	31	C	2.0
12	L	89	PHE	2.0
14	N	181	ASP	2.0
28	2	39	ARG	2.0
6	F	108	VAL	2.0
3	C	131	PHE	2.0
30	0	87	C	2.0
23	W	93	ILE	2.0
30	0	1185	U	2.0
30	0	1949	G	2.0

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

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
30	UR3	0	2619	21/22	0.14	0.95	24,27,31,36	0
30	1MA	0	628	23/24	0.14	0.19	20,22,23,25	0
30	PSU	0	2621	20/21	0.13	-0.89	20,23,27,27	0
30	OMU	0	2587	21/22	0.10	-1.25	22,25,27,28	0
30	OMG	0	2588	24/25	0.12	-1.84	22,25,27,28	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
34	NA	0	8370	1/1	0.60	40.06	70,70,70,70	0
32	MG	0	8082	1/1	0.20	33.50	62,62,62,62	0
34	NA	0	8358	1/1	0.36	31.78	73,73,73,73	0
34	NA	0	8367	1/1	0.28	18.26	46,46,46,46	0
34	NA	0	8366	1/1	0.18	15.53	63,63,63,63	0
34	NA	0	8372	1/1	0.35	15.29	60,60,60,60	0
34	NA	0	8320	1/1	0.20	15.26	37,37,37,37	0
34	NA	0	8371	1/1	0.22	14.17	48,48,48,48	0
34	NA	0	8350	1/1	0.28	13.36	41,41,41,41	0
32	MG	0	8101	1/1	0.18	12.63	44,44,44,44	0
32	MG	0	8087	1/1	0.14	12.57	57,57,57,57	0
34	NA	0	8376	1/1	0.27	10.41	42,42,42,42	0
34	NA	R	8386	1/1	0.38	10.15	80,80,80,80	0
34	NA	0	8340	1/1	0.18	10.03	49,49,49,49	0
35	CL	0	8522	1/1	0.19	9.67	44,44,44,44	0
34	NA	0	8364	1/1	0.20	8.39	40,40,40,40	0
34	NA	L	8380	1/1	0.30	7.79	44,44,44,44	0
34	NA	0	8379	1/1	0.22	7.09	46,46,46,46	0
34	NA	0	8308	1/1	0.19	7.04	45,45,45,45	0
34	NA	0	8363	1/1	0.21	7.02	50,50,50,50	0
34	NA	0	8318	1/1	0.20	6.72	47,47,47,47	0
34	NA	0	8374	1/1	0.15	6.53	47,47,47,47	0
32	MG	0	8066	1/1	0.39	6.22	88,88,88,88	0
32	MG	0	8103	1/1	0.17	5.91	55,55,55,55	0
34	NA	0	8329	1/1	0.13	5.40	55,55,55,55	0
34	NA	0	8382	1/1	0.18	5.25	67,67,67,67	0
32	MG	0	8047	1/1	0.15	5.23	59,59,59,59	0
34	NA	0	8361	1/1	0.19	5.16	41,41,41,41	0
34	NA	0	8307	1/1	0.17	5.16	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	NA	0	8306	1/1	0.21	4.97	29,29,29,29	0
32	MG	0	8049	1/1	0.18	4.79	54,54,54,54	0
34	NA	0	8385	1/1	0.21	4.67	44,44,44,44	0
34	NA	0	8326	1/1	0.15	4.64	37,37,37,37	0
34	NA	0	8373	1/1	0.16	3.90	44,44,44,44	0
34	NA	0	8365	1/1	0.25	3.59	31,31,31,31	0
32	MG	0	8060	1/1	0.19	3.57	33,33,33,33	0
34	NA	0	8311	1/1	0.14	3.48	52,52,52,52	0
34	NA	0	8302	1/1	0.15	3.48	44,44,44,44	0
34	NA	0	8335	1/1	0.18	3.31	31,31,31,31	0
34	NA	0	8362	1/1	0.19	3.29	46,46,46,46	0
34	NA	0	8355	1/1	0.33	3.23	53,53,53,53	0
34	NA	0	8377	1/1	0.16	3.10	50,50,50,50	0
34	NA	0	8314	1/1	0.18	3.05	38,38,38,38	0
34	NA	0	8378	1/1	0.23	3.02	40,40,40,40	0
34	NA	0	8359	1/1	0.18	3.01	39,39,39,39	0
32	MG	0	8057	1/1	0.14	2.80	34,34,34,34	0
32	MG	0	8007	1/1	0.17	2.78	21,21,21,21	0
34	NA	0	8328	1/1	0.14	2.75	31,31,31,31	0
34	NA	9	8383	1/1	0.20	2.69	46,46,46,46	0
32	MG	0	8034	1/1	0.13	2.68	30,30,30,30	0
34	NA	0	8369	1/1	0.18	2.53	42,42,42,42	0
32	MG	0	8041	1/1	0.14	2.11	34,34,34,34	0
34	NA	0	8384	1/1	0.12	1.96	53,53,53,53	0
32	MG	0	8090	1/1	0.28	1.50	56,56,56,56	0
34	NA	0	8360	1/1	0.15	1.48	41,41,41,41	0
34	NA	0	8325	1/1	0.16	1.47	50,50,50,50	0
32	MG	0	8013	1/1	0.15	1.29	22,22,22,22	0
34	NA	0	8324	1/1	0.14	1.17	48,48,48,48	0
34	NA	0	8368	1/1	0.12	1.15	48,48,48,48	0
34	NA	0	8331	1/1	0.17	1.09	35,35,35,35	0
34	NA	0	8342	1/1	0.16	0.99	35,35,35,35	0
32	MG	0	8023	1/1	0.16	0.94	28,28,28,28	0
34	NA	H	8322	1/1	0.21	0.83	54,54,54,54	0
32	MG	0	8015	1/1	0.16	0.71	25,25,25,25	0
34	NA	0	8321	1/1	0.17	0.65	42,42,42,42	0
32	MG	0	8070	1/1	0.15	0.49	44,44,44,44	0
32	MG	0	8080	1/1	0.15	0.47	40,40,40,40	0
32	MG	0	8079	1/1	0.16	0.46	20,20,20,20	0
32	MG	0	8012	1/1	0.12	0.44	30,30,30,30	0
32	MG	0	8104	1/1	0.21	0.42	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	NA	0	8341	1/1	0.11	0.32	41,41,41,41	0
32	MG	0	8099	1/1	0.16	0.26	40,40,40,40	0
34	NA	0	8316	1/1	0.17	0.23	38,38,38,38	0
32	MG	0	8042	1/1	0.10	0.20	31,31,31,31	0
32	MG	0	8102	1/1	0.11	0.08	48,48,48,48	0
32	MG	0	8026	1/1	0.14	-0.09	23,23,23,23	0
32	MG	0	8010	1/1	0.14	-0.17	24,24,24,24	0
32	MG	0	8009	1/1	0.14	-0.17	25,25,25,25	0
32	MG	0	8061	1/1	0.15	-0.28	30,30,30,30	0
32	MG	0	8067	1/1	0.12	-0.42	28,28,28,28	0
35	CL	M	8518	1/1	0.12	-0.49	32,32,32,32	0
32	MG	9	8095	1/1	0.13	-0.52	64,64,64,64	0
35	CL	0	8503	1/1	0.12	-0.74	38,38,38,38	0
34	NA	C	8304	1/1	0.12	-0.75	29,29,29,29	0
34	NA	0	8327	1/1	0.12	-0.85	36,36,36,36	0
32	MG	0	8011	1/1	0.12	-0.89	21,21,21,21	0
32	MG	0	8086	1/1	0.07	-0.98	37,37,37,37	0
35	CL	A	8509	1/1	0.12	-1.03	49,49,49,49	0
34	NA	0	8354	1/1	0.15	-1.04	23,23,23,23	0
32	MG	B	8055	1/1	0.10	-1.09	42,42,42,42	0
32	MG	0	8038	1/1	0.11	-1.15	21,21,21,21	0
35	CL	J	8502	1/1	0.10	-1.22	55,55,55,55	0
32	MG	0	8116	1/1	0.13	-1.25	35,35,35,35	0
32	MG	0	8064	1/1	0.12	-1.30	26,26,26,26	0
34	NA	0	8305	1/1	0.12	-1.31	33,33,33,33	0
32	MG	0	8094	1/1	0.09	-1.33	59,59,59,59	0
35	CL	J	8501	1/1	0.09	-1.41	46,46,46,46	0
36	CD	U	8401	1/1	0.07	-1.42	48,48,48,48	0
34	NA	0	8344	1/1	0.08	-1.49	24,24,24,24	0
34	NA	0	8356	1/1	0.12	-1.54	35,35,35,35	0
32	MG	0	8016	1/1	0.10	-1.55	30,30,30,30	0
35	CL	J	8521	1/1	0.10	-1.60	47,47,47,47	0
32	MG	0	8074	1/1	0.06	-1.72	35,35,35,35	0
35	CL	Y	8520	1/1	0.08	-1.74	35,35,35,35	0
32	MG	0	8077	1/1	0.14	-1.74	22,22,22,22	0
35	CL	0	8511	1/1	0.08	-1.76	37,37,37,37	0
36	CD	1	8402	1/1	0.08	-1.80	45,45,45,45	0
32	MG	0	8100	1/1	0.10	-1.84	63,63,63,63	0
34	NA	M	8347	1/1	0.10	-1.86	19,19,19,19	0
34	NA	0	8375	1/1	0.14	-1.89	38,38,38,38	0
34	NA	0	8315	1/1	0.14	-1.89	30,30,30,30	0
35	CL	0	8516	1/1	0.10	-1.92	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	NA	0	8381	1/1	0.09	-1.94	43,43,43,43	0
34	NA	0	8319	1/1	0.10	-1.97	31,31,31,31	0
32	MG	0	8022	1/1	0.13	-1.99	31,31,31,31	0
34	NA	0	8332	1/1	0.10	-2.06	31,31,31,31	0
36	CD	Z	8403	1/1	0.08	-2.15	43,43,43,43	0
32	MG	0	8098	1/1	0.10	-2.15	25,25,25,25	0
34	NA	J	8346	1/1	0.06	-2.16	37,37,37,37	0
32	MG	0	8024	1/1	0.10	-2.21	22,22,22,22	0
34	NA	A	8345	1/1	0.09	-2.21	43,43,43,43	0
35	CL	O	8508	1/1	0.06	-2.24	51,51,51,51	0
32	MG	0	8045	1/1	0.08	-2.25	55,55,55,55	0
36	CD	O	8405	1/1	0.06	-2.28	71,71,71,71	0
32	MG	0	8096	1/1	0.09	-2.32	34,34,34,34	0
36	CD	3	8404	1/1	0.06	-2.34	45,45,45,45	0
32	MG	0	8106	1/1	0.06	-2.34	31,31,31,31	0
34	NA	S	8312	1/1	0.08	-2.37	28,28,28,28	0
32	MG	0	8031	1/1	0.12	-2.39	24,24,24,24	0
34	NA	0	8339	1/1	0.11	-2.40	19,19,19,19	0
32	MG	0	8020	1/1	0.10	-2.41	22,22,22,22	0
34	NA	9	8351	1/1	0.10	-2.41	45,45,45,45	0
35	CL	N	8507	1/1	0.07	-2.45	44,44,44,44	0
32	MG	0	8053	1/1	0.11	-2.48	33,33,33,33	0
35	CL	0	8505	1/1	0.09	-2.49	41,41,41,41	0
32	MG	0	8001	1/1	0.10	-2.49	24,24,24,24	0
32	MG	0	8083	1/1	0.12	-2.53	33,33,33,33	0
35	CL	0	8512	1/1	0.08	-2.54	35,35,35,35	0
32	MG	0	8085	1/1	0.12	-2.58	37,37,37,37	0
33	K	0	8201	1/1	0.11	-2.76	60,60,60,60	0
35	CL	L	8510	1/1	0.08	-2.82	40,40,40,40	0
34	NA	0	8317	1/1	0.07	-2.82	28,28,28,28	0
32	MG	T	8073	1/1	0.06	-2.84	40,40,40,40	0
34	NA	0	8303	1/1	0.11	-2.89	32,32,32,32	0
32	MG	0	8062	1/1	0.08	-2.96	42,42,42,42	0
34	NA	0	8309	1/1	0.07	-2.97	25,25,25,25	0
35	CL	0	8514	1/1	0.11	-3.02	39,39,39,39	0
32	MG	0	8056	1/1	0.07	-3.09	34,34,34,34	0
34	NA	0	8330	1/1	0.06	-3.12	37,37,37,37	0
34	NA	Q	8348	1/1	0.06	-3.18	30,30,30,30	0
35	CL	3	8504	1/1	0.04	-3.20	43,43,43,43	0
32	MG	0	8054	1/1	0.12	-3.25	16,16,16,16	0
32	MG	0	8115	1/1	0.09	-3.33	41,41,41,41	0
32	MG	0	8058	1/1	0.08	-3.36	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8046	1/1	0.05	-3.38	39,39,39,39	0
34	NA	0	8334	1/1	0.06	-3.41	36,36,36,36	0
32	MG	0	8037	1/1	0.07	-3.44	35,35,35,35	0
34	NA	R	8337	1/1	0.08	-3.45	33,33,33,33	0
32	MG	0	8003	1/1	0.09	-3.48	21,21,21,21	0
35	CL	0	8513	1/1	0.07	-3.50	44,44,44,44	0
32	MG	0	8075	1/1	0.08	-3.50	27,27,27,27	0
34	NA	9	8352	1/1	0.10	-3.52	41,41,41,41	0
35	CL	0	8517	1/1	0.08	-3.54	47,47,47,47	0
32	MG	0	8008	1/1	0.10	-3.65	26,26,26,26	0
34	NA	0	8310	1/1	0.06	-3.66	30,30,30,30	0
35	CL	R	8506	1/1	0.09	-3.69	40,40,40,40	0
32	MG	0	8017	1/1	0.12	-3.80	11,11,11,11	0
32	MG	0	8072	1/1	0.09	-3.84	47,47,47,47	0
35	CL	0	8515	1/1	0.09	-3.85	53,53,53,53	0
34	NA	0	8343	1/1	0.06	-3.91	28,28,28,28	0
32	MG	0	8005	1/1	0.13	-3.91	25,25,25,25	0
34	NA	0	8333	1/1	0.06	-3.97	23,23,23,23	0
32	MG	0	8105	1/1	0.08	-4.02	45,45,45,45	0
32	MG	Y	8108	1/1	0.09	-4.07	25,25,25,25	0
32	MG	0	8035	1/1	0.08	-4.14	34,34,34,34	0
32	MG	A	8065	1/1	0.07	-4.28	23,23,23,23	0
35	CL	B	8519	1/1	0.08	-4.28	34,34,34,34	0
32	MG	0	8081	1/1	0.07	-4.39	39,39,39,39	0
32	MG	3	8078	1/1	0.07	-4.40	37,37,37,37	0
32	MG	0	8088	1/1	0.08	-4.44	24,24,24,24	0
32	MG	0	8051	1/1	0.07	-4.63	54,54,54,54	0
32	MG	0	8109	1/1	0.09	-4.63	25,25,25,25	0
32	MG	0	8107	1/1	0.07	-4.69	68,68,68,68	0
32	MG	0	8068	1/1	0.04	-4.95	46,46,46,46	0
34	NA	0	8353	1/1	0.07	-4.97	17,17,17,17	0
34	NA	0	8338	1/1	0.05	-4.97	41,41,41,41	0
32	MG	0	8084	1/1	0.07	-5.02	38,38,38,38	0
32	MG	0	8030	1/1	0.07	-5.19	21,21,21,21	0
32	MG	0	8014	1/1	0.09	-5.21	25,25,25,25	0
32	MG	0	8113	1/1	0.05	-5.49	31,31,31,31	0
32	MG	0	8029	1/1	0.07	-5.52	34,34,34,34	0
34	NA	0	8349	1/1	0.09	-5.53	32,32,32,32	0
32	MG	0	8004	1/1	0.10	-5.66	19,19,19,19	0
32	MG	0	8071	1/1	0.06	-5.83	61,61,61,61	0
32	MG	0	8032	1/1	0.06	-6.17	26,26,26,26	0
32	MG	0	8033	1/1	0.06	-6.32	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8040	1/1	0.10	-6.37	38,38,38,38	0
32	MG	0	8036	1/1	0.06	-6.44	31,31,31,31	0
32	MG	0	8025	1/1	0.06	-6.53	32,32,32,32	0
32	MG	0	8091	1/1	0.05	-6.69	41,41,41,41	0
32	MG	0	8027	1/1	0.05	-6.76	36,36,36,36	0
32	MG	0	8048	1/1	0.07	-6.80	41,41,41,41	0
32	MG	K	8069	1/1	0.05	-6.91	47,47,47,47	0
32	MG	0	8044	1/1	0.07	-7.06	33,33,33,33	0
32	MG	0	8006	1/1	0.07	-7.13	29,29,29,29	0
32	MG	0	8021	1/1	0.10	-7.14	25,25,25,25	0
32	MG	0	8018	1/1	0.07	-7.26	30,30,30,30	0
34	NA	0	8323	1/1	0.10	-7.29	31,31,31,31	0
32	MG	0	8092	1/1	0.08	-7.50	66,66,66,66	0
32	MG	0	8019	1/1	0.05	-7.54	23,23,23,23	0
32	MG	0	8050	1/1	0.12	-7.80	66,66,66,66	0
32	MG	0	8111	1/1	0.05	-7.94	23,23,23,23	0
32	MG	0	8059	1/1	0.06	-7.96	22,22,22,22	0
34	NA	0	8313	1/1	0.08	-7.97	55,55,55,55	0
34	NA	0	8357	1/1	0.05	-8.36	39,39,39,39	0
33	K	0	8202	1/1	0.06	-8.76	37,37,37,37	0
32	MG	0	8110	1/1	0.05	-8.99	29,29,29,29	0
32	MG	0	8093	1/1	0.07	-9.38	37,37,37,37	0
32	MG	0	8063	1/1	0.10	-9.43	60,60,60,60	0
32	MG	0	8043	1/1	0.05	-9.72	32,32,32,32	0
32	MG	0	8076	1/1	0.04	-10.31	44,44,44,44	0
32	MG	0	8002	1/1	0.05	-10.67	25,25,25,25	0
34	NA	0	8336	1/1	0.03	-11.25	37,37,37,37	0
32	MG	0	8052	1/1	0.04	-13.26	48,48,48,48	0
32	MG	0	8039	1/1	0.05	-13.51	33,33,33,33	0
32	MG	0	8028	1/1	0.07	-16.84	27,27,27,27	0
32	MG	0	8112	1/1	0.11	-17.00	39,39,39,39	0
32	MG	0	8089	1/1	0.07	-18.91	43,43,43,43	0
32	MG	0	8114	1/1	0.05	-21.33	38,38,38,38	0
34	NA	0	8301	1/1	0.10	-21.50	34,34,34,34	0
32	MG	0	8097	1/1	0.06	-21.91	30,30,30,30	0

6.5 Other polymers ⓘ

There are no such residues in this entry.