Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:58 AM GMT

PDB ID	:	3CD6
Title	:	Co-cystal of large Ribosomal Subunit mutant G2616A with CC-Puromycin
Authors	:	Blaha, G.; Gurel, G.
Deposited on	:	2008-02-26
Resolution	:	2.75 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

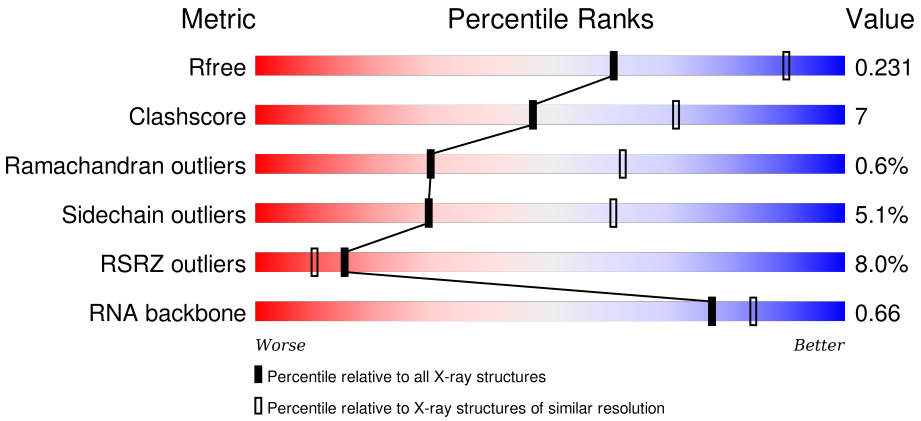
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)
RNA backbone	2183	1006 (3.14-2.38)

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 <=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	11% 88% 10% •
2	B	338	2% 84% 14% •
3	C	246	86% 12% •
4	D	177	46% 64% 14% • 21%

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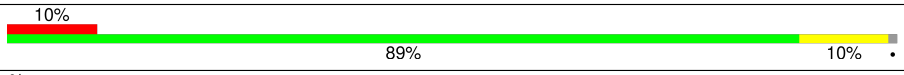
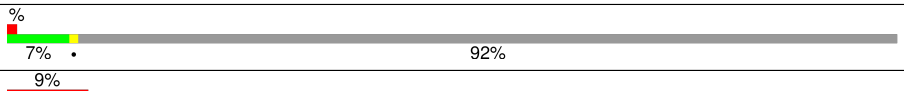
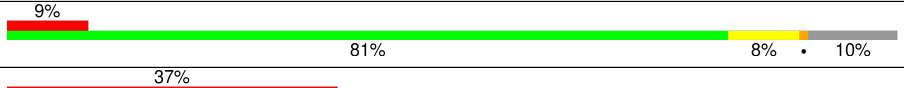
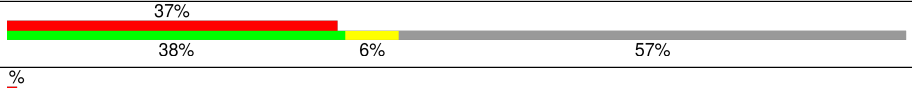
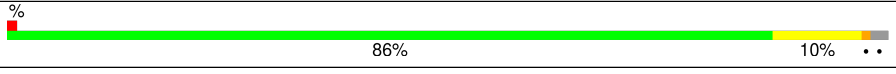
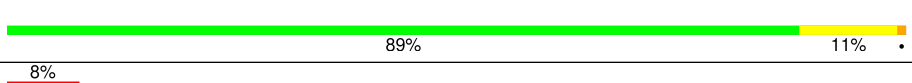
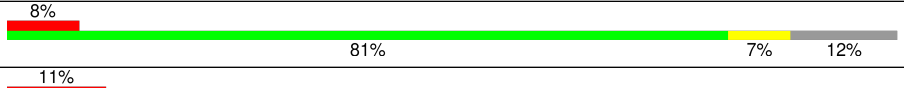
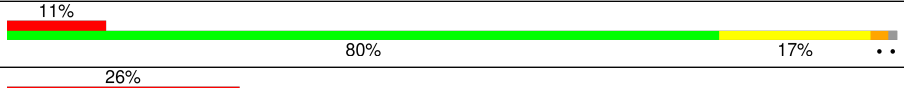
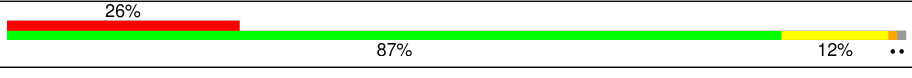
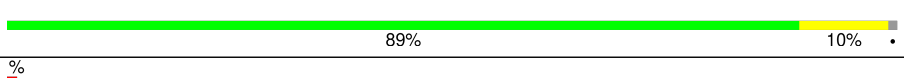
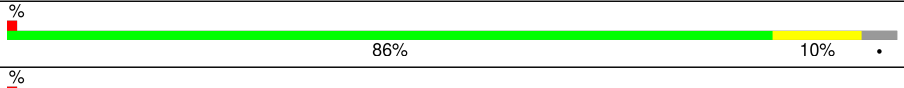
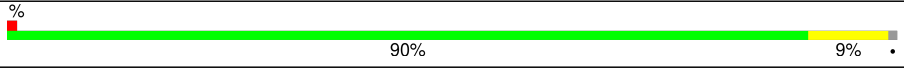
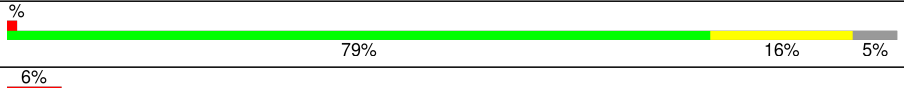
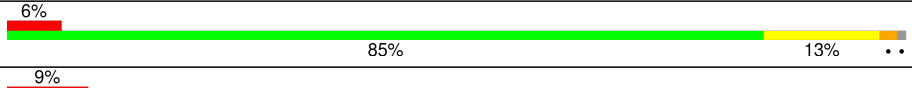
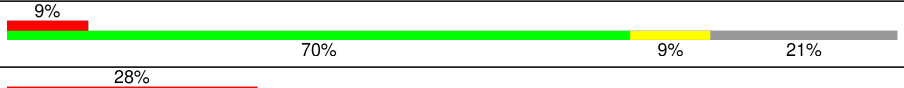
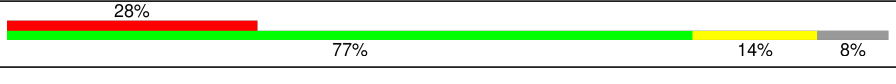
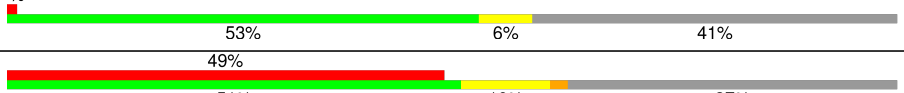
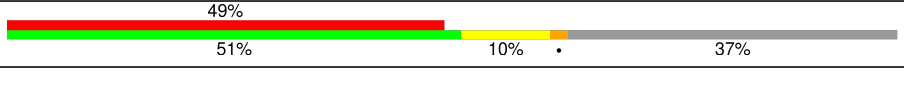
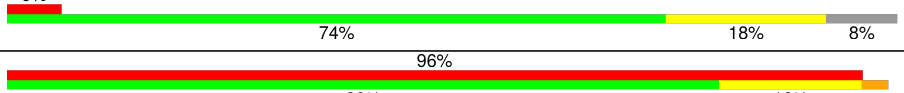
Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	

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Mol	Chain	Length	Quality of chain
30	0	2923	2% 58% 31% 5% 6%
31	9	122	3% 44% 43% 13%
32	4	3	33% 67%

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
33	MG	0	8007	-	-	-	X
33	MG	0	8008	-	-	-	X
33	MG	0	8011	-	-	-	X
33	MG	0	8014	-	-	-	X
33	MG	0	8041	-	-	-	X
33	MG	0	8044	-	-	-	X
33	MG	0	8047	-	-	-	X
33	MG	0	8062	-	-	-	X
33	MG	0	8067	-	-	-	X
33	MG	0	8073	-	-	-	X
33	MG	0	8080	-	-	-	X
33	MG	0	8084	-	-	-	X
33	MG	A	8051	-	-	-	X
34	K	0	8401	-	-	-	X
35	NA	0	8504	-	-	-	X
35	NA	0	8507	-	-	-	X
35	NA	0	8508	-	-	-	X
35	NA	0	8512	-	-	-	X
35	NA	0	8517	-	-	-	X
35	NA	0	8519	-	-	-	X
35	NA	0	8522	-	-	-	X
35	NA	0	8527	-	-	-	X
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	8537	-	-	-	X
35	NA	0	8542	-	-	-	X
35	NA	0	8547	-	-	-	X
35	NA	0	8553	-	-	-	X
35	NA	0	8558	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	NA	0	8559	-	-	-	X
35	NA	0	8562	-	-	-	X
35	NA	0	8563	-	-	-	X
35	NA	0	8564	-	-	-	X
35	NA	0	8565	-	-	-	X
35	NA	0	8568	-	-	-	X
35	NA	0	8575	-	-	-	X
35	NA	9	8572	-	-	-	X
35	NA	B	8552	-	-	-	X
37	SR	0	8903	-	-	-	X
37	SR	0	8904	-	-	-	X
37	SR	0	8923	-	-	-	X
37	SR	0	8957	-	-	-	X
37	SR	0	8969	-	-	-	X
37	SR	0	8975	-	-	-	X
37	SR	0	8987	-	-	-	X
38	CD	3	8704	-	-	-	X

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99180 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
			59019	26349	10873	19052	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 a RNA chain called RNA (5'-R(*CP*CP*(PPU))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	4	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	86	Total	Mg	0	0
			86	86		
33	Y	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	B	1	Total	Mg	0	0
			1	1		
33	A	2	Total	Mg	0	0
			2	2		
33	T	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	9	1	Total Mg 1 1	0	0

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	2	Total K 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	65	Total Na 65 65	0	0
35	J	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	H	1	Total Na 1 1	0	0
35	B	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	R	1	Total Na 1 1	0	0
35	9	2	Total Na 2 2	0	0
35	S	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0

- Molecule 36 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	10	Total Cl 10 10	0	0
36	J	3	Total Cl 3 3	0	0
36	B	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	A	1	Total Cl 1 1	0	0
36	N	1	Total Cl 1 1	0	0
36	O	1	Total Cl 1 1	0	0
36	R	1	Total Cl 1 1	0	0
36	Y	1	Total Cl 1 1	0	0
36	L	1	Total Cl 1 1	0	0
36	3	1	Total Cl 1 1	0	0
36	M	1	Total Cl 1 1	0	0

- Molecule 37 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	93	Total Sr 93 93	0	0
37	J	1	Total Sr 1 1	0	0
37	1	2	Total Sr 2 2	0	0
37	B	1	Total Sr 1 1	0	0
37	3	2	Total Sr 2 2	0	0
37	A	2	Total Sr 2 2	0	0
37	R	1	Total Sr 1 1	0	0
37	9	3	Total Sr 3 3	0	0
37	S	1	Total Sr 1 1	0	0
37	F	1	Total Sr 1 1	0	0

- Molecule 38 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	O	1	Total Cd 1 1	0	0
38	Z	1	Total Cd 1 1	0	0
38	1	1	Total Cd 1 1	0	0
38	3	1	Total Cd 1 1	0	0
38	U	1	Total Cd 1 1	0	0

- Molecule 39 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	0	5949	Total O 5949 5949	0	0
39	9	148	Total O 148 148	0	0
39	A	115	Total O 115 115	0	0
39	B	136	Total O 136 136	0	0
39	C	167	Total O 167 167	0	0
39	D	45	Total O 45 45	0	0
39	E	46	Total O 46 46	0	0
39	F	28	Total O 28 28	0	0
39	G	17	Total O 17 17	0	0
39	H	65	Total O 65 65	0	0
39	I	7	Total O 7 7	0	0
39	J	49	Total O 49 49	0	0
39	K	53	Total O 53 53	0	0
39	L	92	Total O 92 92	0	0
39	M	123	Total O 123 123	0	0

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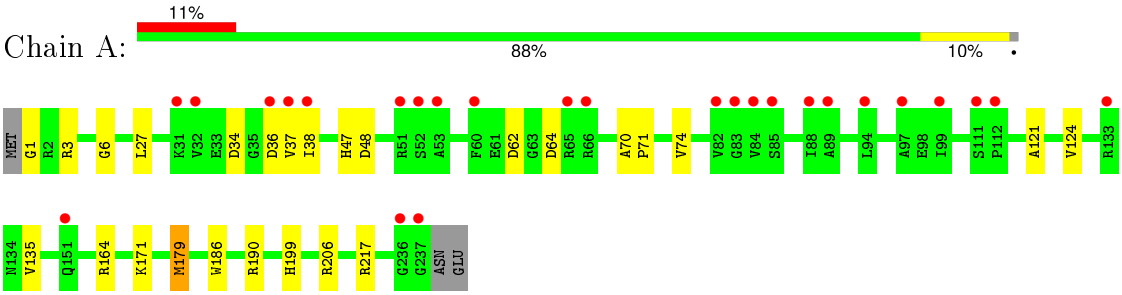
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	N	55	Total O 55 55	0	0
39	O	37	Total O 37 37	0	0
39	P	63	Total O 63 63	0	0
39	Q	51	Total O 51 51	0	0
39	R	78	Total O 78 78	0	0
39	S	31	Total O 31 31	0	0
39	T	38	Total O 38 38	0	0
39	U	30	Total O 30 30	0	0
39	V	10	Total O 10 10	0	0
39	W	67	Total O 67 67	0	0
39	X	23	Total O 23 23	0	0
39	Y	93	Total O 93 93	0	0
39	Z	25	Total O 25 25	0	0
39	1	60	Total O 60 60	0	0
39	2	46	Total O 46 46	0	0
39	3	62	Total O 62 62	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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

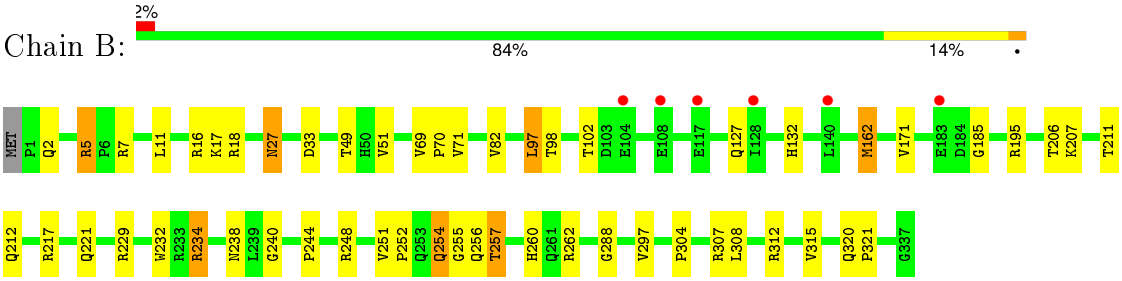
- Molecule 1: 50S ribosomal protein L2P

Chain A:



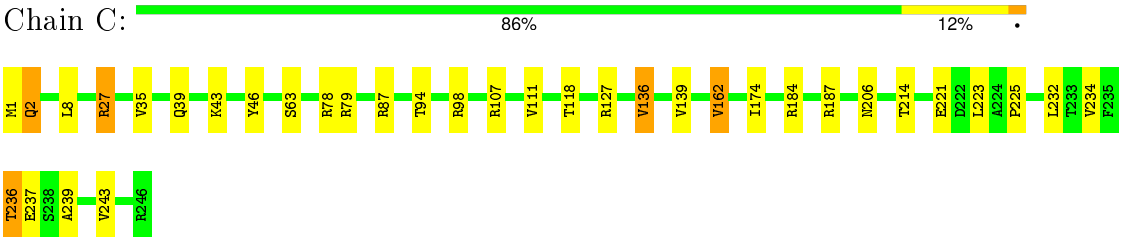
- Molecule 2: 50S ribosomal protein L3P

Chain B:



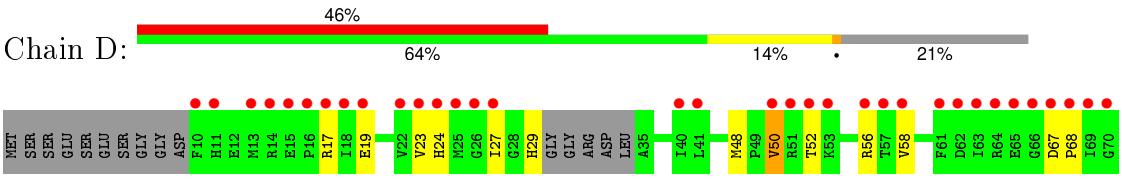
- Molecule 3: 50S ribosomal protein L4P

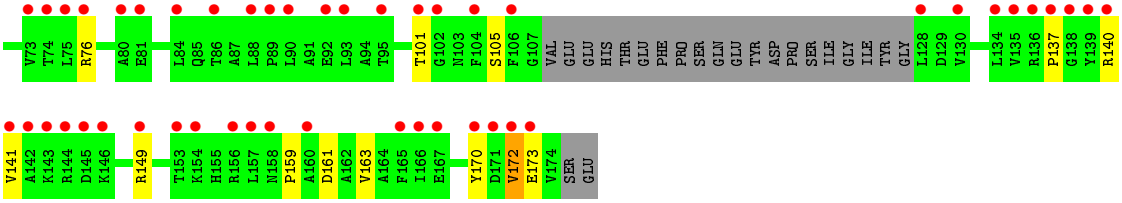
Chain C:



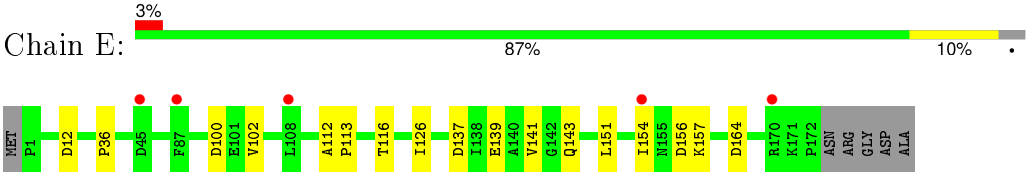
- Molecule 4: 50S ribosomal protein L5P

Chain D:

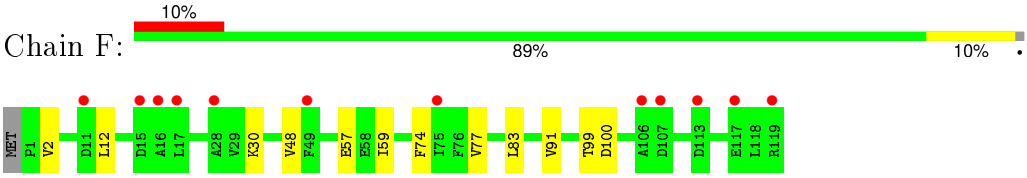




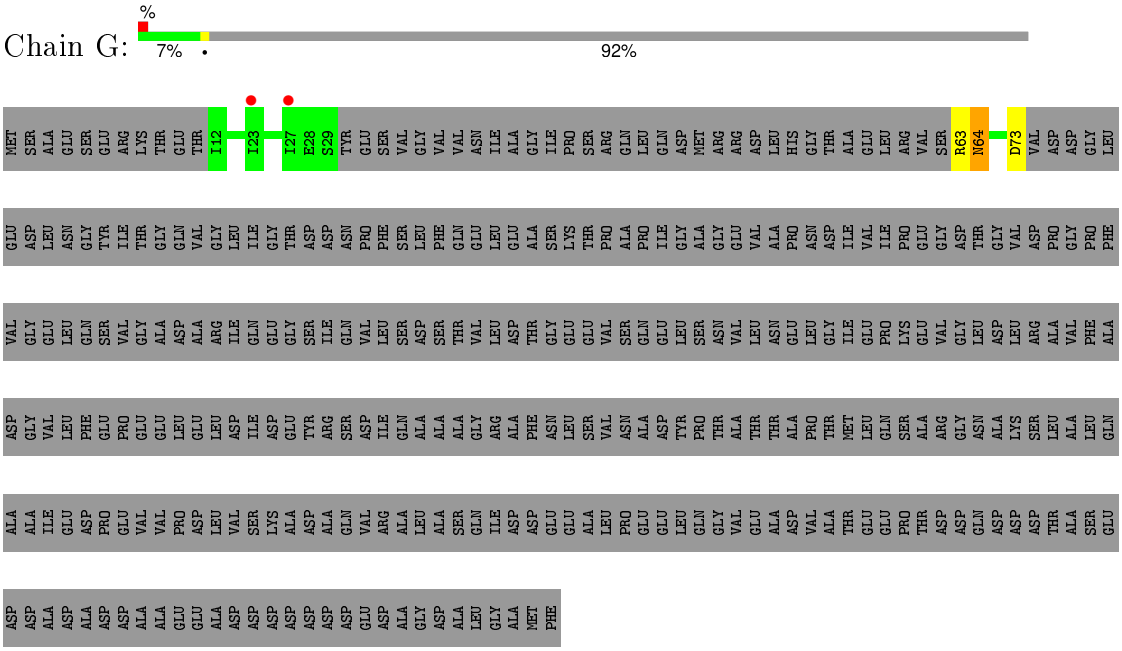
- Molecule 5: 50S ribosomal protein L6P



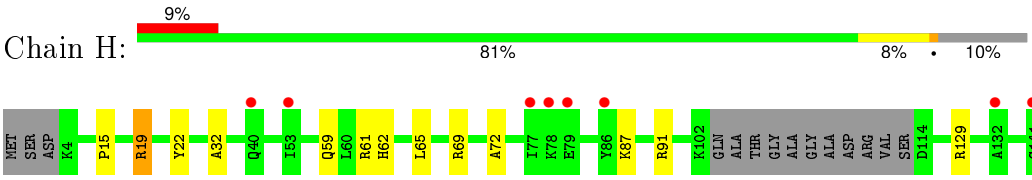
- Molecule 6: 50S ribosomal protein L7Ae

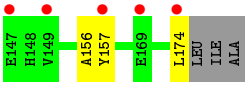


- Molecule 7: 50S ribosomal protein L10E



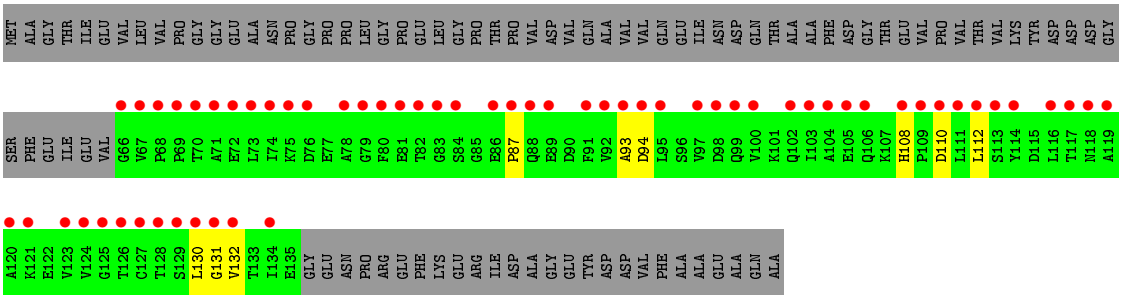
- Molecule 8: 50S ribosomal protein L10e





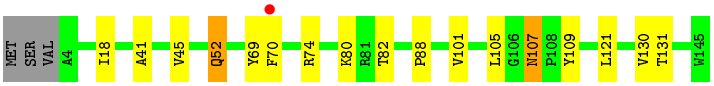
• Molecule 9: 50S ribosomal protein L11P

Chain I:



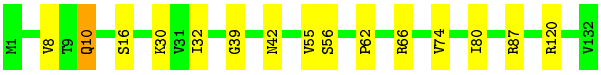
• Molecule 10: 50S ribosomal protein L13P

Chain J:



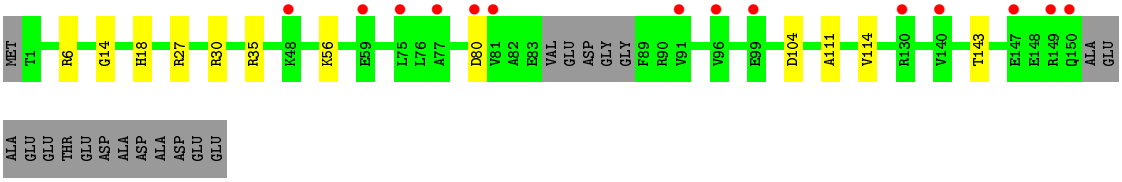
• Molecule 11: 50S ribosomal protein L14P

Chain K:



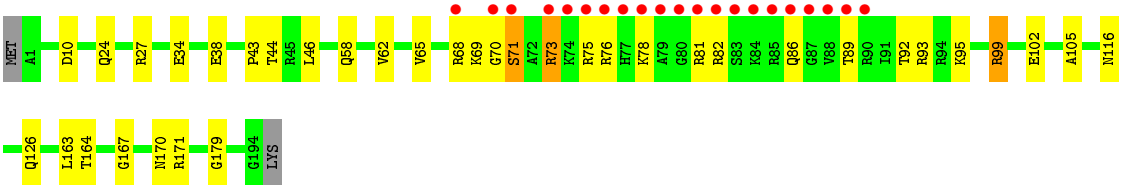
• Molecule 12: 50S ribosomal protein L15P

Chain L:



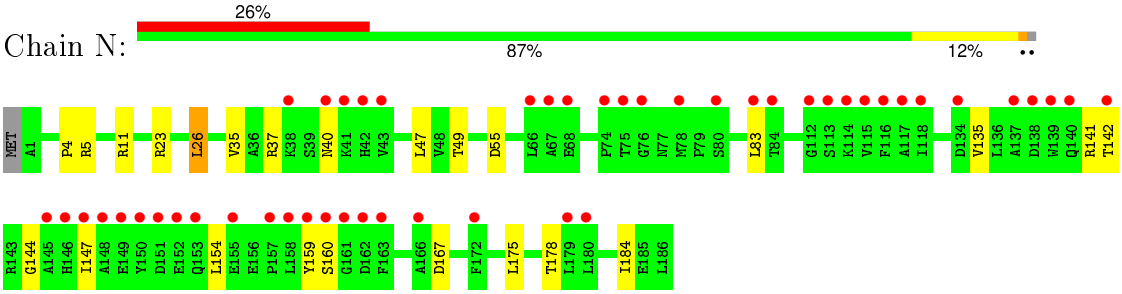
• Molecule 13: 50S ribosomal protein L15e

Chain M:



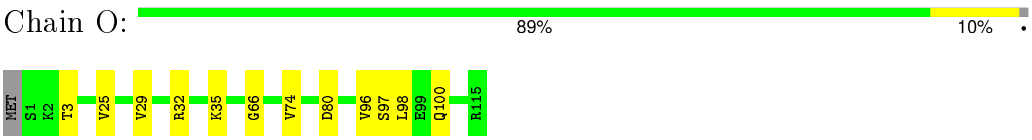
• Molecule 14: 50S ribosomal protein L18P

Chain N:



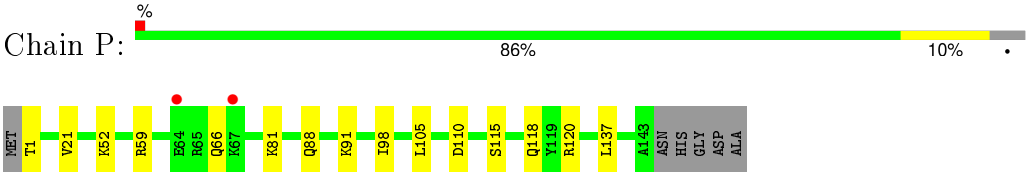
• Molecule 15: 50S ribosomal protein L18e

Chain O:



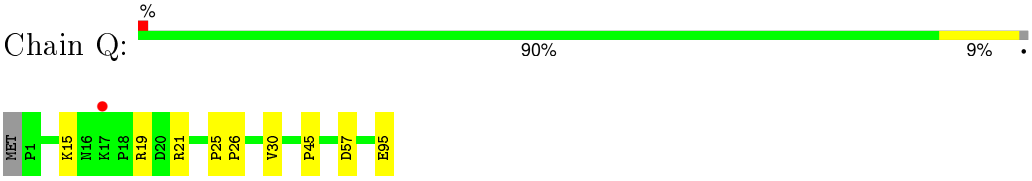
• Molecule 16: 50S ribosomal protein L19e

Chain P:



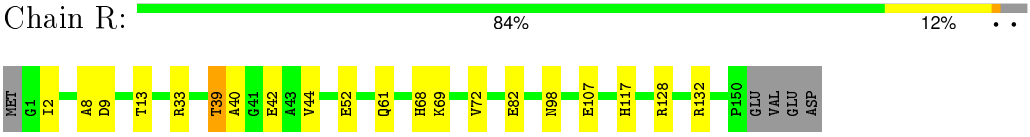
• Molecule 17: 50S ribosomal protein L21e

Chain Q:



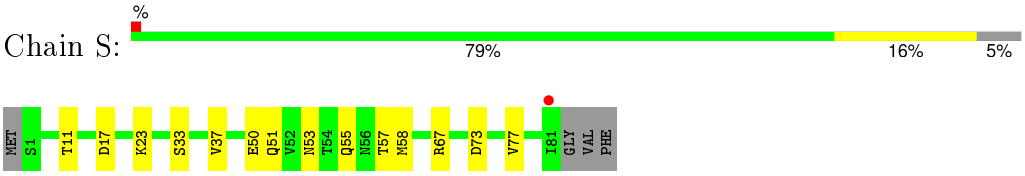
• Molecule 18: 50S ribosomal protein L22P

Chain R:



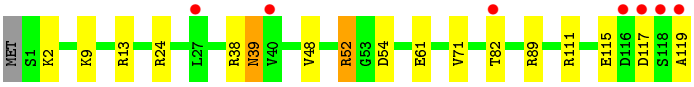
• Molecule 19: 50S ribosomal protein L23P

Chain S:

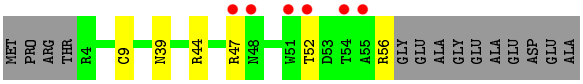


• Molecule 20: 50S ribosomal protein L24P

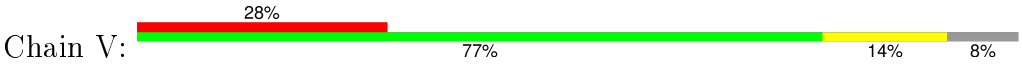
Chain T:

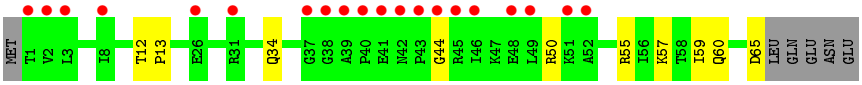


• Molecule 21: 50S ribosomal protein L24e

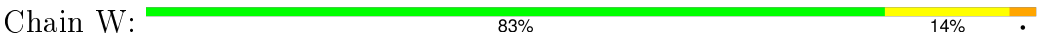


• Molecule 22: 50S ribosomal protein L29P

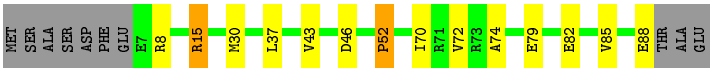




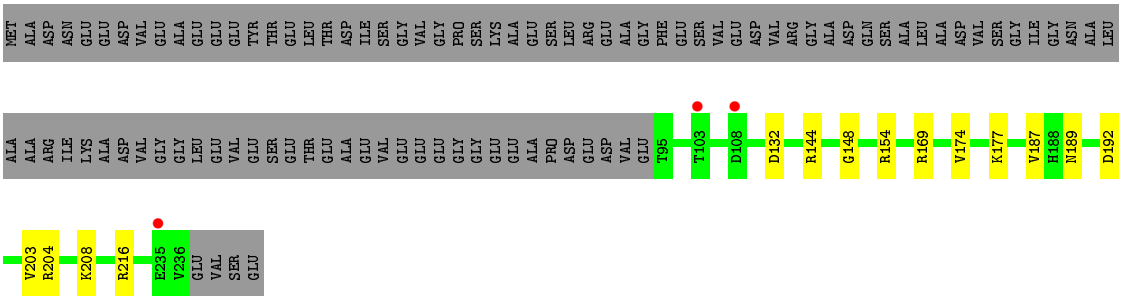
• Molecule 23: 50S ribosomal protein L30P



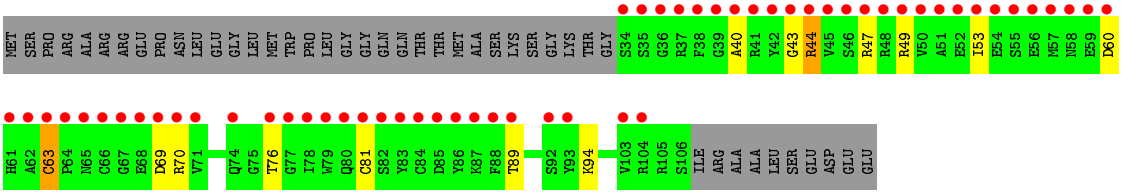
• Molecule 24: 50S ribosomal protein L31e



• Molecule 25: 50S ribosomal protein L32e



• Molecule 26: 50S ribosomal protein L37Ae

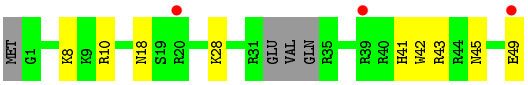


• Molecule 27: 50S ribosomal protein L37e

Chain 1:

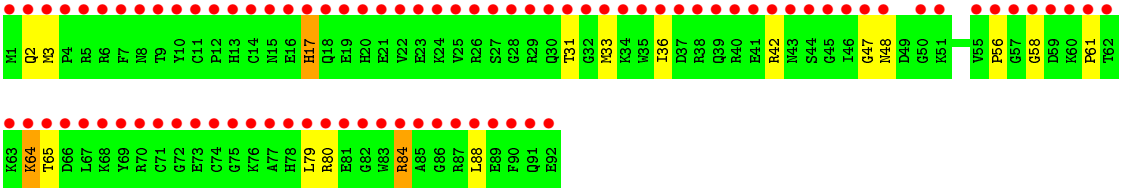
• Molecule 28: 50S ribosomal protein L39e

Chain 2:



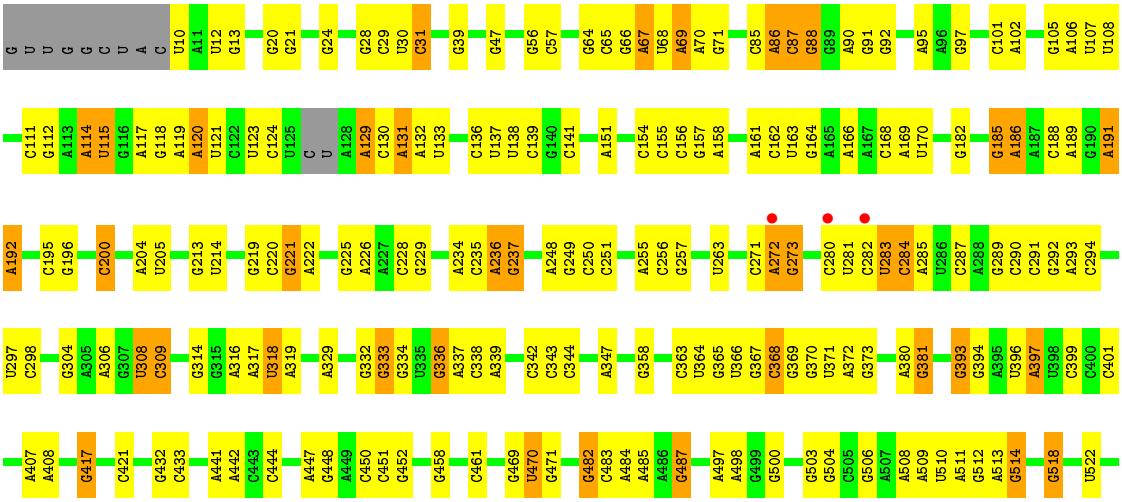
• Molecule 29: 50S ribosomal protein L44E

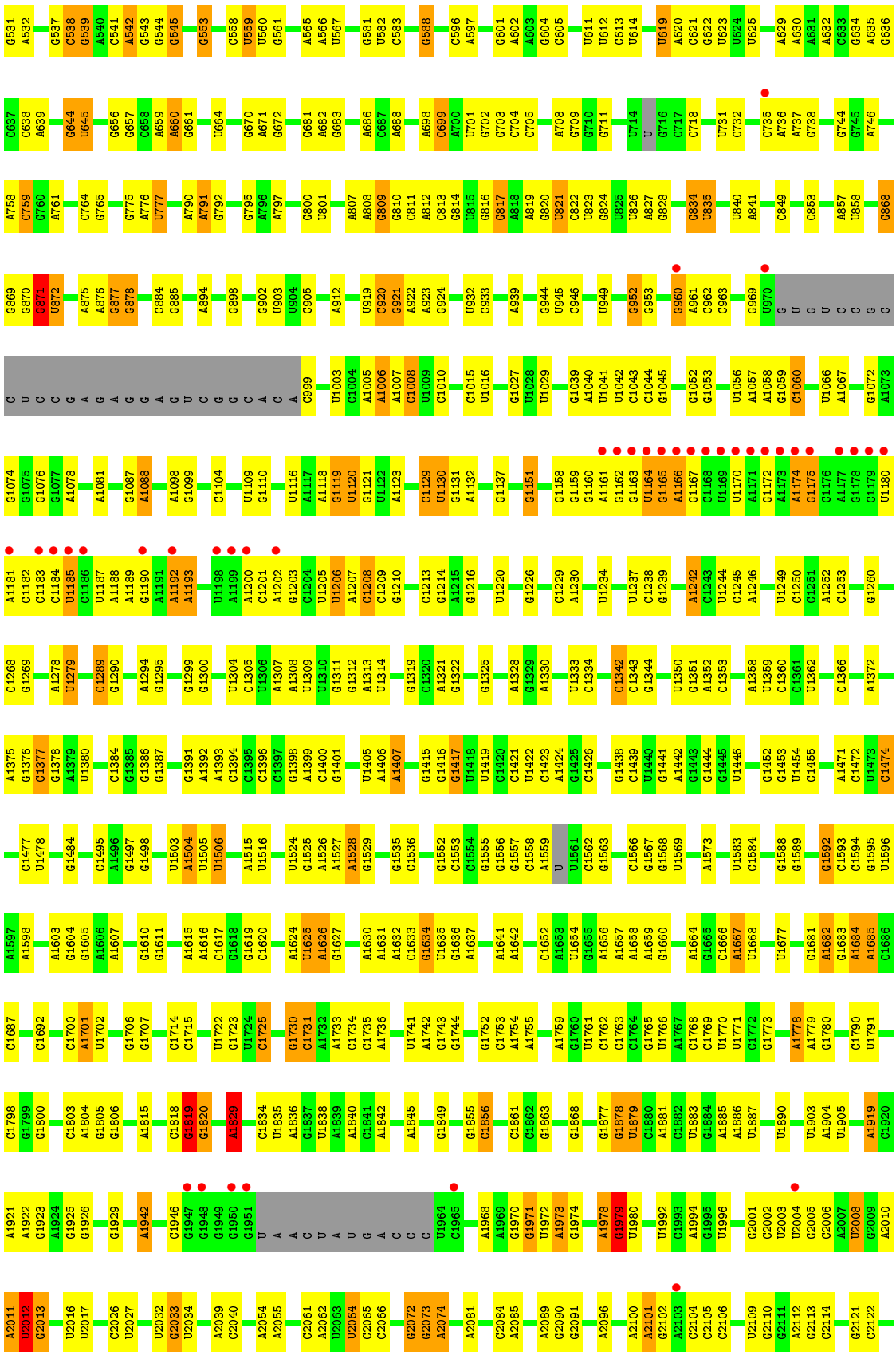
Chain 3:

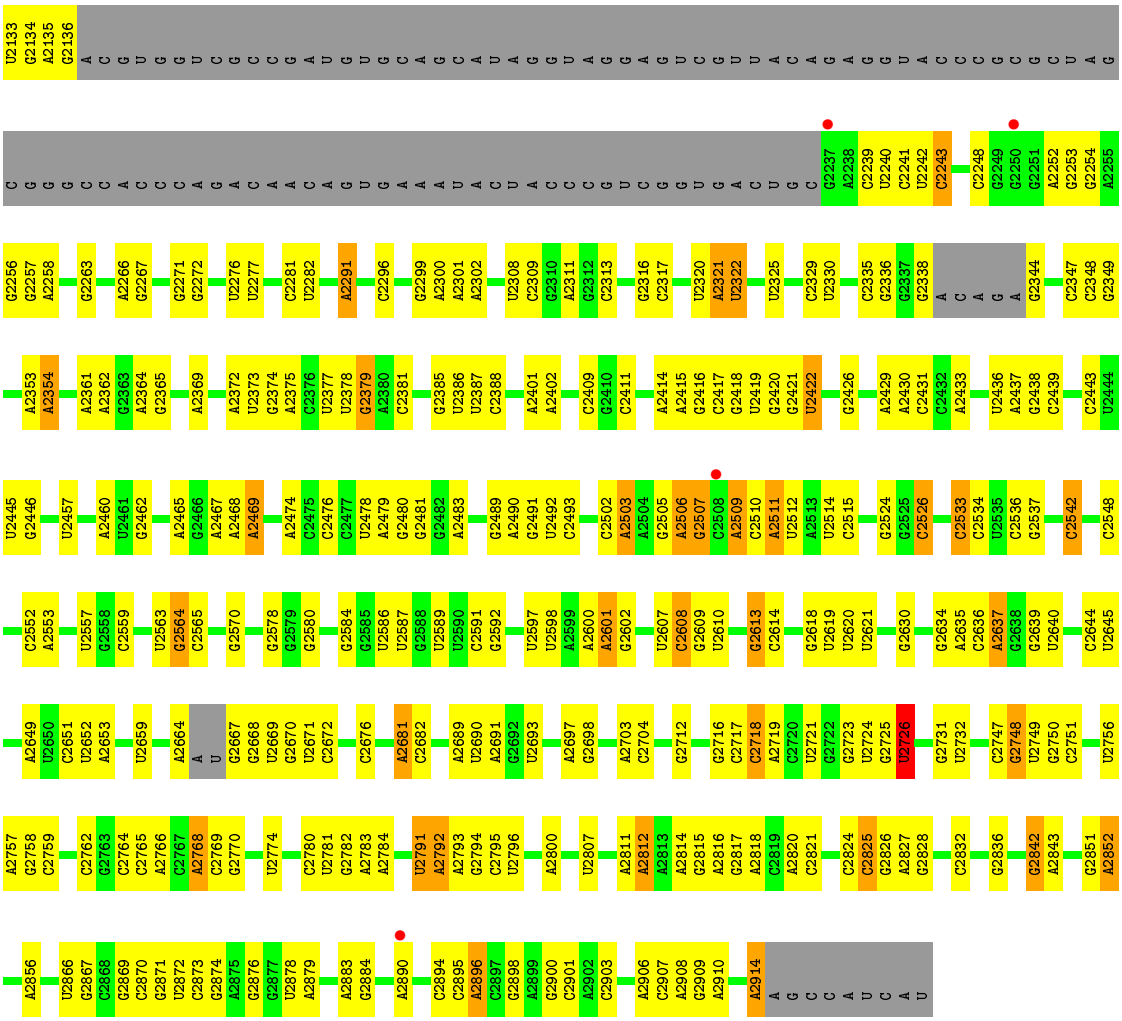


• Molecule 30: 23S RIBOSOMAL RNA

Chain 0:

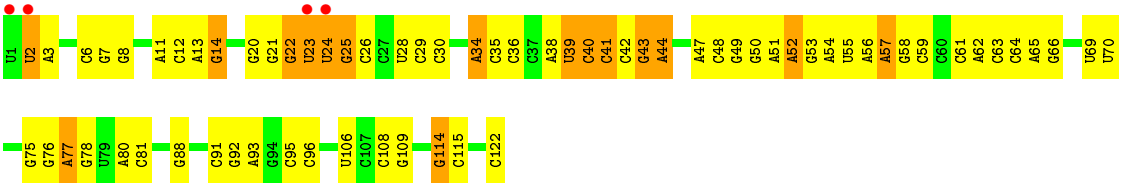






- Molecule 31: 5S RIBOSOMAL RNA

Chain 9:



- Molecule 32: RNA (5'-R(*CP*CP*(PPU))-3')

Chain 4:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	212.81Å 300.00Å 576.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.95 – 2.75 85.82 – 2.41	Depositor EDS
% Data completeness (in resolution range)	91.0 (49.95-2.75) 91.0 (85.82-2.41)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.193 , 0.241 0.189 , 0.231	Depositor DCC
R_{free} test set	4649 reflections (1.09%)	DCC
Wilson B-factor (Å^2)	53.2	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 71.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 667235 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	99180	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.51	0/1786	0.75	0/2408
2	B	0.54	0/2690	0.78	0/3652
3	C	0.56	0/1885	0.78	0/2552
4	D	0.64	0/1111	0.71	1/1498 (0.1%)
5	E	0.60	0/1382	0.67	0/1880
6	F	0.54	0/901	0.70	0/1224
7	G	0.50	0/241	0.66	0/324
8	H	0.61	0/1302	0.78	0/1743
9	I	0.57	0/526	0.63	0/716
10	J	0.64	0/1136	0.73	0/1530
11	K	0.50	0/1004	0.79	0/1351
12	L	0.53	0/1130	0.74	0/1509
13	M	0.52	0/1582	0.76	0/2116
14	N	0.58	0/1474	0.76	0/1999
15	O	0.50	0/874	0.73	1/1181 (0.1%)
16	P	0.52	0/1147	0.67	0/1528
17	Q	0.51	0/749	0.76	0/1005
18	R	0.55	0/1172	0.75	0/1578
19	S	0.54	0/648	0.67	0/875
20	T	0.47	0/958	0.78	1/1289 (0.1%)
21	U	0.64	0/417	0.69	0/562
22	V	0.43	0/502	0.66	0/675
23	W	0.53	0/1219	0.77	1/1655 (0.1%)
24	X	0.53	0/664	0.75	0/895
25	Y	0.53	0/1146	0.72	0/1536
26	Z	0.74	0/584	0.79	0/781
27	1	0.57	0/438	0.74	0/578
28	2	0.47	0/401	0.72	0/529
29	3	0.69	0/771	0.71	0/1024
30	0	0.38	0/65956	0.68	9/102865 (0.0%)
31	9	0.33	0/2904	0.68	0/4526
32	4	0.36	0/40	0.59	0/60

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
All	All	0.44	0/98740	0.70	13/147644 (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	40
All	All	0	41

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	W	4	LEU	CA-CB-CG	6.49	130.22	115.30
30	0	871	G	C5'-C4'-O4'	-6.33	101.50	109.10
20	T	52	ARG	N-CA-C	5.88	126.89	111.00
30	0	1120	U	C5'-C4'-C3'	-5.73	106.83	116.00
30	0	1504	A	N9-C1'-C2'	5.62	121.30	114.00
30	0	1819	G	C5'-C4'-C3'	5.58	124.92	116.00
30	0	1504	A	C1'-O4'-C4'	-5.48	105.52	109.90
30	0	2726	U	N1-C1'-C2'	5.31	120.90	114.00
30	0	841	A	C1'-O4'-C4'	-5.20	105.74	109.90
15	O	66	GLY	N-CA-C	5.17	126.02	113.10
4	D	170	TYR	N-CA-C	5.11	124.79	111.00
30	0	1819	G	C4'-C3'-C2'	-5.09	97.51	102.60
30	0	777	U	O4'-C1'-N1	5.04	112.23	108.20

There are no chirality outliers.

All (41) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1078	A	Sidechain
30	0	115	U	Sidechain
30	0	1309	U	Sidechain
30	0	1417	G	Sidechain
30	0	1829	A	Sidechain
30	0	1863	G	Sidechain
30	0	1878	G	Sidechain

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Mol	Chain	Res	Type	Group
30	0	1970	G	Sidechain
30	0	1978	A	Sidechain
30	0	1979	G	Sidechain
30	0	2012	U	Sidechain
30	0	221	G	Sidechain
30	0	2308	U	Sidechain
30	0	2316	G	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2506	A	Sidechain
30	0	2552	C	Sidechain
30	0	2557	U	Sidechain
30	0	2607	U	Sidechain
30	0	2681	A	Sidechain
30	0	2726	U	Sidechain
30	0	2774	U	Sidechain
30	0	2842	G	Sidechain
30	0	333	G	Sidechain
30	0	393	G	Sidechain
30	0	458	G	Sidechain
30	0	469	G	Sidechain
30	0	470	U	Sidechain
30	0	471	G	Sidechain
30	0	482	G	Sidechain
30	0	518	G	Sidechain
30	0	619	U	Sidechain
30	0	791	A	Sidechain
30	0	795	G	Sidechain
30	0	817	G	Sidechain
30	0	868	G	Sidechain
30	0	872	U	Sidechain
30	0	903	U	Sidechain
30	0	952	G	Sidechain
23	W	90	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	18	0
2	B	2625	0	2533	35	0
3	C	1860	0	1813	19	0
4	D	1094	0	1085	10	0
5	E	1357	0	1266	8	0
6	F	890	0	843	5	0
7	G	240	0	231	2	0
8	H	1282	0	1292	11	0
9	I	519	0	500	5	0
10	J	1120	0	1098	16	0
11	K	994	0	1027	10	0
12	L	1118	0	1076	8	0
13	M	1558	0	1573	23	0
14	N	1445	0	1401	17	0
15	O	865	0	873	6	0
16	P	1136	0	1123	9	0
17	Q	735	0	729	7	0
18	R	1149	0	1122	14	0
19	S	641	0	605	9	0
20	T	950	0	924	8	0
21	U	410	0	364	2	0
22	V	499	0	511	6	0
23	W	1196	0	1137	17	0
24	X	654	0	653	4	0
25	Y	1130	0	1133	10	0
26	Z	573	0	534	11	0
27	1	431	0	426	11	0
28	2	396	0	413	10	0
29	3	755	0	732	14	0
30	0	59019	0	29812	903	0
31	9	2599	0	1325	69	0
32	4	74	0	51	7	0
33	0	86	0	0	0	0
33	9	1	0	0	0	0
33	A	2	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	65	0	0	0	0
35	9	2	0	0	0	0
35	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	C	1	0	0	0	0
35	H	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	0	10	0	0	0	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	0	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	0	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	0	93	0	0	0	0
37	1	2	0	0	0	0
37	3	2	0	0	0	0
37	9	3	0	0	0	0
37	A	2	0	0	0	0
37	B	1	0	0	0	0
37	F	1	0	0	0	0
37	J	1	0	0	0	0
37	R	1	0	0	0	0
37	S	1	0	0	0	0
38	1	1	0	0	0	0
38	3	1	0	0	0	0
38	O	1	0	0	0	0
38	U	1	0	0	0	0
38	Z	1	0	0	0	0
39	0	5949	0	0	114	0
39	1	60	0	0	0	0
39	2	46	0	0	0	0
39	3	62	0	0	0	0
39	9	148	0	0	6	0
39	A	115	0	0	2	0
39	B	136	0	0	5	0
39	C	167	0	0	2	0
39	D	45	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	E	46	0	0	1	0
39	F	28	0	0	0	0
39	G	17	0	0	0	0
39	H	65	0	0	0	0
39	I	7	0	0	1	0
39	J	49	0	0	2	0
39	K	53	0	0	0	0
39	L	92	0	0	2	0
39	M	123	0	0	1	0
39	N	55	0	0	0	0
39	O	37	0	0	0	0
39	P	63	0	0	0	0
39	Q	51	0	0	0	0
39	R	78	0	0	2	0
39	S	31	0	0	0	0
39	T	38	0	0	0	0
39	U	30	0	0	1	0
39	V	10	0	0	0	0
39	W	67	0	0	0	0
39	X	23	0	0	0	0
39	Y	93	0	0	1	0
39	Z	25	0	0	1	0
All	All	99180	0	59971	1124	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 (1124) 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'	1.17	1.08
30:0:1559:A:H1'	39:0:5885:HOH:O	1.55	1.05
31:9:76:G:H3'	31:9:77:A:H5"	1.41	1.00
30:0:871:G:H8	30:0:871:G:H5'	1.25	0.99
30:0:871:G:C8	30:0:871:G:H5'	1.97	0.98
30:0:1701:A:H4'	30:0:1702:U:H5"	1.47	0.96
10:J:82:THR:HG23	30:0:1242:A:H5'	1.49	0.94
30:0:870:G:H2'	30:0:871:G:H5"	1.51	0.91
13:M:171:ARG:HD3	30:0:156:C:H5"	1.49	0.91
16:P:115:SER:H	16:P:118:GLN:HE21	1.19	0.90
30:0:2717:C:C2'	30:0:2718:C:H5"	2.03	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1160:G:C5'	30:0:1161:A:H5'	2.04	0.88
31:9:56:A:H2'	31:9:57:A:H5"	1.52	0.88
10:J:52:GLN:NE2	30:0:1119:G:H2'	1.88	0.88
30:0:1160:G:H5'	30:0:1161:A:C5'	2.02	0.87
30:0:1118:A:H62	30:0:1244:U:H3	1.21	0.87
10:J:52:GLN:HE22	30:0:1119:G:H2'	1.40	0.86
30:0:1835:U:H5	30:0:1840:A:N7	1.73	0.86
30:0:2533:C:H5'	30:0:2533:C:H6	1.41	0.86
30:0:2321:A:H2	30:0:2378:U:H3	1.21	0.85
31:9:29:C:H2'	31:9:30:C:H5'	1.59	0.85
30:0:2717:C:H2'	30:0:2718:C:H5"	1.59	0.84
30:0:1603:A:H5'	30:0:1605:G:O4'	1.77	0.84
30:0:545:G:H8	30:0:545:G:H5'	1.39	0.84
11:K:10:GLN:H	11:K:10:GLN:HE21	1.22	0.84
30:0:2506:A:HO2'	30:0:2507:G:H8	0.87	0.84
30:0:1116:U:HO2'	30:0:1118:A:H2	0.83	0.81
30:0:1116:U:O2'	30:0:1118:A:H2	1.64	0.81
30:0:1118:A:H3'	30:0:1118:A:H8	1.47	0.79
30:0:871:G:H8	30:0:871:G:C5'	1.96	0.79
13:M:163:LEU:HD21	30:0:188:C:H5"	1.62	0.79
30:0:1300:G:H1'	39:0:4703:HOH:O	1.82	0.79
39:B:9053:HOH:O	30:0:2672:C:H1'	1.82	0.78
31:9:14:G:H5'	31:9:14:G:H8	1.47	0.78
30:0:2421:G:H1'	39:0:7053:HOH:O	1.83	0.78
30:0:2812:A:H2	30:0:2814:A:H62	1.32	0.78
30:0:2506:A:O2'	30:0:2507:G:H8	1.66	0.78
30:0:1118:A:H3'	30:0:1118:A:C8	2.19	0.77
30:0:1666:C:O2'	30:0:1667:A:H5"	1.85	0.77
30:0:1474:C:H6	30:0:1474:C:H5'	1.50	0.77
30:0:1667:A:H8	30:0:1667:A:H5'	1.49	0.77
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.31	0.77
2:B:206:THR:HG21	30:0:2716:G:H5"	1.67	0.76
30:0:542:A:H5'	30:0:542:A:H8	1.51	0.76
30:0:1164:U:H3	30:0:1192:A:H2	1.32	0.76
30:0:282:C:H1'	30:0:368:C:N4	2.01	0.76
15:O:3:THR:HG22	30:0:656:G:H5'	1.68	0.76
30:0:506:G:H22	30:0:509:A:C5'	1.98	0.76
30:0:2908:A:H2'	30:0:2909:G:O4'	1.85	0.76
31:9:92:G:H2'	31:9:93:A:C8	2.21	0.75
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.69	0.75
30:0:1183:C:H2'	39:0:6265:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.35	0.74
30:0:1116:U:H3	30:0:1246:A:H62	1.34	0.73
3:C:139:VAL:HG13	39:C:8643:HOH:O	1.88	0.73
30:0:1205:U:H2'	30:0:1206:U:H5'	1.71	0.73
30:0:969:G:H1	30:0:999:C:H42	1.37	0.73
30:0:1741:U:O2'	30:0:2723:G:H4'	1.88	0.72
17:Q:15:LYS:HD3	30:0:2364:A:H5"	1.70	0.72
30:0:544:G:H2'	30:0:545:G:H5"	1.68	0.72
30:0:2717:C:O2'	30:0:2718:C:H5"	1.88	0.72
30:0:559:U:H5'	30:0:559:U:H6	1.53	0.72
30:0:2420:G:O2'	30:0:2421:G:H5'	1.89	0.71
30:0:1183:C:N4	30:0:1184:C:H41	1.88	0.71
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.88	0.71
13:M:102:GLU:OE1	13:M:164:THR:HG21	1.88	0.71
30:0:2637:A:H4'	39:0:4955:HOH:O	1.91	0.71
30:0:1666:C:C2'	30:0:1667:A:H5"	2.21	0.71
30:0:558:C:C2'	30:0:559:U:H5"	2.21	0.71
31:9:7:G:H5'	39:9:9100:HOH:O	1.89	0.71
30:0:2578:G:H5'	30:0:2578:G:H8	1.56	0.70
30:0:1189:A:H1'	30:0:1209:C:O4'	1.91	0.70
30:0:823:U:H3'	39:0:4468:HOH:O	1.90	0.70
30:0:870:G:C2'	30:0:871:G:H5"	2.19	0.70
30:0:1119:G:N2	30:0:1246:A:C2	2.58	0.70
25:Y:204:ARG:HH22	30:0:553:G:P	2.15	0.70
30:0:1206:U:H5'	30:0:1206:U:H6	1.56	0.70
3:C:184:ARG:NH2	30:0:450:C:OP1	2.25	0.70
31:9:56:A:C2'	31:9:57:A:H5"	2.22	0.70
30:0:506:G:H22	30:0:509:A:H5"	1.57	0.70
30:0:2502:C:C2'	30:0:2503:A:H5'	2.22	0.70
30:0:2073:G:H5"	39:0:3843:HOH:O	1.91	0.70
30:0:2534:C:H1'	39:0:3506:HOH:O	1.91	0.70
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.57	0.69
30:0:1372:A:H3'	39:0:7222:HOH:O	1.92	0.69
30:0:1838:U:O2'	30:0:2644:C:H5'	1.92	0.69
4:D:140:ARG:HB3	31:9:29:C:H5"	1.75	0.69
30:0:2321:A:H8	30:0:2322:U:HO2'	1.40	0.69
30:0:2491:G:H1'	39:0:6897:HOH:O	1.92	0.69
30:0:1189:A:H3'	39:0:7712:HOH:O	1.92	0.69
30:0:1205:U:H2'	30:0:1206:U:C5'	2.23	0.69
31:9:24:U:H3'	31:9:25:G:H5'	1.75	0.69
30:0:545:G:C8	30:0:545:G:H5'	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1183:C:H42	30:0:1184:C:H41	1.40	0.68
30:0:2712:G:H5'	39:0:5248:HOH:O	1.92	0.68
3:C:27:ARG:NH2	30:0:657:G:OP1	2.25	0.68
30:0:308:U:H5'	30:0:309:C:OP1	1.93	0.68
30:0:960:G:H3'	30:0:960:G:N3	2.08	0.68
30:0:2502:C:H2'	30:0:2503:A:H5'	1.75	0.68
30:0:2419:U:H5"	30:0:2420:G:H5'	1.74	0.68
30:0:2073:G:OP2	30:0:2490:A:H5'	1.93	0.68
30:0:541:C:H2'	30:0:542:A:C5'	2.23	0.68
30:0:635:A:H2'	30:0:636:G:H5"	1.76	0.68
30:0:853:C:H3'	39:0:4574:HOH:O	1.94	0.67
30:0:1474:C:C6	30:0:1474:C:H5'	2.29	0.67
30:0:1641:A:H2'	30:0:1642:A:H5'	1.76	0.67
30:0:2586:U:H3	30:0:2592:G:H22	1.42	0.67
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.42	0.67
30:0:281:U:H2'	30:0:282:C:O4'	1.94	0.67
30:0:31:C:H4'	39:0:7452:HOH:O	1.94	0.67
30:0:1130:U:H2'	30:0:1131:G:O4'	1.95	0.67
30:0:541:C:C2'	30:0:542:A:H5"	2.24	0.67
30:0:1942:A:H3'	39:0:7377:HOH:O	1.95	0.66
22:V:50:ARG:HH12	30:0:56:G:H5"	1.60	0.66
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.43	0.66
30:0:2613:G:O2'	30:0:2614:C:H5'	1.95	0.66
30:0:1330:A:H4'	39:0:7478:HOH:O	1.95	0.66
13:M:27:ARG:NH2	13:M:44:THR:HG23	2.09	0.66
30:0:182:G:H5'	39:0:5187:HOH:O	1.93	0.66
18:R:128:ARG:NH2	30:0:2054:A:N3	2.43	0.66
30:0:2635:A:O2'	30:0:2636:C:H5'	1.95	0.66
39:Z:395:HOH:O	30:0:1886:A:H4'	1.96	0.66
30:0:541:C:H2'	30:0:542:A:H5"	1.77	0.65
30:0:558:C:H2'	30:0:559:U:H5"	1.77	0.65
30:0:877:G:H5'	30:0:878:G:OP1	1.96	0.65
30:0:2756:U:H3	30:0:2896:A:H2	1.44	0.65
30:0:1666:C:H2'	30:0:1667:A:C5'	2.26	0.65
30:0:2533:C:C6	30:0:2533:C:H5'	2.29	0.65
30:0:659:A:H5"	39:0:7132:HOH:O	1.97	0.65
30:0:2769:C:H2'	30:0:2770:G:O4'	1.97	0.65
30:0:2291:A:C8	30:0:2309:C:H5'	2.31	0.65
30:0:681:G:N3	30:0:681:G:H5'	2.12	0.65
8:H:19:ARG:HH12	30:0:1008:C:H5"	1.62	0.65
30:0:318:U:H5'	30:0:339:A:C2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:812:A:H2'	30:0:813:C:C6	2.32	0.65
30:0:969:G:H1	30:0:999:C:N4	1.95	0.65
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.78	0.64
30:0:1835:U:C5	30:0:1840:A:N7	2.62	0.64
14:N:40:ASN:ND2	31:9:28:U:H5"	2.13	0.64
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.61	0.64
30:0:544:G:C2'	30:0:545:G:H5"	2.26	0.64
30:0:2795:C:O2'	30:0:2796:U:H5'	1.97	0.64
30:0:814:G:H4'	39:0:3146:HOH:O	1.97	0.64
30:0:282:C:O2'	30:0:283:U:H5'	1.98	0.64
30:0:1279:U:O2	30:0:1279:U:H2'	1.98	0.64
26:Z:44:ARG:NH1	30:0:1887:U:H4'	2.12	0.64
30:0:2005:G:H3'	30:0:2005:G:OP2	1.97	0.64
30:0:2827:A:H2'	30:0:2828:G:O4'	1.97	0.63
2:B:238:ASN:HD22	2:B:240:GLY:H	1.47	0.63
30:0:1170:U:H2'	30:0:1172:G:OP2	1.99	0.63
30:0:1701:A:H5"	30:0:1702:U:H3'	1.81	0.63
30:0:2401:A:H2'	30:0:2402:A:C8	2.34	0.63
30:0:2896:A:H5"	39:0:6123:HOH:O	1.99	0.62
30:0:871:G:C8	30:0:871:G:C5'	2.74	0.62
18:R:98:ASN:HD21	30:0:500:G:H21	1.47	0.62
30:0:1087:G:H4'	30:0:1088:A:OP1	1.99	0.62
30:0:2563:U:H2'	30:0:2565:C:O5'	1.99	0.62
30:0:2824:C:H5"	30:0:2825:C:H5'	1.82	0.62
30:0:2851:G:C2'	30:0:2852:A:H5'	2.30	0.62
31:9:13:A:O2'	31:9:14:G:H5"	2.00	0.62
30:0:506:G:H22	30:0:509:A:H5'	1.65	0.62
22:V:50:ARG:NH1	30:0:56:G:H5"	2.13	0.62
30:0:2505:G:O2'	30:0:2506:A:H5'	2.00	0.62
30:0:381:G:H5"	39:0:4338:HOH:O	1.98	0.62
31:9:2:U:OP2	31:9:3:A:H5'	1.99	0.62
30:0:221:G:H5"	39:0:5759:HOH:O	1.99	0.62
30:0:821:U:H3'	39:0:3785:HOH:O	1.99	0.62
30:0:2511:A:H2'	30:0:2512:U:O4'	2.00	0.61
30:0:69:A:H5'	30:0:69:A:C8	2.35	0.61
21:U:39:ASN:ND2	21:U:44:ARG:HH11	1.99	0.61
30:0:582:U:H2'	30:0:583:C:C6	2.35	0.61
30:0:625:U:H5"	30:0:1044:C:N4	2.16	0.61
18:R:39:THR:HG22	18:R:42:GLU:H	1.65	0.61
30:0:1919:A:H4'	39:0:4875:HOH:O	1.99	0.61
10:J:41:ALA:HB3	39:J:9025:HOH:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:10:U:O4	30:0:531:G:H2'	2.01	0.61
30:0:2336:G:H2'	39:0:6318:HOH:O	2.01	0.61
7:G:64:ASN:N	7:G:64:ASN:HD22	1.99	0.61
30:0:1455:C:H3'	39:0:7908:HOH:O	2.01	0.61
28:2:41:HIS:H	28:2:45:ASN:HD22	1.48	0.61
13:M:24:GLN:HE21	13:M:27:ARG:HH11	1.47	0.60
31:9:49:G:O2'	31:9:50:G:H5'	2.01	0.60
30:0:363:C:H1'	39:0:5308:HOH:O	2.00	0.60
13:M:27:ARG:HH22	13:M:44:THR:HG23	1.66	0.60
30:0:2002:C:H2'	30:0:2003:U:H5'	1.83	0.60
30:0:1666:C:H2'	30:0:1667:A:H5'	1.84	0.60
30:0:1278:A:H4'	30:0:1279:U:C4	2.36	0.60
30:0:2426:G:H1'	39:0:6116:HOH:O	2.01	0.60
14:N:37:ARG:NH1	31:9:6:C:OP1	2.34	0.60
30:0:1667:A:C8	30:0:1667:A:H5'	2.36	0.60
11:K:39:GLY:HA2	39:0:5248:HOH:O	2.02	0.60
30:0:1120:U:H5'	30:0:1121:G:OP2	2.02	0.60
29:3:80:ARG:NH2	30:0:2381:C:H4'	2.15	0.60
31:9:12:C:H5'	31:9:70:U:O4'	2.01	0.59
30:0:1132:A:N6	30:0:1229:C:H2'	2.18	0.59
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.18	0.59
23:W:154:ARG:NH1	30:0:588:G:O6	2.35	0.59
30:0:821:U:H2'	30:0:822:C:H6	1.68	0.59
30:0:703:G:O2'	30:0:704:C:H5'	2.03	0.59
30:0:1189:A:H1'	30:0:1209:C:C1'	2.32	0.59
30:0:119:A:H2'	30:0:120:A:H5"	1.85	0.59
30:0:485:A:N3	30:0:487:G:H5"	2.17	0.59
30:0:2769:C:O2'	30:0:2770:G:H5'	2.03	0.59
30:0:1528:A:H2'	30:0:1529:G:O4'	2.03	0.59
30:0:596:C:H2'	30:0:597:A:H8	1.68	0.59
30:0:2820:A:H2'	30:0:2821:C:C6	2.37	0.59
30:0:2748:G:H2'	39:0:7572:HOH:O	2.02	0.58
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.03	0.58
5:E:143:GLN:HE21	30:0:2780:C:C1'	2.16	0.58
30:0:1377:C:H6	30:0:1377:C:H5'	1.68	0.58
31:9:29:C:C2'	31:9:30:C:H5'	2.29	0.58
30:0:164:G:H3'	39:0:3657:HOH:O	2.03	0.58
30:0:195:C:H2'	30:0:196:G:H5'	1.85	0.58
2:B:18:ARG:HE	2:B:256:GLN:NE2	2.02	0.58
27:1:8:GLN:HE22	27:1:11:LYS:HZ2	1.52	0.58
30:0:1778:A:H2'	30:0:1779:A:H5'	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1701:A:H4'	30:0:1702:U:C5'	2.25	0.58
31:9:54:A:O2'	31:9:55:U:H5'	2.03	0.58
30:0:12:U:H2'	30:0:13:G:H5'	1.85	0.58
30:0:2239:C:H2'	30:0:2240:U:C6	2.39	0.58
30:0:1741:U:H5'	30:0:1742:A:OP1	2.04	0.57
30:0:2852:A:H5"	39:0:5259:HOH:O	2.04	0.57
30:0:10:U:O4	30:0:532:A:OP2	2.22	0.57
1:A:199:HIS:HE1	30:0:1881:A:OP1	1.88	0.57
30:0:256:C:H2'	30:0:257:G:O4'	2.04	0.57
30:0:1206:U:H2'	30:0:1207:A:O4'	2.04	0.57
30:0:558:C:H2'	30:0:559:U:C5'	2.33	0.57
1:A:48:ASP:HB3	39:A:9020:HOH:O	2.03	0.57
30:0:1268:C:O2'	30:0:1269:G:H5'	2.05	0.57
29:3:47:GLY:HA2	30:0:2121:G:H4'	1.87	0.57
30:0:2644:C:O2'	30:0:2645:U:H5'	2.04	0.57
29:3:42:ARG:NH1	30:0:396:U:H5'	2.20	0.57
30:0:1595:G:O2'	30:0:1596:U:H5'	2.05	0.57
30:0:371:U:H2'	30:0:372:A:H8	1.69	0.57
31:9:14:G:H5'	31:9:14:G:C8	2.35	0.57
30:0:1592:G:H2'	30:0:1593:C:C6	2.40	0.57
14:N:141:ARG:NH2	31:9:48:C:H4'	2.19	0.57
30:0:282:C:H1'	30:0:368:C:H41	1.68	0.57
30:0:69:A:H5'	30:0:69:A:H8	1.70	0.57
30:0:1562:C:H3'	30:0:1563:G:C8	2.40	0.57
30:0:1426:C:H2'	39:0:9601:HOH:O	2.04	0.57
30:0:2415:A:H2'	30:0:2416:G:H5'	1.86	0.57
30:0:1759:A:N3	30:0:1818:C:H2'	2.20	0.57
26:Z:44:ARG:HH11	30:0:1887:U:H4'	1.69	0.56
30:0:1118:A:H8	30:0:1119:G:H5"	1.70	0.56
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.85	0.56
12:L:6:ARG:HD3	30:0:1299:G:O6	2.05	0.56
16:P:115:SER:H	16:P:118:GLN:NE2	1.97	0.56
30:0:1166:A:H1'	30:0:1192:A:C2	2.40	0.56
30:0:2597:U:H2'	30:0:2598:U:H5'	1.86	0.56
30:0:214:U:H5'	39:0:6165:HOH:O	2.04	0.56
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.70	0.56
30:0:735:C:H5	30:0:736:A:C4	2.24	0.56
31:9:20:G:O2'	31:9:21:G:H5'	2.05	0.56
30:0:1213:C:O2'	30:0:1214:G:H5'	2.06	0.56
3:C:174:ILE:CD1	30:0:338:C:H4'	2.35	0.56
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.86	0.56
30:0:1118:A:C8	30:0:1118:A:C3'	2.84	0.56
30:0:1506:U:H6	30:0:1506:U:H5'	1.71	0.56
30:0:2414:A:H2'	30:0:2415:A:C8	2.41	0.56
30:0:1603:A:H5"	30:0:1604:G:H3'	1.88	0.56
30:0:2505:G:C2'	30:0:2506:A:H5'	2.36	0.56
30:0:2769:C:C2'	30:0:2770:G:H5'	2.36	0.56
30:0:613:C:H2'	30:0:614:U:H6	1.71	0.56
30:0:1666:C:C2'	30:0:1667:A:C5'	2.83	0.55
30:0:2851:G:O2'	30:0:2852:A:H5'	2.06	0.55
30:0:2090:G:H2'	30:0:2091:G:C8	2.41	0.55
19:S:51:GLN:NE2	19:S:53:ASN:HD21	2.04	0.55
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.88	0.55
30:0:2344:G:N3	30:0:2344:G:H2'	2.21	0.55
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.06	0.55
17:Q:19:ARG:HH21	31:9:11:A:P	2.28	0.55
31:9:91:C:H2'	31:9:92:G:O4'	2.06	0.55
29:3:31:THR:O	30:0:1923:G:H4'	2.07	0.55
18:R:117:HIS:HD2	30:0:20:G:H21	1.53	0.55
30:0:28:G:H1'	39:0:4701:HOH:O	2.06	0.55
30:0:421:C:H4'	30:0:1919:A:C6	2.41	0.55
3:C:174:ILE:HD11	30:0:338:C:H4'	1.87	0.55
10:J:45:VAL:HG11	10:J:121:LEU:HD22	1.88	0.55
20:T:52:ARG:O	30:0:317:A:OP1	2.25	0.55
30:0:559:U:H2'	30:0:560:U:O4'	2.06	0.55
19:S:51:GLN:HE21	19:S:53:ASN:HD21	1.53	0.55
30:0:31:C:H2'	39:0:7721:HOH:O	2.07	0.55
30:0:64:G:H2'	30:0:65:C:O4'	2.07	0.55
30:0:2791:U:H1'	30:0:2792:A:H5"	1.88	0.55
30:0:2524:G:H21	30:0:2526:C:N4	2.04	0.55
30:0:660:A:H4'	30:0:661:G:O5'	2.07	0.55
30:0:1189:A:O2'	30:0:1208:C:H2'	2.07	0.55
30:0:2900:G:H2'	30:0:2901:C:O4'	2.06	0.55
14:N:4:PRO:HB2	30:0:1010:C:H4'	1.89	0.55
30:0:1159:G:H21	30:0:1189:A:H8	1.54	0.54
30:0:2748:G:H1'	39:0:7934:HOH:O	2.07	0.54
30:0:2239:C:H2'	30:0:2240:U:H6	1.72	0.54
1:A:70:ALA:HB1	26:Z:89:THR:HG21	1.88	0.54
30:0:670:G:H2'	30:0:671:A:C8	2.41	0.54
30:0:1596:U:H2'	30:0:1598:A:OP2	2.06	0.54
30:0:2241:C:O2'	30:0:2242:U:H5'	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2717:C:H2'	30:0:2718:C:C5'	2.33	0.54
30:0:834:G:H3'	30:0:835:U:H4'	1.89	0.54
31:9:75:G:H1	31:9:106:U:H3	1.55	0.54
30:0:2064:U:H5'	30:0:2652:U:H4'	1.90	0.54
30:0:2248:C:H3'	39:0:5468:HOH:O	2.06	0.54
31:9:49:G:H5"	39:9:9090:HOH:O	2.06	0.54
32:4:76:PPU:C	32:4:76:PPU:H5"	2.37	0.54
30:0:1973:A:H2'	30:0:1974:G:O4'	2.08	0.54
30:0:596:C:H2'	30:0:597:A:C8	2.42	0.54
30:0:90:A:H2'	30:0:91:G:O4'	2.06	0.54
31:9:76:G:C3'	31:9:77:A:H5"	2.28	0.54
30:0:1184:C:H1'	39:0:7498:HOH:O	2.07	0.54
30:0:1130:U:H5'	39:0:7704:HOH:O	2.07	0.54
30:0:2329:C:O2'	30:0:2330:U:H5'	2.07	0.54
30:0:1477:C:O2'	30:0:1478:U:H5'	2.08	0.54
27:1:9:GLY:HA2	30:0:1687:C:O2	2.08	0.54
39:L:8813:HOH:O	30:0:220:C:H2'	2.08	0.54
30:0:1042:U:O2'	30:0:1043:C:H5'	2.08	0.54
30:0:10:U:H6	30:0:10:U:H3'	1.73	0.54
30:0:1377:C:H1'	39:0:7305:HOH:O	2.08	0.54
22:V:34:GLN:HE22	30:0:57:C:H4'	1.72	0.54
30:0:1304:U:H2'	30:0:1305:C:C6	2.43	0.54
30:0:2032:U:H2'	30:0:2033:G:C5'	2.39	0.54
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.07	0.54
13:M:179:GLY:O	30:0:399:C:H5'	2.07	0.54
30:0:1118:A:C8	30:0:1119:G:H5"	2.43	0.53
30:0:582:U:H2'	30:0:583:C:H6	1.73	0.53
30:0:2335:C:H2'	30:0:2336:G:C8	2.42	0.53
30:0:1657:A:H2'	30:0:1658:A:C8	2.44	0.53
30:0:2372:A:H2'	30:0:2373:U:C6	2.44	0.53
15:O:32:ARG:HE	15:O:35:LYS:HD2	1.73	0.53
23:W:108:ARG:HH21	23:W:114:PRO:HG2	1.74	0.53
30:0:200:C:H2'	39:0:3455:HOH:O	2.07	0.53
30:0:2256:G:O2'	30:0:2257:G:H5'	2.08	0.53
30:0:558:C:O2'	30:0:559:U:H5"	2.08	0.53
3:C:127:ARG:NH2	3:C:225:PRO:HG2	2.24	0.53
29:3:48:ASN:HD21	30:0:2468:A:H61	1.56	0.53
30:0:1594:C:O2'	30:0:1607:A:H4'	2.07	0.53
23:W:88:THR:HG22	23:W:89:ASP:H	1.74	0.53
30:0:2559:C:H4'	39:0:7287:HOH:O	2.09	0.53
30:0:2636:C:H3'	30:0:2637:A:H5'	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2004:U:H4'	39:0:5336:HOH:O	2.09	0.53
30:0:1441:G:O2'	30:0:1442:A:H5'	2.07	0.53
27:1:28:HIS:HE1	30:0:776:A:OP1	1.92	0.53
30:0:2377:U:O2'	30:0:2378:U:H5'	2.09	0.53
24:X:74:ALA:HB2	24:X:85:VAL:HG13	1.91	0.53
30:0:1555:G:H4'	30:0:1630:A:H2	1.74	0.53
31:9:92:G:H2'	31:9:93:A:H8	1.73	0.53
30:0:945:U:H2'	30:0:946:C:C6	2.44	0.53
30:0:1730:G:H5"	30:0:1731:C:H6	1.73	0.53
30:0:1702:U:H1'	39:0:5793:HOH:O	2.08	0.52
30:0:2445:U:H2'	30:0:2446:G:C8	2.44	0.52
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.49	0.52
2:B:229:ARG:NH2	30:0:1753:C:O2	2.41	0.52
30:0:1973:A:H5'	30:0:1973:A:H8	1.74	0.52
30:0:952:G:N3	30:0:2302:A:H2'	2.25	0.52
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.90	0.52
30:0:2781:U:H2'	30:0:2782:G:H5'	1.91	0.52
22:V:57:LYS:HA	22:V:60:GLN:HE21	1.74	0.52
30:0:1342:C:C2'	30:0:1343:C:H5'	2.39	0.52
30:0:1904:A:H2'	30:0:1905:U:O4'	2.09	0.52
30:0:2353:A:H4'	30:0:2354:A:O5'	2.09	0.52
30:0:1181:A:H2'	30:0:1182:C:H5'	1.91	0.52
27:1:8:GLN:HE22	27:1:11:LYS:NZ	2.07	0.52
30:0:736:A:H2'	30:0:737:A:O4'	2.09	0.52
30:0:2542:C:H5"	30:0:2608:C:N4	2.24	0.52
30:0:482:G:H4'	30:0:508:A:N1	2.25	0.52
30:0:2718:C:H6	30:0:2718:C:H5'	1.75	0.52
30:0:1116:U:O2'	30:0:1118:A:C2	2.48	0.52
30:0:541:C:H2'	30:0:542:A:H5'	1.89	0.52
31:9:23:U:O2'	31:9:24:U:H4'	2.10	0.52
30:0:819:A:HO2'	30:0:821:U:H6	1.56	0.52
30:0:611:U:H2'	30:0:612:U:C6	2.43	0.52
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.90	0.52
23:W:44:MET:CE	30:0:944:G:H21	2.21	0.52
29:3:36:ILE:HG21	30:0:2433:A:OP1	2.09	0.52
13:M:95:LYS:HE2	30:0:157:G:H4'	1.91	0.52
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.09	0.52
30:0:1066:U:H2'	30:0:1067:A:C8	2.44	0.52
1:A:179:MET:HG2	1:A:186:TRP:HB2	1.91	0.52
30:0:702:G:O2'	30:0:703:G:H5'	2.10	0.52
25:Y:169:ARG:HD2	30:0:1328:A:OP1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1878:G:H1'	39:0:6145:HOH:O	2.10	0.52
1:A:190:ARG:NH1	30:0:1845:A:OP2	2.41	0.52
3:C:27:ARG:HH22	30:0:657:G:P	2.33	0.52
30:0:1972:U:H2'	30:0:1973:A:H5'	1.92	0.52
2:B:162:MET:HE1	2:B:308:LEU:HD21	1.92	0.52
30:0:1471:A:H2'	30:0:1472:C:C6	2.44	0.52
31:9:108:C:H2'	31:9:109:G:C8	2.45	0.52
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.25	0.52
29:3:80:ARG:O	30:0:2457:U:H4'	2.10	0.52
30:0:1174:A:C6	30:0:1201:C:H4'	2.45	0.52
39:D:6783:HOH:O	31:9:59:C:H4'	2.10	0.52
30:0:1187:U:O2'	30:0:1189:A:H2	1.93	0.52
30:0:1377:C:H5'	30:0:1377:C:C6	2.45	0.52
31:9:38:A:H2'	31:9:39:U:C6	2.45	0.52
20:T:38:ARG:NH1	39:0:6710:HOH:O	2.43	0.52
13:M:43:PRO:HG3	13:M:62:VAL:HG21	1.91	0.52
30:0:704:C:H2'	30:0:705:C:H6	1.75	0.52
30:0:1268:C:H2'	30:0:1269:G:H8	1.75	0.52
20:T:9:LYS:HE2	20:T:13:ARG:NH1	2.25	0.52
30:0:1819:G:H2'	30:0:1820:G:C5'	2.40	0.52
30:0:1245:C:O5'	30:0:1245:C:H6	1.93	0.52
30:0:2781:U:C2'	30:0:2782:G:H5'	2.40	0.51
30:0:1819:G:H5'	39:0:4730:HOH:O	2.09	0.51
30:0:162:C:H2'	30:0:163:U:H5'	1.92	0.51
30:0:297:U:H2'	30:0:298:C:C6	2.45	0.51
30:0:192:A:H5'	39:0:7678:HOH:O	2.10	0.51
30:0:2872:U:H2'	30:0:2873:C:H6	1.76	0.51
16:P:1:THR:O	30:0:1396:C:H1'	2.10	0.51
30:0:1736:A:H1'	39:0:7617:HOH:O	2.10	0.51
30:0:221:G:H2'	30:0:222:A:C8	2.46	0.51
16:P:105:LEU:HD21	16:P:137:LEU:HD11	1.92	0.51
31:9:24:U:H3'	31:9:25:G:C5'	2.38	0.51
30:0:236:A:H4'	30:0:237:G:OP1	2.09	0.51
30:0:565:A:H4'	39:0:3972:HOH:O	2.11	0.51
14:N:11:ARG:HD3	31:9:114:G:O6	2.10	0.51
30:0:1453:G:H2'	30:0:1454:U:O4'	2.10	0.51
30:0:1165:G:H4'	30:0:1174:A:O2'	2.11	0.51
30:0:1123:A:C2	30:0:1129:C:H4'	2.45	0.51
30:0:1386:G:O2'	30:0:1387:G:H5'	2.10	0.51
11:K:66:ARG:HH22	30:0:1994:A:P	2.34	0.51
30:0:2002:C:C2'	30:0:2003:U:H5'	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1592:G:H2'	30:0:1593:C:H6	1.76	0.51
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.58	0.51
30:0:291:C:H2'	30:0:292:G:O4'	2.11	0.51
18:R:2:ILE:HG22	30:0:21:G:H4'	1.91	0.51
30:0:522:U:O2'	30:0:1366:C:H5'	2.10	0.51
14:N:35:VAL:HG11	31:9:6:C:H4'	1.91	0.51
30:0:2883:A:H2'	30:0:2884:G:O4'	2.11	0.51
14:N:144:GLY:O	14:N:147:ILE:HG22	2.10	0.51
30:0:1289:C:O2'	30:0:1290:G:H5'	2.11	0.51
2:B:212:GLN:HA	30:0:1733:A:H4'	1.92	0.51
14:N:55:ASP:OD2	31:9:7:G:H4'	2.11	0.51
30:0:1202:A:C2'	30:0:1203:G:H5'	2.40	0.51
23:W:64:THR:O	23:W:68:THR:HG22	2.10	0.51
28:2:42:TRP:HZ2	30:0:1438:G:H1'	1.75	0.51
30:0:185:G:O3'	30:0:186:A:H4'	2.11	0.51
29:3:2:GLN:O	30:0:2320:U:H2'	2.10	0.51
2:B:262:ARG:HG3	30:0:2716:G:H5'	1.91	0.51
31:9:108:C:H2'	31:9:109:G:H8	1.76	0.51
30:0:1201:C:H2'	30:0:1202:A:H5'	1.93	0.51
20:T:38:ARG:HH21	30:0:306:A:P	2.33	0.51
30:0:1249:U:H2'	30:0:1250:C:C6	2.46	0.51
30:0:2016:U:H2'	30:0:2017:U:O4'	2.11	0.51
30:0:2276:U:H2'	30:0:2277:U:C6	2.46	0.50
30:0:638:C:H2'	30:0:639:A:C8	2.47	0.50
30:0:2618:G:N3	32:4:76:PPU:H2	2.25	0.50
30:0:2510:C:H42	30:0:2564:G:H22	1.59	0.50
2:B:221:GLN:HE22	11:K:42:ASN:ND2	2.07	0.50
30:0:2256:G:C2'	30:0:2257:G:H5'	2.41	0.50
5:E:154:ILE:HD11	5:E:157:LYS:HB2	1.94	0.50
30:0:1768:C:H2'	30:0:1769:C:O4'	2.11	0.50
3:C:118:THR:O	3:C:136:VAL:HG13	2.12	0.50
30:0:2703:A:H2'	30:0:2704:C:H6	1.76	0.50
31:9:63:C:O2'	31:9:64:C:H5'	2.12	0.50
15:O:3:THR:CG2	30:0:656:G:H5'	2.39	0.50
30:0:1484:G:H2'	39:0:9108:HOH:O	2.11	0.50
30:0:1174:A:C5	30:0:1201:C:H4'	2.46	0.50
31:9:36:C:H5'	39:9:9050:HOH:O	2.11	0.50
4:D:105:SER:OG	30:0:2338:G:H1'	2.12	0.50
5:E:137:ASP:O	5:E:141:VAL:HG23	2.12	0.50
10:J:70:PHE:CD1	30:0:2676:C:H4'	2.47	0.50
30:0:849:C:H1'	39:0:6642:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2768:A:O2'	30:0:2769:C:H5'	2.11	0.50
18:R:132:ARG:NH2	30:0:2055:A:H4'	2.27	0.50
30:0:2296:C:H4'	30:0:2362:A:H2	1.77	0.50
30:0:2670:G:O2'	30:0:2671:U:H5'	2.11	0.50
30:0:2578:G:C8	30:0:2578:G:H5'	2.43	0.50
30:0:1681:G:H5"	30:0:1682:A:H5'	1.93	0.50
4:D:141:VAL:HG21	31:9:57:A:H8	1.77	0.50
30:0:1535:G:H2'	30:0:1536:C:C6	2.47	0.50
12:L:111:ALA:HB2	30:0:698:A:H5"	1.92	0.50
30:0:366:U:H2'	30:0:367:G:O4'	2.11	0.50
2:B:252:PRO:HD2	30:0:2548:C:H5'	1.94	0.50
39:B:9053:HOH:O	30:0:2818:A:H2	1.95	0.49
30:0:407:A:H2'	30:0:408:A:C8	2.47	0.49
10:J:88:PRO:HD3	30:0:1104:C:H4'	1.92	0.49
30:0:1741:U:H3'	39:0:9773:HOH:O	2.11	0.49
30:0:363:C:O2'	30:0:364:U:H5'	2.12	0.49
30:0:1819:G:H2'	30:0:1820:G:H4'	1.93	0.49
30:0:371:U:H2'	30:0:372:A:C8	2.47	0.49
10:J:107:ASN:HD22	10:J:109:TYR:H	1.60	0.49
30:0:514:G:OP1	30:0:514:G:H2'	2.11	0.49
30:0:1393:A:H2'	30:0:1394:C:C6	2.47	0.49
30:0:1180:U:H2'	30:0:1181:A:C8	2.48	0.49
30:0:2608:C:H3'	39:0:7840:HOH:O	2.13	0.49
4:D:76:ARG:NE	31:9:44:A:O4'	2.44	0.49
24:X:15:ARG:NH2	30:0:2856:A:OP1	2.44	0.49
30:0:1419:U:H2'	30:0:1685:A:C2	2.47	0.49
1:A:171:LYS:HB2	30:0:820:G:C5	2.47	0.49
30:0:1702:U:H5'	39:0:3437:HOH:O	2.12	0.49
26:Z:43:GLY:HA2	30:0:1771:U:O2	2.12	0.49
30:0:2379:G:N3	30:0:2418:G:H2'	2.28	0.49
30:0:711:G:C2	30:0:718:C:C2	3.00	0.49
30:0:1834:C:H2'	30:0:1840:A:N6	2.27	0.49
30:0:1527:A:H1'	30:0:1528:A:C8	2.48	0.49
11:K:32:ILE:HD11	11:K:56:SER:HB2	1.95	0.49
30:0:2266:A:H2'	30:0:2267:G:C8	2.47	0.49
26:Z:63:CYS:SG	26:Z:81:CYS:HB2	2.52	0.49
30:0:107:U:H2'	30:0:108:U:H5'	1.95	0.49
30:0:2507:G:H2'	30:0:2510:C:H42	1.78	0.49
30:0:1666:C:H2'	30:0:1667:A:H5"	1.89	0.49
14:N:4:PRO:HG3	31:9:69:U:OP1	2.13	0.49
30:0:2542:C:H4'	32:4:75:C:O2'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:3:48:ASN:HB3	30:0:170:U:H5'	1.95	0.49
30:0:1946:C:H2'	30:0:1971:G:C8	2.48	0.49
30:0:2348:C:H2'	30:0:2349:G:H8	1.78	0.49
30:0:1226:G:H5'	39:0:4554:HOH:O	2.11	0.49
30:0:1625:U:H4'	39:0:4685:HOH:O	2.13	0.49
30:0:2758:G:H2'	30:0:2759:C:C6	2.48	0.49
3:C:39:GLN:O	3:C:43:LYS:HD3	2.12	0.49
30:0:441:A:H1'	30:0:442:A:N7	2.28	0.49
29:3:79:LEU:HD13	30:0:2457:U:H1'	1.94	0.49
27:1:12:ASN:O	30:0:1415:G:H5'	2.13	0.49
30:0:2421:G:H3'	30:0:2422:U:C5'	2.44	0.48
30:0:2644:C:H5"	39:0:3408:HOH:O	2.13	0.48
30:0:1006:A:N1	30:0:2311:A:H1'	2.28	0.48
10:J:18:ILE:HD13	30:0:1244:U:OP1	2.12	0.48
30:0:2320:U:H4'	30:0:2321:A:O4'	2.13	0.48
30:0:2509:A:H2'	30:0:2510:C:O4'	2.13	0.48
30:0:601:G:O2'	30:0:602:A:H5'	2.13	0.48
13:M:65:VAL:HG21	13:M:105:ALA:HB2	1.94	0.48
30:0:1205:U:C2'	30:0:1206:U:C5'	2.91	0.48
30:0:1131:G:C6	30:0:1230:A:C4	3.01	0.48
30:0:2619:UR3:H5	39:0:5872:HOH:O	2.13	0.48
30:0:1452:G:O2'	30:0:1453:G:H5'	2.13	0.48
30:0:1058:A:H2'	30:0:1060:C:H5"	1.94	0.48
2:B:17:LYS:O	2:B:260:HIS:HD2	1.96	0.48
30:0:2469:A:H1'	39:0:3254:HOH:O	2.13	0.48
30:0:432:G:O2'	30:0:433:C:H5'	2.13	0.48
30:0:1589:G:N2	30:0:1605:G:H1'	2.28	0.48
12:L:27:ARG:HH21	12:L:30:ARG:HG2	1.78	0.48
30:0:249:G:O2'	30:0:250:C:H5'	2.14	0.48
11:K:10:GLN:H	11:K:10:GLN:NE2	2.00	0.48
30:0:372:A:H2'	30:0:373:G:H8	1.78	0.48
30:0:629:A:H2'	30:0:630:A:O4'	2.14	0.48
27:1:16:HIS:HD2	30:0:470:U:O2'	1.96	0.48
30:0:1667:A:H2'	30:0:1668:U:C6	2.48	0.48
30:0:553:G:O4'	30:0:1325:G:H5'	2.14	0.48
30:0:1766:U:O2	30:0:1778:A:H5'	2.14	0.48
30:0:2256:G:H2'	30:0:2257:G:C5'	2.44	0.48
30:0:2445:U:H2'	30:0:2446:G:H8	1.77	0.48
29:3:33:MET:HG2	30:0:1922:A:H2'	1.96	0.48
30:0:2783:A:H2'	30:0:2784:A:C8	2.49	0.48
30:0:2851:G:H2'	30:0:2852:A:H5'	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:661:G:C5	30:0:686:A:C2	3.02	0.48
31:9:34:A:H2'	31:9:35:C:O4'	2.14	0.48
30:0:316:A:N3	30:0:336:G:O2'	2.46	0.48
1:A:206:ARG:NH2	30:0:2630:G:O6	2.46	0.48
30:0:2878:U:H2'	30:0:2879:A:O4'	2.14	0.48
30:0:2812:A:C2	30:0:2814:A:N6	2.79	0.48
30:0:2001:G:O2'	30:0:2002:C:H5'	2.14	0.48
23:W:88:THR:HG22	23:W:110:GLN:HE21	1.79	0.48
30:0:920:C:H5"	30:0:921:G:O5'	2.13	0.48
20:T:2:LYS:HG2	30:0:447:A:OP1	2.14	0.48
30:0:1972:U:H2'	30:0:1973:A:C5'	2.44	0.48
30:0:1477:C:H5'	30:0:1868:G:C5'	2.44	0.48
2:B:211:THR:HG21	39:0:7486:HOH:O	2.14	0.48
31:9:3:A:H2	31:9:21:G:N3	2.12	0.47
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.28	0.47
30:0:2689:A:H2'	30:0:2690:U:H5'	1.96	0.47
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.95	0.47
30:0:158:A:H3'	39:0:7591:HOH:O	2.14	0.47
30:0:2105:C:H2'	30:0:2106:C:C6	2.49	0.47
20:T:111:ARG:HB3	20:T:119:ALA:HB2	1.96	0.47
30:0:1375:A:C2'	30:0:1376:G:H5'	2.43	0.47
31:9:55:U:H4'	31:9:56:A:C8	2.49	0.47
30:0:2506:A:O2'	30:0:2507:G:O5'	2.32	0.47
30:0:1878:G:O2'	30:0:1879:U:OP2	2.32	0.47
23:W:128:VAL:HG22	30:0:1098:A:OP1	2.14	0.47
30:0:2374:G:H2'	30:0:2375:A:C8	2.49	0.47
30:0:2411:C:H4'	39:0:4981:HOH:O	2.13	0.47
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.50	0.47
22:V:44:GLY:HA3	30:0:92:G:H4'	1.95	0.47
30:0:380:A:H2'	39:0:7258:HOH:O	2.14	0.47
30:0:287:C:H42	30:0:365:G:H1	1.62	0.47
30:0:827:A:H2'	30:0:828:G:O4'	2.15	0.47
30:0:67:A:H5"	30:0:69:A:C8	2.50	0.47
18:R:39:THR:HG23	18:R:107:GLU:O	2.14	0.47
30:0:161:A:H2'	30:0:162:C:C6	2.49	0.47
30:0:2321:A:H8	30:0:2322:U:O2'	1.96	0.47
30:0:542:A:H5'	30:0:542:A:C8	2.39	0.47
30:0:2909:G:H2'	30:0:2910:A:H8	1.80	0.47
30:0:1187:U:H2'	39:0:6925:HOH:O	2.13	0.47
31:9:78:G:H5'	39:9:9095:HOH:O	2.13	0.47
30:0:2587:OMU:H6	30:0:2587:OMU:O5'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:105:G:O2'	30:0:106:A:H5'	2.14	0.47
30:0:821:U:H2'	30:0:822:C:C6	2.47	0.47
12:L:6:ARG:NH1	30:0:1299:G:N7	2.62	0.47
30:0:2757:A:H2'	30:0:2758:G:O4'	2.14	0.47
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.96	0.47
30:0:451:C:O2'	30:0:452:G:H5'	2.14	0.47
30:0:308:U:C4	30:0:342:C:H1'	2.50	0.47
30:0:2002:C:H2'	30:0:2003:U:C5'	2.44	0.47
2:B:234:ARG:HG3	30:0:1735:C:OP2	2.15	0.47
30:0:2266:A:H2'	30:0:2267:G:H8	1.79	0.47
30:0:304:G:H1'	30:0:347:A:N6	2.30	0.47
30:0:88:G:H5'	30:0:88:G:H8	1.80	0.47
30:0:790:A:H2'	30:0:791:A:O4'	2.15	0.47
2:B:217:ARG:HG3	2:B:257:THR:HG23	1.97	0.47
6:F:77:VAL:HG21	6:F:83:LEU:HD13	1.96	0.47
30:0:1016:U:H1'	39:0:3672:HOH:O	2.13	0.47
30:0:1903:U:O2'	30:0:1904:A:N7	2.43	0.47
30:0:136:C:H2'	30:0:137:U:O4'	2.15	0.47
6:F:30:LYS:HE2	6:F:99:THR:HG21	1.96	0.47
2:B:27:ASN:H	2:B:27:ASN:HD22	1.63	0.47
30:0:1815:A:H4'	30:0:2751:C:O4'	2.15	0.47
4:D:159:PRO:O	4:D:163:VAL:HG23	2.15	0.47
31:9:95:C:O2'	31:9:96:C:H5'	2.15	0.47
30:0:1160:G:H2'	39:0:5654:HOH:O	2.15	0.47
25:Y:144:ARG:NH1	39:0:7478:HOH:O	2.47	0.47
30:0:137:U:H2'	30:0:139:C:C5	2.50	0.47
30:0:2816:A:H5"	30:0:2817:G:H5'	1.97	0.47
30:0:807:A:O2'	30:0:808:A:H5'	2.15	0.47
2:B:297:VAL:HG23	39:B:9029:HOH:O	2.13	0.47
31:9:3:A:N6	31:9:22:G:H1'	2.29	0.47
3:C:236:THR:HG22	3:C:239:ALA:H	1.80	0.47
30:0:1619:G:H2'	30:0:1620:C:O4'	2.15	0.47
30:0:24:G:N2	30:0:518:G:H1'	2.30	0.47
31:9:80:A:H2'	31:9:81:C:O4'	2.14	0.47
12:L:18:HIS:HD2	30:0:902:G:N7	2.12	0.47
30:0:272:A:H5'	30:0:273:G:OP2	2.15	0.47
30:0:731:U:H2'	30:0:732:C:C6	2.50	0.47
30:0:816:G:H5'	30:0:1598:A:H4'	1.97	0.46
30:0:1202:A:H2'	30:0:1203:G:H5'	1.97	0.46
27:1:25:LYS:HG3	28:2:49:GLU:H	1.80	0.46
3:C:79:ARG:O	3:C:87:ARG:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1804:A:H2'	30:0:1805:G:C8	2.50	0.46
12:L:14:GLY:O	30:0:1295:G:H5"	2.14	0.46
30:0:2563:U:O2'	30:0:2564:G:H3'	2.16	0.46
30:0:372:A:H2'	30:0:373:G:C8	2.51	0.46
30:0:2619:UR3:H5'	32:4:76:PPU:H103	1.98	0.46
30:0:2252:A:H2'	30:0:2253:G:O4'	2.15	0.46
30:0:1188:A:C6	30:0:1189:A:C6	3.03	0.46
3:C:46:TYR:CE1	30:0:450:C:H4'	2.50	0.46
30:0:2300:A:H4'	30:0:2301:A:O5'	2.16	0.46
30:0:1803:C:H2'	30:0:1804:A:C8	2.50	0.46
30:0:800:G:H2'	30:0:801:U:C6	2.50	0.46
30:0:1765:G:H1'	30:0:1780:G:N2	2.30	0.46
30:0:1515:A:H2'	30:0:1516:U:C6	2.50	0.46
30:0:2764:C:H2'	30:0:2765:C:H6	1.80	0.46
30:0:660:A:N6	30:0:746:A:O4'	2.49	0.46
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.44	0.46
30:0:708:A:H2'	30:0:709:G:O4'	2.14	0.46
30:0:2387:U:H2'	30:0:2388:C:C6	2.51	0.46
30:0:101:C:H2'	30:0:102:A:C8	2.51	0.46
30:0:1398:G:O2'	30:0:1399:A:H5'	2.15	0.46
30:0:542:A:H2'	30:0:543:G:O4'	2.16	0.46
30:0:1189:A:H1'	30:0:1209:C:H1'	1.97	0.46
30:0:2591:C:H2'	30:0:2592:G:O4'	2.16	0.46
14:N:159:TYR:HE1	31:9:50:G:H5"	1.80	0.46
30:0:319:A:H4'	30:0:338:C:C4	2.50	0.46
13:M:69:LYS:O	13:M:73:ARG:NH2	2.49	0.46
30:0:2133:U:H4'	30:0:2134:G:H5'	1.98	0.46
30:0:644:G:N3	30:0:644:G:H5'	2.31	0.46
30:0:2691:A:H5'	30:0:2693:U:H1'	1.97	0.46
30:0:1589:G:H22	30:0:1605:G:H1'	1.81	0.46
30:0:1166:A:H61	30:0:1180:U:H3	1.64	0.46
30:0:834:G:H4'	30:0:835:U:OP2	2.16	0.46
2:B:312:ARG:HD3	2:B:315:VAL:HG13	1.98	0.46
31:9:57:A:H2'	31:9:58:G:O4'	2.16	0.46
31:9:29:C:H2'	31:9:30:C:C5'	2.40	0.46
3:C:63:SER:OG	30:0:2101:A:H2'	2.16	0.46
30:0:876:A:N3	30:0:876:A:H2'	2.31	0.46
30:0:1330:A:H2	39:0:4703:HOH:O	1.99	0.46
30:0:1158:G:O2'	30:0:1159:G:H5'	2.15	0.46
30:0:2619:UR3:H3U3	30:0:2620:U:C2	2.50	0.46
23:W:88:THR:CG2	23:W:110:GLN:HE21	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1555:G:H4'	30:0:1630:A:C2	2.51	0.46
30:0:1495:C:H1'	30:0:1573:A:H1'	1.98	0.46
30:0:1056:U:H2'	30:0:1057:A:O4'	2.15	0.46
30:0:2481:G:H5"	39:0:4569:HOH:O	2.15	0.46
25:Y:208:LYS:O	30:0:1313:A:H5'	2.16	0.46
30:0:2421:G:H3'	30:0:2422:U:H5"	1.97	0.46
30:0:542:A:H1'	39:0:4696:HOH:O	2.15	0.46
30:0:560:U:H2'	30:0:561:G:H8	1.80	0.46
30:0:960:G:C3'	30:0:960:G:N3	2.79	0.46
30:0:671:A:O2'	30:0:672:G:H2'	2.16	0.46
31:9:35:C:H5"	39:9:9078:HOH:O	2.15	0.46
3:C:87:ARG:NH2	30:0:894:A:N1	2.63	0.46
30:0:699:C:H2'	30:0:744:G:O4'	2.16	0.46
30:0:1400:C:O2'	30:0:1401:G:H5'	2.16	0.46
25:Y:174:VAL:HG23	25:Y:177:LYS:HD2	1.98	0.46
9:I:130:LEU:CD2	30:0:1167:G:H4'	2.46	0.46
30:0:1634:G:H3'	39:0:3912:HOH:O	2.14	0.46
30:0:2112:A:H2'	30:0:2113:G:C8	2.51	0.46
30:0:1929:G:H1'	39:0:5188:HOH:O	2.15	0.46
30:0:226:A:H1'	30:0:393:G:C5	2.51	0.46
30:0:541:C:O2'	30:0:542:A:H5"	2.17	0.45
30:0:2636:C:H3'	30:0:2637:A:C5'	2.46	0.45
30:0:1120:U:H5"	30:0:1120:U:C6	2.52	0.45
2:B:5:ARG:NH2	30:0:2548:C:OP2	2.49	0.45
30:0:343:C:O2'	30:0:344:C:H5'	2.16	0.45
30:0:396:U:O2'	30:0:397:A:P	2.74	0.45
31:9:114:G:H2'	31:9:115:C:C6	2.51	0.45
17:Q:26:PRO:O	17:Q:30:VAL:HG22	2.17	0.45
30:0:1380:U:H5'	39:0:9222:HOH:O	2.15	0.45
29:3:58:GLY:O	30:0:2460:A:H4'	2.16	0.45
30:0:922:A:N7	30:0:2281:C:H5'	2.31	0.45
30:0:2659:U:H5"	39:0:4146:HOH:O	2.16	0.45
30:0:1183:C:N3	30:0:1184:C:C5	2.85	0.45
30:0:2825:C:H4'	30:0:2826:G:O4'	2.17	0.45
30:0:1342:C:H2'	30:0:1343:C:H5'	1.98	0.45
30:0:1625:U:H5"	39:0:6044:HOH:O	2.16	0.45
22:V:55:ARG:O	22:V:59:ILE:HG12	2.15	0.45
1:A:121:ALA:O	1:A:124:VAL:HG22	2.15	0.45
30:0:1183:C:H41	30:0:1192:A:P	2.40	0.45
30:0:2756:U:N3	30:0:2896:A:H2	2.13	0.45
2:B:234:ARG:NH2	30:0:2039:A:OP2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.52	0.45
30:0:204:A:C2'	30:0:205:U:H5'	2.46	0.45
30:0:503:G:H2'	30:0:504:G:H8	1.81	0.45
30:0:2668:G:H2'	30:0:2669:U:C6	2.51	0.45
30:0:932:U:H2'	30:0:933:C:C6	2.51	0.45
13:M:70:GLY:HA3	30:0:2263:G:H4'	1.97	0.45
16:P:88:GLN:NE2	30:0:1800:G:H1'	2.32	0.45
30:0:29:C:O2'	30:0:30:U:H5'	2.17	0.45
30:0:1244:U:H4'	30:0:1246:A:O4'	2.17	0.45
1:A:171:LYS:HB2	30:0:820:G:C6	2.51	0.45
13:M:99:ARG:HE	13:M:170:ASN:ND2	2.15	0.45
30:0:1583:U:H2'	30:0:1584:C:O4'	2.17	0.45
15:O:97:SER:H	15:O:100:GLN:NE2	2.14	0.45
2:B:244:PRO:HB3	30:0:1234:U:N3	2.31	0.45
30:0:47:G:N3	30:0:114:A:C2	2.85	0.45
31:9:52:A:H2'	31:9:53:G:O4'	2.17	0.45
30:0:1278:A:O2'	30:0:1279:U:H3'	2.17	0.45
30:0:255:A:H2'	30:0:256:C:C6	2.52	0.45
30:0:2281:C:C2'	30:0:2282:U:H5'	2.46	0.45
3:C:107:ARG:O	3:C:111:VAL:HG23	2.16	0.45
6:F:48:VAL:HG23	6:F:74:PHE:HB3	1.98	0.45
30:0:154:C:H2'	30:0:155:C:C6	2.52	0.45
30:0:1925:G:O2'	30:0:1926:G:H5'	2.17	0.45
30:0:39:G:N2	30:0:444:C:C2	2.85	0.45
30:0:2584:G:H4'	39:0:7151:HOH:O	2.16	0.45
30:0:2697:A:H2'	30:0:2698:G:O4'	2.16	0.45
30:0:2505:G:H2'	30:0:2506:A:H5'	1.98	0.45
30:0:297:U:H2'	30:0:298:C:H6	1.81	0.45
16:P:59:ARG:HH22	16:P:66:GLN:NE2	2.14	0.45
30:0:2469:A:H2'	39:0:7506:HOH:O	2.16	0.45
29:3:17:HIS:CG	30:0:2409:C:H4'	2.52	0.45
30:0:129:A:O2'	30:0:131:A:OP1	2.34	0.45
30:0:1362:U:H5'	39:0:3278:HOH:O	2.16	0.45
8:H:61:ARG:HG3	8:H:61:ARG:HH11	1.82	0.45
31:9:55:U:H4'	31:9:56:A:H8	1.81	0.45
30:0:317:A:H4'	39:0:3787:HOH:O	2.16	0.45
30:0:2348:C:H2'	30:0:2349:G:C8	2.52	0.45
30:0:629:A:C2	30:0:2074:A:C2	3.05	0.45
30:0:699:C:C2	30:0:744:G:C2	3.05	0.45
30:0:2437:A:H2'	30:0:2438:G:C8	2.52	0.45
23:W:6:GLN:HB2	23:W:26:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1205:U:H2'	30:0:1206:U:H5"	1.97	0.45
30:0:2256:G:H2'	30:0:2257:G:H5'	1.98	0.45
30:0:1743:G:H1'	39:0:4916:HOH:O	2.16	0.45
14:N:40:ASN:HD21	31:9:28:U:H5"	1.81	0.44
30:0:2748:G:H5'	39:0:7572:HOH:O	2.16	0.44
30:0:2781:U:H2'	30:0:2782:G:C5'	2.47	0.44
14:N:26:LEU:HD13	30:0:2415:A:N3	2.32	0.44
30:0:2598:U:O2	30:0:2600:A:H8	1.99	0.44
26:Z:47:ARG:HH21	30:0:1771:U:H1'	1.82	0.44
30:0:634:G:O2'	30:0:1358:A:OP1	2.31	0.44
30:0:1849:G:H1'	30:0:2011:A:N1	2.33	0.44
30:0:1556:G:O2'	30:0:1557:G:H5'	2.16	0.44
30:0:1166:A:N3	30:0:1166:A:H2'	2.33	0.44
30:0:154:C:H2'	30:0:155:C:H6	1.81	0.44
28:2:10:ARG:NH2	30:0:121:U:OP2	2.35	0.44
30:0:1566:C:H2'	30:0:1567:G:H8	1.83	0.44
30:0:234:A:H2'	30:0:235:C:O4'	2.17	0.44
30:0:1610:G:H2'	30:0:1611:G:O4'	2.17	0.44
19:S:50:GLU:HB3	19:S:67:ARG:HH21	1.82	0.44
3:C:35:VAL:HG13	3:C:221:GLU:HG2	1.99	0.44
30:0:1641:A:C2'	30:0:1642:A:H5'	2.45	0.44
30:0:2089:A:O2'	30:0:2090:G:H5'	2.18	0.44
30:0:1682:A:O2'	30:0:1683:G:H5"	2.17	0.44
8:H:22:TYR:CZ	30:0:1007:A:H2'	2.53	0.44
30:0:566:A:H2'	30:0:567:U:O4'	2.16	0.44
30:0:332:G:O2'	30:0:333:G:H5'	2.17	0.44
30:0:2507:G:H2'	30:0:2510:C:N4	2.33	0.44
30:0:2420:G:H4'	39:0:4115:HOH:O	2.18	0.44
30:0:2073:G:C6	30:0:2489:G:H4'	2.53	0.44
30:0:1343:C:H2'	30:0:1344:G:O5'	2.17	0.44
30:0:1634:G:H2'	30:0:1635:U:C6	2.52	0.44
30:0:962:C:H5"	39:0:4940:HOH:O	2.18	0.44
2:B:16:ARG:NH1	39:B:9041:HOH:O	2.49	0.44
30:0:1636:G:O2'	30:0:1637:A:H5'	2.17	0.44
30:0:1391:G:H2'	30:0:1392:A:H5'	2.00	0.44
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.87	0.44
30:0:228:C:H2'	30:0:229:G:H5'	2.00	0.44
9:I:93:ALA:HB3	9:I:132:VAL:HG22	2.00	0.44
29:3:64:LYS:HA	29:3:84:ARG:HA	1.99	0.44
19:S:57:THR:HG22	19:S:58:MET:N	2.32	0.44
30:0:541:C:C2'	30:0:542:A:C5'	2.89	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:232:TRP:CZ3	30:0:2614:C:H5"	2.52	0.44
30:0:816:G:C6	30:0:817:G:N1	2.86	0.44
30:0:65:C:O2'	30:0:66:G:H5'	2.17	0.44
30:0:1878:G:H5"	39:0:9802:HOH:O	2.18	0.44
30:0:447:A:O2'	30:0:448:G:H5'	2.17	0.44
28:2:28:LYS:O	30:0:87:C:H2'	2.18	0.44
30:0:2724:U:H2'	30:0:2725:G:O4'	2.17	0.44
30:0:2768:A:H5"	39:0:4447:HOH:O	2.16	0.44
30:0:120:A:H2'	30:0:120:A:N3	2.33	0.44
30:0:1202:A:O2'	30:0:1203:G:H5'	2.18	0.44
30:0:2252:A:C5	30:0:2253:G:H1'	2.52	0.44
13:M:58:GLN:HE22	30:0:251:C:H1'	1.83	0.44
13:M:82:ARG:O	13:M:86:GLN:HG3	2.18	0.44
30:0:1202:A:H2'	30:0:1203:G:C5'	2.47	0.44
11:K:30:LYS:HB3	11:K:56:SER:HB3	2.00	0.44
30:0:2894:C:O2'	30:0:2895:C:H5'	2.18	0.44
30:0:213:G:N2	30:0:225:G:H2'	2.33	0.44
30:0:1314:U:H2'	39:0:5894:HOH:O	2.18	0.44
30:0:919:U:H5'	30:0:2465:A:O2'	2.18	0.44
30:0:2533:C:H6	30:0:2533:C:C5'	2.22	0.44
30:0:1268:C:H2'	30:0:1269:G:C8	2.52	0.44
32:4:76:PPU:C9	32:4:76:PPU:N7	2.79	0.44
14:N:11:ARG:NH1	31:9:8:G:O6	2.51	0.44
30:0:2703:A:O2'	30:0:2704:C:H5'	2.17	0.44
30:0:101:C:H2'	30:0:102:A:H8	1.83	0.44
30:0:1552:G:H2'	30:0:1553:C:C6	2.52	0.44
30:0:2564:G:OP2	30:0:2565:C:H5"	2.18	0.43
30:0:1130:U:H4'	39:0:6150:HOH:O	2.18	0.43
30:0:1307:A:H2'	30:0:1308:A:C8	2.53	0.43
30:0:1706:G:C6	30:0:1707:G:C6	3.06	0.43
30:0:293:A:O2'	30:0:294:C:H5'	2.18	0.43
30:0:912:A:C4	30:0:1294:A:C2	3.06	0.43
30:0:2419:U:H5"	30:0:2420:G:C5'	2.44	0.43
30:0:1730:G:C5'	30:0:1731:C:C6	3.00	0.43
30:0:1819:G:H2'	30:0:1820:G:H5'	2.01	0.43
30:0:1883:U:H5'	30:0:2012:U:OP2	2.17	0.43
10:J:80:LYS:HE3	10:J:101:VAL:O	2.18	0.43
18:R:69:LYS:HB2	18:R:72:VAL:HG23	1.99	0.43
7:G:63:ARG:NH1	30:0:1151:G:OP1	2.51	0.43
30:0:168:C:O5'	30:0:168:C:H6	2.01	0.43
2:B:238:ASN:HD22	2:B:240:GLY:N	2.13	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2032:U:H5'	39:0:4537:HOH:O	2.18	0.43
31:9:39:U:H3'	31:9:40:C:H5"	2.00	0.43
2:B:304:PRO:HD2	2:B:307:ARG:HE	1.83	0.43
30:0:2281:C:H2'	30:0:2282:U:H5'	2.00	0.43
30:0:68:U:H4'	39:0:6784:HOH:O	2.19	0.43
30:0:2514:U:H2'	30:0:2515:C:H6	1.83	0.43
30:0:2313:C:H4'	39:0:6597:HOH:O	2.19	0.43
4:D:141:VAL:HG21	31:9:57:A:C8	2.54	0.43
30:0:132:A:H2'	30:0:133:U:C6	2.53	0.43
30:0:1568:G:O2'	30:0:1569:U:H5'	2.18	0.43
30:0:1878:G:O2'	30:0:1879:U:P	2.77	0.43
30:0:2764:C:H2'	30:0:2765:C:C6	2.54	0.43
27:1:1:THR:O	30:0:1836:A:H1'	2.18	0.43
30:0:1790:C:H2'	30:0:1791:U:H6	1.82	0.43
14:N:160:SER:HB3	31:9:51:A:H5'	1.99	0.43
9:I:87:PRO:HD2	30:0:1180:U:H1'	2.01	0.43
30:0:2301:A:H5"	30:0:2302:A:H5'	2.00	0.43
30:0:1743:G:H2'	30:0:1744:G:O4'	2.19	0.43
30:0:1632:A:H2'	30:0:1633:C:H5'	2.00	0.43
1:A:1:GLY:HA2	30:0:2114:C:OP1	2.18	0.43
30:0:1659:A:H2'	30:0:1660:G:O4'	2.18	0.43
10:J:52:GLN:HE22	30:0:1119:G:H8	1.65	0.43
30:0:612:U:H2'	30:0:613:C:C6	2.54	0.43
39:I:6825:HOH:O	30:0:1167:G:H1'	2.17	0.43
30:0:2325:U:H1'	39:0:4167:HOH:O	2.19	0.43
30:0:645:U:O2	30:0:761:A:H2	2.02	0.43
30:0:1175:G:H1'	30:0:1193:A:H2'	2.00	0.43
30:0:483:C:C4	30:0:484:A:C6	3.07	0.43
31:9:53:G:O2'	31:9:54:A:H5'	2.19	0.43
28:2:41:HIS:HE1	30:0:1439:C:H5"	1.84	0.43
30:0:1992:U:H2'	30:0:1994:A:OP2	2.18	0.43
26:Z:76:THR:HG21	30:0:1652:C:H4'	2.00	0.43
30:0:2065:C:O2'	30:0:2066:C:H5'	2.19	0.43
30:0:1406:A:H4'	30:0:1407:A:H5"	2.01	0.43
30:0:1181:A:C2'	30:0:1182:C:H5'	2.48	0.43
30:0:2644:C:O2'	30:0:2645:U:C5'	2.66	0.43
30:0:2064:U:H5'	30:0:2652:U:O3'	2.19	0.43
31:9:39:U:H1'	31:9:44:A:H61	1.83	0.43
30:0:2689:A:C2'	30:0:2690:U:H5'	2.49	0.43
26:Z:40:ALA:HA	30:0:1773:G:C8	2.54	0.43
19:S:33:SER:O	19:S:37:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2832:C:H5	39:0:7245:HOH:O	2.01	0.43
30:0:2502:C:H2'	30:0:2503:A:C5'	2.47	0.43
30:0:1375:A:H2'	30:0:1376:G:H5'	2.00	0.43
30:0:2253:G:H2'	30:0:2254:G:H8	1.83	0.43
2:B:248:ARG:NH1	39:B:9040:HOH:O	2.51	0.43
30:0:2291:A:N9	30:0:2309:C:H5'	2.34	0.42
23:W:44:MET:HE2	30:0:944:G:H21	1.84	0.42
30:0:1098:A:H2'	30:0:1099:G:O4'	2.19	0.42
3:C:1:MET:HG2	3:C:2:GLN:H	1.84	0.42
11:K:8:VAL:HG13	11:K:80:ILE:HG22	2.01	0.42
18:R:40:ALA:O	18:R:44:VAL:HG23	2.18	0.42
30:0:2026:C:O2'	30:0:2027:U:H5'	2.19	0.42
30:0:1700:C:H5"	30:0:1701:A:OP2	2.19	0.42
32:4:75:C:H2'	32:4:76:PPU:N9	2.34	0.42
30:0:1057:A:H1'	30:0:2492:U:O2'	2.18	0.42
30:0:2429:A:H4'	39:0:7769:HOH:O	2.19	0.42
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.84	0.42
30:0:1503:U:H2'	30:0:1504:A:O4'	2.18	0.42
30:0:2769:C:H2'	30:0:2770:G:C5'	2.49	0.42
30:0:1730:G:H5'	30:0:1731:C:C5	2.54	0.42
30:0:248:A:H5'	30:0:249:G:OP2	2.20	0.42
30:0:1015:C:O5'	30:0:1015:C:H6	2.02	0.42
30:0:85:C:H5"	30:0:86:A:OP2	2.18	0.42
2:B:254:GLN:HG2	2:B:255:GLY:N	2.34	0.42
5:E:112:ALA:HA	5:E:113:PRO:HD3	1.91	0.42
30:0:2874:G:H3'	39:0:9585:HOH:O	2.20	0.42
30:0:1730:G:H5"	30:0:1731:C:C6	2.53	0.42
30:0:2758:G:H2'	30:0:2759:C:H6	1.84	0.42
30:0:2436:U:H2'	30:0:2437:A:C8	2.55	0.42
3:C:206:ASN:HB2	30:0:329:A:OP2	2.19	0.42
24:X:30:MET:HG2	30:0:1384:C:H5'	2.02	0.42
30:0:622:G:O2'	30:0:623:U:H5'	2.19	0.42
30:0:2385:G:H2'	30:0:2386:U:C6	2.54	0.42
30:0:10:U:C6	30:0:10:U:H3'	2.54	0.42
31:9:47:A:C2	31:9:48:C:C2	3.08	0.42
30:0:2416:G:H2'	30:0:2417:C:C6	2.55	0.42
1:A:190:ARG:NH2	39:A:9008:HOH:O	2.52	0.42
17:Q:45:PRO:O	30:0:2365:G:H4'	2.19	0.42
30:0:289:G:O2'	30:0:290:C:H5'	2.20	0.42
30:0:1624:A:H5'	30:0:1626:A:O4'	2.18	0.42
30:0:1209:C:H2'	30:0:1210:G:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2896:A:N3	30:0:2896:A:H2'	2.35	0.42
30:0:363:C:H2'	30:0:364:U:C6	2.55	0.42
30:0:2039:A:H2'	30:0:2040:C:C6	2.54	0.42
28:2:42:TRP:CZ2	30:0:1438:G:H1'	2.53	0.42
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.84	0.42
30:0:204:A:H2'	30:0:205:U:H5'	2.01	0.42
30:0:1762:C:H2'	30:0:1763:C:H6	1.84	0.42
4:D:172:VAL:HG12	4:D:173:GLU:H	1.85	0.42
30:0:1422:U:H2'	30:0:1423:C:C6	2.55	0.42
30:0:2667:G:H1'	30:0:2914:A:N3	2.34	0.42
31:9:61:C:H2'	31:9:62:A:H8	1.85	0.42
30:0:1829:A:C8	30:0:1885:A:C8	3.08	0.42
25:Y:204:ARG:NH2	30:0:553:G:P	2.88	0.42
30:0:1015:C:H2'	30:0:1016:U:H6	1.84	0.42
30:0:1557:G:O2'	30:0:1558:C:H5'	2.20	0.42
9:I:112:LEU:HD11	30:0:1162:G:H1'	2.02	0.42
30:0:2533:C:O2'	30:0:2534:C:H5'	2.20	0.42
30:0:1588:G:C6	30:0:1589:G:N1	2.88	0.42
30:0:812:A:H1'	39:0:3977:HOH:O	2.19	0.42
16:P:120:ARG:HD2	30:0:1594:C:OP2	2.19	0.42
30:0:1769:C:O2'	30:0:1770:U:H5'	2.20	0.42
30:0:333:G:O2'	30:0:334:G:H5'	2.19	0.42
30:0:1497:G:H2'	30:0:1498:G:H8	1.85	0.42
6:F:59:ILE:HD13	30:0:263:U:C2	2.54	0.42
30:0:758:A:H2'	30:0:759:C:O4'	2.19	0.42
30:0:2321:A:H2	30:0:2378:U:N3	2.02	0.42
8:H:59:GLN:HE21	8:H:129:ARG:NE	2.09	0.42
30:0:1185:U:H5'	39:0:7498:HOH:O	2.20	0.42
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.53	0.42
30:0:2871:G:H2'	30:0:2872:U:C6	2.55	0.42
30:0:1883:U:H5"	30:0:2013:G:OP2	2.20	0.42
13:M:71:SER:HB2	13:M:92:THR:HG22	2.02	0.42
30:0:95:A:H5"	30:0:97:G:O4'	2.20	0.42
30:0:1890:U:H4'	30:0:2010:A:C6	2.55	0.42
17:Q:95:GLU:HA	30:0:949:U:H4'	2.02	0.42
2:B:288:GLY:HA2	30:0:2898:G:H4'	2.02	0.42
18:R:9:ASP:O	18:R:13:THR:HB	2.20	0.42
30:0:363:C:H2'	30:0:364:U:H6	1.84	0.42
30:0:2430:A:O2'	30:0:2431:C:H5'	2.20	0.42
30:0:1319:G:H1'	39:0:4712:HOH:O	2.20	0.42
30:0:1321:A:H2'	30:0:1322:G:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:C:8655:HOH:O	30:0:2100:A:H5'	2.19	0.42
27:1:10:LYS:HG3	39:0:4369:HOH:O	2.19	0.42
30:0:1181:A:H2'	30:0:1182:C:C5'	2.50	0.41
30:0:1205:U:C2'	30:0:1206:U:H5"	2.50	0.41
30:0:2636:C:C3'	30:0:2637:A:C5'	2.98	0.41
30:0:960:G:H8	39:0:5994:HOH:O	2.02	0.41
1:A:190:ARG:HH11	30:0:1845:A:P	2.43	0.41
30:0:1165:G:C4'	30:0:1174:A:O2'	2.68	0.41
30:0:191:A:H2'	30:0:237:G:O6	2.20	0.41
30:0:2724:U:H6	30:0:2724:U:O5'	2.03	0.41
30:0:2135:A:O2'	30:0:2136:G:H5'	2.19	0.41
30:0:2135:A:O4'	30:0:2243:C:N4	2.53	0.41
1:A:36:ASP:O	1:A:38:ILE:N	2.48	0.41
30:0:1252:A:H2'	30:0:1253:C:O4'	2.19	0.41
30:0:1664:A:OP1	30:0:1664:A:H8	2.02	0.41
30:0:2869:G:H2'	30:0:2870:C:C6	2.55	0.41
30:0:1592:G:O2'	30:0:1593:C:O4'	2.36	0.41
30:0:920:C:H2'	30:0:2109:U:C2	2.55	0.41
30:0:2011:A:H4'	30:0:2012:U:O5'	2.20	0.41
30:0:228:C:C2'	30:0:229:G:H5'	2.50	0.41
30:0:1855:G:H4'	30:0:1856:C:O5'	2.19	0.41
18:R:33:ARG:NH1	39:R:8934:HOH:O	2.52	0.41
15:O:29:VAL:HG11	15:O:98:LEU:HD21	2.02	0.41
30:0:619:U:H3'	39:0:3295:HOH:O	2.19	0.41
30:0:2479:A:H3'	39:0:9847:HOH:O	2.18	0.41
30:0:538:C:H5"	30:0:539:G:C8	2.55	0.41
30:0:939:A:C2	30:0:1027:G:N3	2.88	0.41
10:J:82:THR:CG2	30:0:1242:A:H5'	2.36	0.41
30:0:2580:G:N3	30:0:2600:A:H2	2.17	0.41
30:0:1041:U:H2'	30:0:1042:U:H5'	2.01	0.41
27:1:16:HIS:HE1	30:0:775:G:OP1	2.03	0.41
30:0:1311:G:C2	30:0:1312:G:C8	3.08	0.41
19:S:17:ASP:HB3	19:S:23:LYS:HB2	2.02	0.41
30:0:824:G:H2'	30:0:826:U:OP1	2.20	0.41
30:0:2768:A:H2'	30:0:2769:C:O4'	2.20	0.41
30:0:2781:U:O2'	30:0:2782:G:H5'	2.20	0.41
30:0:1377:C:H6	30:0:1377:C:C5'	2.32	0.41
30:0:613:C:H2'	30:0:614:U:C6	2.54	0.41
30:0:314:G:N1	30:0:317:A:OP2	2.52	0.41
14:N:5:ARG:NH1	30:0:1010:C:OP1	2.53	0.41
30:0:2064:U:H4'	30:0:2653:A:OP1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:ARG:HD3	30:0:1734:C:OP1	2.20	0.41
30:0:1762:C:O2'	30:0:1763:C:H5'	2.20	0.41
30:0:2793:A:H2'	30:0:2794:G:H5'	2.03	0.41
30:0:1039:G:H2'	30:0:1040:A:O4'	2.21	0.41
4:D:50:VAL:HG13	31:9:41:C:O4'	2.20	0.41
30:0:1615:A:H4'	39:0:5906:HOH:O	2.20	0.41
25:Y:216:ARG:HD2	39:Y:8867:HOH:O	2.20	0.41
30:0:284:C:H4'	30:0:285:A:H8	1.85	0.41
21:U:47:ARG:HG3	39:U:4381:HOH:O	2.19	0.41
13:M:76:ARG:HH21	30:0:2122:C:H1'	1.86	0.41
13:M:24:GLN:NE2	13:M:27:ARG:HH11	2.16	0.41
2:B:238:ASN:HD21	30:0:2609:G:N2	2.18	0.41
30:0:737:A:H2'	30:0:738:G:O4'	2.19	0.41
26:Z:47:ARG:NH2	30:0:1771:U:H1'	2.36	0.41
25:Y:148:GLY:HA3	30:0:622:G:P	2.60	0.41
15:O:25:VAL:O	15:O:29:VAL:HG23	2.20	0.41
1:A:6:GLY:O	30:0:1861:C:H4'	2.20	0.41
30:0:2610:U:H4'	39:0:9485:HOH:O	2.20	0.41
4:D:52:THR:HG21	30:0:2347:C:H5'	2.03	0.41
30:0:963:C:O2	30:0:1005:A:N1	2.52	0.41
30:0:512:G:O3'	30:0:513:A:H8	2.04	0.41
30:0:1616:A:H5"	30:0:1617:C:OP1	2.21	0.41
30:0:1350:U:H4'	39:0:5154:HOH:O	2.21	0.41
30:0:1754:A:H2'	30:0:1755:A:O4'	2.20	0.41
30:0:1942:A:H5'	39:0:7377:HOH:O	2.21	0.41
10:J:105:LEU:HD23	39:J:9025:HOH:O	2.20	0.41
30:0:1805:G:O2'	30:0:1806:G:H5'	2.19	0.41
2:B:69:VAL:HA	2:B:70:PRO:HD3	1.92	0.41
30:0:111:C:H2'	30:0:112:G:O4'	2.20	0.41
30:0:2731:G:H2'	30:0:2732:U:O4'	2.20	0.41
18:R:61:GLN:NE2	39:R:8942:HOH:O	2.54	0.41
18:R:68:HIS:O	30:0:2842:G:H5'	2.20	0.41
8:H:32:ALA:HB3	8:H:69:ARG:HH12	1.86	0.41
30:0:705:C:H2'	30:0:705:C:O2	2.19	0.41
30:0:1566:C:H2'	30:0:1567:G:C8	2.56	0.41
30:0:1421:C:O2'	30:0:1422:U:H5'	2.20	0.41
30:0:2842:G:H2'	30:0:2843:A:H5'	2.02	0.41
9:I:110:ASP:O	30:0:1163:G:H5'	2.21	0.41
30:0:682:A:H2'	30:0:683:G:O4'	2.20	0.41
12:L:56:LYS:HE3	30:0:2443:C:H1'	2.02	0.41
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1279:U:O2	30:0:1279:U:C2'	2.67	0.41
30:0:2651:C:H2'	30:0:2652:U:O4'	2.20	0.41
30:0:1819:G:H2'	30:0:1820:G:C4'	2.50	0.41
30:0:921:G:H4'	30:0:924:G:N1	2.36	0.41
23:W:128:VAL:O	23:W:138:LEU:HD11	2.21	0.41
30:0:791:A:H2'	30:0:792:G:O4'	2.21	0.41
30:0:2061:C:C2'	30:0:2062:A:H5'	2.51	0.41
2:B:97:LEU:HD22	2:B:127:GLN:HE21	1.85	0.41
23:W:13:MET:SD	23:W:18:GLN:HG3	2.60	0.41
25:Y:187:VAL:HG23	25:Y:192:ASP:HB2	2.01	0.41
30:0:1160:G:O2'	30:0:1190:G:H1'	2.21	0.41
30:0:1181:A:N1	30:0:1192:A:O2'	2.51	0.41
30:0:664:U:O4	30:0:681:G:H5"	2.21	0.41
14:N:141:ARG:HH21	31:9:48:C:H4'	1.86	0.41
12:L:6:ARG:NH2	39:L:8852:HOH:O	2.54	0.41
30:0:2791:U:C1'	30:0:2792:A:H5"	2.49	0.41
20:T:54:ASP:OD2	30:0:316:A:H5'	2.19	0.41
30:0:1631:A:H2'	30:0:1632:A:C8	2.56	0.41
30:0:1200:A:H3'	39:0:5773:HOH:O	2.20	0.41
1:A:164:ARG:NH2	30:0:1877:G:OP1	2.53	0.41
30:0:2639:G:O2'	30:0:2640:U:H5'	2.21	0.41
30:0:1074:G:H4'	30:0:1260:G:C6	2.54	0.41
30:0:1076:G:H1'	39:0:4473:HOH:O	2.20	0.41
30:0:809:G:H2'	30:0:810:G:H8	1.86	0.41
30:0:369:G:O2'	30:0:370:G:H5'	2.21	0.41
30:0:2866:U:H4'	30:0:2867:G:H5'	2.03	0.41
30:0:810:G:H2'	30:0:811:C:C6	2.55	0.41
30:0:2474:A:N7	30:0:2621:PSU:H4'	2.35	0.41
30:0:2766:A:H5'	39:0:9570:HOH:O	2.20	0.41
30:0:280:C:H2'	30:0:281:U:O4'	2.21	0.41
30:0:2825:C:H4'	30:0:2826:G:O5'	2.21	0.41
30:0:2600:A:H2'	30:0:2601:A:O4'	2.21	0.41
30:0:169:A:HO2'	30:0:170:U:H6	1.67	0.41
30:0:1626:A:H2'	30:0:1627:G:O4'	2.21	0.41
30:0:2478:U:O2'	30:0:2479:A:H5'	2.20	0.41
30:0:764:C:H2'	30:0:765:G:O4'	2.21	0.41
30:0:2836:G:H1'	39:0:6867:HOH:O	2.20	0.41
30:0:1714:C:O2'	30:0:1715:C:H5'	2.21	0.41
8:H:91:ARG:O	30:0:1003:U:H4'	2.20	0.41
30:0:394:G:H1'	30:0:417:G:H22	1.85	0.41
31:9:56:A:C3'	31:9:57:A:H5"	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2072:G:H3'	30:0:2073:G:H5"	2.03	0.40
28:2:41:HIS:CE1	30:0:1439:C:H5"	2.56	0.40
30:0:797:A:N6	30:0:816:G:H1'	2.35	0.40
30:0:1359:U:C5	30:0:2101:A:C8	3.09	0.40
16:P:81:LYS:O	30:0:1761:U:H5'	2.21	0.40
31:9:26:C:H4'	39:9:9052:HOH:O	2.21	0.40
31:9:42:C:H5'	31:9:43:G:OP2	2.21	0.40
30:0:1333:U:H2'	30:0:1334:C:C6	2.57	0.40
8:H:174:LEU:HD21	30:0:1220:U:H4'	2.02	0.40
23:W:130:HIS:NE2	31:9:88:G:OP1	2.52	0.40
19:S:73:ASP:O	19:S:77:VAL:HG23	2.22	0.40
32:4:76:PPU:HM3	32:4:76:PPU:HE1	1.81	0.40
13:M:92:THR:HB	30:0:401:C:O2'	2.22	0.40
19:S:11:THR:HG22	30:0:1444:G:H5"	2.02	0.40
3:C:162:VAL:HG22	3:C:232:LEU:HD21	2.03	0.40
30:0:1603:A:H5'	30:0:1605:G:C4'	2.51	0.40
30:0:2415:A:C2'	30:0:2416:G:H5'	2.51	0.40
30:0:1201:C:H5"	39:0:6256:HOH:O	2.21	0.40
30:0:1393:A:N1	30:0:1725:C:O2'	2.49	0.40
30:0:1006:A:H5"	39:0:3536:HOH:O	2.22	0.40
30:0:1921:A:O2'	30:0:1922:A:H5'	2.21	0.40
2:B:27:ASN:HD21	30:0:2807:U:P	2.44	0.40
30:0:876:A:N3	30:0:876:A:C2'	2.85	0.40
30:0:2438:G:H2'	30:0:2439:C:O4'	2.22	0.40
10:J:80:LYS:NZ	30:0:2815:G:N7	2.70	0.40
30:0:1405:U:H4'	30:0:1406:A:H5"	2.03	0.40
30:0:1416:G:C2'	30:0:1417:G:H5'	2.51	0.40
13:M:34:GLU:HB3	13:M:38:GLU:HG3	2.04	0.40
26:Z:49:ARG:O	26:Z:53:ILE:HD12	2.21	0.40
13:M:75:ARG:HG3	39:M:8868:HOH:O	2.21	0.40
30:0:812:A:H2'	30:0:813:C:H6	1.79	0.40
30:0:1735:C:H2'	30:0:1736:A:C8	2.55	0.40
30:0:117:A:H2'	30:0:118:G:O4'	2.22	0.40
30:0:2084:C:H2'	30:0:2085:A:C8	2.56	0.40
5:E:100:ASP:HB2	39:E:2789:HOH:O	2.20	0.40
30:0:2906:A:H5'	30:0:2907:C:O4'	2.21	0.40
30:0:2299:G:H4'	39:0:6506:HOH:O	2.22	0.40
30:0:1052:G:H2'	30:0:1052:G:N3	2.37	0.40
13:M:171:ARG:NH2	30:0:189:A:OP1	2.55	0.40
30:0:544:G:C3'	30:0:545:G:H5"	2.51	0.40
17:Q:21:ARG:HH12	30:0:2353:A:H1'	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1706:G:C6	30:0:1707:G:N1	2.89	0.40
30:0:1423:C:O2'	30:0:1424:A:H5'	2.21	0.40
30:0:123:U:O2'	30:0:124:C:H5'	2.22	0.40
4:D:67:ASP:HA	4:D:68:PRO:HD3	1.99	0.40
30:0:1980:U:O2	30:0:2008:U:H4'	2.21	0.40
30:0:1842:A:C4	30:0:1979:G:C6	3.10	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%)	221 (94%)	11 (5%)	3 (1%)	15 40
2	B	335/338 (99%)	310 (92%)	23 (7%)	2 (1%)	30 62
3	C	244/246 (99%)	228 (93%)	15 (6%)	1 (0%)	39 72
4	D	134/177 (76%)	114 (85%)	17 (13%)	3 (2%)	8 24
5	E	170/178 (96%)	162 (95%)	8 (5%)	0	100 100
6	F	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	21 52
7	G	25/348 (7%)	25 (100%)	0	0	100 100
8	H	156/177 (88%)	148 (95%)	7 (4%)	1 (1%)	30 62
9	I	68/162 (42%)	61 (90%)	5 (7%)	2 (3%)	6 17
10	J	140/145 (97%)	134 (96%)	6 (4%)	0	100 100
11	K	130/132 (98%)	125 (96%)	5 (4%)	0	100 100
12	L	141/165 (86%)	131 (93%)	10 (7%)	0	100 100
13	M	192/196 (98%)	184 (96%)	7 (4%)	1 (0%)	34 67
14	N	184/187 (98%)	167 (91%)	14 (8%)	3 (2%)	12 34
15	O	113/116 (97%)	112 (99%)	1 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
16	P	141/149 (95%)	140 (99%)	1 (1%)	0	100 100
17	Q	93/96 (97%)	89 (96%)	4 (4%)	0	100 100
18	R	148/155 (96%)	144 (97%)	4 (3%)	0	100 100
19	S	79/85 (93%)	76 (96%)	3 (4%)	0	100 100
20	T	117/120 (98%)	113 (97%)	4 (3%)	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%)	149 (98%)	3 (2%)	0	100 100
24	X	80/92 (87%)	76 (95%)	2 (2%)	2 (2%)	7 21
25	Y	140/241 (58%)	137 (98%)	3 (2%)	0	100 100
26	Z	71/116 (61%)	59 (83%)	10 (14%)	2 (3%)	6 18
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%)	83 (92%)	5 (6%)	2 (2%)	8 24
All	All	3705/4472 (83%)	3502 (94%)	180 (5%)	23 (1%)	30 62

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
4	D	137	PRO
14	N	154	LEU
1	A	27	LEU
8	H	19	ARG
13	M	71	SER
4	D	56	ARG
14	N	167	ASP
26	Z	70	ARG
1	A	74	VAL
2	B	2	GLN
2	B	185	GLY
3	C	8	LEU
6	F	100	ASP
26	Z	44	ARG
4	D	27	ILE
9	I	108	HIS
29	3	64	LYS

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Mol	Chain	Res	Type
14	N	184	ILE
9	I	131	GLY
24	X	70	ILE
29	3	61	PRO
24	X	52	PRO

5.3.2 Protein sidechains (i)

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%)	172 (96%)	7 (4%)	39 72
2	B	282/283 (100%)	262 (93%)	20 (7%)	18 43
3	C	193/193 (100%)	179 (93%)	14 (7%)	17 41
4	D	117/148 (79%)	105 (90%)	12 (10%)	9 23
5	E	152/156 (97%)	146 (96%)	6 (4%)	39 72
6	F	93/94 (99%)	91 (98%)	2 (2%)	60 87
7	G	27/282 (10%)	25 (93%)	2 (7%)	17 40
8	H	134/145 (92%)	130 (97%)	4 (3%)	48 80
9	I	58/130 (45%)	57 (98%)	1 (2%)	68 90
10	J	118/121 (98%)	113 (96%)	5 (4%)	36 68
11	K	106/106 (100%)	100 (94%)	6 (6%)	25 55
12	L	113/127 (89%)	108 (96%)	5 (4%)	35 67
13	M	158/160 (99%)	147 (93%)	11 (7%)	19 44
14	N	149/150 (99%)	142 (95%)	7 (5%)	32 64
15	O	93/94 (99%)	90 (97%)	3 (3%)	46 78
16	P	113/117 (97%)	108 (96%)	5 (4%)	35 67
17	Q	79/80 (99%)	78 (99%)	1 (1%)	76 93
18	R	117/122 (96%)	114 (97%)	3 (3%)	54 84
19	S	71/74 (96%)	71 (100%)	0	100 100
20	T	105/106 (99%)	97 (92%)	8 (8%)	16 39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	U	44/53 (83%)	41 (93%)	3 (7%)	20 46
22	V	51/57 (90%)	48 (94%)	3 (6%)	24 53
23	W	130/130 (100%)	122 (94%)	8 (6%)	23 51
24	X	66/74 (89%)	57 (86%)	9 (14%)	5 12
25	Y	120/196 (61%)	117 (98%)	3 (2%)	55 85
26	Z	60/94 (64%)	58 (97%)	2 (3%)	45 77
27	1	46/47 (98%)	46 (100%)	0	100 100
28	2	42/46 (91%)	41 (98%)	1 (2%)	57 86
29	3	79/79 (100%)	73 (92%)	6 (8%)	16 39
All	All	3095/3646 (85%)	2938 (95%)	157 (5%)	29 61

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	34	ASP
1	A	62	ASP
1	A	64	ASP
1	A	135	VAL
1	A	179	MET
1	A	217	ARG
2	B	5	ARG
2	B	7	ARG
2	B	11	LEU
2	B	27	ASN
2	B	33	ASP
2	B	49	THR
2	B	51	VAL
2	B	71	VAL
2	B	82	VAL
2	B	97	LEU
2	B	98	THR
2	B	102	THR
2	B	132	HIS
2	B	162	MET
2	B	171	VAL
2	B	195	ARG
2	B	234	ARG
2	B	251	VAL

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Mol	Chain	Res	Type
2	B	254	GLN
2	B	257	THR
3	C	2	GLN
3	C	27	ARG
3	C	78	ARG
3	C	94	THR
3	C	98	ARG
3	C	136	VAL
3	C	162	VAL
3	C	187	ARG
3	C	214	THR
3	C	223	LEU
3	C	234	VAL
3	C	236	THR
3	C	237	GLU
3	C	243	VAL
4	D	17	ARG
4	D	19	GLU
4	D	23	VAL
4	D	24	HIS
4	D	29	HIS
4	D	48	MET
4	D	50	VAL
4	D	58	VAL
4	D	101	THR
4	D	149	ARG
4	D	161	ASP
4	D	172	VAL
5	E	12	ASP
5	E	36	PRO
5	E	102	VAL
5	E	126	ILE
5	E	156	ASP
5	E	164	ASP
6	F	12	LEU
6	F	91	VAL
7	G	64	ASN
7	G	73	ASP
8	H	62	HIS
8	H	65	LEU
8	H	87	LYS
8	H	157	TYR

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Mol	Chain	Res	Type
9	I	94	ASP
10	J	52	GLN
10	J	74	ARG
10	J	107	ASN
10	J	130	VAL
10	J	131	THR
11	K	10	GLN
11	K	16	SER
11	K	55	VAL
11	K	62	PRO
11	K	74	VAL
11	K	120	ARG
12	L	35	ARG
12	L	80	ASP
12	L	104	ASP
12	L	114	VAL
12	L	143	THR
13	M	10	ASP
13	M	46	LEU
13	M	68	ARG
13	M	73	ARG
13	M	78	LYS
13	M	81	ARG
13	M	89	THR
13	M	93	ARG
13	M	99	ARG
13	M	116	ASN
13	M	126	GLN
14	N	23	ARG
14	N	26	LEU
14	N	47	LEU
14	N	49	THR
14	N	135	VAL
14	N	142	THR
14	N	178	THR
15	O	74	VAL
15	O	80	ASP
15	O	96	VAL
16	P	21	VAL
16	P	52	LYS
16	P	91	LYS
16	P	98	ILE

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Mol	Chain	Res	Type
16	P	110	ASP
17	Q	57	ASP
18	R	39	THR
18	R	52	GLU
18	R	82	GLU
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	115	GLU
20	T	117	ASP
21	U	9	CYS
21	U	52	THR
21	U	56	ARG
22	V	12	THR
22	V	13	PRO
22	V	65	ASP
23	W	18	GLN
23	W	38	THR
23	W	52	VAL
23	W	88	THR
23	W	120	PRO
23	W	142	ASP
23	W	146	ILE
23	W	154	ARG
24	X	8	ARG
24	X	15	ARG
24	X	43	VAL
24	X	46	ASP
24	X	52	PRO
24	X	72	VAL
24	X	79	GLU
24	X	82	GLU
24	X	88	GLU
25	Y	154	ARG
25	Y	189	ASN
25	Y	203	VAL
26	Z	63	CYS
26	Z	94	LYS
28	2	18	ASN

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Mol	Chain	Res	Type
29	3	3	MET
29	3	17	HIS
29	3	56	PRO
29	3	65	THR
29	3	84	ARG
29	3	88	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	127	GLN
1	A	176	HIS
1	A	199	HIS
2	B	27	ASN
2	B	127	GLN
2	B	145	HIS
2	B	221	GLN
2	B	238	ASN
2	B	256	GLN
2	B	260	HIS
2	B	286	ASN
2	B	320	GLN
2	B	332	ASN
3	C	67	GLN
3	C	73	GLN
3	C	129	HIS
3	C	151	GLN
4	D	85	GLN
4	D	103	ASN
5	E	119	HIS
5	E	143	GLN
7	G	64	ASN
8	H	59	GLN
8	H	73	ASN
10	J	52	GLN
10	J	107	ASN
11	K	10	GLN
11	K	44	HIS
12	L	18	HIS
12	L	41	HIS
13	M	24	GLN

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Mol	Chain	Res	Type
13	M	28	GLN
13	M	58	GLN
13	M	137	ASN
13	M	143	ASN
13	M	170	ASN
14	N	40	ASN
14	N	107	ASN
15	O	100	GLN
16	P	66	GLN
16	P	88	GLN
16	P	118	GLN
17	Q	16	ASN
17	Q	40	HIS
18	R	94	ASN
18	R	98	ASN
18	R	117	HIS
18	R	123	GLN
19	S	44	GLN
19	S	51	GLN
20	T	39	ASN
21	U	39	ASN
22	V	34	GLN
22	V	60	GLN
23	W	12	ASN
23	W	110	GLN
23	W	119	HIS
23	W	141	HIS
24	X	23	HIS
25	Y	119	GLN
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	48	ASN

5.3.3 RNA

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	243 (8%)	23 (0%)
31	9	121/122 (99%)	18 (14%)	1 (0%)
32	4	1/3 (33%)	0	0
All	All	2867/3048 (94%)	261 (9%)	24 (0%)

All (261) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G
30	0	86	A
30	0	87	C
30	0	88	G
30	0	114	A
30	0	115	U
30	0	120	A
30	0	130	C
30	0	131	A
30	0	138	U
30	0	141	C
30	0	151	A
30	0	166	A
30	0	185	G
30	0	186	A
30	0	191	A
30	0	192	A
30	0	200	C
30	0	219	G
30	0	236	A
30	0	237	G
30	0	271	C
30	0	272	A
30	0	273	G
30	0	283	U
30	0	284	C
30	0	308	U
30	0	309	C
30	0	318	U

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Mol	Chain	Res	Type
30	0	336	G
30	0	337	A
30	0	358	G
30	0	368	C
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
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	605	C
30	0	620	A
30	0	632	A
30	0	644	G
30	0	645	U
30	0	660	A
30	0	688	A
30	0	699	C
30	0	701	U
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

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Mol	Chain	Res	Type
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
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	1088	A
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1129	C
30	0	1130	U
30	0	1137	G
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	1208	C

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Mol	Chain	Res	Type
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	1351	G
30	0	1353	C
30	0	1360	C
30	0	1377	C
30	0	1378	G
30	0	1407	A
30	0	1474	C
30	0	1505	U
30	0	1506	U
30	0	1524	U
30	0	1525	G
30	0	1526	A
30	0	1528	A
30	0	1592	G
30	0	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	1752	G
30	0	1778	A
30	0	1798	C
30	0	1819	G
30	0	1820	G

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Mol	Chain	Res	Type
30	0	1829	A
30	0	1856	C
30	0	1879	U
30	0	1919	A
30	0	1942	A
30	0	1968	A
30	0	1971	G
30	0	1973	A
30	0	1978	A
30	0	1979	G
30	0	1996	U
30	0	2006	C
30	0	2008	U
30	0	2011	A
30	0	2012	U
30	0	2013	G
30	0	2033	G
30	0	2034	U
30	0	2064	U
30	0	2072	G
30	0	2073	G
30	0	2074	A
30	0	2096	A
30	0	2101	A
30	0	2102	G
30	0	2104	C
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	2322	U
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	2469	A

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Mol	Chain	Res	Type
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	2542	C
30	0	2553	A
30	0	2564	G
30	0	2570	G
30	0	2589	U
30	0	2601	A
30	0	2602	G
30	0	2608	C
30	0	2613	G
30	0	2634	G
30	0	2637	A
30	0	2649	A
30	0	2664	A
30	0	2681	A
30	0	2682	C
30	0	2719	A
30	0	2726	U
30	0	2747	C
30	0	2748	G
30	0	2749	U
30	0	2750	G
30	0	2762	C
30	0	2768	A
30	0	2792	A
30	0	2800	A
30	0	2811	A
30	0	2812	A
30	0	2825	C
30	0	2852	A
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	0	2903	C
30	0	2914	A

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Mol	Chain	Res	Type
31	9	2	U
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	34	A
31	9	39	U
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 (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	69	A
30	0	129	A
30	0	604	G
30	0	644	G
30	0	834	G
30	0	857	A
30	0	871	G
30	0	877	G
30	0	1237	U
30	0	1352	A
30	0	1377	C
30	0	1684	A
30	0	1685	A
30	0	1692	C
30	0	1730	G
30	0	1856	C
30	0	2011	A
30	0	2467	A
30	0	2526	C
30	0	2536	C

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Mol	Chain	Res	Type
30	0	2649	A
30	0	2718	C
30	0	2791	U
31	9	65	A

5.4 Non-standard residues in protein, DNA, RNA chains (i)

6 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	30,35	12,22,23	1.02	1 (8%)	19,31,34	3.17	2 (10%)
30	OMG	0	2588	32,30	17,26,27	1.04	1 (5%)	21,38,41	2.53	3 (14%)
30	UR3	0	2619	30	12,22,23	0.82	1 (8%)	16,32,35	0.75	0
30	PSU	0	2621	30	13,21,22	1.61	2 (15%)	18,30,33	6.17	4 (22%)
30	1MA	0	628	30,35	14,25,26	0.99	1 (7%)	15,37,40	1.15	1 (6%)
32	PPU	4	76	32,30	30,40,41	2.67	5 (16%)	37,57,60	2.36	8 (21%)

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	30,35	-	0/5/27/28	0/2/2/2
30	OMG	0	2588	32,30	-	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
32	PPU	4	76	32,30	-	0/21/43/44	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	4	76	PPU	C9-N6	-5.41	1.32	1.45
32	4	76	PPU	C10-N6	-5.32	1.32	1.45
30	0	2621	PSU	C5-C1'	-4.81	1.48	1.52
30	0	2619	UR3	C6-C5	-2.04	1.33	1.38
30	0	2587	OMU	C4-N3	2.35	1.37	1.33
30	0	2621	PSU	C4-N3	2.58	1.37	1.33
30	0	628	1MA	C6-N6	2.59	1.33	1.29
32	4	76	PPU	O4'-C1'	2.65	1.44	1.41
30	0	2588	OMG	C6-N1	3.23	1.39	1.33
32	4	76	PPU	C-N3'	5.85	1.47	1.34
32	4	76	PPU	O-C	10.24	1.43	1.23

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	0	2621	PSU	N1-C2-N3	-21.72	114.47	128.33
32	4	76	PPU	N3-C2-N1	-9.54	121.59	128.89
30	0	2588	OMG	C5-C6-N1	-8.72	111.66	123.59
32	4	76	PPU	C3'-N3'-C	-6.83	112.43	123.18
30	0	628	1MA	C2-N3-C4	-3.65	110.74	116.40
30	0	2587	OMU	C5-C4-N3	-3.31	114.64	123.12
32	4	76	PPU	CM-OC-CZ	-2.89	110.76	117.51
32	4	76	PPU	C2'-C3'-C4'	-2.67	98.95	102.27
32	4	76	PPU	C2'-C1'-N9	-2.58	110.35	114.29
30	0	2588	OMG	N3-C2-N1	-2.35	123.87	127.44
32	4	76	PPU	C4-C5-N7	-2.26	107.40	109.48
30	0	2621	PSU	C5-C1'-C2'	-2.00	111.97	115.52
32	4	76	PPU	N1-C6-N6	2.20	119.45	117.05
30	0	2621	PSU	C6-N1-C2	2.72	119.84	115.47
32	4	76	PPU	C2-N1-C6	4.67	121.36	111.43
30	0	2588	OMG	C6-N1-C2	6.60	125.11	115.94
30	0	2587	OMU	C4-N3-C2	13.18	127.19	114.14
30	0	2621	PSU	C4-N3-C2	13.83	127.20	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	1	0
30	0	2619	UR3	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2621	PSU	1	0
32	4	76	PPU	6	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 304 ligands modelled in this entry, 304 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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%)	0.32	26 (10%) 7 4	32, 66, 104, 124	0
2	B	337/338 (99%)	-0.24	6 (1%) 71 66	31, 59, 87, 104	0
3	C	246/246 (100%)	-0.24	0 100 100	19, 47, 71, 81	0
4	D	140/177 (79%)	2.52	81 (57%) 0 0	83, 112, 135, 143	0
5	E	172/178 (96%)	-0.13	5 (2%) 55 48	47, 72, 92, 97	0
6	F	119/120 (99%)	0.45	12 (10%) 9 5	58, 81, 111, 122	0
7	G	29/348 (8%)	0.47	2 (6%) 20 14	76, 97, 108, 110	0
8	H	160/177 (90%)	0.23	16 (10%) 9 6	50, 72, 105, 117	0
9	I	70/162 (43%)	4.72	60 (85%) 0 0	130, 150, 167, 169	0
10	J	142/145 (97%)	-0.49	1 (0%) 89 86	35, 54, 76, 86	0
11	K	132/132 (100%)	-0.45	0 100 100	38, 55, 83, 87	0
12	L	145/165 (87%)	0.43	14 (9%) 10 6	33, 80, 121, 130	0
13	M	194/196 (98%)	0.28	21 (10%) 8 5	31, 48, 108, 117	0
14	N	186/187 (99%)	1.21	49 (26%) 1 0	61, 85, 128, 133	0
15	O	115/116 (99%)	-0.29	0 100 100	39, 58, 75, 79	0
16	P	143/149 (95%)	-0.20	2 (1%) 78 73	42, 60, 83, 90	0
17	Q	95/96 (98%)	-0.32	1 (1%) 82 78	45, 57, 75, 83	0
18	R	150/155 (96%)	-0.44	0 100 100	29, 49, 70, 78	0
19	S	81/85 (95%)	-0.24	1 (1%) 81 76	42, 63, 84, 95	0
20	T	119/120 (99%)	-0.08	7 (5%) 26 19	41, 58, 87, 122	0
21	U	53/67 (79%)	0.35	6 (11%) 7 4	59, 73, 93, 97	0
22	V	65/71 (91%)	1.89	20 (30%) 1 0	51, 77, 123, 129	0
23	W	154/154 (100%)	-0.51	0 100 100	35, 52, 66, 81	0
24	X	82/92 (89%)	-0.24	0 100 100	48, 64, 88, 103	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	Y	142/241 (58%)	-0.33	3 (2%) 67 61	26, 45, 69, 90	0
26	Z	73/116 (62%)	6.42	57 (78%) 0 0	99, 121, 131, 134	0
27	1	56/57 (98%)	-0.05	0 100 100	23, 32, 45, 57	0
28	2	46/50 (92%)	0.12	3 (6%) 22 16	33, 65, 97, 106	0
29	3	92/92 (100%)	8.87	88 (95%) 0 0	112, 127, 133, 140	0
30	0	2749/2923 (94%)	-0.71	47 (1%) 73 68	18, 50, 98, 167	0
31	9	122/122 (100%)	-0.42	4 (3%) 50 43	41, 80, 105, 152	0
32	4	2/3 (66%)	-0.97	0 100 100	70, 70, 70, 74	0
All	All	6648/7520 (88%)	0.00	532 (8%) 15 10	18, 57, 120, 169	0

All (532) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	3	82	GLY	43.1
26	Z	46	SER	30.1
29	3	83	TRP	25.9
26	Z	50	VAL	24.4
26	Z	35	SER	19.6
29	3	1	MET	19.2
26	Z	43	GLY	17.6
26	Z	58	ASN	17.6
26	Z	44	ARG	17.5
13	M	80	GLY	17.5
29	3	81	GLU	17.4
9	I	128	THR	17.2
22	V	1	THR	17.0
26	Z	36	GLY	15.9
26	Z	42	TYR	15.5
29	3	80	ARG	15.1
29	3	38	ARG	14.9
26	Z	49	ARG	14.9
13	M	70	GLY	14.3
29	3	9	THR	14.1
29	3	41	GLU	14.0
29	3	35	TRP	13.8
31	9	1	U	13.7
29	3	65	THR	13.3
29	3	13	HIS	13.3
26	Z	47	ARG	13.2

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Mol	Chain	Res	Type	RSRZ
29	3	33	MET	13.0
26	Z	38	PHE	12.8
26	Z	45	VAL	12.6
9	I	71	ALA	12.6
13	M	89	THR	12.6
29	3	85	ALA	12.6
9	I	74	ILE	12.5
29	3	84	ARG	12.4
29	3	14	CYS	12.2
29	3	10	TYR	11.7
29	3	12	PRO	11.7
29	3	20	HIS	11.7
29	3	64	LYS	11.6
26	Z	34	SER	11.2
29	3	36	ILE	11.1
22	V	39	ALA	11.0
29	3	78	HIS	10.9
26	Z	57	MET	10.8
29	3	39	GLN	10.8
29	3	3	MET	10.8
29	3	69	TYR	10.8
29	3	42	ARG	10.8
29	3	11	CYS	10.8
4	D	63	ILE	10.7
26	Z	40	ALA	10.4
29	3	22	VAL	10.4
29	3	34	LYS	10.4
29	3	74	CYS	10.2
29	3	17	HIS	10.2
29	3	15	ASN	10.1
26	Z	37	ARG	9.9
29	3	31	THR	9.9
29	3	67	LEU	9.7
13	M	71	SER	9.6
4	D	57	THR	9.5
26	Z	59	GLU	9.3
26	Z	55	SER	9.2
1	A	37	VAL	9.0
29	3	60	LYS	8.9
29	3	76	LYS	8.9
9	I	83	GLY	8.8
29	3	75	GLY	8.7

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Mol	Chain	Res	Type	RSRZ
29	3	37	ASP	8.7
30	0	735	C	8.6
29	3	62	THR	8.6
9	I	132	VAL	8.6
29	3	71	CYS	8.4
29	3	18	GLN	8.4
29	3	27	SER	8.4
29	3	44	SER	8.4
29	3	61	PRO	8.3
26	Z	39	GLY	8.2
9	I	112	LEU	8.2
26	Z	82	SER	8.2
22	V	40	PRO	8.2
29	3	16	GLU	8.2
9	I	91	PHE	8.1
29	3	66	ASP	8.1
29	3	45	GLY	8.1
29	3	40	ARG	8.0
29	3	28	GLY	8.0
4	D	18	ILE	8.0
29	3	30	GLN	8.0
29	3	77	ALA	7.9
9	I	92	VAL	7.9
26	Z	56	GLU	7.9
26	Z	69	ASP	7.9
29	3	2	GLN	7.8
13	M	83	SER	7.8
29	3	4	PRO	7.7
26	Z	68	GLU	7.7
29	3	68	LYS	7.7
29	3	59	ASP	7.6
1	A	31	LYS	7.6
26	Z	85	ASP	7.6
29	3	5	ARG	7.6
4	D	40	ILE	7.5
26	Z	60	ASP	7.5
29	3	91	GLN	7.5
9	I	72	GLU	7.5
29	3	23	GLU	7.4
4	D	27	ILE	7.4
29	3	58	GLY	7.4
9	I	104	ALA	7.4

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Mol	Chain	Res	Type	RSRZ
29	3	8	ASN	7.3
1	A	237	GLY	7.3
22	V	43	PRO	7.2
29	3	32	GLY	7.0
29	3	72	GLY	6.9
9	I	82	THR	6.9
9	I	84	SER	6.8
26	Z	77	GLY	6.8
29	3	7	PHE	6.7
14	N	166	ALA	6.7
4	D	135	VAL	6.6
4	D	26	GLY	6.6
4	D	10	PHE	6.6
29	3	88	LEU	6.6
29	3	63	LYS	6.6
9	I	130	LEU	6.5
29	3	43	ASN	6.5
26	Z	70	ARG	6.4
29	3	90	PHE	6.4
29	3	92	GLU	6.4
9	I	108	HIS	6.4
29	3	56	PRO	6.4
4	D	66	GLY	6.3
22	V	46	ILE	6.3
30	0	1173	A	6.2
9	I	127	CYS	6.2
14	N	147	ILE	6.1
9	I	70	THR	6.1
14	N	75	THR	6.1
29	3	6	ARG	6.1
1	A	85	SER	6.1
13	M	74	LYS	6.1
26	Z	53	ILE	6.1
29	3	21	GLU	6.0
26	Z	51	ALA	6.0
29	3	48	ASN	6.0
29	3	19	GLU	6.0
26	Z	83	TYR	5.9
30	0	1170	U	5.9
9	I	69	PRO	5.9
9	I	93	ALA	5.9
29	3	86	GLY	5.9

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Mol	Chain	Res	Type	RSRZ
13	M	81	ARG	5.8
4	D	17	ARG	5.8
29	3	29	ARG	5.8
26	Z	66	CYS	5.8
30	0	1172	G	5.8
29	3	25	VAL	5.7
9	I	111	LEU	5.7
26	Z	54	GLU	5.7
22	V	2	VAL	5.7
9	I	86	GLU	5.6
29	3	79	LEU	5.6
9	I	80	PHE	5.5
30	0	1951	G	5.5
9	I	113	SER	5.5
9	I	126	THR	5.4
9	I	106	GLN	5.4
4	D	154	LYS	5.4
14	N	138	ASP	5.4
9	I	73	LEU	5.4
29	3	51	LYS	5.4
4	D	134	LEU	5.3
4	D	69	ILE	5.3
26	Z	48	ARG	5.3
4	D	143	LYS	5.2
22	V	51	LYS	5.2
29	3	24	LYS	5.2
22	V	45	ARG	5.2
9	I	79	GLY	5.2
14	N	41	LYS	5.2
13	M	82	ARG	5.2
1	A	36	ASP	5.1
30	0	1171	A	5.1
9	I	100	VAL	5.1
26	Z	41	ARG	5.1
20	T	119	ALA	5.1
30	0	1199	A	5.1
26	Z	63	CYS	5.0
30	0	1163	G	5.0
4	D	61	PHE	5.0
22	V	44	GLY	5.0
30	0	282	C	4.9
1	A	38	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
26	Z	67	GLY	4.9
4	D	139	TYR	4.9
30	0	1177	A	4.9
9	I	119	ALA	4.9
29	3	26	ARG	4.8
26	Z	62	ALA	4.8
4	D	58	VAL	4.8
29	3	70	ARG	4.8
4	D	19	GLU	4.8
14	N	159	TYR	4.8
31	9	24	U	4.8
13	M	90	ARG	4.7
14	N	115	VAL	4.7
19	S	81	ILE	4.7
22	V	38	GLY	4.7
9	I	68	PRO	4.7
9	I	88	GLN	4.7
12	L	99	GLU	4.7
13	M	79	ALA	4.7
4	D	142	ALA	4.6
4	D	56	ARG	4.6
28	2	39	ARG	4.6
9	I	66	GLY	4.5
30	0	1198	U	4.5
9	I	76	ASP	4.5
1	A	88	ILE	4.5
29	3	73	GLU	4.5
29	3	46	ILE	4.5
4	D	64	ARG	4.5
22	V	41	GLU	4.4
4	D	144	ARG	4.4
9	I	103	ILE	4.4
14	N	172	PHE	4.4
9	I	75	LYS	4.4
9	I	102	GLN	4.4
26	Z	81	CYS	4.4
30	0	1200	A	4.4
14	N	149	GLU	4.4
26	Z	79	TRP	4.4
4	D	138	GLY	4.4
9	I	129	SER	4.4
14	N	137	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
14	N	74	PRO	4.3
22	V	48	GLU	4.3
30	0	1181	A	4.3
14	N	145	ALA	4.2
25	Y	235	GLU	4.2
9	I	109	PRO	4.2
26	Z	52	GLU	4.2
4	D	141	VAL	4.2
30	0	1178	G	4.2
4	D	156	ARG	4.1
9	I	105	GLU	4.1
4	D	16	PRO	4.1
9	I	81	GLU	4.1
26	Z	71	VAL	4.1
13	M	86	GLN	4.0
1	A	89	ALA	4.0
6	F	75	ILE	4.0
14	N	84	THR	4.0
14	N	114	LYS	4.0
4	D	166	ILE	4.0
9	I	94	ASP	4.0
4	D	11	HIS	4.0
6	F	106	ALA	4.0
4	D	172	VAL	4.0
9	I	125	GLY	3.9
14	N	160	SER	3.9
8	H	146	ALA	3.9
8	H	174	LEU	3.9
1	A	236	GLY	3.9
4	D	88	LEU	3.8
12	L	150	GLN	3.8
9	I	117	THR	3.8
30	0	1169	U	3.8
6	F	17	LEU	3.7
14	N	38	LYS	3.7
4	D	90	LEU	3.7
4	D	137	PRO	3.7
14	N	83	LEU	3.7
9	I	118	ASN	3.7
4	D	128	LEU	3.6
1	A	99	ILE	3.6
9	I	78	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
6	F	119	ARG	3.6
26	Z	78	ILE	3.6
26	Z	65	ASN	3.6
9	I	67	VAL	3.6
30	0	1950	G	3.5
9	I	120	ALA	3.5
4	D	89	PRO	3.5
4	D	65	GLU	3.5
9	I	97	VAL	3.5
30	0	1174	A	3.5
4	D	67	ASP	3.4
9	I	110	ASP	3.4
5	E	154	ILE	3.4
26	Z	76	THR	3.4
30	0	1165	G	3.4
4	D	92	GLU	3.4
9	I	134	ILE	3.4
13	M	84	LYS	3.4
14	N	76	GLY	3.4
20	T	82	THR	3.4
30	0	272	A	3.4
30	0	1167	G	3.4
29	3	57	GLY	3.4
4	D	84	LEU	3.4
30	0	2004	U	3.4
14	N	42	HIS	3.4
30	0	2237	G	3.4
9	I	123	VAL	3.3
9	I	121	LYS	3.3
30	0	1168	C	3.3
9	I	131	GLY	3.3
4	D	62	ASP	3.3
13	M	88	VAL	3.3
1	A	97	ALA	3.3
4	D	101	THR	3.3
14	N	152	GLU	3.3
14	N	161	GLY	3.2
4	D	157	LEU	3.2
26	Z	88	PHE	3.2
9	I	99	GLN	3.2
26	Z	80	GLN	3.2
5	E	108	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
14	N	43	VAL	3.2
21	U	54	THR	3.2
4	D	75	LEU	3.2
1	A	82	VAL	3.2
13	M	78	LYS	3.1
16	P	67	LYS	3.1
31	9	2	U	3.1
22	V	52	ALA	3.1
1	A	94	LEU	3.1
29	3	47	GLY	3.1
30	0	970	U	3.1
26	Z	84	CYS	3.1
6	F	117	GLU	3.1
6	F	28	ALA	3.1
26	Z	74	GLN	3.1
14	N	179	LEU	3.0
7	G	27	ILE	3.0
14	N	150	TYR	3.0
26	Z	61	HIS	3.0
4	D	25	MET	3.0
20	T	118	SER	3.0
13	M	73	ARG	3.0
22	V	8	ILE	3.0
4	D	130	VAL	3.0
1	A	133	ARG	2.9
13	M	75	ARG	2.9
12	L	77	ALA	2.9
26	Z	92	SER	2.9
29	3	89	GLU	2.9
14	N	134	ASP	2.9
12	L	80	ASP	2.9
14	N	40	ASN	2.9
9	I	116	LEU	2.9
14	N	157	PRO	2.9
4	D	51	ARG	2.9
8	H	77	ILE	2.9
4	D	93	LEU	2.9
14	N	80	SER	2.9
14	N	155	GLU	2.9
14	N	78	MET	2.9
4	D	13	MET	2.9
30	0	1190	G	2.8

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Mol	Chain	Res	Type	RSRZ
30	0	1947	G	2.8
4	D	22	VAL	2.8
6	F	15	ASP	2.8
22	V	49	LEU	2.8
13	M	77	HIS	2.8
29	3	55	VAL	2.8
21	U	48	ASN	2.8
26	Z	64	PRO	2.8
12	L	130	ARG	2.8
30	0	1166	A	2.8
9	I	124	VAL	2.8
8	H	169	GLU	2.8
9	I	87	PRO	2.8
4	D	171	ASP	2.8
4	D	14	ARG	2.8
26	Z	89	THR	2.8
30	0	1202	A	2.7
4	D	104	PHE	2.7
20	T	117	ASP	2.7
22	V	37	GLY	2.7
28	2	49	GLU	2.7
12	L	96	VAL	2.7
30	0	1192	A	2.7
4	D	145	ASP	2.7
9	I	95	LEU	2.7
30	0	1164	U	2.7
5	E	45	ASP	2.7
21	U	47	ARG	2.7
26	Z	86	TYR	2.7
1	A	151	GLN	2.7
4	D	102	GLY	2.7
14	N	116	PHE	2.7
1	A	84	VAL	2.7
26	Z	93	TYR	2.7
14	N	66	LEU	2.7
26	Z	104	ARG	2.7
14	N	162	ASP	2.7
1	A	112	PRO	2.7
4	D	68	PRO	2.7
29	3	87	ARG	2.7
1	A	60	PHE	2.7
4	D	153	THR	2.7

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Mol	Chain	Res	Type	RSRZ
4	D	23	VAL	2.6
28	2	20	ARG	2.6
4	D	70	GLY	2.6
14	N	68	GLU	2.6
12	L	81	VAL	2.6
16	P	64	GLU	2.6
4	D	158	ASN	2.6
4	D	167	GLU	2.6
6	F	113	ASP	2.6
14	N	140	GLN	2.6
9	I	89	GLU	2.6
5	E	87	PHE	2.6
6	F	16	ALA	2.5
8	H	145	ASP	2.5
9	I	98	ASP	2.5
10	J	70	PHE	2.5
20	T	27	LEU	2.5
4	D	149	ARG	2.5
21	U	52	THR	2.5
4	D	80	ALA	2.5
8	H	86	TYR	2.5
8	H	132	ALA	2.5
26	Z	103	VAL	2.5
14	N	142	THR	2.5
8	H	147	GLU	2.5
30	0	1185	U	2.5
30	0	2250	G	2.5
8	H	40	GLN	2.5
4	D	106	PHE	2.5
13	M	68	ARG	2.5
14	N	153	GLN	2.5
14	N	139	TRP	2.5
30	0	960	G	2.5
14	N	180	LEU	2.4
20	T	40	VAL	2.4
14	N	118	ILE	2.4
2	B	183	GLU	2.4
22	V	3	LEU	2.4
1	A	52	SER	2.4
14	N	151	ASP	2.4
4	D	140	ARG	2.4
4	D	41	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
4	D	170	TYR	2.4
8	H	157	TYR	2.4
14	N	67	ALA	2.4
30	0	1948	G	2.4
4	D	15	GLU	2.4
6	F	107	ASP	2.4
22	V	42	ASN	2.4
2	B	108	GLU	2.4
8	H	79	GLU	2.4
4	D	146	LYS	2.4
26	Z	87	LYS	2.4
30	0	1180	U	2.4
14	N	158	LEU	2.3
14	N	163	PHE	2.3
30	0	1162	G	2.3
14	N	113	SER	2.3
22	V	26	GLU	2.3
30	0	1184	C	2.3
1	A	51	ARG	2.3
1	A	32	VAL	2.3
4	D	173	GLU	2.3
12	L	59	GLU	2.3
13	M	87	GLY	2.3
1	A	53	ALA	2.3
4	D	24	HIS	2.3
8	H	149	VAL	2.3
4	D	86	THR	2.3
30	0	1175	G	2.3
1	A	83	GLY	2.3
30	0	1161	A	2.3
2	B	128	ILE	2.3
30	0	2103	A	2.3
4	D	81	GLU	2.3
14	N	112	GLY	2.3
4	D	53	LYS	2.3
12	L	75	LEU	2.3
9	I	114	TYR	2.3
4	D	136	ARG	2.2
4	D	50	VAL	2.2
4	D	73	VAL	2.2
20	T	116	ASP	2.2
4	D	160	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
21	U	51	TRP	2.2
2	B	140	LEU	2.2
17	Q	17	LYS	2.2
30	0	1186	C	2.2
4	D	76	ARG	2.2
13	M	76	ARG	2.2
4	D	95	THR	2.2
12	L	91	VAL	2.2
25	Y	108	ASP	2.2
12	L	48	LYS	2.2
1	A	65	ARG	2.2
14	N	148	ALA	2.2
4	D	52	THR	2.2
30	0	1179	C	2.1
12	L	140	VAL	2.1
7	G	23	ILE	2.1
30	0	2890	A	2.1
14	N	146	HIS	2.1
29	3	50	GLY	2.1
8	H	78	LYS	2.1
30	0	2508	C	2.1
12	L	147	GLU	2.1
6	F	49	PHE	2.1
6	F	11	ASP	2.1
5	E	170	ARG	2.1
12	L	149	ARG	2.1
14	N	117	ALA	2.1
1	A	111	SER	2.1
2	B	117	GLU	2.1
8	H	144	GLU	2.1
31	9	23	U	2.1
22	V	31	ARG	2.1
4	D	74	THR	2.1
8	H	141	CYS	2.1
1	A	66	ARG	2.0
4	D	165	PHE	2.0
8	H	53	ILE	2.0
13	M	85	ARG	2.0
30	0	280	C	2.0
30	0	1183	C	2.0
30	0	1965	C	2.0
21	U	55	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	104	GLU	2.0
25	Y	103	THR	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, 95^{th} 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	0.99	0.10	-	37,38,41,42	0
30	UR3	0	2619	21/22	0.98	0.16	-	46,49,53,55	0
30	PSU	0	2621	20/21	0.97	0.18	-	30,37,55,56	0
32	PPU	4	76	37/38	0.94	0.15	-	67,75,88,91	0
30	1MA	0	628	23/24	0.98	0.15	-	28,32,34,36	0
30	OMG	0	2588	24/25	0.99	0.13	-	37,39,41,45	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, 95^{th} 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	8565	1/1	0.88	1.15	62.02	71,71,71,71	0
35	NA	0	8563	1/1	0.69	0.90	42.95	86,86,86,86	0
33	MG	0	8073	1/1	0.63	0.79	40.70	105,105,105,105	0
35	NA	0	8559	1/1	0.79	0.27	36.91	81,81,81,81	0
35	NA	0	8547	1/1	0.97	0.47	36.09	59,59,59,59	0
35	NA	0	8517	1/1	0.81	0.32	24.15	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
35	NA	0	8553	1/1	0.96	0.60	22.10	84,84,84,84	0
35	NA	0	8558	1/1	0.97	0.64	22.04	63,63,63,63	0
35	NA	0	8562	1/1	0.90	0.40	21.88	73,73,73,73	0
35	NA	0	8522	1/1	0.77	1.06	19.10	78,78,78,78	0
35	NA	0	8527	1/1	0.77	0.40	15.89	67,67,67,67	0
35	NA	0	8575	1/1	0.90	0.42	14.76	89,89,89,89	0
35	NA	0	8519	1/1	0.81	0.32	14.61	54,54,54,54	0
37	SR	0	8987	1/1	0.83	0.67	13.30	200,200,200,200	0
33	MG	0	8047	1/1	0.92	0.41	13.16	72,72,72,72	0
35	NA	0	8534	1/1	0.91	0.62	12.05	84,84,84,84	0
34	K	0	8401	1/1	0.63	0.42	11.46	147,147,147,147	0
35	NA	0	8507	1/1	0.56	0.27	11.36	48,48,48,48	0
35	NA	9	8572	1/1	0.97	0.53	11.03	98,98,98,98	0
37	SR	0	8969	1/1	0.77	0.40	10.22	184,184,184,184	0
35	NA	0	8564	1/1	0.94	0.29	10.03	62,62,62,62	0
33	MG	0	8041	1/1	0.98	0.23	8.74	35,35,35,35	0
35	NA	0	8542	1/1	0.90	0.27	8.68	45,45,45,45	0
35	NA	0	8504	1/1	0.94	0.31	7.95	37,37,37,37	0
33	MG	0	8008	1/1	0.83	0.21	6.84	26,26,26,26	0
33	MG	0	8014	1/1	0.99	0.19	6.62	31,31,31,31	0
35	NA	0	8508	1/1	0.93	0.18	5.70	47,47,47,47	0
37	SR	0	8903	1/1	1.00	0.18	5.32	49,49,49,49	0
37	SR	0	8957	1/1	0.69	0.30	5.02	200,200,200,200	0
35	NA	0	8535	1/1	0.89	0.17	5.01	59,59,59,59	0
35	NA	0	8528	1/1	0.90	0.24	4.93	56,56,56,56	0
35	NA	B	8552	1/1	0.96	0.34	4.71	78,78,78,78	0
33	MG	0	8062	1/1	0.97	0.27	4.58	49,49,49,49	0
35	NA	0	8568	1/1	0.96	0.23	4.50	58,58,58,58	0
33	MG	A	8051	1/1	0.68	0.59	4.42	81,81,81,81	0
35	NA	0	8537	1/1	0.91	0.18	3.97	40,40,40,40	0
37	SR	0	8904	1/1	0.99	0.20	3.89	54,54,54,54	0
37	SR	0	8975	1/1	0.93	0.22	3.85	144,144,144,144	0
35	NA	0	8533	1/1	0.48	0.22	3.83	70,70,70,70	0
33	MG	0	8084	1/1	0.99	0.20	3.60	33,33,33,33	0
33	MG	0	8007	1/1	0.64	0.23	3.00	50,50,50,50	0
33	MG	0	8067	1/1	0.91	0.29	2.91	54,54,54,54	0
35	NA	0	8530	1/1	0.75	0.21	2.90	48,48,48,48	0
35	NA	0	8512	1/1	0.81	0.27	2.87	89,89,89,89	0
37	SR	0	8923	1/1	0.93	0.18	2.68	94,94,94,94	0
33	MG	0	8044	1/1	0.93	0.22	2.15	54,54,54,54	0
33	MG	0	8011	1/1	0.98	0.28	2.04	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
33	MG	0	8009	1/1	0.99	0.20	1.76	31,31,31,31	0
35	NA	0	8556	1/1	0.96	0.24	1.68	51,51,51,51	0
33	MG	0	8006	1/1	0.96	0.15	1.52	33,33,33,33	0
33	MG	K	8054	1/1	0.96	0.17	1.33	44,44,44,44	0
33	MG	0	8085	1/1	0.82	0.16	1.15	71,71,71,71	0
33	MG	0	8080	1/1	0.66	0.73	1.09	92,92,92,92	0
37	SR	0	8943	1/1	0.91	0.14	1.09	75,75,75,75	0
33	MG	0	8004	1/1	0.99	0.20	0.95	24,24,24,24	0
33	MG	0	8025	1/1	0.98	0.17	0.91	42,42,42,42	0
37	SR	R	8912	1/1	0.98	0.16	0.90	72,72,72,72	0
35	NA	0	8521	1/1	0.91	0.18	0.62	50,50,50,50	0
35	NA	0	8515	1/1	0.97	0.20	0.42	36,36,36,36	0
33	MG	0	8088	1/1	0.94	0.15	0.32	41,41,41,41	0
34	K	0	8402	1/1	0.99	0.29	0.29	86,86,86,86	0
35	NA	0	8502	1/1	0.83	0.13	0.19	49,49,49,49	0
37	SR	0	8985	1/1	0.91	0.10	-0.22	121,121,121,121	0
37	SR	0	8972	1/1	0.91	0.14	-0.23	143,143,143,143	0
33	MG	0	8087	1/1	0.97	0.16	-0.32	24,24,24,24	0
35	NA	0	8520	1/1	0.88	0.11	-0.34	48,48,48,48	0
33	MG	0	8043	1/1	0.97	0.11	-0.62	44,44,44,44	0
38	CD	3	8704	1/1	0.88	0.76	-0.76	200,200,200,200	0
37	SR	0	8910	1/1	0.84	0.12	-0.78	94,94,94,94	0
37	SR	0	8964	1/1	0.96	0.10	-0.80	121,121,121,121	0
35	NA	J	8538	1/1	0.95	0.12	-0.81	57,57,57,57	0
38	CD	1	8702	1/1	1.00	0.12	-0.90	54,54,54,54	0
35	NA	Q	8540	1/1	0.91	0.10	-0.94	74,74,74,74	0
37	SR	0	8949	1/1	0.73	0.11	-0.95	113,113,113,113	0
37	SR	0	8993	1/1	0.94	0.07	-0.97	167,167,167,167	0
37	SR	A	8929	1/1	0.97	0.10	-1.17	119,119,119,119	0
33	MG	0	8003	1/1	0.99	0.12	-1.20	30,30,30,30	0
37	SR	0	8992	1/1	0.91	0.13	-1.21	136,136,136,136	0
36	CL	O	8808	1/1	0.92	0.11	-1.21	62,62,62,62	0
38	CD	Z	8703	1/1	0.39	0.33	-1.29	200,200,200,200	0
33	MG	A	8050	1/1	0.96	0.11	-1.58	60,60,60,60	0
37	SR	0	8935	1/1	0.99	0.08	-1.65	92,92,92,92	0
37	SR	1	8913	1/1	0.99	0.13	-1.67	79,79,79,79	0
33	MG	0	8065	1/1	0.98	0.11	-1.68	37,37,37,37	0
33	MG	0	8034	1/1	0.84	0.13	-1.68	44,44,44,44	0
37	SR	0	8936	1/1	0.94	0.10	-1.69	95,95,95,95	0
33	MG	Y	8086	1/1	0.97	0.12	-1.76	36,36,36,36	0
36	CL	0	8812	1/1	0.97	0.07	-1.76	49,49,49,49	0
33	MG	0	8002	1/1	0.95	0.13	-1.78	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
33	MG	0	8045	1/1	0.98	0.07	-1.84	38,38,38,38	0
36	CL	J	8821	1/1	0.98	0.07	-1.98	56,56,56,56	0
33	MG	T	8057	1/1	0.83	0.08	-2.01	76,76,76,76	0
38	CD	U	8701	1/1	1.00	0.07	-2.14	78,78,78,78	0
37	SR	0	8981	1/1	0.96	0.06	-2.43	148,148,148,148	0
33	MG	0	8058	1/1	0.99	0.09	-2.45	28,28,28,28	0
33	MG	0	8052	1/1	0.90	0.09	-2.54	50,50,50,50	0
36	CL	B	8819	1/1	0.98	0.12	-2.65	53,53,53,53	0
35	NA	0	8557	1/1	0.94	0.07	-2.69	58,58,58,58	0
35	NA	M	8539	1/1	0.83	0.10	-2.78	38,38,38,38	0
37	SR	0	8970	1/1	0.97	0.05	-3.26	113,113,113,113	0
36	CL	0	8805	1/1	0.99	0.07	-3.32	71,71,71,71	0
33	MG	0	8013	1/1	0.91	0.05	-3.34	30,30,30,30	0
35	NA	0	8523	1/1	0.89	0.08	-3.93	30,30,30,30	0
36	CL	M	8818	1/1	0.99	0.05	-4.26	40,40,40,40	0
37	SR	0	8944	1/1	0.90	0.06	-4.35	167,167,167,167	0
33	MG	0	8075	1/1	0.83	0.07	-6.00	62,62,62,62	0
33	MG	0	8005	1/1	0.95	0.22	-	28,28,28,28	0
33	MG	0	8001	1/1	0.98	0.27	-	20,20,20,20	0
37	SR	0	8926	1/1	0.79	0.12	-	118,118,118,118	0
35	NA	0	8546	1/1	0.95	0.47	-	64,64,64,64	0
37	SR	0	8965	1/1	0.92	0.09	-	118,118,118,118	0
33	MG	0	8083	1/1	0.10	0.12	-	70,70,70,70	0
36	CL	0	8814	1/1	0.99	0.12	-	56,56,56,56	0
33	MG	0	8089	1/1	0.25	0.14	-	49,49,49,49	0
33	MG	0	8046	1/1	0.82	0.10	-	66,66,66,66	0
36	CL	0	8803	1/1	0.96	0.05	-	51,51,51,51	0
37	SR	1	8952	1/1	0.96	0.14	-	73,73,73,73	0
37	SR	0	8928	1/1	0.92	0.07	-	141,141,141,141	0
33	MG	0	8030	1/1	0.94	0.36	-	85,85,85,85	0
37	SR	0	8925	1/1	0.96	0.13	-	89,89,89,89	0
36	CL	A	8809	1/1	0.99	0.34	-	88,88,88,88	0
35	NA	0	8545	1/1	0.96	0.21	-	42,42,42,42	0
37	SR	0	8946	1/1	0.95	0.19	-	102,102,102,102	0
33	MG	0	8018	1/1	0.92	0.24	-	37,37,37,37	0
37	SR	0	8984	1/1	0.87	0.08	-	107,107,107,107	0
33	MG	0	8093	1/1	0.99	0.11	-	37,37,37,37	0
37	SR	0	8995	1/1	0.83	0.15	-	141,141,141,141	0
33	MG	0	8053	1/1	0.96	0.16	-	55,55,55,55	0
33	MG	0	8040	1/1	0.74	0.63	-	84,84,84,84	0
37	SR	0	9002	1/1	0.69	0.14	-	182,182,182,182	0
37	SR	3	8932	1/1	0.89	0.12	-	167,167,167,167	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
33	MG	0	8070	1/1	0.97	0.13	-	58,58,58,58	0
33	MG	0	8017	1/1	0.98	0.26	-	29,29,29,29	0
37	SR	0	8902	1/1	0.99	0.21	-	53,53,53,53	0
37	SR	0	8948	1/1	0.92	0.08	-	105,105,105,105	0
37	SR	0	8947	1/1	-0.04	0.49	-	194,194,194,194	0
37	SR	0	8934	1/1	0.54	0.21	-	133,133,133,133	0
35	NA	9	8543	1/1	0.92	0.19	-	68,68,68,68	0
35	NA	0	8514	1/1	0.97	0.17	-	46,46,46,46	0
36	CL	3	8804	1/1	0.29	0.32	-	114,114,114,114	0
33	MG	0	8081	1/1	0.97	0.17	-	68,68,68,68	0
37	SR	0	8988	1/1	0.72	0.11	-	166,166,166,166	0
37	SR	0	8908	1/1	0.95	0.14	-	87,87,87,87	0
37	SR	0	8933	1/1	0.49	0.11	-	134,134,134,134	0
33	MG	0	8071	1/1	0.86	0.14	-	67,67,67,67	0
37	SR	9	8980	1/1	0.71	0.10	-	185,185,185,185	0
35	NA	0	8561	1/1	0.79	0.54	-	67,67,67,67	0
33	MG	0	8031	1/1	0.84	0.24	-	55,55,55,55	0
33	MG	0	8026	1/1	0.97	0.16	-	38,38,38,38	0
35	NA	0	8531	1/1	0.72	0.17	-	46,46,46,46	0
37	SR	0	8931	1/1	0.96	0.11	-	100,100,100,100	0
37	SR	0	8976	1/1	0.67	0.29	-	181,181,181,181	0
36	CL	0	8816	1/1	0.99	0.09	-	61,61,61,61	0
33	MG	0	8064	1/1	0.92	0.18	-	48,48,48,48	0
33	MG	0	8090	1/1	0.69	0.14	-	87,87,87,87	0
37	SR	0	8982	1/1	0.68	1.16	-	200,200,200,200	0
37	SR	B	8950	1/1	0.91	0.17	-	112,112,112,112	0
33	MG	0	8055	1/1	0.96	0.20	-	59,59,59,59	0
35	NA	H	8518	1/1	0.98	0.09	-	69,69,69,69	0
33	MG	0	8012	1/1	0.96	0.26	-	23,23,23,23	0
35	NA	0	8551	1/1	0.98	0.14	-	36,36,36,36	0
37	SR	0	8958	1/1	0.53	0.10	-	128,128,128,128	0
35	NA	0	8571	1/1	0.85	0.47	-	90,90,90,90	0
33	MG	0	8029	1/1	0.85	0.18	-	43,43,43,43	0
37	SR	0	8971	1/1	0.91	0.07	-	174,174,174,174	0
37	SR	0	9007	1/1	0.92	0.37	-	200,200,200,200	0
37	SR	0	9004	1/1	0.69	0.54	-	200,200,200,200	0
37	SR	0	8921	1/1	0.95	0.14	-	84,84,84,84	0
37	SR	0	8977	1/1	0.72	0.13	-	177,177,177,177	0
35	NA	0	8501	1/1	0.90	0.32	-	39,39,39,39	0
35	NA	0	8573	1/1	0.95	0.19	-	79,79,79,79	0
36	CL	J	8801	1/1	0.96	0.08	-	68,68,68,68	0
36	CL	0	8817	1/1	0.98	0.13	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
36	CL	Y	8820	1/1	0.99	0.04	-	41,41,41,41	0
35	NA	0	8509	1/1	0.84	0.25	-	67,67,67,67	0
37	SR	0	8962	1/1	0.34	0.34	-	194,194,194,194	0
33	MG	0	8022	1/1	0.97	0.21	-	33,33,33,33	0
33	MG	0	8038	1/1	0.95	0.67	-	96,96,96,96	0
37	SR	0	8906	1/1	1.00	0.22	-	56,56,56,56	0
36	CL	0	8822	1/1	0.99	0.26	-	87,87,87,87	0
35	NA	0	8513	1/1	0.94	0.18	-	46,46,46,46	0
37	SR	0	8901	1/1	0.92	0.21	-	57,57,57,57	0
37	SR	0	9000	1/1	0.96	0.08	-	168,168,168,168	0
33	MG	0	8069	1/1	0.97	0.17	-	75,75,75,75	0
35	NA	0	8549	1/1	0.94	0.12	-	53,53,53,53	0
35	NA	0	8506	1/1	0.58	0.20	-	63,63,63,63	0
37	SR	9	8978	1/1	0.78	0.13	-	171,171,171,171	0
37	SR	S	8961	1/1	0.90	0.07	-	118,118,118,118	0
37	SR	0	8914	1/1	0.98	0.27	-	108,108,108,108	0
33	MG	0	8091	1/1	0.99	0.05	-	47,47,47,47	0
37	SR	0	8956	1/1	0.88	0.08	-	141,141,141,141	0
37	SR	0	8955	1/1	0.48	0.10	-	200,200,200,200	0
33	MG	0	8076	1/1	0.86	0.15	-	31,31,31,31	0
35	NA	0	8544	1/1	0.92	0.13	-	71,71,71,71	0
37	SR	0	8994	1/1	0.80	0.49	-	200,200,200,200	0
33	MG	0	8036	1/1	0.99	0.12	-	47,47,47,47	0
37	SR	0	8940	1/1	0.99	0.13	-	89,89,89,89	0
37	SR	F	9005	1/1	0.92	0.08	-	144,144,144,144	0
33	MG	0	8068	1/1	0.95	0.15	-	59,59,59,59	0
37	SR	0	8915	1/1	0.76	0.07	-	127,127,127,127	0
37	SR	0	8997	1/1	0.93	0.26	-	185,185,185,185	0
35	NA	0	8574	1/1	0.97	0.51	-	64,64,64,64	0
37	SR	3	8999	1/1	0.91	0.19	-	200,200,200,200	0
35	NA	C	8503	1/1	0.95	0.20	-	36,36,36,36	0
33	MG	0	8056	1/1	0.88	0.14	-	59,59,59,59	0
37	SR	0	8974	1/1	0.72	0.18	-	163,163,163,163	0
36	CL	R	8806	1/1	0.97	0.16	-	47,47,47,47	0
35	NA	0	8548	1/1	0.75	0.38	-	65,65,65,65	0
36	CL	0	8811	1/1	0.98	0.12	-	64,64,64,64	0
37	SR	0	8938	1/1	0.72	0.23	-	200,200,200,200	0
37	SR	0	9006	1/1	0.49	0.67	-	194,194,194,194	0
37	SR	0	8991	1/1	0.97	0.17	-	182,182,182,182	0
35	NA	0	8570	1/1	0.99	0.07	-	50,50,50,50	0
33	MG	0	8082	1/1	0.94	0.42	-	73,73,73,73	0
33	MG	0	8060	1/1	0.87	0.17	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
33	MG	0	8072	1/1	0.96	0.21	-	58,58,58,58	0
37	SR	0	8998	1/1	0.84	0.37	-	186,186,186,186	0
37	SR	0	8979	1/1	0.53	0.17	-	200,200,200,200	0
37	SR	0	8937	1/1	0.90	0.24	-	102,102,102,102	0
36	CL	L	8810	1/1	0.94	0.06	-	70,70,70,70	0
33	MG	0	8016	1/1	0.93	0.20	-	46,46,46,46	0
37	SR	A	8930	1/1	0.97	0.08	-	128,128,128,128	0
37	SR	0	8927	1/1	0.95	0.04	-	161,161,161,161	0
37	SR	0	8996	1/1	0.93	0.94	-	200,200,200,200	0
33	MG	0	8010	1/1	0.94	0.26	-	47,47,47,47	0
35	NA	0	8526	1/1	0.98	0.05	-	34,34,34,34	0
37	SR	0	8922	1/1	0.90	0.13	-	141,141,141,141	0
37	SR	0	8963	1/1	0.97	0.10	-	129,129,129,129	0
33	MG	0	8015	1/1	0.98	0.18	-	37,37,37,37	0
37	SR	0	8917	1/1	0.96	0.11	-	110,110,110,110	0
33	MG	0	8019	1/1	0.92	0.26	-	33,33,33,33	0
37	SR	0	8939	1/1	0.94	0.07	-	133,133,133,133	0
37	SR	0	8941	1/1	0.87	0.17	-	114,114,114,114	0
33	MG	0	8028	1/1	0.95	0.22	-	27,27,27,27	0
36	CL	0	8815	1/1	0.89	0.21	-	69,69,69,69	0
37	SR	0	8920	1/1	0.90	0.08	-	138,138,138,138	0
37	SR	0	8942	1/1	0.91	0.10	-	126,126,126,126	0
33	MG	B	8042	1/1	0.88	0.10	-	55,55,55,55	0
33	MG	0	8092	1/1	0.84	0.51	-	74,74,74,74	0
33	MG	0	8049	1/1	0.92	0.45	-	56,56,56,56	0
33	MG	0	8037	1/1	0.65	0.21	-	75,75,75,75	0
33	MG	0	8033	1/1	0.92	0.10	-	50,50,50,50	0
35	NA	0	8541	1/1	0.82	0.74	-	73,73,73,73	0
35	NA	0	8511	1/1	0.45	0.17	-	75,75,75,75	0
37	SR	9	9003	1/1	0.80	0.26	-	180,180,180,180	0
33	MG	0	8078	1/1	0.91	0.52	-	59,59,59,59	0
36	CL	N	8807	1/1	0.80	0.23	-	71,71,71,71	0
36	CL	0	8813	1/1	0.98	0.07	-	44,44,44,44	0
33	MG	0	8024	1/1	0.99	0.29	-	44,44,44,44	0
35	NA	0	8516	1/1	0.90	0.29	-	53,53,53,53	0
33	MG	0	8035	1/1	0.93	0.16	-	62,62,62,62	0
33	MG	0	8077	1/1	0.94	0.07	-	42,42,42,42	0
35	NA	0	8569	1/1	0.89	0.24	-	61,61,61,61	0
36	CL	J	8802	1/1	0.96	0.12	-	67,67,67,67	0
37	SR	0	8973	1/1	0.90	0.11	-	124,124,124,124	0
35	NA	0	8555	1/1	0.51	1.25	-	79,79,79,79	0
33	MG	0	8032	1/1	0.99	0.05	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
33	MG	0	8021	1/1	0.92	0.14	-	26,26,26,26	0
37	SR	J	8986	1/1	0.51	0.77	-	200,200,200,200	0
37	SR	0	8951	1/1	0.64	0.08	-	142,142,142,142	0
35	NA	0	8566	1/1	0.94	0.15	-	38,38,38,38	0
33	MG	0	8027	1/1	0.88	0.14	-	38,38,38,38	0
35	NA	0	8505	1/1	0.90	0.50	-	37,37,37,37	0
37	SR	0	8924	1/1	0.79	0.18	-	124,124,124,124	0
37	SR	0	8966	1/1	0.88	0.14	-	103,103,103,103	0
37	SR	0	8990	1/1	0.81	0.23	-	164,164,164,164	0
33	MG	0	8048	1/1	0.99	0.25	-	25,25,25,25	0
33	MG	0	8079	1/1	0.96	0.20	-	60,60,60,60	0
35	NA	0	8529	1/1	0.96	0.07	-	43,43,43,43	0
35	NA	R	8532	1/1	0.87	0.09	-	56,56,56,56	0
33	MG	0	8059	1/1	0.96	0.14	-	47,47,47,47	0
37	SR	0	8918	1/1	0.97	0.13	-	84,84,84,84	0
37	SR	0	8916	1/1	0.61	0.12	-	112,112,112,112	0
35	NA	0	8525	1/1	0.93	0.09	-	70,70,70,70	0
35	NA	0	8567	1/1	0.87	0.81	-	81,81,81,81	0
37	SR	0	8989	1/1	0.77	0.09	-	157,157,157,157	0
37	SR	0	8983	1/1	0.90	0.38	-	183,183,183,183	0
35	NA	S	8510	1/1	0.96	0.11	-	47,47,47,47	0
35	NA	0	8524	1/1	0.97	0.46	-	45,45,45,45	0
38	CD	O	8705	1/1	0.97	0.09	-	88,88,88,88	0
37	SR	0	8967	1/1	0.99	0.03	-	125,125,125,125	0
37	SR	0	9008	1/1	0.98	0.18	-	79,79,79,79	0
33	MG	0	8039	1/1	0.97	0.11	-	62,62,62,62	0
37	SR	0	8959	1/1	0.42	0.60	-	200,200,200,200	0
37	SR	0	8945	1/1	0.92	0.10	-	99,99,99,99	0
37	SR	0	8960	1/1	0.93	0.08	-	138,138,138,138	0
35	NA	0	8536	1/1	0.97	0.10	-	65,65,65,65	0
35	NA	0	8560	1/1	0.94	0.47	-	87,87,87,87	0
33	MG	0	8020	1/1	0.93	0.08	-	42,42,42,42	0
33	MG	0	8066	1/1	0.78	0.20	-	76,76,76,76	0
33	MG	0	8063	1/1	0.77	0.21	-	81,81,81,81	0
37	SR	0	8968	1/1	0.82	0.07	-	175,175,175,175	0
35	NA	0	8554	1/1	0.88	0.62	-	61,61,61,61	0
37	SR	0	8954	1/1	0.96	0.10	-	94,94,94,94	0
33	MG	9	8074	1/1	0.77	0.09	-	79,79,79,79	0
37	SR	0	8905	1/1	0.99	0.24	-	61,61,61,61	0
33	MG	0	8023	1/1	0.97	0.21	-	24,24,24,24	0
37	SR	0	8911	1/1	0.95	0.12	-	82,82,82,82	0
37	SR	0	9001	1/1	0.24	0.23	-	186,186,186,186	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
33	MG	0	8061	1/1	0.93	0.30	-	30,30,30,30	0
35	NA	0	8550	1/1	0.77	0.34	-	63,63,63,63	0
37	SR	0	8953	1/1	0.76	0.17	-	200,200,200,200	0
37	SR	0	8907	1/1	1.00	0.17	-	53,53,53,53	0
37	SR	0	8909	1/1	0.98	0.15	-	84,84,84,84	0

6.5 Other polymers

There are no such residues in this entry.