



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:24 PM GMT

PDB ID : 4WFA
Title : The crystal structure of the large ribosomal subunit of *Staphylococcus aureus* in complex with linezolid
Authors : Eyal, Z.; Matzov, D.; Krupkin, M.; Wekselman, I.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Yonath, A.E.
Deposited on : 2014-09-14
Resolution : 3.39 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

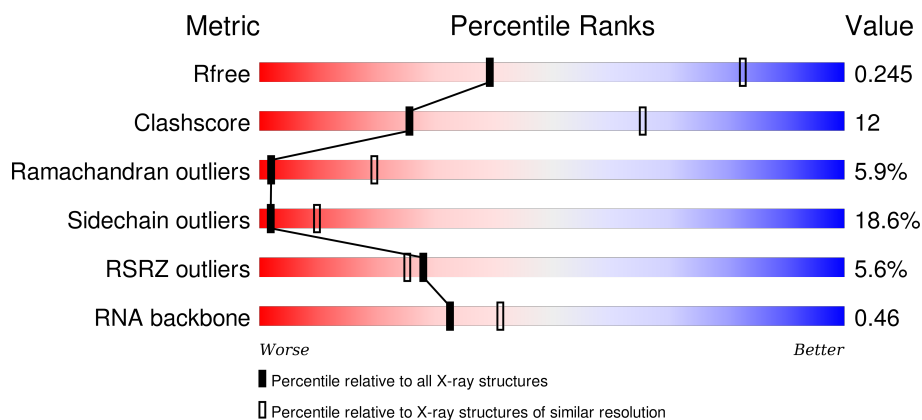
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.39 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)
RNA backbone	2183	1041 (4.00-2.80)

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

Mol	Chain	Length	Quality of chain
1	X	2923	
2	Y	114	
3	A	277	
4	B	220	

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Mol	Chain	Length	Quality of chain
5	C	207	
6	D	179	
7	E	178	
8	G	145	
9	H	122	
10	I	146	
11	J	144	
12	K	122	
13	L	119	
14	M	116	
15	N	118	
16	O	102	
17	P	117	
18	Q	91	
19	R	105	
20	S	217	
21	T	94	
22	U	62	
23	V	69	
24	W	59	
25	Z	58	
26	2	45	
27	3	66	
28	4	37	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	ZLD	X	3001	-	-	-	X
30	MPD	X	3003	-	-	-	X
30	MPD	X	3004	-	-	-	X
30	MPD	X	3006	-	-	-	X
30	MPD	X	3007	-	-	-	X
30	MPD	X	3008	-	-	-	X
30	MPD	X	3009	-	-	-	X
30	MPD	X	3010	-	-	-	X
31	MG	A	302	-	-	-	X
31	MG	X	3021	-	-	-	X
31	MG	X	3024	-	-	-	X
31	MG	X	3032	-	-	-	X
31	MG	X	3035	-	-	-	X
31	MG	X	3037	-	-	-	X
31	MG	X	3062	-	-	-	X
31	MG	X	3063	-	-	-	X
31	MG	X	3249	-	-	-	X
31	MG	X	3287	-	-	-	X
31	MG	X	3294	-	-	-	X
31	MG	X	3308	-	-	-	X
31	MG	X	3310	-	-	-	X
31	MG	X	3314	-	-	-	X
31	MG	X	3319	-	-	-	X
31	MG	X	3323	-	-	-	X
31	MG	X	3335	-	-	-	X
31	MG	X	3344	-	-	-	X
31	MG	X	3345	-	-	-	X
31	MG	X	3384	-	-	-	X
31	MG	X	3415	-	-	-	X
31	MG	X	3418	-	-	-	X
31	MG	X	3420	-	-	-	X
31	MG	X	3441	-	-	-	X
31	MG	Y	206	-	-	-	X
32	MN	X	3079	-	-	-	X
32	MN	X	3084	-	-	-	X
32	MN	X	3119	-	-	-	X
32	MN	X	3124	-	-	-	X
32	MN	X	3130	-	-	-	X
32	MN	X	3131	-	-	-	X
32	MN	X	3132	-	-	-	X
32	MN	X	3133	-	-	-	X
32	MN	X	3142	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MN	X	3143	-	-	-	X
32	MN	X	3146	-	-	-	X
32	MN	X	3147	-	-	-	X
32	MN	X	3148	-	-	-	X
32	MN	X	3150	-	-	-	X
32	MN	X	3151	-	-	-	X
32	MN	X	3152	-	-	-	X
32	MN	X	3153	-	-	-	X
32	MN	X	3154	-	-	-	X
32	MN	X	3157	-	-	-	X
32	MN	X	3159	-	-	-	X
32	MN	X	3161	-	-	-	X
32	MN	X	3162	-	-	-	X
32	MN	X	3168	-	-	-	X
32	MN	X	3172	-	-	-	X
32	MN	X	3176	-	-	-	X
32	MN	X	3184	-	-	-	X
32	MN	X	3187	-	-	-	X
32	MN	X	3195	-	-	-	X
32	MN	X	3199	-	-	-	X
32	MN	X	3215	-	-	-	X
32	MN	X	3220	-	-	-	X
32	MN	X	3221	-	-	-	X
32	MN	X	3223	-	-	-	X
32	MN	X	3224	-	-	-	X
32	MN	X	3227	-	-	-	X
32	MN	X	3231	-	-	-	X
32	MN	X	3239	-	-	-	X
32	MN	X	3240	-	-	-	X
32	MN	X	3442	-	-	-	X
34	EPE	X	3423	-	-	-	X
34	EPE	X	3424	-	-	-	X
34	EPE	X	3425	-	-	-	X
34	EPE	X	3426	-	-	X	X
35	SPD	J	201	-	-	-	X
35	SPD	X	3427	-	-	-	X
35	SPD	X	3428	-	-	-	X
35	SPD	X	3429	-	-	-	X
35	SPD	X	3431	-	-	-	X
35	SPD	X	3432	-	-	-	X
35	SPD	X	3433	-	-	-	X
35	SPD	X	3434	-	-	-	X

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 81465 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2711	Total	C	N	O	P	0	0	0
			58151	25961	10662	18817	2711			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	114	Total	C	N	O	P	0	0	0
			2430	1086	436	794	114			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	268	Total	C	N	O	S	0	0	0
			1620	985	315	316	4			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	215	Total	C	N	O	S	0	0	0
			1531	957	283	286	5			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	199	Total	C	N	O	S	0	0	0
			1321	818	253	248	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	155	Total	C	N	O	S	0	0	0
			794	478	155	160	1			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	157	Total	C	N	O	S	0	0	0
			926	567	172	186	1			

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	145	Total	C	N	O	S	0	0	0
			1087	679	202	203	3			

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	122	Total	C	N	O	S	0	0	0
			840	517	163	157	3			

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	131	Total	C	N	O	S	0	0	0
			817	500	164	152	1			

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	138	Total	C	N	O	S	0	0	0
			1003	642	185	173	3			

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	119	Total	C	N	O	S	0	0	0
			896	551	176	168	1			

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	108	Total	C	N	O	0	0	0
			659	399	134	126			

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	109	Total	C	N	O			
			809	513	158	138	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	116	Total	C	N	O	S			
			932	587	188	153	4	0	0	0

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	101	Total	C	N	O	S			
			751	477	137	136	1	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	112	Total	C	N	O	S			
			862	537	164	158	3	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	88	Total	C	N	O	S			
			586	363	108	113	2	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	100	Total	C	N	O	S			
			680	425	121	133	1	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	167	Total	C	N	O	S			
			1048	656	187	203	2	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	T	75	Total	C	N	O	0	0	0
			530	328	100	102			

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	44	Total	C	N	O	0	0	0
			254	154	52	48			

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	V	65	Total	C	N	O	0	0	0
			414	261	74	79			

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	W	57	Total	C	N	O	0	0	0
			441	274	83	84			

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	44	Total	C	N	O	S	0	0	0
			336	208	70	55	3			

- Molecule 26 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	2	44	Total	C	N	O	S	0	0	0
			368	225	89	53	1			

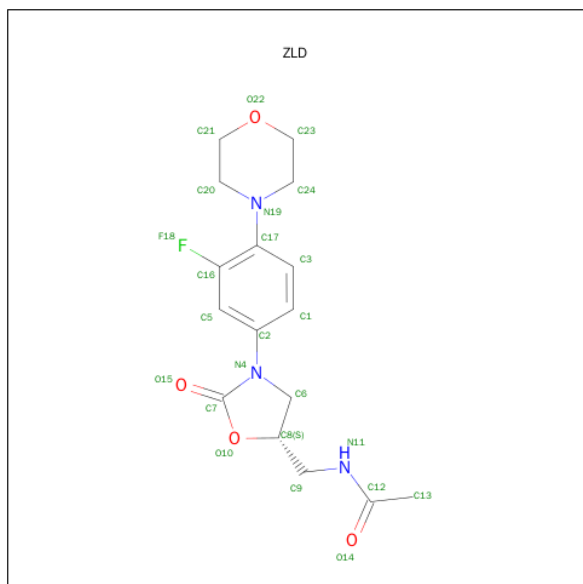
- Molecule 27 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	3	60	Total	C	N	O	S	0	0	0
			414	256	83	73	2			

- Molecule 28 is a protein called 50S ribosomal protein L36.

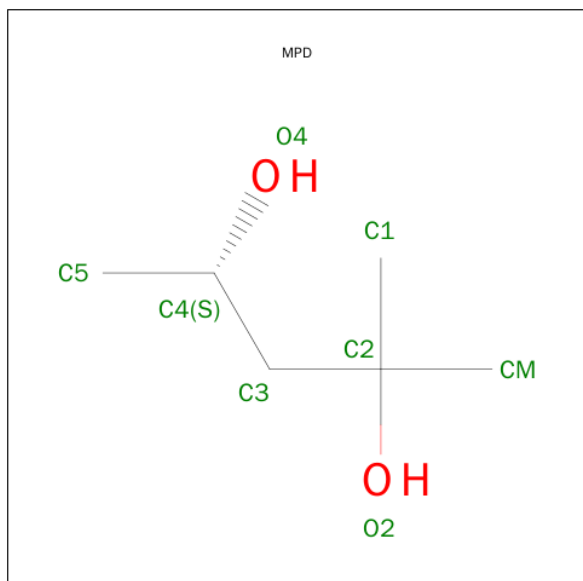
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	4	37	Total	C	N	O	S	0	0	0
			262	164	52	41	5			

- Molecule 29 is N-{[(5S)-3-(3-fluoro-4-morpholin-4-ylphenyl)-2-oxo-1,3-oxazolidin-5-yl]methyl}acetamide (three-letter code: ZLD) (formula: $C_{16}H_{20}FN_3O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	X	1	Total	C	F	N	O	0	0
			24	16	1	3	4		

- Molecule 30 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	G	2	Total Mg 2 2	0	0
31	K	1	Total Mg 1 1	0	0
31	B	1	Total Mg 1 1	0	0
31	I	1	Total Mg 1 1	0	0
31	C	1	Total Mg 1 1	0	0
31	W	1	Total Mg 1 1	0	0
31	Z	2	Total Mg 2 2	0	0
31	A	2	Total Mg 2 2	0	0
31	N	1	Total Mg 1 1	0	0
31	X	226	Total Mg 226 226	0	0
31	O	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	Y	6	Total 6	Mg 6	0	0

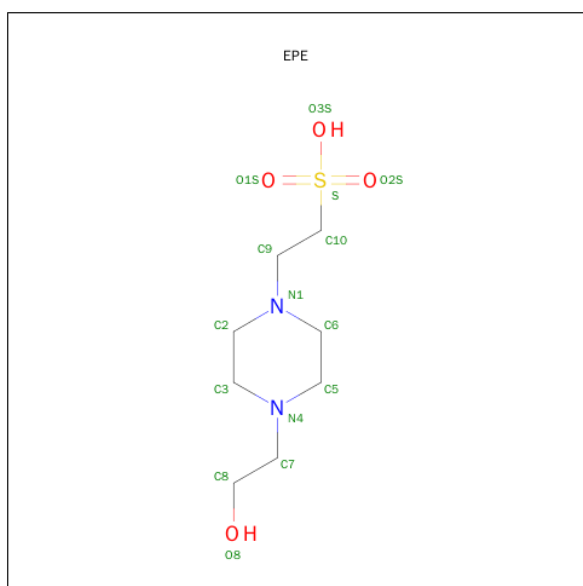
- Molecule 32 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	X	191	Total 191	Mn 191	0	0
32	Z	1	Total 1	Mn 1	0	0
32	Y	2	Total 2	Mn 2	0	0
32	M	1	Total 1	Mn 1	0	0

- Molecule 33 is SODIUM ION (three-letter code: NA) (formula: Na).

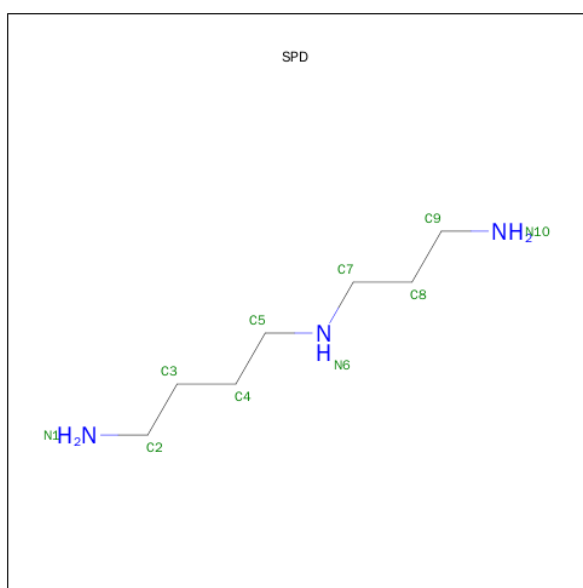
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	X	1	Total 1	Na 1	0	0

- Molecule 34 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
34	X	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
34	X	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
34	X	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
34	X	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 35 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



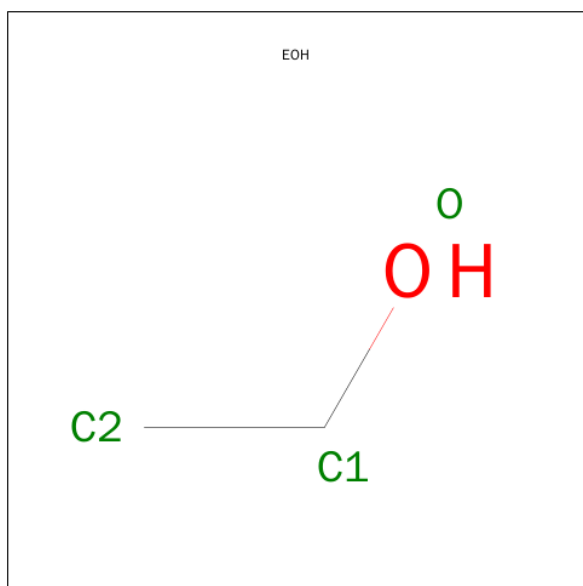
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	J	1	Total	C	N	0	0
			10	7	3		

- Molecule 36 is ETHANOL (three-letter code: EOH) (formula: C₂H₆O).

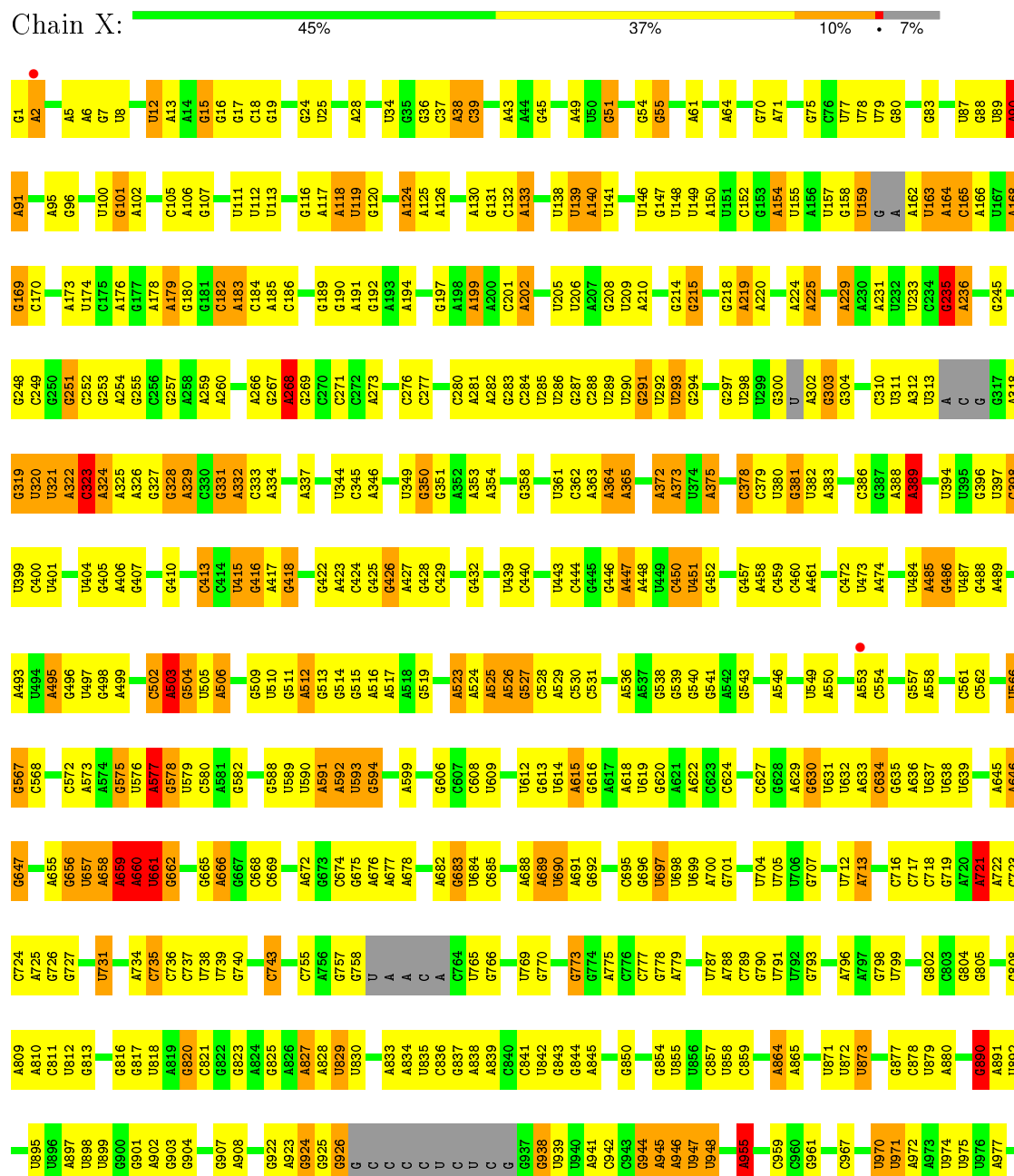


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	X	1	Total	C	O	0	0
			3	2	1		
36	X	1	Total	C	O	0	0
			3	2	1		
36	X	1	Total	C	O	0	0
			3	2	1		
36	X	1	Total	C	O	0	0
			3	2	1		
36	Y	1	Total	C	O	0	0
			3	2	1		

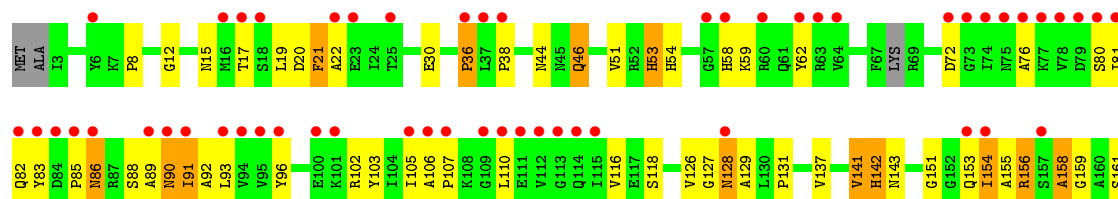
3 Residue-property plots

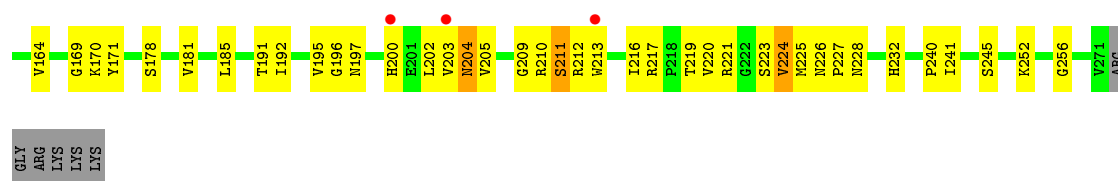
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 23S rRNA

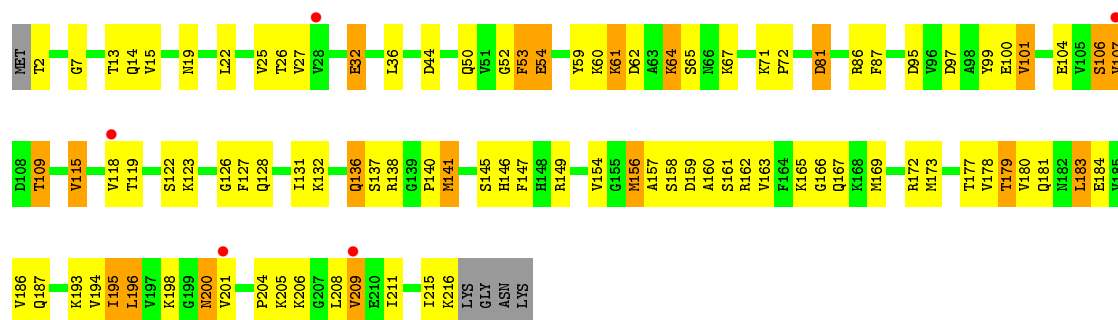




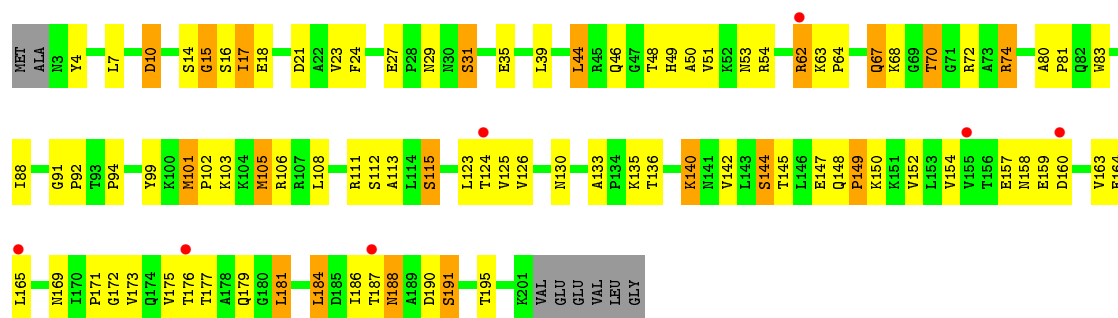




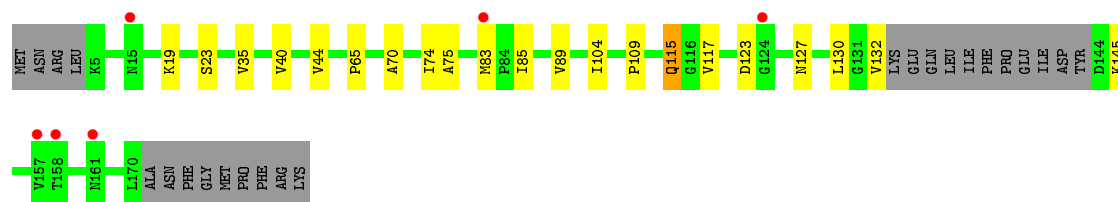
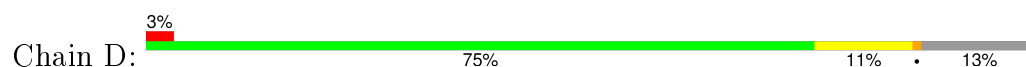
• Molecule 4: 50S ribosomal protein L3



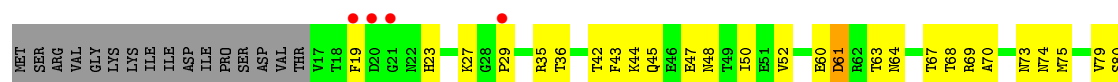
• Molecule 5: 50S ribosomal protein L4

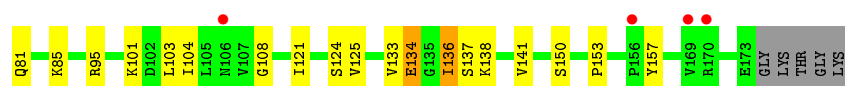


• Molecule 6: 50S ribosomal protein L5

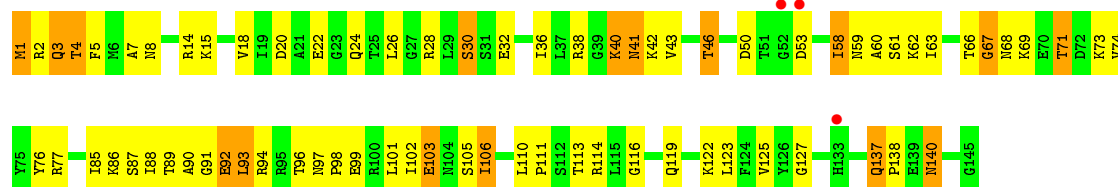


• Molecule 7: 50S ribosomal protein L6

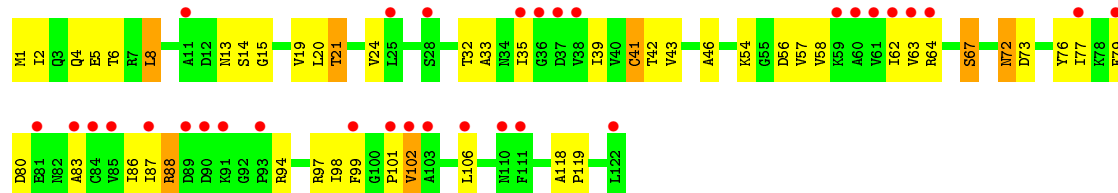




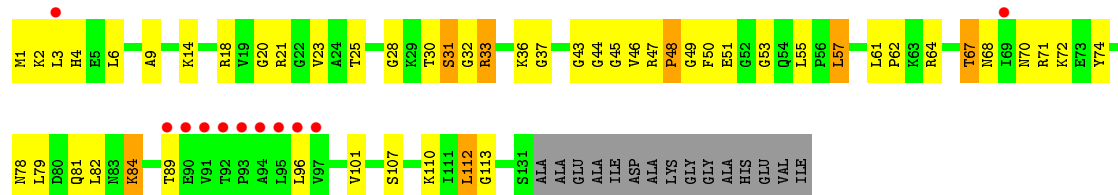
• Molecule 8: 50S ribosomal protein L13



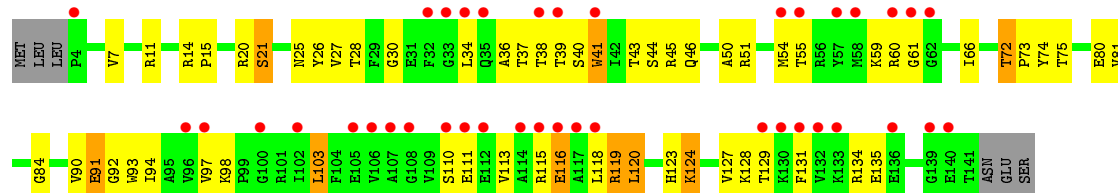
• Molecule 9: 50S ribosomal protein L14



• Molecule 10: 50S ribosomal protein L15

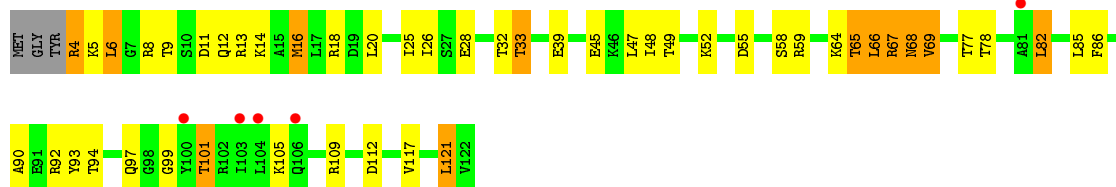


• Molecule 11: 50S ribosomal protein L16

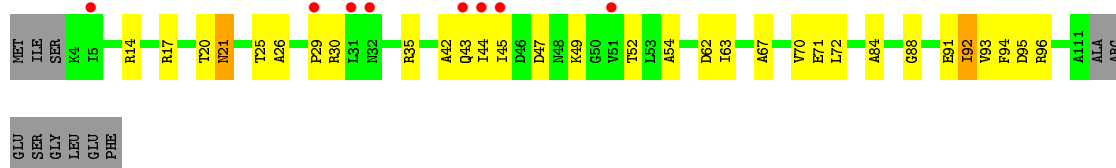


• Molecule 12: 50S ribosomal protein L17

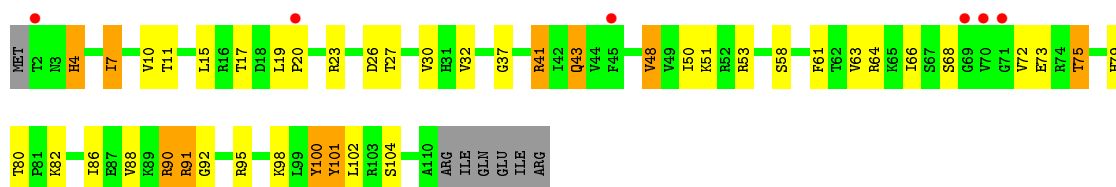




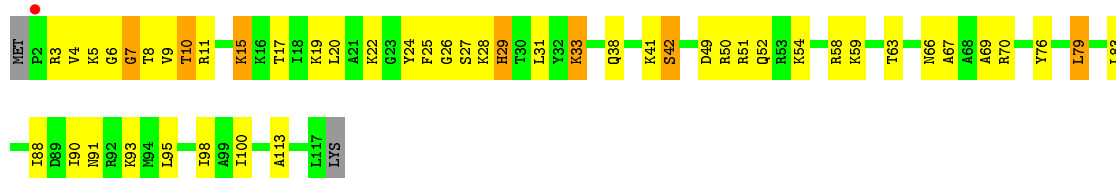
• Molecule 13: 50S ribosomal protein L18



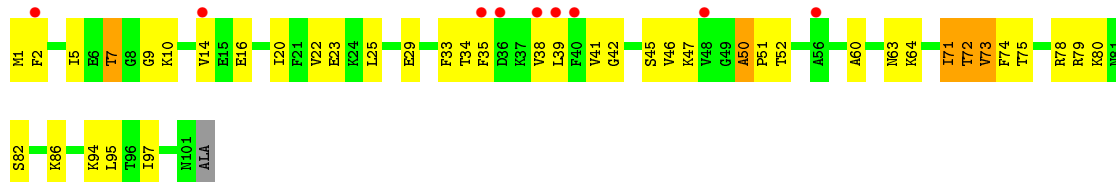
• Molecule 14: 50S ribosomal protein L19



• Molecule 15: 50S ribosomal protein L20

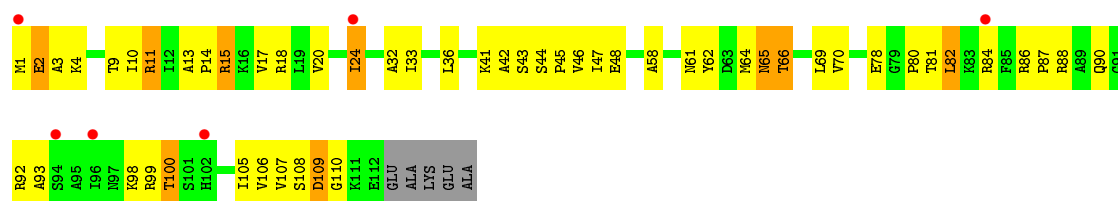


• Molecule 16: 50S ribosomal protein L21

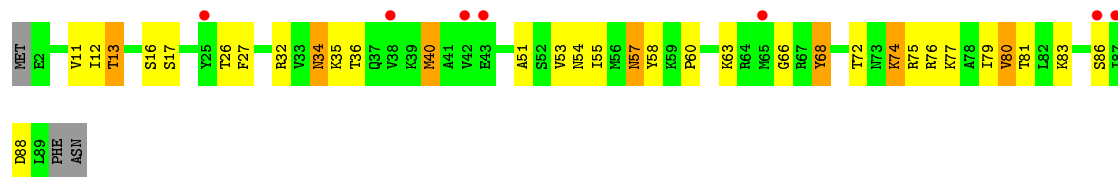


• Molecule 17: 50S ribosomal protein L22

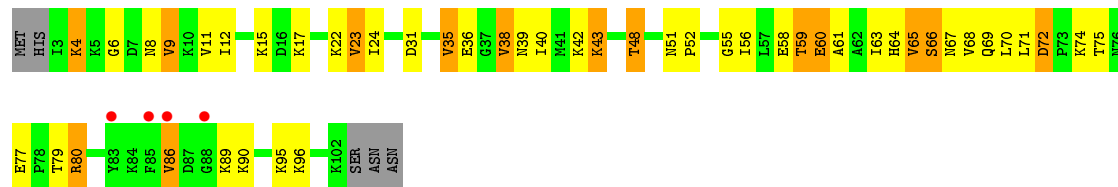




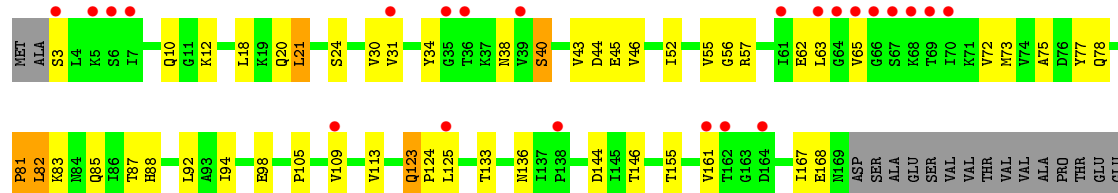
• Molecule 18: 50S ribosomal protein L23



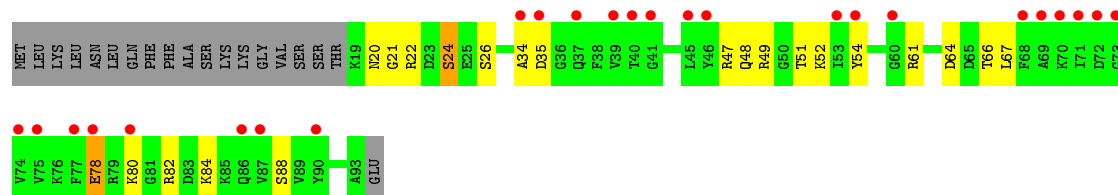
• Molecule 19: 50S ribosomal protein L24



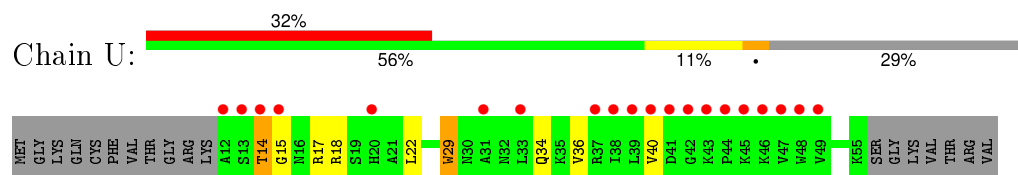
• Molecule 20: 50S ribosomal protein L25



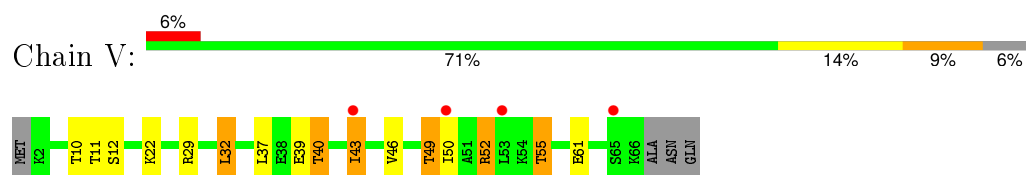
• Molecule 21: 50S ribosomal protein L27



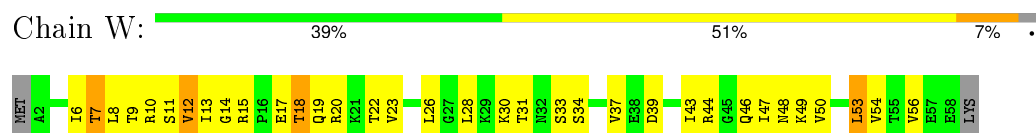
- Molecule 22: 50S ribosomal protein L28



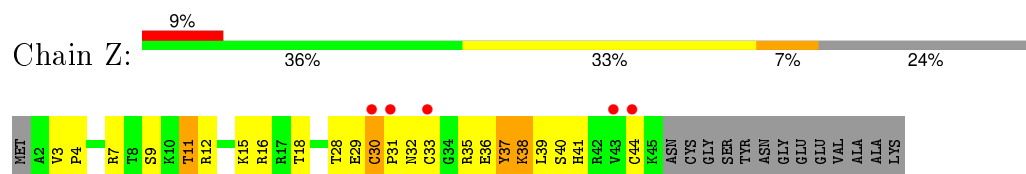
- Molecule 23: 50S ribosomal protein L29



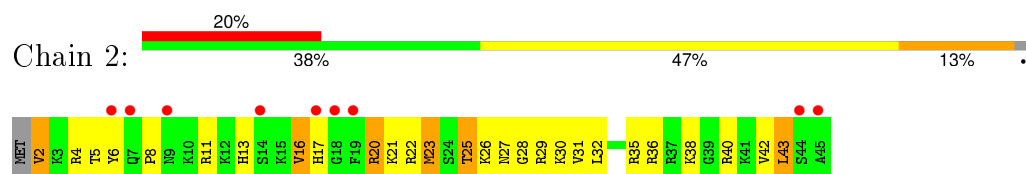
- Molecule 24: 50S ribosomal protein L30



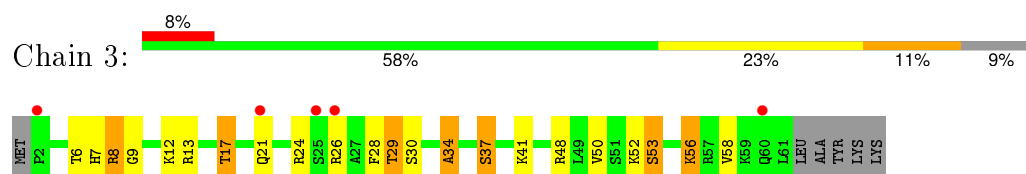
- Molecule 25: 50S ribosomal protein L32



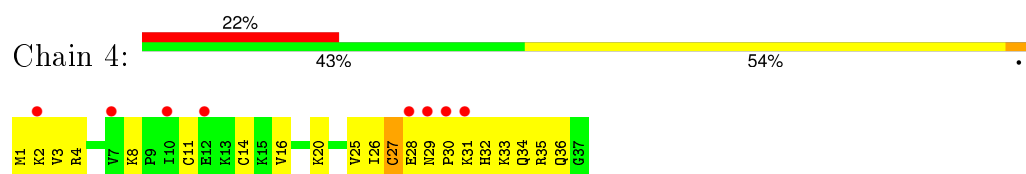
- Molecule 26: 50S ribosomal protein L34



- Molecule 27: 50S ribosomal protein L35



- Molecule 28: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	279.92Å 279.92Å 870.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	64.88 – 3.39 100.73 – 3.39	Depositor EDS
% Data completeness (in resolution range)	88.9 (64.88-3.39) 88.9 (100.73-3.39)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 3.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.202 , 0.243 0.205 , 0.245	Depositor DCC
R_{free} test set	12433 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	109.3	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 88.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 245649 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	81465	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZLD, MG, MN, NA, EOH, MPD, EPE, SPD

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	X	0.53	7/65113 (0.0%)	1.03	150/101510 (0.1%)
2	Y	0.50	0/2717	1.03	10/4232 (0.2%)
3	A	0.36	0/1652	0.67	0/2280
4	B	0.49	0/1554	0.76	0/2101
5	C	0.49	0/1339	0.76	0/1832
6	D	0.27	0/796	0.54	0/1104
7	E	0.36	0/937	0.64	0/1296
8	G	0.45	0/1109	0.69	0/1504
9	H	0.47	0/847	0.68	0/1150
10	I	0.56	0/825	0.90	1/1119 (0.1%)
11	J	0.47	0/1026	0.70	0/1390
12	K	0.44	0/899	0.71	0/1204
13	L	0.36	0/664	0.67	0/907
14	M	0.43	0/821	0.71	0/1110
15	N	0.53	0/944	0.73	0/1252
16	O	0.47	0/761	0.73	0/1022
17	P	0.48	0/870	0.69	0/1171
18	Q	0.35	0/591	0.60	0/809
19	R	0.36	0/686	0.63	0/934
20	S	0.45	0/1060	0.71	2/1461 (0.1%)
21	T	0.42	0/536	0.64	0/720
22	U	0.30	0/257	0.59	0/356
23	V	0.35	0/415	0.55	0/569
24	W	0.44	0/443	0.66	0/597
25	Z	0.57	0/342	0.89	0/457
26	2	0.41	0/372	0.63	0/487
27	3	0.50	0/418	0.80	0/558
28	4	0.37	0/265	0.58	0/356
All	All	0.51	7/88259 (0.0%)	0.97	163/133488 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying

if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	1
4	B	0	1
9	H	0	1
All	All	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	577	A	N9-C4	-8.16	1.32	1.37
1	X	1065	A	N9-C4	-7.99	1.33	1.37
1	X	577	A	C5-C6	-6.29	1.35	1.41
1	X	350	G	N9-C4	5.82	1.42	1.38
1	X	2845	G	N9-C4	-5.62	1.33	1.38
1	X	2048	G	N9-C4	-5.20	1.33	1.38
1	X	1065	A	N3-C4	-5.05	1.31	1.34

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	577	A	N1-C6-N6	13.04	126.42	118.60
1	X	577	A	C2-N3-C4	-11.54	104.83	110.60
1	X	2845	G	N3-C4-N9	-11.21	119.27	126.00
1	X	2845	G	N3-C4-C5	11.11	134.15	128.60
1	X	2048	G	C4-C5-N7	10.77	115.11	110.80
1	X	2048	G	C5-N7-C8	-10.48	99.06	104.30
1	X	1065	A	C2-N3-C4	-10.08	105.56	110.60
1	X	2808	A	O5'-P-OP1	-9.66	97.00	105.70
1	X	577	A	C6-C5-N7	-9.62	125.57	132.30
1	X	1659	C	C2-N1-C1'	9.57	129.33	118.80
1	X	350	G	N3-C4-C5	-9.37	123.92	128.60
1	X	577	A	C4-C5-N7	9.09	115.24	110.70
1	X	2845	G	C2-N3-C4	-8.88	107.46	111.90
2	Y	93	C	N3-C2-O2	-8.44	115.99	121.90
2	Y	93	C	N1-C2-O2	8.43	123.96	118.90
1	X	577	A	C5-N7-C8	-8.36	99.72	103.90
1	X	1953	U	C2-N1-C1'	8.14	127.47	117.70
1	X	350	G	C4-N9-C1'	8.14	137.08	126.50
1	X	350	G	N3-C4-N9	8.09	130.85	126.00
1	X	12	U	N3-C2-O2	-8.04	116.57	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2048	G	N3-C4-C5	7.84	132.52	128.60
1	X	2048	G	C2-N3-C4	-7.82	107.99	111.90
1	X	1186	A	C2-N3-C4	-7.75	106.72	110.60
1	X	1065	A	C5-N7-C8	-7.65	100.07	103.90
1	X	1659	C	C5-C6-N1	7.65	124.83	121.00
1	X	1030	C	C6-N1-C2	7.64	123.36	120.30
1	X	12	U	N1-C2-O2	7.43	128.00	122.80
1	X	577	A	C5-C6-N1	-7.40	114.00	117.70
1	X	577	A	N9-C4-C5	-7.39	102.84	105.80
1	X	2048	G	N7-C8-N9	7.35	116.78	113.10
1	X	12	U	C2-N1-C1'	7.33	126.49	117.70
1	X	428	G	N3-C4-C5	-7.27	124.97	128.60
1	X	268	A	O4'-C1'-N9	7.25	114.00	108.20
1	X	373	A	C2-N3-C4	-7.23	106.98	110.60
1	X	1200	A	N1-C6-N6	7.11	122.87	118.60
1	X	496	G	C4-N9-C1'	7.10	135.73	126.50
1	X	1065	A	N7-C8-N9	7.03	117.32	113.80
1	X	1568	U	P-O3'-C3'	7.02	128.12	119.70
2	Y	99	U	N3-C2-O2	-6.97	117.32	122.20
1	X	2716	U	C5-C4-O4	6.94	130.06	125.90
1	X	2845	G	N3-C2-N2	-6.93	115.05	119.90
1	X	657	U	C2-N1-C1'	6.92	126.01	117.70
1	X	1065	A	N1-C2-N3	6.92	132.76	129.30
1	X	721	A	C2-N3-C4	-6.90	107.15	110.60
1	X	2844	U	N1-C2-N3	6.88	119.03	114.90
1	X	1953	U	N1-C2-O2	6.85	127.59	122.80
2	Y	88	U	N3-C2-O2	-6.81	117.43	122.20
1	X	1659	C	C6-N1-C1'	-6.77	112.68	120.80
1	X	496	G	C8-N9-C1'	-6.76	118.21	127.00
1	X	512	A	N1-C6-N6	6.75	122.65	118.60
1	X	350	G	C8-N9-C4	-6.75	103.70	106.40
1	X	2024	A	C8-N9-C4	-6.55	103.18	105.80
1	X	2845	G	C8-N9-C1'	6.54	135.50	127.00
1	X	2048	G	C6-C5-N7	-6.52	126.49	130.40
1	X	1395	G	N3-C4-C5	-6.46	125.37	128.60
1	X	634	C	C6-N1-C2	-6.45	117.72	120.30
1	X	2787	C	C2-N1-C1'	6.44	125.89	118.80
1	X	1806	U	C5-C6-N1	-6.40	119.50	122.70
1	X	657	U	C6-N1-C1'	-6.38	112.27	121.20
1	X	1659	C	C6-N1-C2	-6.37	117.75	120.30
1	X	1659	C	N1-C2-O2	6.32	122.69	118.90
1	X	660	A	P-O3'-C3'	6.31	127.27	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	721	A	N1-C6-N6	6.31	122.39	118.60
20	S	21	LEU	CA-CB-CG	6.24	129.65	115.30
1	X	721	A	C6-C5-N7	-6.20	127.96	132.30
1	X	1065	A	C8-N9-C4	-6.16	103.33	105.80
1	X	428	G	N3-C4-N9	6.14	129.68	126.00
1	X	2048	G	N1-C6-O6	6.06	123.54	119.90
1	X	2483	C	C6-N1-C2	6.06	122.72	120.30
1	X	2716	U	N3-C4-O4	-6.05	115.17	119.40
1	X	350	G	C8-N9-C1'	-6.03	119.16	127.00
1	X	1200	A	C5-C6-N6	-6.02	118.89	123.70
1	X	634	C	C5-C6-N1	5.99	123.99	121.00
10	I	37	GLY	N-CA-C	-5.95	98.22	113.10
1	X	2479	C	C6-N1-C2	-5.95	117.92	120.30
1	X	890	G	P-O3'-C3'	5.94	126.82	119.70
1	X	1289	A	C2-N3-C4	-5.91	107.65	110.60
1	X	1395	G	C2-N3-C4	5.90	114.85	111.90
1	X	373	A	N1-C2-N3	5.89	132.25	129.30
1	X	577	A	N3-C4-C5	5.87	130.91	126.80
1	X	182	C	N1-C2-O2	5.86	122.42	118.90
1	X	1953	U	N3-C2-O2	-5.85	118.11	122.20
1	X	323	C	C6-N1-C2	-5.84	117.96	120.30
1	X	1453	G	C4-N9-C1'	-5.82	118.94	126.50
1	X	656	G	C8-N9-C4	-5.81	104.08	106.40
1	X	496	G	C4-C5-C6	5.80	122.28	118.80
1	X	659	A	O4'-C1'-N9	5.80	112.84	108.20
1	X	1305	U	N3-C2-O2	-5.79	118.15	122.20
1	X	2845	G	C5-N7-C8	-5.76	101.42	104.30
1	X	630	G	C4-C5-N7	5.72	113.09	110.80
1	X	955	A	N1-C6-N6	5.72	122.03	118.60
1	X	2534	C	N3-C2-O2	-5.71	117.90	121.90
1	X	496	G	C6-C5-N7	-5.70	126.98	130.40
1	X	2599	A	N1-C6-N6	5.70	122.02	118.60
1	X	1953	U	C6-N1-C1'	-5.68	113.25	121.20
1	X	657	U	C5-C4-O4	-5.68	122.49	125.90
1	X	1568	U	OP2-P-O3'	5.67	117.67	105.20
2	Y	92	G	N3-C4-C5	5.66	131.43	128.60
1	X	743	C	C6-N1-C2	5.61	122.54	120.30
1	X	113	U	C2-N1-C1'	5.58	124.39	117.70
1	X	2583	C	N1-C2-O2	5.56	122.23	118.90
2	Y	79	C	C2-N1-C1'	5.55	124.91	118.80
1	X	90	A	P-O3'-C3'	5.55	126.36	119.70
2	Y	108	G	O4'-C1'-N9	5.54	112.63	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	428	G	C4-N9-C1'	5.54	133.69	126.50
1	X	502	C	C6-N1-C2	5.53	122.51	120.30
1	X	2418	G	O4'-C1'-N9	5.52	112.61	108.20
1	X	2682	G	O4'-C1'-N9	5.50	112.60	108.20
1	X	793	G	O4'-C1'-N9	5.50	112.60	108.20
1	X	350	G	C2-N3-C4	5.48	114.64	111.90
1	X	350	G	O4'-C1'-N9	5.48	112.58	108.20
1	X	1350	U	C2-N1-C1'	5.48	124.27	117.70
1	X	1453	G	N3-C4-N9	-5.46	122.72	126.00
1	X	1566	G	C5-C6-N1	-5.45	108.78	111.50
1	X	496	G	N3-C4-N9	5.44	129.26	126.00
2	Y	79	C	C5-C4-N4	-5.42	116.41	120.20
1	X	16	G	C2-N3-C4	-5.41	109.19	111.90
1	X	428	G	C2-N3-C4	5.38	114.59	111.90
1	X	890	G	OP1-P-O3'	5.38	117.04	105.20
1	X	2845	G	C4-N9-C1'	-5.38	119.50	126.50
1	X	1065	A	N1-C6-N6	5.37	121.83	118.60
1	X	1491	C	C6-N1-C2	-5.36	118.16	120.30
1	X	955	A	O4'-C1'-N9	5.34	112.47	108.20
1	X	381	G	N3-C4-N9	5.33	129.20	126.00
1	X	1086	G	O4'-C1'-N9	5.33	112.46	108.20
1	X	1453	G	C8-N9-C1'	5.32	133.92	127.00
1	X	2752	A	C8-N9-C4	-5.32	103.67	105.80
1	X	557	G	O4'-C1'-N9	5.32	112.45	108.20
1	X	2534	C	N1-C2-O2	5.30	122.08	118.90
1	X	389	A	N7-C8-N9	5.28	116.44	113.80
1	X	1499	U	N3-C2-O2	-5.27	118.51	122.20
1	X	2716	U	C2-N1-C1'	-5.27	111.38	117.70
1	X	2081	A	C2-N3-C4	-5.26	107.97	110.60
20	S	63	LEU	CA-CB-CG	5.25	127.37	115.30
1	X	428	G	N1-C6-O6	-5.23	116.76	119.90
1	X	1065	A	N3-C4-N9	-5.22	123.22	127.40
1	X	503	A	C5-N7-C8	-5.21	101.29	103.90
1	X	378	C	C5-C6-N1	5.18	123.59	121.00
1	X	496	G	N3-C4-C5	-5.18	126.01	128.60
2	Y	79	C	C6-N1-C1'	-5.17	114.60	120.80
1	X	1395	G	N3-C4-N9	5.16	129.09	126.00
1	X	577	A	C5-C6-N6	-5.16	119.58	123.70
1	X	1593	G	C4-N9-C1'	5.14	133.19	126.50
1	X	661	U	C5-C6-N1	5.13	125.27	122.70
1	X	2740	A	N1-C6-N6	5.13	121.68	118.60
1	X	2667	G	C6-C5-N7	-5.13	127.32	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	43	A	O4'-C1'-N9	5.12	112.30	108.20
1	X	721	A	C5-N7-C8	-5.12	101.34	103.90
1	X	116	G	N3-C4-C5	-5.11	126.05	128.60
1	X	1294	G	C4-N9-C1'	5.11	133.14	126.50
1	X	2583	C	C2-N1-C1'	5.09	124.40	118.80
1	X	568	C	C6-N1-C2	5.09	122.33	120.30
1	X	2061	U	N3-C4-O4	5.08	122.96	119.40
1	X	350	G	N7-C8-N9	5.07	115.63	113.10
2	Y	90	C	C6-N1-C2	-5.07	118.27	120.30
1	X	660	A	OP1-P-OP2	-5.05	112.03	119.60
1	X	961	G	C4-C5-N7	5.04	112.81	110.80
1	X	582	G	N1-C6-O6	5.03	122.92	119.90
1	X	612	U	N1-C2-N3	5.02	117.91	114.90
1	X	496	G	N1-C6-O6	5.01	122.91	119.90
1	X	1017	A	C8-N9-C4	-5.01	103.80	105.80
1	X	235	G	P-O3'-C3'	5.00	125.71	119.70
1	X	1566	G	N3-C4-C5	5.00	131.10	128.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	128	ASN	Peptide
4	B	166	GLY	Peptide
9	H	83	ALA	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	58151	0	29248	918	0
2	Y	2430	0	1229	37	0
3	A	1620	0	1213	57	0
4	B	1531	0	1483	66	0
5	C	1321	0	1184	54	0
6	D	794	0	415	4	0
7	E	926	0	656	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	G	1087	0	1022	47	0
9	H	840	0	802	35	0
10	I	817	0	688	27	0
11	J	1003	0	970	44	0
12	K	896	0	921	35	0
13	L	659	0	505	17	0
14	M	809	0	811	23	0
15	N	932	0	997	45	0
16	O	751	0	744	24	0
17	P	862	0	920	45	0
18	Q	586	0	493	24	0
19	R	680	0	650	32	0
20	S	1048	0	847	15	0
21	T	530	0	494	19	0
22	U	254	0	165	4	0
23	V	414	0	354	9	0
24	W	441	0	478	20	0
25	Z	336	0	340	22	0
26	2	368	0	409	20	0
27	3	414	0	392	12	0
28	4	262	0	266	19	0
29	X	24	0	20	5	0
30	X	72	0	126	5	0
31	A	2	0	0	0	0
31	B	1	0	0	0	0
31	C	1	0	0	0	0
31	G	2	0	0	0	0
31	I	1	0	0	0	0
31	K	1	0	0	0	0
31	N	1	0	0	0	0
31	O	2	0	0	0	0
31	W	1	0	0	0	0
31	X	226	0	0	0	0
31	Y	6	0	0	0	0
31	Z	2	0	0	0	0
32	M	1	0	0	0	0
32	X	191	0	0	0	0
32	Y	2	0	0	0	0
32	Z	1	0	0	0	0
33	X	1	0	0	0	0
34	X	60	0	68	20	0
35	J	10	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	X	80	0	152	11	0
36	X	12	0	24	0	0
36	Y	3	0	6	0	0
All	All	81465	0	49111	1518	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1518) 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)
3:A:116:VAL:HG11	3:A:127:GLY:HA3	1.41	0.97
34:X:3426:EPE:H52	15:N:7:GLY:HA2	1.50	0.94
1:X:1521:A:N6	1:X:1560:A:N3	2.17	0.93
1:X:1247:G:O2'	1:X:1275:A:N6	2.02	0.92
5:C:17:ILE:HD11	5:C:124:THR:HG21	1.56	0.88
5:C:7:LEU:HG	5:C:124:THR:HG22	1.57	0.87
2:Y:18:G:H1	2:Y:61:U:H3	1.16	0.87
28:4:14:CYS:SG	28:4:32:HIS:ND1	2.49	0.86
1:X:1302:G:OP1	25:Z:16:ARG:NH2	2.08	0.85
1:X:1663:G:HO2'	26:2:2:VAL:N	1.74	0.85
2:Y:80:A:H61	2:Y:91:C:H42	1.23	0.85
1:X:2649:U:O2'	1:X:2845:G:N2	2.10	0.83
1:X:498:G:H21	1:X:503:A:H8	1.23	0.82
17:P:11:ARG:HH11	17:P:98:LYS:HD2	1.44	0.82
20:S:75:ALA:HB2	20:S:92:LEU:HB2	1.62	0.82
1:X:1515:G:H1	1:X:1565:U:H3	1.25	0.82
1:X:2505:A:H5'	28:4:31:LYS:HE3	1.62	0.82
1:X:1513:A:H3'	1:X:1514:A:H8	1.43	0.81
30:X:3010:MPD:HO2	30:X:3010:MPD:HO4	1.28	0.81
9:H:4:GLN:HG2	9:H:5:GLU:HG2	1.63	0.81
1:X:1472:C:N4	1:X:1617:A:OP2	2.14	0.81
19:R:80:ARG:NH1	19:R:95:LYS:O	2.14	0.80
1:X:329:A:H61	1:X:397:U:H3	1.28	0.80
8:G:20:ASP:HA	8:G:58:ILE:HG22	1.64	0.80
1:X:1039:C:OP2	15:N:54:LYS:NZ	2.14	0.79
3:A:92:ALA:H	3:A:106:ALA:HB2	1.46	0.79
4:B:7:GLY:HA2	4:B:53:PHE:CZ	2.17	0.79
9:H:1:MET:N	9:H:67:SER:OG	2.16	0.78
20:S:105:PRO:HD2	20:S:124:PRO:HA	1.63	0.78
1:X:1683:U:H2'	1:X:1684:A:H5''	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1518:G:N2	1:X:1562:C:N3	2.32	0.78
5:C:63:LYS:HE3	5:C:67:GLN:HG2	1.66	0.78
2:Y:79:C:H42	2:Y:92:G:H1	1.30	0.78
8:G:40:LYS:O	8:G:42:LYS:N	2.17	0.77
26:2:36:ARG:HG3	26:2:43:LEU:HD21	1.66	0.77
1:X:1467:G:HO2'	1:X:1543:G:HO2'	1.27	0.77
12:K:109:ARG:NH1	12:K:112:ASP:OD2	2.19	0.76
2:Y:4:G:H1	2:Y:111:A:H62	1.32	0.76
1:X:591:A:H4'	1:X:592:A:H5'	1.67	0.76
1:X:1300:G:OP2	17:P:99:ARG:NH2	2.18	0.76
1:X:1092:A:OP2	1:X:1154:G:N2	2.17	0.76
1:X:268:A:N6	1:X:473:U:O2'	2.19	0.76
28:4:27:CYS:O	28:4:29:ASN:N	2.17	0.76
1:X:615:A:OP2	16:O:79:ARG:NH2	2.18	0.76
1:X:719:G:H1'	5:C:74:ARG:HE	1.50	0.76
17:P:65:ASN:OD1	17:P:65:ASN:N	2.18	0.75
1:X:1275:A:H4'	1:X:1275:A:OP1	1.86	0.75
1:X:636:A:H62	30:X:3009:MPD:HM2	1.51	0.75
1:X:696:G:H5''	27:3:17:THR:HB	1.69	0.75
1:X:529:A:H1'	19:R:55:GLY:HA2	1.65	0.75
25:Z:15:LYS:O	25:Z:18:THR:HG23	1.87	0.75
1:X:2049:U:OP2	25:Z:12:ARG:NH2	2.20	0.75
1:X:2331:G:H22	1:X:2339:U:H3	1.32	0.75
1:X:2860:U:H5''	12:K:49:THR:HG21	1.67	0.74
11:J:116:GLU:OE1	11:J:119:ARG:NH1	2.20	0.74
8:G:7:ALA:H	8:G:46:THR:HG21	1.51	0.74
1:X:2618:C:H2'	1:X:2619:G:H8	1.51	0.74
1:X:120:G:H4'	1:X:150:A:H5'	1.70	0.74
17:P:80:PRO:O	17:P:100:THR:OG1	2.06	0.74
20:S:81:PRO:O	20:S:83:LYS:N	2.20	0.74
2:Y:65:G:O6	2:Y:105:G:N2	2.21	0.74
1:X:2419:A:H2	1:X:2451:C:H42	1.34	0.74
19:R:38:VAL:HB	19:R:61:ALA:HB3	1.70	0.73
21:T:47:ARG:HE	21:T:66:THR:HG21	1.53	0.73
1:X:460:C:O2	1:X:1891:U:O2'	2.06	0.73
16:O:9:GLY:H	16:O:10:LYS:HE3	1.54	0.73
1:X:743:C:O2'	1:X:779:A:N6	2.20	0.73
3:A:209:GLY:HA2	3:A:212:ARG:HB2	1.71	0.73
11:J:51:ARG:HA	11:J:54:MET:HE2	1.70	0.73
1:X:629:A:H62	1:X:1289:A:H2	1.36	0.72
1:X:1528:G:N2	1:X:1547:C:N3	2.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:73:ASP:HB3	14:M:82:LYS:HD3	1.71	0.72
1:X:627:C:OP2	34:X:3426:EPE:O1S	2.08	0.72
5:C:108:LEU:O	5:C:112:SER:OG	2.05	0.72
6:D:65:PRO:HD2	6:D:83:MET:HA	1.71	0.72
11:J:43:THR:N	11:J:46:GLN:OE1	2.18	0.72
1:X:1512:U:H2'	1:X:1513:A:C8	2.25	0.72
1:X:624:C:OP2	15:N:33:LYS:NZ	2.23	0.72
10:I:43:GLY:O	10:I:45:GLY:N	2.21	0.71
1:X:2779:C:H3'	1:X:2780:A:H8	1.55	0.71
1:X:2072:C:H5''	25:Z:15:LYS:HD2	1.70	0.71
17:P:11:ARG:O	17:P:11:ARG:NH2	2.18	0.71
16:O:42:GLY:HA2	16:O:46:VAL:HG12	1.71	0.71
1:X:2817:A:O2'	1:X:2818:A:OP2	2.09	0.71
19:R:59:THR:OG1	19:R:60:GLU:N	2.24	0.71
1:X:235:G:O2'	1:X:236:A:O5'	2.08	0.71
10:I:67:THR:OG1	10:I:68:ASN:N	2.22	0.71
2:Y:74:G:H22	2:Y:97:A:H61	1.39	0.70
4:B:119:THR:HG23	4:B:179:THR:HG22	1.74	0.70
11:J:90:VAL:HG12	11:J:91:GLU:H	1.56	0.70
13:L:17:ARG:NH1	13:L:92:ILE:O	2.24	0.70
1:X:659:A:H1'	1:X:660:A:H5'	1.73	0.70
1:X:735:C:O2'	1:X:825:G:OP1	2.09	0.70
12:K:28:GLU:HB3	12:K:121:LEU:HD11	1.72	0.70
19:R:6:GLY:HA2	19:R:23:VAL:HG22	1.74	0.70
13:L:70:VAL:O	13:L:72:LEU:N	2.25	0.70
4:B:59:TYR:O	4:B:61:LYS:N	2.25	0.70
28:4:27:CYS:SG	28:4:32:HIS:ND1	2.61	0.70
1:X:1758:A:N7	1:X:1772:G:N1	2.40	0.70
1:X:721:A:H8	1:X:2096:G:H21	1.38	0.69
4:B:26:THR:HG21	4:B:201:VAL:HG22	1.74	0.69
9:H:64:ARG:NH1	9:H:101:PRO:O	2.25	0.69
8:G:85:ILE:O	8:G:87:SER:N	2.26	0.69
4:B:118:VAL:HG21	4:B:201:VAL:HG12	1.73	0.69
1:X:2360:A:H5'	1:X:2362:A:H1'	1.73	0.69
3:A:107:PRO:HA	3:A:195:VAL:HA	1.75	0.69
1:X:2808:A:H5''	1:X:2809:G:O5'	1.91	0.69
1:X:738:U:O2'	1:X:1390:A:N3	2.25	0.69
11:J:30:GLY:O	11:J:134:ARG:NH2	2.26	0.69
1:X:2314:A:O2'	1:X:2315:A:H2'	1.93	0.69
1:X:201:C:H42	1:X:251:G:H1	1.41	0.69
1:X:396:G:H2'	1:X:397:U:H5'	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1185:U:H2'	8:G:66:THR:HG21	1.75	0.68
8:G:63:ILE:O	8:G:94:ARG:NH1	2.26	0.68
7:E:70:ALA:O	7:E:74:ASN:ND2	2.20	0.68
1:X:318:A:C6	1:X:319:G:H1'	2.29	0.68
1:X:388:A:H1'	1:X:389:A:H2	1.58	0.68
1:X:1440:A:O2'	1:X:1514:A:O2'	2.12	0.68
20:S:105:PRO:HG3	20:S:125:LEU:HG	1.75	0.68
1:X:787:U:H2'	1:X:788:A:C8	2.29	0.68
9:H:21:THR:HB	9:H:39:ILE:HD12	1.76	0.68
1:X:1518:G:H1	1:X:1562:C:H42	1.42	0.67
1:X:51:G:O2'	1:X:118:A:N1	2.28	0.67
2:Y:69:C:H42	2:Y:102:A:H61	1.41	0.67
21:T:54:TYR:CE2	21:T:84:LYS:HD3	2.29	0.67
16:O:5:ILE:HG22	16:O:38:VAL:HG22	1.76	0.67
1:X:1400:C:O2'	1:X:1836:A:H1'	1.94	0.67
4:B:107:VAL:HG21	4:B:193:LYS:HA	1.75	0.67
5:C:190:ASP:OD1	5:C:191:SER:N	2.27	0.67
4:B:132:LYS:HG2	4:B:173:MET:HE1	1.75	0.67
1:X:923:A:N6	1:X:925:G:N7	2.42	0.67
3:A:15:ASN:O	3:A:204:ASN:ND2	2.28	0.67
21:T:54:TYR:HE2	21:T:84:LYS:HD3	1.58	0.67
18:Q:13:THR:O	18:Q:17:SER:N	2.27	0.67
18:Q:53:VAL:HA	18:Q:80:VAL:HG12	1.76	0.67
1:X:2355:A:H2'	1:X:2356:A:C8	2.30	0.67
1:X:1836:A:H2'	1:X:1837:A:C8	2.29	0.67
5:C:51:VAL:HG11	5:C:91:GLY:HA3	1.77	0.67
3:A:171:TYR:HD1	3:A:185:LEU:HA	1.60	0.67
1:X:1818:A:N6	1:X:1855:G:O2'	2.28	0.66
1:X:2007:G:O2'	1:X:2009:U:OP2	2.12	0.66
1:X:2495:A:O2'	1:X:2496:A:H8	1.78	0.66
4:B:159:ASP:O	4:B:161:SER:N	2.28	0.66
22:U:14:THR:OG1	22:U:15:GLY:N	2.29	0.66
1:X:2717:A:N6	12:K:13:ARG:HD2	2.10	0.66
14:M:26:ASP:HB3	14:M:92:GLY:H	1.61	0.66
9:H:101:PRO:HD3	14:M:68:SER:HB2	1.78	0.66
12:K:105:LYS:HA	12:K:117:VAL:HG12	1.78	0.66
4:B:156:MET:HB2	4:B:160:ALA:HB3	1.76	0.66
1:X:1826:G:H5'	1:X:1846:A:H61	1.61	0.66
17:P:86:ARG:HG3	17:P:87:PRO:HD2	1.78	0.66
24:W:8:LEU:HB2	24:W:28:LEU:HD23	1.78	0.66
1:X:1465:G:H2'	1:X:1466:G:H8	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2668:A:P	8:G:77:ARG:HH21	2.18	0.66
5:C:157:GLU:O	5:C:159:GLU:N	2.28	0.66
1:X:858:U:H2'	1:X:859:C:C6	2.31	0.66
1:X:2712:G:OP2	14:M:51:LYS:NZ	2.25	0.66
1:X:1065:A:H62	1:X:1185:U:H3	1.42	0.65
1:X:1644:C:OP1	18:Q:76:ARG:NH2	2.29	0.65
11:J:14:ARG:HD3	11:J:72:THR:HG22	1.77	0.65
9:H:88:ARG:HG2	9:H:94:ARG:HG2	1.79	0.65
1:X:364:A:O2'	1:X:383:A:O2'	2.14	0.65
1:X:638:U:H2'	1:X:639:U:C6	2.30	0.65
1:X:2835:C:H1'	25:Z:39:LEU:HD23	1.77	0.65
19:R:70:LEU:HD12	19:R:71:LEU:H	1.60	0.65
24:W:8:LEU:HD23	24:W:31:THR:HA	1.78	0.65
21:T:80:LYS:HB3	21:T:84:LYS:HB2	1.79	0.65
28:4:2:LYS:HB2	28:4:34:GLN:HG2	1.78	0.65
1:X:131:G:N1	1:X:148:U:O2	2.17	0.65
17:P:11:ARG:NH1	17:P:98:LYS:HD2	2.11	0.65
1:X:1013:U:O3'	24:W:14:GLY:HA2	1.97	0.65
1:X:1575:A:H2'	1:X:1576:A:H5'	1.79	0.65
3:A:90:ASN:N	3:A:90:ASN:OD1	2.30	0.64
8:G:14:ARG:NH1	8:G:50:ASP:O	2.30	0.64
1:X:1082:C:H42	1:X:1161:A:H61	1.44	0.64
17:P:2:GLU:HB3	17:P:108:SER:HA	1.80	0.64
15:N:98:ILE:HG12	16:O:2:PHE:HZ	1.61	0.64
10:I:112:LEU:HD22	10:I:112:LEU:H	1.62	0.64
5:C:111:ARG:O	5:C:115:SER:OG	2.15	0.64
24:W:50:VAL:HB	24:W:53:LEU:HD11	1.80	0.64
13:L:43:GLN:HA	13:L:54:ALA:HB3	1.77	0.64
20:S:55:VAL:HG22	20:S:56:GLY:H	1.63	0.64
1:X:955:A:C4	11:J:15:PRO:HG3	2.32	0.64
1:X:1091:G:H4'	1:X:1092:A:O5'	1.98	0.64
1:X:645:A:O2'	1:X:647:G:O2'	2.12	0.64
34:X:3426:EPE:H61	15:N:10:THR:HG23	1.79	0.64
28:4:25:VAL:HB	28:4:34:GLN:HB2	1.79	0.64
5:C:4:TYR:HA	5:C:18:GLU:HA	1.80	0.64
1:X:658:A:H3'	1:X:659:A:H5''	1.80	0.64
1:X:1448:U:H3'	1:X:1449:A:H5''	1.80	0.64
1:X:2856:U:H2'	1:X:2857:A:C8	2.32	0.64
3:A:200:HIS:O	3:A:203:VAL:HG22	1.97	0.64
1:X:1250:G:H2'	1:X:1274:G:N2	2.13	0.64
5:C:123:LEU:HD12	5:C:188:ASN:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:22:ARG:HB3	26:2:32:LEU:HD11	1.80	0.64
1:X:707:G:O2'	10:I:14:LYS:NZ	2.30	0.63
23:V:10:THR:O	23:V:12:SER:N	2.31	0.63
1:X:139:U:O2'	1:X:140:A:O5'	2.17	0.63
1:X:2757:U:H2'	1:X:2758:G:H8	1.61	0.63
1:X:83:G:H1	1:X:101:G:HO2'	1.44	0.63
1:X:2618:C:H2'	1:X:2619:G:C8	2.31	0.63
1:X:718:C:OP1	5:C:54:ARG:NH1	2.30	0.63
1:X:1353:A:H2'	1:X:1354:G:C8	2.32	0.63
3:A:211:SER:O	3:A:216:ILE:HB	1.98	0.63
1:X:2706:A:H4'	4:B:178:VAL:HG21	1.81	0.63
4:B:187:GLN:HB3	4:B:196:LEU:HD22	1.79	0.63
1:X:2817:A:N6	1:X:2825:U:O4	2.32	0.63
1:X:503:A:H62	1:X:516:A:H5''	1.64	0.62
1:X:1565:U:H2'	1:X:1566:G:C8	2.34	0.62
11:J:14:ARG:HD2	11:J:73:PRO:HD2	1.79	0.62
1:X:695:C:N4	1:X:696:G:O6	2.32	0.62
1:X:700:A:H4'	1:X:701:G:H5'	1.81	0.62
1:X:2060:A:O2'	1:X:2062:G:OP2	2.17	0.62
1:X:630:G:OP2	10:I:21:ARG:NH1	2.32	0.62
1:X:613:G:H2'	1:X:2057:A:N7	2.15	0.62
1:X:2249:G:O3'	3:A:171:TYR:OH	2.18	0.62
1:X:2024:A:H8	4:B:138:ARG:NH1	1.97	0.62
1:X:739:U:OP1	3:A:59:LYS:NZ	2.33	0.62
1:X:485:A:H2'	1:X:486:G:O4'	1.99	0.62
1:X:2231:C:N3	1:X:2248:G:N2	2.48	0.62
1:X:498:G:N2	1:X:503:A:H8	1.94	0.62
1:X:90:A:H8	1:X:90:A:OP1	1.83	0.62
24:W:26:LEU:HD21	24:W:46:GLN:HB3	1.81	0.62
9:H:80:ASP:OD2	14:M:64:ARG:NH2	2.31	0.62
1:X:1835:U:H2'	1:X:1836:A:H5''	1.80	0.61
3:A:169:GLY:O	3:A:171:TYR:N	2.32	0.61
23:V:22:LYS:HG2	23:V:50:ILE:HD13	1.81	0.61
1:X:1250:G:O2'	1:X:1275:A:N1	2.31	0.61
1:X:24:G:H2'	1:X:25:U:C6	2.35	0.61
1:X:2717:A:H62	12:K:13:ARG:HD2	1.65	0.61
1:X:637:U:H2'	1:X:638:U:C6	2.36	0.61
1:X:89:U:H3'	1:X:90:A:H2'	1.82	0.61
1:X:83:G:H21	1:X:102:A:H2	1.48	0.61
34:X:3426:EPE:H31	34:X:3426:EPE:O1S	2.00	0.61
3:A:210:ARG:HA	3:A:213:TRP:CE3	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:364:A:HO2'	1:X:383:A:HO2'	1.46	0.61
28:4:1:MET:HB2	28:4:33:LYS:HB3	1.83	0.61
17:P:4:LYS:HB2	17:P:106:VAL:HG22	1.81	0.61
9:H:13:ASN:HD21	9:H:97:ARG:H	1.49	0.61
1:X:1821:U:H2'	1:X:1822:C:C6	2.35	0.61
17:P:90:GLN:OE1	17:P:92:ARG:NH2	2.33	0.61
1:X:1830:A:N1	1:X:1849:G:O2'	2.32	0.61
13:L:21:ASN:OD1	13:L:30:ARG:NH1	2.33	0.61
1:X:926:G:H21	1:X:941:A:H62	1.49	0.61
1:X:1337:A:H4'	1:X:1338:U:H5''	1.81	0.61
14:M:26:ASP:HB2	14:M:90:ARG:O	2.00	0.61
1:X:2740:A:O2'	1:X:2742:C:OP2	2.14	0.61
1:X:1468:G:H1	1:X:1621:C:H42	1.49	0.60
1:X:513:G:OP2	26:2:35:ARG:NH1	2.30	0.60
9:H:72:ASN:N	9:H:72:ASN:OD1	2.32	0.60
1:X:459:C:HO2'	1:X:1907:U:HO2'	1.49	0.60
1:X:24:G:H2'	1:X:25:U:H6	1.66	0.60
1:X:1869:G:H1	1:X:1925:U:H3	1.48	0.60
1:X:2088:G:O6	29:X:3001:ZLD:H9	2.00	0.60
26:2:16:VAL:H	26:2:21:LYS:HG3	1.65	0.60
9:H:63:VAL:HG12	9:H:106:LEU:HD11	1.82	0.60
1:X:633:A:H2'	1:X:634:C:C6	2.36	0.60
1:X:1423:C:H2'	1:X:1424:A:C8	2.37	0.60
1:X:1488:A:H61	1:X:1595:C:H42	1.50	0.60
13:L:45:ILE:HG23	13:L:52:THR:HG22	1.82	0.60
17:P:14:PRO:O	17:P:18:ARG:HG3	2.02	0.60
1:X:877:G:H2'	1:X:878:C:C6	2.37	0.60
1:X:1885:G:H1'	1:X:1911:A:N6	2.17	0.60
1:X:1518:G:H1	1:X:1562:C:N4	1.99	0.60
1:X:2314:A:H2	1:X:2373:A:H62	1.49	0.60
1:X:922:G:O6	1:X:942:C:N4	2.34	0.60
1:X:575:G:HO2'	1:X:577:A:H2	1.49	0.60
1:X:1359:A:N1	1:X:1370:C:O2'	2.30	0.60
1:X:503:A:H2	1:X:517:A:H62	1.50	0.60
12:K:59:ARG:HA	12:K:86:PHE:CZ	2.35	0.60
1:X:229:A:O2'	1:X:231:A:N1	2.33	0.60
15:N:26:GLY:O	15:N:29:HIS:ND1	2.34	0.60
1:X:788:A:O2'	1:X:1703:U:OP1	2.15	0.59
1:X:2000:G:H2'	1:X:2001:C:H6	1.66	0.59
1:X:1636:U:N3	1:X:1637:A:N7	2.49	0.59
1:X:1280:U:H2'	1:X:1281:U:C6	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:57:LEU:HA	27:3:12:LYS:HB3	1.84	0.59
20:S:105:PRO:HG2	20:S:123:GLN:O	2.02	0.59
1:X:1780:G:H5''	14:M:95:ARG:HD2	1.83	0.59
5:C:147:GLU:O	5:C:148:GLN:NE2	2.20	0.59
8:G:92:GLU:O	8:G:94:ARG:N	2.36	0.59
1:X:2717:A:H5''	12:K:4:ARG:HH22	1.67	0.59
1:X:1826:G:N7	3:A:178:SER:OG	2.35	0.59
1:X:2566:C:H5'	28:4:3:VAL:HG21	1.83	0.59
1:X:1568:U:O2'	1:X:1569:G:OP2	2.17	0.59
5:C:149:PRO:HD2	5:C:186:ILE:O	2.03	0.59
4:B:123:LYS:HG2	4:B:204:PRO:HB3	1.83	0.59
1:X:1563:U:H2'	1:X:1564:G:C8	2.37	0.59
1:X:1398:G:O2'	1:X:2242:G:O2'	2.19	0.59
12:K:52:LYS:HE3	12:K:94:THR:HA	1.85	0.59
1:X:1710:G:O3'	9:H:6:THR:HG23	2.02	0.59
1:X:1806:U:H5	1:X:1811:A:N7	2.01	0.59
1:X:1514:A:N6	1:X:1566:G:H1	2.01	0.59
3:A:128:ASN:HA	3:A:191:THR:HG23	1.84	0.59
1:X:1482:U:H3	1:X:1601:U:H5	1.50	0.59
2:Y:64:A:N6	2:Y:104:C:H2'	2.18	0.59
1:X:273:A:N1	1:X:415:U:O2'	2.35	0.59
1:X:1063:U:H3	1:X:1186:A:H62	1.50	0.58
1:X:1560:A:H4'	30:X:3005:MPD:H12	1.85	0.58
1:X:106:A:H2'	1:X:107:G:H8	1.68	0.58
1:X:1241:A:H2'	1:X:1242:A:C8	2.38	0.58
1:X:2757:U:H2'	1:X:2758:G:C8	2.37	0.58
1:X:164:A:O2'	1:X:165:C:H5'	2.02	0.58
1:X:827:A:C8	3:A:220:VAL:HG21	2.38	0.58
17:P:24:ILE:HG13	17:P:32:ALA:HB1	1.86	0.58
1:X:1758:A:H3'	1:X:1758:A:N3	2.18	0.58
1:X:2313:A:H4'	1:X:2314:A:O4'	2.04	0.58
1:X:89:U:OP2	1:X:90:A:O2'	2.19	0.58
24:W:6:ILE:HG12	24:W:56:VAL:HG12	1.84	0.58
1:X:1512:U:H2'	1:X:1513:A:H8	1.67	0.58
11:J:51:ARG:HD3	11:J:66:ILE:HD11	1.86	0.58
3:A:83:TYR:HA	3:A:90:ASN:HB3	1.84	0.58
1:X:1490:G:O2'	1:X:1491:C:O5'	2.21	0.58
34:X:3423:EPE:H62	4:B:146:HIS:CE1	2.38	0.58
1:X:841:C:H2'	1:X:842:U:H6	1.68	0.58
1:X:2319:U:H2'	1:X:2320:C:C6	2.38	0.58
1:X:132:C:H42	1:X:147:G:H1	1.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2024:A:H2'	1:X:2025:A:H8	1.69	0.58
1:X:1436:C:HO2'	1:X:1437:U:H6	1.52	0.58
1:X:1378:U:H3'	1:X:1434:U:O2	2.04	0.58
9:H:6:THR:O	9:H:21:THR:HG22	2.04	0.58
1:X:1053:A:H5''	15:N:63:THR:HG22	1.85	0.58
1:X:2851:G:N7	4:B:64:LYS:HG3	2.19	0.58
34:X:3425:EPE:H101	21:T:24:SER:OG	2.04	0.58
20:S:10:GLN:HB2	20:S:40:SER:HB3	1.86	0.58
1:X:2495:A:OP1	11:J:119:ARG:NH2	2.37	0.58
1:X:319:G:N2	1:X:320:U:O3'	2.37	0.58
1:X:1501:G:H22	1:X:2729:G:H1	1.51	0.58
1:X:1882:G:H2'	1:X:1883:A:H8	1.69	0.58
24:W:19:GLN:O	24:W:23:VAL:HG23	2.04	0.58
17:P:11:ARG:HE	17:P:98:LYS:HB3	1.68	0.57
4:B:126:GLY:O	4:B:128:GLN:HG2	2.03	0.57
1:X:1830:A:N6	1:X:1841:G:O2'	2.35	0.57
19:R:64:HIS:O	19:R:66:SER:N	2.37	0.57
1:X:955:A:C6	11:J:15:PRO:HD3	2.39	0.57
1:X:1023:A:H2'	1:X:1026:C:H42	1.70	0.57
34:X:3426:EPE:H81	15:N:11:ARG:H	1.70	0.57
1:X:1302:G:C6	1:X:1303:A:N6	2.72	0.57
1:X:2760:A:N1	4:B:216:LYS:HB2	2.19	0.57
5:C:103:LYS:HA	5:C:106:ARG:NE	2.19	0.57
1:X:38:A:O2'	1:X:39:C:OP1	2.13	0.57
24:W:10:ARG:HB2	24:W:53:LEU:HA	1.85	0.57
1:X:901:G:H2'	1:X:902:A:C8	2.39	0.57
12:K:18:ARG:NE	12:K:65:THR:O	2.31	0.57
8:G:85:ILE:HG12	8:G:87:SER:CB	2.35	0.57
11:J:39:THR:HG23	11:J:98:LYS:HA	1.87	0.57
1:X:503:A:N6	1:X:516:A:H5''	2.18	0.57
1:X:1383:G:N2	1:X:1644:C:O2	2.33	0.57
17:P:69:LEU:HD22	17:P:107:VAL:HB	1.86	0.57
34:X:3426:EPE:H82	15:N:8:THR:H	1.68	0.57
1:X:2818:A:H2'	1:X:2819:C:O4'	2.04	0.57
12:K:47:LEU:HB3	12:K:85:LEU:HD21	1.87	0.57
8:G:93:LEU:HD22	8:G:101:LEU:HB2	1.87	0.57
1:X:2098:A:H2'	1:X:2099:G:H8	1.69	0.57
3:A:91:ILE:HG22	3:A:105:ILE:HA	1.86	0.57
1:X:1725:G:N3	1:X:1789:A:O2'	2.34	0.57
8:G:15:LYS:N	8:G:53:ASP:OD1	2.37	0.57
1:X:105:C:O2	1:X:337:A:O2'	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1567:A:H5''	1:X:1568:U:H2'	1.86	0.57
26:2:22:ARG:O	26:2:28:GLY:HA3	2.05	0.57
1:X:577:A:O2'	1:X:578:G:OP1	2.19	0.57
1:X:716:C:H2'	1:X:717:C:H6	1.70	0.57
11:J:59:LYS:O	11:J:61:GLY:N	2.37	0.57
1:X:363:A:H4'	1:X:365:A:N7	2.20	0.57
5:C:39:LEU:HD11	5:C:99:TYR:O	2.05	0.57
1:X:2098:A:H2'	1:X:2099:G:C8	2.40	0.56
8:G:68:ASN:HB3	8:G:71:THR:HB	1.85	0.56
1:X:1515:G:N2	1:X:1565:U:O2	2.37	0.56
1:X:49:A:N7	1:X:119:U:H5	2.02	0.56
1:X:1398:G:HO2'	1:X:2242:G:HO2'	1.53	0.56
5:C:124:THR:HG23	5:C:190:ASP:O	2.05	0.56
1:X:15:G:H4'	25:Z:18:THR:HB	1.87	0.56
1:X:1436:C:O2'	1:X:1437:U:O5'	2.23	0.56
11:J:38:THR:HG23	11:J:128:LYS:HB2	1.86	0.56
9:H:98:ILE:HB	9:H:118:ALA:HB2	1.87	0.56
1:X:2554:C:H5''	28:4:30:PRO:HB3	1.88	0.56
1:X:439:U:H2'	1:X:440:C:C6	2.40	0.56
1:X:1460:U:H3	1:X:1628:A:H61	1.52	0.56
1:X:1039:C:N3	8:G:4:THR:HG22	2.21	0.56
7:E:150:SER:HA	7:E:153:PRO:HG3	1.87	0.56
1:X:2549:U:O2'	1:X:2674:U:OP1	2.20	0.56
15:N:83:LEU:HD22	15:N:88:ILE:HG13	1.87	0.56
1:X:1605:A:N3	30:X:3005:MPD:HM1	2.21	0.56
10:I:81:GLN:CB	10:I:110:LYS:H	2.18	0.56
16:O:14:VAL:HG12	16:O:20:ILE:HG21	1.87	0.56
19:R:86:VAL:HG23	19:R:90:LYS:HD3	1.88	0.56
1:X:1424:A:H2'	1:X:1425:G:C8	2.41	0.56
3:A:36:PRO:HD2	3:A:62:TYR:O	2.06	0.56
1:X:2425:U:H2'	1:X:2426:G:C8	2.40	0.56
5:C:125:VAL:HG12	5:C:190:ASP:HA	1.88	0.56
1:X:214:G:H2'	1:X:215:G:O4'	2.05	0.56
1:X:1356:G:H3'	1:X:1357:G:N2	2.20	0.55
9:H:20:LEU:HB3	9:H:42:THR:HG22	1.87	0.55
12:K:32:THR:HG22	12:K:33:THR:H	1.72	0.55
4:B:141:MET:N	4:B:141:MET:SD	2.78	0.55
1:X:504:G:C8	26:2:38:LYS:HG2	2.41	0.55
1:X:878:C:H1'	10:I:48:PRO:HB3	1.87	0.55
1:X:1511:C:O2	1:X:1571:G:N2	2.39	0.55
1:X:2039:G:OP1	17:P:11:ARG:NH1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:658:A:H3'	1:X:659:A:C5'	2.36	0.55
4:B:140:PRO:HG2	4:B:145:SER:HB2	1.89	0.55
1:X:1609:U:H2'	1:X:1610:G:C8	2.42	0.55
5:C:14:SER:OG	5:C:15:GLY:N	2.35	0.55
26:2:20:ARG:HB2	26:2:20:ARG:HH11	1.72	0.55
1:X:2234:C:H2'	1:X:2235:A:C8	2.41	0.55
25:Z:31:PRO:O	25:Z:33:CYS:N	2.38	0.55
28:4:3:VAL:HA	28:4:35:ARG:O	2.06	0.55
10:I:70:ASN:O	10:I:72:LYS:N	2.32	0.55
1:X:1696:C:OP1	12:K:5:LYS:HD3	2.07	0.55
1:X:2351:U:H3	1:X:2358:G:H1	1.53	0.55
1:X:506:A:H2	1:X:515:G:H21	1.54	0.55
19:R:36:GLU:CD	19:R:36:GLU:H	2.09	0.55
24:W:11:SER:OG	24:W:13:ILE:HG13	2.07	0.55
34:X:3426:EPE:H62	15:N:6:GLY:C	2.27	0.55
34:X:3426:EPE:H82	15:N:8:THR:N	2.21	0.55
1:X:2650:G:O5'	1:X:2845:G:N2	2.39	0.55
1:X:1013:U:H2'	1:X:1014:U:C6	2.42	0.55
1:X:1352:C:H42	1:X:1374:G:H1	1.55	0.55
1:X:1424:A:H2'	1:X:1425:G:H8	1.72	0.55
1:X:1501:G:C4	1:X:1502:A:H2	2.24	0.55
12:K:45:GLU:OE1	12:K:101:THR:HB	2.07	0.55
1:X:1226:G:HO2'	1:X:1227:U:H6	1.55	0.55
20:S:73:MET:HG3	20:S:94:ILE:HD13	1.88	0.55
1:X:1700:C:H2'	1:X:1701:U:H6	1.71	0.55
1:X:660:A:H1'	1:X:661:U:H5''	1.87	0.55
7:E:63:THR:O	7:E:67:THR:HG23	2.06	0.55
1:X:2470:C:H2'	1:X:2471:G:C8	2.42	0.55
1:X:2559:G:O2'	1:X:2684:A:N1	2.40	0.55
1:X:1739:G:H8	3:A:8:PRO:HB2	1.72	0.55
7:E:80:SER:OG	7:E:81:GLN:N	2.39	0.55
28:4:27:CYS:HB3	28:4:32:HIS:HB2	1.89	0.55
1:X:460:C:H2'	1:X:461:A:H8	1.71	0.55
1:X:2533:U:H1'	29:X:3001:ZLD:H24A	1.88	0.55
1:X:841:C:H2'	1:X:842:U:C6	2.41	0.55
1:X:1378:U:OP1	1:X:1434:U:N3	2.40	0.55
19:R:11:VAL:HA	19:R:67:ASN:HB2	1.88	0.55
1:X:2851:G:C8	4:B:64:LYS:HG3	2.42	0.55
19:R:11:VAL:HG13	19:R:17:LYS:HA	1.89	0.55
5:C:163:VAL:O	5:C:165:LEU:N	2.40	0.55
1:X:2642:U:C2	25:Z:4:PRO:HA	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:38:GLN:O	15:N:42:SER:HB2	2.07	0.55
1:X:579:U:H2'	1:X:580:C:C6	2.42	0.55
1:X:1700:C:H2'	1:X:1701:U:C6	2.42	0.55
5:C:102:PRO:HB2	5:C:105:MET:HG3	1.88	0.55
1:X:677:A:H2'	1:X:678:A:C8	2.42	0.55
1:X:1037:A:OP1	15:N:50:ARG:NH1	2.40	0.55
20:S:44:ASP:OD1	20:S:45:GLU:N	2.39	0.54
1:X:2052:C:H2'	1:X:2053:U:C6	2.42	0.54
25:Z:39:LEU:O	25:Z:41:HIS:ND1	2.35	0.54
1:X:1769:C:N4	1:X:1770:C:H41	2.05	0.54
1:X:1352:C:H2'	1:X:1353:A:C8	2.41	0.54
1:X:1072:A:N6	1:X:1169:G:H2'	2.21	0.54
8:G:60:ALA:HB3	8:G:127:GLY:HA2	1.88	0.54
4:B:67:LYS:HA	4:B:86:ARG:NH2	2.22	0.54
1:X:631:U:H2'	1:X:632:U:C6	2.42	0.54
1:X:577:A:H8	15:N:28:LYS:HE3	1.72	0.54
19:R:11:VAL:HA	19:R:67:ASN:CB	2.38	0.54
1:X:1833:C:N4	1:X:1839:G:O6	2.40	0.54
1:X:1658:A:H61	17:P:88:ARG:H	1.54	0.54
1:X:2112:C:H42	1:X:2261:A:H61	1.54	0.54
2:Y:60:C:H2'	2:Y:61:U:H6	1.72	0.54
12:K:32:THR:HG22	12:K:33:THR:N	2.22	0.54
5:C:50:ALA:HB2	5:C:94:PRO:HD3	1.89	0.54
1:X:1487:G:H1	1:X:1597:U:H3	1.53	0.54
1:X:1698:A:H1'	1:X:2843:A:H5'	1.90	0.54
1:X:1304:G:N7	17:P:15:ARG:HG2	2.22	0.54
3:A:171:TYR:CD1	3:A:185:LEU:HA	2.42	0.54
1:X:1315:C:OP1	12:K:32:THR:HG23	2.07	0.54
1:X:2330:G:H4'	6:D:115:GLN:H	1.72	0.54
1:X:77:U:H2'	1:X:78:U:H6	1.72	0.54
17:P:66:THR:HA	17:P:69:LEU:HD12	1.89	0.54
1:X:273:A:OP2	1:X:297:G:N2	2.33	0.54
11:J:39:THR:HA	11:J:97:VAL:O	2.08	0.54
1:X:725:A:OP1	1:X:821:C:N4	2.41	0.54
1:X:566:U:H2'	1:X:567:G:N7	2.23	0.54
8:G:20:ASP:OD1	8:G:59:ASN:ND2	2.29	0.54
8:G:94:ARG:HA	8:G:98:PRO:HB3	1.88	0.54
1:X:1826:G:N2	1:X:1845:U:O2'	2.39	0.54
19:R:36:GLU:OE1	19:R:36:GLU:N	2.31	0.54
1:X:1452:C:O2	1:X:1631:G:N2	2.40	0.54
1:X:1765:A:O2'	1:X:1766:C:O4'	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1065:A:H3'	1:X:1065:A:C8	2.43	0.54
1:X:2047:A:H5'	25:Z:9:SER:HB3	1.90	0.54
1:X:1214:C:H42	1:X:1218:G:H1	1.54	0.54
1:X:13:A:O2'	1:X:15:G:N7	2.31	0.54
1:X:1885:G:H1'	1:X:1911:A:H62	1.73	0.54
1:X:1813:A:H1'	1:X:1965:A:N6	2.22	0.54
1:X:657:U:O4	1:X:659:A:N6	2.40	0.53
1:X:2116:U:H2'	1:X:2117:A:C8	2.43	0.53
14:M:20:PRO:HD2	14:M:86:ILE:HB	1.90	0.53
3:A:89:ALA:HB2	3:A:158:ALA:HA	1.90	0.53
1:X:2784:A:N1	7:E:67:THR:HG21	2.24	0.53
1:X:630:G:P	10:I:21:ARG:HH22	2.31	0.53
1:X:19:G:OP1	15:N:29:HIS:HD2	1.92	0.53
1:X:2645:G:O2'	4:B:162:ARG:HB2	2.08	0.53
17:P:11:ARG:HA	17:P:100:THR:HG22	1.90	0.53
1:X:333:C:H2'	1:X:334:A:H8	1.71	0.53
1:X:1800:A:C5	1:X:1856:A:H1'	2.43	0.53
1:X:705:U:O4	35:X:3433:SPD:N6	2.41	0.53
1:X:1092:A:O2'	1:X:1093:C:O5'	2.26	0.53
1:X:1352:C:H2'	1:X:1353:A:H8	1.74	0.53
1:X:633:A:H2'	1:X:634:C:H6	1.72	0.53
1:X:804:G:H2'	1:X:805:G:H8	1.73	0.53
1:X:897:A:H2'	1:X:898:U:C6	2.44	0.53
1:X:1039:C:C5	8:G:1:MET:HA	2.43	0.53
12:K:109:ARG:HD2	12:K:112:ASP:OD1	2.09	0.53
2:Y:74:G:H22	2:Y:97:A:N6	2.07	0.53
17:P:109:ASP:OD1	17:P:109:ASP:N	2.41	0.53
16:O:35:PHE:HZ	16:O:95:LEU:HD13	1.73	0.53
1:X:139:U:HO2'	1:X:140:A:H8	1.53	0.53
1:X:1848:A:H2'	1:X:1849:G:C8	2.44	0.53
1:X:372:A:N6	19:R:15:LYS:HB2	2.24	0.53
25:Z:28:THR:HG23	25:Z:37:TYR:HE1	1.73	0.53
1:X:2494:C:H4'	11:J:123:HIS:ND1	2.24	0.53
3:A:105:ILE:O	3:A:107:PRO:HD3	2.08	0.53
1:X:1761:G:O2'	1:X:1762:U:O4'	2.27	0.53
1:X:1609:U:H2'	1:X:1610:G:H8	1.73	0.53
7:E:95:ARG:CB	7:E:104:ILE:HA	2.38	0.53
4:B:215:ILE:O	4:B:216:LYS:HG2	2.09	0.53
1:X:562:C:O2'	17:P:18:ARG:NH2	2.42	0.53
1:X:327:G:O2'	1:X:328:G:H8	1.93	0.52
1:X:1521:A:N1	1:X:1559:G:N2	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:459:C:O2'	1:X:1907:U:O2'	2.21	0.52
15:N:59:LYS:O	15:N:63:THR:HG23	2.09	0.52
11:J:40:SER:OG	11:J:41:TRP:N	2.40	0.52
4:B:127:PHE:HA	4:B:172:ARG:HA	1.90	0.52
3:A:118:SER:HA	3:A:129:ALA:HB3	1.91	0.52
3:A:53:HIS:ND1	3:A:219:THR:HG21	2.23	0.52
1:X:331:G:HO2'	1:X:332:A:H8	1.56	0.52
1:X:1683:U:C2'	1:X:1684:A:H5''	2.37	0.52
18:Q:55:ILE:HD13	18:Q:76:ARG:HH11	1.75	0.52
1:X:540:G:N3	17:P:61:ASN:ND2	2.51	0.52
1:X:2872:G:H2'	1:X:2873:C:O4'	2.09	0.52
7:E:136:ILE:HG13	7:E:137:SER:N	2.25	0.52
16:O:7:THR:OG1	16:O:22:VAL:HG21	2.08	0.52
1:X:1275:A:H2'	1:X:1276:G:O4'	2.09	0.52
1:X:1567:A:OP2	1:X:1568:U:O2'	2.26	0.52
1:X:1815:C:H5''	3:A:224:VAL:HG11	1.91	0.52
4:B:71:LYS:N	4:B:72:PRO:HD2	2.24	0.52
1:X:811:C:N4	1:X:812:U:O4	2.42	0.52
2:Y:14:G:C6	2:Y:67:G:C2	2.98	0.52
1:X:2231:C:H42	1:X:2248:G:H1	1.57	0.52
1:X:901:G:H2'	1:X:902:A:H8	1.75	0.52
27:3:13:ARG:HA	27:3:21:GLN:O	2.09	0.52
4:B:106:SER:O	4:B:109:THR:OG1	2.28	0.52
1:X:1022:G:O2'	1:X:1046:G:O2'	2.24	0.52
1:X:199:A:H62	10:I:36:LYS:HZ2	1.58	0.52
3:A:91:ILE:CG2	3:A:105:ILE:HA	2.40	0.52
1:X:2758:G:C2	1:X:2759:G:C6	2.97	0.52
1:X:1507:A:H2'	1:X:1508:C:H5'	1.92	0.52
1:X:37:C:H2'	1:X:38:A:C8	2.45	0.52
4:B:86:ARG:O	4:B:86:ARG:HG2	2.10	0.52
24:W:12:VAL:HG12	24:W:20:ARG:HG2	1.92	0.52
1:X:345:C:H2'	1:X:346:A:H8	1.73	0.52
9:H:19:VAL:HB	9:H:41:CYS:SG	2.49	0.52
1:X:1056:U:OP2	15:N:70:ARG:NH2	2.43	0.52
1:X:1063:U:HO2'	1:X:1065:A:H2	1.58	0.52
1:X:245:G:O2'	1:X:257:G:O6	2.24	0.52
4:B:95:ASP:O	4:B:97:ASP:N	2.42	0.52
1:X:674:C:H2'	1:X:675:G:C8	2.45	0.52
1:X:2632:U:H2'	1:X:2633:C:C6	2.45	0.52
14:M:4:HIS:HB2	14:M:7:ILE:HG23	1.90	0.52
1:X:1845:U:C4	3:A:153:GLN:HB2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1436:C:O2'	1:X:1437:U:H6	1.93	0.52
1:X:898:U:H2'	1:X:899:U:H6	1.75	0.52
16:O:72:THR:O	16:O:74:PHE:N	2.43	0.52
1:X:967:C:O2'	21:T:34:ALA:HB2	2.09	0.52
13:L:95:ASP:O	13:L:96:ARG:HB3	2.08	0.52
1:X:124:A:OP2	26:2:20:ARG:HD3	2.10	0.52
1:X:1732:U:H1'	1:X:1745:A:C6	2.45	0.52
28:4:4:ARG:O	28:4:36:GLN:HA	2.09	0.52
14:M:98:LYS:HB3	14:M:100:TYR:HE1	1.73	0.52
1:X:790:G:H2'	1:X:791:U:H5'	1.91	0.52
1:X:926:G:N2	1:X:941:A:H62	2.07	0.51
12:K:48:ILE:HA	12:K:85:LEU:HD11	1.91	0.51
3:A:89:ALA:HB1	3:A:196:GLY:HA3	1.92	0.51
1:X:253:G:H2'	1:X:254:A:C8	2.45	0.51
1:X:280:C:H42	1:X:291:G:H1	1.58	0.51
1:X:439:U:H2'	1:X:440:C:H6	1.75	0.51
5:C:113:ALA:HB1	5:C:181:LEU:HD22	1.92	0.51
10:I:78:ASN:HA	10:I:107:SER:HB3	1.90	0.51
14:M:15:LEU:HG	14:M:79:HIS:HE1	1.74	0.51
11:J:34:LEU:HD11	11:J:129:THR:HB	1.90	0.51
9:H:2:ILE:HG22	9:H:21:THR:HG21	1.92	0.51
28:4:1:MET:HE3	28:4:33:LYS:HD2	1.92	0.51
5:C:149:PRO:HA	5:C:169:ASN:O	2.10	0.51
1:X:523:A:H2'	1:X:524:A:C8	2.46	0.51
1:X:898:U:H2'	1:X:899:U:C6	2.46	0.51
17:P:82:LEU:HB2	17:P:84:ARG:NH1	2.26	0.51
1:X:2457:A:H2'	1:X:2457:A:N3	2.25	0.51
26:2:25:THR:OG1	26:2:26:LYS:N	2.43	0.51
1:X:1490:G:O2'	1:X:1491:C:O4'	2.29	0.51
12:K:25:ILE:HD11	12:K:85:LEU:HD13	1.93	0.51
1:X:2470:C:H2'	1:X:2471:G:H8	1.75	0.51
1:X:345:C:H2'	1:X:346:A:C8	2.44	0.51
3:A:232:HIS:CE1	3:A:241:ILE:HD12	2.45	0.51
1:X:1293:U:H5''	1:X:1294:G:H5''	1.93	0.51
2:Y:22:G:O5'	2:Y:22:G:H8	1.93	0.51
2:Y:92:G:H8	2:Y:92:G:O5'	1.94	0.51
1:X:2495:A:O2'	1:X:2496:A:O5'	2.28	0.51
1:X:1418:G:H1'	1:X:1618:A:N1	2.25	0.51
9:H:76:TYR:HB2	14:M:75:THR:HG22	1.91	0.51
1:X:1186:A:H4'	8:G:28:ARG:HH22	1.76	0.51
1:X:132:C:N4	1:X:147:G:H1	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1563:U:H2'	1:X:1564:G:H8	1.75	0.51
1:X:138:U:N3	1:X:141:U:OP2	2.34	0.51
1:X:525:A:H4'	1:X:526:A:OP1	2.11	0.51
1:X:1699:A:H1'	4:B:127:PHE:CE1	2.45	0.51
1:X:655:A:H2'	1:X:656:G:O4'	2.11	0.51
11:J:11:ARG:HB3	11:J:14:ARG:HH22	1.76	0.51
1:X:2361:U:O2'	1:X:2362:A:OP1	2.28	0.51
1:X:1998:A:O2'	1:X:1999:G:OP1	2.29	0.51
1:X:1711:G:H22	1:X:2018:U:H2'	1.76	0.51
1:X:1630:A:H2'	1:X:1631:G:H5''	1.93	0.51
1:X:1523:G:C2	1:X:1524:C:H1'	2.46	0.51
1:X:530:C:H2'	1:X:531:C:C6	2.46	0.51
1:X:2886:G:C2	1:X:2888:A:H1'	2.45	0.51
1:X:1305:U:C5	1:X:2040:A:N7	2.79	0.51
1:X:1304:G:OP2	25:Z:16:ARG:NH1	2.44	0.51
12:K:93:TYR:OH	12:K:121:LEU:O	2.29	0.51
28:4:16:VAL:HG22	28:4:25:VAL:HG22	1.93	0.51
14:M:50:ILE:HG22	14:M:98:LYS:O	2.11	0.51
1:X:2558:A:H5''	7:E:157:TYR:CZ	2.46	0.51
1:X:1810:A:H5'	1:X:2635:G:H4'	1.93	0.51
1:X:1733:A:H2'	1:X:1734:A:C8	2.46	0.51
1:X:493:A:OP1	15:N:5:LYS:NZ	2.38	0.51
1:X:1528:G:H1	1:X:1547:C:H42	1.59	0.51
1:X:661:U:O2'	1:X:662:G:OP2	2.24	0.51
1:X:100:U:H3'	1:X:101:G:H5'	1.93	0.51
1:X:2769:G:OP1	28:4:35:ARG:NE	2.38	0.51
1:X:1376:G:OP1	18:Q:13:THR:HG21	2.11	0.50
1:X:1831:A:H61	1:X:1840:U:H3	1.59	0.50
1:X:1008:C:O2'	1:X:2300:A:N3	2.37	0.50
1:X:705:U:O4	35:X:3433:SPD:N10	2.44	0.50
19:R:8:ASN:HA	19:R:22:LYS:HA	1.93	0.50
1:X:1747:G:H2'	1:X:1748:G:H8	1.76	0.50
2:Y:1:U:O2'	2:Y:2:C:OP2	2.29	0.50
1:X:2081:A:C2	1:X:2643:C:N3	2.79	0.50
4:B:53:PHE:CG	4:B:54:GLU:N	2.79	0.50
1:X:2354:A:H2'	1:X:2355:A:C8	2.46	0.50
11:J:110:SER:HB3	11:J:113:VAL:HB	1.94	0.50
1:X:378:C:H2'	1:X:379:C:H6	1.76	0.50
21:T:78:GLU:OE1	21:T:88:SER:OG	2.27	0.50
1:X:1518:G:HO2'	1:X:1519:U:H6	1.59	0.50
1:X:201:C:H2'	1:X:202:A:H5''	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:970:U:H1'	1:X:971:U:H5''	1.93	0.50
1:X:12:U:H2'	1:X:12:U:O2	2.11	0.50
1:X:460:C:H2'	1:X:461:A:C8	2.46	0.50
1:X:2391:C:H2'	1:X:2392:G:H8	1.77	0.50
1:X:579:U:H2'	1:X:580:C:H6	1.77	0.50
1:X:2000:G:H2'	1:X:2001:C:C6	2.44	0.50
35:X:3430:SPD:H101	5:C:62:ARG:HH22	1.58	0.50
1:X:302:A:N6	1:X:450:C:C2	2.80	0.50
1:X:322:A:C2'	1:X:323:C:H5'	2.42	0.50
1:X:1521:A:H61	1:X:1560:A:H1'	1.76	0.50
1:X:1575:A:H2'	1:X:1576:A:C5'	2.42	0.50
1:X:879:U:H2'	1:X:880:A:H8	1.76	0.50
25:Z:28:THR:O	25:Z:30:CYS:N	2.45	0.50
1:X:17:G:OP1	25:Z:11:THR:HB	2.11	0.50
1:X:293:U:H2'	1:X:294:G:C8	2.47	0.50
8:G:41:ASN:O	15:N:67:ALA:HB1	2.11	0.50
4:B:131:ILE:HA	4:B:136:GLN:HB2	1.94	0.50
8:G:22:GLU:HA	8:G:62:LYS:HB2	1.94	0.50
9:H:15:GLY:O	9:H:46:ALA:HB1	2.12	0.50
1:X:1487:G:N2	1:X:1597:U:H3	2.09	0.50
8:G:74:VAL:HB	8:G:76:TYR:CE1	2.47	0.50
5:C:140:LYS:N	5:C:140:LYS:HD3	2.27	0.50
1:X:1039:C:H1'	15:N:93:LYS:HE2	1.94	0.49
1:X:683:G:C6	1:X:696:G:C6	2.99	0.49
8:G:77:ARG:H	8:G:87:SER:CB	2.25	0.49
1:X:2520:U:O2'	11:J:80:GLU:OE2	2.25	0.49
8:G:119:GLN:HA	8:G:122:LYS:HD3	1.94	0.49
1:X:646:A:H5''	1:X:700:A:H61	1.77	0.49
1:X:77:U:H2'	1:X:78:U:C6	2.46	0.49
7:E:29:PRO:HG3	7:E:75:MET:HG2	1.94	0.49
18:Q:66:GLY:O	18:Q:68:TYR:N	2.36	0.49
4:B:118:VAL:HG12	4:B:211:ILE:HG12	1.95	0.49
1:X:1354:G:H1	1:X:1372:C:H42	1.60	0.49
5:C:101:MET:HG2	5:C:102:PRO:HD2	1.94	0.49
1:X:2286:G:C6	1:X:2287:C:C4	3.00	0.49
8:G:32:GLU:O	8:G:36:ILE:HG12	2.12	0.49
9:H:35:ILE:HG23	9:H:63:VAL:HA	1.93	0.49
1:X:24:G:O2'	17:P:78:GLU:O	2.30	0.49
1:X:1501:G:C4	1:X:1502:A:C2	3.01	0.49
1:X:2720:A:H2'	1:X:2721:G:H8	1.77	0.49
1:X:2833:U:H2'	1:X:2834:C:H6	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1922:C:H2'	1:X:1923:A:H8	1.77	0.49
2:Y:79:C:N4	2:Y:92:G:H1	2.05	0.49
1:X:472:C:H2'	1:X:473:U:H6	1.77	0.49
1:X:2774:G:O2'	7:E:67:THR:HG22	2.12	0.49
1:X:638:U:H2'	1:X:639:U:H6	1.78	0.49
17:P:69:LEU:HD23	17:P:108:SER:O	2.11	0.49
1:X:1353:A:H2'	1:X:1354:G:H8	1.75	0.49
1:X:1152:U:H2'	1:X:1153:C:O4'	2.12	0.49
5:C:31:SER:HB3	10:I:9:ALA:HB2	1.93	0.49
1:X:333:C:H2'	1:X:334:A:C8	2.47	0.49
1:X:1760:G:H1	1:X:1770:C:H42	1.60	0.49
1:X:1510:U:H2'	1:X:1511:C:O4'	2.12	0.49
1:X:2391:C:C5'	21:T:64:ASP:HB2	2.42	0.49
1:X:2359:C:OP1	21:T:84:LYS:NZ	2.40	0.49
21:T:49:ARG:NH2	21:T:64:ASP:OD1	2.46	0.49
1:X:690:U:O2'	1:X:691:A:H5'	2.12	0.49
1:X:2731:C:H2'	1:X:2732:A:O4'	2.13	0.49
34:X:3426:EPE:H52	15:N:7:GLY:CA	2.32	0.49
4:B:27:VAL:HG13	4:B:194:VAL:HG11	1.93	0.49
1:X:695:C:N4	1:X:696:G:C6	2.81	0.49
17:P:86:ARG:HG3	17:P:87:PRO:CD	2.41	0.49
1:X:282:A:H2'	1:X:283:G:H8	1.76	0.49
1:X:2228:C:H2'	1:X:2229:C:H6	1.77	0.49
1:X:487:U:H2'	1:X:488:G:C8	2.48	0.49
1:X:267:G:H2'	1:X:268:A:H5''	1.95	0.49
5:C:53:ASN:OD1	5:C:54:ARG:N	2.46	0.49
1:X:259:A:H2'	1:X:260:A:H8	1.78	0.49
18:Q:54:ASN:HB3	18:Q:79:ILE:HG13	1.95	0.49
19:R:48:THR:HG23	19:R:51:ASN:HB3	1.94	0.49
1:X:1304:G:O5'	17:P:15:ARG:NH2	2.45	0.48
1:X:83:G:O6	19:R:89:LYS:HD3	2.13	0.48
1:X:363:A:H4'	1:X:365:A:C8	2.47	0.48
1:X:259:A:H2'	1:X:260:A:C8	2.47	0.48
1:X:1346:G:H4'	26:2:8:PRO:HG2	1.94	0.48
1:X:2581:U:H2'	1:X:2582:U:C6	2.48	0.48
1:X:676:A:N3	1:X:2442:G:O2'	2.34	0.48
1:X:1494:G:N7	1:X:1495:C:H5	2.10	0.48
1:X:1185:U:H4'	1:X:1186:A:O4'	2.13	0.48
4:B:128:GLN:HG3	4:B:173:MET:HE3	1.96	0.48
1:X:2356:A:H2'	1:X:2357:G:C8	2.47	0.48
1:X:302:A:H1'	1:X:303:G:H5''	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2682:G:O2'	1:X:2683:U:H5	1.95	0.48
1:X:484:U:H2'	1:X:485:A:C8	2.49	0.48
1:X:1473:G:H2'	1:X:1474:C:C6	2.48	0.48
1:X:54:G:H2'	1:X:55:G:O4'	2.14	0.48
1:X:1726:A:H61	1:X:1750:U:H3	1.61	0.48
21:T:20:ASN:OD1	21:T:21:GLY:N	2.45	0.48
5:C:23:VAL:HG12	5:C:24:PHE:CD1	2.48	0.48
1:X:1391:A:H2'	1:X:1392:G:O4'	2.13	0.48
1:X:1733:A:H2'	1:X:1734:A:H8	1.79	0.48
1:X:619:U:H2'	1:X:620:G:C8	2.48	0.48
18:Q:51:ALA:HB3	18:Q:81:THR:O	2.13	0.48
1:X:1:G:H3'	1:X:2:A:H4'	1.95	0.48
1:X:668:C:H2'	1:X:669:C:C6	2.49	0.48
1:X:923:A:H2'	1:X:924:G:H8	1.78	0.48
17:P:86:ARG:HH11	17:P:86:ARG:HB2	1.79	0.48
1:X:2842:G:H2'	1:X:2843:A:H5''	1.94	0.48
1:X:1053:A:N3	1:X:1197:C:O2'	2.41	0.48
1:X:38:A:H2'	1:X:39:C:O4'	2.13	0.48
1:X:897:A:H2'	1:X:898:U:H6	1.78	0.48
1:X:2719:C:H2'	1:X:2720:A:O4'	2.14	0.48
1:X:2377:C:H2'	1:X:2378:G:O4'	2.14	0.48
1:X:2037:G:P	17:P:41:LYS:HE2	2.54	0.48
1:X:418:G:O2'	1:X:446:G:O6	2.18	0.48
1:X:1529:U:O4	1:X:1530:A:N6	2.46	0.48
1:X:2725:U:H2'	1:X:2726:C:C6	2.49	0.48
1:X:271:C:H5'	1:X:324:A:O2'	2.14	0.48
8:G:2:ARG:O	8:G:3:GLN:HG2	2.13	0.48
1:X:1440:A:HO2'	1:X:1514:A:HO2'	1.52	0.48
18:Q:55:ILE:HG13	18:Q:77:LYS:O	2.14	0.48
1:X:2478:A:H2'	29:X:3001:ZLD:H20	1.96	0.48
1:X:2669:G:O6	35:X:3428:SPD:N1	2.46	0.48
2:Y:46:A:OP1	13:L:35:ARG:NH2	2.46	0.48
14:M:48:VAL:O	14:M:63:VAL:HA	2.14	0.48
1:X:154:A:O2'	1:X:155:U:H5''	2.13	0.48
1:X:2813:U:O2'	4:B:72:PRO:O	2.28	0.48
14:M:98:LYS:HB3	14:M:100:TYR:CE1	2.49	0.48
20:S:3:SER:O	20:S:62:GLU:N	2.31	0.48
1:X:955:A:N3	11:J:15:PRO:HG3	2.29	0.48
1:X:878:C:H2'	1:X:879:U:C6	2.48	0.48
27:3:7:HIS:CE1	27:3:9:GLY:HA3	2.48	0.48
1:X:1537:A:N3	1:X:1537:A:H2'	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:215:ILE:HD12	4:B:216:LYS:H	1.79	0.47
9:H:13:ASN:ND2	9:H:97:ARG:HB3	2.29	0.47
1:X:1422:A:O2'	1:X:1423:C:O4'	2.22	0.47
1:X:1741:G:O2'	1:X:2005:A:OP1	2.30	0.47
12:K:5:LYS:HB2	12:K:39:GLU:OE2	2.14	0.47
1:X:789:C:H2'	1:X:790:G:O4'	2.13	0.47
17:P:10:ILE:HD13	17:P:46:VAL:HG11	1.96	0.47
1:X:1781:C:H5'	14:M:101:TYR:CE2	2.49	0.47
16:O:50:ALA:O	16:O:52:THR:N	2.47	0.47
18:Q:88:ASP:OD1	18:Q:88:ASP:N	2.45	0.47
2:Y:91:C:H2'	2:Y:92:G:C8	2.50	0.47
19:R:80:ARG:NH2	19:R:96:LYS:HA	2.28	0.47
1:X:119:U:H4'	1:X:120:G:H5''	1.96	0.47
2:Y:15:C:H42	2:Y:105:G:N2	2.11	0.47
2:Y:68:A:O5'	2:Y:68:A:H8	1.97	0.47
12:K:14:LYS:O	12:K:18:ARG:HG3	2.14	0.47
18:Q:26:THR:HG22	18:Q:79:ILE:HG22	1.96	0.47
18:Q:51:ALA:HB2	18:Q:83:LYS:N	2.29	0.47
1:X:2771:G:H1	1:X:2787:C:H5	1.61	0.47
1:X:312:A:N3	1:X:312:A:H2'	2.30	0.47
9:H:1:MET:HG2	9:H:32:THR:OG1	2.15	0.47
8:G:7:ALA:N	8:G:46:THR:HG21	2.24	0.47
1:X:1906:C:H2'	1:X:1907:U:O4'	2.15	0.47
1:X:1854:U:H2'	1:X:1855:G:O4'	2.14	0.47
3:A:76:ALA:HB2	3:A:96:TYR:CD1	2.48	0.47
1:X:1953:U:N3	1:X:1955:A:N7	2.62	0.47
1:X:1229:G:OP1	10:I:31:SER:HA	2.13	0.47
1:X:133:A:H61	1:X:146:U:H3	1.63	0.47
3:A:228:ASN:N	3:A:228:ASN:OD1	2.47	0.47
13:L:92:ILE:HD12	13:L:94:PHE:O	2.14	0.47
19:R:9:VAL:HG22	19:R:23:VAL:HG12	1.97	0.47
1:X:1013:U:OP1	24:W:17:GLU:HG2	2.13	0.47
1:X:2851:G:H2'	4:B:64:LYS:HE3	1.96	0.47
1:X:124:A:H5'	26:2:20:ARG:HD2	1.97	0.47
16:O:63:ASN:HB2	16:O:94:LYS:O	2.14	0.47
1:X:2401:C:H42	1:X:2406:G:H1	1.61	0.47
1:X:1395:G:O2'	1:X:1396:A:OP2	2.32	0.47
1:X:1068:G:C6	1:X:1069:G:C6	3.03	0.47
1:X:325:A:H2'	1:X:326:A:H8	1.79	0.47
17:P:11:ARG:HH11	17:P:98:LYS:HB3	1.79	0.47
1:X:2773:U:O4	1:X:2782:C:H4'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:154:ILE:HG22	3:A:155:ALA:N	2.30	0.47
1:X:1227:U:OP1	16:O:82:SER:HB3	2.14	0.47
1:X:1851:G:OP2	3:A:53:HIS:CE1	2.67	0.47
1:X:349:U:H2'	1:X:350:G:O4'	2.13	0.47
5:C:133:ALA:HB1	5:C:135:LYS:H	1.77	0.47
9:H:58:VAL:HG21	9:H:86:ILE:HD12	1.95	0.47
1:X:1740:G:H2'	1:X:1741:G:O4'	2.15	0.47
1:X:1737:U:O2'	1:X:1739:G:O6	2.22	0.47
4:B:194:VAL:HG12	4:B:195:ILE:H	1.79	0.47
18:Q:74:LYS:H	18:Q:74:LYS:HG3	1.44	0.47
5:C:10:ASP:OD1	5:C:10:ASP:N	2.46	0.47
1:X:2495:A:O2'	1:X:2496:A:P	2.72	0.47
19:R:39:ASN:HA	19:R:59:THR:O	2.15	0.47
5:C:51:VAL:HG12	5:C:92:PRO:O	2.15	0.47
28:4:8:LYS:O	28:4:34:GLN:NE2	2.48	0.47
1:X:2856:U:H2'	1:X:2857:A:H8	1.76	0.47
1:X:18:C:OP1	15:N:26:GLY:N	2.46	0.47
1:X:1437:U:H2'	1:X:1438:G:C8	2.49	0.47
1:X:1981:G:N1	1:X:2013:G:OP1	2.39	0.47
1:X:2850:G:OP1	4:B:86:ARG:NH2	2.47	0.47
4:B:27:VAL:HG13	4:B:194:VAL:CG1	2.44	0.47
2:Y:49:G:C6	2:Y:50:A:C6	3.02	0.47
1:X:1310:A:H3'	1:X:1311:A:C8	2.50	0.47
5:C:68:LYS:HB3	5:C:68:LYS:HE3	1.73	0.47
1:X:528:C:H4'	19:R:43:LYS:HD3	1.96	0.47
1:X:589:U:C4	1:X:591:A:C6	3.03	0.47
1:X:2382:C:H1'	21:T:47:ARG:NH1	2.30	0.47
8:G:97:ASN:HA	8:G:98:PRO:HD2	1.53	0.47
4:B:138:ARG:HG3	4:B:138:ARG:HH11	1.80	0.47
1:X:2018:U:O2'	1:X:2019:G:H5'	2.14	0.47
1:X:974:U:H2'	1:X:975:U:O4'	2.15	0.47
1:X:2391:C:H2'	1:X:2392:G:C8	2.50	0.47
1:X:2679:U:H2'	1:X:2680:U:C6	2.50	0.47
7:E:138:LYS:HA	7:E:141:VAL:HB	1.96	0.47
1:X:1973:U:H2'	1:X:1974:C:C6	2.49	0.47
25:Z:38:LYS:HE2	25:Z:38:LYS:HB2	1.30	0.47
1:X:2495:A:O2'	1:X:2496:A:C8	2.66	0.47
15:N:24:TYR:CE2	15:N:38:GLN:HG3	2.50	0.47
1:X:579:U:H5'	15:N:42:SER:OG	2.15	0.47
1:X:877:G:H2'	1:X:878:C:H6	1.79	0.47
5:C:149:PRO:HG2	5:C:187:THR:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:716:C:H2'	1:X:717:C:C6	2.48	0.47
1:X:249:C:N4	27:3:8:ARG:HG2	2.30	0.47
10:I:84:LYS:HG3	10:I:84:LYS:H	1.52	0.47
1:X:1513:A:H3'	1:X:1514:A:C8	2.35	0.47
9:H:35:ILE:HA	9:H:62:ILE:HG22	1.97	0.47
1:X:575:G:N3	1:X:575:G:H2'	2.30	0.47
11:J:127:VAL:HG12	11:J:128:LYS:O	2.14	0.47
1:X:1394:U:H2'	1:X:1395:G:H5'	1.96	0.47
2:Y:77:G:H1	2:Y:94:U:H3	1.63	0.47
1:X:1539:A:N3	1:X:1539:A:H2'	2.29	0.47
1:X:1071:A:C6	1:X:1170:A:C4	3.03	0.46
1:X:2850:G:P	4:B:86:ARG:HH22	2.39	0.46
1:X:1174:U:O2	4:B:162:ARG:NH2	2.48	0.46
7:E:85:LYS:H	7:E:133:VAL:CG1	2.27	0.46
1:X:608:C:H2'	1:X:609:U:O4'	2.14	0.46
1:X:422:G:H2'	1:X:423:A:C8	2.50	0.46
1:X:1867:G:N2	1:X:1929:C:O2	2.42	0.46
1:X:158:G:N1	1:X:159:U:O2	2.49	0.46
1:X:91:A:H8	1:X:91:A:O5'	1.98	0.46
11:J:73:PRO:HB3	11:J:93:TRP:CZ3	2.50	0.46
1:X:79:U:O2'	1:X:389:A:H8	1.98	0.46
1:X:2774:G:O6	1:X:2782:C:H5''	2.15	0.46
1:X:577:A:N6	1:X:2062:G:N2	2.63	0.46
1:X:2019:G:C2	1:X:2024:A:C5	3.03	0.46
1:X:1848:A:H2'	1:X:1849:G:H8	1.80	0.46
1:X:1508:C:N3	1:X:1509:G:N1	2.63	0.46
1:X:514:G:H21	35:X:3430:SPD:H51	1.80	0.46
1:X:379:C:C2	1:X:380:U:C5	3.04	0.46
1:X:1183:G:H5'	8:G:105:SER:OG	2.14	0.46
1:X:773:G:OP2	1:X:773:G:H8	1.97	0.46
1:X:268:A:O2'	1:X:269:G:H4'	2.15	0.46
1:X:49:A:C5	1:X:179:A:C6	3.03	0.46
13:L:17:ARG:HH12	13:L:91:GLU:CB	2.28	0.46
1:X:2784:A:OP2	28:4:20:LYS:HA	2.14	0.46
1:X:718:C:H5''	5:C:81:PRO:HD2	1.97	0.46
1:X:577:A:H61	1:X:2062:G:N2	2.13	0.46
1:X:2531:U:H5	29:X:3001:ZLD:H13B	1.80	0.46
17:P:36:LEU:HD13	17:P:48:GLU:HA	1.98	0.46
1:X:627:C:OP2	34:X:3426:EPE:H91	2.16	0.46
35:X:3432:SPD:N6	35:X:3432:SPD:H22	2.31	0.46
1:X:2845:G:H8	1:X:2845:G:OP2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:18:VAL:HG23	8:G:138:PRO:HB2	1.98	0.46
1:X:2418:G:C6	1:X:2454:C:H1'	2.51	0.46
1:X:688:A:H2'	1:X:689:A:H5'	1.96	0.46
1:X:1644:C:P	18:Q:76:ARG:NH2	2.89	0.46
3:A:210:ARG:HA	3:A:213:TRP:CD2	2.51	0.46
2:Y:13:A:H1'	2:Y:106:U:N1	2.31	0.46
3:A:19:LEU:O	3:A:21:PHE:N	2.48	0.46
1:X:2043:U:H2'	1:X:2044:C:C6	2.51	0.46
3:A:85:PRO:HG2	3:A:86:ASN:OD1	2.15	0.46
1:X:1468:G:H2'	1:X:1469:G:O4'	2.15	0.46
13:L:30:ARG:NH2	13:L:47:ASP:OD1	2.48	0.46
17:P:108:SER:OG	17:P:109:ASP:N	2.48	0.46
1:X:575:G:O2'	1:X:577:A:H2	1.98	0.46
1:X:879:U:H5'	27:3:52:LYS:HD3	1.97	0.46
1:X:804:G:H2'	1:X:805:G:C8	2.51	0.46
1:X:1306:A:C2	1:X:2040:A:C4	3.04	0.46
1:X:361:U:H2'	1:X:362:C:H6	1.81	0.46
7:E:64:ASN:O	7:E:68:THR:OG1	2.31	0.46
1:X:2507:C:H2'	1:X:2508:G:H5'	1.98	0.46
1:X:2882:A:H2'	1:X:2883:U:H6	1.80	0.46
1:X:125:A:N7	1:X:126:A:C6	2.84	0.46
1:X:683:G:C6	1:X:696:G:N1	2.84	0.46
5:C:147:GLU:HB2	5:C:184:LEU:O	2.16	0.46
4:B:154:VAL:HG21	4:B:169:MET:HE3	1.98	0.46
16:O:22:VAL:HG22	16:O:23:GLU:H	1.79	0.46
17:P:82:LEU:HB2	17:P:84:ARG:HH12	1.79	0.46
1:X:1854:U:OP1	1:X:1998:A:H4'	2.16	0.46
1:X:173:A:H2'	1:X:174:U:C6	2.50	0.46
1:X:1269:A:H2'	1:X:1270:U:C6	2.50	0.46
24:W:7:THR:OG1	24:W:34:SER:HB3	2.15	0.46
1:X:890:G:H8	1:X:890:G:O5'	1.99	0.46
13:L:44:ILE:HB	13:L:54:ALA:H	1.81	0.46
34:X:3425:EPE:H62	34:X:3425:EPE:H71	1.82	0.46
1:X:971:U:H2'	1:X:972:A:C8	2.50	0.46
1:X:2877:G:H5'	1:X:2878:U:OP2	2.15	0.46
1:X:2023:C:H4'	1:X:2024:A:OP1	2.15	0.46
1:X:1806:U:C5	1:X:1811:A:N7	2.82	0.46
1:X:2117:A:H2	22:U:34:GLN:HE22	1.64	0.46
1:X:1642:C:H4'	18:Q:34:ASN:OD1	2.16	0.46
1:X:622:A:C2	1:X:1300:G:C5	3.04	0.45
1:X:397:U:O2'	1:X:398:C:H5''	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:43:THR:HA	11:J:94:ILE:HD13	1.98	0.45
1:X:659:A:O2'	1:X:660:A:H4'	2.16	0.45
1:X:2008:A:H5''	1:X:2009:U:OP2	2.16	0.45
34:X:3425:EPE:H61	21:T:24:SER:OG	2.16	0.45
11:J:20:ARG:N	11:J:98:LYS:HE2	2.30	0.45
1:X:2370:U:H2'	1:X:2371:U:C6	2.51	0.45
1:X:509:G:N2	1:X:511:G:H3'	2.31	0.45
1:X:489:A:N3	1:X:1240:U:H1'	2.31	0.45
1:X:331:G:C6	1:X:396:G:C6	3.04	0.45
4:B:53:PHE:HB3	4:B:87:PHE:HB2	1.97	0.45
1:X:684:U:H2'	1:X:685:C:C6	2.52	0.45
1:X:2314:A:HO2'	1:X:2315:A:H2'	1.82	0.45
1:X:1063:U:O2'	1:X:1065:A:H2	1.98	0.45
1:X:139:U:O2'	1:X:140:A:H8	1.99	0.45
5:C:160:ASP:O	5:C:163:VAL:HG13	2.16	0.45
14:M:15:LEU:HG	14:M:79:HIS:CE1	2.49	0.45
1:X:1697:G:O6	12:K:6:LEU:HB2	2.17	0.45
1:X:45:G:H21	1:X:183:A:H61	1.63	0.45
27:3:56:LYS:HE3	27:3:56:LYS:H	1.80	0.45
1:X:2305:A:N6	21:T:22:ARG:O	2.48	0.45
1:X:2622:G:N2	1:X:2625:A:OP2	2.47	0.45
20:S:78:GLN:HB2	20:S:88:HIS:HB3	1.98	0.45
1:X:15:G:O2'	25:Z:18:THR:HG21	2.16	0.45
14:M:27:THR:HB	14:M:90:ARG:HG2	1.98	0.45
1:X:1465:G:H2'	1:X:1466:G:C8	2.45	0.45
1:X:1508:C:HO2'	1:X:1509:G:C5'	2.28	0.45
1:X:712:U:H2'	1:X:713:A:O4'	2.16	0.45
1:X:828:A:H2'	1:X:829:U:H4'	1.99	0.45
4:B:36:LEU:N	4:B:50:GLN:O	2.38	0.45
10:I:1:MET:HG3	10:I:6:LEU:HD23	1.98	0.45
1:X:1467:G:H2'	1:X:1468:G:H8	1.81	0.45
11:J:51:ARG:O	11:J:55:THR:HG23	2.16	0.45
23:V:46:VAL:O	23:V:50:ILE:HG13	2.16	0.45
5:C:39:LEU:HD12	5:C:39:LEU:O	2.15	0.45
10:I:72:LYS:C	10:I:74:TYR:H	2.20	0.45
1:X:199:A:H62	10:I:36:LYS:NZ	2.14	0.45
1:X:1098:A:N7	1:X:1099:G:N2	2.65	0.45
2:Y:26:C:H2'	2:Y:27:A:O4'	2.16	0.45
1:X:266:A:H2'	1:X:267:G:O4'	2.16	0.45
11:J:50:ALA:O	11:J:54:MET:HB2	2.16	0.45
12:K:92:ARG:HD2	12:K:93:TYR:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:83:G:N2	1:X:101:G:H1'	2.30	0.45
1:X:2076:A:C2'	1:X:2077:C:H5'	2.46	0.45
7:E:29:PRO:HD2	7:E:35:ARG:O	2.17	0.45
1:X:691:A:H2'	1:X:692:G:O4'	2.17	0.45
1:X:157:U:H2'	1:X:158:G:C8	2.52	0.45
1:X:1614:A:H2'	3:A:85:PRO:HG3	1.98	0.45
27:3:53:SER:HA	27:3:56:LYS:CE	2.46	0.45
1:X:1889:G:C6	1:X:1908:A:C6	3.05	0.45
1:X:986:G:H5''	10:I:32:GLY:HA2	1.98	0.45
8:G:66:THR:HG22	8:G:67:GLY:H	1.80	0.45
1:X:1037:A:H4'	16:O:71:ILE:HD11	1.98	0.45
1:X:354:A:C8	1:X:375:A:C5	3.05	0.45
1:X:1332:C:H4'	12:K:67:ARG:CZ	2.47	0.45
2:Y:48:A:P	13:L:67:ALA:HB3	2.56	0.45
3:A:159:GLY:N	3:A:197:ASN:O	2.50	0.45
1:X:865:A:N3	1:X:987:U:O2'	2.45	0.45
1:X:1092:A:N6	1:X:1155:A:C4	2.85	0.45
1:X:1449:A:H4'	1:X:1449:A:OP1	2.17	0.45
1:X:895:U:O2	24:W:46:GLN:NE2	2.50	0.45
8:G:60:ALA:HB2	8:G:125:VAL:HG12	1.98	0.45
2:Y:14:G:N2	2:Y:67:G:H1'	2.32	0.45
1:X:292:U:H2'	1:X:293:U:C6	2.52	0.45
9:H:79:PHE:CD1	14:M:72:VAL:HG22	2.51	0.45
24:W:39:ASP:OD1	24:W:44:ARG:NH2	2.50	0.45
1:X:2289:U:H2'	1:X:2290:C:H6	1.81	0.45
1:X:1337:A:H4'	1:X:1338:U:C5'	2.47	0.45
1:X:325:A:H2'	1:X:326:A:C8	2.52	0.45
24:W:18:THR:HB	24:W:49:LYS:NZ	2.31	0.45
13:L:17:ARG:NH2	13:L:30:ARG:HD2	2.32	0.45
1:X:148:U:H2'	1:X:149:U:C6	2.52	0.45
1:X:1501:G:H2'	1:X:1502:A:C2	2.52	0.45
3:A:53:HIS:CE1	3:A:219:THR:HG21	2.52	0.45
1:X:1332:C:H4'	12:K:67:ARG:NH2	2.32	0.45
1:X:1720:A:H2'	1:X:1721:A:O4'	2.17	0.45
2:Y:6:U:OP1	13:L:14:ARG:NH2	2.38	0.45
6:D:35:VAL:HA	6:D:85:ILE:O	2.16	0.45
1:X:558:A:O2'	15:N:11:ARG:HD2	2.17	0.45
1:X:1211:G:O2'	1:X:1212:U:H5'	2.17	0.45
1:X:168:A:H3'	1:X:169:G:H5'	1.97	0.45
1:X:192:G:O2'	1:X:210:A:N6	2.48	0.45
16:O:60:ALA:HB2	16:O:97:ILE:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2050:A:H2'	1:X:2051:C:H6	1.82	0.45
1:X:947:U:H2'	1:X:948:U:C6	2.52	0.45
34:X:3426:EPE:H62	15:N:6:GLY:O	2.15	0.44
1:X:660:A:H4'	1:X:661:U:OP1	2.18	0.44
1:X:321:U:H1'	1:X:322:A:H5''	1.98	0.44
2:Y:13:A:H1'	2:Y:106:U:C6	2.52	0.44
1:X:2878:U:H6	1:X:2878:U:OP1	2.00	0.44
1:X:1962:G:H1'	1:X:1991:G:N2	2.32	0.44
1:X:162:A:H5''	1:X:163:U:H2'	2.00	0.44
15:N:66:ASN:HA	15:N:76:TYR:HB2	1.99	0.44
15:N:20:LEU:HD23	15:N:20:LEU:HA	1.86	0.44
1:X:2325:A:C2	1:X:2326:G:H1'	2.52	0.44
11:J:36:ALA:HB2	11:J:103:LEU:HD21	1.99	0.44
1:X:2829:A:C6	1:X:2830:A:C6	3.05	0.44
2:Y:15:C:N4	2:Y:105:G:H21	2.15	0.44
1:X:378:C:H2'	1:X:379:C:C6	2.52	0.44
1:X:293:U:H2'	1:X:294:G:H8	1.81	0.44
1:X:1992:C:H3'	1:X:1993:A:C8	2.52	0.44
1:X:1445:C:H2'	1:X:1446:U:C6	2.53	0.44
1:X:1887:G:O6	1:X:1910:G:N2	2.50	0.44
1:X:2594:G:H2'	1:X:2595:C:C6	2.52	0.44
1:X:1466:G:O2'	1:X:1537:A:N6	2.50	0.44
1:X:903:G:N3	1:X:2295:A:H2'	2.33	0.44
1:X:2494:C:O2	11:J:124:LYS:HE2	2.18	0.44
1:X:2026:C:O2	1:X:2714:U:O2'	2.28	0.44
1:X:2599:A:N7	4:B:158:SER:HB3	2.32	0.44
1:X:2466:A:N6	1:X:2612:U:H4'	2.33	0.44
1:X:1064:A:C2	1:X:1185:U:C2	3.05	0.44
1:X:1574:G:H2'	1:X:1575:A:O4'	2.18	0.44
26:2:27:ASN:O	26:2:31:VAL:HG23	2.16	0.44
1:X:514:G:H2'	1:X:515:G:O4'	2.18	0.44
1:X:524:A:C6	1:X:526:A:C6	3.05	0.44
1:X:1723:A:H2	1:X:1791:G:C8	2.36	0.44
1:X:2341:A:H2'	1:X:2342:U:C6	2.52	0.44
1:X:416:G:OP2	1:X:416:G:H8	2.01	0.44
1:X:817:G:H2'	1:X:818:U:H6	1.82	0.44
1:X:1197:C:H2'	1:X:1198:G:O4'	2.18	0.44
15:N:17:THR:O	15:N:20:LEU:HB2	2.17	0.44
14:M:41:ARG:NH1	14:M:43:GLN:HG3	2.32	0.44
1:X:2446:U:H2'	1:X:2447:C:C6	2.53	0.44
1:X:2419:A:H2	1:X:2451:C:N4	2.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:102:VAL:HG13	9:H:106:LEU:HD12	2.00	0.44
1:X:406:A:H2'	1:X:407:G:H8	1.82	0.44
1:X:140:A:H2'	1:X:141:U:C6	2.52	0.44
23:V:22:LYS:HE2	23:V:22:LYS:HB3	1.67	0.44
1:X:2858:G:H2'	1:X:2859:G:O4'	2.17	0.44
18:Q:75:ARG:HD3	18:Q:75:ARG:HA	1.62	0.44
5:C:80:ALA:HB3	5:C:83:TRP:CD1	2.53	0.44
3:A:20:ASP:O	3:A:22:ALA:N	2.51	0.44
22:U:17:ARG:O	22:U:29:TRP:N	2.41	0.44
16:O:29:GLU:OE1	16:O:64:LYS:HA	2.17	0.44
1:X:871:U:H2'	1:X:873:U:O4'	2.18	0.44
1:X:1289:A:OP2	15:N:10:THR:HG21	2.18	0.44
34:X:3426:EPE:H72	15:N:10:THR:OG1	2.18	0.44
1:X:1770:C:O2'	1:X:1771:A:H5'	2.18	0.44
1:X:1315:C:H2'	1:X:1316:G:H8	1.82	0.44
20:S:44:ASP:OD2	20:S:46:VAL:HG12	2.17	0.44
7:E:101:LYS:O	7:E:103:LEU:N	2.49	0.44
18:Q:60:PRO:HB3	18:Q:72:THR:O	2.18	0.44
1:X:769:U:H2'	1:X:770:G:O4'	2.18	0.44
21:T:48:GLN:HE21	21:T:67:LEU:HD13	1.83	0.44
1:X:2656:A:C2	1:X:2914:A:C8	3.06	0.44
1:X:1471:A:C4	1:X:1472:C:N4	2.85	0.44
1:X:1845:U:OP2	3:A:156:ARG:HD3	2.18	0.44
19:R:70:LEU:HD12	19:R:71:LEU:N	2.29	0.44
5:C:14:SER:HG	5:C:15:GLY:H	1.64	0.44
1:X:1867:G:C8	1:X:1954:A:C2	3.06	0.44
1:X:688:A:C2'	1:X:689:A:H5'	2.48	0.44
18:Q:58:TYR:HB2	18:Q:75:ARG:HB2	2.00	0.44
1:X:1526:G:N3	1:X:1526:G:H3'	2.33	0.44
15:N:69:ALA:HB2	15:N:79:LEU:HD12	1.99	0.44
5:C:179:GLN:N	5:C:179:GLN:OE1	2.50	0.44
16:O:25:LEU:HD13	16:O:33:PHE:CZ	2.53	0.44
17:P:20:VAL:HG21	17:P:43:SER:HB2	2.00	0.44
15:N:95:LEU:HA	15:N:95:LEU:HD12	1.85	0.44
26:2:23:MET:CE	26:2:29:ARG:HG3	2.48	0.44
11:J:93:TRP:O	11:J:94:ILE:HD13	2.18	0.44
1:X:955:A:C2	11:J:15:PRO:HG3	2.53	0.44
3:A:142:HIS:CD2	3:A:143:ASN:HB2	2.53	0.44
1:X:2077:C:H1'	4:B:169:MET:HE1	2.00	0.44
1:X:351:G:O2'	19:R:15:LYS:HE2	2.18	0.44
1:X:189:G:H2'	1:X:190:G:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:41:VAL:HG22	16:O:47:LYS:H	1.82	0.44
1:X:982:G:C2	1:X:983:G:N7	2.86	0.44
8:G:113:THR:OG1	8:G:116:GLY:N	2.45	0.44
1:X:1066:G:N2	1:X:1186:A:C2	2.85	0.43
1:X:1826:G:H5'	1:X:1846:A:N6	2.31	0.43
1:X:1013:U:H2'	1:X:1014:U:H6	1.82	0.43
1:X:1739:G:C8	3:A:8:PRO:HB2	2.51	0.43
1:X:704:U:H2'	1:X:705:U:O4'	2.18	0.43
3:A:72:ASP:HA	3:A:118:SER:CB	2.48	0.43
2:Y:76:A:H2'	2:Y:77:G:O4'	2.17	0.43
1:X:1086:G:O6	1:X:1158:G:C5	2.71	0.43
1:X:1659:C:H2'	1:X:1659:C:O2	2.18	0.43
1:X:2449:C:H6	1:X:2449:C:H2'	1.54	0.43
3:A:81:ILE:HG12	3:A:92:ALA:HB2	2.00	0.43
20:S:105:PRO:HA	20:S:136:ASN:HB2	2.00	0.43
2:Y:16:A:N1	2:Y:105:G:N2	2.66	0.43
11:J:54:MET:HE3	11:J:54:MET:HB3	1.79	0.43
1:X:2024:A:H2'	1:X:2025:A:C8	2.50	0.43
10:I:57:LEU:HD23	10:I:57:LEU:N	2.33	0.43
1:X:525:A:N3	1:X:527:G:H5''	2.33	0.43
1:X:2833:U:H2'	1:X:2834:C:C6	2.53	0.43
1:X:1091:G:H1'	1:X:1154:G:N2	2.33	0.43
1:X:179:A:OP2	1:X:179:A:H8	2.01	0.43
1:X:809:A:H5''	3:A:209:GLY:HA3	2.00	0.43
1:X:2717:A:H5''	12:K:4:ARG:NH2	2.33	0.43
1:X:2770:U:OP1	28:4:33:LYS:NZ	2.49	0.43
11:J:40:SER:HB3	11:J:127:VAL:HG22	2.00	0.43
1:X:1487:G:N2	1:X:1597:U:O2	2.50	0.43
1:X:566:U:H2'	1:X:567:G:C8	2.53	0.43
1:X:327:G:H2'	1:X:327:G:N3	2.33	0.43
1:X:280:C:H2'	1:X:281:A:H8	1.83	0.43
1:X:2908:U:H2'	1:X:2909:C:H6	1.83	0.43
3:A:54:HIS:HA	3:A:217:ARG:H	1.83	0.43
1:X:2687:A:H2'	1:X:2688:G:O4'	2.18	0.43
1:X:1238:U:H1'	15:N:4:VAL:HG22	2.00	0.43
8:G:73:LYS:O	8:G:91:GLY:N	2.40	0.43
8:G:140:ASN:N	8:G:140:ASN:OD1	2.51	0.43
1:X:331:G:O2'	1:X:332:A:H8	2.01	0.43
1:X:661:U:HO2'	1:X:662:G:P	2.39	0.43
19:R:9:VAL:HG12	19:R:69:GLN:HA	2.01	0.43
4:B:14:GLN:NE2	4:B:22:LEU:HD21	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:11:A:O2'	2:Y:13:A:OP2	2.35	0.43
16:O:25:LEU:HD13	16:O:33:PHE:CE2	2.52	0.43
11:J:115:ARG:HA	11:J:131:PHE:CE1	2.53	0.43
1:X:1605:A:O4'	30:X:3005:MPD:H32	2.18	0.43
4:B:119:THR:O	4:B:209:VAL:HA	2.19	0.43
11:J:28:THR:O	11:J:30:GLY:N	2.51	0.43
1:X:1998:A:C5	3:A:240:PRO:HD3	2.53	0.43
29:X:3001:ZLD:O15	29:X:3001:ZLD:H5	2.18	0.43
1:X:561:C:C2'	1:X:562:C:H5'	2.49	0.43
1:X:2350:G:C6	1:X:2351:U:C4	3.07	0.43
14:M:61:PHE:HD2	14:M:63:VAL:HG23	1.82	0.43
1:X:593:U:OP2	16:O:64:LYS:NZ	2.51	0.43
1:X:1016:G:H3'	1:X:1017:A:H5''	2.00	0.43
1:X:588:G:N2	1:X:594:G:C6	2.87	0.43
5:C:88:ILE:HD13	5:C:88:ILE:HA	1.82	0.43
1:X:504:G:O2'	26:2:40:ARG:HD3	2.19	0.43
1:X:719:G:H1'	5:C:74:ARG:NE	2.26	0.43
1:X:2758:G:N1	1:X:2759:G:O6	2.51	0.43
1:X:1599:G:OP1	1:X:1761:G:N2	2.47	0.43
1:X:926:G:H21	1:X:941:A:N6	2.17	0.43
1:X:2646:U:O2'	1:X:2647:C:H5'	2.19	0.43
1:X:674:C:H2'	1:X:675:G:H8	1.82	0.43
1:X:2634:G:H2'	1:X:2635:G:O4'	2.19	0.43
1:X:2883:U:H2'	1:X:2884:G:H8	1.83	0.43
24:W:44:ARG:HA	24:W:47:ILE:HD12	2.01	0.43
18:Q:36:THR:O	18:Q:40:MET:HG2	2.19	0.43
26:2:4:ARG:HA	26:2:4:ARG:HD3	1.64	0.43
19:R:4:LYS:HB3	19:R:4:LYS:NZ	2.33	0.43
1:X:2844:U:H2'	1:X:2845:G:O4'	2.18	0.43
1:X:225:A:N6	1:X:235:G:H1'	2.33	0.43
1:X:1998:A:HO2'	1:X:1999:G:P	2.40	0.43
5:C:188:ASN:O	5:C:188:ASN:ND2	2.42	0.43
1:X:1507:A:N7	1:X:1508:C:H5	2.15	0.43
19:R:12:ILE:H	19:R:67:ASN:HA	1.84	0.43
1:X:2720:A:H2'	1:X:2721:G:C8	2.54	0.43
1:X:2378:G:H1'	1:X:2394:G:N2	2.34	0.43
4:B:36:LEU:HD12	4:B:52:GLY:HA3	1.99	0.43
1:X:538:G:H2'	1:X:539:G:O4'	2.18	0.43
16:O:78:ARG:O	16:O:80:LYS:N	2.43	0.43
1:X:2587:C:C4	1:X:2588:A:N7	2.87	0.43
1:X:1461:C:N4	1:X:1462:G:N7	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1329:G:H2'	1:X:1330:U:C6	2.54	0.43
4:B:81:ASP:N	4:B:81:ASP:OD1	2.52	0.43
11:J:120:LEU:HD12	11:J:120:LEU:HA	1.87	0.43
1:X:1088:C:H4'	1:X:1092:A:C8	2.53	0.43
1:X:2807:G:H2'	1:X:2808:A:OP1	2.18	0.43
1:X:1712:A:H4'	1:X:1713:A:O5'	2.19	0.43
1:X:879:U:H2'	1:X:880:A:C8	2.54	0.43
1:X:1494:G:C8	1:X:1495:C:H5	2.36	0.43
1:X:2670:G:OP2	35:X:3428:SPD:H92	2.18	0.43
1:X:2050:A:H2'	1:X:2051:C:C6	2.54	0.43
1:X:2652:G:H2'	1:X:2653:C:C6	2.54	0.43
1:X:2102:U:H1'	1:X:2624:G:H21	1.84	0.43
1:X:2479:C:H2'	1:X:2480:A:C8	2.54	0.43
23:V:32:LEU:HB2	23:V:37:LEU:HD12	2.01	0.43
1:X:510:U:C2	1:X:833:A:C6	3.07	0.43
5:C:46:GLN:HG3	5:C:48:THR:HG23	2.01	0.43
12:K:12:GLN:O	12:K:16:MET:HB2	2.19	0.43
1:X:2511:G:OP1	11:J:45:ARG:HD3	2.19	0.43
15:N:49:ASP:HA	15:N:52:GLN:HG2	2.01	0.43
8:G:40:LYS:HG2	8:G:40:LYS:H	1.56	0.43
1:X:2359:C:H5''	21:T:54:TYR:OH	2.18	0.43
4:B:156:MET:HB2	4:B:160:ALA:CB	2.47	0.43
1:X:526:A:OP2	19:R:42:LYS:HD3	2.19	0.43
1:X:327:G:O2'	1:X:328:G:O5'	2.37	0.43
1:X:971:U:H2'	1:X:972:A:H8	1.84	0.43
2:Y:13:A:H1'	2:Y:106:U:C2	2.54	0.43
18:Q:57:ASN:O	18:Q:58:TYR:HD1	2.01	0.43
3:A:226:ASN:HB3	3:A:227:PRO:HD2	2.01	0.43
17:P:47:ILE:HG23	17:P:105:ILE:HD11	2.01	0.43
27:3:24:ARG:HD2	27:3:24:ARG:HA	1.82	0.43
1:X:1760:G:C6	1:X:1761:G:C8	3.07	0.43
1:X:443:U:OP1	22:U:34:GLN:HB3	2.19	0.43
23:V:49:THR:HA	23:V:52:ARG:HB2	2.00	0.43
2:Y:24:C:H2'	2:Y:25:A:O4'	2.19	0.43
27:3:48:ARG:HA	27:3:50:VAL:HG22	2.01	0.43
1:X:938:G:H2'	1:X:939:U:C6	2.53	0.43
1:X:2440:G:C6	1:X:2441:G:N7	2.87	0.43
34:X:3426:EPE:H72	34:X:3426:EPE:H61	1.74	0.42
1:X:329:A:C6	1:X:398:C:C4	3.07	0.42
2:Y:15:C:N4	2:Y:105:G:N2	2.67	0.42
5:C:29:ASN:HB3	5:C:108:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2357:G:H4'	21:T:52:LYS:HE3	2.00	0.42
24:W:22:THR:HG23	24:W:46:GLN:HG2	2.00	0.42
1:X:1168:C:H2'	1:X:1169:G:O4'	2.19	0.42
1:X:525:A:C2	1:X:526:A:C5	3.07	0.42
7:E:133:VAL:HG11	7:E:141:VAL:HG13	2.01	0.42
4:B:36:LEU:HD23	4:B:36:LEU:HA	1.75	0.42
1:X:192:G:H2'	1:X:208:G:N2	2.34	0.42
17:P:62:TYR:HB2	17:P:64:MET:HG3	2.01	0.42
1:X:736:C:H2'	1:X:737:C:C6	2.54	0.42
1:X:796:A:C6	1:X:834:A:C5	3.06	0.42
1:X:1379:A:C6	1:X:1382:C:C2	3.07	0.42
8:G:5:PHE:HD2	15:N:100:ILE:HD13	1.83	0.42
17:P:13:ALA:O	17:P:17:VAL:HG23	2.18	0.42
4:B:208:LEU:HA	4:B:208:LEU:HD12	1.81	0.42
8:G:90:ALA:C	8:G:92:GLU:N	2.72	0.42
1:X:2646:U:H4'	4:B:163:VAL:HG12	2.01	0.42
1:X:2882:A:H2'	1:X:2883:U:C6	2.54	0.42
1:X:1753:U:H2'	1:X:1754:C:C6	2.54	0.42
10:I:33:ARG:NH1	10:I:33:ARG:HB2	2.34	0.42
1:X:946:A:O2'	1:X:947:U:O4'	2.35	0.42
12:K:11:ASP:OD1	12:K:12:GLN:HG3	2.19	0.42
1:X:2838:C:O2'	1:X:2839:A:H5'	2.19	0.42
10:I:2:LYS:O	10:I:4:HIS:N	2.44	0.42
1:X:459:C:H2'	1:X:460:C:C6	2.54	0.42
1:X:1840:U:H2'	1:X:1841:G:O4'	2.19	0.42
11:J:41:TRP:O	11:J:41:TRP:HD1	2.02	0.42
1:X:1747:G:H2'	1:X:1748:G:C8	2.54	0.42
1:X:2827:A:H2'	1:X:2828:U:O4'	2.19	0.42
23:V:37:LEU:HD22	23:V:39:GLU:O	2.20	0.42
18:Q:11:VAL:HG23	18:Q:27:PHE:HA	2.01	0.42
1:X:798:G:H2'	1:X:799:U:C6	2.54	0.42
6:D:123:ASP:CB	6:D:145:LYS:HA	2.50	0.42
3:A:93:LEU:HD12	3:A:102:ARG:O	2.19	0.42
1:X:2734:C:H4'	12:K:64:LYS:HE3	2.01	0.42
1:X:1547:C:H2'	1:X:1548:U:C6	2.54	0.42
1:X:734:A:H2'	1:X:735:C:C6	2.54	0.42
12:K:92:ARG:HD2	12:K:93:TYR:CE2	2.54	0.42
1:X:2360:A:H5''	1:X:2361:U:H5'	2.02	0.42
1:X:1169:G:C6	1:X:1170:A:N6	2.87	0.42
11:J:34:LEU:HB2	11:J:118:LEU:HD13	2.01	0.42
26:2:23:MET:HE2	26:2:29:ARG:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:5:A:H2'	1:X:6:A:C8	2.54	0.42
1:X:87:U:H5''	1:X:88:G:H5'	2.00	0.42
9:H:43:VAL:HB	9:H:54:LYS:HA	2.01	0.42
9:H:43:VAL:HG23	9:H:56:ASP:O	2.20	0.42
1:X:28:A:H1'	1:X:558:A:C2	2.54	0.42
20:S:72:VAL:HG23	20:S:92:LEU:O	2.20	0.42
13:L:17:ARG:HH22	13:L:91:GLU:CB	2.32	0.42
1:X:83:G:N2	1:X:102:A:H2	2.16	0.42
4:B:154:VAL:HA	4:B:167:GLN:NE2	2.34	0.42
1:X:1315:C:H2'	1:X:1316:G:C8	2.55	0.42
27:3:34:ALA:HB1	27:3:37:SER:OG	2.19	0.42
1:X:276:C:H2'	1:X:277:C:C6	2.55	0.42
1:X:1055:A:H1'	1:X:1057:A:O4'	2.19	0.42
15:N:19:LYS:HA	15:N:19:LYS:HD2	1.88	0.42
1:X:2385:A:N1	10:I:50:PHE:HZ	2.17	0.42
1:X:901:G:H1'	21:T:35:ASP:HB3	2.01	0.42
1:X:218:G:H4'	1:X:219:A:H4'	2.01	0.42
1:X:1032:A:C8	24:W:13:ILE:HD12	2.55	0.42
18:Q:35:LYS:HE2	18:Q:54:ASN:HA	2.02	0.42
1:X:1781:C:H2'	1:X:1782:A:C8	2.54	0.42
1:X:1069:G:C4	1:X:1179:C:H1'	2.54	0.42
2:Y:6:U:H3	2:Y:109:C:H42	1.66	0.42
1:X:1463:A:H3'	1:X:1464:U:H5''	2.01	0.42
1:X:2567:C:O2'	1:X:2767:A:N3	2.47	0.42
12:K:55:ASP:OD1	12:K:58:SER:OG	2.31	0.42
26:2:13:HIS:O	26:2:17:HIS:HB2	2.20	0.42
1:X:1300:G:C6	1:X:1301:U:C4	3.07	0.42
1:X:1440:A:H2'	1:X:1441:C:C6	2.55	0.42
19:R:40:ILE:HB	19:R:59:THR:HG23	2.02	0.42
1:X:1834:G:N1	1:X:1835:U:H1'	2.34	0.42
1:X:2759:G:H3'	1:X:2760:A:O4'	2.19	0.42
1:X:577:A:H4'	1:X:578:G:C8	2.55	0.42
1:X:2232:A:N1	1:X:2247:G:C2	2.88	0.42
1:X:1831:A:N6	1:X:1840:U:H3	2.18	0.42
1:X:1510:U:H3	1:X:1571:G:H1	1.67	0.42
1:X:2235:A:H2'	1:X:2236:C:C6	2.55	0.42
35:X:3430:SPD:H52	35:X:3430:SPD:HN11	1.84	0.42
1:X:322:A:H2'	1:X:323:C:H5'	2.01	0.42
5:C:177:THR:HB	5:C:179:GLN:OE1	2.19	0.42
20:S:113:VAL:HG22	20:S:144:ASP:H	1.85	0.42
1:X:447:A:H2'	1:X:448:A:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:304:G:H1	1:X:413:C:H42	1.68	0.42
15:N:91:ASN:OD1	15:N:91:ASN:C	2.58	0.42
1:X:622:A:OP1	35:X:3432:SPD:N10	2.51	0.42
1:X:907:G:H2'	1:X:908:A:O4'	2.20	0.42
19:R:23:VAL:HA	19:R:35:VAL:HB	2.01	0.42
1:X:1065:A:C8	1:X:1066:G:H4'	2.54	0.42
1:X:1241:A:C6	1:X:1242:A:C6	3.08	0.42
1:X:1736:U:O2'	1:X:1737:U:H2'	2.19	0.42
1:X:810:A:H2'	1:X:811:C:C6	2.55	0.42
1:X:2883:U:H2'	1:X:2884:G:C8	2.54	0.42
1:X:731:U:O2'	26:2:6:TYR:HA	2.20	0.42
1:X:1301:U:H2'	1:X:1302:G:O4'	2.19	0.42
1:X:683:G:H2'	1:X:684:U:C6	2.55	0.42
11:J:74:TYR:CE2	11:J:92:GLY:HA3	2.55	0.42
9:H:39:ILE:HD13	9:H:62:ILE:HD11	2.02	0.42
1:X:2075:G:C5	1:X:2076:A:C8	3.08	0.42
1:X:2843:A:OP1	4:B:127:PHE:HB2	2.20	0.42
1:X:777:C:H2'	1:X:778:G:O4'	2.19	0.42
1:X:1288:G:O6	10:I:18:ARG:NH2	2.28	0.42
1:X:1000:G:H2'	1:X:1001:A:H2'	2.02	0.42
14:M:102:LEU:C	14:M:104:SER:H	2.23	0.42
11:J:74:TYR:CD2	11:J:94:ILE:HG12	2.55	0.42
1:X:2231:C:HO2'	1:X:2232:A:H8	1.65	0.42
1:X:1280:U:H2'	1:X:1281:U:H6	1.84	0.42
5:C:101:MET:HE3	5:C:101:MET:HB3	1.81	0.42
1:X:328:G:O6	1:X:400:C:H1'	2.20	0.42
19:R:72:ASP:OD1	19:R:72:ASP:N	2.53	0.42
19:R:24:ILE:HG12	19:R:35:VAL:HA	2.01	0.41
4:B:26:THR:OG1	4:B:200:ASN:HA	2.20	0.41
4:B:163:VAL:HG13	4:B:167:GLN:HG3	2.01	0.41
1:X:2580:G:C4	1:X:2581:U:H1'	2.55	0.41
1:X:361:U:H2'	1:X:362:C:C6	2.55	0.41
1:X:1223:A:OP1	24:W:30:LYS:HE2	2.20	0.41
8:G:38:ARG:HG2	8:G:110:LEU:HD22	2.01	0.41
4:B:165:LYS:HB2	4:B:165:LYS:HE2	1.71	0.41
1:X:332:A:H2'	1:X:333:C:C6	2.55	0.41
8:G:1:MET:N	8:G:1:MET:SD	2.84	0.41
1:X:1542:C:H5'	1:X:1543:G:OP2	2.20	0.41
9:H:2:ILE:HB	9:H:33:ALA:HB3	2.02	0.41
1:X:2017:C:H5''	1:X:2018:U:OP2	2.19	0.41
3:A:142:HIS:CD2	3:A:191:THR:HB	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1482:U:H2'	1:X:1483:A:C8	2.54	0.41
15:N:83:LEU:HD23	15:N:113:ALA:HB2	2.02	0.41
1:X:2711:U:H5'	9:H:76:TYR:CE1	2.55	0.41
24:W:30:LYS:O	24:W:33:SER:OG	2.33	0.41
1:X:1078:G:C6	1:X:1079:U:C4	3.09	0.41
8:G:99:GLU:O	8:G:103:GLU:HB3	2.20	0.41
1:X:2105:C:H2'	1:X:2106:U:O4'	2.19	0.41
1:X:1540:U:H1'	1:X:1625:U:H4'	2.02	0.41
14:M:88:VAL:HG11	14:M:91:ARG:NH2	2.35	0.41
1:X:1044:A:H2'	1:X:1045:A:C8	2.55	0.41
1:X:546:A:O5'	1:X:546:A:H8	2.04	0.41
1:X:2903:A:H5'	1:X:2904:U:H5'	2.03	0.41
1:X:1564:G:H2'	1:X:1565:U:H6	1.84	0.41
5:C:63:LYS:HA	5:C:64:PRO:HD3	1.84	0.41
1:X:659:A:N3	1:X:659:A:H2'	2.34	0.41
1:X:1281:U:H2'	1:X:1282:A:O4'	2.20	0.41
1:X:902:A:C6	1:X:903:G:C6	3.08	0.41
5:C:80:ALA:HB3	5:C:83:TRP:HD1	1.83	0.41
1:X:2567:C:O2	1:X:2767:A:H2	2.03	0.41
1:X:843:G:H2'	1:X:844:G:C8	2.55	0.41
1:X:1335:C:H2'	1:X:1336:G:O4'	2.20	0.41
1:X:1492:G:N3	1:X:1593:G:N2	2.68	0.41
1:X:499:A:N3	1:X:503:A:O2'	2.48	0.41
1:X:1065:A:H2'	1:X:1067:U:H5'	2.02	0.41
4:B:22:LEU:N	9:H:72:ASN:O	2.48	0.41
3:A:86:ASN:OD1	3:A:86:ASN:N	2.54	0.41
1:X:2876:G:H2'	1:X:2877:G:O4'	2.20	0.41
1:X:1463:A:OP2	1:X:1624:C:N4	2.53	0.41
1:X:185:A:C6	1:X:186:C:C4	3.08	0.41
1:X:696:G:H2'	1:X:697:U:C6	2.55	0.41
1:X:235:G:O2'	1:X:236:A:P	2.78	0.41
4:B:118:VAL:HG22	4:B:183:LEU:HD11	2.02	0.41
1:X:923:A:C2'	1:X:924:G:H8	2.34	0.41
1:X:577:A:C8	15:N:28:LYS:HE3	2.55	0.41
10:I:20:GLY:O	10:I:21:ARG:HD3	2.20	0.41
1:X:2241:C:H2'	1:X:2242:G:O4'	2.20	0.41
12:K:47:LEU:HD13	12:K:66:LEU:HD12	2.03	0.41
16:O:35:PHE:CZ	16:O:95:LEU:HD13	2.53	0.41
1:X:450:C:H4'	1:X:451:U:H5'	2.01	0.41
16:O:41:VAL:CG2	16:O:47:LYS:H	2.32	0.41
10:I:2:LYS:HE3	10:I:2:LYS:HB2	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:723:C:H2'	1:X:724:C:C6	2.55	0.41
1:X:424:C:N4	1:X:425:G:O6	2.54	0.41
25:Z:35:ARG:O	25:Z:36:GLU:HG2	2.20	0.41
1:X:2854:A:O3'	4:B:67:LYS:NZ	2.53	0.41
9:H:8:LEU:HD12	9:H:19:VAL:HG23	2.03	0.41
1:X:1908:A:H5'	1:X:1909:C:OP2	2.21	0.41
1:X:426:G:H2'	1:X:427:A:O4'	2.20	0.41
1:X:944:G:H1'	1:X:945:A:H2'	2.02	0.41
1:X:1249:U:O4	35:X:3434:SPD:N1	2.54	0.41
1:X:2709:U:O4	1:X:2755:U:H1'	2.20	0.41
11:J:74:TYR:HD2	11:J:94:ILE:HG12	1.86	0.41
17:P:1:MET:HB3	17:P:2:GLU:H	1.66	0.41
3:A:143:ASN:H	3:A:155:ALA:HB3	1.86	0.41
1:X:1791:G:H2'	1:X:1792:C:O4'	2.21	0.41
18:Q:51:ALA:HB2	18:Q:83:LYS:H	1.84	0.41
1:X:1754:C:H4'	1:X:2878:U:O2	2.21	0.41
1:X:1086:G:O2'	1:X:1087:C:P	2.79	0.41
1:X:197:G:C2	1:X:205:U:H1'	2.55	0.41
2:Y:68:A:H2'	2:Y:69:C:H6	1.85	0.41
1:X:864:A:C4	1:X:1228:A:C2	3.07	0.41
1:X:1071:A:C2	1:X:2515:A:H5'	2.56	0.41
1:X:372:A:H61	19:R:15:LYS:HB2	1.84	0.41
1:X:2510:C:N3	11:J:124:LYS:NZ	2.69	0.41
1:X:190:G:C6	1:X:191:A:C5	3.09	0.41
17:P:3:ALA:HB3	17:P:58:ALA:HB2	2.02	0.41
1:X:2539:C:H2'	1:X:2540:A:O4'	2.20	0.41
1:X:2416:G:H5''	1:X:2417:U:O4'	2.21	0.41
1:X:1317:G:N2	1:X:1328:C:C2	2.88	0.41
5:C:44:LEU:HA	5:C:44:LEU:HD12	1.74	0.41
34:X:3424:EPE:H61	34:X:3424:EPE:H102	1.79	0.41
28:4:11:CYS:SG	28:4:32:HIS:HE1	2.44	0.41
8:G:66:THR:HG22	8:G:67:GLY:N	2.36	0.41
3:A:17:THR:OG1	3:A:204:ASN:N	2.54	0.41
18:Q:13:THR:HG23	18:Q:16:SER:HB3	2.03	0.41
1:X:2717:A:H4'	1:X:2718:C:OP2	2.21	0.41
1:X:2905:C:H42	25:Z:39:LEU:HD11	1.86	0.41
1:X:2289:U:OP1	1:X:2414:U:O2'	2.34	0.41
1:X:1762:U:H5'	1:X:1763:U:OP2	2.20	0.41
1:X:1711:G:N2	1:X:2018:U:H2'	2.35	0.41
26:2:31:VAL:O	26:2:35:ARG:HG3	2.21	0.41
1:X:1356:G:C5	1:X:1357:G:C6	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:90:ALA:O	12:K:94:THR:HG23	2.21	0.41
1:X:1436:C:O2'	1:X:1437:U:P	2.79	0.41
1:X:864:A:OP2	1:X:1226:G:N2	2.51	0.41
1:X:1800:A:N7	1:X:1856:A:H1'	2.35	0.41
25:Z:28:THR:CG2	25:Z:37:TYR:HE1	2.34	0.41
1:X:987:U:OP1	10:I:33:ARG:HG3	2.21	0.41
1:X:1444:C:H2'	1:X:1445:C:C6	2.55	0.41
17:P:44:SER:N	17:P:45:PRO:HD2	2.36	0.41
1:X:1267:A:H2'	1:X:1268:C:H6	1.86	0.41
1:X:2889:G:H2'	1:X:2890:C:O4'	2.21	0.41
1:X:1322:G:C5	1:X:1366:U:C4	3.09	0.41
1:X:2763:G:C2	1:X:2764:G:C8	3.09	0.41
8:G:106:ILE:HG21	8:G:123:LEU:HD22	2.03	0.41
8:G:26:LEU:O	8:G:30:SER:HB2	2.21	0.41
1:X:1862:G:O6	1:X:1957:G:N2	2.54	0.41
13:L:29:PRO:O	13:L:88:GLY:HA3	2.20	0.41
1:X:1411:G:C4	1:X:1412:G:C8	3.09	0.41
1:X:672:A:H8	1:X:672:A:P	2.44	0.41
34:X:3426:EPE:H21	34:X:3426:EPE:H102	1.48	0.41
1:X:1091:G:H1'	1:X:1154:G:H22	1.86	0.41
1:X:624:C:OP1	15:N:31:LEU:HB3	2.20	0.41
1:X:2783:U:H4'	1:X:2784:A:OP1	2.21	0.41
34:X:3425:EPE:H61	34:X:3425:EPE:H101	1.72	0.41
1:X:1511:C:H1'	1:X:1571:G:N2	2.36	0.41
1:X:2642:U:N1	25:Z:4:PRO:HA	2.36	0.41
1:X:665:G:H4'	1:X:666:A:H5''	2.02	0.41
1:X:2286:G:C5	1:X:2287:C:C5	3.09	0.41
1:X:208:G:O2'	1:X:209:U:OP2	2.38	0.41
1:X:2830:A:H2'	1:X:2831:G:O4'	2.20	0.41
8:G:111:PRO:HB2	8:G:113:THR:HG23	2.03	0.41
23:V:52:ARG:O	23:V:55:THR:OG1	2.38	0.41
17:P:42:ALA:O	17:P:45:PRO:HD2	2.21	0.41
1:X:820:G:C4	1:X:839:A:C8	3.09	0.41
1:X:1429:G:C6	1:X:1430:A:N6	2.89	0.41
1:X:1658:A:N1	17:P:93:ALA:HB2	2.37	0.40
1:X:2112:C:H42	1:X:2261:A:N6	2.18	0.40
1:X:173:A:H2'	1:X:174:U:H6	1.86	0.40
1:X:2047:A:P	25:Z:7:ARG:HH21	2.44	0.40
1:X:2672:G:O6	35:X:3428:SPD:N10	2.55	0.40
1:X:1525:U:H2'	1:X:1526:G:C8	2.56	0.40
1:X:1893:A:C6	1:X:1903:A:N7	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1272:U:H2'	1:X:1273:G:O4'	2.21	0.40
1:X:7:G:O2'	1:X:8:U:H5'	2.21	0.40
16:O:39:LEU:HA	16:O:39:LEU:HD23	1.85	0.40
15:N:11:ARG:O	15:N:15:LYS:HB2	2.22	0.40
1:X:236:A:N3	1:X:236:A:H2'	2.36	0.40
17:P:109:ASP:HB2	17:P:110:GLY:H	1.66	0.40
1:X:505:U:H2'	1:X:506:A:H5''	2.02	0.40
8:G:102:ILE:HB	8:G:125:VAL:HG11	2.03	0.40
1:X:525:A:HO2'	1:X:527:G:H8	1.69	0.40
21:T:49:ARG:HA	21:T:49:ARG:NE	2.36	0.40
1:X:2391:C:H2'	1:X:2392:G:O4'	2.21	0.40
7:E:133:VAL:HG13	7:E:134:GLU:H	1.86	0.40
1:X:1331:C:H2'	1:X:1332:C:C6	2.56	0.40
1:X:1086:G:O6	1:X:1158:G:C6	2.73	0.40
8:G:30:SER:HA	8:G:106:ILE:HG13	2.03	0.40
7:E:69:ARG:O	7:E:73:ASN:HB2	2.21	0.40
1:X:498:G:N2	1:X:504:G:C4	2.89	0.40
1:X:1440:A:H1'	1:X:1513:A:H2	1.86	0.40
5:C:150:LYS:HA	5:C:188:ASN:ND2	2.36	0.40
1:X:1770:C:C2	1:X:1771:A:C8	3.10	0.40
1:X:2319:U:H2'	1:X:2320:C:H6	1.86	0.40
1:X:2112:C:N4	1:X:2261:A:H61	2.18	0.40
1:X:1965:A:C6	1:X:2617:A:H1'	2.56	0.40
1:X:2871:A:H2'	1:X:2872:G:C8	2.57	0.40
2:Y:22:G:C6	2:Y:54:U:C2	3.08	0.40
1:X:1078:G:H2'	1:X:1079:U:O4'	2.21	0.40
3:A:44:ASN:OD1	3:A:46:GLN:N	2.54	0.40
1:X:267:G:C2'	1:X:268:A:H5''	2.51	0.40
13:L:17:ARG:HA	13:L:20:THR:HG22	2.04	0.40
9:H:24:VAL:HG13	9:H:33:ALA:HB2	2.03	0.40
1:X:1482:U:H2'	1:X:1483:A:H8	1.86	0.40
1:X:2616:A:H2'	1:X:2617:A:C8	2.56	0.40
1:X:344:U:C2	1:X:345:C:C5	3.09	0.40
1:X:280:C:H2'	1:X:281:A:C8	2.57	0.40
15:N:25:PHE:CZ	25:Z:11:THR:HG21	2.56	0.40
23:V:40:THR:O	23:V:43:ILE:HG12	2.21	0.40
3:A:221:ARG:O	3:A:225:MET:HE3	2.21	0.40
5:C:70:THR:HB	5:C:72:ARG:H	1.86	0.40
1:X:2678:C:C2	1:X:2697:G:C2	3.09	0.40
1:X:381:G:N2	1:X:382:U:H1'	2.37	0.40
12:K:68:ASN:HB3	12:K:69:VAL:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:495:A:H4'	15:N:3:ARG:NH1	2.37	0.40
4:B:115:VAL:HG23	4:B:184:GLU:HB3	2.03	0.40
9:H:99:PHE:CD1	9:H:99:PHE:N	2.89	0.40
4:B:7:GLY:O	4:B:209:VAL:HB	2.20	0.40
1:X:2705:U:H2'	1:X:2706:A:C8	2.56	0.40
1:X:540:G:N2	17:P:61:ASN:HD21	2.20	0.40
1:X:2660:A:H2'	1:X:2661:A:O4'	2.21	0.40
1:X:511:G:H2'	1:X:512:A:C8	2.56	0.40
27:3:56:LYS:HE3	27:3:56:LYS:HB2	1.72	0.40
1:X:1823:U:H2'	1:X:1824:C:C6	2.57	0.40
1:X:854:G:C6	1:X:855:U:C4	3.09	0.40
1:X:1775:G:H2'	1:X:1776:A:C8	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	266/277 (96%)	208 (78%)	35 (13%)	23 (9%)	1	10
4	B	213/220 (97%)	183 (86%)	17 (8%)	13 (6%)	2	18
5	C	197/207 (95%)	162 (82%)	18 (9%)	17 (9%)	1	10
6	D	151/179 (84%)	118 (78%)	20 (13%)	13 (9%)	1	10
7	E	155/178 (87%)	109 (70%)	30 (19%)	16 (10%)	1	7
8	G	143/145 (99%)	122 (85%)	12 (8%)	9 (6%)	2	18
9	H	120/122 (98%)	109 (91%)	10 (8%)	1 (1%)	24	67
10	I	129/146 (88%)	91 (70%)	23 (18%)	15 (12%)	0	5
11	J	136/144 (94%)	119 (88%)	11 (8%)	6 (4%)	3	28
12	K	117/122 (96%)	106 (91%)	5 (4%)	6 (5%)	2	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	L	106/119 (89%)	82 (77%)	15 (14%)	9 (8%)	1	11
14	M	107/116 (92%)	95 (89%)	9 (8%)	3 (3%)	6	41
15	N	114/118 (97%)	110 (96%)	3 (3%)	1 (1%)	21	65
16	O	99/102 (97%)	86 (87%)	8 (8%)	5 (5%)	2	24
17	P	110/117 (94%)	106 (96%)	4 (4%)	0	100	100
18	Q	86/91 (94%)	75 (87%)	9 (10%)	2 (2%)	8	45
19	R	98/105 (93%)	77 (79%)	15 (15%)	6 (6%)	2	18
20	S	165/217 (76%)	130 (79%)	25 (15%)	10 (6%)	2	18
21	T	73/94 (78%)	67 (92%)	5 (7%)	1 (1%)	14	55
22	U	42/62 (68%)	32 (76%)	6 (14%)	4 (10%)	1	8
23	V	63/69 (91%)	52 (82%)	10 (16%)	1 (2%)	12	53
24	W	55/59 (93%)	52 (94%)	3 (6%)	0	100	100
25	Z	42/58 (72%)	36 (86%)	2 (5%)	4 (10%)	1	8
26	2	42/45 (93%)	36 (86%)	5 (12%)	1 (2%)	7	44
27	3	58/66 (88%)	47 (81%)	7 (12%)	4 (7%)	1	15
28	4	35/37 (95%)	30 (86%)	3 (9%)	2 (6%)	2	20
All	All	2922/3215 (91%)	2440 (84%)	310 (11%)	172 (6%)	2	19

All (172) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	141	VAL
3	A	154	ILE
3	A	192	ILE
4	B	60	LYS
4	B	61	LYS
4	B	62	ASP
5	C	126	VAL
5	C	154	VAL
5	C	171	PRO
5	C	175	VAL
5	C	184	LEU
6	D	44	VAL
6	D	74	ILE
6	D	104	ILE
6	D	109	PRO

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Mol	Chain	Res	Type
6	D	117	VAL
7	E	27	LYS
7	E	125	VAL
8	G	40	LYS
8	G	93	LEU
9	H	119	PRO
10	I	30	THR
10	I	46	VAL
10	I	48	PRO
10	I	62	PRO
10	I	101	VAL
11	J	60	ARG
12	K	26	ILE
12	K	78	THR
12	K	82	LEU
12	K	97	GLN
13	L	25	THR
13	L	63	ILE
13	L	71	GLU
14	M	101	TYR
16	O	50	ALA
19	R	65	VAL
20	S	12	LYS
21	T	82	ARG
22	U	14	THR
23	V	11	THR
26	2	16	VAL
27	3	30	SER
3	A	21	PHE
3	A	82	GLN
3	A	88	SER
3	A	126	VAL
3	A	158	ALA
4	B	53	PHE
4	B	101	VAL
5	C	15	GLY
5	C	130	ASN
6	D	40	VAL
6	D	70	ALA
6	D	127	ASN
7	E	47	GLU
7	E	61	ASP

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Mol	Chain	Res	Type
7	E	134	GLU
8	G	41	ASN
8	G	67	GLY
8	G	86	LYS
10	I	44	GLY
10	I	51	GLU
10	I	53	GLY
10	I	71	ARG
10	I	113	GLY
11	J	84	GLY
11	J	91	GLU
11	J	135	GLU
13	L	26	ALA
13	L	84	ALA
13	L	92	ILE
16	O	45	SER
16	O	73	VAL
18	Q	86	SER
20	S	34	TYR
20	S	65	VAL
20	S	109	VAL
20	S	146	THR
20	S	167	ILE
22	U	22	LEU
25	Z	29	GLU
3	A	51	VAL
3	A	151	GLY
3	A	156	ARG
3	A	170	LYS
4	B	32	GLU
4	B	106	SER
4	B	195	ILE
4	B	209	VAL
5	C	145	THR
5	C	149	PRO
5	C	173	VAL
5	C	191	SER
6	D	19	LYS
6	D	130	LEU
7	E	23	HIS
7	E	44	LYS
7	E	45	GLN

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Mol	Chain	Res	Type
7	E	60	GLU
7	E	108	GLY
8	G	89	THR
10	I	3	LEU
10	I	28	GLY
10	I	49	GLY
11	J	21	SER
11	J	25	ASN
13	L	93	VAL
15	N	7	GLY
19	R	52	PRO
19	R	58	GLU
19	R	75	THR
20	S	82	LEU
25	Z	32	ASN
25	Z	44	CYS
28	4	28	GLU
3	A	30	GLU
3	A	38	PRO
3	A	110	LEU
3	A	245	SER
4	B	157	ALA
4	B	186	VAL
5	C	10	ASP
5	C	27	GLU
5	C	144	SER
5	C	158	ASN
5	C	164	GLU
6	D	75	ALA
6	D	89	VAL
6	D	115	GLN
7	E	19	PHE
7	E	43	PHE
7	E	48	ASN
7	E	50	ILE
7	E	121	ILE
7	E	124	SER
8	G	69	LYS
12	K	99	GLY
13	L	42	ALA
19	R	77	GLU
20	S	81	PRO

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Mol	Chain	Res	Type
20	S	98	GLU
20	S	168	GLU
22	U	29	TRP
27	3	34	ALA
3	A	131	PRO
3	A	224	VAL
3	A	252	LYS
4	B	99	TYR
4	B	122	SER
8	G	137	GLN
10	I	64	ARG
12	K	77	THR
13	L	62	ASP
16	O	16	GLU
18	Q	63	LYS
22	U	40	VAL
27	3	28	PHE
28	4	27	CYS
5	C	172	GLY
10	I	79	LEU
14	M	37	GLY
19	R	74	LYS
27	3	29	THR
3	A	12	GLY
3	A	36	PRO
3	A	256	GLY
25	Z	30	CYS
8	G	88	ILE
14	M	66	ILE
16	O	51	PRO
3	A	164	VAL

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	102/224 (46%)	84 (82%)	18 (18%)	2 12
4	B	148/177 (84%)	115 (78%)	33 (22%)	1 5
5	C	107/169 (63%)	84 (78%)	23 (22%)	1 6
6	D	13/158 (8%)	11 (85%)	2 (15%)	3 18
7	E	53/155 (34%)	47 (89%)	6 (11%)	7 32
8	G	105/123 (85%)	87 (83%)	18 (17%)	2 14
9	H	77/100 (77%)	66 (86%)	11 (14%)	4 22
10	I	54/112 (48%)	40 (74%)	14 (26%)	0 3
11	J	91/119 (76%)	75 (82%)	16 (18%)	2 12
12	K	88/102 (86%)	73 (83%)	15 (17%)	2 14
13	L	35/95 (37%)	33 (94%)	2 (6%)	25 65
14	M	78/102 (76%)	58 (74%)	20 (26%)	0 3
15	N	93/98 (95%)	80 (86%)	13 (14%)	4 23
16	O	72/86 (84%)	64 (89%)	8 (11%)	8 33
17	P	91/94 (97%)	78 (86%)	13 (14%)	4 22
18	Q	44/82 (54%)	35 (80%)	9 (20%)	1 7
19	R	64/90 (71%)	45 (70%)	19 (30%)	0 2
20	S	75/190 (40%)	56 (75%)	19 (25%)	1 3
21	T	47/75 (63%)	42 (89%)	5 (11%)	8 36
22	U	10/52 (19%)	8 (80%)	2 (20%)	1 8
23	V	30/62 (48%)	22 (73%)	8 (27%)	0 3
24	W	51/53 (96%)	41 (80%)	10 (20%)	1 8
25	Z	35/51 (69%)	30 (86%)	5 (14%)	4 22
26	2	38/40 (95%)	29 (76%)	9 (24%)	1 4
27	3	35/57 (61%)	25 (71%)	10 (29%)	0 2
28	4	27/35 (77%)	26 (96%)	1 (4%)	41 77
All	All	1663/2701 (62%)	1354 (81%)	309 (19%)	2 10

All (309) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	46	GLN
3	A	53	HIS
3	A	58	HIS
3	A	80	SER
3	A	86	ASN
3	A	90	ASN
3	A	91	ILE
3	A	103	TYR
3	A	137	VAL
3	A	141	VAL
3	A	142	HIS
3	A	161	SER
3	A	181	VAL
3	A	202	LEU
3	A	204	ASN
3	A	205	VAL
3	A	211	SER
3	A	223	SER
4	B	2	THR
4	B	13	THR
4	B	15	VAL
4	B	19	ASN
4	B	25	VAL
4	B	32	GLU
4	B	44	ASP
4	B	54	GLU
4	B	64	LYS
4	B	65	SER
4	B	81	ASP
4	B	100	GLU
4	B	101	VAL
4	B	104	GLU
4	B	107	VAL
4	B	109	THR
4	B	115	VAL
4	B	136	GLN
4	B	137	SER
4	B	141	MET
4	B	147	PHE
4	B	149	ARG
4	B	156	MET
4	B	177	THR
4	B	179	THR

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Mol	Chain	Res	Type
4	B	180	VAL
4	B	181	GLN
4	B	183	LEU
4	B	196	LEU
4	B	198	LYS
4	B	200	ASN
4	B	205	LYS
4	B	206	LYS
5	C	16	SER
5	C	17	ILE
5	C	21	ASP
5	C	31	SER
5	C	35	GLU
5	C	44	LEU
5	C	49	HIS
5	C	62	ARG
5	C	67	GLN
5	C	70	THR
5	C	74	ARG
5	C	101	MET
5	C	105	MET
5	C	115	SER
5	C	136	THR
5	C	140	LYS
5	C	142	VAL
5	C	144	SER
5	C	152	VAL
5	C	176	THR
5	C	181	LEU
5	C	188	ASN
5	C	195	THR
6	D	23	SER
6	D	132	VAL
7	E	36	THR
7	E	42	THR
7	E	52	VAL
7	E	61	ASP
7	E	79	VAL
7	E	136	ILE
8	G	1	MET
8	G	3	GLN
8	G	4	THR

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Mol	Chain	Res	Type
8	G	8	ASN
8	G	24	GLN
8	G	30	SER
8	G	43	VAL
8	G	46	THR
8	G	58	ILE
8	G	61	SER
8	G	71	THR
8	G	92	GLU
8	G	96	THR
8	G	103	GLU
8	G	106	ILE
8	G	114	ARG
8	G	137	GLN
8	G	140	ASN
9	H	8	LEU
9	H	14	SER
9	H	21	THR
9	H	41	CYS
9	H	57	VAL
9	H	67	SER
9	H	72	ASN
9	H	77	ILE
9	H	87	ILE
9	H	88	ARG
9	H	102	VAL
10	I	23	VAL
10	I	25	THR
10	I	31	SER
10	I	33	ARG
10	I	47	ARG
10	I	55	LEU
10	I	57	LEU
10	I	61	LEU
10	I	67	THR
10	I	82	LEU
10	I	84	LYS
10	I	89	THR
10	I	96	LEU
10	I	112	LEU
11	J	7	VAL
11	J	21	SER

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Mol	Chain	Res	Type
11	J	26	TYR
11	J	27	VAL
11	J	37	THR
11	J	41	TRP
11	J	44	SER
11	J	72	THR
11	J	75	THR
11	J	81	VAL
11	J	103	LEU
11	J	111	GLU
11	J	116	GLU
11	J	119	ARG
11	J	120	LEU
11	J	124	LYS
12	K	4	ARG
12	K	6	LEU
12	K	8	ARG
12	K	9	THR
12	K	16	MET
12	K	20	LEU
12	K	33	THR
12	K	65	THR
12	K	66	LEU
12	K	67	ARG
12	K	68	ASN
12	K	69	VAL
12	K	82	LEU
12	K	101	THR
12	K	121	LEU
13	L	21	ASN
13	L	49	LYS
14	M	4	HIS
14	M	7	ILE
14	M	10	VAL
14	M	11	THR
14	M	17	THR
14	M	19	LEU
14	M	23	ARG
14	M	30	VAL
14	M	32	VAL
14	M	41	ARG
14	M	43	GLN

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Mol	Chain	Res	Type
14	M	48	VAL
14	M	53	ARG
14	M	58	SER
14	M	73	GLU
14	M	75	THR
14	M	80	THR
14	M	90	ARG
14	M	91	ARG
14	M	100	TYR
15	N	9	VAL
15	N	10	THR
15	N	15	LYS
15	N	22	LYS
15	N	27	SER
15	N	29	HIS
15	N	33	LYS
15	N	41	LYS
15	N	42	SER
15	N	51	ARG
15	N	58	ARG
15	N	79	LEU
15	N	90	ILE
16	O	1	MET
16	O	7	THR
16	O	34	THR
16	O	71	ILE
16	O	72	THR
16	O	73	VAL
16	O	75	THR
16	O	86	LYS
17	P	2	GLU
17	P	9	THR
17	P	11	ARG
17	P	15	ARG
17	P	24	ILE
17	P	33	ILE
17	P	65	ASN
17	P	66	THR
17	P	70	VAL
17	P	81	THR
17	P	82	LEU
17	P	100	THR

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Mol	Chain	Res	Type
17	P	109	ASP
18	Q	12	ILE
18	Q	13	THR
18	Q	32	ARG
18	Q	34	ASN
18	Q	40	MET
18	Q	57	ASN
18	Q	68	TYR
18	Q	74	LYS
18	Q	80	VAL
19	R	4	LYS
19	R	9	VAL
19	R	23	VAL
19	R	31	ASP
19	R	35	VAL
19	R	38	VAL
19	R	43	LYS
19	R	48	THR
19	R	56	ILE
19	R	59	THR
19	R	60	GLU
19	R	63	ILE
19	R	65	VAL
19	R	66	SER
19	R	68	VAL
19	R	72	ASP
19	R	79	THR
19	R	80	ARG
19	R	86	VAL
20	S	18	LEU
20	S	20	GLN
20	S	21	LEU
20	S	24	SER
20	S	30	VAL
20	S	31	VAL
20	S	38	ASN
20	S	40	SER
20	S	43	VAL
20	S	52	ILE
20	S	57	ARG
20	S	77	TYR
20	S	82	LEU

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Mol	Chain	Res	Type
20	S	85	GLN
20	S	87	THR
20	S	123	GLN
20	S	133	THR
20	S	155	THR
20	S	161	VAL
21	T	24	SER
21	T	26	SER
21	T	51	THR
21	T	61	ARG
21	T	78	GLU
22	U	18	ARG
22	U	36	VAL
23	V	29	ARG
23	V	32	LEU
23	V	40	THR
23	V	43	ILE
23	V	49	THR
23	V	52	ARG
23	V	55	THR
23	V	61	GLU
24	W	7	THR
24	W	9	THR
24	W	12	VAL
24	W	15	ARG
24	W	18	THR
24	W	37	VAL
24	W	43	ILE
24	W	48	ASN
24	W	53	LEU
24	W	54	VAL
25	Z	3	VAL
25	Z	11	THR
25	Z	37	TYR
25	Z	38	LYS
25	Z	40	SER
26	2	2	VAL
26	2	5	THR
26	2	11	ARG
26	2	20	ARG
26	2	23	MET
26	2	25	THR

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Mol	Chain	Res	Type
26	2	30	LYS
26	2	42	VAL
26	2	43	LEU
27	3	6	THR
27	3	8	ARG
27	3	17	THR
27	3	26	ARG
27	3	29	THR
27	3	37	SER
27	3	41	LYS
27	3	53	SER
27	3	56	LYS
27	3	58	VAL
28	4	26	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
24	W	40	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2691/2923 (92%)	627 (23%)	33 (1%)
2	Y	113/114 (99%)	14 (12%)	0
All	All	2804/3037 (92%)	641 (22%)	33 (1%)

All (641) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	A
1	X	15	G
1	X	34	U
1	X	36	G
1	X	39	C
1	X	51	G
1	X	55	G
1	X	61	A
1	X	64	A
1	X	70	G

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Mol	Chain	Res	Type
1	X	71	A
1	X	75	G
1	X	80	G
1	X	90	A
1	X	91	A
1	X	95	A
1	X	96	G
1	X	101	G
1	X	111	U
1	X	112	U
1	X	117	A
1	X	118	A
1	X	119	U
1	X	124	A
1	X	130	A
1	X	133	A
1	X	139	U
1	X	140	A
1	X	152	C
1	X	154	A
1	X	159	U
1	X	163	U
1	X	164	A
1	X	165	C
1	X	166	A
1	X	168	A
1	X	169	G
1	X	170	C
1	X	176	A
1	X	178	A
1	X	179	A
1	X	180	G
1	X	182	C
1	X	183	A
1	X	184	C
1	X	194	A
1	X	199	A
1	X	202	A
1	X	206	U
1	X	215	G
1	X	219	A
1	X	220	A

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Mol	Chain	Res	Type
1	X	224	A
1	X	225	A
1	X	229	A
1	X	233	U
1	X	235	G
1	X	236	A
1	X	248	G
1	X	251	G
1	X	252	C
1	X	255	G
1	X	268	A
1	X	284	C
1	X	285	U
1	X	286	U
1	X	287	G
1	X	288	C
1	X	289	U
1	X	290	U
1	X	291	G
1	X	293	U
1	X	298	U
1	X	300	G
1	X	303	G
1	X	310	C
1	X	311	U
1	X	313	U
1	X	319	G
1	X	320	U
1	X	321	U
1	X	322	A
1	X	323	C
1	X	324	A
1	X	328	G
1	X	329	A
1	X	331	G
1	X	332	A
1	X	353	A
1	X	358	G
1	X	364	A
1	X	365	A
1	X	372	A
1	X	373	A

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Mol	Chain	Res	Type
1	X	375	A
1	X	386	C
1	X	389	A
1	X	394	U
1	X	398	C
1	X	399	U
1	X	401	U
1	X	404	U
1	X	405	G
1	X	410	G
1	X	413	C
1	X	415	U
1	X	416	G
1	X	417	A
1	X	418	G
1	X	426	G
1	X	429	C
1	X	432	G
1	X	444	C
1	X	447	A
1	X	450	C
1	X	451	U
1	X	452	G
1	X	457	G
1	X	458	A
1	X	474	A
1	X	486	G
1	X	495	A
1	X	497	U
1	X	502	C
1	X	503	A
1	X	504	G
1	X	506	A
1	X	519	G
1	X	523	A
1	X	525	A
1	X	526	A
1	X	527	G
1	X	536	A
1	X	541	G
1	X	543	G
1	X	549	U

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Mol	Chain	Res	Type
1	X	550	A
1	X	553	A
1	X	554	C
1	X	566	U
1	X	567	G
1	X	572	C
1	X	573	A
1	X	575	G
1	X	576	U
1	X	577	A
1	X	578	G
1	X	590	U
1	X	591	A
1	X	592	A
1	X	593	U
1	X	594	G
1	X	599	A
1	X	606	G
1	X	615	A
1	X	616	G
1	X	618	A
1	X	635	G
1	X	646	A
1	X	647	G
1	X	658	A
1	X	659	A
1	X	660	A
1	X	661	U
1	X	662	G
1	X	666	A
1	X	682	A
1	X	683	G
1	X	689	A
1	X	690	U
1	X	697	U
1	X	698	U
1	X	699	U
1	X	713	A
1	X	721	A
1	X	722	A
1	X	726	G
1	X	727	G

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Mol	Chain	Res	Type
1	X	731	U
1	X	735	C
1	X	740	G
1	X	755	C
1	X	757	G
1	X	758	G
1	X	765	U
1	X	766	G
1	X	773	G
1	X	775	A
1	X	802	G
1	X	808	G
1	X	813	G
1	X	816	G
1	X	820	G
1	X	823	G
1	X	827	A
1	X	829	U
1	X	830	U
1	X	835	U
1	X	836	C
1	X	837	G
1	X	838	A
1	X	845	A
1	X	850	G
1	X	857	C
1	X	864	A
1	X	872	U
1	X	873	U
1	X	891	A
1	X	892	U
1	X	904	G
1	X	924	G
1	X	926	G
1	X	938	G
1	X	944	G
1	X	945	A
1	X	946	A
1	X	947	U
1	X	948	U
1	X	955	A
1	X	959	C

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Mol	Chain	Res	Type
1	X	970	U
1	X	971	U
1	X	977	A
1	X	985	A
1	X	989	A
1	X	990	G
1	X	1005	G
1	X	1017	A
1	X	1018	A
1	X	1027	A
1	X	1040	A
1	X	1047	G
1	X	1055	A
1	X	1056	U
1	X	1057	A
1	X	1066	G
1	X	1067	U
1	X	1069	G
1	X	1070	A
1	X	1077	U
1	X	1085	U
1	X	1086	G
1	X	1087	C
1	X	1091	G
1	X	1092	A
1	X	1093	C
1	X	1145	U
1	X	1146	C
1	X	1150	A
1	X	1151	G
1	X	1156	G
1	X	1157	U
1	X	1176	U
1	X	1177	A
1	X	1178	C
1	X	1179	C
1	X	1180	G
1	X	1183	G
1	X	1186	A
1	X	1187	A
1	X	1192	A
1	X	1195	A

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Mol	Chain	Res	Type
1	X	1200	A
1	X	1212	U
1	X	1218	G
1	X	1220	A
1	X	1221	C
1	X	1235	C
1	X	1250	G
1	X	1275	A
1	X	1278	G
1	X	1285	A
1	X	1287	U
1	X	1288	G
1	X	1291	A
1	X	1293	U
1	X	1294	G
1	X	1309	G
1	X	1310	A
1	X	1311	A
1	X	1312	A
1	X	1313	G
1	X	1337	A
1	X	1338	U
1	X	1349	U
1	X	1358	A
1	X	1362	C
1	X	1366	U
1	X	1389	U
1	X	1401	G
1	X	1402	A
1	X	1405	G
1	X	1415	A
1	X	1416	U
1	X	1421	A
1	X	1422	A
1	X	1432	A
1	X	1433	U
1	X	1437	U
1	X	1445	C
1	X	1448	U
1	X	1449	A
1	X	1450	A
1	X	1451	U

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Mol	Chain	Res	Type
1	X	1452	C
1	X	1453	G
1	X	1454	U
1	X	1463	A
1	X	1464	U
1	X	1465	G
1	X	1467	G
1	X	1471	A
1	X	1472	C
1	X	1475	A
1	X	1477	U
1	X	1481	A
1	X	1491	C
1	X	1492	G
1	X	1493	U
1	X	1494	G
1	X	1495	C
1	X	1496	G
1	X	1497	A
1	X	1498	U
1	X	1502	A
1	X	1505	G
1	X	1508	C
1	X	1509	G
1	X	1510	U
1	X	1511	C
1	X	1512	U
1	X	1513	A
1	X	1514	A
1	X	1515	G
1	X	1516	C
1	X	1519	U
1	X	1522	G
1	X	1525	U
1	X	1526	G
1	X	1527	A
1	X	1530	A
1	X	1538	A
1	X	1539	A
1	X	1541	C
1	X	1542	C
1	X	1543	G

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Mol	Chain	Res	Type
1	X	1544	G
1	X	1546	A
1	X	1547	C
1	X	1557	C
1	X	1559	G
1	X	1561	G
1	X	1562	C
1	X	1568	U
1	X	1569	G
1	X	1570	G
1	X	1575	A
1	X	1576	A
1	X	1577	G
1	X	1593	G
1	X	1594	U
1	X	1595	C
1	X	1597	U
1	X	1599	G
1	X	1602	U
1	X	1603	U
1	X	1605	A
1	X	1613	G
1	X	1616	A
1	X	1617	A
1	X	1619	A
1	X	1623	U
1	X	1625	U
1	X	1628	A
1	X	1629	U
1	X	1631	G
1	X	1636	U
1	X	1637	A
1	X	1638	G
1	X	1651	C
1	X	1652	A
1	X	1653	A
1	X	1654	A
1	X	1657	G
1	X	1659	C
1	X	1660	A
1	X	1662	A
1	X	1663	G

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Mol	Chain	Res	Type
1	X	1684	A
1	X	1690	A
1	X	1691	G
1	X	1692	C
1	X	1695	G
1	X	1699	A
1	X	1718	G
1	X	1719	C
1	X	1732	U
1	X	1738	C
1	X	1744	A
1	X	1745	A
1	X	1746	G
1	X	1747	G
1	X	1751	G
1	X	1756	U
1	X	1757	U
1	X	1758	A
1	X	1759	G
1	X	1760	G
1	X	1761	G
1	X	1762	U
1	X	1763	U
1	X	1765	A
1	X	1766	C
1	X	1768	C
1	X	1770	C
1	X	1771	A
1	X	1772	G
1	X	1783	G
1	X	1787	A
1	X	1789	A
1	X	1790	G
1	X	1791	G
1	X	1800	A
1	X	1808	U
1	X	1813	A
1	X	1818	A
1	X	1826	G
1	X	1827	C
1	X	1828	U
1	X	1835	U

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Mol	Chain	Res	Type
1	X	1836	A
1	X	1837	A
1	X	1843	U
1	X	1845	U
1	X	1846	A
1	X	1847	U
1	X	1856	A
1	X	1865	C
1	X	1877	G
1	X	1891	U
1	X	1902	G
1	X	1903	A
1	X	1908	A
1	X	1909	C
1	X	1911	A
1	X	1912	A
1	X	1926	A
1	X	1930	G
1	X	1932	C
1	X	1933	G
1	X	1935	C
1	X	1953	U
1	X	1954	A
1	X	1956	G
1	X	1963	A
1	X	1964	A
1	X	1967	U
1	X	1982	U
1	X	1991	G
1	X	1994	C
1	X	1997	A
1	X	1998	A
1	X	1999	G
1	X	2009	U
1	X	2017	C
1	X	2018	U
1	X	2019	G
1	X	2020	U
1	X	2024	A
1	X	2048	G
1	X	2050	A
1	X	2054	G

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Mol	Chain	Res	Type
1	X	2058	A
1	X	2059	G
1	X	2060	A
1	X	2061	U
1	X	2070	C
1	X	2077	C
1	X	2079	G
1	X	2082	C
1	X	2083	G
1	X	2087	A
1	X	2088	G
1	X	2089	A
1	X	2094	G
1	X	2096	G
1	X	2117	A
1	X	2119	U
1	X	2123	A
1	X	2124	U
1	X	2218	G
1	X	2225	A
1	X	2230	G
1	X	2231	C
1	X	2232	A
1	X	2233	C
1	X	2234	C
1	X	2235	A
1	X	2237	U
1	X	2238	U
1	X	2239	A
1	X	2240	U
1	X	2241	C
1	X	2245	G
1	X	2246	U
1	X	2251	G
1	X	2252	A
1	X	2265	G
1	X	2266	G
1	X	2270	U
1	X	2293	A
1	X	2295	A
1	X	2296	A
1	X	2306	G

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Mol	Chain	Res	Type
1	X	2310	C
1	X	2314	A
1	X	2332	U
1	X	2334	G
1	X	2335	G
1	X	2338	A
1	X	2347	A
1	X	2348	G
1	X	2352	G
1	X	2354	A
1	X	2361	U
1	X	2362	A
1	X	2363	A
1	X	2374	C
1	X	2377	C
1	X	2398	G
1	X	2399	G
1	X	2406	G
1	X	2410	G
1	X	2412	C
1	X	2429	U
1	X	2432	G
1	X	2433	C
1	X	2434	A
1	X	2440	G
1	X	2449	C
1	X	2450	U
1	X	2452	A
1	X	2456	G
1	X	2457	A
1	X	2468	C
1	X	2472	G
1	X	2474	G
1	X	2475	A
1	X	2486	A
1	X	2496	A
1	X	2497	G
1	X	2500	U
1	X	2501	U
1	X	2503	A
1	X	2505	A
1	X	2514	G

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Mol	Chain	Res	Type
1	X	2519	U
1	X	2525	C
1	X	2526	C
1	X	2528	C
1	X	2529	G
1	X	2532	G
1	X	2545	A
1	X	2546	U
1	X	2547	C
1	X	2556	G
1	X	2561	C
1	X	2565	C
1	X	2591	A
1	X	2593	A
1	X	2594	G
1	X	2600	C
1	X	2603	G
1	X	2609	G
1	X	2612	U
1	X	2613	C
1	X	2636	U
1	X	2640	U
1	X	2642	U
1	X	2656	A
1	X	2661	A
1	X	2681	A
1	X	2682	G
1	X	2690	G
1	X	2698	A
1	X	2709	U
1	X	2712	G
1	X	2716	U
1	X	2717	A
1	X	2740	A
1	X	2745	G
1	X	2753	U
1	X	2760	A
1	X	2766	U
1	X	2775	A
1	X	2779	C
1	X	2787	C
1	X	2788	A

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Mol	Chain	Res	Type
1	X	2792	A
1	X	2805	A
1	X	2807	G
1	X	2808	A
1	X	2809	G
1	X	2817	A
1	X	2818	A
1	X	2819	C
1	X	2821	U
1	X	2824	G
1	X	2828	U
1	X	2832	A
1	X	2840	A
1	X	2845	G
1	X	2853	U
1	X	2854	A
1	X	2855	A
1	X	2856	U
1	X	2857	A
1	X	2863	G
1	X	2868	G
1	X	2887	G
1	X	2892	G
1	X	2899	A
1	X	2900	C
1	X	2903	A
1	X	2905	C
1	X	2913	G
1	X	2920	U
2	Y	10	U
2	Y	13	A
2	Y	23	U
2	Y	24	C
2	Y	39	G
2	Y	40	C
2	Y	42	G
2	Y	54	U
2	Y	55	A
2	Y	87	G
2	Y	88	U
2	Y	94	U
2	Y	106	U

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Mol	Chain	Res	Type
2	Y	114	C

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	38	A
1	X	90	A
1	X	165	C
1	X	179	A
1	X	235	G
1	X	285	U
1	X	485	A
1	X	525	A
1	X	614	U
1	X	660	A
1	X	890	G
1	X	944	G
1	X	1028	G
1	X	1091	G
1	X	1311	A
1	X	1432	A
1	X	1466	G
1	X	1490	G
1	X	1510	U
1	X	1521	A
1	X	1568	U
1	X	1575	A
1	X	1576	A
1	X	1627	G
1	X	1789	A
1	X	1901	C
1	X	2062	G
1	X	2234	C
1	X	2457	A
1	X	2495	A
1	X	2778	G
1	X	2787	C
1	X	2807	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 470 ligands modelled in this entry, 442 are monoatomic - leaving 28 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	SPD	J	201	-	9,9,9	0.18	0	8,8,8	0.20	0
29	ZLD	X	3001	-	26,26,26	1.05	1 (3%)	36,36,36	1.42	7 (19%)
30	MPD	X	3002	-	6,7,7	0.28	0	6,10,10	0.13	0
30	MPD	X	3003	-	6,7,7	0.45	0	6,10,10	0.23	0
30	MPD	X	3004	-	6,7,7	0.33	0	6,10,10	0.11	0
30	MPD	X	3005	-	6,7,7	0.30	0	6,10,10	0.33	0
30	MPD	X	3006	-	6,7,7	0.40	0	6,10,10	0.21	0
30	MPD	X	3007	-	6,7,7	0.48	0	6,10,10	0.24	0
30	MPD	X	3008	-	6,7,7	0.29	0	6,10,10	0.09	0
30	MPD	X	3009	-	6,7,7	0.33	0	6,10,10	0.10	0
30	MPD	X	3010	-	6,7,7	0.32	0	6,10,10	0.14	0
34	EPE	X	3423	-	15,15,15	1.21	1 (6%)	19,20,20	0.75	1 (5%)
34	EPE	X	3424	-	15,15,15	1.38	1 (6%)	19,20,20	0.95	1 (5%)
34	EPE	X	3425	-	15,15,15	1.01	1 (6%)	19,20,20	0.71	1 (5%)
34	EPE	X	3426	-	15,15,15	2.86	1 (6%)	19,20,20	0.87	0
35	SPD	X	3427	-	9,9,9	0.22	0	8,8,8	0.38	0
35	SPD	X	3428	-	9,9,9	0.20	0	8,8,8	0.18	0
35	SPD	X	3429	-	9,9,9	0.23	0	8,8,8	0.16	0
35	SPD	X	3430	-	9,9,9	0.15	0	8,8,8	0.20	0
35	SPD	X	3431	-	9,9,9	0.19	0	8,8,8	0.18	0
35	SPD	X	3432	-	9,9,9	0.24	0	8,8,8	0.24	0
35	SPD	X	3433	-	9,9,9	0.19	0	8,8,8	0.23	0
35	SPD	X	3434	-	9,9,9	0.19	0	8,8,8	0.22	0
36	EOH	X	3435	-	2,2,2	0.63	0	1,1,1	0.38	0
36	EOH	X	3436	-	2,2,2	0.52	0	1,1,1	0.67	0
36	EOH	X	3437	-	2,2,2	0.51	0	1,1,1	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	EOH	X	3438	-	2,2,2	0.60	0	1,1,1	0.54	0
36	EOH	Y	209	-	2,2,2	0.52	0	1,1,1	0.67	0

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
35	SPD	J	201	-	-	0/7/7/7	0/0/0/0
29	ZLD	X	3001	-	-	0/13/33/33	0/3/3/3
30	MPD	X	3002	-	-	0/5/5/5	0/0/0/0
30	MPD	X	3003	-	-	0/5/5/5	0/0/0/0
30	MPD	X	3004	-	-	0/5/5/5	0/0/0/0
30	MPD	X	3005	-	-	0/5/5/5	0/0/0/0
30	MPD	X	3006	-	-	0/5/5/5	0/0/0/0
30	MPD	X	3007	-	-	0/5/5/5	0/0/0/0
30	MPD	X	3008	-	-	0/5/5/5	0/0/0/0
30	MPD	X	3009	-	-	0/5/5/5	0/0/0/0
30	MPD	X	3010	-	-	0/5/5/5	0/0/0/0
34	EPE	X	3423	-	-	0/9/19/19	0/1/1/1
34	EPE	X	3424	-	-	0/9/19/19	0/1/1/1
34	EPE	X	3425	-	-	0/9/19/19	0/1/1/1
34	EPE	X	3426	-	-	0/9/19/19	0/1/1/1
35	SPD	X	3427	-	-	0/7/7/7	0/0/0/0
35	SPD	X	3428	-	-	0/7/7/7	0/0/0/0
35	SPD	X	3429	-	-	0/7/7/7	0/0/0/0
35	SPD	X	3430	-	-	0/7/7/7	0/0/0/0
35	SPD	X	3431	-	-	0/7/7/7	0/0/0/0
35	SPD	X	3432	-	-	0/7/7/7	0/0/0/0
35	SPD	X	3433	-	-	0/7/7/7	0/0/0/0
35	SPD	X	3434	-	-	0/7/7/7	0/0/0/0
36	EOH	X	3435	-	-	0/0/0/0	0/0/0/0
36	EOH	X	3436	-	-	0/0/0/0	0/0/0/0
36	EOH	X	3437	-	-	0/0/0/0	0/0/0/0
36	EOH	X	3438	-	-	0/0/0/0	0/0/0/0
36	EOH	Y	209	-	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	X	3426	EPE	C10-S	-10.95	1.61	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	X	3424	EPE	C10-S	-5.24	1.69	1.77
34	X	3423	EPE	C10-S	-4.54	1.70	1.77
34	X	3425	EPE	C10-S	-3.77	1.71	1.77
29	X	3001	ZLD	C7-N4	4.23	1.41	1.36

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	X	3424	EPE	O2S-S-C10	-3.66	104.28	106.87
29	X	3001	ZLD	O10-C7-N4	-2.98	107.98	109.97
29	X	3001	ZLD	O15-C7-N4	-2.67	126.68	128.84
29	X	3001	ZLD	C6-C8-C9	-2.63	109.24	114.64
34	X	3423	EPE	O2S-S-C10	-2.55	105.07	106.87
34	X	3425	EPE	O1S-S-C10	-2.48	105.12	106.87
29	X	3001	ZLD	C24-N19-C17	2.08	121.10	116.32
29	X	3001	ZLD	O10-C7-O15	2.52	125.30	122.43
29	X	3001	ZLD	C8-C9-N11	3.19	119.60	112.10
29	X	3001	ZLD	C8-O10-C7	3.90	113.36	110.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	X	3001	ZLD	5	0
30	X	3005	MPD	3	0
30	X	3009	MPD	1	0
30	X	3010	MPD	1	0
34	X	3423	EPE	1	0
34	X	3424	EPE	1	0
34	X	3425	EPE	4	0
34	X	3426	EPE	14	0
35	X	3428	SPD	3	0
35	X	3430	SPD	3	0
35	X	3432	SPD	2	0
35	X	3433	SPD	2	0
35	X	3434	SPD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	X	2711/2923 (92%)	-0.50	9 (0%) 94 92	39, 91, 192, 340	0
2	Y	114/114 (100%)	-0.79	0 100 100	61, 106, 172, 208	0
3	A	268/277 (96%)	0.74	57 (21%) 1 1	64, 121, 176, 224	0
4	B	215/220 (97%)	-0.04	5 (2%) 64 58	50, 66, 114, 194	0
5	C	199/207 (96%)	0.02	7 (3%) 48 42	56, 82, 132, 163	0
6	D	155/179 (86%)	-0.26	6 (3%) 43 38	96, 156, 222, 311	0
7	E	157/178 (88%)	-0.36	8 (5%) 32 28	88, 136, 197, 264	0
8	G	145/145 (100%)	0.01	3 (2%) 67 61	47, 63, 98, 129	0
9	H	122/122 (100%)	0.95	32 (26%) 1 1	66, 89, 129, 146	0
10	I	131/146 (89%)	0.24	11 (8%) 14 13	34, 94, 152, 175	0
11	J	138/144 (95%)	1.10	39 (28%) 1 1	54, 83, 183, 312	0
12	K	119/122 (97%)	-0.03	5 (4%) 40 35	37, 74, 127, 175	0
13	L	108/119 (90%)	-0.31	8 (7%) 17 17	68, 109, 149, 173	0
14	M	109/116 (93%)	0.10	6 (5%) 29 26	54, 86, 155, 201	0
15	N	116/118 (98%)	-0.14	1 (0%) 85 81	35, 60, 98, 125	0
16	O	101/102 (99%)	0.10	9 (8%) 12 11	38, 73, 127, 149	0
17	P	112/117 (95%)	0.45	6 (5%) 29 27	43, 63, 114, 179	0
18	Q	88/91 (96%)	0.11	7 (7%) 15 14	84, 110, 167, 193	0
19	R	100/105 (95%)	-0.31	4 (4%) 42 37	60, 110, 228, 298	0
20	S	167/217 (76%)	0.22	23 (13%) 4 4	55, 104, 213, 309	0
21	T	75/94 (79%)	1.29	25 (33%) 0 1	66, 78, 132, 178	0
22	U	44/62 (70%)	2.31	20 (45%) 0 0	89, 163, 227, 254	0
23	V	65/69 (94%)	-0.12	4 (6%) 24 22	75, 114, 166, 228	0
24	W	57/59 (96%)	-0.29	0 100 100	37, 62, 114, 159	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Z	44/58 (75%)	0.44	5 (11%) 7 7	34, 74, 140, 227	0
26	2	44/45 (97%)	0.84	9 (20%) 1 1	57, 83, 118, 145	0
27	3	60/66 (90%)	0.14	5 (8%) 14 13	41, 77, 118, 148	0
28	4	37/37 (100%)	0.86	8 (21%) 1 1	96, 104, 144, 162	0
All	All	5801/6252 (92%)	-0.13	322 (5%) 28 25	34, 92, 181, 340	0

All (322) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	U	42	GLY	12.5
3	A	82	GLN	12.3
22	U	41	ASP	10.0
20	S	164	ASP	8.6
22	U	39	LEU	8.6
3	A	81	ILE	7.8
3	A	38	PRO	7.3
3	A	113	GLY	7.2
22	U	38	ILE	6.9
1	X	2629	A	6.7
25	Z	44	CYS	6.6
3	A	112	VAL	6.5
3	A	83	TYR	6.1
22	U	14	THR	6.0
3	A	95	VAL	5.8
3	A	60	ARG	5.7
3	A	94	VAL	5.7
3	A	18	SER	5.6
20	S	63	LEU	5.5
10	I	95	LEU	5.3
11	J	131	PHE	5.2
3	A	114	GLN	5.1
3	A	58	HIS	5.0
20	S	67	SER	5.0
22	U	45	LYS	5.0
9	H	111	PHE	5.0
11	J	33	GLY	5.0
3	A	79	ASP	5.0
22	U	40	VAL	4.9
3	A	23	GLU	4.8
22	U	47	VAL	4.8
3	A	93	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
17	P	1	MET	4.7
3	A	36	PRO	4.6
3	A	90	ASN	4.6
11	J	115	ARG	4.5
14	M	70	VAL	4.5
20	S	3	SER	4.5
21	T	75	VAL	4.4
13	L	45	ILE	4.4
3	A	63	ARG	4.3
3	A	80	SER	4.3
7	E	20	ASP	4.3
11	J	32	PHE	4.2
3	A	110	LEU	4.2
10	I	92	THR	4.2
20	S	6	SER	4.2
21	T	72	ASP	4.1
5	C	187	THR	4.1
20	S	36	THR	4.0
13	L	31	LEU	4.0
3	A	115	ILE	4.0
3	A	84	ASP	4.0
3	A	111	GLU	4.0
3	A	78	VAL	4.0
22	U	15	GLY	4.0
19	R	85	PHE	3.9
11	J	58	MET	3.9
9	H	36	GLY	3.9
3	A	89	ALA	3.9
28	4	12	GLU	3.8
11	J	118	LEU	3.8
21	T	69	ALA	3.8
11	J	117	ALA	3.8
6	D	83	MET	3.7
9	H	122	LEU	3.7
9	H	84	CYS	3.7
9	H	106	LEU	3.7
11	J	34	LEU	3.7
9	H	102	VAL	3.7
22	U	46	LYS	3.7
21	T	74	VAL	3.7
11	J	111	GLU	3.6
21	T	77	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
9	H	11	ALA	3.6
1	X	1613	G	3.6
21	T	34	ALA	3.6
9	H	90	ASP	3.6
9	H	91	LYS	3.6
3	A	16	MET	3.6
22	U	44	PRO	3.5
22	U	43	LYS	3.5
21	T	73	GLY	3.5
9	H	81	GLU	3.4
3	A	25	THR	3.4
11	J	106	VAL	3.4
11	J	97	VAL	3.4
27	3	25	SER	3.4
17	P	94	SER	3.4
20	S	35	GLY	3.4
20	S	64	GLY	3.4
3	A	157	SER	3.4
21	T	37	GLN	3.4
6	D	157	VAL	3.4
10	I	3	LEU	3.4
12	K	104	LEU	3.3
3	A	107	PRO	3.3
9	H	85	VAL	3.3
20	S	70	ILE	3.3
1	X	2	A	3.3
3	A	213	TRP	3.3
7	E	21	GLY	3.3
20	S	66	GLY	3.3
18	Q	38	VAL	3.3
9	H	62	ILE	3.3
13	L	32	ASN	3.3
8	G	53	ASP	3.3
16	O	38	VAL	3.2
11	J	114	ALA	3.2
21	T	86	GLN	3.2
11	J	57	TYR	3.2
9	H	63	VAL	3.2
18	Q	87	ILE	3.2
9	H	38	VAL	3.2
11	J	38	THR	3.2
1	X	1614	A	3.2

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Mol	Chain	Res	Type	RSRZ
28	4	31	LYS	3.2
5	C	124	THR	3.2
3	A	62	TYR	3.2
22	U	13	SER	3.1
12	K	100	TYR	3.1
3	A	128	ASN	3.1
8	G	52	GLY	3.1
21	T	40	THR	3.1
3	A	75	ASN	3.1
26	2	19	PHE	3.1
3	A	101	LYS	3.1
10	I	93	PRO	3.0
9	H	87	ILE	3.0
10	I	90	GLU	3.0
9	H	60	ALA	3.0
3	A	153	GLN	3.0
11	J	110	SER	3.0
11	J	54	MET	3.0
21	T	35	ASP	3.0
6	D	158	THR	3.0
25	Z	31	PRO	3.0
3	A	91	ILE	2.9
21	T	78	GLU	2.9
21	T	39	VAL	2.9
18	Q	25	TYR	2.9
3	A	22	ALA	2.9
11	J	108	GLY	2.9
16	O	35	PHE	2.9
11	J	4	PRO	2.9
20	S	138	PRO	2.8
21	T	80	LYS	2.8
20	S	162	THR	2.8
10	I	94	ALA	2.8
19	R	83	TYR	2.8
4	B	28	VAL	2.8
28	4	28	GLU	2.8
22	U	31	ALA	2.8
11	J	102	ILE	2.8
28	4	10	ILE	2.8
11	J	55	THR	2.8
9	H	37	ASP	2.8
7	E	106	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
20	S	5	LYS	2.8
3	A	74	ILE	2.8
13	L	29	PRO	2.8
4	B	201	VAL	2.8
20	S	125	LEU	2.8
11	J	96	VAL	2.8
16	O	36	ASP	2.8
3	A	106	ALA	2.7
11	J	139	GLY	2.7
1	X	2612	U	2.7
3	A	64	VAL	2.7
10	I	69	ILE	2.7
20	S	7	ILE	2.7
9	H	83	ALA	2.7
13	L	44	ILE	2.7
17	P	102	HIS	2.7
9	H	61	VAL	2.7
14	M	20	PRO	2.7
26	2	18	GLY	2.7
26	2	44	SER	2.7
11	J	133	LYS	2.7
16	O	2	PHE	2.7
15	N	2	PRO	2.7
11	J	132	VAL	2.6
11	J	140	GLU	2.6
3	A	73	GLY	2.6
9	H	77	ILE	2.6
12	K	81	ALA	2.6
9	H	64	ARG	2.6
3	A	105	ILE	2.6
20	S	65	VAL	2.6
27	3	60	GLN	2.6
26	2	14	SER	2.6
3	A	77	LYS	2.6
3	A	154	ILE	2.6
21	T	71	ILE	2.6
27	3	21	GLN	2.6
14	M	71	GLY	2.6
19	R	86	VAL	2.6
20	S	69	THR	2.6
7	E	169	VAL	2.6
3	A	85	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
11	J	41	TRP	2.5
7	E	170	ARG	2.5
19	R	88	GLY	2.5
9	H	89	ASP	2.5
10	I	91	VAL	2.5
28	4	7	VAL	2.5
25	Z	30	CYS	2.5
12	K	103	ILE	2.5
23	V	43	ILE	2.5
9	H	28	SER	2.5
3	A	100	GLU	2.5
5	C	160	ASP	2.5
25	Z	43	VAL	2.5
22	U	33	LEU	2.5
16	O	14	VAL	2.5
28	4	29	ASN	2.5
13	L	51	VAL	2.5
16	O	56	ALA	2.5
18	Q	42	VAL	2.5
11	J	39	THR	2.5
7	E	29	PRO	2.5
9	H	103	ALA	2.5
21	T	54	TYR	2.5
3	A	109	GLY	2.4
3	A	17	THR	2.4
4	B	118	VAL	2.4
6	D	124	GLY	2.4
9	H	99	PHE	2.4
26	2	6	TYR	2.4
1	X	2216	U	2.4
10	I	89	THR	2.4
3	A	6	TYR	2.4
3	A	37	LEU	2.4
9	H	101	PRO	2.4
11	J	130	LYS	2.4
22	U	37	ARG	2.4
9	H	110	ASN	2.4
16	O	48	VAL	2.4
14	M	2	THR	2.4
13	L	5	ILE	2.4
10	I	97	VAL	2.4
11	J	129	THR	2.4

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Mol	Chain	Res	Type	RSRZ
28	4	30	PRO	2.4
3	A	200	HIS	2.4
11	J	61	GLY	2.4
20	S	161	VAL	2.4
12	K	106	GLN	2.4
21	T	60	GLY	2.4
9	H	59	LYS	2.4
21	T	46	TYR	2.4
28	4	2	LYS	2.3
21	T	41	GLY	2.3
22	U	48	TRP	2.3
17	P	96	ILE	2.3
7	E	156	PRO	2.3
21	T	53	ILE	2.3
3	A	203	VAL	2.3
27	3	2	PRO	2.3
11	J	105	GLU	2.3
26	2	45	ALA	2.3
3	A	57	GLY	2.3
21	T	45	LEU	2.3
9	H	25	LEU	2.3
14	M	45	PHE	2.3
20	S	61	ILE	2.2
9	H	35	ILE	2.2
21	T	68	PHE	2.2
11	J	116	GLU	2.2
18	Q	65	MET	2.2
3	A	72	ASP	2.2
11	J	35	GLN	2.2
1	X	553	A	2.2
11	J	136	GLU	2.2
17	P	84	ARG	2.2
16	O	40	PHE	2.2
20	S	109	VAL	2.2
21	T	87	VAL	2.2
5	C	165	LEU	2.2
18	Q	43	GLU	2.2
20	S	39	VAL	2.2
16	O	39	LEU	2.2
27	3	26	ARG	2.2
13	L	43	GLN	2.2
17	P	24	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
10	I	96	LEU	2.2
7	E	19	PHE	2.2
11	J	112	GLU	2.2
22	U	49	VAL	2.2
26	2	9	ASN	2.2
23	V	53	LEU	2.1
22	U	12	ALA	2.1
18	Q	86	SER	2.1
20	S	68	LYS	2.1
3	A	96	TYR	2.1
3	A	76	ALA	2.1
9	H	79	PHE	2.1
26	2	7	GLN	2.1
4	B	107	VAL	2.1
8	G	133	HIS	2.1
5	C	62	ARG	2.1
26	2	17	HIS	2.1
1	X	2501	U	2.1
11	J	107	ALA	2.1
5	C	155	VAL	2.1
11	J	60	ARG	2.1
25	Z	33	CYS	2.1
11	J	100	GLY	2.1
21	T	70	LYS	2.1
14	M	69	GLY	2.1
23	V	65	SER	2.1
3	A	86	ASN	2.1
22	U	20	HIS	2.1
6	D	15	ASN	2.0
20	S	31	VAL	2.0
21	T	90	TYR	2.0
23	V	50	ILE	2.0
6	D	161	ASN	2.0
4	B	209	VAL	2.0
11	J	62	GLY	2.0
9	H	93	PRO	2.0
1	X	1090	A	2.0
5	C	176	THR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
31	MG	X	3418	1/1	0.65	0.76	62.14	81,81,81,81	0
31	MG	X	3420	1/1	0.47	0.64	36.08	79,79,79,79	0
31	MG	X	3287	1/1	0.91	0.93	28.89	67,67,67,67	0
30	MPD	X	3008	8/8	0.80	0.51	27.69	144,144,144,144	0
32	MN	X	3151	1/1	0.85	0.62	23.92	106,106,106,106	0
32	MN	X	3231	1/1	0.97	0.75	23.57	135,135,135,135	0
32	MN	X	3119	1/1	0.83	0.70	23.18	155,155,155,155	0
31	MG	X	3384	1/1	0.94	0.54	21.93	81,81,81,81	0
32	MN	X	3161	1/1	0.85	0.58	20.51	98,98,98,98	0
32	MN	X	3146	1/1	0.95	0.34	18.58	100,100,100,100	0
35	SPD	X	3431	10/10	0.75	0.39	17.60	98,98,98,98	0
35	SPD	X	3429	10/10	0.61	0.64	17.39	106,106,106,106	0
31	MG	X	3344	1/1	0.69	0.68	16.44	92,92,92,92	0
32	MN	X	3079	1/1	0.98	0.47	14.54	71,71,71,71	0
32	MN	X	3172	1/1	0.89	0.57	14.26	82,82,82,82	0
31	MG	X	3294	1/1	0.97	0.36	14.02	51,51,51,51	0
31	MG	X	3032	1/1	0.78	0.48	13.90	64,64,64,64	0
32	MN	X	3221	1/1	0.79	0.35	13.31	130,130,130,130	0
32	MN	X	3224	1/1	0.96	0.35	13.12	99,99,99,99	0
32	MN	X	3150	1/1	0.99	0.40	12.86	39,39,39,39	0
30	MPD	X	3006	8/8	0.65	0.42	12.63	133,133,133,133	0
32	MN	X	3159	1/1	0.99	0.43	11.41	61,61,61,61	0
31	MG	Y	206	1/1	0.82	0.42	10.89	65,65,65,65	0
35	SPD	X	3434	10/10	0.84	0.26	10.53	98,98,98,98	0
32	MN	X	3133	1/1	0.99	0.35	10.22	58,58,58,58	0
32	MN	X	3148	1/1	0.87	0.39	9.99	102,102,102,102	0
32	MN	X	3124	1/1	0.98	0.36	9.52	80,80,80,80	0
31	MG	X	3314	1/1	0.97	0.34	9.40	45,45,45,45	0
31	MG	X	3037	1/1	0.85	0.23	9.26	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MN	X	3152	1/1	0.98	0.38	9.21	60,60,60,60	0
32	MN	X	3168	1/1	0.93	0.42	9.19	85,85,85,85	0
32	MN	X	3239	1/1	0.96	0.44	8.90	60,60,60,60	0
32	MN	X	3157	1/1	0.94	0.42	8.39	85,85,85,85	0
31	MG	X	3345	1/1	0.98	0.34	8.32	78,78,78,78	0
32	MN	X	3153	1/1	0.97	0.32	8.22	75,75,75,75	0
32	MN	X	3154	1/1	0.95	0.39	7.84	46,46,46,46	0
31	MG	X	3063	1/1	0.83	0.32	7.23	49,49,49,49	0
35	SPD	X	3427	10/10	0.85	0.33	6.77	56,56,56,56	0
32	MN	X	3184	1/1	0.95	0.34	6.73	86,86,86,86	0
32	MN	X	3220	1/1	0.97	0.21	6.48	111,111,111,111	0
35	SPD	X	3428	10/10	0.91	0.22	6.45	82,82,82,82	0
31	MG	X	3021	1/1	0.92	0.31	6.44	76,76,76,76	0
30	MPD	X	3009	8/8	0.84	0.42	6.39	107,107,107,107	0
31	MG	X	3308	1/1	0.94	0.24	6.09	39,39,39,39	0
32	MN	X	3195	1/1	0.97	0.27	6.08	90,90,90,90	0
32	MN	X	3187	1/1	0.97	0.33	5.98	89,89,89,89	0
30	MPD	X	3007	8/8	0.89	0.19	5.78	114,114,114,114	0
31	MG	X	3310	1/1	0.95	0.23	5.74	66,66,66,66	0
32	MN	X	3132	1/1	0.99	0.30	5.70	66,66,66,66	0
32	MN	X	3143	1/1	0.99	0.32	5.64	76,76,76,76	0
30	MPD	X	3004	8/8	0.87	0.24	5.29	109,109,109,109	0
35	SPD	X	3433	10/10	0.94	0.22	5.10	93,93,93,93	0
32	MN	X	3084	1/1	0.98	0.28	4.96	81,81,81,81	0
32	MN	X	3215	1/1	0.95	0.37	4.91	154,154,154,154	0
31	MG	X	3323	1/1	0.93	0.27	4.82	76,76,76,76	0
31	MG	X	3062	1/1	0.86	0.32	4.63	56,56,56,56	0
32	MN	X	3162	1/1	0.92	0.28	4.53	74,74,74,74	0
31	MG	X	3335	1/1	0.97	0.67	4.47	260,260,260,260	0
32	MN	X	3130	1/1	0.98	0.26	3.82	70,70,70,70	0
31	MG	X	3024	1/1	0.92	0.32	3.78	67,67,67,67	0
32	MN	X	3442	1/1	0.96	0.32	3.71	51,51,51,51	0
32	MN	X	3147	1/1	0.98	0.33	3.67	82,82,82,82	0
32	MN	X	3227	1/1	0.88	0.23	3.61	107,107,107,107	0
30	MPD	X	3003	8/8	0.95	0.20	3.39	92,92,92,92	0
30	MPD	X	3010	8/8	0.90	0.31	3.33	122,122,122,122	0
31	MG	X	3415	1/1	0.98	0.29	3.06	45,45,45,45	0
32	MN	X	3199	1/1	0.99	0.30	2.94	93,93,93,93	0
31	MG	X	3249	1/1	0.98	0.38	2.78	16,16,16,16	0
31	MG	X	3319	1/1	0.98	0.26	2.75	26,26,26,26	0
35	SPD	X	3432	10/10	0.87	0.25	2.67	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
29	ZLD	X	3001	24/24	0.92	0.40	2.65	87,88,90,91	0
32	MN	X	3240	1/1	0.82	0.36	2.52	123,123,123,123	0
34	EPE	X	3424	15/15	0.77	0.39	2.51	194,194,194,194	0
32	MN	X	3131	1/1	0.97	0.23	2.46	66,66,66,66	0
31	MG	X	3035	1/1	0.94	0.27	2.43	39,39,39,39	0
35	SPD	J	201	10/10	0.75	0.27	2.43	82,82,82,82	0
34	EPE	X	3425	15/15	0.72	0.33	2.41	152,152,152,152	0
32	MN	X	3223	1/1	0.96	0.15	2.40	127,127,127,127	0
34	EPE	X	3423	15/15	0.86	0.32	2.26	152,152,152,152	0
32	MN	X	3142	1/1	0.98	0.18	2.18	108,108,108,108	0
31	MG	A	302	1/1	0.86	0.33	2.16	58,58,58,58	0
34	EPE	X	3426	15/15	0.94	0.27	2.11	101,101,101,101	3
32	MN	X	3176	1/1	0.96	0.31	2.09	80,80,80,80	0
31	MG	X	3039	1/1	0.88	0.19	2.00	53,53,53,53	0
31	MG	X	3441	1/1	0.89	0.76	1.88	72,72,72,72	0
32	MN	X	3439	1/1	0.94	0.29	1.77	97,97,97,97	0
31	MG	X	3352	1/1	0.94	0.16	1.60	50,50,50,50	0
32	MN	X	3111	1/1	0.95	0.27	1.51	125,125,125,125	0
32	MN	X	3126	1/1	0.98	0.21	1.50	96,96,96,96	0
32	MN	X	3087	1/1	0.98	0.20	1.34	104,104,104,104	0
30	MPD	X	3005	8/8	0.90	0.14	1.32	64,64,64,64	0
31	MG	X	3406	1/1	0.93	0.21	1.19	55,55,55,55	0
32	MN	X	3268	1/1	0.94	0.19	1.13	94,94,94,94	0
32	MN	X	3201	1/1	0.98	0.19	0.96	49,49,49,49	0
32	MN	X	3189	1/1	0.98	0.28	0.89	53,53,53,53	0
32	MN	X	3066	1/1	0.96	0.26	0.83	64,64,64,64	0
31	MG	X	3440	1/1	0.85	0.21	0.51	37,37,37,37	0
32	MN	X	3123	1/1	0.91	0.25	0.47	97,97,97,97	0
31	MG	X	3349	1/1	0.91	0.12	0.37	45,45,45,45	0
31	MG	X	3211	1/1	0.84	0.23	0.34	32,32,32,32	0
35	SPD	X	3430	10/10	0.91	0.28	0.26	80,80,80,80	0
31	MG	N	201	1/1	0.95	0.27	0.22	25,25,25,25	0
31	MG	X	3209	1/1	0.91	0.29	0.21	34,34,34,34	0
31	MG	X	3444	1/1	0.85	0.24	0.10	44,44,44,44	0
32	MN	X	3099	1/1	0.98	0.14	0.09	128,128,128,128	0
32	MN	X	3103	1/1	0.99	0.16	0.08	81,81,81,81	0
32	MN	X	3262	1/1	0.77	0.10	-0.01	191,191,191,191	0
32	MN	X	3120	1/1	0.98	0.14	-0.02	75,75,75,75	0
32	MN	X	3136	1/1	0.99	0.21	-0.04	84,84,84,84	0
31	MG	X	3252	1/1	0.66	0.30	-0.15	50,50,50,50	0
32	MN	X	3416	1/1	0.91	0.13	-0.41	111,111,111,111	0
31	MG	X	3304	1/1	0.84	0.18	-0.48	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	MG	X	3332	1/1	1.00	0.17	-0.81	28,28,28,28	0
31	MG	X	3338	1/1	0.97	0.15	-1.03	43,43,43,43	0
32	MN	X	3205	1/1	0.87	0.14	-1.17	113,113,113,113	0
31	MG	Z	103	1/1	0.97	0.11	-1.42	39,39,39,39	0
32	MN	X	3228	1/1	0.94	0.13	-	110,110,110,110	0
31	MG	X	3419	1/1	0.70	1.75	-	100,100,100,100	0
31	MG	X	3034	1/1	0.76	0.39	-	75,75,75,75	0
31	MG	X	3011	1/1	0.84	0.38	-	85,85,85,85	0
31	MG	G	202	1/1	0.84	0.28	-	77,77,77,77	0
31	MG	X	3041	1/1	0.96	0.36	-	68,68,68,68	0
31	MG	X	3060	1/1	0.99	0.44	-	16,16,16,16	0
31	MG	X	3290	1/1	0.88	0.40	-	46,46,46,46	0
32	MN	X	3095	1/1	0.93	0.25	-	133,133,133,133	0
31	MG	X	3023	1/1	0.93	0.23	-	56,56,56,56	0
32	MN	X	3140	1/1	0.87	0.33	-	111,111,111,111	0
31	MG	X	3040	1/1	0.97	0.91	-	58,58,58,58	0
31	MG	X	3289	1/1	0.95	0.31	-	27,27,27,27	0
31	MG	X	3208	1/1	0.56	0.43	-	78,78,78,78	0
32	MN	X	3102	1/1	0.96	0.29	-	96,96,96,96	0
32	MN	X	3192	1/1	0.91	0.20	-	85,85,85,85	0
32	MN	X	3180	1/1	0.99	0.27	-	70,70,70,70	0
31	MG	X	3348	1/1	0.75	0.41	-	85,85,85,85	0
31	MG	X	3320	1/1	0.98	0.43	-	43,43,43,43	0
31	MG	X	3316	1/1	0.82	0.86	-	88,88,88,88	0
32	MN	X	3100	1/1	0.95	0.76	-	129,129,129,129	0
32	MN	X	3179	1/1	0.99	0.28	-	77,77,77,77	0
31	MG	X	3411	1/1	0.71	0.42	-	83,83,83,83	0
36	EOH	X	3437	3/3	0.89	0.21	-	92,92,92,92	0
31	MG	X	3256	1/1	0.87	1.16	-	82,82,82,82	0
31	MG	X	3347	1/1	0.86	0.19	-	77,77,77,77	0
31	MG	X	3372	1/1	0.81	0.18	-	49,49,49,49	0
31	MG	Y	204	1/1	0.91	0.46	-	63,63,63,63	0
32	MN	X	3074	1/1	0.97	0.24	-	98,98,98,98	0
31	MG	X	3363	1/1	0.75	0.46	-	81,81,81,81	0
32	MN	X	3443	1/1	0.95	0.35	-	91,91,91,91	0
36	EOH	X	3438	3/3	0.83	0.31	-	63,63,63,63	0
31	MG	X	3412	1/1	0.91	1.01	-	82,82,82,82	0
31	MG	X	3312	1/1	0.73	1.02	-	57,57,57,57	0
31	MG	X	3043	1/1	0.97	0.41	-	64,64,64,64	0
32	MN	X	3219	1/1	0.91	0.22	-	139,139,139,139	0
32	MN	X	3078	1/1	0.99	0.25	-	56,56,56,56	0
31	MG	X	3306	1/1	0.82	0.31	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	MG	X	3355	1/1	0.97	0.19	-	71,71,71,71	0
32	MN	X	3108	1/1	0.93	0.50	-	182,182,182,182	0
31	MG	X	3390	1/1	0.96	0.20	-	47,47,47,47	0
31	MG	X	3044	1/1	0.90	0.39	-	20,20,20,20	1
31	MG	X	3400	1/1	0.78	0.37	-	50,50,50,50	0
31	MG	X	3025	1/1	0.90	0.46	-	10,10,10,10	1
32	MN	X	3125	1/1	0.96	0.80	-	122,122,122,122	0
32	MN	X	3182	1/1	0.94	0.37	-	88,88,88,88	0
32	MN	X	3077	1/1	0.96	0.21	-	61,61,61,61	0
32	MN	X	3113	1/1	0.67	0.24	-	123,123,123,123	0
31	MG	X	3027	1/1	0.91	0.59	-	66,66,66,66	0
32	MN	X	3417	1/1	0.93	0.23	-	156,156,156,156	0
32	MN	X	3169	1/1	0.95	0.51	-	76,76,76,76	0
31	MG	X	3309	1/1	0.81	0.10	-	53,53,53,53	0
31	MG	Y	207	1/1	0.65	0.54	-	101,101,101,101	0
36	EOH	X	3436	3/3	0.83	0.36	-	92,92,92,92	0
32	MN	X	3139	1/1	0.98	0.42	-	143,143,143,143	0
31	MG	X	3018	1/1	0.86	0.87	-	76,76,76,76	0
32	MN	X	3232	1/1	0.90	0.25	-	105,105,105,105	0
31	MG	X	3038	1/1	0.79	0.22	-	75,75,75,75	0
31	MG	X	3413	1/1	0.92	0.38	-	57,57,57,57	0
32	MN	X	3267	1/1	0.83	0.43	-	140,140,140,140	0
31	MG	X	3272	1/1	0.88	1.14	-	69,69,69,69	0
31	MG	X	3377	1/1	0.90	0.21	-	73,73,73,73	0
31	MG	X	3058	1/1	0.93	0.69	-	45,45,45,45	0
32	MN	X	3217	1/1	0.76	0.54	-	113,113,113,113	0
32	MN	Y	202	1/1	0.96	0.18	-	92,92,92,92	0
31	MG	X	3245	1/1	0.46	0.39	-	93,93,93,93	0
31	MG	X	3045	1/1	0.75	0.34	-	87,87,87,87	0
32	MN	X	3264	1/1	0.76	0.29	-	128,128,128,128	0
31	MG	X	3284	1/1	0.49	0.77	-	94,94,94,94	0
31	MG	X	3206	1/1	0.87	0.52	-	74,74,74,74	0
31	MG	X	3303	1/1	0.94	0.44	-	63,63,63,63	0
31	MG	X	3343	1/1	0.61	0.67	-	108,108,108,108	0
32	MN	X	3144	1/1	0.91	0.48	-	143,143,143,143	0
31	MG	X	3210	1/1	0.97	0.32	-	57,57,57,57	0
31	MG	X	3399	1/1	0.53	1.35	-	101,101,101,101	0
31	MG	X	3033	1/1	0.84	0.56	-	12,12,12,12	1
32	MN	X	3097	1/1	0.88	0.51	-	118,118,118,118	0
31	MG	X	3251	1/1	0.96	0.39	-	47,47,47,47	0
31	MG	X	3396	1/1	0.87	0.81	-	85,85,85,85	0
31	MG	X	3351	1/1	0.41	0.56	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	MG	X	3405	1/1	0.86	0.97	-	79,79,79,79	0
31	MG	X	3339	1/1	0.93	0.23	-	59,59,59,59	0
31	MG	X	3361	1/1	0.65	1.08	-	76,76,76,76	0
31	MG	X	3054	1/1	0.99	0.24	-	20,20,20,20	0
30	MPD	X	3002	8/8	0.84	0.38	-	132,132,132,132	0
31	MG	X	3329	1/1	0.94	0.28	-	60,60,60,60	0
31	MG	X	3280	1/1	0.68	1.21	-	87,87,87,87	0
31	MG	X	3315	1/1	0.96	0.86	-	87,87,87,87	0
31	MG	X	3042	1/1	0.97	0.69	-	59,59,59,59	0
32	MN	X	3177	1/1	0.88	0.14	-	56,56,56,56	0
31	MG	X	3395	1/1	0.95	0.90	-	93,93,93,93	0
32	MN	X	3271	1/1	0.87	0.20	-	117,117,117,117	0
32	MN	X	3109	1/1	0.90	0.39	-	145,145,145,145	0
31	MG	X	3402	1/1	0.94	0.17	-	84,84,84,84	0
31	MG	Z	102	1/1	0.92	0.26	-	68,68,68,68	0
31	MG	A	301	1/1	0.90	0.16	-	81,81,81,81	0
31	MG	X	3274	1/1	0.94	0.27	-	79,79,79,79	0
32	MN	X	3235	1/1	0.72	0.16	-	134,134,134,134	0
31	MG	X	3031	1/1	0.88	0.28	-	70,70,70,70	0
31	MG	X	3055	1/1	0.92	0.54	-	53,53,53,53	0
31	MG	X	3253	1/1	0.94	0.41	-	45,45,45,45	0
31	MG	X	3292	1/1	0.54	0.17	-	70,70,70,70	0
31	MG	X	3414	1/1	0.92	0.35	-	59,59,59,59	0
32	MN	X	3263	1/1	0.96	0.18	-	80,80,80,80	0
31	MG	X	3340	1/1	0.72	0.43	-	56,56,56,56	0
31	MG	X	3404	1/1	0.98	0.34	-	78,78,78,78	0
31	MG	G	201	1/1	0.50	0.98	-	68,68,68,68	0
31	MG	X	3026	1/1	0.83	0.24	-	64,64,64,64	0
31	MG	X	3276	1/1	0.88	0.55	-	85,85,85,85	0
31	MG	Y	205	1/1	0.92	0.16	-	77,77,77,77	0
31	MG	X	3048	1/1	0.91	0.41	-	31,31,31,31	1
32	MN	X	3122	1/1	0.97	0.18	-	123,123,123,123	0
31	MG	X	3030	1/1	0.75	0.23	-	38,38,38,38	1
31	MG	X	3305	1/1	0.93	0.47	-	68,68,68,68	0
31	MG	X	3394	1/1	0.80	0.30	-	80,80,80,80	0
32	MN	X	3194	1/1	0.96	0.36	-	93,93,93,93	0
31	MG	X	3358	1/1	0.96	0.35	-	46,46,46,46	0
32	MN	X	3265	1/1	0.15	0.89	-	158,158,158,158	0
31	MG	X	3255	1/1	0.84	0.63	-	69,69,69,69	0
32	MN	X	3203	1/1	0.96	0.33	-	69,69,69,69	0
32	MN	X	3089	1/1	0.94	0.13	-	92,92,92,92	0
31	MG	X	3371	1/1	0.88	1.00	-	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MN	X	3261	1/1	0.95	0.35	-	132,132,132,132	0
31	MG	X	3017	1/1	0.92	0.31	-	75,75,75,75	0
32	MN	X	3233	1/1	0.99	0.34	-	66,66,66,66	0
32	MN	Y	203	1/1	0.75	0.18	-	99,99,99,99	0
31	MG	X	3353	1/1	0.98	0.16	-	81,81,81,81	0
32	MN	X	3067	1/1	0.82	0.36	-	166,166,166,166	0
31	MG	X	3354	1/1	0.92	0.33	-	64,64,64,64	0
32	MN	X	3118	1/1	0.98	0.36	-	123,123,123,123	0
32	MN	X	3080	1/1	0.94	0.39	-	130,130,130,130	0
32	MN	X	3164	1/1	0.95	0.32	-	92,92,92,92	0
31	MG	X	3250	1/1	0.92	0.57	-	70,70,70,70	0
31	MG	X	3356	1/1	0.94	0.22	-	70,70,70,70	0
32	MN	X	3128	1/1	0.98	0.23	-	77,77,77,77	0
32	MN	X	3197	1/1	0.90	0.20	-	102,102,102,102	0
31	MG	X	3056	1/1	0.72	0.80	-	55,55,55,55	1
32	MN	X	3075	1/1	0.95	0.31	-	116,116,116,116	0
32	MN	X	3137	1/1	0.99	0.26	-	108,108,108,108	0
32	MN	X	3214	1/1	0.79	0.28	-	163,163,163,163	0
32	MN	X	3163	1/1	0.96	0.37	-	61,61,61,61	0
32	MN	X	3098	1/1	0.69	0.26	-	131,131,131,131	0
32	MN	X	3135	1/1	0.96	0.27	-	76,76,76,76	0
32	MN	X	3200	1/1	0.97	0.21	-	126,126,126,126	0
32	MN	X	3186	1/1	0.97	0.28	-	69,69,69,69	0
32	MN	X	3064	1/1	0.93	0.25	-	145,145,145,145	0
31	MG	X	3301	1/1	0.99	0.12	-	43,43,43,43	0
31	MG	X	3241	1/1	0.83	0.67	-	66,66,66,66	0
31	MG	X	3328	1/1	0.92	0.50	-	59,59,59,59	0
31	MG	O	201	1/1	0.92	0.33	-	41,41,41,41	0
32	MN	X	3085	1/1	0.71	0.59	-	128,128,128,128	0
32	MN	X	3106	1/1	0.95	0.24	-	96,96,96,96	0
32	MN	X	3259	1/1	0.84	0.12	-	140,140,140,140	0
31	MG	X	3248	1/1	0.33	0.26	-	65,65,65,65	0
31	MG	X	3047	1/1	0.62	0.35	-	71,71,71,71	0
31	MG	C	301	1/1	0.92	0.25	-	46,46,46,46	0
31	MG	X	3383	1/1	0.93	0.66	-	58,58,58,58	0
31	MG	X	3288	1/1	0.99	0.26	-	79,79,79,79	0
32	MN	X	3069	1/1	0.97	0.22	-	121,121,121,121	0
31	MG	X	3213	1/1	0.92	0.38	-	22,22,22,22	0
32	MN	X	3237	1/1	0.98	0.27	-	71,71,71,71	0
31	MG	X	3330	1/1	0.96	0.16	-	55,55,55,55	0
31	MG	I	201	1/1	0.86	0.63	-	47,47,47,47	0
32	MN	X	3173	1/1	0.98	0.14	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	MG	X	3409	1/1	0.90	1.05	-	67,67,67,67	0
31	MG	X	3388	1/1	0.88	0.22	-	65,65,65,65	0
31	MG	X	3293	1/1	0.94	0.16	-	91,91,91,91	0
32	MN	X	3191	1/1	0.86	0.18	-	107,107,107,107	0
31	MG	X	3365	1/1	0.99	0.09	-	63,63,63,63	0
31	MG	X	3019	1/1	0.79	0.63	-	69,69,69,69	0
31	MG	X	3050	1/1	0.88	0.80	-	2,2,2,2	1
32	MN	X	3091	1/1	0.92	0.41	-	100,100,100,100	0
31	MG	X	3334	1/1	0.91	0.21	-	57,57,57,57	0
32	MN	X	3065	1/1	0.99	0.19	-	78,78,78,78	0
31	MG	X	3013	1/1	0.98	0.75	-	61,61,61,61	0
32	MN	X	3141	1/1	0.82	0.48	-	100,100,100,100	0
31	MG	X	3242	1/1	0.62	0.72	-	90,90,90,90	0
32	MN	X	3117	1/1	0.75	0.52	-	166,166,166,166	0
31	MG	X	3401	1/1	0.58	0.54	-	63,63,63,63	0
31	MG	W	101	1/1	0.97	0.61	-	84,84,84,84	0
31	MG	X	3307	1/1	0.95	0.51	-	67,67,67,67	0
32	MN	X	3138	1/1	0.92	0.25	-	120,120,120,120	0
32	MN	X	3202	1/1	0.85	0.27	-	117,117,117,117	0
32	MN	X	3145	1/1	0.99	0.19	-	47,47,47,47	0
31	MG	X	3333	1/1	0.98	0.95	-	71,71,71,71	0
31	MG	X	3380	1/1	0.57	0.43	-	83,83,83,83	0
31	MG	X	3300	1/1	0.93	0.76	-	80,80,80,80	0
31	MG	X	3061	1/1	0.92	0.28	-	41,41,41,41	0
31	MG	X	3368	1/1	0.85	0.37	-	70,70,70,70	0
32	MN	X	3238	1/1	0.93	0.17	-	174,174,174,174	0
31	MG	X	3366	1/1	0.12	0.38	-	69,69,69,69	0
31	MG	X	3350	1/1	0.92	0.12	-	28,28,28,28	0
31	MG	X	3318	1/1	0.75	0.36	-	65,65,65,65	0
31	MG	X	3364	1/1	0.85	0.33	-	80,80,80,80	0
32	MN	X	3178	1/1	0.97	0.39	-	92,92,92,92	0
31	MG	X	3286	1/1	0.80	0.57	-	82,82,82,82	0
32	MN	X	3134	1/1	0.96	0.41	-	57,57,57,57	0
31	MG	X	3311	1/1	0.67	0.12	-	86,86,86,86	0
31	MG	X	3020	1/1	0.96	0.23	-	53,53,53,53	0
32	MN	X	3226	1/1	0.77	0.22	-	112,112,112,112	0
36	EOH	Y	209	3/3	0.66	0.27	-	93,93,93,93	0
31	MG	X	3403	1/1	0.97	0.08	-	52,52,52,52	0
31	MG	X	3410	1/1	0.90	0.37	-	78,78,78,78	0
31	MG	X	3393	1/1	0.80	0.12	-	67,67,67,67	0
32	MN	X	3090	1/1	0.85	0.14	-	123,123,123,123	0
31	MG	X	3298	1/1	0.94	0.30	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MN	X	3422	1/1	0.57	1.08	-	201,201,201,201	0
32	MN	X	3104	1/1	0.98	0.42	-	88,88,88,88	0
31	MG	X	3302	1/1	0.72	0.21	-	51,51,51,51	0
31	MG	Y	201	1/1	0.96	0.42	-	24,24,24,24	1
32	MN	X	3092	1/1	0.90	0.29	-	104,104,104,104	0
32	MN	Z	101	1/1	0.98	0.38	-	88,88,88,88	0
31	MG	X	3015	1/1	0.89	0.40	-	36,36,36,36	1
32	MN	X	3170	1/1	0.96	0.28	-	95,95,95,95	0
32	MN	X	3129	1/1	0.94	0.60	-	106,106,106,106	0
31	MG	X	3378	1/1	0.83	0.23	-	83,83,83,83	0
31	MG	X	3370	1/1	0.58	0.34	-	103,103,103,103	0
31	MG	X	3036	1/1	0.95	0.65	-	85,85,85,85	0
36	EOH	X	3435	3/3	0.90	0.23	-	36,36,36,36	0
32	MN	X	3185	1/1	0.92	0.84	-	132,132,132,132	0
32	MN	X	3072	1/1	0.80	0.20	-	91,91,91,91	0
31	MG	X	3283	1/1	0.93	0.13	-	62,62,62,62	0
32	MN	X	3258	1/1	0.95	0.20	-	98,98,98,98	0
31	MG	X	3317	1/1	0.95	0.24	-	39,39,39,39	0
32	MN	X	3110	1/1	0.95	0.21	-	103,103,103,103	0
31	MG	X	3376	1/1	0.95	0.27	-	93,93,93,93	0
31	MG	X	3046	1/1	0.92	0.23	-	43,43,43,43	1
31	MG	X	3243	1/1	0.77	0.36	-	82,82,82,82	0
32	MN	X	3160	1/1	0.99	0.28	-	39,39,39,39	0
31	MG	X	3049	1/1	0.95	0.54	-	14,14,14,14	1
31	MG	X	3254	1/1	0.76	0.86	-	47,47,47,47	1
32	MN	X	3269	1/1	0.96	0.33	-	131,131,131,131	0
31	MG	X	3022	1/1	0.91	0.30	-	83,83,83,83	0
32	MN	X	3193	1/1	0.96	0.17	-	87,87,87,87	0
32	MN	X	3174	1/1	0.98	0.34	-	81,81,81,81	0
32	MN	X	3114	1/1	0.56	0.85	-	150,150,150,150	0
31	MG	X	3052	1/1	0.98	0.28	-	27,27,27,27	0
32	MN	X	3225	1/1	0.96	0.86	-	133,133,133,133	0
31	MG	B	301	1/1	0.85	0.28	-	65,65,65,65	0
32	MN	X	3071	1/1	0.60	0.15	-	134,134,134,134	0
31	MG	X	3331	1/1	0.98	0.20	-	60,60,60,60	0
32	MN	X	3070	1/1	0.83	0.18	-	148,148,148,148	0
32	MN	X	3266	1/1	0.78	0.14	-	104,104,104,104	0
31	MG	X	3285	1/1	0.78	0.30	-	73,73,73,73	0
32	MN	X	3234	1/1	0.97	0.06	-	91,91,91,91	0
32	MN	X	3260	1/1	0.87	0.26	-	126,126,126,126	0
31	MG	X	3016	1/1	0.91	0.43	-	81,81,81,81	0
31	MG	X	3408	1/1	0.87	0.24	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MN	X	3073	1/1	0.90	0.09	-	105,105,105,105	0
31	MG	X	3327	1/1	0.63	0.47	-	103,103,103,103	0
31	MG	X	3326	1/1	0.99	0.25	-	32,32,32,32	0
31	MG	X	3341	1/1	0.83	0.47	-	43,43,43,43	0
32	MN	X	3086	1/1	0.87	0.21	-	82,82,82,82	0
31	MG	X	3359	1/1	0.58	1.18	-	87,87,87,87	0
32	MN	X	3183	1/1	0.97	0.22	-	63,63,63,63	0
31	MG	X	3297	1/1	0.68	0.47	-	85,85,85,85	0
32	MN	X	3083	1/1	0.84	0.31	-	150,150,150,150	0
31	MG	X	3281	1/1	0.90	0.40	-	72,72,72,72	0
32	MN	X	3165	1/1	0.98	0.25	-	79,79,79,79	0
32	MN	X	3188	1/1	0.93	0.38	-	100,100,100,100	0
32	MN	X	3204	1/1	0.95	0.15	-	126,126,126,126	0
31	MG	X	3028	1/1	0.84	0.24	-	58,58,58,58	0
31	MG	X	3379	1/1	0.98	0.20	-	40,40,40,40	0
31	MG	X	3324	1/1	0.95	0.66	-	88,88,88,88	0
31	MG	X	3279	1/1	0.94	0.29	-	68,68,68,68	0
31	MG	X	3277	1/1	0.94	0.07	-	55,55,55,55	0
31	MG	X	3059	1/1	0.86	0.26	-	35,35,35,35	0
31	MG	X	3386	1/1	0.40	1.38	-	112,112,112,112	0
32	MN	X	3196	1/1	0.97	0.26	-	77,77,77,77	0
32	MN	X	3236	1/1	0.95	0.17	-	104,104,104,104	0
32	MN	X	3107	1/1	0.98	0.15	-	71,71,71,71	0
31	MG	X	3369	1/1	0.76	0.80	-	76,76,76,76	0
31	MG	X	3382	1/1	0.78	0.72	-	68,68,68,68	0
31	MG	X	3257	1/1	0.96	0.26	-	71,71,71,71	0
32	MN	X	3190	1/1	0.98	0.47	-	91,91,91,91	0
31	MG	X	3296	1/1	0.77	0.30	-	75,75,75,75	0
31	MG	X	3346	1/1	0.91	0.92	-	81,81,81,81	0
31	MG	X	3029	1/1	0.41	0.41	-	65,65,65,65	1
32	MN	X	3374	1/1	0.92	0.21	-	153,153,153,153	0
31	MG	X	3357	1/1	0.75	0.65	-	56,56,56,56	0
33	NA	X	3367	1/1	0.83	0.36	-	64,64,64,64	0
31	MG	X	3014	1/1	0.70	1.10	-	85,85,85,85	0
31	MG	X	3381	1/1	0.86	0.31	-	82,82,82,82	0
32	MN	X	3155	1/1	0.97	0.35	-	75,75,75,75	0
31	MG	X	3291	1/1	0.80	0.97	-	62,62,62,62	0
31	MG	X	3360	1/1	0.85	0.61	-	123,123,123,123	0
32	MN	X	3101	1/1	0.99	0.17	-	86,86,86,86	0
31	MG	K	201	1/1	0.65	0.34	-	72,72,72,72	0
32	MN	X	3158	1/1	0.98	0.36	-	58,58,58,58	0
31	MG	X	3421	1/1	0.94	0.26	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MN	X	3121	1/1	0.83	0.38	-	126,126,126,126	0
31	MG	X	3278	1/1	0.90	0.24	-	67,67,67,67	0
31	MG	O	202	1/1	0.34	0.74	-	67,67,67,67	0
31	MG	X	3407	1/1	0.85	0.52	-	89,89,89,89	0
31	MG	X	3244	1/1	0.81	0.44	-	78,78,78,78	0
32	MN	X	3181	1/1	0.96	0.27	-	73,73,73,73	0
32	MN	X	3270	1/1	0.88	0.11	-	109,109,109,109	0
31	MG	X	3337	1/1	0.97	0.31	-	44,44,44,44	0
32	MN	X	3216	1/1	0.93	0.13	-	112,112,112,112	0
32	MN	X	3096	1/1	0.75	0.10	-	153,153,153,153	0
31	MG	X	3313	1/1	0.99	0.41	-	59,59,59,59	0
31	MG	X	3362	1/1	0.89	0.23	-	47,47,47,47	0
32	MN	X	3149	1/1	0.96	0.37	-	64,64,64,64	0
31	MG	X	3057	1/1	0.94	0.45	-	41,41,41,41	0
32	MN	X	3229	1/1	0.93	0.43	-	135,135,135,135	0
32	MN	X	3082	1/1	0.96	0.19	-	109,109,109,109	0
31	MG	Y	208	1/1	0.79	0.52	-	81,81,81,81	0
31	MG	X	3282	1/1	0.96	0.29	-	68,68,68,68	0
31	MG	X	3273	1/1	0.84	0.25	-	79,79,79,79	0
31	MG	X	3392	1/1	0.92	0.16	-	91,91,91,91	0
31	MG	X	3398	1/1	0.94	1.58	-	107,107,107,107	0
32	MN	X	3105	1/1	0.73	0.37	-	87,87,87,87	0
32	MN	X	3076	1/1	0.93	0.47	-	148,148,148,148	0
32	MN	X	3112	1/1	0.82	0.12	-	155,155,155,155	0
31	MG	X	3275	1/1	0.33	0.22	-	73,73,73,73	0
31	MG	X	3295	1/1	0.99	0.06	-	56,56,56,56	0
32	MN	X	3116	1/1	0.91	0.17	-	84,84,84,84	0
32	MN	X	3156	1/1	0.95	0.26	-	83,83,83,83	0
32	MN	X	3171	1/1	0.97	0.39	-	88,88,88,88	0
32	MN	X	3127	1/1	0.97	0.22	-	108,108,108,108	0
31	MG	X	3325	1/1	0.98	0.39	-	93,93,93,93	0
32	MN	X	3093	1/1	0.95	0.14	-	122,122,122,122	0
31	MG	X	3246	1/1	0.92	0.37	-	69,69,69,69	0
31	MG	X	3212	1/1	0.96	0.71	-	40,40,40,40	0
32	MN	X	3198	1/1	0.99	0.42	-	73,73,73,73	0
31	MG	X	3053	1/1	0.90	0.70	-	42,42,42,42	1
31	MG	X	3322	1/1	0.95	0.50	-	50,50,50,50	0
31	MG	X	3051	1/1	0.85	0.51	-	14,14,14,14	1
32	MN	X	3167	1/1	0.91	0.42	-	91,91,91,91	0
32	MN	M	201	1/1	0.65	0.16	-	122,122,122,122	0
32	MN	X	3094	1/1	0.90	0.18	-	139,139,139,139	0
31	MG	X	3336	1/1	0.97	0.09	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	MG	X	3385	1/1	0.94	0.18	-	63,63,63,63	0
31	MG	X	3012	1/1	0.74	1.29	-	13,13,13,13	1
31	MG	X	3342	1/1	0.96	0.18	-	67,67,67,67	0
32	MN	X	3373	1/1	0.91	0.29	-	94,94,94,94	0
32	MN	X	3218	1/1	0.93	0.53	-	151,151,151,151	0
31	MG	X	3247	1/1	0.94	0.20	-	49,49,49,49	0
32	MN	X	3230	1/1	0.95	0.30	-	100,100,100,100	0
31	MG	X	3207	1/1	0.97	0.12	-	56,56,56,56	0
32	MN	X	3166	1/1	0.99	0.30	-	90,90,90,90	0
31	MG	X	3321	1/1	0.89	0.52	-	80,80,80,80	0
32	MN	X	3175	1/1	0.98	0.20	-	86,86,86,86	0
31	MG	X	3397	1/1	0.79	0.40	-	95,95,95,95	0
31	MG	X	3387	1/1	0.86	0.29	-	60,60,60,60	0
31	MG	X	3391	1/1	0.83	0.35	-	73,73,73,73	0
31	MG	X	3375	1/1	0.87	0.18	-	69,69,69,69	0
32	MN	X	3222	1/1	0.79	1.24	-	171,171,171,171	0
31	MG	X	3299	1/1	0.90	0.07	-	38,38,38,38	0
32	MN	X	3068	1/1	0.77	0.15	-	130,130,130,130	0
32	MN	X	3115	1/1	0.70	0.28	-	135,135,135,135	0
31	MG	X	3389	1/1	0.62	0.29	-	66,66,66,66	0
32	MN	X	3088	1/1	0.86	0.15	-	110,110,110,110	0
32	MN	X	3081	1/1	0.98	0.30	-	95,95,95,95	0

6.5 Other polymers

There are no such residues in this entry.