



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2017 – 06:52 PM EDT

PDB ID : 3CC4
Title : Co-crystal Structure of Anisomycin Bound to the 50S Ribosomal Subunit
Authors : Blaha, G.; Gurel, G.
Deposited on : unknown
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

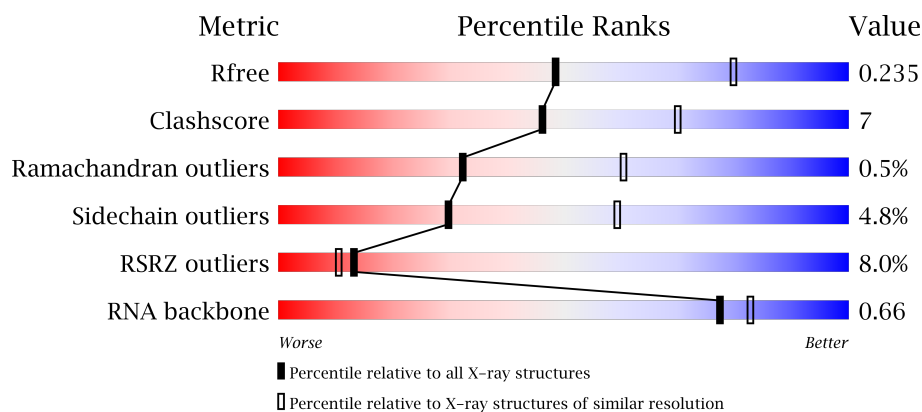
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)
RNA backbone	2435	1011 (3.06-2.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	240	<div> <div>10%</div> <div> <div>84%</div> <div>14%</div> <div>..</div> </div> </div>
2	B	338	<div> <div>3%</div> <div> <div>87%</div> <div>12%</div> <div>.</div> </div> </div>
3	C	246	<div> <div>%</div> <div> <div>83%</div> <div>14%</div> <div>.</div> </div> </div>
4	D	177	<div> <div>40%</div> <div> <div>66%</div> <div>14%</div> <div>21%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
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	

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Mol	Chain	Length	Quality of chain
30	0	2923	
31	9	122	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	0	8001	-	-	-	X
32	MG	0	8004	-	-	-	X
32	MG	0	8006	-	-	-	X
32	MG	0	8009	-	-	-	X
32	MG	0	8011	-	-	-	X
32	MG	0	8012	-	-	-	X
32	MG	0	8014	-	-	-	X
32	MG	0	8016	-	-	-	X
32	MG	0	8028	-	-	-	X
32	MG	0	8041	-	-	-	X
32	MG	0	8047	-	-	-	X
32	MG	0	8055	-	-	-	X
32	MG	0	8062	-	-	-	X
32	MG	0	8085	-	-	-	X
32	MG	0	8087	-	-	-	X
32	MG	A	8051	-	-	-	X
34	SR	0	8949	-	-	-	X
34	SR	0	8957	-	-	-	X
34	SR	0	8962	-	-	-	X
34	SR	0	8969	-	-	-	X
34	SR	0	8986	-	-	-	X
34	SR	0	8992	-	-	-	X
34	SR	A	8929	-	-	-	X
34	SR	B	8987	-	-	-	X
35	NA	0	8504	-	-	-	X
35	NA	0	8507	-	-	-	X
35	NA	0	8508	-	-	-	X
35	NA	0	8517	-	-	-	X
35	NA	0	8519	-	-	-	X
35	NA	0	8521	-	-	-	X
35	NA	0	8522	-	-	-	X
35	NA	0	8523	-	-	-	X
35	NA	0	8527	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	NA	0	8528	-	-	-	X
35	NA	0	8530	-	-	-	X
35	NA	0	8533	-	-	-	X
35	NA	0	8534	-	-	-	X
35	NA	0	8535	-	-	-	X
35	NA	0	8542	-	-	-	X
35	NA	0	8546	-	-	-	X
35	NA	0	8547	-	-	-	X
35	NA	0	8553	-	-	-	X
35	NA	0	8555	-	-	-	X
35	NA	0	8556	-	-	-	X
35	NA	0	8557	-	-	-	X
35	NA	0	8558	-	-	-	X
35	NA	0	8559	-	-	-	X
35	NA	0	8560	-	-	-	X
35	NA	0	8562	-	-	-	X
35	NA	0	8563	-	-	-	X
35	NA	0	8564	-	-	-	X
35	NA	0	8565	-	-	-	X
35	NA	0	8567	-	-	-	X
35	NA	0	8568	-	-	-	X
35	NA	0	8569	-	-	-	X
35	NA	0	8575	-	-	-	X
35	NA	9	8572	-	-	-	X
35	NA	B	8552	-	-	-	X
35	NA	M	8539	-	-	-	X
37	K	0	8401	-	-	-	X
38	ANM	0	2924	-	-	-	X

2 Entry composition [i](#)

There are 39 unique types of molecules in this entry. The entry contains 99135 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a 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	87	Total	Mg	0	0
			87	87		
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		

- Molecule 33 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	10	Total Cl 10 10	0	0
33	J	3	Total Cl 3 3	0	0
33	B	1	Total Cl 1 1	0	0
33	A	1	Total Cl 1 1	0	0
33	N	1	Total Cl 1 1	0	0
33	O	1	Total Cl 1 1	0	0
33	R	1	Total Cl 1 1	0	0
33	Y	1	Total Cl 1 1	0	0
33	L	1	Total Cl 1 1	0	0
33	3	1	Total Cl 1 1	0	0
33	M	1	Total Cl 1 1	0	0

- Molecule 34 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	92	Total Sr 92 92	0	0
34	1	2	Total Sr 2 2	0	0
34	H	1	Total Sr 1 1	0	0
34	B	2	Total Sr 2 2	0	0
34	3	2	Total Sr 2 2	0	0
34	A	3	Total Sr 3 3	0	0
34	R	1	Total Sr 1 1	0	0
34	9	3	Total Sr 3 3	0	0
34	S	1	Total Sr 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	F	1	Total	Sr	0	0
			1	1		

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	66	Total	Na	0	0
			66	66		
35	J	1	Total	Na	0	0
			1	1		
35	Q	1	Total	Na	0	0
			1	1		
35	B	1	Total	Na	0	0
			1	1		
35	C	1	Total	Na	0	0
			1	1		
35	R	1	Total	Na	0	0
			1	1		
35	9	2	Total	Na	0	0
			2	2		
35	S	1	Total	Na	0	0
			1	1		
35	M	1	Total	Na	0	0
			1	1		

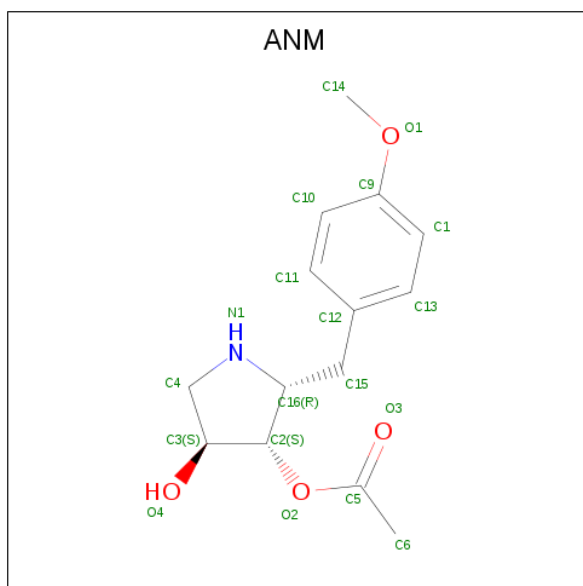
- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

- Molecule 37 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	2	Total K 2 2	0	0

- Molecule 38 is ANISOMYCIN (three-letter code: ANM) (formula: $C_{14}H_{19}NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	0	1	Total C N O 19 14 1 4	0	0

- Molecule 39 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	A	110	Total O 110 110	0	0
39	B	140	Total O 140 140	0	0
39	C	163	Total O 163 163	0	0
39	D	46	Total O 46 46	0	0
39	E	44	Total O 44 44	0	0
39	F	26	Total O 26 26	0	0
39	G	17	Total O 17 17	0	0
39	H	67	Total O 67 67	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	I	6	Total 6	O 6	0	0
39	J	49	Total 49	O 49	0	0
39	K	56	Total 56	O 56	0	0
39	L	85	Total 85	O 85	0	0
39	M	121	Total 121	O 121	0	0
39	N	61	Total 61	O 61	0	0
39	O	44	Total 44	O 44	0	0
39	P	62	Total 62	O 62	0	0
39	Q	48	Total 48	O 48	0	0
39	R	78	Total 78	O 78	0	0
39	S	32	Total 32	O 32	0	0
39	T	39	Total 39	O 39	0	0
39	U	27	Total 27	O 27	0	0
39	V	13	Total 13	O 13	0	0
39	W	65	Total 65	O 65	0	0
39	X	23	Total 23	O 23	0	0
39	Y	92	Total 92	O 92	0	0
39	Z	31	Total 31	O 31	0	0
39	1	48	Total 48	O 48	0	0
39	2	38	Total 38	O 38	0	0
39	3	66	Total 66	O 66	0	0

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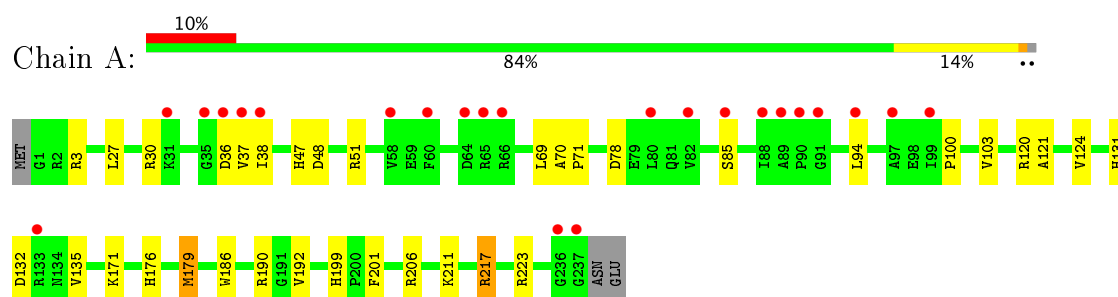
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	5972	Total 5972	O 5972	0	0
39	9	147	Total 147	O 147	0	0

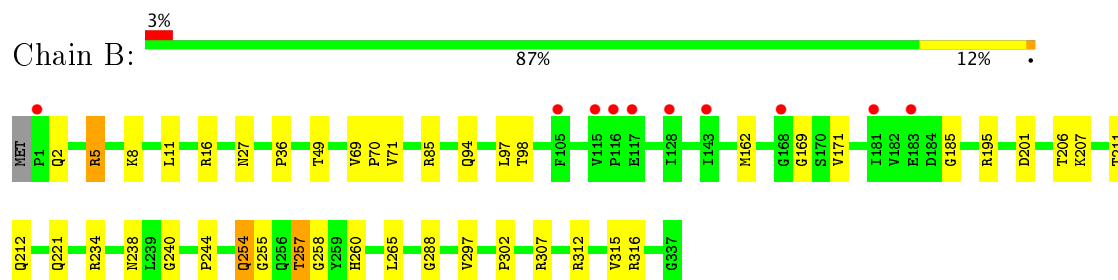
3 Residue-property plots [i](#)

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

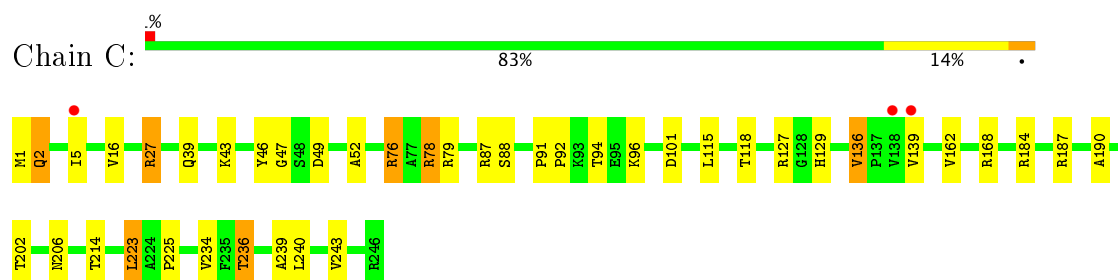
- Molecule 1: 50S ribosomal protein L2P



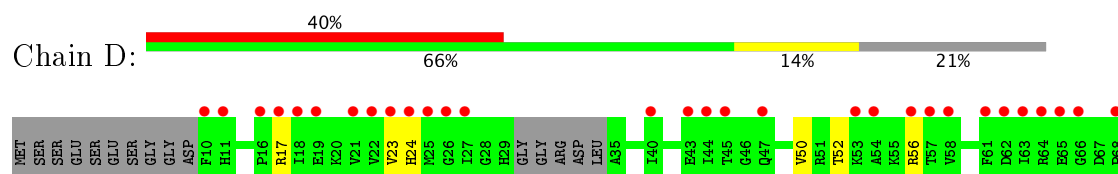
- Molecule 2: 50S ribosomal protein L3P

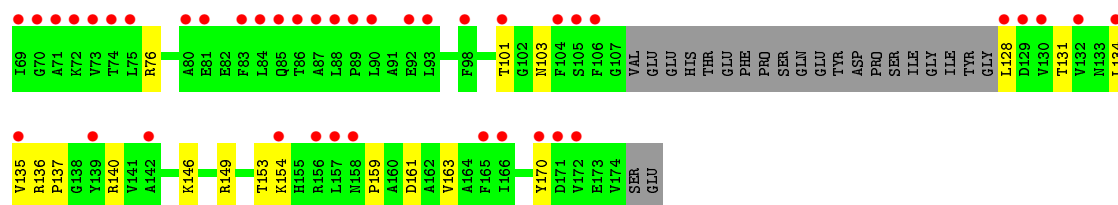


- Molecule 3: 50S ribosomal protein L4P

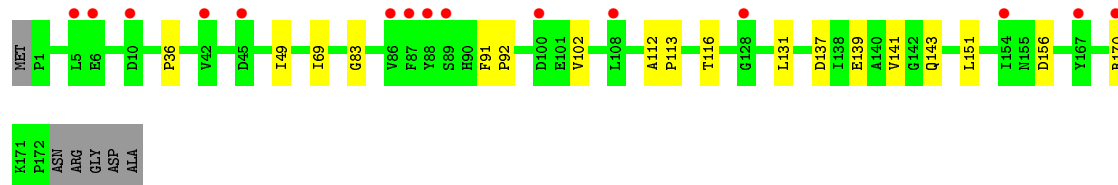
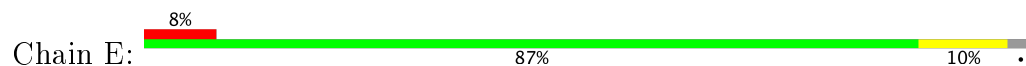


- Molecule 4: 50S ribosomal protein L5P

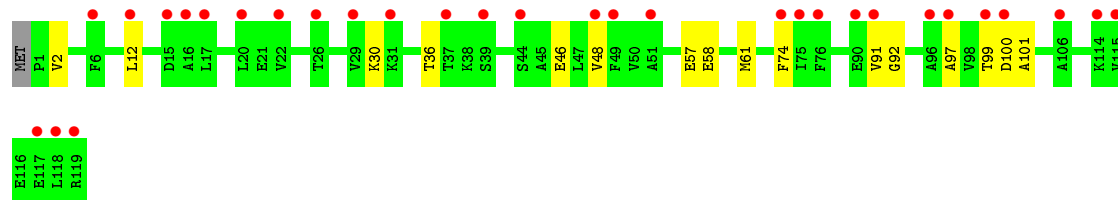
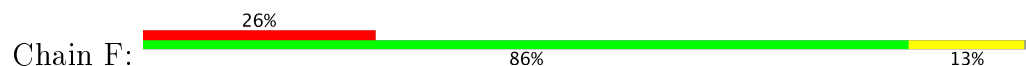




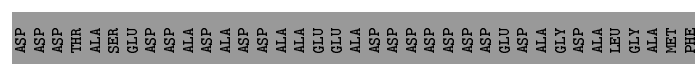
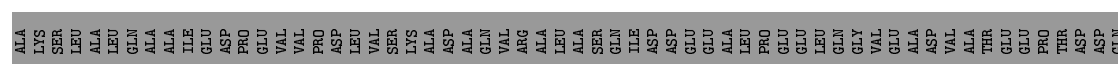
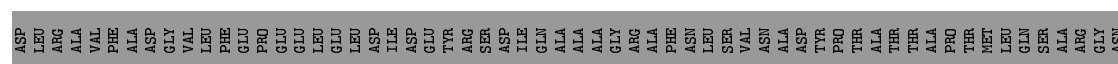
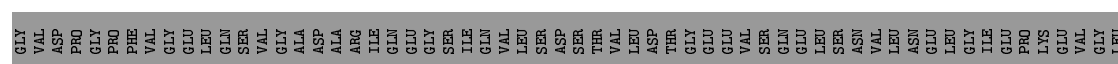
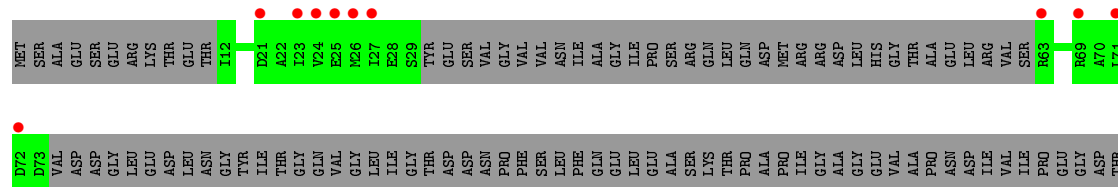
• Molecule 5: 50S ribosomal protein L6P



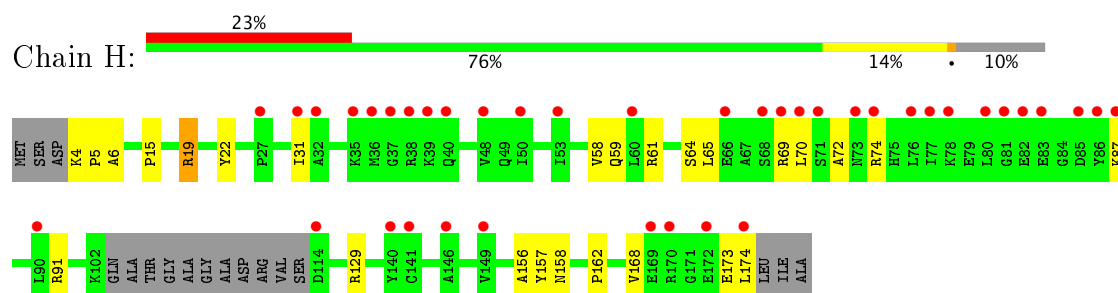
• Molecule 6: 50S ribosomal protein L7Ae



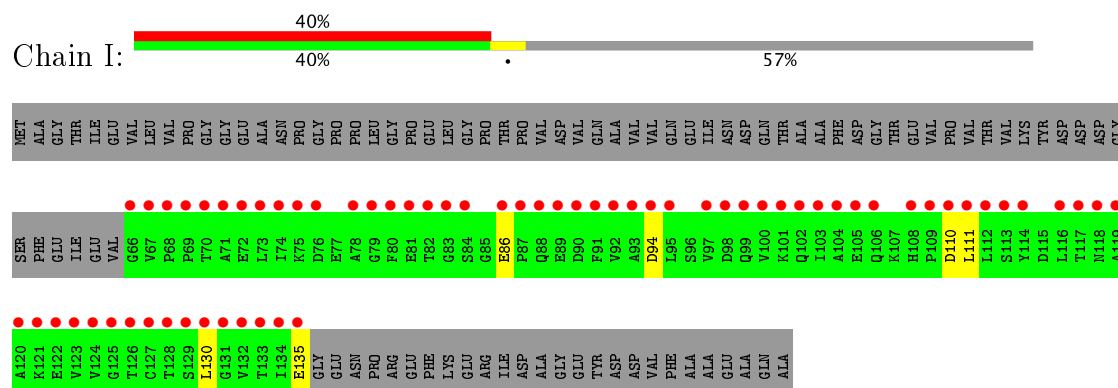
• Molecule 7: 50S ribosomal protein L10E



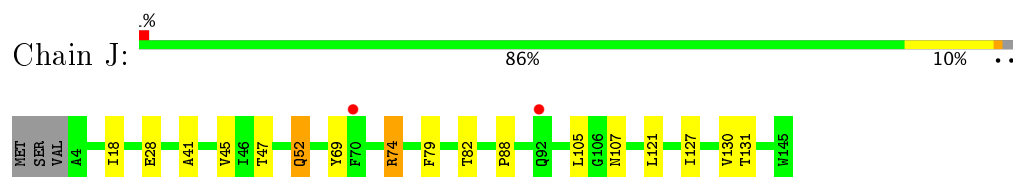
• Molecule 8: 50S ribosomal protein L10e



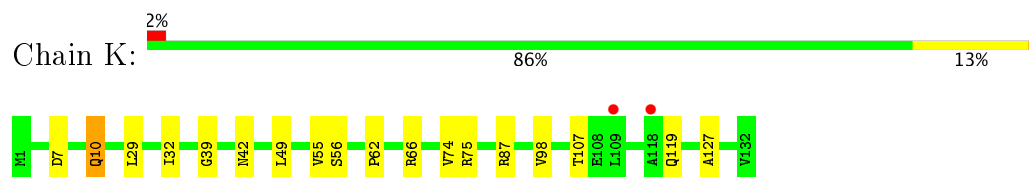
- Molecule 9: 50S ribosomal protein L11P



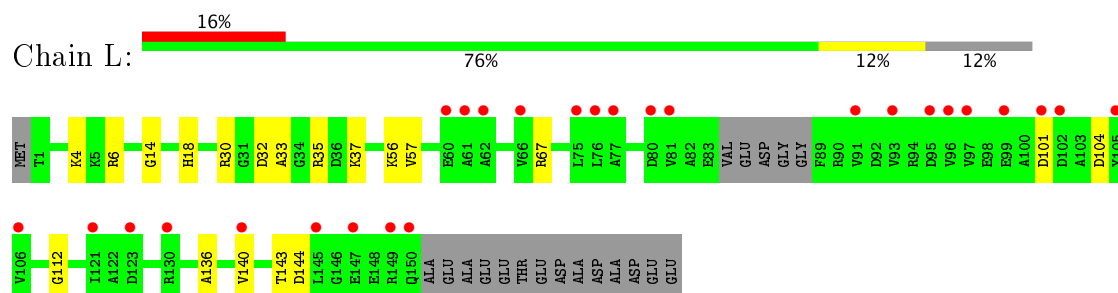
- Molecule 10: 50S ribosomal protein L13P



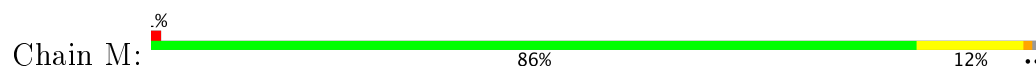
- Molecule 11: 50S ribosomal protein L14P

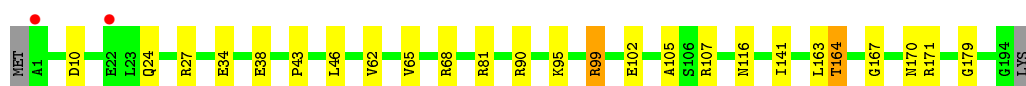


- Molecule 12: 50S ribosomal protein L15P

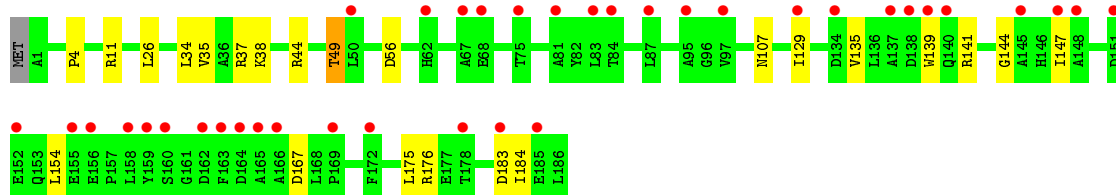
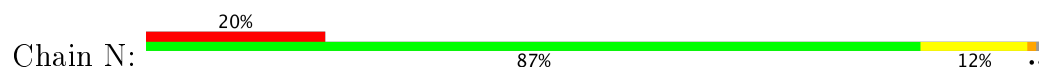


- Molecule 13: 50S ribosomal protein L15e





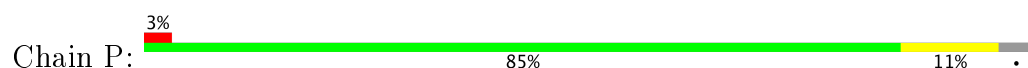
- Molecule 14: 50S ribosomal protein L18P



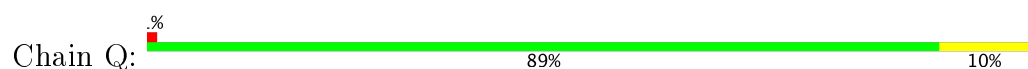
- Molecule 15: 50S ribosomal protein L18e



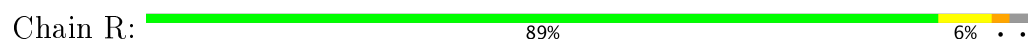
- Molecule 16: 50S ribosomal protein L19e



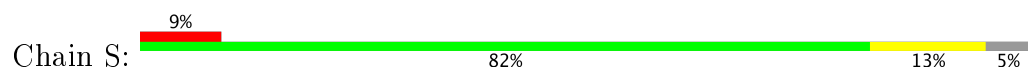
- Molecule 17: 50S ribosomal protein L21e



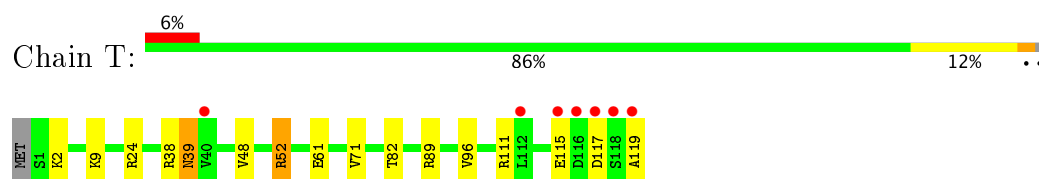
- Molecule 18: 50S ribosomal protein L22P



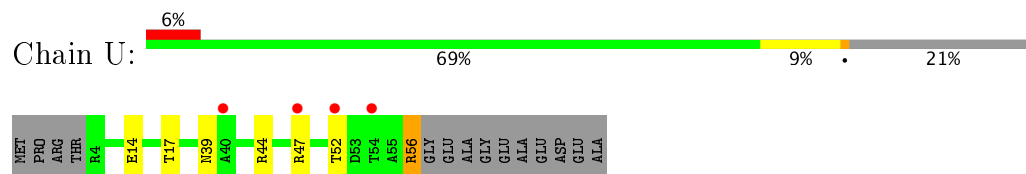
- Molecule 19: 50S ribosomal protein L23P



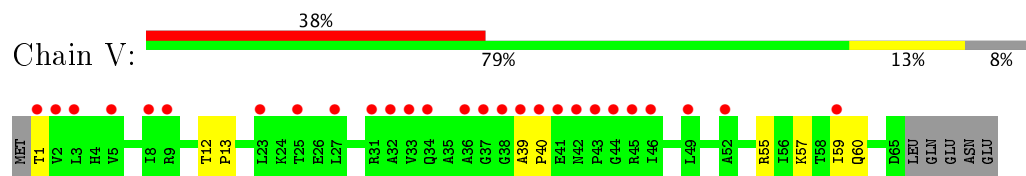
- Molecule 20: 50S ribosomal protein L24P



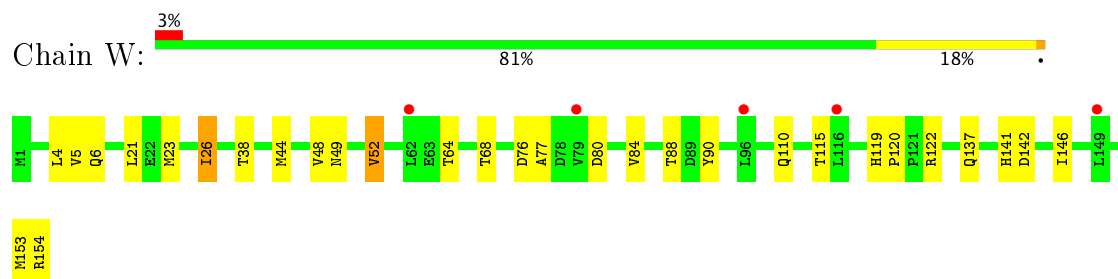
- Molecule 21: 50S ribosomal protein L24e



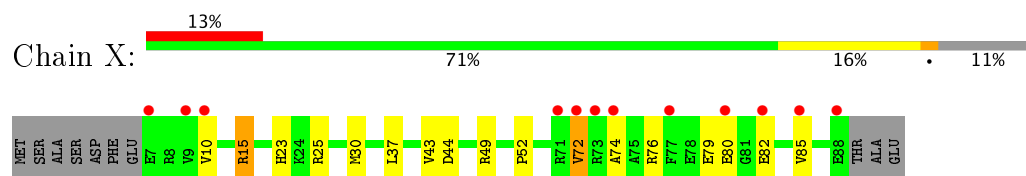
- Molecule 22: 50S ribosomal protein L29P



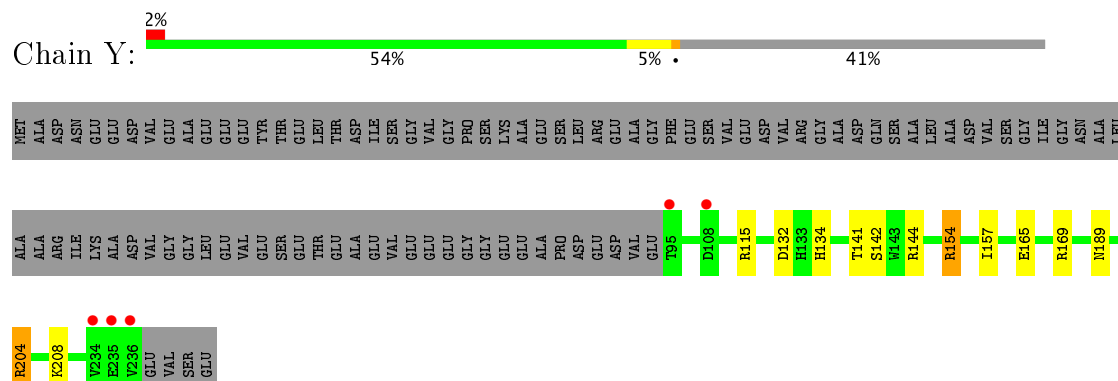
- Molecule 23: 50S ribosomal protein L30P



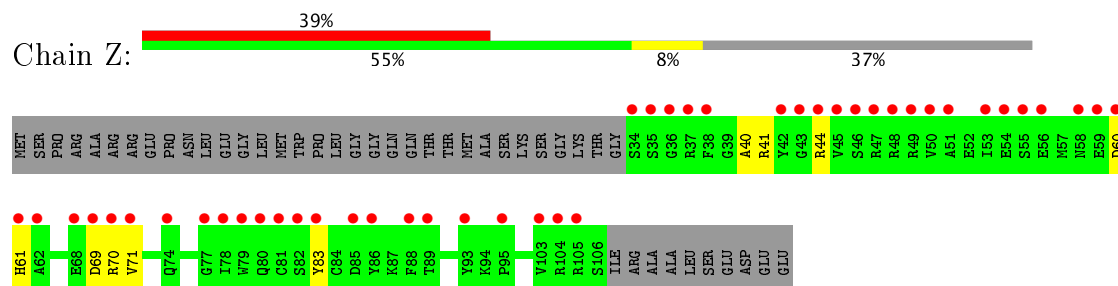
- Molecule 24: 50S ribosomal protein L31e



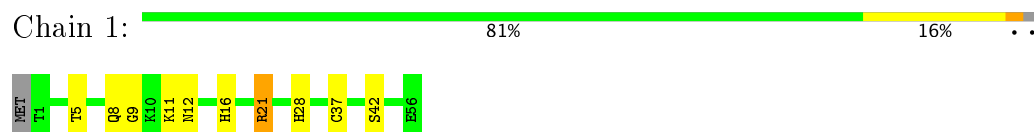
- Molecule 25: 50S ribosomal protein L32e



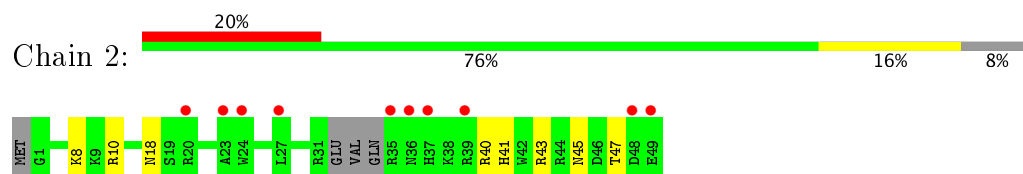
- Molecule 26: 50S ribosomal protein L37Ae



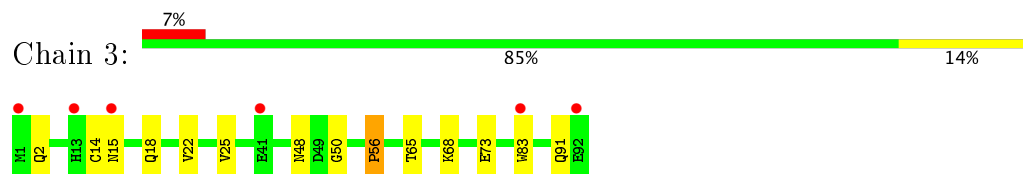
- Molecule 27: 50S ribosomal protein L37e



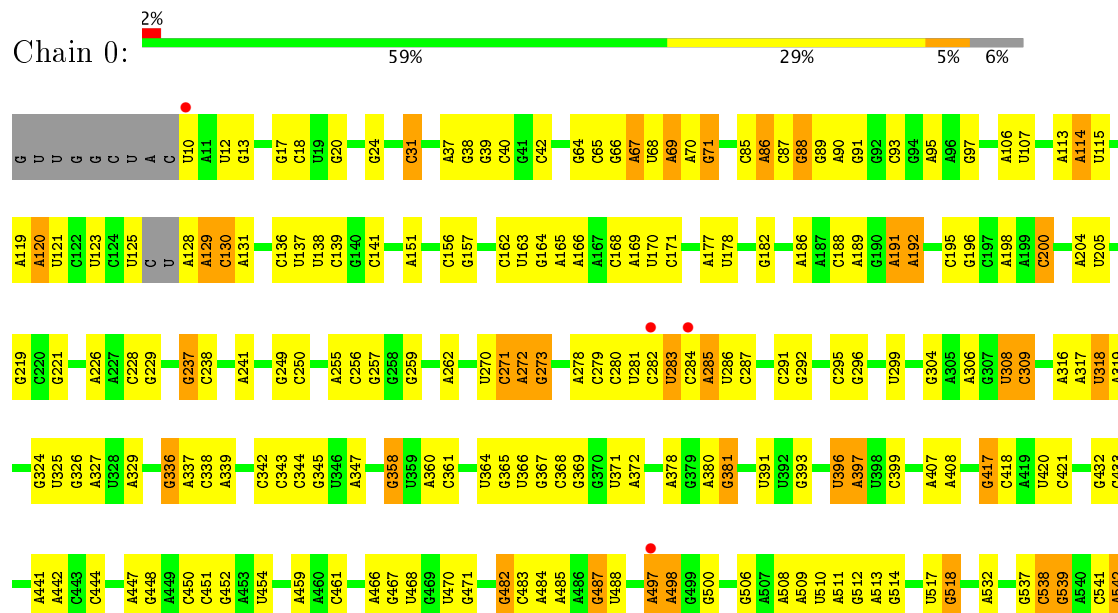
- Molecule 28: 50S ribosomal protein L39e



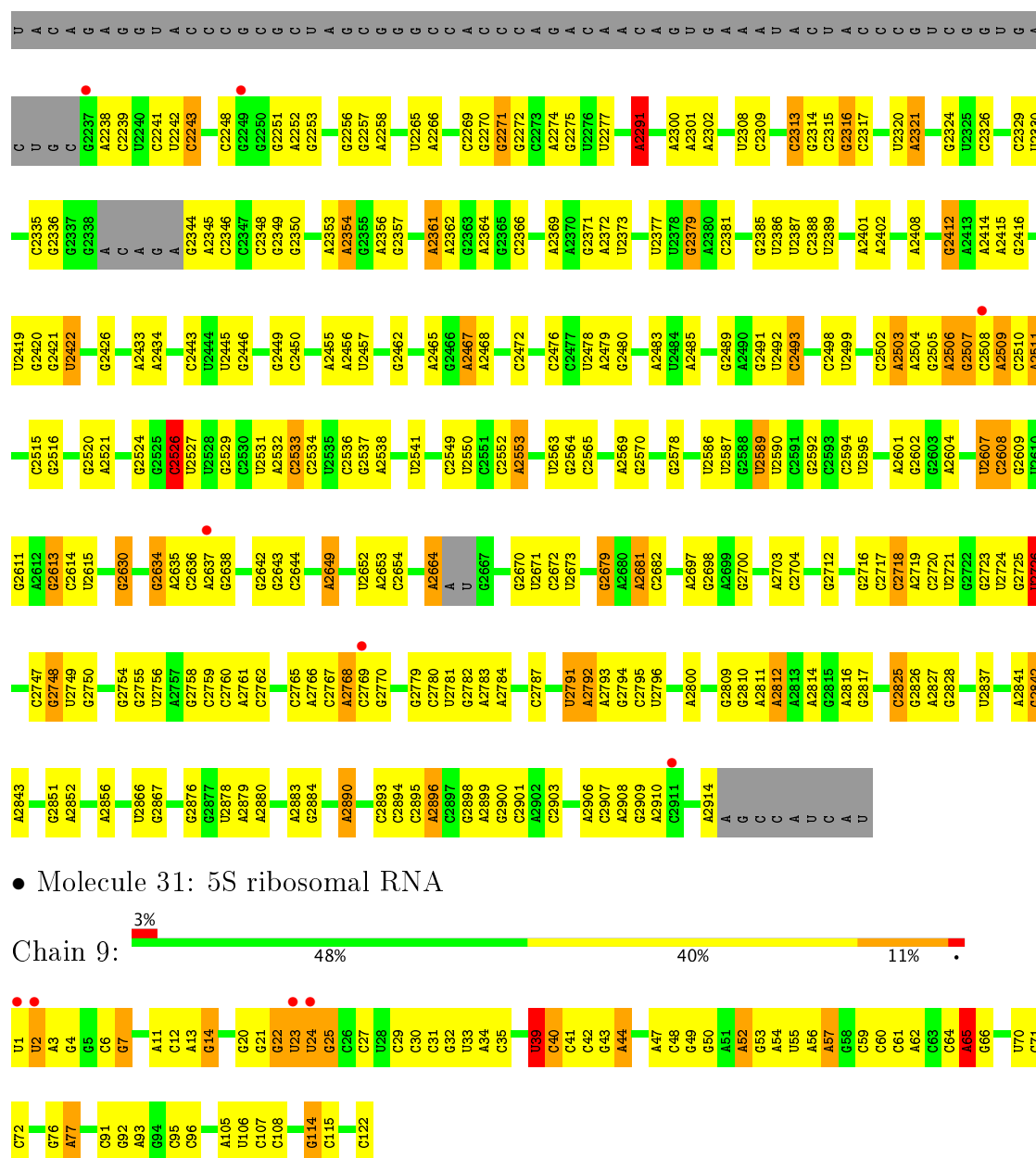
- Molecule 29: 50S ribosomal protein L44E



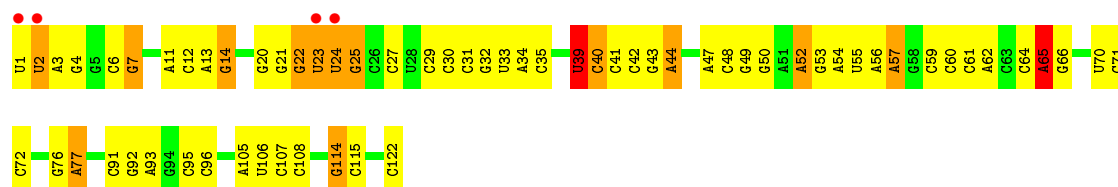
- Molecule 30: 23S ribosomal RNA



A2089	G1971	G1863	A1755	G1634	U8506	G1391	U1266	U1185	G1087	G	A791	A660	G543
G2090	U1972	G1863	G1756	U1635	A1516	A1392	C1267	C1186	A1088	A	G792	A661	G544
G2091	A1973	G1636	C1762	A1637	U1516	C1396	G1268	A1187	U1096	G	A793	A666	G545
G2092	G1974	G1975	C1763	A1637	U1516	C1397	G1269	A1188	U1097	C	U794	A667	A553
A2096	G1976	G1877	U1766	A1641	U1524	A1398	A1278	A1189	A1097	C	A807	G668	A558
A2100	U1977	G1878	A1766	A1642	G1525	A1399	U1279	A1191	A1098	C	A808	G669	C558
A2101	A1978	U1879	U1771	U1654	A1527	A1406	C1289	A1193	G1099	C	A809	A671	U560
G2102	G1979	G1772	G1773	G1655	A1528	A1407	G1290	A1194	C1104	A	A812	G672	G561
A2103	U1980	A1881	G1773	A1656	G1529	G1409	A1294	G1195	U1109	C	G814	G677	G564
C2104	C1993	G1882	A1778	A1657	A1533	A1413	G1295	G1196	G1110	C	U815	G678	U567
C2105	U1982	U1883	A1779	A1658	C1534	A1414	G1299	U1198	U1116	A1005	G816	G681	G581
C2106	G1995	G1884	A1779	G1663	C1536	A1415	G1300	A1199	A1117	A1006	G817	A682	U582
G2110	U1996	A1885	A1779	G1663	C1537	G1416	G1300	C1201	A1118	A1007	G818	G683	U582
G2111	A1997	A1886	U1784	G1666	U1544	G1417	U1304	C1202	G1119	C1008	G820	U582	G588
G2121	G2000	C1894	U1787	G1667	C1545	U1418	C1305	G1203	U1121	C1010	U821	A686	G588
G2122	G2001	A1895	U1788	A1667	C1546	U1419	A1313	C1204	G1135	A1014	U822	A687	U595
G2123	C2002	U1896	U1788	U1668	G1546	C1420	G1314	U1205	U1136	A1015	U823	A688	C596
G2134	U2004	A1919	U1790	U1677	A1559	U1421	G1315	U1206	G1131	U1016	A827	G689	U595
A2135	G2005	U1920	U1791	A1678	U	U1422	G1316	A1207	G1131	U1016	U827	G690	C596
G2136	G2006	C1921	C1798	G1679	U1561	C1423	G1316	C1208	A1132	C1023	U832	A694	A602
A	U2008	A1921	C1799	G1680	C1562	A1427	A1321	C1209	G1151	G1040	U833	C695	A603
C	G2009	A1922	G1799	G1681	C1562	A1427	G1322	G1210	U1135	U1041	U834	U701	A604
G	A2010	U1897	A1804	A1682	A1573	G1430	G1328	C1211	U1136	U1042	U835	G702	A605
U	A2011	G1925	G1805	A1683	A1573	G1430	G1329	C1212	U1137	U1043	U836	G703	U612
C	U2012	A1942	A1809	A1684	U1587	U1440	G1330	C1213	U1138	U1044	U837	G704	U613
G	G2013	A1927	G1809	A1685	G1588	G1441	G1331	C1214	U1139	C1045	U838	G705	U614
U	U2016	U1839	A1815	C1686	G1589	A1442	G1332	C1215	G1151	G1046	U839	G706	U615
C	C2033	C1940	C1816	G1687	G1688	C1451	G1333	G1216	C1157	G952	C847	G707	U619
C	U2034	A1942	G1819	C1692	C1692	C1456	U1334	U1218	G1163	G953	C848	G708	A620
G	A2039	C1943	G1820	A1693	C1594	U1457	G1339	U1219	U1164	C959	C849	G709	A621
U	C2040	U1947	A1829	U1702	U1596	U1457	G1340	U1220	A1161	G960	U850	G710	A622
G	G2044	G1948	A1830	A1710	A1598	U1473	A1341	C1229	G1162	A961	C853	G711	U623
C	G2050	G1949	C1834	A1710	A1598	C1474	A1342	A1230	U1163	C962	G856	U714	U625
A	A2054	U1951	U1835	C1714	A1603	C1477	A1343	A1231	U1164	C963	A857	U	A629
C	A2055	A	G1836	C1715	G1604	U1478	A1351	A1232	A1165	G1052	U858	G716	A630
C	A2056	A	G1837	U1722	G1605	U1481	A1352	A1233	C1166	G1053	G868	G722	A631
A	U2064	C	U1838	U1723	A1606	A1482	A1353	A1234	U1169	U1056	G869	G722	A632
U	A2067	U	A1839	U1724	A1607	A1482	C1353	U1235	U1170	A1057	G870	G735	A635
A	G2068	A	A1840	C1725	A1613	A1485	C1360	G1239	A1171	G1058	U872	A736	A636
G	G2072	U	G1848	C1725	G1614	A1485	C1363	A1242	G1172	C1060	A875	A737	A637
A	G2073	C	U1850	C1730	A1615	G1490	G1363	C1243	A1173	U1066	A876	G738	A638
G	A2074	C	G1851	C1731	G1622	C1495	A1372	U1244	G1175	A1067	G877	C741	A639
A	G2075	C	A1852	A1733	C1623	A1496	A1377	A1246	C1176	G1071	G878	G759	A644
G	A2078	C	C1853	A1733	A1624	G1497	C1377	A1246	G1177	U1072	C884	G760	U645
A	U2078	U1964	C1854	U1741	U1625	U1500	C1384	U1249	A1178	G1072	G885	A761	U653
G	A2081	C1865	G1855	A1742	G1626	G1627	G1385	C1250	U1180	A1078	U888	A776	A654
C	U1967	U1966	C1856	A1742	G1627	U1503	G1386	C1251	A1181	A1079	U889	U777	A655
G	C2088	A1857	A1857	G1752	A1632	A1504	G1387	A1253	C1182	C1080	G998	A	A657
U					A1633	A1505		C1253	C1184	A1082	C999	A790	



- Molecule 31: 5S ribosomal RNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.78Å 299.08Å 573.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.85 – 2.70 85.45 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.9 (49.85-2.70) 96.9 (85.45-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.202 , 0.244 0.197 , 0.235	Depositor DCC
R_{free} test set	4704 reflections (0.99%)	DCC
Wilson B-factor (Å ²)	47.7	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 63.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99135	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, SR, NA, K, CD, OMU, UR3, 1MA, ANM, 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	0.51	0/1786	0.78	0/2408
2	B	0.53	0/2690	0.78	0/3652
3	C	0.54	0/1885	0.77	0/2552
4	D	0.65	0/1111	0.71	1/1498 (0.1%)
5	E	0.60	0/1382	0.68	0/1880
6	F	0.54	0/901	0.71	0/1224
7	G	0.51	0/241	0.67	0/324
8	H	0.60	0/1302	0.79	0/1743
9	I	0.59	0/526	0.62	0/716
10	J	0.61	0/1136	0.72	0/1530
11	K	0.51	0/1004	0.80	0/1351
12	L	0.49	0/1130	0.76	0/1509
13	M	0.51	0/1582	0.77	0/2116
14	N	0.55	0/1474	0.77	0/1999
15	O	0.47	0/874	0.73	1/1181 (0.1%)
16	P	0.52	0/1147	0.67	0/1528
17	Q	0.49	0/749	0.77	0/1005
18	R	0.54	0/1172	0.74	0/1578
19	S	0.54	0/648	0.67	0/875
20	T	0.46	0/958	0.76	1/1289 (0.1%)
21	U	0.57	0/417	0.71	0/562
22	V	0.44	0/502	0.67	0/675
23	W	0.52	0/1219	0.78	1/1655 (0.1%)
24	X	0.52	0/664	0.72	0/895
25	Y	0.52	0/1146	0.74	0/1536
26	Z	0.69	0/584	0.74	0/781
27	1	0.55	0/438	0.75	0/578
28	2	0.45	0/401	0.70	0/529
29	3	0.59	0/771	0.70	0/1024
30	0	0.37	0/65958	0.68	15/102869 (0.0%)
31	9	0.32	0/2904	0.69	1/4526 (0.0%)
All	All	0.43	0/98702	0.70	20/147588 (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
23	W	0	1
30	0	0	42
31	9	0	2
All	All	0	45

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	4	LEU	CA-CB-CG	7.59	132.77	115.30
30	0	1942	A	C5'-C4'-C3'	6.82	126.92	116.00
30	0	871	G	C5'-C4'-O4'	-6.64	101.13	109.10
30	0	1504	A	N9-C1'-C2'	5.91	121.68	114.00
30	0	2726	U	N1-C1'-C2'	5.85	121.60	114.00
31	9	39	U	N1-C1'-C2'	5.84	121.59	114.00
30	0	1504	A	C1'-O4'-C4'	-5.62	105.40	109.90
15	O	66	GLY	N-CA-C	5.61	127.11	113.10
30	0	1592	G	N9-C1'-C2'	5.49	121.14	114.00
30	0	1819	G	C5'-C4'-C3'	5.49	124.78	116.00
30	0	2467	A	C1'-O4'-C4'	-5.47	105.52	109.90
20	T	52	ARG	N-CA-C	5.42	125.64	111.00
30	0	1829	A	N9-C1'-C2'	-5.39	106.08	112.00
30	0	2313	C	C5'-C4'-O4'	5.32	115.48	109.10
30	0	1120	U	C5'-C4'-C3'	-5.21	107.66	116.00
4	D	170	TYR	N-CA-C	5.14	124.87	111.00
30	0	1165	G	C1'-O4'-C4'	-5.12	105.80	109.90
30	0	777	U	O4'-C1'-N1	5.12	112.29	108.20
30	0	2316	G	C5'-C4'-C3'	-5.09	107.86	116.00
30	0	2291	A	N9-C1'-C2'	5.05	120.56	114.00

There are no chirality outliers.

All (45) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
30	0	1342	C	Sidechain
30	0	1351	G	Sidechain
30	0	1417	G	Sidechain
30	0	1430	G	Sidechain
30	0	1677	U	Sidechain
30	0	1702	U	Sidechain
30	0	1809	G	Sidechain
30	0	1829	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	1993	C	Sidechain
30	0	221	G	Sidechain
30	0	2308	U	Sidechain
30	0	2316	G	Sidechain
30	0	2412	G	Sidechain
30	0	2465	A	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2506	A	Sidechain
30	0	2526	C	Sidechain
30	0	2552	C	Sidechain
30	0	2607	U	Sidechain
30	0	2630	G	Sidechain
30	0	2679	G	Sidechain
30	0	270	U	Sidechain
30	0	2726	U	Sidechain
30	0	2842	G	Sidechain
30	0	391	U	Sidechain
30	0	396	U	Sidechain
30	0	471	G	Sidechain
30	0	482	G	Sidechain
30	0	518	G	Sidechain
30	0	619	U	Sidechain
30	0	817	G	Sidechain
30	0	888	U	Sidechain
31	9	39	U	Sidechain
31	9	65	A	Sidechain
23	W	90	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	21	0
2	B	2625	0	2533	29	0
3	C	1860	0	1813	22	0
4	D	1094	0	1085	11	0
5	E	1357	0	1266	10	0
6	F	890	0	843	8	0
7	G	240	0	231	0	0
8	H	1282	0	1292	18	0
9	I	519	0	500	4	0
10	J	1120	0	1098	14	0
11	K	994	0	1027	11	0
12	L	1118	0	1076	12	0
13	M	1558	0	1573	19	0
14	N	1445	0	1401	16	0
15	O	865	0	873	4	0
16	P	1136	0	1123	11	0
17	Q	735	0	729	6	0
18	R	1149	0	1122	11	0
19	S	641	0	605	5	0
20	T	950	0	924	8	0
21	U	410	0	364	3	0
22	V	499	0	511	4	0
23	W	1196	0	1137	22	0
24	X	654	0	653	11	0
25	Y	1130	0	1133	13	0
26	Z	573	0	532	6	0
27	1	431	0	426	10	0
28	2	396	0	413	5	0
29	3	755	0	729	7	0
30	0	59021	0	29812	846	0
31	9	2599	0	1325	64	0
32	0	87	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	Y	1	0	0	0	0
33	0	10	0	0	0	0
33	3	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	J	3	0	0	1	0
33	L	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	0	0
33	O	1	0	0	0	0
33	R	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	92	0	0	0	0
34	1	2	0	0	0	0
34	3	2	0	0	0	0
34	9	3	0	0	0	0
34	A	3	0	0	0	0
34	B	2	0	0	0	0
34	F	1	0	0	0	0
34	H	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	66	0	0	0	0
35	9	2	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
35	S	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	2	0	0	0	0
38	0	19	0	19	5	0
39	0	5972	0	0	121	0
39	1	48	0	0	0	0
39	2	38	0	0	0	0
39	3	66	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	9	147	0	0	5	0
39	A	110	0	0	4	0
39	B	140	0	0	5	0
39	C	163	0	0	2	0
39	D	46	0	0	0	0
39	E	44	0	0	0	0
39	F	26	0	0	0	0
39	G	17	0	0	0	0
39	H	67	0	0	3	0
39	I	6	0	0	1	0
39	J	49	0	0	1	0
39	K	56	0	0	0	0
39	L	85	0	0	2	0
39	M	121	0	0	1	0
39	N	61	0	0	1	0
39	O	44	0	0	0	0
39	P	62	0	0	0	0
39	Q	48	0	0	0	0
39	R	78	0	0	0	0
39	S	32	0	0	0	0
39	T	39	0	0	0	0
39	U	27	0	0	0	0
39	V	13	0	0	0	0
39	W	65	0	0	2	0
39	X	23	0	0	1	0
39	Y	92	0	0	3	0
39	Z	31	0	0	1	0
All	All	99135	0	59934	1085	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (1085) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1160:G:H5'	30:0:1161:A:H5'	1.22	1.16
31:9:76:G:H3'	31:9:77:A:H5''	1.34	1.02
15:O:3:THR:HG22	30:0:656:G:H5'	1.43	1.00
30:0:871:G:H8	30:0:871:G:H5'	1.27	0.98
30:0:871:G:C8	30:0:871:G:H5'	1.98	0.97
30:0:2717:C:H2'	30:0:2718:C:H5''	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:171:ARG:HD3	30:0:156:C:H5''	1.44	0.96
10:J:82:THR:HG23	30:0:1242:A:H5'	1.47	0.96
30:0:2717:C:C2'	30:0:2718:C:H5''	1.97	0.94
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.15	0.93
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.13	0.93
14:N:37:ARG:NH1	31:9:6:C:H5''	1.83	0.93
31:9:56:A:H2'	31:9:57:A:H5''	1.48	0.92
30:0:542:A:H5'	30:0:542:A:H8	1.35	0.91
30:0:870:G:H2'	30:0:871:G:H5''	1.53	0.90
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.54	0.90
16:P:115:SER:H	16:P:118:GLN:HE21	1.20	0.89
30:0:1474:C:H6	30:0:1474:C:H5'	1.37	0.89
30:0:1116:U:HO2'	30:0:1118:A:H2	0.87	0.87
30:0:1160:G:H5'	30:0:1161:A:C5'	2.04	0.87
30:0:1160:G:C5'	30:0:1161:A:H5'	2.03	0.86
30:0:2506:A:HO2'	30:0:2507:G:H8	0.89	0.86
30:0:2812:A:H2	30:0:2814:A:H62	1.24	0.85
30:0:1667:A:H8	30:0:1667:A:H5'	1.42	0.85
30:0:1603:A:H5'	30:0:1605:G:O4'	1.75	0.85
30:0:1118:A:H62	30:0:1244:U:H3	1.25	0.84
30:0:1701:A:H4'	30:0:1702:U:H5''	1.56	0.84
30:0:2586:U:H3	30:0:2592:G:H22	1.21	0.83
11:K:10:GLN:H	11:K:10:GLN:HE21	1.25	0.83
39:N:8843:HOH:O	31:9:49:G:H5''	1.77	0.83
30:0:1835:U:H5	30:0:1840:A:N7	1.76	0.83
30:0:381:G:H5''	39:0:4352:HOH:O	1.77	0.83
3:C:5:ILE:HD11	3:C:16:VAL:HG23	1.61	0.82
30:0:541:C:H2'	30:0:542:A:H5''	1.61	0.82
30:0:559:U:H5'	30:0:559:U:H6	1.45	0.81
30:0:545:G:H8	30:0:545:G:H5'	1.44	0.81
30:0:2533:C:H5'	30:0:2533:C:H6	1.46	0.81
30:0:1979:G:H2'	39:0:3320:HOH:O	1.82	0.79
30:0:2291:A:C8	30:0:2309:C:H5'	2.18	0.78
30:0:871:G:C5'	30:0:871:G:H8	1.96	0.78
30:0:2908:A:H2'	30:0:2909:G:O4'	1.83	0.78
38:0:2924:ANM:H63	38:0:2924:ANM:H151	1.63	0.78
30:0:506:G:H22	30:0:509:A:C5'	1.97	0.78
30:0:1300:G:H1'	39:0:4716:HOH:O	1.82	0.77
30:0:1205:U:H2'	30:0:1206:U:H5''	1.66	0.77
13:M:102:GLU:OE1	13:M:164:THR:HG21	1.85	0.77
30:0:506:G:H22	30:0:509:A:H5''	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:853:C:H3'	39:0:4586:HOH:O	1.83	0.77
30:0:541:C:C2'	30:0:542:A:H5''	2.15	0.76
30:0:1666:C:O2'	30:0:1667:A:H5''	1.86	0.75
28:2:41:HIS:H	28:2:45:ASN:HD22	1.34	0.75
31:9:29:C:H2'	31:9:30:C:H5'	1.68	0.75
30:0:1116:U:H3	30:0:1246:A:H62	1.34	0.75
30:0:1118:A:H3'	30:0:1118:A:C8	2.22	0.75
30:0:1118:A:H3'	30:0:1118:A:H8	1.51	0.75
30:0:2506:A:O2'	30:0:2507:G:H8	1.69	0.75
3:C:27:ARG:NH2	30:0:657:G:OP1	2.20	0.75
30:0:182:G:H5'	39:0:5189:HOH:O	1.86	0.74
31:9:14:G:H5'	31:9:14:G:H8	1.51	0.74
30:0:1474:C:C6	30:0:1474:C:H5'	2.22	0.74
30:0:1120:U:H5'	30:0:1121:G:OP2	1.89	0.73
13:M:163:LEU:HD21	30:0:188:C:H5''	1.71	0.73
30:0:1209:C:H2'	30:0:1210:G:H8	1.53	0.73
18:R:98:ASN:HD21	30:0:500:G:H21	1.34	0.73
22:V:1:THR:HB	30:0:93:C:H5''	1.70	0.73
30:0:877:G:H5'	30:0:878:G:OP1	1.90	0.72
30:0:1166:A:H61	30:0:1180:U:H3	1.35	0.72
30:0:544:G:H2'	30:0:545:G:H5''	1.72	0.72
30:0:1973:A:H5'	30:0:1973:A:H8	1.55	0.72
31:9:56:A:C2'	31:9:57:A:H5''	2.20	0.72
30:0:282:C:H1'	30:0:368:C:N4	2.04	0.72
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.37	0.71
30:0:1189:A:H1'	30:0:1209:C:O4'	1.90	0.71
30:0:1206:U:H6	30:0:1206:U:H5'	1.53	0.71
31:9:92:G:H2'	31:9:93:A:C8	2.26	0.71
10:J:52:GLN:NE2	30:0:1119:G:H2'	2.05	0.71
30:0:1878:G:H1'	39:0:6168:HOH:O	1.91	0.71
30:0:2491:G:H1'	39:0:6923:HOH:O	1.91	0.70
30:0:2534:C:H1'	39:0:3522:HOH:O	1.91	0.70
30:0:1741:U:H5'	30:0:1742:A:OP1	1.91	0.70
3:C:184:ARG:NH2	30:0:450:C:OP1	2.24	0.70
30:0:1183:C:H2'	39:0:6292:HOH:O	1.91	0.70
30:0:281:U:H2'	30:0:282:C:O4'	1.91	0.70
2:B:5:ARG:HH11	2:B:8:LYS:HE2	1.56	0.70
30:0:1701:A:H5'	39:0:6332:HOH:O	1.92	0.69
1:A:211:LYS:HB2	39:A:9075:HOH:O	1.91	0.69
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.57	0.69
30:0:823:U:H3'	39:0:4481:HOH:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:116:SER:O	30:0:1593:C:H5'	1.92	0.69
2:B:206:THR:HG21	30:0:2716:G:H5''	1.72	0.69
30:0:2851:G:O2'	30:0:2852:A:H5'	1.92	0.69
30:0:541:C:H2'	30:0:542:A:C5'	2.23	0.69
30:0:1159:G:H21	30:0:1189:A:H8	1.39	0.69
31:9:39:U:H1'	31:9:44:A:H61	1.57	0.68
30:0:870:G:C2'	30:0:871:G:H5''	2.21	0.68
30:0:1527:A:H1'	30:0:1528:A:C8	2.29	0.68
30:0:2533:C:C6	30:0:2533:C:H5'	2.27	0.68
30:0:12:U:H2'	30:0:13:G:H5'	1.75	0.68
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.58	0.68
30:0:1119:G:N2	30:0:1246:A:C2	2.58	0.68
30:0:2769:C:C2'	30:0:2770:G:H5'	2.23	0.68
3:C:139:VAL:HG13	39:C:8643:HOH:O	1.92	0.68
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.75	0.67
30:0:603:A:H5''	30:0:604:G:OP1	1.94	0.67
30:0:2783:A:H3'	39:0:5264:HOH:O	1.93	0.67
30:0:681:G:N3	30:0:681:G:H5'	2.09	0.67
30:0:1641:A:H2'	30:0:1642:A:H5'	1.76	0.67
30:0:1205:U:H2'	30:0:1206:U:C5'	2.24	0.67
30:0:1666:C:C2'	30:0:1667:A:H5''	2.25	0.67
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.78	0.66
30:0:2538:A:H8	38:0:2924:ANM:H61	1.61	0.65
30:0:1701:A:H4'	30:0:1702:U:C5'	2.23	0.65
30:0:558:C:C2'	30:0:559:U:H5''	2.26	0.65
21:U:39:ASN:ND2	21:U:44:ARG:HH11	1.93	0.65
30:0:1377:C:H6	30:0:1377:C:H5'	1.61	0.65
30:0:1667:A:C8	30:0:1667:A:H5'	2.29	0.65
30:0:2613:G:O2'	30:0:2614:C:H5'	1.96	0.65
11:K:39:GLY:HA2	39:0:5253:HOH:O	1.97	0.65
10:J:52:GLN:HE22	30:0:1119:G:H8	1.43	0.65
30:0:2073:G:H5''	39:0:3853:HOH:O	1.95	0.65
30:0:2827:A:H2'	30:0:2828:G:O4'	1.97	0.65
12:L:136:ALA:HB3	39:L:8874:HOH:O	1.96	0.65
31:9:23:U:O2'	31:9:24:U:H4'	1.96	0.65
18:R:128:ARG:NH2	30:0:2054:A:N3	2.44	0.65
30:0:119:A:H2'	30:0:120:A:H5''	1.78	0.65
30:0:2005:G:H3'	30:0:2005:G:OP2	1.97	0.64
2:B:238:ASN:HD22	2:B:240:GLY:H	1.44	0.64
30:0:2766:A:H5'	39:0:9579:HOH:O	1.96	0.64
30:0:1183:C:N4	30:0:1184:C:H41	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2578:G:H5'	30:0:2578:G:H8	1.62	0.64
30:0:2765:C:H4'	39:0:5557:HOH:O	1.98	0.64
30:0:542:A:H5'	30:0:542:A:C8	2.24	0.64
30:0:545:G:C8	30:0:545:G:H5'	2.29	0.64
2:B:212:GLN:HA	30:0:1733:A:H4'	1.80	0.64
30:0:1947:G:H2'	30:0:1948:G:H8	1.62	0.64
25:Y:204:ARG:HH22	30:0:553:G:P	2.21	0.64
30:0:2637:A:H5'	39:0:9282:HOH:O	1.96	0.64
23:W:88:THR:HG23	23:W:110:GLN:HE21	1.62	0.64
30:0:1701:A:H5''	30:0:1702:U:H3'	1.79	0.64
30:0:2635:A:O2'	30:0:2636:C:H5'	1.98	0.64
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.80	0.64
30:0:2756:U:H3	30:0:2896:A:H2	1.45	0.63
30:0:2878:U:H2'	30:0:2879:A:O4'	1.97	0.63
30:0:871:G:C8	30:0:871:G:C5'	2.73	0.63
30:0:1189:A:H3'	39:0:7737:HOH:O	1.97	0.63
30:0:2502:C:C2'	30:0:2503:A:H5'	2.28	0.63
30:0:2717:C:O2'	30:0:2718:C:H5''	1.98	0.63
30:0:1116:U:O2'	30:0:1118:A:H2	1.70	0.63
30:0:544:G:C2'	30:0:545:G:H5''	2.28	0.63
30:0:2426:G:H1'	39:0:6139:HOH:O	1.97	0.62
4:D:154:LYS:HD2	4:D:154:LYS:H	1.63	0.62
30:0:1165:G:H4'	30:0:1174:A:O2'	1.99	0.62
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.92	0.62
1:A:223:ARG:NH1	30:0:2270:G:H4'	2.15	0.62
30:0:90:A:H2'	30:0:91:G:O4'	1.98	0.62
30:0:1166:A:H1'	30:0:1192:A:C2	2.34	0.62
30:0:1205:U:C2'	30:0:1206:U:H5''	2.30	0.62
30:0:2004:U:H4'	39:0:5340:HOH:O	1.99	0.62
30:0:1666:C:H2'	30:0:1667:A:C5'	2.29	0.62
30:0:2679:G:H2'	30:0:2681:A:OP2	1.99	0.62
30:0:2896:A:H5''	39:0:6146:HOH:O	1.99	0.62
1:A:223:ARG:HH12	30:0:2270:G:H4'	1.65	0.62
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.82	0.62
30:0:1184:C:H1'	39:0:7526:HOH:O	1.99	0.62
31:9:7:G:H5'	39:9:9098:HOH:O	2.00	0.62
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.65	0.62
30:0:832:U:OP2	39:0:7839:HOH:O	2.16	0.62
31:9:20:G:O2'	31:9:21:G:H5'	1.99	0.61
25:Y:169:ARG:HD2	30:0:1328:A:OP1	2.00	0.61
23:W:154:ARG:NH1	30:0:588:G:O6	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1441:G:O2'	30:0:1442:A:H5'	1.99	0.61
30:0:123:U:H5'	39:0:6705:HOH:O	2.00	0.61
20:T:52:ARG:HD2	30:0:317:A:H5''	1.82	0.61
6:F:91:VAL:HG12	6:F:92:GLY:H	1.64	0.61
30:0:1666:C:H2'	30:0:1667:A:H5'	1.83	0.61
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.48	0.61
30:0:2768:A:H2'	30:0:2769:C:O4'	2.00	0.61
30:0:1189:A:H1'	30:0:1209:C:C1'	2.30	0.61
3:C:115:LEU:HD13	3:C:223:LEU:HD21	1.82	0.61
30:0:69:A:H5'	30:0:69:A:C8	2.36	0.61
11:K:29:LEU:HB3	11:K:55:VAL:HG11	1.81	0.61
30:0:2717:C:H2'	30:0:2718:C:C5'	2.26	0.61
30:0:282:C:O2'	30:0:283:U:H5'	2.00	0.61
11:K:87:ARG:NH2	30:0:2720:C:O2	2.34	0.60
29:3:48:ASN:HD21	30:0:2468:A:H61	1.49	0.60
30:0:848:C:H5'	39:0:7329:HOH:O	2.00	0.60
12:L:56:LYS:HE3	30:0:2443:C:H1'	1.83	0.60
31:9:14:G:H5'	31:9:14:G:C8	2.35	0.60
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.83	0.60
30:0:1209:C:H2'	30:0:1210:G:C8	2.36	0.60
30:0:558:C:O2'	30:0:559:U:H5''	2.02	0.60
30:0:1819:G:H2'	30:0:1820:G:H4'	1.81	0.60
30:0:1278:A:H4'	30:0:1279:U:C4	2.37	0.60
30:0:2502:C:H2'	30:0:2503:A:H5'	1.83	0.60
30:0:2587:OMU:H2'	30:0:2589:U:H5''	1.84	0.60
31:9:39:U:H3'	31:9:40:C:H5''	1.84	0.60
18:R:39:THR:HG22	18:R:42:GLU:H	1.67	0.60
30:0:905:C:H3'	39:0:5219:HOH:O	2.00	0.60
13:M:24:GLN:NE2	13:M:27:ARG:HH11	1.99	0.60
30:0:2241:C:O2'	30:0:2242:U:H5'	2.01	0.59
30:0:2563:U:H2'	30:0:2565:C:O5'	2.01	0.59
30:0:1372:A:H3'	39:0:7247:HOH:O	2.02	0.59
30:0:2064:U:H5'	30:0:2652:U:H4'	1.85	0.59
30:0:920:C:H5''	30:0:921:G:O5'	2.02	0.59
13:M:99:ARG:HH21	13:M:170:ASN:HD22	1.50	0.59
14:N:144:GLY:O	14:N:147:ILE:HG22	2.02	0.59
30:0:447:A:O2'	30:0:448:G:H5'	2.03	0.59
30:0:2507:G:H2'	30:0:2510:C:H42	1.67	0.59
30:0:2638:G:H5'	39:0:4962:HOH:O	2.02	0.59
30:0:2851:G:C2'	30:0:2852:A:H5'	2.32	0.58
30:0:2748:G:H5'	39:0:7599:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:969:G:H1	30:0:999:C:H42	1.50	0.58
30:0:1182:C:H1'	30:0:1192:A:H8	1.69	0.58
30:0:69:A:H5'	30:0:69:A:H8	1.68	0.58
9:I:86:GLU:HG2	30:0:1180:U:H4'	1.86	0.58
30:0:1681:G:H5''	30:0:1682:A:H5'	1.84	0.58
31:9:29:C:C2'	31:9:30:C:H5'	2.34	0.58
30:0:292:G:H2'	30:0:358:G:N2	2.19	0.58
30:0:316:A:N3	30:0:336:G:O2'	2.36	0.58
30:0:2769:C:H2'	30:0:2770:G:H5'	1.85	0.57
30:0:2816:A:H5''	30:0:2817:G:H5'	1.86	0.57
31:9:71:C:H2'	31:9:72:C:H6	1.69	0.57
30:0:2372:A:H2'	30:0:2373:U:C6	2.39	0.57
30:0:506:G:H22	30:0:509:A:H5'	1.70	0.57
30:0:1201:C:H5''	39:0:6282:HOH:O	2.03	0.57
30:0:1632:A:H2'	30:0:1633:C:H5'	1.86	0.57
31:9:76:G:C3'	31:9:77:A:H5''	2.20	0.57
30:0:2372:A:H2'	30:0:2373:U:H6	1.69	0.57
30:0:558:C:H2'	30:0:559:U:C5'	2.33	0.57
10:J:45:VAL:HG11	10:J:121:LEU:HD22	1.85	0.57
30:0:1947:G:H2'	30:0:1948:G:C8	2.40	0.57
8:H:6:ALA:HA	8:H:61:ARG:HH12	1.70	0.57
16:P:115:SER:H	16:P:118:GLN:NE2	1.98	0.57
30:0:2529:G:H3'	39:0:7241:HOH:O	2.05	0.57
30:0:2712:G:H5'	39:0:5253:HOH:O	2.05	0.57
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.05	0.57
30:0:2795:C:O2'	30:0:2796:U:H5'	2.05	0.56
14:N:37:ARG:NH1	31:9:6:C:OP1	2.34	0.56
30:0:2769:C:H2'	30:0:2770:G:O4'	2.05	0.56
31:9:64:C:C2'	31:9:65:A:H5'	2.34	0.56
16:P:105:LEU:HD21	16:P:137:LEU:HD11	1.87	0.56
30:0:2301:A:H5''	30:0:2302:A:H5'	1.86	0.56
30:0:317:A:H5'	39:0:3798:HOH:O	2.05	0.56
30:0:1080:C:H4'	30:0:1081:A:OP1	2.05	0.56
30:0:1118:A:C8	30:0:1118:A:C3'	2.85	0.56
30:0:1835:U:C5	30:0:1840:A:N7	2.66	0.56
5:E:143:GLN:NE2	30:0:2779:G:H21	2.03	0.56
30:0:1116:U:O2'	30:0:1118:A:C2	2.52	0.56
11:K:66:ARG:HH22	30:0:1994:A:P	2.28	0.56
30:0:2505:G:O2'	30:0:2506:A:H5'	2.05	0.56
19:S:51:GLN:HE21	19:S:53:ASN:HD21	1.53	0.56
30:0:1175:G:H1'	30:0:1193:A:H2'	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1790:C:H2'	30:0:1791:U:H6	1.71	0.56
30:0:625:U:H5''	30:0:1044:C:N4	2.21	0.56
28:2:10:ARG:NH2	30:0:121:U:OP2	2.36	0.56
30:0:1406:A:H4'	30:0:1407:A:H5''	1.87	0.56
30:0:2700:G:H3'	39:0:3609:HOH:O	2.06	0.56
30:0:441:A:H1'	30:0:442:A:N7	2.21	0.56
30:0:711:G:H1'	39:0:7152:HOH:O	2.06	0.56
31:9:39:U:H1'	31:9:44:A:N6	2.20	0.56
30:0:1377:C:H5'	30:0:1377:C:C6	2.41	0.55
30:0:1972:U:H2'	30:0:1973:A:C5'	2.36	0.55
3:C:127:ARG:NH2	3:C:225:PRO:HG2	2.21	0.55
30:0:2748:G:H1'	39:0:7956:HOH:O	2.06	0.55
30:0:1187:U:O2'	30:0:1189:A:H2	1.89	0.55
30:0:2472:C:O2'	30:0:2634:G:H4'	2.07	0.55
30:0:2670:G:O2'	30:0:2671:U:H5'	2.06	0.55
30:0:644:G:N3	30:0:644:G:H5'	2.20	0.55
11:K:32:ILE:HD11	11:K:56:SER:HB3	1.88	0.55
30:0:907:A:H4'	30:0:1328:A:C2	2.41	0.55
10:J:88:PRO:HD3	30:0:1104:C:H4'	1.87	0.55
30:0:2768:A:H5''	39:0:4460:HOH:O	2.06	0.55
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.22	0.55
30:0:138:U:H5''	30:0:139:C:OP2	2.07	0.55
30:0:669:G:O2'	30:0:670:G:H5'	2.06	0.55
30:0:2769:C:O2'	30:0:2770:G:H5'	2.07	0.55
29:3:2:GLN:HE21	29:3:91:GLN:HE21	1.54	0.55
14:N:4:PRO:HB2	30:0:1010:C:H4'	1.88	0.55
30:0:602:A:O2'	30:0:605:C:H4'	2.07	0.54
30:0:2718:C:H6	30:0:2718:C:H5'	1.72	0.54
3:C:76:ARG:HG2	3:C:78:ARG:NH1	2.22	0.54
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.05	0.54
30:0:272:A:H3'	39:0:7588:HOH:O	2.07	0.54
30:0:595:U:H2'	30:0:596:C:H6	1.72	0.54
4:D:146:LYS:NZ	14:N:107:ASN:HD21	2.05	0.54
30:0:1625:U:H4'	39:0:4699:HOH:O	2.06	0.54
30:0:1666:C:C2'	30:0:1667:A:C5'	2.85	0.54
30:0:1682:A:H5''	39:0:9470:HOH:O	2.06	0.54
23:W:64:THR:O	23:W:68:THR:HG22	2.07	0.54
30:0:1174:A:C5	30:0:1201:C:H4'	2.43	0.54
30:0:1741:U:O2'	30:0:2723:G:H4'	2.07	0.54
31:9:49:G:O2'	31:9:50:G:H5'	2.08	0.54
30:0:1130:U:H2'	30:0:1131:G:O4'	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:18:ILE:HD13	30:0:1244:U:OP1	2.07	0.54
23:W:88:THR:HG23	23:W:110:GLN:NE2	2.23	0.54
30:0:1528:A:H2'	30:0:1529:G:O4'	2.08	0.53
30:0:1634:G:H3'	39:0:3923:HOH:O	2.06	0.53
30:0:2419:U:H5''	30:0:2420:G:H5'	1.90	0.53
30:0:2769:C:H2'	30:0:2770:G:C5'	2.38	0.53
21:U:56:ARG:NH2	30:0:2890:A:H1'	2.22	0.53
9:I:111:LEU:HD23	30:0:1163:G:H4'	1.89	0.53
1:A:199:HIS:HE1	30:0:1881:A:OP1	1.89	0.53
30:0:1289:C:O2'	30:0:1290:G:H5'	2.09	0.53
30:0:1477:C:H5'	30:0:1868:G:C5'	2.38	0.53
30:0:2420:G:O2'	30:0:2421:G:H5'	2.08	0.53
31:9:54:A:O2'	31:9:55:U:H5'	2.08	0.53
23:W:84:VAL:HG12	39:W:6679:HOH:O	2.07	0.53
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.08	0.53
30:0:1058:A:H2'	30:0:1060:C:H5''	1.89	0.53
30:0:821:U:H2'	30:0:822:C:H6	1.74	0.53
29:3:48:ASN:ND2	29:3:50:GLY:H	2.06	0.53
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.43	0.53
14:N:37:ARG:NH1	31:9:6:C:C5'	2.67	0.53
30:0:2265:U:H2'	30:0:2266:A:C8	2.44	0.53
30:0:2768:A:O2'	30:0:2769:C:H5'	2.08	0.53
30:0:380:A:H2'	39:0:7284:HOH:O	2.09	0.53
30:0:272:A:H5'	30:0:273:G:OP2	2.09	0.53
30:0:671:A:O2'	30:0:672:G:H2'	2.09	0.53
30:0:899:C:H5'	39:0:3228:HOH:O	2.08	0.53
30:0:1641:A:C2'	30:0:1642:A:H5'	2.39	0.53
30:0:31:C:H2'	39:0:7745:HOH:O	2.08	0.53
31:9:64:C:H2'	31:9:65:A:H5'	1.90	0.53
17:Q:95:GLU:HA	30:0:949:U:H4'	1.90	0.53
30:0:2346:C:O5'	30:0:2346:C:H6	1.92	0.53
29:3:65:THR:HB	29:3:83:TRP:H	1.73	0.53
10:J:52:GLN:HE22	30:0:1119:G:H2'	1.71	0.53
30:0:1456:C:H2'	30:0:1457:U:C6	2.44	0.53
30:0:2526:C:H5'	30:0:2526:C:C6	2.44	0.53
22:V:55:ARG:O	22:V:59:ILE:HG12	2.09	0.53
30:0:1279:U:O2	30:0:1279:U:H2'	2.08	0.52
30:0:2251:G:H2'	30:0:2252:A:C8	2.44	0.52
30:0:558:C:H2'	30:0:559:U:H5''	1.90	0.52
30:0:952:G:N3	30:0:2302:A:H2'	2.24	0.52
30:0:17:G:H2'	30:0:18:C:C6	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:2:U:OP2	31:9:3:A:H5'	2.09	0.52
39:Z:8706:HOH:O	30:0:1886:A:H4'	2.10	0.52
30:0:2787:C:H5	39:0:4665:HOH:O	1.92	0.52
30:0:10:U:O4	30:0:532:A:OP2	2.28	0.52
30:0:849:C:H1'	39:0:6667:HOH:O	2.10	0.52
39:I:1549:HOH:O	30:0:1180:U:H1'	2.08	0.52
30:0:2353:A:H4'	30:0:2354:A:O5'	2.09	0.52
30:0:482:G:H4'	30:0:508:A:N1	2.24	0.52
30:0:814:G:H4'	39:0:3158:HOH:O	2.09	0.52
30:0:1766:U:O2	30:0:1778:A:H5'	2.10	0.52
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.92	0.52
30:0:343:C:O2'	30:0:344:C:H5'	2.08	0.52
30:0:304:G:H1'	30:0:347:A:N6	2.24	0.52
30:0:1118:A:H8	30:0:1119:G:H5''	1.73	0.52
30:0:468:U:H3'	39:0:7628:HOH:O	2.10	0.52
1:A:48:ASP:HB3	39:A:9064:HOH:O	2.08	0.52
3:C:76:ARG:HH22	30:0:1363:G:P	2.32	0.52
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.92	0.52
12:L:6:ARG:HD3	30:0:1299:G:O6	2.09	0.52
15:O:3:THR:CG2	30:0:656:G:H5'	2.30	0.52
3:C:236:THR:HG22	3:C:239:ALA:H	1.75	0.52
20:T:52:ARG:O	30:0:317:A:OP1	2.27	0.52
30:0:1314:U:H2'	39:0:5916:HOH:O	2.08	0.52
30:0:2010:A:H2'	39:0:6002:HOH:O	2.09	0.52
30:0:88:G:H2'	30:0:89:G:C8	2.44	0.52
4:D:146:LYS:HZ1	14:N:38:LYS:HE2	1.75	0.52
30:0:1714:C:O2'	30:0:1715:C:H5'	2.10	0.52
30:0:2320:U:H4'	30:0:2321:A:O4'	2.10	0.52
30:0:2538:A:C8	38:0:2924:ANM:H61	2.44	0.52
2:B:307:ARG:HH11	2:B:307:ARG:HG3	1.75	0.52
30:0:1250:C:O2'	30:0:1251:C:H5'	2.10	0.51
30:0:1506:U:H6	30:0:1506:U:H5'	1.74	0.51
30:0:1972:U:H2'	30:0:1973:A:H5''	1.92	0.51
30:0:2748:G:H2'	39:0:7599:HOH:O	2.10	0.51
30:0:280:C:H2'	30:0:281:U:O4'	2.10	0.51
31:9:12:C:H5'	31:9:70:U:O4'	2.10	0.51
30:0:2111:G:H1'	39:0:9050:HOH:O	2.10	0.51
30:0:1131:G:C6	30:0:1230:A:C4	2.98	0.51
30:0:2783:A:H2'	30:0:2784:A:C8	2.46	0.51
30:0:512:G:O3'	30:0:513:A:H8	1.94	0.51
30:0:1333:U:H2'	30:0:1334:C:C6	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:103:ASN:HD22	4:D:134:LEU:H	1.57	0.51
22:V:57:LYS:HA	22:V:60:GLN:HE21	1.75	0.51
23:W:80:ASP:O	23:W:84:VAL:HG23	2.11	0.51
30:0:1014:A:H2'	30:0:1015:C:H5'	1.92	0.51
30:0:1132:A:N6	30:0:1229:C:H2'	2.25	0.51
30:0:1189:A:O2'	30:0:1208:C:H2'	2.10	0.51
30:0:1268:C:O2'	30:0:1269:G:H5'	2.11	0.51
30:0:2604:A:H5'	39:0:5833:HOH:O	2.10	0.51
4:D:76:ARG:NE	31:9:44:A:O4'	2.42	0.51
1:A:199:HIS:HD2	1:A:201:PHE:H	1.58	0.51
30:0:136:C:H2'	30:0:137:U:O4'	2.11	0.51
30:0:794:U:H3	30:0:819:A:H61	1.57	0.51
12:L:18:HIS:HD2	30:0:902:G:N7	2.09	0.51
12:L:143:THR:HG22	12:L:144:ASP:H	1.76	0.51
30:0:1249:U:H2'	30:0:1250:C:C6	2.45	0.51
30:0:2243:C:H5''	39:0:3776:HOH:O	2.11	0.51
30:0:820:G:O2'	30:0:856:G:H4'	2.11	0.51
30:0:2344:G:N3	30:0:2344:G:H2'	2.25	0.51
31:9:54:A:H2	39:9:9064:HOH:O	1.93	0.51
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.91	0.51
30:0:1755:A:H2'	30:0:1756:G:O4'	2.10	0.51
25:Y:144:ARG:NH1	30:0:905:C:OP1	2.43	0.51
30:0:1211:G:O2'	30:0:1212:C:H5'	2.11	0.50
30:0:182:G:H5''	39:0:3749:HOH:O	2.11	0.50
30:0:2385:G:H2'	30:0:2386:U:C6	2.46	0.50
30:0:67:A:H5''	30:0:69:A:C8	2.46	0.50
13:M:24:GLN:HE21	13:M:27:ARG:HH11	1.57	0.50
18:R:117:HIS:HD2	30:0:20:G:H21	1.59	0.50
24:X:30:MET:HG2	30:0:1384:C:H5'	1.93	0.50
30:0:1667:A:H2'	30:0:1668:U:C6	2.46	0.50
30:0:396:U:O2'	30:0:418:C:H4'	2.12	0.50
14:N:141:ARG:NH2	31:9:48:C:H4'	2.26	0.50
30:0:1015:C:H2'	30:0:1016:U:C6	2.46	0.50
30:0:1200:A:H3'	39:0:5796:HOH:O	2.10	0.50
30:0:71:G:H5''	39:0:3940:HOH:O	2.10	0.50
30:0:1940:C:H4'	39:0:7406:HOH:O	2.10	0.50
30:0:407:A:H5'	39:0:6070:HOH:O	2.10	0.50
30:0:1172:G:H5''	39:0:7316:HOH:O	2.11	0.50
30:0:1596:U:H2'	30:0:1598:A:OP2	2.11	0.50
14:N:11:ARG:HD3	31:9:114:G:O6	2.11	0.50
8:H:168:VAL:HG13	39:H:9008:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:74:VAL:HG12	11:K:75:ARG:HG3	1.92	0.50
23:W:6:GLN:HB2	23:W:26:ILE:HD12	1.93	0.50
30:0:1778:A:H2'	30:0:1779:A:H5'	1.93	0.50
30:0:271:C:H41	30:0:378:A:H2	1.58	0.50
30:0:396:U:H1'	39:0:7686:HOH:O	2.09	0.50
30:0:969:G:H1	30:0:999:C:N4	2.10	0.50
23:W:21:LEU:HD22	23:W:26:ILE:HD11	1.92	0.50
30:0:1185:U:H2'	30:0:1186:C:C6	2.46	0.50
30:0:125:U:H2'	39:0:3792:HOH:O	2.10	0.50
30:0:1925:G:O2'	30:0:1926:G:H5'	2.12	0.50
30:0:2252:A:C5	30:0:2253:G:H1'	2.46	0.50
30:0:1819:G:H2'	30:0:1820:G:C5'	2.42	0.50
30:0:1972:U:C2'	30:0:1973:A:H5''	2.42	0.50
30:0:2415:A:H2'	30:0:2416:G:H5'	1.94	0.50
30:0:485:A:N3	30:0:487:G:H5''	2.27	0.50
27:1:12:ASN:O	30:0:1415:G:H5'	2.11	0.50
31:9:95:C:O2'	31:9:96:C:H5'	2.12	0.50
30:0:2104:C:O2	30:0:2485:A:N1	2.45	0.50
30:0:255:A:H2'	30:0:256:C:C6	2.46	0.50
30:0:559:U:H5'	30:0:559:U:C6	2.36	0.50
30:0:1562:C:O2	30:0:1562:C:H2'	2.12	0.49
1:A:121:ALA:O	1:A:124:VAL:HG22	2.12	0.49
30:0:2498:C:O2'	30:0:2499:U:H5'	2.12	0.49
30:0:564:G:H1'	39:0:6359:HOH:O	2.12	0.49
1:A:192:VAL:HG12	39:A:9054:HOH:O	2.11	0.49
12:L:14:GLY:O	30:0:1295:G:H5''	2.12	0.49
31:9:52:A:H2'	31:9:53:G:O4'	2.12	0.49
31:9:92:G:H2'	31:9:93:A:H8	1.76	0.49
30:0:1350:U:H4'	39:0:5156:HOH:O	2.12	0.49
30:0:2256:G:O2'	30:0:2257:G:H5'	2.12	0.49
30:0:2300:A:H4'	30:0:2301:A:O5'	2.13	0.49
8:H:31:ILE:HG23	39:H:9028:HOH:O	2.13	0.49
30:0:1181:A:N1	30:0:1192:A:O2'	2.44	0.49
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.38	0.49
30:0:660:A:H4'	30:0:661:G:O5'	2.13	0.49
30:0:1419:U:H2'	30:0:1685:A:C2	2.47	0.49
30:0:249:G:O2'	30:0:250:C:H5'	2.13	0.49
30:0:958:G:H2'	30:0:959:C:C6	2.47	0.49
30:0:120:A:H2'	30:0:120:A:N3	2.28	0.49
30:0:1894:C:N4	30:0:1939:U:H2'	2.27	0.49
30:0:2508:C:H2'	39:0:6808:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:91:VAL:HG11	30:0:262:A:OP2	2.13	0.49
39:B:9096:HOH:O	30:0:2672:C:H1'	2.12	0.49
30:0:2825:C:H4'	30:0:2826:G:O5'	2.13	0.49
30:0:2756:U:N3	30:0:2896:A:H2	2.08	0.49
31:9:34:A:H2'	31:9:35:C:O4'	2.12	0.49
31:9:35:C:H5''	39:9:9077:HOH:O	2.12	0.49
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.95	0.49
30:0:1135:G:H5'	39:0:5971:HOH:O	2.13	0.49
30:0:1838:U:O2'	30:0:2644:C:H5'	2.13	0.49
30:0:2758:G:H2'	30:0:2759:C:C6	2.48	0.49
31:9:61:C:H2'	31:9:62:A:H8	1.77	0.49
2:B:221:GLN:HE22	11:K:42:ASN:ND2	1.94	0.49
30:0:1046:G:N3	30:0:1082:A:H2	2.11	0.49
30:0:1632:A:C2'	30:0:1633:C:H5'	2.43	0.49
30:0:1919:A:H4'	39:0:4884:HOH:O	2.12	0.49
30:0:2248:C:H3'	39:0:5478:HOH:O	2.13	0.49
30:0:459:A:H5''	39:0:9053:HOH:O	2.13	0.49
24:X:74:ALA:HB2	24:X:85:VAL:HG13	1.95	0.49
30:0:1603:A:H5''	30:0:1605:G:H5'	1.95	0.49
30:0:567:U:OP1	39:0:5320:HOH:O	2.19	0.49
30:0:64:G:H2'	30:0:65:C:O4'	2.13	0.49
2:B:288:GLY:HA2	30:0:2898:G:H4'	1.95	0.49
4:D:159:PRO:O	4:D:163:VAL:HG23	2.13	0.49
23:W:48:VAL:HG12	23:W:52:VAL:HB	1.94	0.49
30:0:1189:A:H1'	30:0:1209:C:H1'	1.94	0.48
30:0:2649:A:H5'	30:0:2649:A:H8	1.77	0.48
5:E:137:ASP:O	5:E:141:VAL:HG23	2.12	0.48
8:H:70:LEU:O	8:H:74:ARG:HB2	2.13	0.48
30:0:1044:C:H5	39:0:6654:HOH:O	1.94	0.48
9:I:130:LEU:HD21	30:0:1167:G:H4'	1.95	0.48
39:Y:8908:HOH:O	30:0:1330:A:H5''	2.12	0.48
30:0:1946:C:H2'	30:0:1971:G:C8	2.48	0.48
30:0:2090:G:H2'	30:0:2091:G:C8	2.48	0.48
2:B:16:ARG:NH1	39:B:9082:HOH:O	2.45	0.48
30:0:1441:G:H1'	39:0:7823:HOH:O	2.11	0.48
31:9:114:G:H2'	31:9:115:C:C6	2.49	0.48
13:M:164:THR:HG22	13:M:167:GLY:H	1.78	0.48
14:N:44:ARG:NH1	31:9:4:G:H21	2.11	0.48
30:0:1119:G:N2	30:0:1246:A:N1	2.61	0.48
30:0:324:G:O2'	30:0:325:U:H5'	2.13	0.48
25:Y:142:SER:OG	30:0:1331:G:OP2	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:432:G:O2'	30:0:433:C:H5'	2.14	0.48
30:0:558:C:H2'	30:0:559:U:H5'	1.95	0.48
30:0:947:U:O2'	30:0:948:G:H5'	2.13	0.48
20:T:38:ARG:HH21	30:0:306:A:P	2.37	0.48
30:0:1819:G:H2'	30:0:1820:G:C4'	2.44	0.48
30:0:318:U:H5'	30:0:339:A:C2	2.49	0.48
30:0:42:C:H1'	39:0:4709:HOH:O	2.13	0.48
30:0:932:U:H2'	30:0:933:C:C6	2.49	0.48
6:F:91:VAL:HG12	6:F:92:GLY:N	2.29	0.48
18:R:40:ALA:O	18:R:44:VAL:HG23	2.13	0.48
30:0:2011:A:H4'	30:0:2012:U:O5'	2.14	0.48
30:0:2361:A:H2'	30:0:2362:A:C8	2.49	0.48
30:0:2608:C:H2'	39:0:7867:HOH:O	2.14	0.48
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.14	0.48
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.28	0.48
30:0:1066:U:H2'	30:0:1067:A:C8	2.49	0.48
30:0:1183:C:H42	30:0:1184:C:H41	1.61	0.48
30:0:2000:G:O2'	30:0:2001:G:H5'	2.14	0.48
24:X:43:VAL:HG22	24:X:76:ARG:NH1	2.29	0.48
30:0:1087:G:H4'	30:0:1088:A:OP1	2.14	0.47
30:0:1206:U:H2'	30:0:1207:A:O4'	2.13	0.47
16:P:41:ARG:HH22	30:0:1500:U:P	2.37	0.47
30:0:1613:C:H2'	30:0:1614:G:O4'	2.14	0.47
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.78	0.47
30:0:1855:G:H4'	30:0:1856:C:O5'	2.13	0.47
30:0:2135:A:O2'	30:0:2136:G:H5'	2.14	0.47
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.14	0.47
30:0:622:G:O2'	30:0:623:U:H5'	2.14	0.47
27:1:28:HIS:HE1	30:0:776:A:OP1	1.97	0.47
30:0:2649:A:H5'	30:0:2649:A:C8	2.50	0.47
30:0:790:A:H1'	30:0:1710:A:H2'	1.96	0.47
30:0:2329:C:O2'	30:0:2330:U:H5'	2.13	0.47
30:0:24:G:N2	30:0:518:G:H1'	2.29	0.47
30:0:2526:C:O2'	30:0:2527:U:H5'	2.14	0.47
30:0:2755:G:H1'	39:0:4715:HOH:O	2.14	0.47
30:0:635:A:H2'	30:0:636:G:H5''	1.95	0.47
1:A:51:ARG:NH1	1:A:120:ARG:O	2.47	0.47
2:B:5:ARG:NH1	2:B:8:LYS:HE2	2.27	0.47
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.95	0.47
30:0:1166:A:OP1	30:0:1174:A:H4'	2.14	0.47
30:0:1926:G:H2'	30:0:1927:A:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2842:G:H2'	30:0:2843:A:H5'	1.95	0.47
30:0:961:A:H4'	39:0:6826:HOH:O	2.14	0.47
2:B:244:PRO:HB3	30:0:1234:U:N3	2.28	0.47
14:N:49:THR:HG22	14:N:56:ASP:HB2	1.97	0.47
21:U:14:GLU:O	21:U:17:THR:HB	2.15	0.47
30:0:1181:A:C2'	30:0:1182:C:H5'	2.45	0.47
30:0:1342:C:C2'	30:0:1343:C:H5'	2.45	0.47
30:0:1603:A:H5'	30:0:1605:G:C4'	2.44	0.47
30:0:677:C:O2'	30:0:678:G:H5'	2.15	0.47
31:9:107:C:O2'	31:9:108:C:H5'	2.14	0.47
30:0:1829:A:H2'	30:0:1830:C:H5'	1.97	0.47
30:0:2064:U:H5'	30:0:2652:U:O3'	2.15	0.47
30:0:2105:C:H2'	30:0:2106:C:C6	2.49	0.47
30:0:368:C:H2'	30:0:369:G:H5'	1.97	0.47
31:9:39:U:HO2'	31:9:42:C:H5	1.57	0.47
23:W:23:MET:O	30:0:1025:C:H5'	2.15	0.47
30:0:1535:G:H2'	30:0:1536:C:C6	2.50	0.47
13:M:95:LYS:HE2	30:0:157:G:H4'	1.97	0.47
30:0:1622:G:H2'	30:0:1623:C:H5'	1.97	0.47
29:3:15:ASN:O	30:0:2408:A:H4'	2.15	0.47
16:P:83:LYS:HG2	30:0:793:A:H5"	1.97	0.47
20:T:38:ARG:NH1	39:0:6736:HOH:O	2.47	0.47
30:0:2414:A:H2'	30:0:2415:A:C8	2.50	0.47
30:0:560:U:H2'	30:0:561:G:H8	1.79	0.47
30:0:714:U:H3'	39:0:6997:HOH:O	2.15	0.47
27:1:16:HIS:HD2	30:0:470:U:O2'	1.97	0.47
30:0:1016:U:H1'	39:0:3685:HOH:O	2.13	0.47
30:0:1588:G:C6	30:0:1589:G:N1	2.83	0.47
30:0:1662:C:H2'	30:0:1663:G:O4'	2.15	0.47
30:0:170:U:H2'	30:0:171:C:H5'	1.95	0.47
30:0:653:U:H2'	30:0:654:A:C8	2.49	0.47
30:0:920:C:H4'	30:0:921:G:C2	2.49	0.47
8:H:22:TYR:CZ	30:0:1007:A:H2'	2.49	0.47
30:0:1406:A:H4'	30:0:1407:A:C5'	2.45	0.47
30:0:1595:G:O2'	30:0:1596:U:H5'	2.15	0.47
30:0:1815:A:H2'	30:0:1816:C:O4'	2.15	0.47
30:0:255:A:H2'	30:0:256:C:H6	1.80	0.47
3:C:118:THR:O	3:C:136:VAL:HG13	2.15	0.47
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.97	0.47
17:Q:15:LYS:HD3	30:0:2364:A:H5"	1.97	0.47
26:Z:40:ALA:HA	30:0:1773:G:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2064:U:H4'	30:0:2653:A:OP1	2.14	0.46
30:0:299:U:H5'	39:0:7395:HOH:O	2.16	0.46
2:B:211:THR:HG21	39:0:7515:HOH:O	2.14	0.46
14:N:141:ARG:HH21	31:9:48:C:H4'	1.79	0.46
30:0:1515:A:H2'	30:0:1516:U:C6	2.50	0.46
30:0:256:C:H2'	30:0:257:G:O4'	2.15	0.46
30:0:559:U:H2'	30:0:560:U:O4'	2.15	0.46
30:0:704:C:H2'	30:0:705:C:H6	1.80	0.46
30:0:951:A:O2'	30:0:952:G:H5'	2.15	0.46
30:0:960:G:N3	30:0:960:G:C2'	2.78	0.46
17:Q:19:ARG:HH21	31:9:11:A:P	2.37	0.46
30:0:1592:G:H2'	30:0:1593:C:C6	2.51	0.46
30:0:1603:A:C5'	30:0:1605:G:H5'	2.45	0.46
30:0:595:U:H2'	30:0:596:C:C6	2.49	0.46
30:0:834:G:H3'	30:0:835:U:H4'	1.98	0.46
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.15	0.46
20:T:111:ARG:HB3	20:T:119:ALA:HB2	1.97	0.46
30:0:1057:A:H1'	30:0:2492:U:O2'	2.15	0.46
30:0:192:A:H5'	39:0:7700:HOH:O	2.16	0.46
30:0:2072:G:C6	30:0:2533:C:H1'	2.51	0.46
30:0:2909:G:H2'	30:0:2910:A:H8	1.80	0.46
23:W:6:GLN:HB2	23:W:26:ILE:CD1	2.45	0.46
30:0:1137:G:H1'	39:0:3907:HOH:O	2.15	0.46
30:0:2781:U:C2'	30:0:2782:G:H5'	2.45	0.46
30:0:694:A:H2'	30:0:695:C:H5'	1.97	0.46
19:S:33:SER:O	19:S:37:VAL:HG23	2.15	0.46
23:W:21:LEU:HD22	23:W:26:ILE:CD1	2.44	0.46
30:0:1118:A:C8	30:0:1119:G:H5''	2.51	0.46
30:0:12:U:C2'	30:0:13:G:H5'	2.46	0.46
30:0:1973:A:H5'	30:0:1973:A:C8	2.42	0.46
30:0:821:U:H3'	39:0:3796:HOH:O	2.15	0.46
14:N:34:LEU:HD22	14:N:129:ILE:HD13	1.98	0.46
30:0:1158:G:O2'	30:0:1159:G:H5'	2.16	0.46
30:0:1218:U:H2'	30:0:1219:U:C6	2.51	0.46
30:0:1804:A:H2'	30:0:1805:G:C8	2.50	0.46
30:0:2361:A:H8	30:0:2361:A:H5'	1.81	0.46
30:0:2531:U:O2'	30:0:2532:A:H5'	2.15	0.46
30:0:702:G:O2'	30:0:703:G:H5'	2.16	0.46
30:0:645:U:O2	30:0:761:A:H2	1.98	0.46
30:0:1060:C:H6	30:0:1060:C:H5'	1.81	0.46
30:0:1614:G:H2'	39:0:4660:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1771:U:O2'	30:0:1773:G:N7	2.48	0.46
30:0:2445:U:H2'	30:0:2446:G:C8	2.50	0.46
30:0:2879:A:H2'	30:0:2880:A:O4'	2.16	0.46
30:0:2894:C:O2'	30:0:2895:C:H5'	2.15	0.46
30:0:2900:G:H2'	30:0:2901:C:O4'	2.16	0.46
30:0:407:A:H2'	30:0:408:A:C8	2.51	0.46
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.55	0.46
30:0:113:A:OP2	30:0:114:A:H2'	2.15	0.46
30:0:807:A:O2'	30:0:808:A:H5'	2.16	0.46
2:B:238:ASN:HD22	2:B:240:GLY:N	2.11	0.46
6:F:58:GLU:CD	13:M:27:ARG:HH22	2.19	0.46
39:C:8656:HOH:O	30:0:2100:A:H5'	2.15	0.46
30:0:538:C:H5''	30:0:539:G:C8	2.50	0.46
30:0:612:U:H2'	30:0:613:C:C6	2.51	0.46
28:2:40:ARG:HD2	28:2:47:THR:HG22	1.97	0.46
1:A:179:MET:HG2	1:A:186:TRP:HB2	1.97	0.46
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.64	0.46
26:Z:70:ARG:HD3	26:Z:83:TYR:HB2	1.97	0.46
30:0:1641:A:H2'	30:0:1642:A:C5'	2.44	0.45
30:0:1657:A:H2'	30:0:1658:A:C8	2.51	0.45
30:0:1972:U:H2'	30:0:1973:A:H5'	1.98	0.45
30:0:2421:G:H3'	30:0:2422:U:C5'	2.46	0.45
30:0:2509:A:OP2	30:0:2510:C:H5	1.97	0.45
30:0:2852:A:H5''	39:0:5266:HOH:O	2.17	0.45
30:0:876:A:N3	30:0:876:A:H2'	2.31	0.45
8:H:174:LEU:HD21	30:0:1220:U:H4'	1.97	0.45
30:0:1056:U:H2'	30:0:1057:A:O4'	2.16	0.45
30:0:1413:A:H2'	30:0:1414:A:O4'	2.16	0.45
30:0:2326:C:H4'	30:0:2412:G:C4'	2.47	0.45
30:0:319:A:H4'	30:0:338:C:C4	2.52	0.45
30:0:95:A:H5''	30:0:97:G:O4'	2.16	0.45
30:0:960:G:H3'	30:0:960:G:N3	2.31	0.45
8:H:64:SER:OG	30:0:2520:G:H5'	2.16	0.45
30:0:1201:C:H2'	30:0:1202:A:H5'	1.99	0.45
30:0:2314:G:C2'	30:0:2315:C:H5'	2.46	0.45
30:0:629:A:H2'	30:0:630:A:O4'	2.16	0.45
3:C:168:ARG:NH2	3:C:190:ALA:O	2.49	0.45
11:K:55:VAL:HG12	11:K:56:SER:N	2.32	0.45
14:N:35:VAL:HG11	31:9:6:C:H4'	1.97	0.45
15:O:25:VAL:HG13	30:0:709:G:O2'	2.16	0.45
25:Y:115:ARG:HH21	30:0:1266:U:H4'	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1485:A:H8	39:0:9975:HOH:O	1.99	0.45
30:0:1592:G:O2'	30:0:1593:C:O5'	2.34	0.45
30:0:1973:A:H2'	30:0:1974:G:O4'	2.16	0.45
30:0:2766:A:O2'	30:0:2767:C:H5'	2.16	0.45
30:0:281:U:O2'	30:0:282:C:H5'	2.16	0.45
30:0:1787:C:H4'	30:0:2883:A:O4'	2.17	0.45
38:0:2924:ANM:H62	38:0:2924:ANM:H2	1.87	0.45
31:9:13:A:O2'	31:9:14:G:H5''	2.17	0.45
31:9:24:U:H3'	31:9:25:G:H5'	1.97	0.45
1:A:51:ARG:HB2	39:A:9064:HOH:O	2.17	0.45
10:J:127:ILE:HG22	33:J:8801:CL:CL	2.53	0.45
18:R:39:THR:HG23	18:R:107:GLU:O	2.17	0.45
30:0:1304:U:H2'	30:0:1305:C:C6	2.52	0.45
30:0:1497:G:H4'	30:0:1627:G:O2'	2.16	0.45
30:0:17:G:H2'	30:0:18:C:H6	1.81	0.45
30:0:2781:U:H2'	30:0:2782:G:H5'	1.98	0.45
30:0:812:A:H1'	39:0:3988:HOH:O	2.16	0.45
8:H:69:ARG:HD3	39:H:9028:HOH:O	2.16	0.45
30:0:1391:G:H2'	30:0:1392:A:H5'	1.99	0.45
30:0:2589:U:H2'	30:0:2590:U:C6	2.52	0.45
30:0:2758:G:H2'	30:0:2759:C:H6	1.82	0.45
30:0:777:U:OP2	30:0:777:U:H4'	2.16	0.45
27:1:8:GLN:HE22	27:1:11:LYS:HZ2	1.65	0.45
31:9:49:G:H2'	31:9:50:G:O4'	2.17	0.45
6:F:48:VAL:HG23	6:F:74:PHE:HB3	1.99	0.45
30:0:1181:A:H2'	30:0:1182:C:H5'	1.98	0.45
30:0:1160:G:HO2'	30:0:1190:G:H8	1.64	0.45
30:0:1333:U:H2'	30:0:1334:C:H6	1.82	0.45
30:0:1398:G:H2'	30:0:1399:A:C8	2.51	0.45
30:0:1503:U:H2'	30:0:1504:A:O4'	2.16	0.45
30:0:2387:U:H2'	30:0:2388:C:C6	2.51	0.45
30:0:2883:A:H2'	30:0:2884:G:O4'	2.17	0.45
30:0:295:C:H2'	30:0:296:G:O4'	2.15	0.45
30:0:366:U:H2'	30:0:367:G:O4'	2.16	0.45
3:C:88:SER:HB3	3:C:91:PRO:HB3	1.99	0.45
30:0:1015:C:H2'	30:0:1016:U:H6	1.80	0.45
30:0:2456:A:H2'	30:0:2457:U:C6	2.52	0.45
30:0:308:U:H5'	30:0:309:C:OP1	2.16	0.45
13:M:43:PRO:HG3	13:M:62:VAL:HG21	1.97	0.45
30:0:1427:A:H61	30:0:1440:U:C1'	2.30	0.45
30:0:168:C:O5'	30:0:168:C:H6	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2401:A:H2'	30:0:2402:A:C8	2.52	0.45
30:0:847:C:H4'	39:0:3779:HOH:O	2.16	0.45
2:B:94:GLN:O	30:0:2673:U:H4'	2.17	0.45
4:D:140:ARG:HB3	31:9:29:C:H5''	1.99	0.45
13:M:107:ARG:NH1	39:M:8871:HOH:O	2.49	0.45
30:0:2509:A:H2'	30:0:2510:C:O4'	2.17	0.45
30:0:2594:C:O2'	30:0:2595:U:H5'	2.16	0.45
30:0:291:C:H2'	30:0:292:G:O4'	2.17	0.45
30:0:397:A:O2'	30:0:417:G:N3	2.37	0.45
3:C:127:ARG:HD3	3:C:129:HIS:HE1	1.82	0.45
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.97	0.45
24:X:43:VAL:HG12	24:X:44:ASP:N	2.32	0.45
2:B:234:ARG:NH2	30:0:2039:A:OP2	2.51	0.44
30:0:2371:G:H5'	39:0:5043:HOH:O	2.17	0.44
30:0:2510:C:H5'	30:0:2511:A:OP2	2.18	0.44
30:0:2607:U:H4'	39:0:9455:HOH:O	2.16	0.44
30:0:638:C:H2'	30:0:639:A:C8	2.53	0.44
30:0:907:A:H2'	30:0:908:A:H8	1.80	0.44
31:9:22:G:H5'	31:9:23:U:OP1	2.17	0.44
1:A:36:ASP:O	1:A:38:ILE:N	2.44	0.44
2:B:254:GLN:HG2	2:B:255:GLY:N	2.32	0.44
19:S:11:THR:H	19:S:14:ALA:HB3	1.80	0.44
30:0:1204:C:H2'	30:0:1205:U:O4'	2.17	0.44
30:0:2866:U:H4'	30:0:2867:G:H5'	1.99	0.44
23:W:44:MET:CE	30:0:944:G:H21	2.31	0.44
30:0:1167:G:H2'	30:0:1168:C:C6	2.51	0.44
30:0:1878:G:O2'	30:0:1879:U:C6	2.68	0.44
30:0:1942:A:H3'	39:0:7406:HOH:O	2.17	0.44
30:0:2524:G:H21	30:0:2526:C:N4	2.16	0.44
1:A:206:ARG:NH2	30:0:2630:G:O6	2.50	0.44
30:0:737:A:H2'	30:0:738:G:O4'	2.17	0.44
30:0:821:U:H2'	30:0:822:C:C6	2.53	0.44
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.99	0.44
25:Y:154:ARG:NH2	30:0:1071:G:H4'	2.32	0.44
30:0:1594:C:O2'	30:0:1607:A:H4'	2.17	0.44
30:0:168:C:H5'	30:0:2277:U:OP1	2.17	0.44
30:0:1878:G:O2'	30:0:1879:U:P	2.74	0.44
30:0:690:G:H4'	30:0:741:C:O2	2.17	0.44
30:0:960:G:H2'	30:0:960:G:N3	2.31	0.44
4:D:135:VAL:HG22	4:D:136:ARG:H	1.82	0.44
30:0:1996:U:O2'	30:0:1997:A:H5'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2754:G:H2'	30:0:2755:G:O4'	2.17	0.44
27:1:5:THR:HG23	30:0:1688:G:O2'	2.18	0.44
12:L:30:ARG:NH2	39:L:8818:HOH:O	2.51	0.44
30:0:2421:G:H3'	30:0:2422:U:H5''	2.00	0.44
12:L:57:VAL:HG21	30:0:2443:C:H5'	1.99	0.44
30:0:454:U:H5''	39:0:7834:HOH:O	2.17	0.44
29:3:73:GLU:HB3	39:3:9051:HOH:O	2.17	0.44
31:9:3:A:OP2	31:9:25:G:N2	2.51	0.44
3:C:115:LEU:O	3:C:118:THR:HB	2.18	0.44
12:L:33:ALA:HB2	30:0:165:A:H5''	2.00	0.44
25:Y:165:GLU:HB3	39:Y:8889:HOH:O	2.17	0.44
30:0:1252:A:H2'	30:0:1253:C:O4'	2.18	0.44
30:0:128:A:O2'	30:0:129:A:H5'	2.17	0.44
30:0:1477:C:H5'	30:0:1868:G:H5''	2.00	0.44
30:0:162:C:H2'	30:0:163:U:H5'	1.99	0.44
30:0:1683:G:C2	30:0:1693:A:O4'	2.71	0.44
30:0:2256:G:C2'	30:0:2257:G:H5'	2.48	0.44
30:0:2092:G:H2'	30:0:2613:G:OP1	2.18	0.44
30:0:2899:A:O2'	30:0:2900:G:H5'	2.18	0.44
30:0:666:A:H2'	30:0:667:C:O4'	2.18	0.44
30:0:951:A:C2'	30:0:952:G:H5'	2.48	0.44
1:A:132:ASP:HB3	1:A:135:VAL:H	1.82	0.44
30:0:1172:G:H1'	39:0:5007:HOH:O	2.17	0.44
30:0:1165:G:H1'	30:0:1174:A:H1'	1.98	0.44
30:0:137:U:OP1	30:0:259:G:O2'	2.36	0.44
30:0:1422:U:H2'	30:0:1423:C:C6	2.52	0.44
4:D:131:THR:HG21	30:0:2348:C:H1'	1.99	0.44
30:0:2379:G:N7	30:0:2408:A:N1	2.65	0.44
30:0:2809:G:H2'	30:0:2810:G:O4'	2.18	0.44
30:0:542:A:H2'	30:0:543:G:O4'	2.18	0.44
30:0:71:G:H8	39:0:3940:HOH:O	2.00	0.44
30:0:1130:U:H5'	39:0:7729:HOH:O	2.17	0.44
30:0:138:U:OP2	30:0:139:C:H5	2.00	0.44
30:0:1592:G:H2'	30:0:1593:C:H6	1.83	0.44
30:0:2039:A:H2'	30:0:2040:C:C6	2.52	0.44
30:0:920:C:H5'	30:0:921:G:C4	2.53	0.44
30:0:1421:C:O2'	30:0:1422:U:H5'	2.17	0.43
30:0:1790:C:H2'	30:0:1791:U:C6	2.52	0.43
30:0:2326:C:H4'	30:0:2412:G:H4'	2.00	0.43
8:H:74:ARG:NH1	30:0:2504:A:H4'	2.33	0.43
30:0:2703:A:H2'	30:0:2704:C:H6	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:466:A:H2'	30:0:467:G:O4'	2.18	0.43
30:0:484:A:N1	30:0:506:G:H4'	2.33	0.43
30:0:941:G:C5	30:0:942:U:C4	3.06	0.43
31:9:91:C:H2'	31:9:92:G:O4'	2.18	0.43
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.90	0.43
2:B:315:VAL:HG23	2:B:316:ARG:HG2	2.00	0.43
30:0:1762:C:H2'	30:0:1763:C:H6	1.84	0.43
30:0:2088:C:H1'	30:0:2841:A:N1	2.33	0.43
30:0:2533:C:H6	30:0:2533:C:C5'	2.24	0.43
30:0:2578:G:C8	30:0:2578:G:H5'	2.49	0.43
30:0:558:C:C2'	30:0:559:U:C5'	2.92	0.43
3:C:47:GLY:HA2	3:C:92:PRO:HB2	2.00	0.43
18:R:128:ARG:NH2	30:0:2054:A:C2	2.83	0.43
16:P:1:THR:O	30:0:1396:C:H1'	2.18	0.43
30:0:2765:C:H2'	30:0:2766:A:C8	2.54	0.43
30:0:371:U:H2'	30:0:372:A:H8	1.83	0.43
19:S:17:ASP:HB3	19:S:23:LYS:HB2	2.00	0.43
30:0:1377:C:H1'	39:0:9041:HOH:O	2.18	0.43
30:0:1504:A:H5'	39:0:4450:HOH:O	2.19	0.43
30:0:1544:U:H2'	30:0:1545:C:C6	2.54	0.43
13:M:171:ARG:CD	30:0:156:C:H5''	2.31	0.43
30:0:1837:G:H3'	39:0:7851:HOH:O	2.18	0.43
18:R:132:ARG:NH2	30:0:2055:A:H4'	2.33	0.43
30:0:2569:A:H2'	30:0:2570:G:O5'	2.18	0.43
30:0:603:A:H1'	30:0:605:C:C2	2.53	0.43
27:1:8:GLN:HE22	27:1:11:LYS:NZ	2.16	0.43
16:P:120:ARG:HD2	30:0:1594:C:OP2	2.19	0.43
16:P:88:GLN:HE22	30:0:1799:G:H21	1.65	0.43
23:W:119:HIS:HE1	39:0:9570:HOH:O	2.01	0.43
30:0:1039:G:H2'	30:0:1040:A:O4'	2.19	0.43
30:0:1042:U:O2'	30:0:1043:C:H5'	2.18	0.43
30:0:1138:G:H4'	39:0:5749:HOH:O	2.18	0.43
30:0:1213:C:O2'	30:0:1214:G:H5'	2.18	0.43
30:0:1788:U:O2'	30:0:1789:G:H5'	2.19	0.43
30:0:2072:G:H3'	30:0:2073:G:C5'	2.49	0.43
30:0:2274:A:O2'	30:0:2275:G:H5'	2.18	0.43
30:0:191:A:C4	30:0:237:G:N7	2.87	0.43
30:0:2697:A:H2'	30:0:2698:G:O4'	2.18	0.43
30:0:2791:U:H1'	30:0:2792:A:H5''	2.00	0.43
30:0:417:G:P	39:0:7478:HOH:O	2.75	0.43
30:0:790:A:H2'	30:0:791:A:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:33:U:H2'	39:9:9068:HOH:O	2.19	0.43
5:E:112:ALA:HA	5:E:113:PRO:HD3	1.88	0.43
13:M:171:ARG:NH2	30:0:189:A:OP1	2.52	0.43
30:0:1096:U:O2'	30:0:1097:A:H5'	2.18	0.43
30:0:271:C:H4'	30:0:272:A:OP1	2.18	0.43
30:0:364:U:H2'	30:0:365:G:O4'	2.19	0.43
30:0:407:A:H8	39:0:4495:HOH:O	2.00	0.43
30:0:497:A:H2'	30:0:498:A:C5'	2.49	0.43
12:L:37:LYS:NZ	30:0:919:U:O3'	2.50	0.43
24:X:15:ARG:NH1	30:0:2896:A:OP1	2.52	0.43
25:Y:208:LYS:O	30:0:1313:A:H5'	2.18	0.43
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.99	0.43
30:0:1477:C:O2'	30:0:1478:U:H5'	2.18	0.43
30:0:1921:A:O2'	30:0:1922:A:H5'	2.19	0.43
30:0:195:C:H2'	30:0:196:G:H5'	2.00	0.43
30:0:2653:A:H2'	30:0:2654:C:C6	2.54	0.43
30:0:37:A:H2'	30:0:38:G:C8	2.53	0.43
30:0:603:A:H4'	30:0:604:G:O5'	2.18	0.43
30:0:722:G:H22	30:0:938:G:P	2.41	0.43
2:B:297:VAL:HG23	39:B:9071:HOH:O	2.17	0.43
30:0:815:U:O2'	30:0:1598:A:H4'	2.18	0.43
30:0:1926:G:H2'	30:0:1927:A:H8	1.84	0.43
30:0:2039:A:H4'	30:0:2760:C:O2'	2.19	0.43
30:0:488:U:H2'	39:0:4037:HOH:O	2.18	0.43
18:R:98:ASN:ND2	30:0:500:G:H21	2.10	0.43
30:0:517:U:H1'	39:0:7636:HOH:O	2.19	0.43
31:9:47:A:C2	31:9:48:C:C2	3.07	0.43
24:X:43:VAL:HG12	24:X:44:ASP:H	1.83	0.43
10:J:52:GLN:NE2	30:0:1119:G:H8	2.13	0.43
30:0:1278:A:H4'	30:0:1279:U:N3	2.34	0.43
30:0:1481:G:H2'	30:0:1482:A:O4'	2.19	0.43
30:0:1634:G:H2'	30:0:1635:U:C6	2.54	0.43
30:0:2001:G:O2'	30:0:2002:C:H5'	2.18	0.43
30:0:2256:G:H2'	30:0:2257:G:C5'	2.49	0.43
2:B:36:PRO:HG3	2:B:169:GLY:H	1.83	0.43
30:0:1342:C:O2'	30:0:1343:C:H5'	2.19	0.43
30:0:1451:C:H5'	30:0:1505:U:C5	2.54	0.43
30:0:285:A:H2'	30:0:286:U:O4'	2.19	0.43
30:0:238:C:H4'	30:0:287:C:OP1	2.19	0.43
30:0:65:C:O2'	30:0:66:G:H5'	2.19	0.43
5:E:83:GLY:HA3	5:E:170:ARG:HE	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:39:ALA:N	22:V:40:PRO:HD2	2.34	0.43
25:Y:141:THR:HG23	39:Y:8884:HOH:O	2.18	0.43
1:A:217:ARG:NH2	30:0:1853:C:O2'	2.52	0.42
30:0:2121:G:O2'	30:0:2122:C:H5'	2.19	0.42
30:0:420:U:H2'	30:0:421:C:C6	2.54	0.42
27:1:42:SER:HB3	30:0:1473:U:O4'	2.18	0.42
30:0:1490:G:H4'	30:0:1533:A:OP1	2.18	0.42
30:0:1762:C:H2'	30:0:1763:C:C6	2.54	0.42
30:0:1834:C:H2'	30:0:1840:A:N6	2.34	0.42
13:M:90:ARG:NH2	30:0:2266:A:OP2	2.51	0.42
30:0:2515:C:H2'	30:0:2516:G:O4'	2.19	0.42
30:0:2672:C:H2'	30:0:2673:U:C6	2.53	0.42
3:C:46:TYR:CE1	30:0:450:C:H4'	2.53	0.42
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.18	0.42
23:W:5:VAL:HG11	23:W:153:MET:HE3	2.00	0.42
30:0:1187:U:H2'	39:0:6950:HOH:O	2.18	0.42
30:0:164:G:H3'	39:0:3671:HOH:O	2.18	0.42
30:0:204:A:C2'	30:0:205:U:H5'	2.49	0.42
30:0:2526:C:H5'	30:0:2526:C:H6	1.84	0.42
30:0:255:A:H2'	30:0:256:C:O4'	2.19	0.42
30:0:2793:A:H2'	30:0:2794:G:H5'	2.01	0.42
30:0:85:C:H5''	30:0:86:A:OP2	2.19	0.42
31:9:59:C:H2'	31:9:60:C:C6	2.54	0.42
30:0:1159:G:H1	30:0:1208:C:H42	1.68	0.42
30:0:2324:G:N2	30:0:2377:U:H1'	2.34	0.42
30:0:2433:A:H2'	30:0:2434:A:C8	2.54	0.42
30:0:2906:A:H5'	30:0:2907:C:O4'	2.19	0.42
30:0:952:G:H4'	39:0:4063:HOH:O	2.18	0.42
23:W:115:THR:HG23	39:W:5420:HOH:O	2.18	0.42
30:0:1339:G:C6	30:0:1340:G:N1	2.87	0.42
30:0:1427:A:H61	30:0:1440:U:H1'	1.84	0.42
30:0:1850:U:H2'	30:0:1851:G:H8	1.84	0.42
30:0:1942:A:O2'	30:0:1943:C:H5'	2.20	0.42
30:0:2614:C:O2'	30:0:2615:U:H5'	2.20	0.42
30:0:661:G:C5	30:0:686:A:C2	3.08	0.42
10:J:52:GLN:NE2	30:0:1119:G:C8	2.87	0.42
17:Q:53:HIS:CD2	30:0:2389:U:H4'	2.54	0.42
25:Y:134:HIS:CD2	25:Y:134:HIS:H	2.37	0.42
30:0:1079:A:H4'	30:0:2078:U:H5'	2.02	0.42
30:0:1622:G:C2'	30:0:1623:C:H5'	2.49	0.42
30:0:1839:A:H5'	30:0:2643:G:H4'	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:56:A:C3'	31:9:57:A:H5''	2.49	0.42
23:W:44:MET:HE2	30:0:944:G:H21	1.84	0.42
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.55	0.42
30:0:129:A:O2'	30:0:131:A:OP1	2.37	0.42
30:0:1386:G:O2'	30:0:1387:G:H5'	2.19	0.42
30:0:204:A:H2'	30:0:205:U:H5'	2.01	0.42
30:0:278:A:H2'	30:0:279:C:O4'	2.20	0.42
30:0:451:C:O2'	30:0:452:G:H5'	2.19	0.42
3:C:96:LYS:NZ	30:0:1351:G:OP1	2.39	0.42
30:0:1525:G:H5'	30:0:1526:A:OP2	2.19	0.42
30:0:1682:A:H2'	39:0:9817:HOH:O	2.20	0.42
30:0:2269:C:C2'	30:0:2270:G:H5'	2.50	0.42
31:9:27:C:H1'	39:9:9053:HOH:O	2.17	0.42
1:A:190:ARG:HD2	30:0:1884:G:O6	2.20	0.42
10:J:41:ALA:HB3	39:J:5907:HOH:O	2.20	0.42
12:L:30:ARG:HD3	30:0:164:G:H4'	2.01	0.42
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.88	0.42
30:0:1052:G:H2'	30:0:1052:G:N3	2.35	0.42
30:0:1058:A:H2'	30:0:1060:C:C5'	2.50	0.42
30:0:1186:C:H42	30:0:1190:G:H22	1.68	0.42
30:0:1243:C:H3'	39:0:4869:HOH:O	2.20	0.42
30:0:1537:C:H1'	39:0:6638:HOH:O	2.19	0.42
30:0:2672:C:H2'	30:0:2673:U:H6	1.85	0.42
30:0:816:G:C6	30:0:817:G:N1	2.88	0.42
2:B:258:GLY:H	2:B:260:HIS:CE1	2.38	0.42
30:0:1023:C:O2'	30:0:1024:G:H5'	2.20	0.42
10:J:82:THR:CG2	30:0:1242:A:H5'	2.34	0.42
30:0:1406:A:H5'	30:0:1407:A:C8	2.55	0.42
30:0:1477:C:C5'	30:0:1868:G:H5''	2.49	0.42
30:0:1544:U:H2'	30:0:1545:C:H6	1.85	0.42
30:0:1883:U:H5'	30:0:2012:U:OP2	2.19	0.42
30:0:200:C:H2'	39:0:3470:HOH:O	2.19	0.42
30:0:2356:A:H2'	30:0:2357:G:O4'	2.19	0.42
30:0:2724:U:H2'	30:0:2725:G:O4'	2.19	0.42
30:0:304:G:H1'	30:0:347:A:H61	1.84	0.42
30:0:39:G:N2	30:0:444:C:C2	2.88	0.42
30:0:567:U:O5'	30:0:567:U:H6	2.02	0.42
3:C:79:ARG:O	3:C:87:ARG:HG2	2.20	0.42
5:E:143:GLN:HE21	30:0:2780:C:C1'	2.28	0.42
10:J:74:ARG:NH1	10:J:105:LEU:HD11	2.35	0.42
24:X:23:HIS:HE1	30:0:2044:G:OP1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1098:A:H2'	30:0:1099:G:O4'	2.20	0.41
30:0:1587:U:H2'	30:0:1588:G:O4'	2.20	0.41
30:0:1679:C:H5'	39:0:9335:HOH:O	2.20	0.41
30:0:1856:C:H5'	30:0:1858:A:O4'	2.20	0.41
30:0:1878:G:O2'	30:0:1879:U:OP2	2.37	0.41
18:R:80:TYR:O	30:0:2050:G:H5''	2.20	0.41
30:0:2134:G:N2	30:0:2242:U:C2	2.88	0.41
30:0:2335:C:H2'	30:0:2336:G:C8	2.55	0.41
30:0:2842:G:C2'	30:0:2843:A:H5'	2.50	0.41
30:0:360:A:H2'	30:0:361:C:O4'	2.19	0.41
30:0:821:U:H5''	39:0:3074:HOH:O	2.20	0.41
31:9:60:C:O2'	31:9:61:C:H5'	2.19	0.41
30:0:177:A:H2'	30:0:178:U:O4'	2.20	0.41
30:0:2506:A:O2'	30:0:2507:G:O5'	2.38	0.41
30:0:2664:A:OP1	30:0:2664:A:H8	2.02	0.41
30:0:344:C:H2'	30:0:345:G:O4'	2.20	0.41
30:0:68:U:O2'	30:0:69:A:H5''	2.20	0.41
3:C:39:GLN:O	3:C:43:LYS:HD3	2.20	0.41
4:D:103:ASN:ND2	4:D:134:LEU:H	2.17	0.41
4:D:146:LYS:HZ1	14:N:107:ASN:HD21	1.68	0.41
24:X:10:VAL:HG23	24:X:72:VAL:HG12	2.03	0.41
25:Y:134:HIS:HE1	30:0:538:C:OP2	2.02	0.41
30:0:1615:A:H4'	39:0:5927:HOH:O	2.20	0.41
31:9:1:U:H5''	31:9:3:A:OP1	2.20	0.41
2:B:5:ARG:HB3	2:B:5:ARG:HE	1.69	0.41
8:H:4:LYS:HA	8:H:5:PRO:HD3	1.96	0.41
24:X:25:ARG:HD2	39:X:5356:HOH:O	2.19	0.41
30:0:1315:G:H4'	30:0:1316:G:OP2	2.20	0.41
30:0:2073:G:C6	30:0:2489:G:H4'	2.55	0.41
30:0:2366:C:O5'	30:0:2366:C:H6	2.03	0.41
2:B:238:ASN:HD21	30:0:2609:G:N2	2.18	0.41
2:B:302:PRO:HA	30:0:2717:C:H5'	2.02	0.41
38:0:2924:ANM:H63	38:0:2924:ANM:C15	2.43	0.41
30:0:308:U:C4	30:0:342:C:H1'	2.55	0.41
31:9:31:C:H2'	31:9:32:G:O4'	2.21	0.41
2:B:69:VAL:HA	2:B:70:PRO:HD3	1.93	0.41
20:T:9:LYS:HD3	39:0:3781:HOH:O	2.20	0.41
23:W:122:ARG:HH12	23:W:154:ARG:N	2.19	0.41
30:0:1636:G:O2'	30:0:1637:A:H5'	2.20	0.41
30:0:241:A:C2	30:0:378:A:H4'	2.55	0.41
30:0:932:U:H2'	30:0:933:C:H6	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:105:A:H2'	31:9:106:U:O4'	2.21	0.41
30:0:1205:U:C2'	30:0:1206:U:C5'	2.95	0.41
30:0:2379:G:H5'	30:0:2381:C:O4'	2.21	0.41
30:0:2506:A:O2'	30:0:2507:G:P	2.79	0.41
30:0:2672:C:O2'	30:0:2673:U:H5'	2.20	0.41
30:0:2781:U:H2'	30:0:2782:G:C5'	2.50	0.41
31:9:29:C:H2'	31:9:30:C:C5'	2.45	0.41
6:F:36:THR:HG23	6:F:97:ALA:HB2	2.03	0.41
30:0:1603:A:H5''	30:0:1604:G:H3'	2.03	0.41
30:0:1377:C:H2'	30:0:1723:G:O6	2.21	0.41
30:0:1896:G:C6	30:0:1897:U:C4	3.09	0.41
30:0:2349:G:O2'	30:0:2350:G:H5'	2.20	0.41
30:0:2455:A:H2'	30:0:2456:A:O4'	2.20	0.41
30:0:326:G:O2'	30:0:327:A:H5'	2.20	0.41
30:0:612:U:H2'	30:0:613:C:H6	1.85	0.41
30:0:963:C:O2	30:0:1005:A:N1	2.54	0.41
31:9:23:U:C2'	31:9:24:U:H4'	2.51	0.41
19:S:37:VAL:O	19:S:41:VAL:HG23	2.21	0.41
30:0:1495:C:H1'	30:0:1573:A:H1'	2.03	0.41
30:0:2238:A:O2'	30:0:2239:C:H5'	2.21	0.41
30:0:629:A:C2	30:0:2074:A:C2	3.09	0.41
31:9:24:U:H3'	31:9:25:G:C5'	2.51	0.41
31:9:39:U:H3'	31:9:40:C:C5'	2.50	0.41
15:O:39:THR:O	15:O:115:ARG:NH2	2.54	0.41
26:Z:41:ARG:HH12	30:0:821:U:H4'	1.86	0.41
30:0:1829:A:C2'	30:0:1830:C:H5'	2.50	0.41
30:0:2067:A:H2'	30:0:2068:G:O4'	2.21	0.41
30:0:2837:U:H2'	39:0:6892:HOH:O	2.21	0.41
20:T:2:LYS:HG2	30:0:447:A:OP1	2.21	0.41
1:A:171:LYS:HB2	30:0:820:G:C5	2.56	0.41
3:C:49:ASP:HB3	3:C:52:ALA:HB2	2.02	0.41
30:0:1321:A:H2'	30:0:1322:G:C8	2.56	0.41
27:1:9:GLY:HA2	30:0:1687:C:O2	2.21	0.41
13:M:163:LEU:CD2	30:0:188:C:H5''	2.45	0.41
30:0:1976:G:O2'	30:0:1977:U:H5'	2.21	0.41
30:0:2271:G:N3	30:0:2271:G:H2'	2.36	0.41
30:0:2896:A:N3	30:0:2896:A:H2'	2.36	0.41
30:0:682:A:H2'	30:0:683:G:O4'	2.20	0.41
2:B:254:GLN:NE2	39:B:9055:HOH:O	2.54	0.41
2:B:85:ARG:NH1	39:B:9096:HOH:O	2.53	0.41
30:0:1398:G:O2'	30:0:1399:A:H5'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1783:A:O2'	30:0:1784:U:H5'	2.21	0.41
30:0:2016:U:H6	30:0:2016:U:O5'	2.03	0.41
30:0:2553:A:H2'	30:0:2553:A:N3	2.35	0.41
30:0:581:G:O2'	30:0:582:U:H5'	2.20	0.41
1:A:176:HIS:CD2	30:0:857:A:H4'	2.55	0.41
3:C:206:ASN:HB2	30:0:329:A:OP2	2.21	0.41
5:E:91:PHE:HA	5:E:92:PRO:HD3	1.88	0.41
30:0:1165:G:H4'	30:0:1174:A:HO2'	1.86	0.40
30:0:130:C:H2'	39:0:3186:HOH:O	2.21	0.40
30:0:2385:G:H2'	30:0:2386:U:H6	1.83	0.40
30:0:2493:C:O2	30:0:2493:C:H2'	2.21	0.40
30:0:2549:C:H2'	30:0:2550:U:O4'	2.22	0.40
30:0:2642:G:H2'	30:0:2643:G:O4'	2.21	0.40
30:0:226:A:H1'	30:0:393:G:C5	2.56	0.40
13:M:179:GLY:O	30:0:399:C:H5'	2.22	0.40
30:0:827:A:H1'	39:0:6263:HOH:O	2.20	0.40
16:P:117:SER:HB3	30:0:1593:C:OP1	2.21	0.40
9:I:110:ASP:O	30:0:1163:G:H5'	2.21	0.40
30:0:1185:U:H5'	39:0:7526:HOH:O	2.21	0.40
30:0:1268:C:H2'	30:0:1269:G:H8	1.86	0.40
30:0:1972:U:C2'	30:0:1973:A:C5'	2.99	0.40
30:0:228:C:H2'	30:0:229:G:H5'	2.03	0.40
30:0:2449:G:H2'	30:0:2450:C:O4'	2.21	0.40
30:0:2812:A:C2	30:0:2814:A:N6	2.75	0.40
30:0:613:C:H2'	30:0:614:U:H6	1.87	0.40
30:0:912:A:C4	30:0:1294:A:C2	3.09	0.40
12:L:67:ARG:HB2	12:L:112:GLY:HA3	2.04	0.40
13:M:65:VAL:HG21	13:M:105:ALA:HB2	2.04	0.40
30:0:106:A:H2'	30:0:107:U:O4'	2.22	0.40
30:0:2419:U:H5''	30:0:2420:G:C5'	2.51	0.40
30:0:849:C:O2'	30:0:850:U:H5'	2.21	0.40
30:0:876:A:N3	30:0:876:A:C2'	2.85	0.40
6:F:30:LYS:HE2	6:F:99:THR:HG21	2.04	0.40
14:N:147:ILE:HD11	31:9:50:G:OP1	2.22	0.40
26:Z:41:ARG:NH1	30:0:821:U:H4'	2.37	0.40
30:0:1080:C:O5'	30:0:1080:C:H6	2.04	0.40
30:0:1299:G:N2	39:0:4716:HOH:O	2.54	0.40
30:0:1545:C:H2'	30:0:1546:G:O4'	2.22	0.40
30:0:1762:C:O2'	30:0:1763:C:H5'	2.21	0.40
30:0:2291:A:N9	30:0:2309:C:H5'	2.35	0.40
30:0:39:G:H2'	30:0:40:C:O4'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:441:A:H8	30:0:441:A:O5'	2.04	0.40
27:1:16:HIS:CD2	30:0:470:U:O2'	2.73	0.40
3:C:1:MET:HG2	3:C:2:GLN:H	1.87	0.40
23:W:21:LEU:HD23	23:W:21:LEU:HA	1.86	0.40
30:0:1051:C:H2'	30:0:1052:G:O4'	2.21	0.40
30:0:1119:G:C5	30:0:1243:C:C4	3.10	0.40
30:0:2478:U:O2'	30:0:2479:A:H5'	2.21	0.40
8:H:158:ASN:ND2	30:0:2502:C:H4'	2.36	0.40
24:X:15:ARG:NH2	30:0:2856:A:OP1	2.55	0.40
30:0:2893:C:O2'	30:0:2894:C:H5'	2.21	0.40
30:0:396:U:HO2'	30:0:397:A:P	2.45	0.40
30:0:483:C:C4	30:0:484:A:C6	3.10	0.40
30:0:877:G:C5'	30:0:878:G:OP1	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/240 (98%)	220 (94%)	13 (6%)	2 (1%)	20	46
2	B	335/338 (99%)	314 (94%)	19 (6%)	2 (1%)	28	56
3	C	244/246 (99%)	229 (94%)	15 (6%)	0	100	100
4	D	134/177 (76%)	121 (90%)	11 (8%)	2 (2%)	12	30
5	E	170/178 (96%)	159 (94%)	11 (6%)	0	100	100
6	F	117/120 (98%)	110 (94%)	4 (3%)	3 (3%)	6	15
7	G	25/348 (7%)	25 (100%)	0	0	100	100
8	H	156/177 (88%)	148 (95%)	7 (4%)	1 (1%)	28	56
9	I	68/162 (42%)	60 (88%)	8 (12%)	0	100	100
10	J	140/145 (97%)	131 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	130/132 (98%)	123 (95%)	6 (5%)	1 (1%)	22	49
12	L	141/165 (86%)	134 (95%)	7 (5%)	0	100	100
13	M	192/196 (98%)	188 (98%)	4 (2%)	0	100	100
14	N	184/187 (98%)	174 (95%)	5 (3%)	5 (3%)	6	15
15	O	113/116 (97%)	112 (99%)	1 (1%)	0	100	100
16	P	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
17	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
18	R	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
19	S	79/85 (93%)	76 (96%)	3 (4%)	0	100	100
20	T	117/120 (98%)	111 (95%)	6 (5%)	0	100	100
21	U	51/67 (76%)	50 (98%)	1 (2%)	0	100	100
22	V	63/71 (89%)	61 (97%)	2 (3%)	0	100	100
23	W	152/154 (99%)	148 (97%)	2 (1%)	2 (1%)	14	35
24	X	80/92 (87%)	76 (95%)	4 (5%)	0	100	100
25	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100
26	Z	71/116 (61%)	64 (90%)	6 (8%)	1 (1%)	13	33
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%)	2 (2%)	1 (1%)	17	40
All	All	3705/4472 (83%)	3524 (95%)	161 (4%)	20 (0%)	32	60

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
14	N	154	LEU
14	N	184	ILE
14	N	183	ASP
1	A	27	LEU
4	D	56	ARG
8	H	19	ARG
14	N	139	TRP
14	N	167	ASP
23	W	77	ALA
2	B	2	GLN

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Mol	Chain	Res	Type
6	F	100	ASP
6	F	101	ALA
11	K	127	ALA
2	B	185	GLY
4	D	137	PRO
23	W	49	ASN
26	Z	44	ARG
6	F	61	MET
29	3	56	PRO

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%)	170 (95%)	9 (5%)	28	57
2	B	282/283 (100%)	269 (95%)	13 (5%)	31	61
3	C	193/193 (100%)	177 (92%)	16 (8%)	13	30
4	D	117/148 (79%)	107 (92%)	10 (8%)	12	28
5	E	152/156 (97%)	148 (97%)	4 (3%)	51	81
6	F	93/94 (99%)	91 (98%)	2 (2%)	57	84
7	G	27/282 (10%)	27 (100%)	0	100	100
8	H	134/145 (92%)	127 (95%)	7 (5%)	27	55
9	I	58/130 (45%)	56 (97%)	2 (3%)	42	73
10	J	118/121 (98%)	110 (93%)	8 (7%)	18	41
11	K	106/106 (100%)	99 (93%)	7 (7%)	19	43
12	L	113/127 (89%)	107 (95%)	6 (5%)	26	54
13	M	158/160 (99%)	150 (95%)	8 (5%)	28	56
14	N	149/150 (99%)	144 (97%)	5 (3%)	42	73
15	O	93/94 (99%)	91 (98%)	2 (2%)	57	84
16	P	113/117 (97%)	109 (96%)	4 (4%)	41	72
17	Q	79/80 (99%)	76 (96%)	3 (4%)	38	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	R	117/122 (96%)	114 (97%)	3 (3%)	51	81
19	S	71/74 (96%)	69 (97%)	2 (3%)	49	79
20	T	105/106 (99%)	96 (91%)	9 (9%)	12	28
21	U	44/53 (83%)	41 (93%)	3 (7%)	18	41
22	V	51/57 (90%)	49 (96%)	2 (4%)	37	68
23	W	130/130 (100%)	123 (95%)	7 (5%)	26	54
24	X	66/74 (89%)	59 (89%)	7 (11%)	8	18
25	Y	120/196 (61%)	116 (97%)	4 (3%)	43	73
26	Z	60/94 (64%)	60 (100%)	0	100	100
27	1	46/47 (98%)	45 (98%)	1 (2%)	57	84
28	2	42/46 (91%)	41 (98%)	1 (2%)	54	83
29	3	79/79 (100%)	75 (95%)	4 (5%)	28	56
All	All	3095/3646 (85%)	2946 (95%)	149 (5%)	30	59

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	30	ARG
1	A	69	LEU
1	A	78	ASP
1	A	85	SER
1	A	94	LEU
1	A	131	HIS
1	A	179	MET
1	A	217	ARG
2	B	5	ARG
2	B	11	LEU
2	B	27	ASN
2	B	49	THR
2	B	71	VAL
2	B	97	LEU
2	B	98	THR
2	B	162	MET
2	B	171	VAL
2	B	195	ARG
2	B	254	GLN
2	B	257	THR

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Mol	Chain	Res	Type
2	B	265	LEU
3	C	2	GLN
3	C	27	ARG
3	C	76	ARG
3	C	78	ARG
3	C	94	THR
3	C	101	ASP
3	C	136	VAL
3	C	162	VAL
3	C	187	ARG
3	C	202	THR
3	C	214	THR
3	C	223	LEU
3	C	234	VAL
3	C	236	THR
3	C	240	LEU
3	C	243	VAL
4	D	17	ARG
4	D	23	VAL
4	D	24	HIS
4	D	50	VAL
4	D	52	THR
4	D	101	THR
4	D	128	LEU
4	D	149	ARG
4	D	153	THR
4	D	161	ASP
5	E	36	PRO
5	E	102	VAL
5	E	131	LEU
5	E	156	ASP
6	F	12	LEU
6	F	46	GLU
8	H	58	VAL
8	H	65	LEU
8	H	87	LYS
8	H	91	ARG
8	H	157	TYR
8	H	162	PRO
8	H	173	GLU
9	I	94	ASP
9	I	135	GLU

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Mol	Chain	Res	Type
10	J	28	GLU
10	J	47	THR
10	J	52	GLN
10	J	74	ARG
10	J	79	PHE
10	J	107	ASN
10	J	130	VAL
10	J	131	THR
11	K	7	ASP
11	K	10	GLN
11	K	49	LEU
11	K	62	PRO
11	K	98	VAL
11	K	107	THR
11	K	119	GLN
12	L	4	LYS
12	L	32	ASP
12	L	35	ARG
12	L	101	ASP
12	L	104	ASP
12	L	140	VAL
13	M	10	ASP
13	M	46	LEU
13	M	68	ARG
13	M	81	ARG
13	M	99	ARG
13	M	116	ASN
13	M	141	ILE
13	M	164	THR
14	N	26	LEU
14	N	49	THR
14	N	135	VAL
14	N	175	LEU
14	N	176	ARG
15	O	3	THR
15	O	25	VAL
16	P	21	VAL
16	P	52	LYS
16	P	91	LYS
16	P	98	ILE
17	Q	16	ASN
17	Q	18	PRO

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Mol	Chain	Res	Type
17	Q	57	ASP
18	R	13	THR
18	R	39	THR
18	R	132	ARG
19	S	10	VAL
19	S	81	ILE
20	T	39	ASN
20	T	48	VAL
20	T	61	GLU
20	T	71	VAL
20	T	82	THR
20	T	89	ARG
20	T	96	VAL
20	T	115	GLU
20	T	117	ASP
21	U	47	ARG
21	U	52	THR
21	U	56	ARG
22	V	12	THR
22	V	13	PRO
23	W	26	ILE
23	W	38	THR
23	W	52	VAL
23	W	76	ASP
23	W	120	PRO
23	W	142	ASP
23	W	146	ILE
24	X	15	ARG
24	X	49	ARG
24	X	52	PRO
24	X	72	VAL
24	X	79	GLU
24	X	80	GLU
24	X	82	GLU
25	Y	154	ARG
25	Y	157	ILE
25	Y	189	ASN
25	Y	204	ARG
27	1	21	ARG
28	2	18	ASN
29	3	14	CYS
29	3	18	GLN

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Mol	Chain	Res	Type
29	3	22	VAL
29	3	56	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	199	HIS
2	B	27	ASN
2	B	145	HIS
2	B	238	ASN
2	B	260	HIS
2	B	332	ASN
3	C	73	GLN
3	C	129	HIS
4	D	103	ASN
5	E	143	GLN
7	G	64	ASN
8	H	34	HIS
8	H	59	GLN
8	H	62	HIS
10	J	52	GLN
10	J	107	ASN
11	K	10	GLN
11	K	42	ASN
11	K	44	HIS
12	L	18	HIS
12	L	41	HIS
12	L	42	ASN
13	M	24	GLN
13	M	58	GLN
13	M	137	ASN
13	M	170	ASN
14	N	107	ASN
14	N	140	GLN
16	P	50	GLN
16	P	66	GLN
16	P	88	GLN
16	P	118	GLN
17	Q	16	ASN
17	Q	40	HIS
18	R	22	GLN

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Mol	Chain	Res	Type
18	R	94	ASN
18	R	98	ASN
18	R	117	HIS
18	R	122	GLN
18	R	123	GLN
19	S	9	HIS
19	S	44	GLN
19	S	51	GLN
20	T	39	ASN
21	U	39	ASN
22	V	60	GLN
23	W	12	ASN
23	W	110	GLN
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS
24	X	23	HIS
25	Y	119	GLN
25	Y	133	HIS
25	Y	134	HIS
25	Y	189	ASN
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	41	HIS
28	2	45	ASN
29	3	2	GLN
29	3	48	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	232 (8%)	28 (1%)
31	9	121/122 (99%)	17 (14%)	1 (0%)
All	All	2866/3045 (94%)	249 (8%)	29 (1%)

All (249) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A

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Mol	Chain	Res	Type
30	0	69	A
30	0	70	A
30	0	71	G
30	0	86	A
30	0	87	C
30	0	88	G
30	0	114	A
30	0	115	U
30	0	120	A
30	0	130	C
30	0	141	C
30	0	151	A
30	0	166	A
30	0	186	A
30	0	191	A
30	0	192	A
30	0	198	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	285	A
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	497	A
30	0	498	A
30	0	510	U
30	0	511	A
30	0	514	G

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Mol	Chain	Res	Type
30	0	537	G
30	0	538	C
30	0	539	G
30	0	542	A
30	0	545	G
30	0	553	G
30	0	559	U
30	0	581	G
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	857	A
30	0	858	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	920	C
30	0	921	G
30	0	923	A
30	0	953	G
30	0	960	G
30	0	961	A

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Mol	Chain	Res	Type
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
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1130	U
30	0	1151	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	1237	U
30	0	1238	C
30	0	1239	G
30	0	1242	A
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

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Mol	Chain	Res	Type
30	0	1525	G
30	0	1526	A
30	0	1592	G
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
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	1730	G
30	0	1731	C
30	0	1732	A
30	0	1752	G
30	0	1778	A
30	0	1798	C
30	0	1819	G
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	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

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Mol	Chain	Res	Type
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	2110	G
30	0	2243	C
30	0	2258	A
30	0	2271	G
30	0	2272	G
30	0	2291	A
30	0	2317	C
30	0	2321	A
30	0	2345	A
30	0	2354	A
30	0	2361	A
30	0	2369	A
30	0	2379	G
30	0	2422	U
30	0	2462	G
30	0	2467	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	2611	G
30	0	2613	G
30	0	2634	G
30	0	2649	A
30	0	2664	A

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Mol	Chain	Res	Type
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
30	0	2812	A
30	0	2825	C
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	7	G
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

All (29) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	69	A

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Mol	Chain	Res	Type
30	0	129	A
30	0	169	A
30	0	603	A
30	0	699	C
30	0	834	G
30	0	857	A
30	0	871	G
30	0	877	G
30	0	1080	C
30	0	1232	A
30	0	1237	U
30	0	1246	A
30	0	1352	A
30	0	1377	C
30	0	1684	A
30	0	1692	C
30	0	1856	C
30	0	1942	A
30	0	2313	C
30	0	2467	A
30	0	2526	C
30	0	2536	C
30	0	2649	A
30	0	2718	C
30	0	2726	U
30	0	2761	A
30	0	2791	U
31	9	65	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	OMU	0	2587	30	14,22,23	0.95	1 (7%)	18,31,34	3.74	2 (11%)
30	OMG	0	2588	30	18,26,27	1.04	2 (11%)	22,38,41	2.46	5 (22%)
30	UR3	0	2619	30	14,22,23	0.75	0	16,32,35	0.74	0
30	PSU	0	2621	30	16,21,22	1.57	3 (18%)	20,30,33	6.13	4 (20%)
30	1MA	0	628	30,35	16,25,26	1.06	1 (6%)	13,37,40	1.19	1 (7%)

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	-	0/5/27/28	0/2/2/2
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3
30	UR3	0	2619	30	-	0/3/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	1MA	0	628	30,35	-	0/3/25/26	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-4.86	1.48	1.52
30	0	2588	OMG	C8-N7	-2.12	1.30	1.34
30	0	2621	PSU	C2-N1	2.22	1.42	1.38
30	0	2587	OMU	C4-N3	2.42	1.37	1.33
30	0	2621	PSU	C4-N3	2.67	1.37	1.33
30	0	628	1MA	C6-N6	2.97	1.34	1.27
30	0	2588	OMG	C6-N1	3.24	1.38	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-19.13	114.64	128.40
30	0	2621	PSU	C5-C4-N3	-13.01	114.76	125.43
30	0	2588	OMG	C5-C6-N1	-8.34	111.60	123.48
30	0	628	1MA	C2-N3-C4	-3.60	110.89	116.41
30	0	2587	OMU	C5-C4-N3	-3.53	114.70	123.12
30	0	2588	OMG	C2-N3-C4	-2.81	111.87	115.16
30	0	2588	OMG	N3-C2-N1	-2.38	123.99	127.46
30	0	2588	OMG	C6-C5-C4	-2.01	118.85	120.84
30	0	2621	PSU	C6-N1-C2	2.90	120.00	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2588	OMG	C6-N1-C2	6.29	125.11	116.06
30	0	2621	PSU	C4-N3-C2	13.93	127.35	115.16
30	0	2587	OMU	C4-N3-C2	15.30	127.28	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 306 ligands modelled in this entry, 305 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
38	ANM	0	2924	37	19,20,20	0.48	0	22,27,27	1.93	6 (27%)

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
38	ANM	0	2924	37	-	0/10/23/23	0/2/2/2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
38	0	2924	ANM	C4-C3-C2	-3.74	98.31	103.22
38	0	2924	ANM	C2-O2-C5	-3.70	111.92	117.72
38	0	2924	ANM	C3-C2-C16	-2.94	99.95	104.21
38	0	2924	ANM	C14-O1-C9	-2.76	111.46	117.50
38	0	2924	ANM	O2-C5-O3	-2.02	118.84	122.94
38	0	2924	ANM	O2-C5-C6	5.12	120.72	111.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	0	2924	ANM	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	237/240 (98%)	0.63	23 (9%) 8 6	24, 49, 88, 107	0
2	B	337/338 (99%)	0.37	10 (2%) 51 50	27, 53, 82, 95	0
3	C	246/246 (100%)	0.29	3 (1%) 79 80	21, 42, 65, 78	0
4	D	140/177 (79%)	2.48	71 (50%) 0 0	61, 99, 124, 134	0
5	E	172/178 (96%)	0.70	15 (8%) 11 8	44, 69, 88, 94	0
6	F	119/120 (99%)	1.32	31 (26%) 1 0	43, 69, 99, 114	0
7	G	29/348 (8%)	1.77	10 (34%) 0 0	77, 95, 103, 106	0
8	H	160/177 (90%)	1.29	40 (25%) 1 0	44, 61, 96, 101	0
9	I	70/162 (43%)	5.13	65 (92%) 0 0	131, 146, 163, 164	0
10	J	142/145 (97%)	0.31	2 (1%) 75 76	35, 50, 71, 91	0
11	K	132/132 (100%)	0.15	2 (1%) 74 75	32, 49, 72, 77	0
12	L	145/165 (87%)	0.94	27 (18%) 1 1	25, 63, 109, 125	0
13	M	194/196 (98%)	0.12	2 (1%) 82 82	28, 40, 56, 63	0
14	N	186/187 (99%)	1.13	37 (19%) 1 1	42, 64, 112, 121	0
15	O	115/116 (99%)	0.50	3 (2%) 56 56	33, 53, 69, 80	0
16	P	143/149 (95%)	0.42	4 (2%) 53 54	38, 53, 67, 74	0
17	Q	95/96 (98%)	0.28	1 (1%) 80 81	34, 45, 62, 73	0
18	R	150/155 (96%)	0.14	0 100 100	30, 43, 63, 71	0
19	S	81/85 (95%)	0.91	8 (9%) 8 6	42, 56, 79, 90	0
20	T	119/120 (99%)	0.65	7 (5%) 23 21	35, 54, 84, 109	0
21	U	53/67 (79%)	0.62	4 (7%) 15 12	40, 56, 78, 84	0
22	V	65/71 (91%)	2.56	27 (41%) 0 0	52, 73, 117, 123	0
23	W	154/154 (100%)	0.54	5 (3%) 48 48	33, 49, 65, 75	0
24	X	82/92 (89%)	0.86	12 (14%) 3 2	43, 60, 85, 101	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	0.18	5 (3%) 44 44	22, 41, 64, 89	0
26	Z	73/116 (62%)	2.49	45 (61%) 0 0	58, 76, 89, 100	0
27	1	56/57 (98%)	0.04	0 100 100	24, 30, 36, 43	0
28	2	46/50 (92%)	1.02	10 (21%) 1 1	34, 60, 91, 101	0
29	3	92/92 (100%)	0.69	6 (6%) 20 17	36, 59, 72, 86	0
30	0	2749/2923 (94%)	-0.32	56 (2%) 65 66	18, 43, 87, 165	0
31	9	122/122 (100%)	-0.29	4 (3%) 47 46	34, 65, 86, 145	0
All	All	6646/7517 (88%)	0.31	535 (8%) 13 10	18, 50, 99, 165	0

All (535) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	V	39	ALA	14.7
22	V	1	THR	12.8
22	V	40	PRO	12.0
9	I	74	ILE	11.7
14	N	166	ALA	10.9
4	D	63	ILE	10.8
9	I	97	VAL	10.4
9	I	70	THR	9.8
9	I	72	GLU	9.0
9	I	66	GLY	8.9
9	I	132	VAL	8.9
9	I	128	THR	8.9
9	I	100	VAL	8.6
4	D	57	THR	8.5
26	Z	35	SER	8.5
22	V	43	PRO	8.2
9	I	91	PHE	7.9
31	9	1	U	7.9
9	I	108	HIS	7.8
26	Z	58	ASN	7.8
9	I	99	GLN	7.7
9	I	71	ALA	7.6
4	D	90	LEU	7.4
22	V	37	GLY	7.1
9	I	79	GLY	7.1
9	I	102	GLN	7.0
9	I	117	THR	7.0
9	I	104	ALA	6.8

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Mol	Chain	Res	Type	RSRZ
9	I	106	GLN	6.7
9	I	98	ASP	6.7
4	D	10	PHE	6.5
20	T	119	ALA	6.5
9	I	109	PRO	6.5
9	I	80	PHE	6.5
9	I	111	LEU	6.3
30	0	1198	U	6.2
4	D	134	LEU	6.2
4	D	18	ILE	6.1
9	I	112	LEU	6.1
4	D	85	GLN	6.1
19	S	81	ILE	6.1
4	D	64	ARG	6.0
9	I	127	CYS	6.0
9	I	78	ALA	5.8
1	A	237	GLY	5.8
26	Z	46	SER	5.7
9	I	73	LEU	5.7
30	0	1172	G	5.7
22	V	38	GLY	5.7
9	I	88	GLN	5.7
9	I	105	GLU	5.6
4	D	89	PRO	5.6
26	Z	45	VAL	5.6
1	A	37	VAL	5.5
4	D	44	ILE	5.5
9	I	130	LEU	5.4
6	F	49	PHE	5.4
9	I	103	ILE	5.4
22	V	41	GLU	5.4
9	I	113	SER	5.4
9	I	120	ALA	5.3
9	I	69	PRO	5.3
4	D	40	ILE	5.2
4	D	128	LEU	5.2
30	0	1199	A	5.1
4	D	88	LEU	5.1
26	Z	44	ARG	5.1
26	Z	104	ARG	5.1
4	D	75	LEU	5.1
9	I	116	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
4	D	69	ILE	5.0
25	Y	235	GLU	5.0
9	I	121	LYS	4.9
9	I	86	GLU	4.8
9	I	76	ASP	4.8
4	D	104	PHE	4.7
26	Z	34	SER	4.7
22	V	36	ALA	4.7
9	I	94	ASP	4.7
9	I	82	THR	4.6
9	I	83	GLY	4.6
8	H	77	ILE	4.6
30	0	1202	A	4.5
9	I	92	VAL	4.5
4	D	130	VAL	4.5
24	X	88	GLU	4.5
4	D	61	PHE	4.5
9	I	93	ALA	4.5
12	L	60	GLU	4.5
5	E	45	ASP	4.5
9	I	133	THR	4.4
26	Z	78	ILE	4.4
6	F	75	ILE	4.4
30	0	735	C	4.4
4	D	56	ARG	4.4
26	Z	49	ARG	4.4
9	I	110	ASP	4.3
14	N	155	GLU	4.3
9	I	118	ASN	4.3
4	D	27	ILE	4.3
26	Z	69	ASP	4.3
19	S	76	GLU	4.3
8	H	76	LEU	4.3
9	I	131	GLY	4.3
7	G	23	ILE	4.3
9	I	75	LYS	4.2
4	D	157	LEU	4.2
4	D	84	LEU	4.2
14	N	160	SER	4.2
24	X	7	GLU	4.2
26	Z	55	SER	4.2
12	L	106	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
30	0	1169	U	4.1
30	0	1171	A	4.1
30	0	1163	G	4.1
8	H	40	GLN	4.1
26	Z	82	SER	4.1
9	I	67	VAL	4.1
14	N	152	GLU	4.1
4	D	26	GLY	4.1
22	V	2	VAL	4.1
4	D	106	PHE	4.1
30	0	970	U	4.1
8	H	86	TYR	4.1
30	0	1173	A	4.0
8	H	141	CYS	4.0
4	D	23	VAL	4.0
26	Z	60	ASP	4.0
24	X	74	ALA	4.0
26	Z	83	TYR	3.9
31	9	24	U	3.9
26	Z	50	VAL	3.9
26	Z	62	ALA	3.9
28	2	20	ARG	3.9
9	I	126	THR	3.9
28	2	49	GLU	3.9
28	2	39	ARG	3.8
6	F	17	LEU	3.8
3	C	139	VAL	3.8
4	D	58	VAL	3.8
24	X	77	PHE	3.8
14	N	165	ALA	3.8
24	X	71	ARG	3.8
22	V	3	LEU	3.7
4	D	92	GLU	3.7
4	D	22	VAL	3.7
4	D	70	GLY	3.7
4	D	170	TYR	3.7
4	D	24	HIS	3.7
24	X	80	GLU	3.6
10	J	70	PHE	3.6
9	I	123	VAL	3.6
30	0	282	C	3.6
4	D	62	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
22	V	46	ILE	3.6
7	G	27	ILE	3.6
5	E	108	LEU	3.6
8	H	37	GLY	3.6
30	O	1170	U	3.5
21	U	47	ARG	3.5
12	L	75	LEU	3.5
8	H	81	GLY	3.5
12	L	96	VAL	3.5
6	F	99	THR	3.5
9	I	119	ALA	3.5
26	Z	54	GLU	3.4
26	Z	61	HIS	3.4
30	O	1181	A	3.4
9	I	124	VAL	3.4
30	O	1177	A	3.4
4	D	154	LYS	3.4
20	T	118	SER	3.4
6	F	106	ALA	3.4
22	V	32	ALA	3.4
26	Z	53	ILE	3.4
4	D	25	MET	3.4
7	G	26	MET	3.3
14	N	172	PHE	3.3
22	V	44	GLY	3.3
1	A	94	LEU	3.3
8	H	70	LEU	3.3
8	H	174	LEU	3.3
26	Z	68	GLU	3.3
4	D	19	GLU	3.3
7	G	71	LEU	3.3
5	E	87	PHE	3.3
4	D	68	PRO	3.3
8	H	35	LYS	3.3
6	F	91	VAL	3.3
1	A	99	ILE	3.3
9	I	68	PRO	3.3
4	D	86	THR	3.2
4	D	87	ALA	3.2
12	L	80	ASP	3.2
26	Z	79	TRP	3.2
1	A	58	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
22	V	33	VAL	3.2
12	L	105	TYR	3.2
26	Z	42	TYR	3.2
4	D	158	ASN	3.2
8	H	140	TYR	3.2
9	I	114	TYR	3.2
9	I	84	SER	3.2
4	D	73	VAL	3.2
4	D	101	THR	3.2
12	L	81	VAL	3.2
28	2	27	LEU	3.2
25	Y	108	ASP	3.2
11	K	118	ALA	3.2
6	F	12	LEU	3.2
4	D	47	GLN	3.2
30	0	10	U	3.1
5	E	154	ILE	3.1
20	T	116	ASP	3.1
28	2	37	HIS	3.1
4	D	45	THR	3.1
8	H	73	ASN	3.1
4	D	43	GLU	3.1
9	I	89	GLU	3.1
4	D	165	PHE	3.1
9	I	90	ASP	3.1
2	B	181	ILE	3.1
12	L	145	LEU	3.1
14	N	83	LEU	3.1
1	A	90	PRO	3.1
26	Z	48	ARG	3.1
29	3	15	ASN	3.1
14	N	62	HIS	3.1
29	3	13	HIS	3.1
8	H	82	GLU	3.1
19	S	77	VAL	3.1
30	0	1186	C	3.1
4	D	129	ASP	3.1
8	H	85	ASP	3.1
30	0	1951	G	3.1
4	D	171	ASP	3.1
9	I	81	GLU	3.1
1	A	35	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
9	I	122	GLU	3.0
22	V	8	ILE	3.0
30	0	1200	A	3.0
30	0	2637	A	3.0
14	N	159	TYR	3.0
4	D	98	PHE	3.0
28	2	36	ASN	3.0
28	2	35	ARG	3.0
22	V	52	ALA	3.0
28	2	23	ALA	3.0
22	V	59	ILE	3.0
30	0	1203	G	3.0
8	H	38	ARG	3.0
12	L	91	VAL	3.0
14	N	138	ASP	3.0
24	X	85	VAL	3.0
8	H	53	ILE	3.0
30	0	497	A	3.0
4	D	93	LEU	2.9
6	F	29	VAL	2.9
26	Z	43	GLY	2.9
14	N	145	ALA	2.9
12	L	99	GLU	2.9
30	0	1178	G	2.9
14	N	158	LEU	2.9
22	V	45	ARG	2.9
26	Z	47	ARG	2.9
9	I	95	LEU	2.9
7	G	24	VAL	2.9
30	0	1947	G	2.9
26	Z	38	PHE	2.9
4	D	65	GLU	2.9
4	D	74	THR	2.9
6	F	20	LEU	2.9
30	0	1279	U	2.9
20	T	117	ASP	2.9
9	I	129	SER	2.9
6	F	26	THR	2.9
1	A	31	LYS	2.9
9	I	101	LYS	2.9
28	2	48	ASP	2.9
12	L	150	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	38	ILE	2.8
30	0	2769	C	2.8
6	F	119	ARG	2.8
5	E	100	ASP	2.8
19	S	78	ALA	2.8
30	0	1168	C	2.8
8	H	69	ARG	2.8
10	J	92	GLN	2.8
5	E	10	ASP	2.8
14	N	163	PHE	2.8
3	C	138	VAL	2.8
24	X	10	VAL	2.8
24	X	72	VAL	2.8
8	H	78	LYS	2.8
30	0	1948	G	2.8
8	H	169	GLU	2.8
19	S	20	PHE	2.8
8	H	36	MET	2.7
4	D	11	HIS	2.7
30	0	1165	G	2.7
30	0	1197	G	2.7
6	F	97	ALA	2.7
8	H	114	ASP	2.7
14	N	164	ASP	2.7
1	A	65	ARG	2.7
14	N	147	ILE	2.7
26	Z	89	THR	2.7
30	0	1190	G	2.7
1	A	91	GLY	2.7
30	0	1164	U	2.7
22	V	34	GLN	2.7
5	E	170	ARG	2.7
4	D	135	VAL	2.7
26	Z	70	ARG	2.7
4	D	139	TYR	2.7
1	A	64	ASP	2.7
17	Q	95	GLU	2.7
6	F	90	GLU	2.7
8	H	66	GLU	2.7
6	F	44	SER	2.7
12	L	149	ARG	2.7
30	0	1180	U	2.7

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Mol	Chain	Res	Type	RSRZ
14	N	95	ALA	2.7
14	N	169	PRO	2.7
22	V	49	LEU	2.7
7	G	21	ASP	2.7
26	Z	93	TYR	2.7
1	A	236	GLY	2.6
6	F	16	ALA	2.6
1	A	60	PHE	2.6
26	Z	59	GLU	2.6
4	D	66	GLY	2.6
4	D	132	VAL	2.6
1	A	85	SER	2.6
9	I	125	GLY	2.6
1	A	82	VAL	2.6
12	L	97	VAL	2.6
4	D	156	ARG	2.6
24	X	73	ARG	2.6
31	9	23	U	2.6
30	0	1965	C	2.6
8	H	39	LYS	2.6
14	N	178	THR	2.6
25	Y	95	THR	2.6
14	N	67	ALA	2.6
22	V	31	ARG	2.6
8	H	172	GLU	2.6
24	X	82	GLU	2.6
26	Z	56	GLU	2.6
2	B	116	PRO	2.6
13	M	1	ALA	2.6
1	A	80	LEU	2.6
30	0	1964	U	2.6
31	9	2	U	2.6
4	D	17	ARG	2.6
8	H	48	VAL	2.6
4	D	83	PHE	2.6
29	3	41	GLU	2.6
12	L	121	ILE	2.6
22	V	42	ASN	2.6
4	D	166	ILE	2.5
14	N	81	ALA	2.5
8	H	83	GLU	2.5
14	N	97	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	143	ILE	2.5
4	D	71	ALA	2.5
14	N	139	TRP	2.5
19	S	45	TYR	2.5
23	W	62	LEU	2.5
19	S	80	ARG	2.5
6	F	51	ALA	2.5
6	F	96	ALA	2.5
8	H	50	ILE	2.5
21	U	54	THR	2.5
22	V	23	LEU	2.5
2	B	105	PHE	2.5
26	Z	81	CYS	2.5
16	P	67	LYS	2.5
25	Y	236	VAL	2.5
8	H	68	SER	2.5
29	3	92	GLU	2.5
8	H	149	VAL	2.5
4	D	105	SER	2.5
30	0	1966	U	2.5
8	H	74	ARG	2.5
6	F	6	PHE	2.5
6	F	114	LYS	2.5
22	V	25	THR	2.5
14	N	183	ASP	2.5
29	3	1	MET	2.5
4	D	16	PRO	2.4
8	H	27	PRO	2.4
30	0	1179	C	2.4
22	V	5	VAL	2.4
9	I	135	GLU	2.4
14	N	68	GLU	2.4
6	F	115	VAL	2.4
26	Z	36	GLY	2.4
26	Z	77	GLY	2.4
30	0	1192	A	2.4
12	L	147	GLU	2.4
4	D	172	VAL	2.4
30	0	2237	G	2.4
7	G	72	ASP	2.4
8	H	31	ILE	2.4
6	F	74	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
25	Y	234	VAL	2.4
4	D	142	ALA	2.4
1	A	88	ILE	2.4
12	L	66	VAL	2.4
14	N	140	GLN	2.3
8	H	146	ALA	2.3
14	N	87	LEU	2.3
20	T	112	LEU	2.3
30	0	1185	U	2.3
6	F	117	GLU	2.3
30	0	284	C	2.3
26	Z	80	GLN	2.3
4	D	53	LYS	2.3
12	L	62	ALA	2.3
3	C	5	ILE	2.3
30	0	1196	C	2.3
30	0	1174	A	2.3
6	F	48	VAL	2.3
23	W	79	VAL	2.3
26	Z	85	ASP	2.3
1	A	133	ARG	2.3
8	H	71	SER	2.3
26	Z	37	ARG	2.3
14	N	84	THR	2.3
14	N	137	ALA	2.3
30	0	2508	C	2.3
14	N	185	GLU	2.3
8	H	170	ARG	2.3
5	E	5	LEU	2.3
26	Z	86	TYR	2.3
30	0	1625	U	2.3
30	0	1967	U	2.3
1	A	36	ASP	2.3
14	N	162	ASP	2.3
30	0	1162	G	2.3
30	0	1950	G	2.3
4	D	54	ALA	2.3
12	L	102	ASP	2.3
2	B	168	GLY	2.3
16	P	108	LEU	2.3
26	Z	105	ARG	2.3
12	L	101	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
6	F	39	SER	2.2
23	W	96	LEU	2.2
30	0	960	G	2.2
30	0	2004	U	2.2
6	F	118	LEU	2.2
8	H	60	LEU	2.2
23	W	116	LEU	2.2
19	S	15	MET	2.2
26	Z	51	ALA	2.2
5	E	88	TYR	2.2
5	E	6	GLU	2.2
22	V	27	LEU	2.2
2	B	183	GLU	2.2
12	L	130	ARG	2.2
26	Z	74	GLN	2.2
6	F	22	VAL	2.2
9	I	134	ILE	2.2
24	X	9	VAL	2.2
5	E	89	SER	2.2
1	A	89	ALA	2.2
12	L	77	ALA	2.2
4	D	81	GLU	2.2
4	D	21	VAL	2.2
26	Z	95	PRO	2.2
6	F	15	ASP	2.2
7	G	69	ARG	2.2
5	E	128	GLY	2.2
6	F	37	THR	2.2
30	0	1157	C	2.2
20	T	40	VAL	2.1
8	H	80	LEU	2.1
12	L	123	ASP	2.1
21	U	52	THR	2.1
5	E	86	VAL	2.1
15	O	89	ILE	2.1
2	B	1	PRO	2.1
6	F	100	ASP	2.1
22	V	9	ARG	2.1
2	B	117	GLU	2.1
13	M	22	GLU	2.1
14	N	156	GLU	2.1
30	0	2103	A	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	115	VAL	2.1
5	E	42	VAL	2.1
26	Z	71	VAL	2.1
16	P	48	ALA	2.1
14	N	75	THR	2.1
26	Z	88	PHE	2.1
12	L	76	LEU	2.1
14	N	134	ASP	2.1
16	P	116	SER	2.1
15	O	98	LEU	2.1
30	0	1175	G	2.1
1	A	97	ALA	2.1
4	D	80	ALA	2.1
8	H	87	LYS	2.1
30	0	1195	G	2.1
30	0	2249	G	2.1
7	G	63	ARG	2.1
6	F	76	PHE	2.1
2	B	128	ILE	2.1
12	L	93	VAL	2.1
14	N	129	ILE	2.1
4	D	72	LYS	2.1
20	T	115	GLU	2.1
12	L	95	ASP	2.1
6	F	31	LYS	2.0
8	H	90	LEU	2.0
14	N	50	LEU	2.0
23	W	149	LEU	2.0
12	L	140	VAL	2.0
30	0	1201	C	2.0
7	G	25	GLU	2.0
12	L	61	ALA	2.0
14	N	148	ALA	2.0
21	U	40	ALA	2.0
14	N	151	ASP	2.0
28	2	24	TRP	2.0
9	I	87	PRO	2.0
30	0	2911	C	2.0
1	A	66	ARG	2.0
26	Z	103	VAL	2.0
15	O	102	ILE	2.0
5	E	167	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
8	H	32	ALA	2.0
29	3	83	TRP	2.0
11	K	109	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
30	OMU	0	2587	21/22	0.98	0.15	-	31,33,35,37	0
30	UR3	0	2619	21/22	0.98	0.17	-	30,34,36,39	0
30	PSU	0	2621	20/21	0.98	0.16	-	22,26,34,34	0
30	1MA	0	628	23/24	0.98	0.18	-	25,28,29,31	0
30	OMG	0	2588	24/25	0.98	0.15	-	27,30,33,35	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
35	NA	0	8562	1/1	0.78	0.85	129.99	69,69,69,69	0
34	SR	0	8986	1/1	0.51	1.98	59.83	200,200,200,200	0
34	SR	0	8957	1/1	0.28	0.75	35.92	200,200,200,200	0
35	NA	0	8555	1/1	0.77	0.73	32.48	54,54,54,54	0
35	NA	0	8519	1/1	0.88	0.42	30.94	39,39,39,39	0
37	K	0	8401	1/1	0.83	0.41	27.28	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8547	1/1	0.94	0.42	25.98	54,54,54,54	0
32	MG	0	8041	1/1	0.95	0.33	24.70	24,24,24,24	0
32	MG	0	8047	1/1	0.93	0.44	24.18	49,49,49,49	0
35	NA	0	8565	1/1	0.82	0.54	23.56	62,62,62,62	0
35	NA	0	8542	1/1	0.87	0.42	21.24	42,42,42,42	0
35	NA	0	8553	1/1	0.73	0.42	20.74	79,79,79,79	0
35	NA	0	8567	1/1	0.85	0.43	18.54	78,78,78,78	0
35	NA	0	8517	1/1	0.94	0.32	14.25	30,30,30,30	0
35	NA	0	8535	1/1	0.95	0.25	13.97	52,52,52,52	0
34	SR	0	8969	1/1	0.72	0.39	13.38	150,150,150,150	0
35	NA	9	8572	1/1	0.38	0.43	13.28	76,76,76,76	0
35	NA	0	8507	1/1	0.95	0.29	12.86	45,45,45,45	0
35	NA	0	8546	1/1	0.57	1.03	12.54	95,95,95,95	0
35	NA	0	8563	1/1	0.92	0.38	12.44	60,60,60,60	0
35	NA	B	8552	1/1	0.92	0.34	11.53	56,56,56,56	0
35	NA	0	8522	1/1	0.67	0.53	11.43	78,78,78,78	0
35	NA	0	8521	1/1	0.89	0.29	11.19	61,61,61,61	0
35	NA	0	8523	1/1	0.88	0.26	11.03	48,48,48,48	0
35	NA	0	8568	1/1	0.79	0.39	10.32	47,47,47,47	0
35	NA	0	8527	1/1	0.96	0.26	9.97	52,52,52,52	0
32	MG	0	8028	1/1	0.99	0.26	9.01	22,22,22,22	0
32	MG	0	8016	1/1	0.85	0.33	8.80	49,49,49,49	0
35	NA	0	8559	1/1	0.91	0.23	8.75	75,75,75,75	0
34	SR	B	8987	1/1	0.68	0.68	8.66	200,200,200,200	0
35	NA	0	8560	1/1	0.78	0.47	7.71	69,69,69,69	0
35	NA	0	8504	1/1	0.87	0.28	7.23	26,26,26,26	0
35	NA	0	8556	1/1	0.87	0.50	7.17	44,44,44,44	0
32	MG	0	8009	1/1	0.97	0.26	7.10	21,21,21,21	0
34	SR	0	8992	1/1	0.90	0.24	7.05	123,123,123,123	0
35	NA	0	8530	1/1	0.89	0.27	7.02	42,42,42,42	0
35	NA	0	8534	1/1	0.96	0.28	6.42	32,32,32,32	0
32	MG	0	8014	1/1	0.96	0.22	6.34	30,30,30,30	0
35	NA	0	8508	1/1	0.89	0.23	6.20	37,37,37,37	0
34	SR	0	8962	1/1	0.94	0.25	6.15	167,167,167,167	0
32	MG	0	8011	1/1	0.96	0.29	6.10	23,23,23,23	0
32	MG	A	8051	1/1	0.77	0.50	5.70	81,81,81,81	0
35	NA	0	8528	1/1	0.95	0.20	5.59	45,45,45,45	0
32	MG	0	8085	1/1	0.88	0.28	5.39	80,80,80,80	0
35	NA	0	8558	1/1	0.96	0.26	5.37	44,44,44,44	0
35	NA	0	8575	1/1	0.81	0.35	4.85	94,94,94,94	0
35	NA	0	8569	1/1	0.94	0.26	4.41	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8564	1/1	0.92	0.19	4.32	65,65,65,65	0
32	MG	0	8006	1/1	0.85	0.21	3.87	30,30,30,30	0
34	SR	0	8949	1/1	0.76	0.20	3.67	110,110,110,110	0
32	MG	0	8062	1/1	0.78	0.23	3.58	34,34,34,34	0
38	ANM	0	2924	19/19	0.95	0.22	3.54	31,37,40,40	0
32	MG	0	8004	1/1	0.97	0.24	3.51	25,25,25,25	0
32	MG	0	8012	1/1	0.94	0.23	3.16	21,21,21,21	0
35	NA	M	8539	1/1	0.74	0.25	3.06	41,41,41,41	0
32	MG	0	8055	1/1	0.86	0.27	2.82	38,38,38,38	0
35	NA	0	8557	1/1	0.72	0.16	2.75	67,67,67,67	0
32	MG	0	8087	1/1	0.96	0.20	2.63	42,42,42,42	0
32	MG	0	8001	1/1	0.96	0.20	2.38	25,25,25,25	0
35	NA	0	8533	1/1	0.77	0.25	2.31	63,63,63,63	0
34	SR	A	8929	1/1	0.91	0.27	2.08	131,131,131,131	0
32	MG	0	8003	1/1	0.97	0.19	1.96	30,30,30,30	0
34	SR	0	8904	1/1	0.99	0.20	1.91	52,52,52,52	0
32	MG	0	8070	1/1	0.94	0.17	1.86	45,45,45,45	0
32	MG	0	8084	1/1	0.95	0.18	1.54	31,31,31,31	0
32	MG	0	8008	1/1	0.91	0.19	1.30	25,25,25,25	0
33	CL	0	8816	1/1	0.96	0.19	0.91	60,60,60,60	0
35	NA	0	8515	1/1	0.95	0.23	0.74	33,33,33,33	0
35	NA	0	8520	1/1	0.89	0.18	0.66	54,54,54,54	0
35	NA	Q	8540	1/1	0.84	0.22	0.65	60,60,60,60	0
33	CL	0	8805	1/1	0.93	0.15	0.41	59,59,59,59	0
32	MG	0	8045	1/1	0.95	0.17	0.22	32,32,32,32	0
32	MG	0	8050	1/1	0.73	0.18	0.05	37,37,37,37	0
34	SR	H	8972	1/1	0.92	0.20	-0.13	130,130,130,130	0
32	MG	0	8043	1/1	0.85	0.15	-0.22	49,49,49,49	0
35	NA	J	8538	1/1	0.89	0.20	-0.41	56,56,56,56	0
32	MG	0	8088	1/1	0.82	0.16	-0.62	37,37,37,37	0
34	SR	0	8985	1/1	0.93	0.13	-0.65	110,110,110,110	0
37	K	0	8402	1/1	0.93	0.17	-0.67	64,64,64,64	0
33	CL	O	8808	1/1	0.94	0.17	-0.82	61,61,61,61	0
32	MG	0	8002	1/1	0.98	0.17	-0.83	22,22,22,22	0
32	MG	0	8021	1/1	0.98	0.13	-0.94	32,32,32,32	0
32	MG	0	8053	1/1	0.94	0.16	-1.08	61,61,61,61	0
33	CL	J	8821	1/1	0.95	0.15	-1.19	56,56,56,56	0
32	MG	0	8058	1/1	0.96	0.12	-1.29	23,23,23,23	0
32	MG	0	8025	1/1	0.97	0.13	-1.64	24,24,24,24	0
33	CL	0	8812	1/1	0.98	0.11	-1.67	48,48,48,48	0
32	MG	0	8065	1/1	0.97	0.13	-1.73	33,33,33,33	0
32	MG	0	8044	1/1	0.88	0.12	-1.74	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	CD	3	8704	1/1	0.99	0.09	-1.82	66,66,66,66	0
36	CD	U	8701	1/1	0.99	0.12	-1.94	58,58,58,58	0
33	CL	M	8818	1/1	0.97	0.15	-1.94	37,37,37,37	0
36	CD	Z	8703	1/1	0.93	0.06	-1.95	81,81,81,81	0
34	SR	3	8932	1/1	0.96	0.13	-2.02	73,73,73,73	0
32	MG	T	8057	1/1	0.90	0.15	-2.19	57,57,57,57	0
35	NA	0	8537	1/1	0.95	0.12	-2.19	34,34,34,34	0
34	SR	0	8975	1/1	0.83	0.11	-2.27	134,134,134,134	0
34	SR	0	8910	1/1	0.85	0.12	-2.32	97,97,97,97	0
33	CL	B	8819	1/1	0.99	0.12	-3.12	46,46,46,46	0
34	SR	0	8943	1/1	0.92	0.08	-3.25	95,95,95,95	0
34	SR	0	8935	1/1	0.97	0.11	-3.44	79,79,79,79	0
33	CL	3	8804	1/1	0.98	0.05	-3.78	54,54,54,54	0
34	SR	0	8902	1/1	0.96	0.15	-3.91	69,69,69,69	0
32	MG	0	8052	1/1	0.98	0.11	-4.04	40,40,40,40	0
36	CD	1	8702	1/1	0.99	0.08	-4.08	57,57,57,57	0
34	SR	0	8936	1/1	0.93	0.13	-4.43	89,89,89,89	0
34	SR	1	8913	1/1	0.96	0.09	-4.97	85,85,85,85	0
33	CL	0	8815	1/1	0.96	0.11	-5.30	57,57,57,57	0
32	MG	0	8075	1/1	0.89	0.08	-5.33	45,45,45,45	0
32	MG	0	8034	1/1	0.93	0.11	-5.71	32,32,32,32	0
34	SR	0	8970	1/1	0.87	0.07	-6.71	131,131,131,131	0
32	MG	0	8013	1/1	0.97	0.08	-7.06	26,26,26,26	0
32	MG	Y	8086	1/1	0.97	0.11	-10.05	39,39,39,39	0
32	MG	0	8080	1/1	0.85	0.29	-	57,57,57,57	0
32	MG	K	8054	1/1	0.95	0.16	-	39,39,39,39	0
34	SR	0	8966	1/1	0.83	0.08	-	110,110,110,110	0
35	NA	9	8543	1/1	0.80	0.08	-	70,70,70,70	0
34	SR	0	8968	1/1	0.90	0.11	-	143,143,143,143	0
32	MG	0	8056	1/1	0.93	0.20	-	42,42,42,42	0
34	SR	0	8982	1/1	0.76	0.85	-	180,180,180,180	0
32	MG	0	8005	1/1	0.98	0.30	-	26,26,26,26	0
32	MG	B	8042	1/1	0.86	0.12	-	50,50,50,50	0
34	SR	A	8977	1/1	0.54	0.18	-	172,172,172,172	0
34	SR	0	8955	1/1	0.16	0.34	-	200,200,200,200	0
34	SR	0	8917	1/1	0.78	0.18	-	119,119,119,119	0
35	NA	0	8511	1/1	0.78	0.32	-	59,59,59,59	0
32	MG	0	8020	1/1	0.92	0.20	-	54,54,54,54	0
32	MG	0	8032	1/1	0.94	0.09	-	40,40,40,40	0
33	CL	0	8811	1/1	0.96	0.11	-	53,53,53,53	0
34	SR	0	8926	1/1	0.85	0.12	-	115,115,115,115	0
34	SR	0	8940	1/1	0.97	0.10	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	SR	0	8971	1/1	0.71	0.17	-	170,170,170,170	0
32	MG	0	8079	1/1	0.80	0.24	-	47,47,47,47	0
34	SR	0	9006	1/1	0.14	1.93	-	200,200,200,200	0
34	SR	0	8922	1/1	0.48	0.37	-	159,159,159,159	0
35	NA	0	8505	1/1	0.85	0.57	-	39,39,39,39	0
32	MG	0	8081	1/1	0.88	0.24	-	54,54,54,54	0
35	NA	0	8536	1/1	0.96	0.12	-	50,50,50,50	0
34	SR	0	8960	1/1	0.74	0.11	-	145,145,145,145	0
34	SR	0	8954	1/1	0.95	0.08	-	105,105,105,105	0
32	MG	0	8072	1/1	0.84	0.28	-	52,52,52,52	0
32	MG	0	8082	1/1	0.97	0.33	-	48,48,48,48	0
34	SR	0	8974	1/1	0.80	0.29	-	166,166,166,166	0
34	SR	0	8921	1/1	0.93	0.12	-	92,92,92,92	0
32	MG	0	8007	1/1	0.94	0.30	-	26,26,26,26	0
35	NA	0	8570	1/1	0.94	0.17	-	49,49,49,49	0
34	SR	0	8915	1/1	0.99	0.07	-	117,117,117,117	0
34	SR	0	8941	1/1	0.85	0.19	-	115,115,115,115	0
32	MG	0	8073	1/1	0.90	0.14	-	76,76,76,76	0
32	MG	0	8019	1/1	0.96	0.30	-	24,24,24,24	0
33	CL	Y	8820	1/1	0.95	0.11	-	38,38,38,38	0
34	SR	0	8947	1/1	0.53	0.48	-	200,200,200,200	0
34	SR	0	8937	1/1	0.96	0.21	-	100,100,100,100	0
34	SR	0	8945	1/1	0.86	0.11	-	99,99,99,99	0
32	MG	0	8022	1/1	0.96	0.21	-	29,29,29,29	0
34	SR	0	8963	1/1	0.78	0.12	-	133,133,133,133	0
32	MG	0	8068	1/1	0.93	0.09	-	47,47,47,47	0
34	SR	0	8920	1/1	0.88	0.11	-	124,124,124,124	0
35	NA	S	8510	1/1	0.36	0.43	-	79,79,79,79	0
34	SR	0	8983	1/1	0.65	0.23	-	164,164,164,164	0
35	NA	C	8503	1/1	0.92	0.28	-	37,37,37,37	0
35	NA	0	8506	1/1	0.83	0.24	-	47,47,47,47	0
34	SR	0	8927	1/1	0.95	0.15	-	167,167,167,167	0
32	MG	0	8037	1/1	0.90	0.22	-	83,83,83,83	0
34	SR	0	8993	1/1	0.70	0.16	-	168,168,168,168	0
32	MG	0	8067	1/1	0.95	0.28	-	34,34,34,34	0
33	CL	0	8803	1/1	0.98	0.07	-	46,46,46,46	0
35	NA	0	8513	1/1	0.97	0.27	-	44,44,44,44	0
34	SR	0	9007	1/1	0.83	0.40	-	200,200,200,200	0
32	MG	0	8061	1/1	0.94	0.39	-	37,37,37,37	0
32	MG	0	8010	1/1	0.93	0.17	-	26,26,26,26	0
35	NA	0	8518	1/1	0.86	0.41	-	79,79,79,79	0
32	MG	0	8029	1/1	0.94	0.18	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	SR	S	8961	1/1	0.67	0.10	-	114,114,114,114	0
34	SR	0	8973	1/1	0.83	0.10	-	137,137,137,137	0
34	SR	0	8907	1/1	0.99	0.32	-	76,76,76,76	0
32	MG	0	8024	1/1	0.82	0.57	-	85,85,85,85	0
32	MG	0	8076	1/1	0.92	0.22	-	35,35,35,35	0
32	MG	0	8036	1/1	0.93	0.12	-	49,49,49,49	0
32	MG	0	8071	1/1	0.86	0.27	-	55,55,55,55	0
33	CL	J	8802	1/1	0.97	0.15	-	60,60,60,60	0
32	MG	0	8083	1/1	0.91	0.16	-	56,56,56,56	0
34	SR	0	8944	1/1	0.70	0.26	-	185,185,185,185	0
34	SR	A	8930	1/1	0.87	0.08	-	116,116,116,116	0
34	SR	0	9008	1/1	0.90	0.14	-	90,90,90,90	0
35	NA	0	8548	1/1	0.87	0.38	-	57,57,57,57	0
34	SR	0	8903	1/1	0.98	0.20	-	53,53,53,53	0
32	MG	0	8023	1/1	0.96	0.18	-	22,22,22,22	0
32	MG	0	8038	1/1	0.86	0.12	-	58,58,58,58	0
34	SR	0	8990	1/1	0.77	0.22	-	118,118,118,118	0
33	CL	0	8813	1/1	0.97	0.08	-	48,48,48,48	0
34	SR	0	8956	1/1	0.75	0.14	-	142,142,142,142	0
35	NA	0	8561	1/1	0.69	0.83	-	74,74,74,74	0
34	SR	0	9001	1/1	0.84	0.24	-	169,169,169,169	0
34	SR	9	8980	1/1	0.77	0.27	-	182,182,182,182	0
33	CL	0	8822	1/1	0.95	0.25	-	68,68,68,68	0
35	NA	0	8551	1/1	0.97	0.23	-	46,46,46,46	0
34	SR	0	8911	1/1	0.89	0.08	-	78,78,78,78	0
34	SR	0	8946	1/1	0.95	0.16	-	108,108,108,108	0
34	SR	0	8938	1/1	0.80	0.08	-	159,159,159,159	0
32	MG	9	8074	1/1	0.95	0.13	-	67,67,67,67	0
32	MG	0	8077	1/1	0.90	0.16	-	32,32,32,32	0
34	SR	0	8959	1/1	0.54	0.26	-	169,169,169,169	0
34	SR	0	8998	1/1	0.82	0.41	-	173,173,173,173	0
34	SR	0	8979	1/1	0.56	0.29	-	194,194,194,194	0
36	CD	O	8705	1/1	0.90	0.06	-	124,124,124,124	0
34	SR	0	8988	1/1	0.80	0.08	-	163,163,163,163	0
32	MG	0	8017	1/1	0.93	0.19	-	56,56,56,56	0
34	SR	0	8906	1/1	0.99	0.21	-	56,56,56,56	0
32	MG	0	8018	1/1	0.95	0.24	-	38,38,38,38	0
34	SR	3	8999	1/1	0.94	0.08	-	95,95,95,95	0
32	MG	0	8027	1/1	0.97	0.14	-	34,34,34,34	0
35	NA	0	8502	1/1	0.87	0.34	-	67,67,67,67	0
34	SR	0	8909	1/1	0.89	0.14	-	94,94,94,94	0
34	SR	F	9005	1/1	0.94	0.06	-	136,136,136,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	SR	0	8948	1/1	0.82	0.17	-	102,102,102,102	0
35	NA	0	8571	1/1	0.72	0.32	-	83,83,83,83	0
32	MG	0	8093	1/1	0.95	0.11	-	29,29,29,29	0
32	MG	0	8046	1/1	0.96	0.16	-	28,28,28,28	0
34	SR	0	8967	1/1	0.89	0.11	-	133,133,133,133	0
35	NA	0	8554	1/1	0.74	0.75	-	65,65,65,65	0
33	CL	N	8807	1/1	0.96	0.13	-	61,61,61,61	0
34	SR	0	8965	1/1	0.91	0.12	-	120,120,120,120	0
32	MG	0	8015	1/1	0.98	0.19	-	27,27,27,27	0
32	MG	0	8048	1/1	0.95	0.28	-	28,28,28,28	0
35	NA	0	8531	1/1	0.77	0.16	-	40,40,40,40	0
32	MG	0	8090	1/1	0.96	0.13	-	54,54,54,54	0
35	NA	0	8529	1/1	0.93	0.09	-	37,37,37,37	0
34	SR	0	9000	1/1	0.83	0.17	-	159,159,159,159	0
34	SR	0	8942	1/1	0.87	0.15	-	121,121,121,121	0
34	SR	0	8981	1/1	0.78	0.23	-	167,167,167,167	0
34	SR	0	8931	1/1	0.95	0.11	-	108,108,108,108	0
33	CL	0	8817	1/1	0.92	0.12	-	53,53,53,53	0
35	NA	0	8574	1/1	0.87	0.43	-	53,53,53,53	0
32	MG	0	8049	1/1	0.93	0.37	-	55,55,55,55	0
34	SR	0	8901	1/1	0.96	0.16	-	58,58,58,58	0
32	MG	0	8039	1/1	0.89	0.33	-	69,69,69,69	0
35	NA	0	8514	1/1	0.90	0.28	-	42,42,42,42	0
34	SR	0	8991	1/1	0.82	0.23	-	191,191,191,191	0
32	MG	0	8089	1/1	0.43	0.17	-	48,48,48,48	0
32	MG	0	8040	1/1	0.74	0.34	-	83,83,83,83	0
33	CL	A	8809	1/1	0.94	0.15	-	57,57,57,57	0
32	MG	0	8064	1/1	0.94	0.27	-	38,38,38,38	0
35	NA	0	8512	1/1	0.72	0.51	-	43,43,43,43	0
35	NA	0	8501	1/1	0.86	0.20	-	39,39,39,39	0
35	NA	0	8566	1/1	0.96	0.29	-	37,37,37,37	0
34	SR	0	8976	1/1	0.41	0.45	-	186,186,186,186	0
35	NA	0	8526	1/1	0.96	0.09	-	32,32,32,32	0
34	SR	0	8994	1/1	0.60	0.60	-	190,190,190,190	0
34	SR	0	8919	1/1	0.46	0.24	-	178,178,178,178	0
32	MG	0	8031	1/1	0.81	0.20	-	61,61,61,61	0
33	CL	L	8810	1/1	0.95	0.09	-	49,49,49,49	0
32	MG	0	8091	1/1	0.94	0.07	-	42,42,42,42	0
35	NA	0	8516	1/1	0.94	0.23	-	30,30,30,30	0
34	SR	0	8984	1/1	0.66	0.10	-	128,128,128,128	0
34	SR	0	8951	1/1	0.81	0.07	-	146,146,146,146	0
34	SR	0	8916	1/1	0.71	0.15	-	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	SR	B	8950	1/1	0.88	0.19	-	108,108,108,108	0
34	SR	0	8933	1/1	0.76	0.52	-	138,138,138,138	0
35	NA	0	8509	1/1	0.88	0.34	-	64,64,64,64	0
34	SR	0	9002	1/1	0.78	0.15	-	184,184,184,184	0
32	MG	0	8092	1/1	0.72	0.14	-	61,61,61,61	0
34	SR	0	8989	1/1	0.66	0.39	-	187,187,187,187	0
34	SR	R	8912	1/1	0.97	0.16	-	84,84,84,84	0
32	MG	0	8063	1/1	0.82	0.28	-	72,72,72,72	0
34	SR	0	8924	1/1	0.64	0.13	-	145,145,145,145	0
32	MG	0	8078	1/1	0.93	0.37	-	51,51,51,51	0
34	SR	0	8958	1/1	0.81	0.11	-	108,108,108,108	0
34	SR	0	8996	1/1	0.50	0.82	-	200,200,200,200	0
32	MG	0	8060	1/1	0.96	0.11	-	42,42,42,42	0
32	MG	0	8030	1/1	0.85	0.37	-	55,55,55,55	0
35	NA	0	8525	1/1	0.87	0.12	-	69,69,69,69	0
33	CL	0	8814	1/1	0.96	0.17	-	47,47,47,47	0
32	MG	0	8026	1/1	0.98	0.14	-	31,31,31,31	0
35	NA	0	8550	1/1	0.94	0.25	-	54,54,54,54	0
32	MG	0	8033	1/1	0.93	0.11	-	45,45,45,45	0
35	NA	0	8541	1/1	0.94	0.34	-	53,53,53,53	0
34	SR	0	8997	1/1	0.81	0.63	-	184,184,184,184	0
34	SR	0	8928	1/1	0.83	0.20	-	138,138,138,138	0
35	NA	0	8549	1/1	0.74	0.42	-	81,81,81,81	0
34	SR	9	8978	1/1	0.09	0.14	-	144,144,144,144	0
32	MG	0	8069	1/1	0.69	0.57	-	47,47,47,47	0
34	SR	0	8908	1/1	0.89	0.18	-	107,107,107,107	0
34	SR	0	8905	1/1	0.99	0.26	-	57,57,57,57	0
35	NA	0	8544	1/1	0.89	0.30	-	64,64,64,64	0
34	SR	0	8953	1/1	0.77	0.24	-	160,160,160,160	0
32	MG	0	8035	1/1	0.95	0.10	-	44,44,44,44	0
34	SR	0	8914	1/1	0.80	0.34	-	118,118,118,118	0
32	MG	0	8059	1/1	0.91	0.09	-	36,36,36,36	0
33	CL	J	8801	1/1	0.95	0.13	-	62,62,62,62	0
33	CL	R	8806	1/1	0.99	0.17	-	43,43,43,43	0
35	NA	0	8545	1/1	0.90	0.30	-	37,37,37,37	0
34	SR	0	8939	1/1	0.82	0.18	-	152,152,152,152	0
34	SR	0	8918	1/1	0.94	0.14	-	79,79,79,79	0
35	NA	0	8573	1/1	0.68	0.63	-	69,69,69,69	0
34	SR	0	8995	1/1	0.83	0.19	-	136,136,136,136	0
34	SR	0	8923	1/1	0.92	0.19	-	101,101,101,101	0
32	MG	0	8066	1/1	0.88	0.21	-	52,52,52,52	0
35	NA	R	8532	1/1	0.89	0.18	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	SR	9	9003	1/1	0.60	0.10	-	162,162,162,162	0
34	SR	0	8925	1/1	0.98	0.12	-	90,90,90,90	0
34	SR	0	9004	1/1	0.86	0.42	-	200,200,200,200	0
34	SR	0	8934	1/1	0.64	0.13	-	90,90,90,90	0
34	SR	1	8952	1/1	0.97	0.12	-	79,79,79,79	0
34	SR	0	8964	1/1	0.88	0.08	-	126,126,126,126	0
35	NA	0	8524	1/1	0.96	0.26	-	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.