



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:33 PM UTC

PDB ID : 5HL7 / pdb_00005hl7
Title : The crystal structure of the large ribosomal subunit of *Staphylococcus aureus* in complex with lefamulin
Authors : Eyal, Z.; Matzov, D.; Krupkin, M.; Rozenberg, H.; Zimmerman, E.; Bashan, A.; Yonath, A.
Deposited on : 2016-01-14
Resolution : 3.55 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

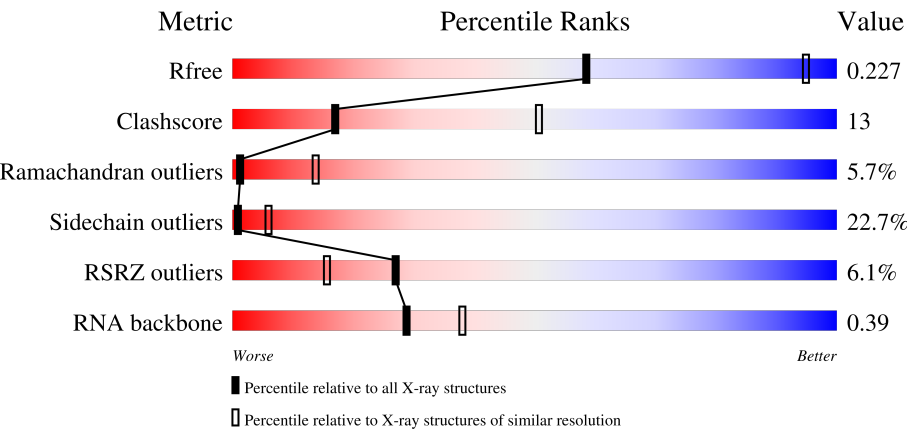
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 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}	180053	1410 (3.62-3.50)
Clashscore	190562	1480 (3.62-3.50)
Ramachandran outliers	187476	1440 (3.62-3.50)
Sidechain outliers	187428	1441 (3.62-3.50)
RSRZ outliers	180081	1409 (3.62-3.50)
RNA backbone	3983	1006 (4.02-3.06)

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

Mol	Chain	Length	Quality of chain
1	A	277	10% 66% 24% 6% ••
2	X	2923	3% 44% 39% 10% 7%
3	Y	114	3% 43% 52% 5%

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Mol	Chain	Length	Quality of chain
4	B	220	
5	C	207	
6	D	179	
7	E	178	
8	G	145	
9	H	122	
10	I	140	
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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	MG	A	303	-	-	-	X
30	MG	A	304	-	-	-	X
30	MG	X	3002	-	-	-	X
30	MG	X	3165	-	-	-	X
30	MG	X	3250	-	-	-	X
30	MG	X	3265	-	-	-	X
30	MG	X	3287	-	-	-	X
30	MG	X	3291	-	-	-	X
30	MG	X	3327	-	-	-	X
30	MG	X	3342	-	-	-	X
30	MG	X	3347	-	-	-	X
30	MG	X	3349	-	-	-	X
30	MG	X	3351	-	-	-	X
30	MG	X	3358	-	-	-	X
30	MG	X	3370	-	-	-	X
30	MG	X	3385	-	-	-	X
30	MG	X	3417	-	-	-	X
30	MG	X	3424	-	-	-	X
30	MG	X	3488	-	-	-	X
30	MG	Y	205	-	-	-	X
35	EPE	N	201	-	-	X	-

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 81462 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			1667	1007	331	324	5			

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	2705	Total	C	N	O	P	0	0	0
			57983	25884	10620	18774	2705			

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

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

- 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
			1547	967	289	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
			1324	823	250	249	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	165	Total	C	N	O	S	0	0	0
			853	512	165	174	2			

- 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
			915	559	172	182	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	174	LYS	GLY	conflict	UNP Q2FW21

- 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
			1090	682	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
			884	548	167	165	4			

- 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
			819	498	164	156	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
			1001	641	187	170	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
			906	556	175	174	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	109	Total	C	N	O	0	0	0
			673	411	134	128			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	110	Total	C	N	O	0	0	0
			807	510	162	135			

- 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	0	0	0
			922	581	183	154	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	102	Total	C	N	O	S	0	0	0
			751	477	138	135	1			

- 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	0	0	0
			853	531	161	158	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	90	Total	C	N	O	S	0	0	0
			583	365	103	112	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	102	Total	C	N	O	S	0	0	0
			627	382	120	124	1			

- 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	0	0	0
			1087	682	191	212	2			

- 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
			559	349	110	100				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	U	42	Total	C	N	O		0	0	0
			242	149	48	45				

- 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
			486	299	89	98				

- 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
			437	271	82	84				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	43	Total	C	N	O	S	0	0	0
			339	208	70	57	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	2	43	Total	C	N	O	S	0	0	0
			350	213	85	51	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
			405	248	81	74	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	4	36	Total	C	N	O	S	0	0	0
			181	107	36	36	2			

- Molecule 29 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	1	Total	Mn	0	0
			1	1		
29	X	268	Total	Mn	0	0
			268	268		
29	Y	2	Total	Mn	0	0
			2	2		
29	R	1	Total	Mn	0	0
			1	1		
29	T	1	Total	Mn	0	0
			1	1		
29	Z	1	Total	Mn	0	0
			1	1		

- Molecule 30 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

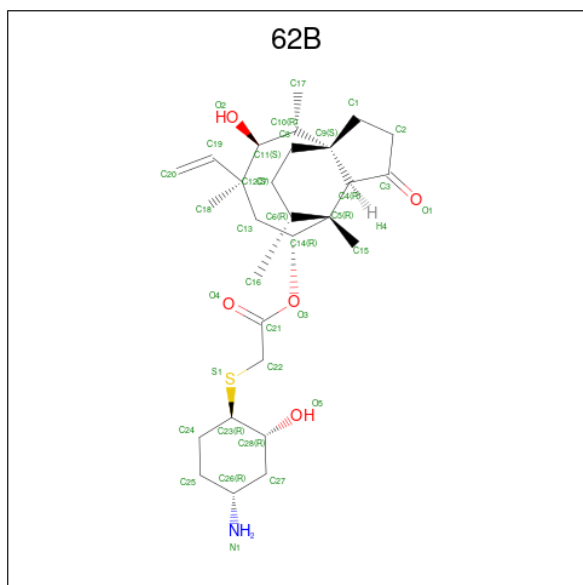
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	3	Total	Mg	0	0
			3	3		
30	X	218	Total	Mg	0	0
			218	218		
30	Y	10	Total	Mg	0	0
			10	10		
30	C	2	Total	Mg	0	0
			2	2		
30	G	2	Total	Mg	0	0
			2	2		
30	I	1	Total	Mg	0	0
			1	1		
30	J	1	Total	Mg	0	0
			1	1		

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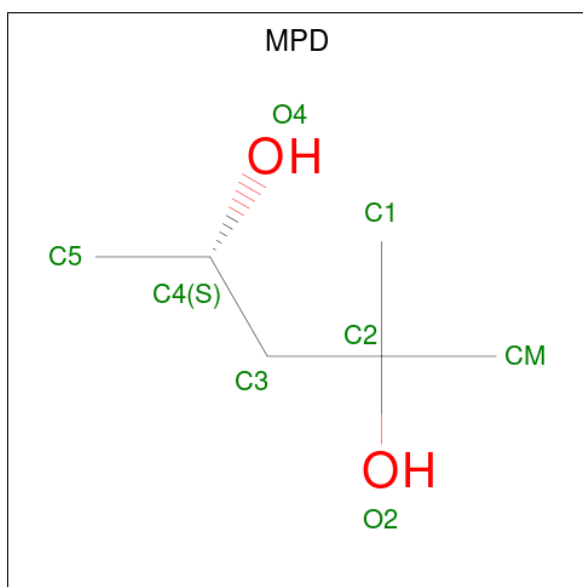
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	M	1	Total	Mg	0	0
			1	1		
30	O	1	Total	Mg	0	0
			1	1		
30	P	1	Total	Mg	0	0
			1	1		

- Molecule 31 is Lefamulin (CCD ID: 62B) (formula: $C_{28}H_{45}NO_5S$).



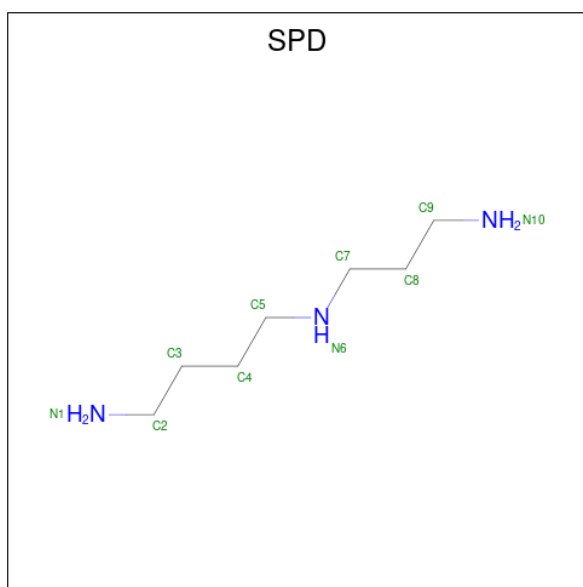
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
31	X	1	Total	C	N	O	S	0	0
			35	28	1	5	1		

- Molecule 32 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



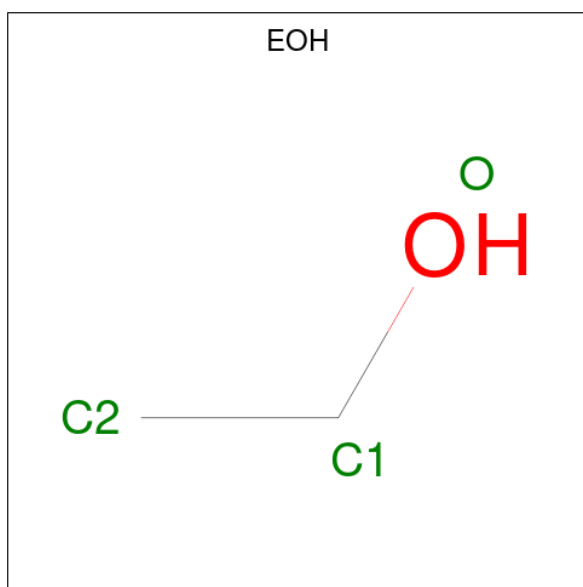
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	X	1	Total	C	O	0	0
			8	6	2		
32	X	1	Total	C	O	0	0
			8	6	2		
32	X	1	Total	C	O	0	0
			8	6	2		
32	X	1	Total	C	O	0	0
			8	6	2		
32	X	1	Total	C	O	0	0
			8	6	2		
32	X	1	Total	C	O	0	0
			8	6	2		
32	X	1	Total	C	O	0	0
			8	6	2		
32	J	1	Total	C	O	0	0
			8	6	2		
32	Q	1	Total	C	O	0	0
			8	6	2		
32	Z	1	Total	C	O	0	0
			8	6	2		

- Molecule 33 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



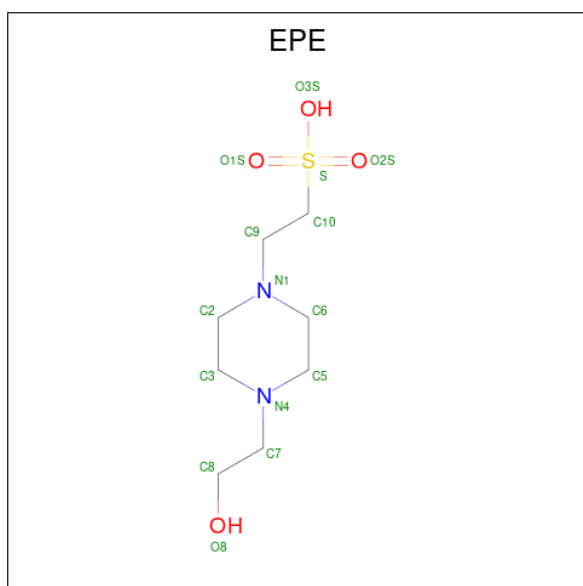
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	X	1	Total C N 10 7 3	0	0
33	X	1	Total C N 10 7 3	0	0
33	X	1	Total C N 10 7 3	0	0
33	X	1	Total C N 10 7 3	0	0
33	X	1	Total C N 10 7 3	0	0
33	X	1	Total C N 10 7 3	0	0
33	X	1	Total C N 10 7 3	0	0
33	Y	1	Total C N 10 7 3	0	0

- Molecule 34 is ETHANOL (CCD ID: EOH) (formula: C₂H₆O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	S	1	Total	C	O	0	0
			3	2	1		

- Molecule 35 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).

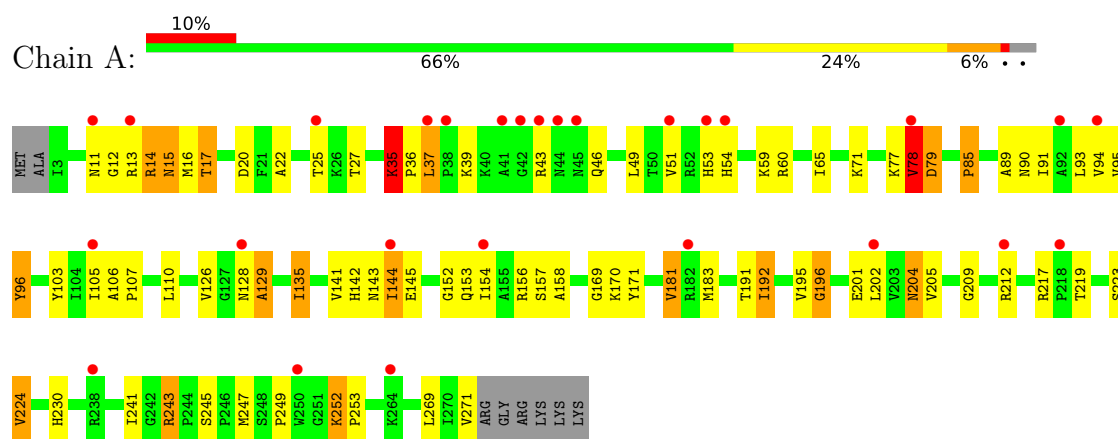


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
35	N	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

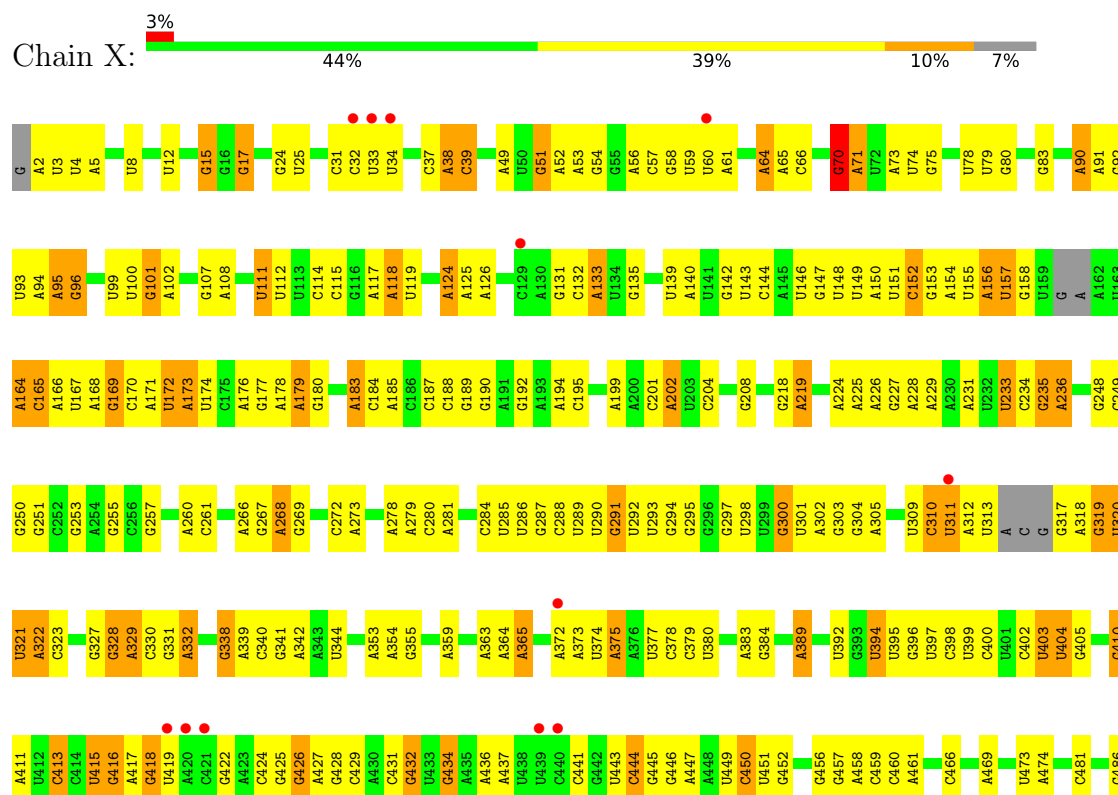
3 Residue-property plots [i](#)

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

• Molecule 1: 50S ribosomal protein L2

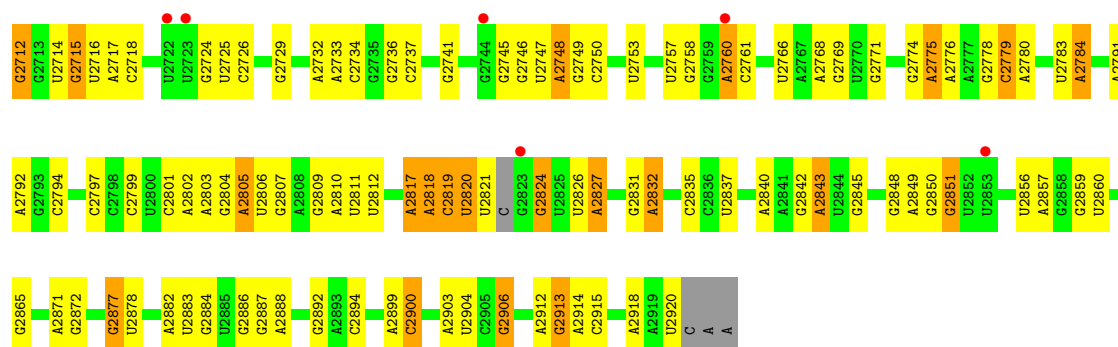


• Molecule 2: 23S ribosomal RNA

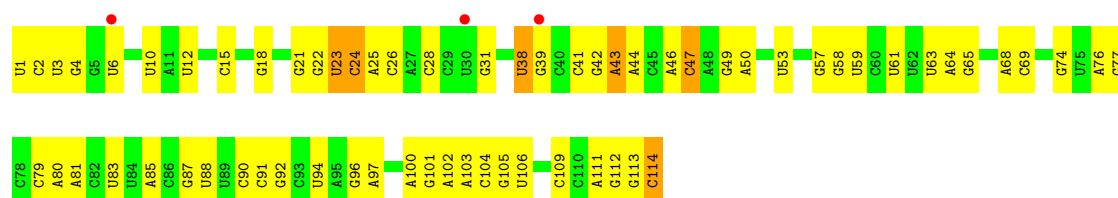




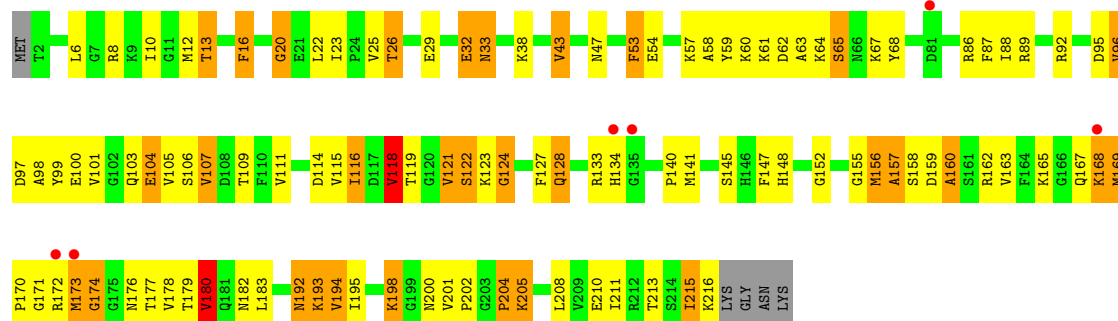




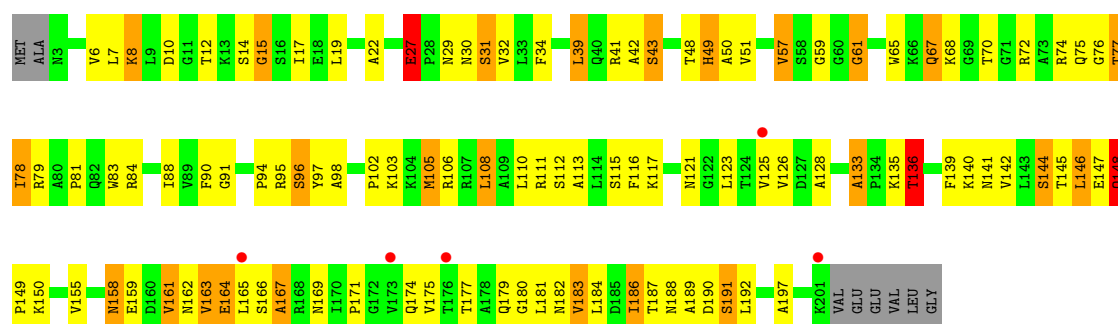
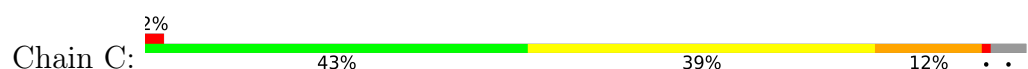
• Molecule 3: 5S ribosomal RNA



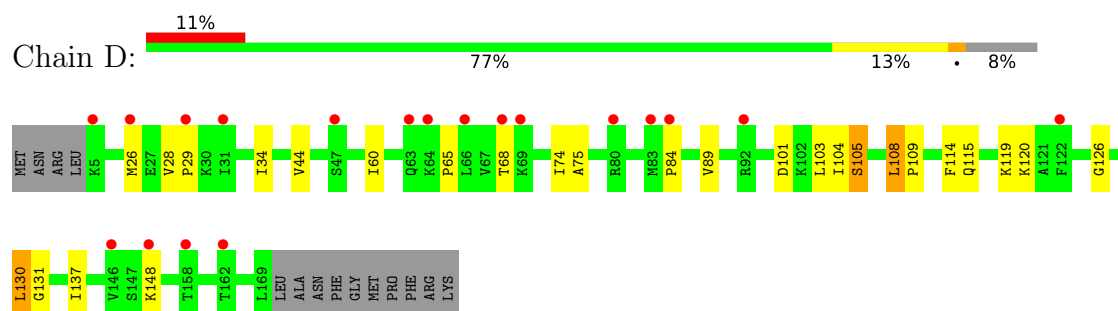
• Molecule 4: 50S ribosomal protein L3



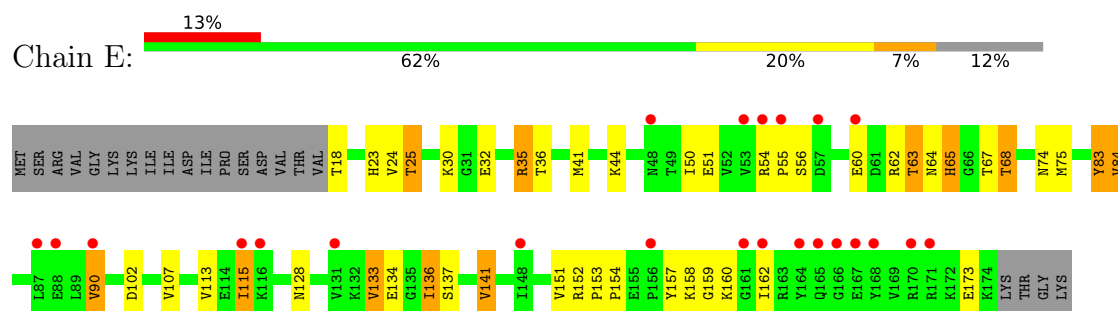
• Molecule 5: 50S ribosomal protein L4



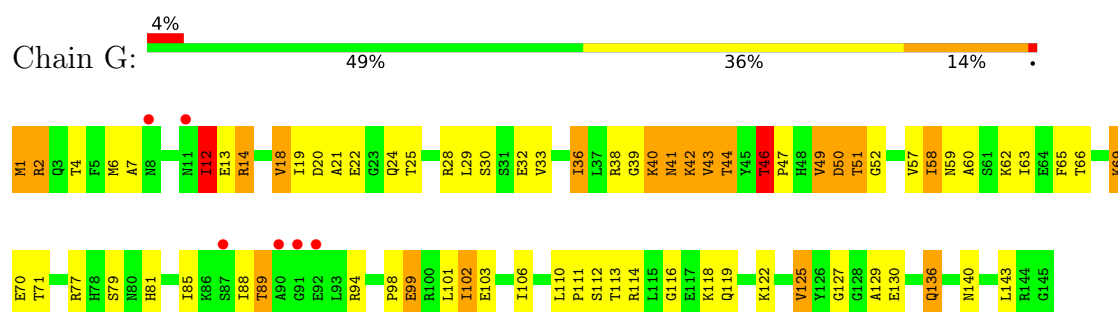
- Molecule 6: 50S ribosomal protein L5



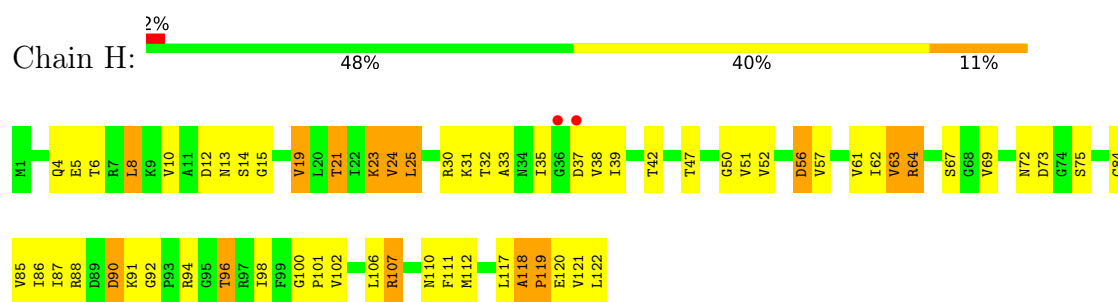
- Molecule 7: 50S ribosomal protein L6



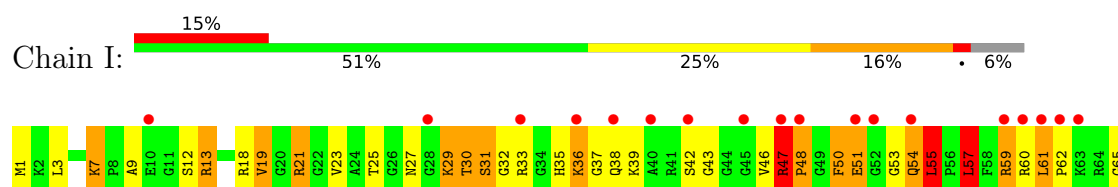
- Molecule 8: 50S ribosomal protein L13

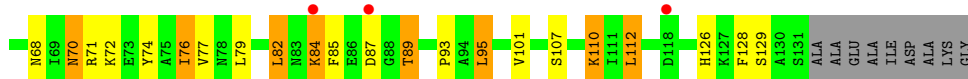


- Molecule 9: 50S ribosomal protein L14

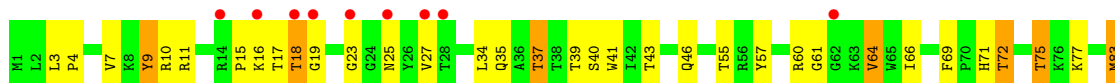


- Molecule 10: 50S ribosomal protein L15

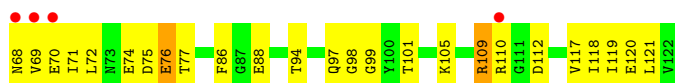




- Molecule 11: 50S ribosomal protein L16



- Molecule 12: 50S ribosomal protein L17



- Molecule 13: 50S ribosomal protein L18

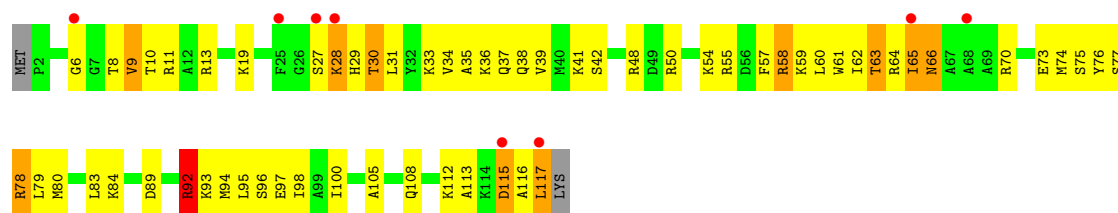


- Molecule 14: 50S ribosomal protein L19

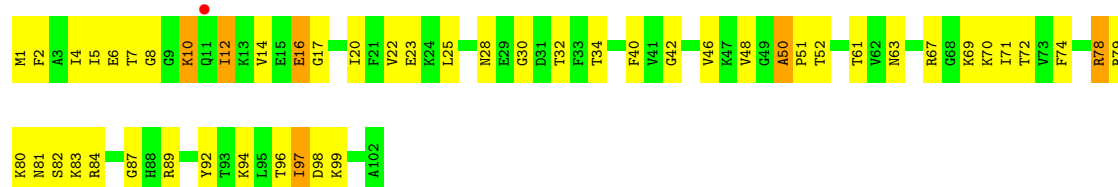


- Molecule 15: 50S ribosomal protein L20

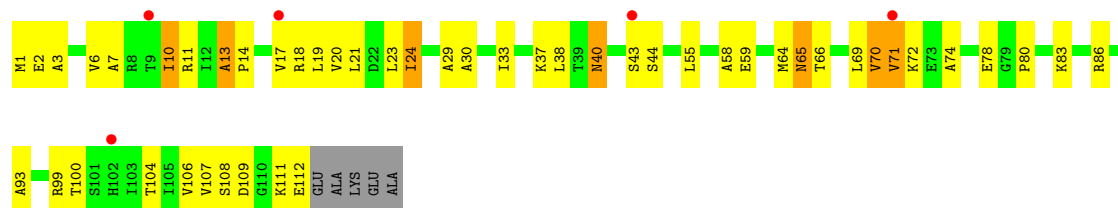




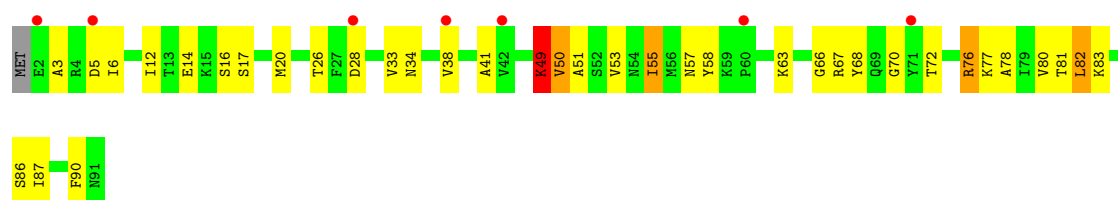
• Molecule 16: 50S ribosomal protein L21



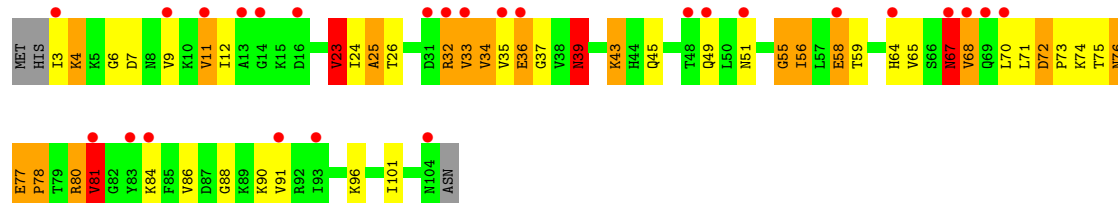
• Molecule 17: 50S ribosomal protein L22



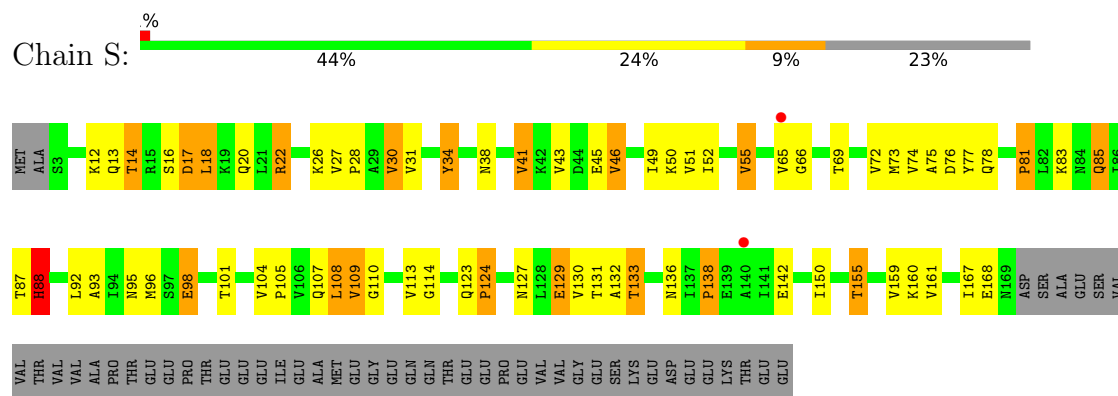
• Molecule 18: 50S ribosomal protein L23



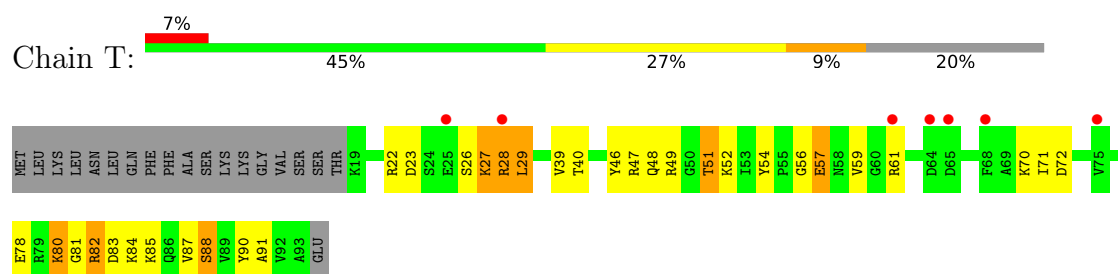
• Molecule 19: 50S ribosomal protein L24



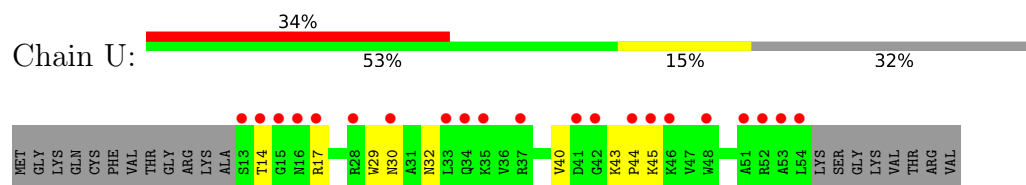
- Molecule 20: 50S ribosomal protein L25



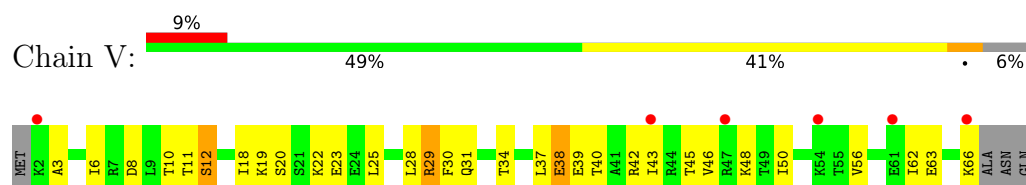
- Molecule 21: 50S ribosomal protein L27



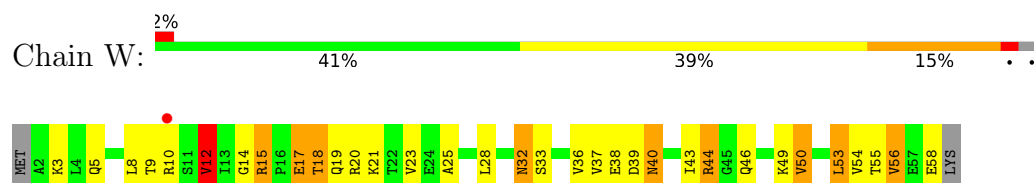
- Molecule 22: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L30

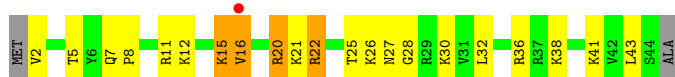


- Molecule 25: 50S ribosomal protein L32





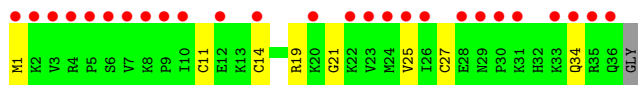
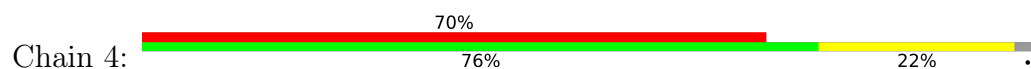
- Molecule 26: 50S ribosomal protein L34



- 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	282.11Å 282.11Å 875.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.93 – 3.55 49.93 – 3.55	Depositor EDS
% Data completeness (in resolution range)	95.4 (49.93-3.55) 95.6 (49.93-3.55)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 3.57Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.187 , 0.227 0.189 , 0.227	Depositor DCC
R_{free} test set	11848 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	105.6	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 59.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	81462	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MN, EOH, MG, 62B, SPD, MPD, EPE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.39	0/1697	1.00	8/2332 (0.3%)
2	X	0.50	1/64923 (0.0%)	0.70	5/101215 (0.0%)
3	Y	0.46	0/2717	0.65	0/4232
4	B	0.91	2/1570 (0.1%)	1.33	23/2117 (1.1%)
5	C	1.02	3/1343 (0.2%)	1.52	24/1838 (1.3%)
6	D	0.56	0/855	1.04	3/1185 (0.3%)
7	E	0.71	1/925 (0.1%)	1.10	3/1279 (0.2%)
8	G	1.02	3/1112 (0.3%)	1.34	11/1507 (0.7%)
9	H	0.81	0/891	1.17	6/1203 (0.5%)
10	I	1.12	4/827 (0.5%)	1.57	16/1121 (1.4%)
11	J	0.85	1/1023 (0.1%)	1.34	14/1388 (1.0%)
12	K	0.48	0/909	0.91	0/1217
13	L	0.75	0/678	1.18	5/927 (0.5%)
14	M	0.94	1/819 (0.1%)	1.29	5/1107 (0.5%)
15	N	1.05	1/934 (0.1%)	1.33	7/1241 (0.6%)
16	O	1.00	0/761	1.58	9/1022 (0.9%)
17	P	0.59	0/861	1.00	4/1160 (0.3%)
18	Q	0.84	1/589 (0.2%)	1.27	5/808 (0.6%)
19	R	1.13	3/631 (0.5%)	1.32	3/863 (0.3%)
20	S	0.86	2/1099 (0.2%)	1.29	9/1509 (0.6%)
21	T	0.78	0/565	1.15	2/751 (0.3%)
22	U	0.58	0/247	1.03	1/344 (0.3%)
23	V	0.56	0/487	1.03	2/654 (0.3%)
24	W	0.95	1/439 (0.2%)	1.25	1/593 (0.2%)
25	Z	0.96	0/345	1.19	4/460 (0.9%)
26	2	0.85	0/353	1.29	3/463 (0.6%)
27	3	1.06	0/409	1.50	8/550 (1.5%)
28	4	0.80	0/180	1.38	1/249 (0.4%)
All	All	0.60	24/88189 (0.0%)	0.85	182/133335 (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
1	A	0	1
4	B	0	2
5	C	0	2
10	I	0	1
16	O	0	1
17	P	0	1
20	S	0	1
27	3	0	2
All	All	0	11

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	R	68	VAL	CA-CB	14.12	1.68	1.54
19	R	67	ASN	CA-C	6.44	1.61	1.52
15	N	34	VAL	CA-CB	-6.04	1.47	1.54
8	G	50	ASP	CA-C	-6.04	1.45	1.52
10	I	55	LEU	CA-C	5.92	1.60	1.52
10	I	39	LYS	N-CA	5.89	1.53	1.46
10	I	76	ILE	CA-CB	5.84	1.60	1.54
4	B	180	VAL	CA-CB	-5.83	1.47	1.54
5	C	177	THR	CA-CB	5.80	1.62	1.53
19	R	81	VAL	CA-CB	5.75	1.62	1.54
20	S	14	THR	CA-CB	5.65	1.61	1.53
14	M	32	VAL	CA-CB	5.62	1.60	1.54
2	X	660	A	O3'-P	5.36	1.69	1.61
5	C	136	THR	CA-CB	5.33	1.61	1.53
5	C	163	VAL	CA-CB	5.27	1.61	1.54
11	J	18	THR	CA-CB	5.16	1.61	1.53
24	W	12	VAL	CA-CB	-5.12	1.48	1.54
4	B	194	VAL	CA-CB	-5.11	1.48	1.54
10	I	54	GLN	CA-C	5.09	1.58	1.52
20	S	88	HIS	CA-C	5.08	1.59	1.52
18	Q	53	VAL	CA-C	5.06	1.59	1.52
7	E	54	ARG	CA-C	5.05	1.58	1.52
8	G	49	VAL	CA-CB	-5.02	1.46	1.54
8	G	122	LYS	CA-C	5.01	1.59	1.52

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	O	50	ALA	CA-C-N	-19.29	100.36	119.85
16	O	50	ALA	C-N-CA	-19.29	100.36	119.85
5	C	184	LEU	N-CA-C	10.59	122.91	111.36
8	G	46	THR	CA-C-N	10.29	130.59	119.28
8	G	46	THR	C-N-CA	10.29	130.59	119.28
10	I	51	GLU	N-CA-C	9.80	124.87	111.54
5	C	189	ALA	N-CA-C	-9.79	96.04	110.23
10	I	29	LYS	N-CA-C	-9.30	101.01	111.71
11	J	3	LEU	CA-C-N	9.26	131.41	119.84
11	J	3	LEU	C-N-CA	9.26	131.41	119.84
11	J	98	LYS	CA-C-N	9.24	131.39	119.84
11	J	98	LYS	C-N-CA	9.24	131.39	119.84
20	S	73	MET	N-CA-C	9.09	123.94	112.03
13	L	28	LYS	CA-C-N	8.89	128.82	119.85
13	L	28	LYS	C-N-CA	8.89	128.82	119.85
5	C	180	GLY	N-CA-C	-8.83	101.67	113.24
27	3	11	ALA	N-CA-C	-8.48	103.05	112.72
16	O	82	SER	N-CA-C	8.40	121.98	107.28
19	R	55	GLY	N-CA-C	-8.35	102.71	112.73
4	B	92	ARG	N-CA-C	-8.34	98.49	110.59
20	S	108	LEU	N-CA-C	8.31	118.05	108.49
1	A	135	ILE	CA-C-N	8.22	128.15	119.85
1	A	135	ILE	C-N-CA	8.22	128.15	119.85
20	S	104	VAL	N-CA-C	8.21	117.09	107.73
10	I	55	LEU	CA-C-N	-7.97	109.88	119.84
10	I	55	LEU	C-N-CA	-7.97	109.88	119.84
5	C	197	ALA	N-CA-C	-7.95	102.62	111.28
18	Q	49	LYS	N-CA-C	7.85	122.03	108.76
5	C	96	SER	N-CA-C	7.82	120.70	111.71
2	X	660	A	P-O3'-C3'	7.75	131.82	120.20
23	V	8	ASP	N-CA-C	-7.69	105.06	114.75
27	3	59	LYS	N-CA-C	-7.67	103.92	113.20
10	I	54	GLN	N-CA-C	7.65	120.96	108.26
5	C	159	GLU	N-CA-C	-7.58	103.02	111.28
10	I	7	LYS	CA-C-N	7.49	127.42	119.85
10	I	7	LYS	C-N-CA	7.49	127.42	119.85
4	B	204	PRO	N-CA-C	-7.34	97.35	112.47
5	C	192	LEU	N-CA-C	-7.33	103.23	111.07
10	I	47	ARG	N-CA-C	7.33	114.81	108.22
23	V	12	SER	N-CA-C	-7.26	106.35	114.62
14	M	14	GLN	N-CA-C	-7.25	105.61	114.75
5	C	183	VAL	N-CA-C	-7.22	103.61	113.00
10	I	39	LYS	N-CA-C	7.16	118.73	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	174	GLY	N-CA-C	7.14	124.67	115.32
20	S	41	VAL	N-CA-C	7.13	119.00	108.45
16	O	81	ASN	N-CA-C	6.98	120.48	109.39
8	G	70	GLU	N-CA-C	-6.91	103.76	111.71
4	B	64	LYS	N-CA-C	6.90	118.88	111.36
5	C	174	GLN	N-CA-C	-6.89	104.75	113.01
16	O	92	TYR	N-CA-C	6.86	117.33	108.34
13	L	90	LYS	N-CA-C	6.83	119.57	111.71
13	L	35	ARG	N-CA-C	6.83	119.74	111.40
18	Q	55	ILE	N-CA-C	6.83	117.36	108.35
27	3	43	GLN	N-CA-C	6.80	118.97	109.31
5	C	148	GLN	N-CA-C	6.78	114.23	108.13
21	T	22	ARG	N-CA-C	6.74	120.11	109.39
9	H	118	ALA	CA-C-N	6.73	128.25	119.84
9	H	118	ALA	C-N-CA	6.73	128.25	119.84
4	B	32	GLU	N-CA-C	6.72	120.93	111.52
9	H	92	GLY	CA-C-N	6.70	126.68	119.78
9	H	92	GLY	C-N-CA	6.70	126.68	119.78
18	Q	82	LEU	N-CA-C	6.66	120.37	109.72
4	B	122	SER	N-CA-C	6.66	120.13	107.75
20	S	49	ILE	N-CA-C	-6.59	103.90	110.62
11	J	94	ILE	N-CA-C	6.54	117.54	108.12
10	I	59	ARG	N-CA-C	6.52	118.46	108.42
1	A	196	GLY	N-CA-C	6.46	122.91	111.73
11	J	77	LYS	CA-C-N	6.45	126.43	119.78
11	J	77	LYS	C-N-CA	6.45	126.43	119.78
5	C	30	ASN	N-CA-C	6.44	118.38	111.36
20	S	30	VAL	CB-CA-C	-6.40	102.42	111.19
18	Q	53	VAL	N-CA-C	6.29	116.69	107.37
8	G	12	ILE	N-CA-C	6.27	116.63	108.35
9	H	38	VAL	CB-CA-C	-6.25	102.36	111.68
21	T	23	ASP	CB-CA-C	-6.19	108.81	117.23
16	O	17	GLY	N-CA-C	-6.14	105.63	115.08
19	R	39	ASN	N-CA-C	6.12	118.39	107.80
20	S	168	GLU	N-CA-C	6.09	117.57	108.31
1	A	195	VAL	N-CA-C	6.08	117.33	108.58
4	B	12	MET	N-CA-C	6.07	119.94	110.17
1	A	35	LYS	CA-C-N	6.05	127.40	119.84
1	A	35	LYS	C-N-CA	6.05	127.40	119.84
5	C	116	PHE	N-CA-C	-6.04	104.69	111.28
15	N	36	LYS	N-CA-C	-6.02	104.62	111.07
15	N	115	ASP	N-CA-C	-6.02	102.01	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	4	21	GLY	N-CA-C	-5.96	106.95	115.64
10	I	68	ASN	N-CA-C	5.94	118.34	109.25
16	O	5	ILE	N-CA-C	5.92	116.45	108.17
25	Z	3	VAL	CB-CA-C	-5.91	103.53	109.33
27	3	44	LEU	CA-CB-CG	5.85	136.76	116.30
10	I	37	GLY	N-CA-C	-5.82	99.39	113.18
27	3	22	LEU	N-CA-C	5.80	118.67	109.50
15	N	92	ARG	N-CA-C	-5.80	100.72	109.60
4	B	98	ALA	N-CA-C	-5.79	101.27	109.96
11	J	129	THR	N-CA-C	5.78	117.86	109.07
5	C	141	ASN	N-CA-C	-5.77	106.01	113.16
8	G	110	LEU	CA-C-N	5.76	125.69	119.76
8	G	110	LEU	C-N-CA	5.76	125.69	119.76
26	2	7	GLN	CA-C-N	5.74	125.64	119.85
26	2	7	GLN	C-N-CA	5.74	125.64	119.85
5	C	167	ALA	N-CA-C	5.74	119.54	112.54
14	M	7	ILE	CB-CA-C	-5.71	104.66	111.97
14	M	99	LEU	N-CA-C	5.67	120.01	113.38
11	J	72	THR	CA-C-N	5.64	125.57	119.76
11	J	72	THR	C-N-CA	5.64	125.57	119.76
10	I	57	LEU	N-CA-C	5.64	118.41	109.50
1	A	129	ALA	N-CA-C	5.63	118.81	110.48
5	C	121	ASN	N-CA-C	5.61	118.59	109.06
11	J	83	MET	N-CA-C	5.60	119.74	113.02
19	R	23	VAL	N-CA-C	5.59	116.79	108.23
11	J	25	ASN	N-CA-C	5.58	122.69	110.80
15	N	34	VAL	CB-CA-C	-5.57	104.83	111.97
22	U	14	THR	CB-CA-C	-5.57	108.54	116.34
10	I	43	GLY	N-CA-C	-5.57	105.64	112.77
5	C	27	GLU	CA-C-N	5.56	125.49	119.76
5	C	27	GLU	C-N-CA	5.56	125.49	119.76
4	B	101	VAL	N-CA-C	5.54	116.28	110.62
8	G	118	LYS	N-CA-C	-5.54	105.24	111.28
11	J	9	TYR	N-CA-C	5.54	122.60	110.80
25	Z	16	ARG	N-CA-C	-5.54	105.34	111.71
15	N	11	ARG	N-CA-C	-5.53	105.35	111.71
6	D	108	LEU	CA-C-N	5.53	126.75	119.84
6	D	108	LEU	C-N-CA	5.53	126.75	119.84
5	C	84	ARG	N-CA-C	-5.50	101.91	110.10
4	B	16	PHE	N-CA-C	5.49	117.92	109.07
2	X	627	C	O5'-P-OP2	-5.48	91.57	108.00
2	X	1568	U	P-O3'-C3'	5.43	128.35	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	95	ARG	N-CA-C	5.43	116.40	108.14
14	M	54	GLY	N-CA-C	5.43	126.05	113.18
4	B	47	ASN	N-CA-C	5.43	117.81	109.07
2	X	70	G	N9-C1'-C2'	5.37	120.06	112.00
10	I	53	GLY	N-CA-C	-5.35	107.22	115.73
11	J	23	GLY	N-CA-C	-5.35	108.32	115.32
27	3	50	VAL	N-CA-C	-5.34	104.57	112.04
5	C	133	ALA	CA-C-N	5.33	126.50	119.84
5	C	133	ALA	C-N-CA	5.33	126.50	119.84
4	B	155	GLY	N-CA-C	5.33	119.72	111.08
5	C	67	GLN	N-CA-C	5.32	117.08	111.28
4	B	128	GLN	N-CA-C	5.31	117.90	109.50
20	S	16	SER	N-CA-C	-5.31	105.50	112.41
16	O	28	ASN	N-CA-C	5.30	117.52	110.53
8	G	99	GLU	N-CA-C	-5.29	105.51	111.28
27	3	24	ARG	N-CA-C	5.28	118.06	109.24
18	Q	12	ILE	N-CA-C	5.27	115.67	107.28
4	B	43	VAL	CB-CA-C	-5.26	105.59	111.80
7	E	152	ARG	CA-C-N	-5.26	114.96	120.38
7	E	152	ARG	C-N-CA	-5.26	114.96	120.38
27	3	3	LYS	N-CA-C	-5.25	102.51	110.28
4	B	23	ILE	N-CA-C	5.24	113.21	107.60
2	X	1568	U	C2'-C3'-O3'	5.23	117.35	109.50
4	B	160	ALA	N-CA-C	-5.22	100.28	108.63
1	A	12	GLY	N-CA-C	-5.22	105.07	112.37
16	O	6	GLU	N-CA-C	-5.21	102.57	110.28
20	S	18	LEU	N-CA-C	-5.21	106.76	113.01
25	Z	8	THR	N-CA-C	5.21	117.99	110.28
17	P	13	ALA	CA-C-N	5.19	124.99	119.28
17	P	13	ALA	C-N-CA	5.19	124.99	119.28
4	B	205	LYS	N-CA-C	-5.16	101.24	109.23
26	2	15	LYS	N-CA-C	-5.16	103.72	110.53
15	N	28	LYS	N-CA-C	-5.15	106.83	113.01
10	I	95	LEU	N-CA-C	5.15	117.76	107.62
24	W	56	VAL	N-CA-C	5.12	116.65	108.87
4	B	63	ALA	N-CA-C	5.12	115.80	108.74
7	E	173	GLU	N-CA-C	5.12	117.09	108.96
13	L	81	ALA	N-CA-C	-5.12	105.70	111.28
15	N	66	ASN	N-CA-C	-5.11	105.60	111.07
4	B	20	GLY	N-CA-C	-5.10	108.57	115.36
5	C	162	ASN	CA-C-N	5.09	128.02	120.74
5	C	162	ASN	C-N-CA	5.09	128.02	120.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	H	110	ASN	N-CA-C	5.08	118.78	112.58
4	B	118	VAL	N-CA-C	5.08	115.77	107.24
6	D	68	THR	N-CA-C	5.08	116.62	111.14
25	Z	8	THR	CB-CA-C	-5.08	100.97	109.65
4	B	157	ALA	CA-C-O	5.07	120.88	117.94
8	G	14	ARG	N-CA-C	5.07	117.17	107.75
4	B	65	SER	N-CA-C	5.05	117.37	110.55
14	M	44	VAL	N-CA-C	5.05	116.55	108.87
17	P	44	SER	CA-C-N	-5.05	113.45	119.05
17	P	44	SER	C-N-CA	-5.05	113.45	119.05
8	G	47	PRO	N-CA-C	5.01	120.42	113.65
4	B	163	VAL	N-CA-C	-5.01	101.15	108.17
8	G	136	GLN	N-CA-C	-5.01	107.12	113.18

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	3	10	ALA	Peptide
27	3	17	THR	Peptide
1	A	77	LYS	Peptide
4	B	104	GLU	Peptide
4	B	57	LYS	Peptide
5	C	161	VAL	Peptide
5	C	27	GLU	Peptide
10	I	35	HIS	Peptide
16	O	80	LYS	Peptide
17	P	70	VAL	Peptide
20	S	17	ASP	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	A	1667	0	1292	50	0
2	X	57983	0	29161	924	0
3	Y	2430	0	1229	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1547	0	1514	68	0
5	C	1324	0	1175	62	0
6	D	853	0	444	7	0
7	E	915	0	648	24	0
8	G	1090	0	1034	51	0
9	H	884	0	902	45	0
10	I	819	0	687	45	0
11	J	1001	0	971	37	0
12	K	906	0	930	37	0
13	L	673	0	538	20	0
14	M	807	0	803	32	0
15	N	922	0	973	63	0
16	O	751	0	743	23	0
17	P	853	0	900	31	0
18	Q	583	0	472	21	0
19	R	627	0	510	24	0
20	S	1087	0	934	26	0
21	T	559	0	569	24	0
22	U	242	0	141	5	0
23	V	486	0	469	11	0
24	W	437	0	467	25	0
25	Z	339	0	350	24	0
26	2	350	0	383	12	0
27	3	405	0	363	20	0
28	4	181	0	76	5	0
29	A	1	0	0	0	0
29	R	1	0	0	0	0
29	T	1	0	0	0	0
29	X	268	0	0	0	0
29	Y	2	0	0	0	0
29	Z	1	0	0	0	0
30	A	3	0	0	0	0
30	C	2	0	0	0	0
30	G	2	0	0	0	0
30	I	1	0	0	0	0
30	J	1	0	0	0	0
30	M	1	0	0	0	0
30	O	1	0	0	0	0
30	P	1	0	0	0	0
30	X	218	0	0	0	0
30	Y	10	0	0	0	0
31	X	35	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	J	8	0	14	1	0
32	Q	8	0	14	0	0
32	X	64	0	112	7	0
32	Z	8	0	14	0	0
33	X	70	0	133	9	0
33	Y	10	0	19	1	0
34	S	3	0	6	0	0
34	X	6	0	12	0	0
35	N	15	0	17	17	0
All	All	81462	0	49019	1593	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 13.

All (1593) 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)
19:R:11:VAL:HA	19:R:67:ASN:HB2	1.48	0.96
2:X:956:A:H2'	11:J:11:ARG:HH11	1.30	0.96
2:X:83:G:H21	2:X:102:A:H2	1.15	0.93
4:B:124:GLY:HA2	4:B:174:GLY:HA3	1.53	0.91
3:Y:21:G:H1	3:Y:58:G:H1	1.08	0.91
2:X:498:G:H21	2:X:503:A:H8	1.19	0.90
23:V:10:THR:O	23:V:12:SER:N	2.05	0.89
8:G:65:PHE:HB3	8:G:69:LYS:HD3	1.55	0.89
10:I:57:LEU:HD11	27:3:12:LYS:CB	2.03	0.88
2:X:304:G:H1	2:X:413:C:H42	1.18	0.87
2:X:2775:A:H1'	7:E:67:THR:HG22	1.54	0.87
13:L:45:ILE:HG23	13:L:52:THR:HB	1.55	0.87
9:H:31:LYS:HG3	9:H:32:THR:HG22	1.54	0.87
3:Y:15:C:H42	3:Y:105:G:H21	1.17	0.87
2:X:1290:G:OP2	15:N:13:ARG:NH2	2.07	0.86
15:N:10:THR:HG21	35:N:201:EPE:H32	1.58	0.86
2:X:1063:U:H3	2:X:1186:A:H62	1.24	0.85
2:X:657:U:O4	2:X:659:A:N6	2.10	0.85
2:X:501:C:H3'	2:X:502:C:H5''	1.59	0.84
5:C:113:ALA:HB1	5:C:181:LEU:HD22	1.61	0.83
2:X:591:A:H4'	2:X:592:A:H5'	1.59	0.82
2:X:2649:U:O2'	2:X:2845:G:N2	2.13	0.82
2:X:1460:U:H3	2:X:1628:A:H61	1.24	0.82
9:H:101:PRO:HD3	14:M:68:SER:HB2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:63:VAL:HG21	9:H:102:VAL:HG22	1.62	0.81
11:J:116:GLU:OE1	11:J:119:ARG:NH1	2.13	0.81
1:A:89:ALA:HB2	1:A:158:ALA:HA	1.63	0.81
15:N:61:TRP:CE2	15:N:93:LYS:HB2	2.16	0.80
2:X:627:C:OP2	35:N:201:EPE:H61	1.82	0.80
6:D:101:ASP:HA	6:D:130:LEU:HD11	1.62	0.80
2:X:1605:A:H1'	32:X:3004:MPD:HM1	1.64	0.80
2:X:1487:G:H1	2:X:1597:U:H3	1.27	0.79
2:X:2419:A:H2	2:X:2451:C:H42	1.28	0.79
3:Y:15:C:N4	3:Y:105:G:H21	1.81	0.79
5:C:147:GLU:HA	5:C:167:ALA:HB1	1.64	0.79
3:Y:77:G:H1	3:Y:94:U:H3	1.28	0.79
14:M:24:PRO:HA	14:M:49:VAL:HB	1.63	0.79
20:S:81:PRO:O	20:S:83:LYS:N	2.16	0.79
5:C:8:LYS:HZ2	5:C:8:LYS:HB2	1.48	0.78
25:Z:15:LYS:O	25:Z:18:THR:HG23	1.83	0.78
2:X:2382:C:O2	2:X:2389:G:N2	2.16	0.78
2:X:1302:G:OP1	25:Z:16:ARG:NH2	2.15	0.78
2:X:1467:G:O2'	2:X:1543:G:O2'	2.02	0.78
14:M:106:ARG:CZ	14:M:106:ARG:HA	2.13	0.78
2:X:1952:C:N3	2:X:1956:G:N2	2.30	0.77
12:K:105:LYS:HA	12:K:117:VAL:HG12	1.66	0.77
2:X:2850:G:H5'	4:B:67:LYS:HE3	1.63	0.77
8:G:57:VAL:HB	8:G:125:VAL:HG13	1.65	0.77
11:J:135:GLU:OE2	32:J:201:MPD:O4	2.01	0.77
2:X:1876:G:N2	2:X:1920:C:O2	2.18	0.77
2:X:2470:C:H2'	2:X:2471:G:H8	1.50	0.77
8:G:14:ARG:NH1	8:G:50:ASP:O	2.17	0.77
5:C:108:LEU:O	5:C:112:SER:OG	2.02	0.77
26:2:36:ARG:HG3	26:2:43:LEU:HD21	1.66	0.77
2:X:1894:G:O6	2:X:1902:G:N2	2.17	0.77
17:P:21:LEU:HD22	17:P:74:ALA:HB1	1.67	0.77
15:N:10:THR:HG23	35:N:201:EPE:H71	1.65	0.76
2:X:1726:A:H61	2:X:1750:U:H3	1.33	0.76
15:N:27:SER:HA	15:N:30:THR:HG23	1.67	0.76
2:X:1289:A:OP1	15:N:13:ARG:NH1	2.19	0.76
2:X:1796:A:O2'	2:X:1985:C:OP1	2.03	0.76
3:Y:15:C:H42	3:Y:105:G:N2	1.83	0.75
3:Y:79:C:H42	3:Y:92:G:H1	1.33	0.75
8:G:7:ALA:H	8:G:46:THR:HG21	1.48	0.75
5:C:31:SER:HB3	10:I:9:ALA:HB2	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:272:C:N3	2:X:416:G:N2	2.33	0.75
2:X:1346:G:H4'	26:2:8:PRO:HG2	1.69	0.75
9:H:4:GLN:HG2	9:H:5:GLU:HG2	1.66	0.75
24:W:40:ASN:HB3	24:W:43:ILE:H	1.52	0.75
1:A:78:VAL:HG12	1:A:79:ASP:H	1.52	0.74
5:C:61:GLY:HA2	5:C:77:THR:HG23	1.68	0.74
2:X:589:U:O4	2:X:592:A:N6	2.19	0.74
2:X:1472:C:N4	2:X:1617:A:OP2	2.19	0.74
2:X:2860:U:H5''	12:K:49:THR:HG21	1.70	0.74
2:X:2331:G:H22	2:X:2339:U:H3	1.36	0.74
14:M:102:LEU:O	14:M:103:ARG:NH2	2.21	0.74
2:X:2761:C:H41	2:X:2797:C:H6	1.32	0.74
1:A:171:TYR:OH	2:X:2250:A:OP1	2.05	0.73
2:X:629:A:H62	2:X:1289:A:H2	1.33	0.73
2:X:1501:G:H2'	2:X:1502:A:H8	1.52	0.73
3:Y:18:G:H1	3:Y:61:U:H3	1.35	0.73
2:X:864:A:OP2	2:X:1226:G:N2	2.17	0.73
2:X:1501:G:H22	2:X:2729:G:H22	1.36	0.73
2:X:903:G:OP2	21:T:85:LYS:NZ	2.22	0.73
2:X:683:G:C6	2:X:696:G:C6	2.77	0.73
2:X:995:U:OP1	33:Y:213:SPD:N1	2.22	0.72
2:X:1400:C:O2'	2:X:1836:A:H1'	1.90	0.72
2:X:1013:U:O3'	24:W:14:GLY:HA2	1.88	0.72
4:B:53:PHE:HB3	4:B:87:PHE:HB2	1.72	0.72
2:X:1711:G:N2	2:X:2020:U:O4	2.18	0.71
2:X:1490:G:O2'	2:X:1491:C:O5'	2.07	0.71
2:X:229:A:O2'	2:X:231:A:N1	2.22	0.71
2:X:1881:A:H62	2:X:1915:G:H8	1.38	0.71
1:A:183:MET:HE2	1:A:269:LEU:HA	1.73	0.71
2:X:1810:A:H5'	2:X:2635:G:H4'	1.73	0.71
4:B:10:ILE:HD12	14:M:6:LEU:HD22	1.71	0.71
2:X:2007:G:O2'	2:X:2009:U:OP2	2.05	0.70
7:E:133:VAL:HG11	7:E:141:VAL:HG13	1.71	0.70
2:X:1293:U:H5''	2:X:1294:G:H5''	1.73	0.70
2:X:659:A:H1'	2:X:660:A:H5'	1.73	0.70
2:X:1487:G:N2	2:X:1597:U:O2	2.24	0.70
18:Q:57:ASN:O	18:Q:58:TYR:HD1	1.74	0.70
2:X:460:C:O2	2:X:1891:U:O2'	2.09	0.70
2:X:1185:U:OP2	8:G:66:THR:OG1	2.05	0.70
3:Y:38:U:O2'	3:Y:43:A:N6	2.25	0.70
2:X:956:A:C6	11:J:11:ARG:HD2	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:44:THR:O	8:G:44:THR:OG1	2.01	0.70
2:X:788:A:O2'	2:X:1703:U:OP1	2.09	0.69
2:X:2604:A:H5''	2:X:2605:G:H5'	1.75	0.69
5:C:158:ASN:HA	5:C:161:VAL:HG22	1.75	0.69
2:X:164:A:H1'	2:X:165:C:H5'	1.74	0.68
2:X:634:C:HO2'	27:3:2:PRO:N	1.91	0.68
11:J:69:PHE:HB3	11:J:71:HIS:CE1	2.27	0.68
2:X:1261:G:OP1	16:O:67:ARG:NH2	2.26	0.68
5:C:14:SER:OG	5:C:15:GLY:N	2.22	0.68
13:L:73:ALA:HB1	13:L:107:ALA:HB2	1.72	0.68
5:C:43:SER:HA	5:C:98:ALA:HB2	1.75	0.68
1:A:224:VAL:HG11	2:X:1815:C:H5''	1.76	0.68
2:X:1063:U:H3	2:X:1186:A:N6	1.90	0.68
2:X:1494:G:C8	2:X:1495:C:H5	2.11	0.68
2:X:878:C:H2'	2:X:879:U:C6	2.28	0.68
2:X:2290:C:OP2	21:T:27:LYS:NZ	2.25	0.68
9:H:51:VAL:HG12	9:H:94:ARG:HH21	1.58	0.68
2:X:1460:U:H3	2:X:1628:A:N6	1.92	0.68
4:B:38:LYS:NZ	4:B:96:VAL:O	2.19	0.68
3:Y:31:G:H1	3:Y:47:C:H42	1.38	0.68
18:Q:55:ILE:HG13	18:Q:78:ALA:HB2	1.76	0.68
2:X:2314:A:O2'	2:X:2315:A:H2'	1.93	0.68
4:B:156:MET:HB2	4:B:160:ALA:HB3	1.75	0.68
13:L:36:SER:OG	13:L:37:ASN:N	2.24	0.68
2:X:715:A:H4'	2:X:716:C:H5'	1.74	0.67
2:X:2906:G:C2	25:Z:39:LEU:HD21	2.29	0.67
2:X:878:C:H1'	10:I:48:PRO:HB3	1.76	0.67
2:X:2101:U:H2'	2:X:2102:U:C6	2.28	0.67
2:X:2707:C:H5'	4:B:202:PRO:HA	1.76	0.67
1:A:78:VAL:HA	1:A:94:VAL:HA	1.76	0.67
3:Y:46:A:OP1	13:L:35:ARG:NH1	2.27	0.67
5:C:136:THR:HG22	5:C:140:LYS:NZ	2.10	0.67
2:X:321:U:O2'	2:X:322:A:OP2	2.13	0.67
2:X:2334:G:O2'	2:X:2337:A:N6	2.21	0.67
11:J:40:SER:OG	11:J:41:TRP:N	2.27	0.67
12:K:105:LYS:HB2	25:Z:41:HIS:HA	1.75	0.67
2:X:1826:G:N2	2:X:1845:U:O2'	2.27	0.66
2:X:2672:G:O6	33:X:3493:SPD:H81	1.95	0.66
2:X:1518:G:H1	2:X:1562:C:H42	1.42	0.66
19:R:72:ASP:OD1	19:R:72:ASP:N	2.29	0.66
2:X:2805:A:O2'	2:X:2807:G:O2'	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:LYS:O	1:A:37:LEU:N	2.27	0.66
4:B:192:ASN:HB2	4:B:194:VAL:HG23	1.77	0.66
18:Q:49:LYS:HD3	18:Q:50:VAL:HG12	1.78	0.66
2:X:183:A:H5'	2:X:481:C:H1'	1.77	0.66
15:N:80:MET:HE1	15:N:95:LEU:HD23	1.78	0.66
2:X:1683:U:H2'	2:X:1684:A:H5''	1.76	0.65
9:H:75:SER:OG	14:M:74:ARG:NH2	2.27	0.65
2:X:1835:U:H2'	2:X:1836:A:H5''	1.79	0.65
1:A:217:ARG:NH1	2:X:736:C:OP1	2.29	0.65
2:X:1501:G:H2'	2:X:1502:A:C8	2.32	0.65
18:Q:50:VAL:HG13	18:Q:51:ALA:H	1.61	0.65
2:X:280:C:H2'	2:X:281:A:H8	1.62	0.65
3:Y:80:A:H61	3:Y:91:C:H42	1.45	0.65
19:R:80:ARG:NH2	19:R:96:LYS:HA	2.12	0.65
14:M:102:LEU:O	14:M:103:ARG:CZ	2.45	0.65
26:2:16:VAL:H	26:2:21:LYS:HG2	1.62	0.65
8:G:18:VAL:HG23	8:G:140:ASN:HA	1.78	0.65
2:X:718:C:H5''	5:C:81:PRO:HD2	1.79	0.65
2:X:1710:G:O3'	9:H:6:THR:HG23	1.96	0.64
2:X:2817:A:O2'	2:X:2818:A:OP2	2.14	0.64
15:N:93:LYS:O	15:N:97:GLU:N	2.22	0.64
15:N:29:HIS:CD2	15:N:30:THR:HG22	2.33	0.64
2:X:1313:G:OP2	2:X:1689:G:O2'	2.16	0.64
3:Y:21:G:H22	3:Y:58:G:N2	1.95	0.64
1:A:78:VAL:O	1:A:95:VAL:HG12	1.98	0.64
3:Y:4:G:H1	3:Y:111:A:H62	1.46	0.64
2:X:503:A:H2	2:X:517:A:H62	1.44	0.64
2:X:1041:G:H5''	15:N:92:ARG:HH12	1.63	0.64
2:X:1723:A:H2	2:X:1791:G:C8	2.16	0.64
12:K:8:ARG:O	12:K:13:ARG:NH1	2.31	0.64
1:A:60:ARG:HD3	1:A:85:PRO:HB2	1.80	0.64
2:X:630:G:C6	10:I:30:THR:HG21	2.33	0.64
2:X:2682:G:HO2'	2:X:2691:G:H1	1.45	0.64
17:P:20:VAL:HA	17:P:23:LEU:HD12	1.79	0.64
21:T:54:TYR:HD2	21:T:80:LYS:HE3	1.63	0.64
1:A:107:PRO:HA	1:A:196:GLY:H	1.63	0.63
11:J:18:THR:OG1	11:J:19:GLY:N	2.32	0.63
1:A:15:ASN:O	1:A:204:ASN:ND2	2.31	0.63
2:X:876:G:O2'	10:I:36:LYS:HD2	1.97	0.63
2:X:78:U:H2'	2:X:79:U:C6	2.32	0.63
2:X:1663:G:HO2'	26:2:2:VAL:N	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:679:G:H2'	2:X:680:C:C6	2.34	0.63
20:S:75:ALA:HB2	20:S:92:LEU:HB2	1.80	0.63
1:A:209:GLY:HA2	1:A:212:ARG:HB2	1.80	0.63
2:X:2646:U:O2	4:B:169:MET:HE1	1.97	0.63
3:Y:46:A:P	13:L:35:ARG:HH12	2.22	0.63
2:X:1805:U:H2'	2:X:1811:A:H62	1.64	0.63
2:X:418:G:O2'	2:X:419:U:OP2	2.17	0.63
2:X:1089:C:O2	2:X:1091:G:N1	2.31	0.63
2:X:621:A:O2'	2:X:623:C:OP2	2.15	0.63
25:Z:38:LYS:H	25:Z:38:LYS:HZ2	1.46	0.63
2:X:1037:A:OP1	15:N:50:ARG:NH1	2.32	0.62
2:X:1526:G:N2	2:X:1550:G:H1	1.96	0.62
7:E:136:ILE:HD12	7:E:137:SER:H	1.63	0.62
8:G:14:ARG:HG2	8:G:52:GLY:O	1.99	0.62
20:S:28:PRO:O	20:S:88:HIS:HA	2.00	0.62
2:X:268:A:N6	2:X:473:U:O2'	2.32	0.62
5:C:103:LYS:HA	5:C:106:ARG:NE	2.15	0.62
24:W:5:GLN:HG3	24:W:36:VAL:HG22	1.81	0.62
2:X:956:A:H2'	11:J:11:ARG:NH1	2.10	0.62
2:X:1887:G:H22	2:X:1910:G:H1'	1.63	0.62
2:X:2553:G:O2'	28:4:1:MET:N	2.32	0.62
5:C:149:PRO:HD2	5:C:187:THR:HA	1.82	0.62
18:Q:28:ASP:HA	18:Q:77:LYS:HA	1.80	0.62
2:X:1875:A:H2'	2:X:1876:G:C8	2.34	0.62
3:Y:6:U:OP1	13:L:11:ARG:NH2	2.32	0.62
11:J:69:PHE:HB3	11:J:71:HIS:HE1	1.64	0.62
9:H:88:ARG:O	9:H:90:ASP:N	2.33	0.62
2:X:817:G:H2'	2:X:818:U:H6	1.64	0.62
2:X:1836:A:O2'	2:X:1837:A:O4'	2.17	0.62
2:X:1492:G:O2'	2:X:1574:G:N2	2.32	0.62
1:A:59:LYS:HG2	2:X:1615:G:H4'	1.81	0.61
2:X:501:C:H3'	2:X:502:C:C5'	2.29	0.61
1:A:145:GLU:HA	1:A:152:GLY:HA2	1.82	0.61
2:X:2848:G:H2'	2:X:2849:A:H8	1.63	0.61
2:X:1515:G:O2'	2:X:1516:C:O5'	2.16	0.61
10:I:128:PHE:HD1	10:I:129:SER:H	1.48	0.61
5:C:50:ALA:HB2	5:C:94:PRO:HD3	1.83	0.61
2:X:1332:C:H4'	12:K:67:ARG:NH2	2.16	0.61
2:X:1599:G:OP1	2:X:1761:G:N2	2.28	0.61
2:X:2050:A:H5'	2:X:2644:C:H4'	1.83	0.61
4:B:26:THR:HG21	4:B:201:VAL:HG12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:92:ARG:O	15:N:93:LYS:HB3	1.98	0.61
2:X:2470:C:H2'	2:X:2471:G:C8	2.33	0.61
15:N:9:VAL:HG23	15:N:10:THR:HG23	1.82	0.61
4:B:140:PRO:HG2	4:B:145:SER:HB2	1.83	0.61
15:N:59:LYS:O	15:N:63:THR:HG23	2.01	0.61
2:X:1515:G:H22	2:X:1565:U:H3	1.48	0.61
28:4:14:CYS:HA	28:4:27:CYS:HA	1.82	0.61
4:B:8:ARG:NH2	4:B:54:GLU:OE2	2.33	0.60
2:X:124:A:OP2	26:2:20:ARG:HD3	2.01	0.60
7:E:18:THR:N	7:E:32:GLU:OE2	2.34	0.60
2:X:609:U:O4	16:O:79:ARG:HD3	2.01	0.60
2:X:1041:G:OP1	15:N:92:ARG:HG2	2.01	0.60
2:X:661:U:H1'	2:X:662:G:C8	2.37	0.60
3:Y:79:C:N4	3:Y:92:G:H1	1.99	0.60
8:G:4:THR:HG23	15:N:61:TRP:CZ3	2.36	0.60
9:H:15:GLY:HA3	9:H:50:GLY:HA3	1.84	0.60
2:X:1065:A:H2'	2:X:1067:U:H5'	1.82	0.60
25:Z:28:THR:HG23	25:Z:37:TYR:CE1	2.37	0.60
4:B:95:ASP:O	4:B:97:ASP:N	2.31	0.60
8:G:113:THR:O	8:G:116:GLY:N	2.33	0.60
16:O:22:VAL:HG22	16:O:23:GLU:H	1.66	0.60
20:S:72:VAL:HG12	20:S:93:ALA:HA	1.83	0.60
3:Y:74:G:H22	3:Y:97:A:H61	1.47	0.60
14:M:105:LEU:O	14:M:106:ARG:NH1	2.35	0.60
2:X:528:C:H5''	2:X:529:A:OP1	2.01	0.60
2:X:1773:A:H2'	2:X:1774:A:H8	1.66	0.60
1:A:243:ARG:HD3	1:A:247:MET:HE1	1.82	0.59
2:X:329:A:N6	2:X:398:C:H42	1.99	0.59
2:X:665:G:H4'	2:X:666:A:H5''	1.82	0.59
2:X:1512:U:H2'	2:X:1513:A:C8	2.37	0.59
2:X:1886:A:N6	2:X:1910:G:O2'	2.35	0.59
2:X:460:C:H2'	2:X:461:A:C8	2.38	0.59
2:X:125:A:N7	2:X:126:A:C6	2.71	0.59
2:X:107:G:H2'	2:X:108:A:H8	1.67	0.59
2:X:630:G:P	10:I:21:ARG:HH22	2.24	0.59
2:X:1147:A:H2'	2:X:1148:C:O4'	2.02	0.59
2:X:1836:A:H2'	2:X:1837:A:C8	2.37	0.59
2:X:2549:U:O2'	2:X:2674:U:OP1	2.20	0.59
2:X:424:C:H2'	2:X:425:G:C8	2.37	0.59
2:X:1487:G:N2	2:X:1597:U:C2	2.71	0.59
2:X:1793:C:H2'	2:X:1794:C:H6	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:338:G:H2'	2:X:339:A:H8	1.67	0.59
2:X:999:U:H5''	11:J:87:LYS:HD2	1.85	0.59
2:X:1362:C:OP1	2:X:1691:G:O2'	2.18	0.59
2:X:1488:A:N6	2:X:1595:C:H42	2.00	0.59
2:X:1916:A:H1'	2:X:2114:G:H5'	1.85	0.59
3:Y:113:G:H2'	3:Y:114:C:H5'	1.85	0.59
11:J:134:ARG:HH12	20:S:123:GLN:CD	2.11	0.59
4:B:100:GLU:O	4:B:103:GLN:HG2	2.02	0.59
2:X:1150:A:H4'	2:X:1150:A:OP1	2.01	0.59
2:X:1440:A:HO2'	2:X:1514:A:HO2'	1.40	0.59
2:X:1513:A:H3'	2:X:1514:A:H8	1.67	0.59
5:C:102:PRO:HB2	5:C:105:MET:HG3	1.83	0.59
15:N:10:THR:CG2	35:N:201:EPE:H71	2.32	0.59
16:O:42:GLY:HA2	16:O:46:VAL:HG12	1.85	0.59
2:X:1415:A:O2'	2:X:1417:G:N7	2.30	0.59
5:C:150:LYS:HA	5:C:188:ASN:OD1	2.02	0.59
8:G:136:GLN:N	8:G:136:GLN:OE1	2.35	0.59
16:O:2:PHE:CE1	16:O:42:GLY:HA3	2.38	0.58
2:X:904:G:O2'	2:X:961:G:O6	2.15	0.58
2:X:2120:G:H21	2:X:2225:A:N6	2.00	0.58
2:X:1422:A:O2'	2:X:1423:C:O5'	2.21	0.58
9:H:87:ILE:HG12	9:H:88:ARG:H	1.69	0.58
24:W:50:VAL:HB	24:W:53:LEU:HD11	1.85	0.58
2:X:3:U:H2'	2:X:4:U:C6	2.38	0.58
4:B:111:VAL:O	4:B:114:ASP:HB2	2.02	0.58
11:J:34:LEU:HB2	11:J:118:LEU:HD13	1.85	0.58
22:U:43:LYS:O	22:U:45:LYS:N	2.36	0.58
25:Z:38:LYS:H	25:Z:38:LYS:NZ	2.00	0.58
2:X:268:A:O2'	2:X:269:G:H4'	2.04	0.58
2:X:1507:A:H2'	2:X:1508:C:H5'	1.85	0.58
2:X:90:A:H8	2:X:90:A:OP1	1.86	0.58
2:X:355:G:O2'	33:X:3498:SPD:H72	2.04	0.58
2:X:1180:G:H1'	2:X:2065:G:H4'	1.86	0.58
2:X:2495:A:O2'	2:X:2496:A:H8	1.87	0.58
2:X:994:A:H5''	3:Y:85:A:N6	2.19	0.58
2:X:1875:A:H2'	2:X:1876:G:H8	1.68	0.58
2:X:2465:U:O2'	2:X:2466:A:H5''	2.03	0.58
9:H:13:ASN:CG	9:H:96:THR:H	2.11	0.58
14:M:83:ILE:HD13	14:M:86:ILE:HD11	1.84	0.58
12:K:27:SER:O	12:K:29:ARG:N	2.37	0.58
2:X:95:A:H5'	2:X:96:G:OP2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:59:TYR:O	4:B:61:LYS:N	2.37	0.58
7:E:74:ASN:O	7:E:83:TYR:OH	2.21	0.58
10:I:57:LEU:HD21	27:3:11:ALA:HB3	1.86	0.58
17:P:7:ALA:HB1	17:P:10:ILE:HD11	1.85	0.58
2:X:187:C:H2'	2:X:188:C:H6	1.69	0.57
2:X:1492:G:N7	2:X:1493:U:H5	2.01	0.57
21:T:57:GLU:HB2	21:T:88:SER:HB3	1.86	0.57
2:X:1300:G:OP2	17:P:99:ARG:NH2	2.37	0.57
2:X:1628:A:H4'	2:X:1628:A:OP1	2.02	0.57
2:X:2331:G:N2	2:X:2339:U:H3	2.02	0.57
12:K:24:LEU:HG	12:K:121:LEU:HD23	1.86	0.57
2:X:133:A:H61	2:X:146:U:H3	1.52	0.57
2:X:1885:G:H1'	2:X:1911:A:H62	1.69	0.57
9:H:98:ILE:HB	9:H:118:ALA:HA	1.86	0.57
2:X:83:G:H1	2:X:101:G:HO2'	1.53	0.57
2:X:318:A:C6	2:X:319:G:H1'	2.38	0.57
2:X:418:G:O2'	2:X:446:G:N1	2.34	0.57
16:O:74:PHE:HE1	16:O:83:LYS:HB2	1.68	0.57
2:X:811:C:H2'	2:X:812:U:H5'	1.85	0.57
2:X:1821:U:H2'	2:X:1822:C:H6	1.70	0.57
2:X:1998:A:O2'	2:X:1999:G:OP1	2.22	0.57
2:X:2843:A:OP1	4:B:127:PHE:HB2	2.04	0.57
8:G:39:GLY:C	8:G:41:ASN:H	2.12	0.57
16:O:98:ASP:OD1	16:O:98:ASP:N	2.38	0.57
2:X:498:G:N2	2:X:503:A:H8	1.96	0.57
2:X:506:A:N1	2:X:515:G:H8	2.02	0.57
17:P:71:VAL:HA	17:P:107:VAL:HA	1.86	0.57
18:Q:6:ILE:HG23	18:Q:33:VAL:HG11	1.87	0.57
19:R:4:LYS:HB3	19:R:4:LYS:HZ2	1.69	0.57
2:X:302:A:N6	2:X:450:C:C2	2.72	0.57
2:X:568:C:O2	2:X:597:U:O2'	2.21	0.57
7:E:25:THR:HG22	7:E:41:MET:HE3	1.86	0.57
20:S:98:GLU:HA	20:S:129:GLU:O	2.05	0.57
23:V:39:GLU:HG2	23:V:42:ARG:HE	1.70	0.57
1:A:156:ARG:N	2:X:1846:A:OP1	2.38	0.57
2:X:15:G:H4'	25:Z:18:THR:HB	1.85	0.57
2:X:2904:U:C5	25:Z:40:SER:HA	2.40	0.57
2:X:645:A:O2'	2:X:647:G:O2'	2.18	0.57
2:X:1498:U:HO2'	2:X:1499:U:H5	1.53	0.57
2:X:319:G:N7	2:X:400:C:N4	2.53	0.57
2:X:1353:A:H2'	2:X:1354:G:C8	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1780:G:OP1	14:M:95:ARG:HD2	2.05	0.57
8:G:4:THR:OG1	15:N:61:TRP:HH2	1.88	0.57
9:H:24:VAL:HB	9:H:30:ARG:HD2	1.87	0.57
24:W:39:ASP:OD2	24:W:44:ARG:NH2	2.37	0.57
2:X:529:A:H1'	19:R:55:GLY:HA2	1.87	0.56
2:X:2241:C:H2'	2:X:2242:G:O4'	2.05	0.56
2:X:2370:U:O2'	2:X:2400:U:O2'	2.22	0.56
14:M:26:ASP:O	14:M:49:VAL:HG23	2.05	0.56
15:N:6:GLY:O	35:N:201:EPE:H72	2.04	0.56
16:O:63:ASN:HD21	16:O:96:THR:HB	1.69	0.56
21:T:82:ARG:HH12	21:T:84:LYS:HG3	1.69	0.56
2:X:300:G:N2	2:X:302:A:N7	2.52	0.56
2:X:579:U:H5'	15:N:42:SER:OG	2.04	0.56
2:X:1563:U:H2'	2:X:1564:G:C8	2.40	0.56
2:X:2807:G:N1	8:G:103:GLU:OE1	2.34	0.56
17:P:70:VAL:O	17:P:71:VAL:O	2.23	0.56
2:X:311:U:H3	2:X:404:U:H3	1.54	0.56
2:X:342:A:N1	2:X:365:A:O2'	2.33	0.56
2:X:459:C:O2'	2:X:1907:U:O2'	2.23	0.56
2:X:1055:A:H5''	15:N:77:SER:HB2	1.87	0.56
2:X:2784:A:N1	7:E:67:THR:HG21	2.19	0.56
4:B:67:LYS:HA	4:B:86:ARG:NH2	2.19	0.56
7:E:113:VAL:HG21	7:E:151:VAL:HG11	1.87	0.56
19:R:23:VAL:HA	19:R:35:VAL:HA	1.86	0.56
2:X:2290:C:H4'	2:X:2356:A:H4'	1.88	0.56
11:J:40:SER:HB3	11:J:127:VAL:HG12	1.87	0.56
15:N:10:THR:CG2	35:N:201:EPE:H32	2.33	0.56
24:W:10:ARG:HG3	24:W:10:ARG:HH11	1.70	0.56
2:X:107:G:H2'	2:X:108:A:C8	2.41	0.56
7:E:102:ASP:H	7:E:115:ILE:HD13	1.71	0.56
9:H:63:VAL:HB	9:H:106:LEU:HD11	1.86	0.56
10:I:57:LEU:CD1	27:3:12:LYS:CB	2.80	0.56
10:I:95:LEU:H	10:I:112:LEU:HD23	1.71	0.56
2:X:1518:G:H1	2:X:1562:C:N4	2.03	0.56
2:X:2682:G:O2'	2:X:2683:U:OP2	2.22	0.56
15:N:38:GLN:O	15:N:42:SER:HB2	2.06	0.56
2:X:99:U:O2	2:X:101:G:N1	2.37	0.56
2:X:955:A:C4	11:J:15:PRO:HG3	2.40	0.56
2:X:2835:C:H1'	25:Z:39:LEU:HD22	1.88	0.56
11:J:43:THR:N	11:J:46:GLN:OE1	2.33	0.56
2:X:322:A:O2'	2:X:323:C:H5'	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:2507:C:H2'	2:X:2508:G:H5'	1.87	0.56
8:G:22:GLU:HA	8:G:62:LYS:HB2	1.88	0.56
5:C:135:LYS:O	5:C:139:PHE:N	2.39	0.56
27:3:24:ARG:HD2	27:3:42:ARG:O	2.06	0.56
2:X:657:U:C4	2:X:659:A:N6	2.74	0.56
2:X:2358:G:O2'	2:X:2363:A:N1	2.31	0.56
5:C:7:LEU:HD23	5:C:8:LYS:N	2.20	0.56
2:X:575:G:N3	2:X:575:G:H2'	2.21	0.55
2:X:715:A:H4'	2:X:716:C:C5'	2.36	0.55
2:X:2082:C:OP1	25:Z:5:LYS:NZ	2.38	0.55
2:X:2807:G:C8	32:X:3006:MPD:H13	2.40	0.55
2:X:2877:G:H5'	2:X:2878:U:OP2	2.07	0.55
1:A:65:ILE:HA	1:A:103:TYR:HB2	1.88	0.55
2:X:273:A:OP2	2:X:297:G:N2	2.29	0.55
2:X:638:U:H2'	2:X:639:U:C6	2.40	0.55
2:X:1405:G:H2'	2:X:1406:G:C8	2.41	0.55
2:X:2403:A:C5	13:L:96:ARG:HD2	2.41	0.55
17:P:55:LEU:HD23	17:P:69:LEU:HD12	1.88	0.55
2:X:2026:C:O2	2:X:2714:U:O2'	2.24	0.55
8:G:60:ALA:HB3	8:G:127:GLY:HA2	1.88	0.55
21:T:71:ILE:HD13	21:T:91:ALA:HB2	1.89	0.55
2:X:1053:A:OP2	8:G:40:LYS:NZ	2.35	0.55
2:X:1758:A:N1	2:X:1759:G:N2	2.54	0.55
4:B:128:GLN:HB2	4:B:173:MET:HG3	1.88	0.55
7:E:62:ARG:HA	7:E:65:HIS:HD2	1.72	0.55
2:X:135:G:H1	2:X:144:C:H42	1.53	0.55
2:X:383:A:H2'	2:X:384:G:O4'	2.06	0.55
2:X:1526:G:N2	2:X:1550:G:H22	2.05	0.55
2:X:2479:C:H2'	2:X:2480:A:C8	2.41	0.55
9:H:8:LEU:HD12	9:H:19:VAL:HG23	1.89	0.55
2:X:955:A:N3	11:J:15:PRO:HG3	2.22	0.55
10:I:128:PHE:HD1	10:I:129:SER:N	2.03	0.55
2:X:613:G:H2'	2:X:2057:A:N7	2.22	0.55
2:X:2112:C:H42	2:X:2261:A:H61	1.54	0.55
9:H:73:ASP:HB3	14:M:82:LYS:HE3	1.88	0.55
2:X:627:C:C5	35:N:201:EPE:H102	2.42	0.55
8:G:4:THR:HG23	15:N:61:TRP:HZ3	1.70	0.55
14:M:98:LYS:HB3	14:M:100:TYR:HE1	1.72	0.55
2:X:2313:A:H4'	2:X:2314:A:O4'	2.07	0.55
24:W:8:LEU:HB2	24:W:28:LEU:HD13	1.89	0.55
2:X:955:A:N7	2:X:956:A:C5	2.74	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:43:VAL:HG23	15:N:100:ILE:HG12	1.88	0.54
16:O:32:THR:HG22	16:O:61:THR:HG23	1.88	0.54
2:X:1836:A:O2'	2:X:1837:A:O5'	2.24	0.54
8:G:2:ARG:NH2	8:G:2:ARG:HA	2.22	0.54
16:O:20:ILE:HG23	16:O:97:ILE:HD11	1.88	0.54
2:X:870:C:H1'	10:I:50:PHE:CE2	2.42	0.54
2:X:1072:A:N3	2:X:2513:G:O2'	2.36	0.54
2:X:1488:A:H61	2:X:1595:C:H42	1.54	0.54
2:X:1576:A:N3	2:X:1577:G:C8	2.76	0.54
16:O:16:GLU:HA	16:O:97:ILE:HB	1.88	0.54
2:X:1400:C:HO2'	2:X:1836:A:H1'	1.73	0.54
10:I:60:ARG:O	10:I:61:LEU:HG	2.08	0.54
19:R:36:GLU:OE2	19:R:37:GLY:N	2.41	0.54
20:S:51:VAL:O	20:S:55:VAL:HG23	2.07	0.54
1:A:156:ARG:HB2	2:X:1845:U:H3'	1.89	0.54
2:X:111:U:H5'	2:X:112:U:OP2	2.08	0.54
2:X:1821:U:H2'	2:X:1822:C:C6	2.42	0.54
2:X:2725:U:H2'	2:X:2726:C:C6	2.43	0.54
17:P:71:VAL:C	17:P:108:SER:H	2.16	0.54
26:2:32:LEU:HD22	26:2:43:LEU:HD23	1.89	0.54
2:X:37:C:H2'	2:X:38:A:C8	2.42	0.54
2:X:627:C:OP2	35:N:201:EPE:O2S	2.24	0.54
2:X:1885:G:HO2'	2:X:1886:A:P	2.30	0.54
4:B:16:PHE:CE1	4:B:22:LEU:HD13	2.43	0.54
22:U:17:ARG:O	22:U:29:TRP:HD1	1.90	0.54
2:X:267:G:H2'	2:X:268:A:H5''	1.89	0.54
2:X:2361:U:OP2	13:L:17:ARG:NH1	2.41	0.54
14:M:94:VAL:HG11	14:M:99:LEU:HD21	1.89	0.54
17:P:11:ARG:HA	17:P:100:THR:HG22	1.89	0.54
2:X:986:G:H5''	10:I:32:GLY:HA2	1.89	0.54
2:X:1658:A:N1	17:P:93:ALA:HB2	2.23	0.54
2:X:1813:A:H1'	2:X:1965:A:N6	2.23	0.54
27:3:22:LEU:CB	27:3:44:LEU:HB3	2.37	0.54
2:X:100:U:H3'	2:X:101:G:H5'	1.89	0.54
2:X:218:G:H4'	2:X:219:A:H4'	1.90	0.54
2:X:1576:A:H4'	2:X:1577:G:OP1	2.08	0.54
2:X:1762:U:H5'	2:X:1763:U:OP2	2.08	0.54
10:I:85:PHE:HA	10:I:89:THR:HG23	1.89	0.54
2:X:618:A:O2'	2:X:619:U:H5'	2.08	0.53
2:X:1983:U:H1'	2:X:2579:U:OP1	2.07	0.53
2:X:1366:U:H5''	2:X:1367:C:H5	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1733:A:H2'	2:X:1734:A:C8	2.43	0.53
1:A:142:HIS:N	1:A:192:ILE:O	2.41	0.53
2:X:1065:A:H3'	2:X:1065:A:C8	2.44	0.53
2:X:1474:C:H2'	2:X:1475:A:H8	1.73	0.53
9:H:56:ASP:OD1	9:H:56:ASP:N	2.36	0.53
2:X:499:A:N3	2:X:503:A:O2'	2.41	0.53
2:X:2231:C:O2'	2:X:2232:A:H8	1.92	0.53
5:C:8:LYS:HB2	5:C:8:LYS:NZ	2.17	0.53
2:X:2232:A:H5'	2:X:2233:C:P	2.48	0.53
2:X:2457:A:N3	2:X:2457:A:H2'	2.24	0.53
2:X:687:G:N2	2:X:690:U:OP2	2.42	0.53
2:X:730:A:C8	2:X:819:A:C6	2.96	0.53
2:X:2732:A:H2'	2:X:2733:A:O4'	2.08	0.53
8:G:21:ALA:HB1	8:G:63:ILE:HD13	1.91	0.53
10:I:29:LYS:O	10:I:30:THR:HB	2.09	0.53
2:X:148:U:H2'	2:X:149:U:C6	2.44	0.53
2:X:1352:C:O2'	2:X:1429:G:O2'	2.25	0.53
2:X:1423:C:O2'	2:X:1512:U:O2	2.17	0.53
27:3:22:LEU:CB	27:3:44:LEU:HD22	2.39	0.53
2:X:59:U:O2'	2:X:74:U:OP2	2.22	0.53
2:X:155:U:H5'	2:X:156:A:OP2	2.09	0.53
20:S:155:THR:O	20:S:155:THR:OG1	2.23	0.53
1:A:201:GLU:HG3	1:A:202:LEU:HD12	1.91	0.53
2:X:1306:A:C2	2:X:2040:A:C4	2.97	0.53
2:X:1523:G:H1	2:X:1557:C:H42	1.56	0.53
2:X:2058:A:C6	2:X:2525:C:H1'	2.44	0.53
4:B:134:HIS:CE1	4:B:168:LYS:HB2	2.44	0.53
19:R:26:THR:HA	19:R:33:VAL:HG12	1.91	0.53
23:V:25:LEU:HD11	23:V:29:ARG:NH1	2.24	0.53
2:X:309:U:O2'	2:X:310:C:OP2	2.19	0.53
2:X:415:U:H5'	2:X:416:G:OP1	2.09	0.52
2:X:620:G:C6	2:X:621:A:N6	2.77	0.52
2:X:1514:A:H3'	2:X:1515:G:H8	1.74	0.52
2:X:1518:G:N2	2:X:1562:C:N3	2.52	0.52
4:B:119:THR:CB	4:B:179:THR:HG22	2.38	0.52
4:B:182:ASN:O	4:B:183:LEU:HD23	2.09	0.52
18:Q:16:SER:O	18:Q:20:MET:HG3	2.10	0.52
2:X:955:A:C6	11:J:15:PRO:HD3	2.44	0.52
2:X:1349:U:H4'	2:X:1350:U:O5'	2.08	0.52
2:X:1508:C:O2'	2:X:1509:G:O5'	2.28	0.52
2:X:1823:U:H2'	2:X:1824:C:C6	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:2271:U:O2'	2:X:2272:U:H5'	2.09	0.52
2:X:2507:C:C2'	2:X:2508:G:H5'	2.39	0.52
3:Y:69:C:H42	3:Y:102:A:H61	1.58	0.52
20:S:76:ASP:CG	20:S:77:TYR:H	2.18	0.52
2:X:460:C:H2'	2:X:461:A:H8	1.72	0.52
2:X:1930:G:H2'	2:X:1931:G:H8	1.75	0.52
2:X:870:C:H1'	10:I:50:PHE:HE2	1.74	0.52
2:X:2268:A:H2'	2:X:2269:G:C8	2.44	0.52
2:X:858:U:H2'	2:X:859:C:C6	2.44	0.52
2:X:2760:A:C2	4:B:216:LYS:HB2	2.45	0.52
4:B:119:THR:HA	4:B:179:THR:HG22	1.90	0.52
17:P:30:ALA:HA	17:P:33:ILE:HD12	1.90	0.52
21:T:81:GLY:O	21:T:82:ARG:NE	2.42	0.52
2:X:38:A:H2'	2:X:39:C:O4'	2.10	0.52
2:X:416:G:OP2	2:X:469:A:N6	2.42	0.52
2:X:668:C:H2'	2:X:669:C:C6	2.45	0.52
2:X:1733:A:H2'	2:X:1734:A:H8	1.74	0.52
2:X:1862:G:H1	2:X:1957:G:H21	1.58	0.52
2:X:2819:C:H42	2:X:2824:G:H1	1.58	0.52
3:Y:74:G:H1	3:Y:97:A:H62	1.57	0.52
2:X:142:G:N2	2:X:1640:U:O3'	2.29	0.52
2:X:627:C:OP2	35:N:201:EPE:C6	2.57	0.52
2:X:719:G:H1'	5:C:74:ARG:HE	1.73	0.52
2:X:1516:C:H42	2:X:1564:G:H1	1.56	0.52
2:X:1074:G:OP2	11:J:128:LYS:NZ	2.41	0.52
2:X:1211:G:H2'	2:X:1212:U:C6	2.44	0.52
2:X:1770:C:O2'	2:X:1771:A:H8	1.93	0.52
2:X:2018:U:O2'	2:X:2019:G:H5'	2.09	0.52
2:X:2581:U:H2'	2:X:2582:U:C6	2.45	0.52
6:D:105:SER:O	6:D:105:SER:OG	2.27	0.52
7:E:90:VAL:O	7:E:160:LYS:HA	2.10	0.52
11:J:55:THR:HG22	11:J:64:VAL:HG11	1.92	0.52
15:N:61:TRP:CD2	15:N:93:LYS:HB2	2.45	0.52
2:X:721:A:H8	2:X:2096:G:H21	1.57	0.52
18:Q:49:LYS:HE2	18:Q:50:VAL:H	1.74	0.52
2:X:17:G:H5''	25:Z:11:THR:HG21	1.92	0.52
2:X:1013:U:H2'	2:X:1014:U:C6	2.45	0.52
2:X:2286:G:H1'	2:X:2454:C:C2	2.44	0.52
4:B:20:GLY:O	9:H:73:ASP:HA	2.10	0.52
1:A:169:GLY:O	1:A:171:TYR:N	2.43	0.51
2:X:955:A:N7	2:X:956:A:C6	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:30:ARG:HD2	13:L:45:ILE:HD12	1.92	0.51
15:N:6:GLY:HA3	35:N:201:EPE:H52	1.92	0.51
2:X:1315:C:OP1	12:K:32:THR:HG23	2.10	0.51
3:Y:3:U:H3	3:Y:112:G:H1	1.58	0.51
14:M:48:VAL:O	14:M:63:VAL:HA	2.10	0.51
2:X:1492:G:C8	2:X:1493:U:H5	2.29	0.51
4:B:215:ILE:O	4:B:216:LYS:HG2	2.10	0.51
5:C:8:LYS:NZ	5:C:12:THR:O	2.43	0.51
5:C:190:ASP:OD1	5:C:191:SER:N	2.39	0.51
17:P:14:PRO:O	17:P:18:ARG:HG3	2.10	0.51
1:A:43:ARG:HG3	1:A:49:LEU:HA	1.93	0.51
2:X:1336:G:N1	2:X:1684:A:OP2	2.36	0.51
2:X:1471:A:H1'	2:X:1472:C:C4	2.45	0.51
2:X:2109:A:H2'	2:X:2110:G:O4'	2.10	0.51
4:B:67:LYS:HA	4:B:86:ARG:HH22	1.76	0.51
4:B:169:MET:HB2	4:B:170:PRO:CD	2.41	0.51
9:H:100:GLY:H	9:H:119:PRO:HG2	1.76	0.51
10:I:70:ASN:C	10:I:72:LYS:H	2.17	0.51
1:A:156:ARG:NH1	2:X:1844:G:OP2	2.43	0.51
2:X:804:G:O2'	2:X:805:G:H5'	2.10	0.51
4:B:107:VAL:HG21	4:B:193:LYS:HA	1.93	0.51
2:X:234:C:O2'	2:X:235:G:C8	2.59	0.51
2:X:280:C:H2'	2:X:281:A:C8	2.44	0.51
2:X:1383:G:N2	2:X:1644:C:O2	2.26	0.51
2:X:1526:G:C8	2:X:1527:A:C6	2.98	0.51
2:X:2126:C:H2'	2:X:2127:G:H8	1.75	0.51
2:X:2736:G:H2'	2:X:2737:C:C6	2.46	0.51
2:X:179:A:OP2	2:X:179:A:H8	1.94	0.51
2:X:1353:A:H2'	2:X:1354:G:H8	1.75	0.51
2:X:2052:C:H5'	4:B:162:ARG:HH21	1.75	0.51
2:X:2687:A:H2'	2:X:2688:G:O4'	2.11	0.51
5:C:65:TRP:CZ2	5:C:75:GLN:HG3	2.45	0.51
12:K:29:ARG:HB3	12:K:120:GLU:HB3	1.93	0.51
15:N:10:THR:HA	15:N:13:ARG:HB2	1.93	0.51
2:X:895:U:O2	24:W:46:GLN:NE2	2.43	0.51
2:X:1000:G:H2'	2:X:1001:A:H2'	1.93	0.51
2:X:1017:A:H8	2:X:1017:A:OP1	1.93	0.51
2:X:1526:G:H21	2:X:1550:G:H22	1.58	0.51
3:Y:4:G:N3	3:Y:112:G:N2	2.59	0.51
2:X:51:G:O2'	2:X:118:A:N1	2.31	0.51
2:X:774:G:H2'	2:X:1802:U:H1'	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1185:U:H4'	2:X:1186:A:O4'	2.10	0.51
2:X:1490:G:O2'	2:X:1491:C:O4'	2.29	0.51
2:X:1507:A:C2'	2:X:1508:C:H5'	2.40	0.51
2:X:2442:G:H4'	10:I:59:ARG:O	2.11	0.51
2:X:173:A:H2'	2:X:174:U:C6	2.46	0.51
2:X:363:A:H4'	2:X:365:A:C8	2.46	0.51
2:X:1378:U:H3'	2:X:1434:U:O2	2.11	0.51
2:X:2059:G:N2	2:X:2599:A:OP2	2.43	0.51
15:N:10:THR:OG1	35:N:201:EPE:H31	2.11	0.51
2:X:657:U:O2	2:X:657:U:H2'	2.10	0.50
3:Y:22:G:N2	3:Y:26:C:N3	2.59	0.50
9:H:4:GLN:OE1	9:H:23:LYS:NZ	2.45	0.50
12:K:61:ASN:HA	12:K:64:LYS:HE3	1.93	0.50
17:P:65:ASN:HD22	17:P:65:ASN:H	1.59	0.50
1:A:43:ARG:HE	1:A:49:LEU:HD12	1.77	0.50
2:X:658:A:H3'	2:X:659:A:C5'	2.41	0.50
2:X:1176:U:H6	2:X:1176:U:H5'	1.77	0.50
2:X:1887:G:O6	2:X:1910:G:N2	2.45	0.50
2:X:2289:U:H2'	2:X:2290:C:H6	1.76	0.50
2:X:2479:C:C4	2:X:2480:A:C6	2.99	0.50
10:I:19:VAL:CG2	10:I:30:THR:HG23	2.42	0.50
2:X:1542:C:H3'	2:X:1543:G:H5''	1.94	0.50
2:X:2257:G:H2'	2:X:2258:U:H6	1.76	0.50
2:X:2811:U:H2'	2:X:2812:U:C6	2.46	0.50
3:Y:91:C:H2'	3:Y:92:G:C8	2.46	0.50
4:B:88:ILE:O	4:B:89:ARG:NH2	2.43	0.50
4:B:119:THR:CA	4:B:179:THR:HG22	2.41	0.50
14:M:82:LYS:NZ	14:M:82:LYS:HB3	2.26	0.50
14:M:98:LYS:HB3	14:M:100:TYR:CE1	2.46	0.50
2:X:201:C:H5'	2:X:2271:U:OP1	2.12	0.50
5:C:29:ASN:OD1	5:C:32:VAL:HG23	2.12	0.50
8:G:112:SER:O	8:G:112:SER:OG	2.25	0.50
12:K:70:GLU:O	12:K:72:LEU:N	2.45	0.50
15:N:76:TYR:CZ	15:N:80:MET:HG3	2.46	0.50
20:S:105:PRO:HD2	20:S:124:PRO:HA	1.93	0.50
2:X:17:G:OP1	25:Z:11:THR:HG22	2.11	0.50
2:X:422:G:H1	2:X:444:C:H42	1.58	0.50
2:X:1041:G:H5''	15:N:92:ARG:NH1	2.26	0.50
2:X:1746:G:H2'	2:X:1747:G:H8	1.76	0.50
19:R:39:ASN:O	19:R:39:ASN:ND2	2.41	0.50
27:3:53:SER:O	27:3:56:LYS:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:2043:U:H2'	2:X:2044:C:C6	2.47	0.50
2:X:2539:C:H2'	2:X:2540:A:O4'	2.12	0.50
2:X:2900:C:O2'	12:K:99:GLY:O	2.24	0.50
9:H:120:GLU:OE1	14:M:67:SER:OG	2.28	0.50
15:N:27:SER:HB2	15:N:31:LEU:HG	1.94	0.50
27:3:24:ARG:HG2	27:3:24:ARG:HH11	1.77	0.50
2:X:581:A:H4'	15:N:57:PHE:HE1	1.76	0.50
2:X:704:U:H2'	2:X:705:U:O4'	2.12	0.50
2:X:1337:A:H4'	2:X:1338:U:H5''	1.94	0.50
2:X:1405:G:H2'	2:X:1406:G:H8	1.75	0.50
2:X:1922:C:H2'	2:X:1923:A:H8	1.76	0.50
21:T:56:GLY:H	21:T:59:VAL:HB	1.76	0.50
1:A:241:ILE:HG13	2:X:1929:C:H5''	1.94	0.50
2:X:132:C:H2'	2:X:133:A:O4'	2.12	0.50
2:X:1392:G:C6	2:X:1393:C:C4	3.00	0.50
2:X:1873:G:O2'	2:X:1874:A:O4'	2.20	0.50
19:R:49:GLN:O	19:R:51:ASN:N	2.42	0.50
2:X:64:A:H2	18:Q:68:TYR:CD2	2.30	0.50
2:X:683:G:C2	2:X:696:G:C4	3.00	0.50
2:X:897:A:H2'	2:X:898:U:H6	1.75	0.50
2:X:90:A:OP1	2:X:90:A:C8	2.65	0.49
2:X:194:A:H2'	2:X:195:C:C6	2.47	0.49
2:X:1336:G:O2'	2:X:1684:A:N6	2.45	0.49
2:X:1378:U:OP1	2:X:1434:U:N3	2.41	0.49
2:X:2904:U:H5	25:Z:40:SER:HA	1.75	0.49
5:C:8:LYS:HA	5:C:14:SER:H	1.77	0.49
9:H:64:ARG:NH1	9:H:101:PRO:O	2.41	0.49
14:M:51:LYS:HD3	14:M:100:TYR:OH	2.12	0.49
26:2:22:ARG:O	26:2:28:GLY:HA3	2.12	0.49
2:X:896:U:H2'	2:X:897:A:H8	1.77	0.49
2:X:1514:A:H3'	2:X:1515:G:C8	2.47	0.49
2:X:2803:A:C2	2:X:2805:A:C4	3.01	0.49
11:J:75:THR:HG21	11:J:87:LYS:HB2	1.94	0.49
12:K:23:SER:O	12:K:24:LEU:HB3	2.11	0.49
24:W:8:LEU:HD12	24:W:53:LEU:O	2.11	0.49
2:X:2:A:H4'	2:X:3:U:O4'	2.13	0.49
4:B:16:PHE:HB2	14:M:14:GLN:HE21	1.77	0.49
8:G:88:ILE:O	8:G:89:THR:HB	2.12	0.49
11:J:66:ILE:HG12	11:J:104:PHE:HE1	1.75	0.49
2:X:204:C:H1'	2:X:253:G:O6	2.12	0.49
2:X:683:G:N1	2:X:696:G:C5	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:799:U:H2'	2:X:800:G:H8	1.76	0.49
2:X:1197:C:H2'	2:X:1198:G:O4'	2.12	0.49
2:X:1261:G:OP2	16:O:89:ARG:NH1	2.45	0.49
2:X:1635:A:H2'	2:X:1635:A:N3	2.26	0.49
2:X:1986:G:H2'	2:X:1987:A:O4'	2.13	0.49
8:G:77:ARG:O	8:G:85:ILE:HD12	2.12	0.49
14:M:106:ARG:HA	14:M:106:ARG:NH1	2.27	0.49
15:N:8:THR:H	35:N:201:EPE:H81	1.78	0.49
1:A:181:VAL:HG23	1:A:271:VAL:HB	1.95	0.49
2:X:379:C:H2'	2:X:380:U:H6	1.77	0.49
2:X:787:U:H2'	2:X:788:A:C8	2.48	0.49
2:X:955:A:C2	11:J:15:PRO:HB3	2.47	0.49
2:X:2299:U:H5''	2:X:2300:A:OP1	2.11	0.49
10:I:65:GLY:O	10:I:93:PRO:HB2	2.11	0.49
12:K:53:LYS:HB3	12:K:55:ASP:OD1	2.13	0.49
19:R:56:ILE:HB	19:R:58:GLU:HG2	1.94	0.49
21:T:88:SER:HB2	21:T:90:TYR:HE1	1.76	0.49
24:W:18:THR:HB	24:W:49:LYS:NZ	2.28	0.49
2:X:633:A:H2'	2:X:634:C:O4'	2.13	0.49
11:J:93:TRP:O	11:J:94:ILE:HD13	2.12	0.49
1:A:230:HIS:CD2	1:A:249:PRO:HG3	2.48	0.49
2:X:609:U:H2'	2:X:610:U:O4'	2.13	0.49
2:X:635:G:O2'	27:3:3:LYS:HA	2.13	0.49
2:X:747:U:H2'	2:X:748:U:C6	2.47	0.49
2:X:1259:U:H2'	2:X:1260:C:H6	1.78	0.49
2:X:1527:A:H2	2:X:1549:C:C4	2.31	0.49
5:C:181:LEU:HD23	5:C:181:LEU:O	2.13	0.49
7:E:44:LYS:HE3	7:E:56:SER:CB	2.43	0.49
8:G:39:GLY:O	8:G:41:ASN:N	2.42	0.49
13:L:44:ILE:O	13:L:53:LEU:HD12	2.12	0.49
18:Q:34:ASN:O	18:Q:38:VAL:HG23	2.12	0.49
19:R:80:ARG:CZ	19:R:96:LYS:HA	2.43	0.49
19:R:84:LYS:HA	19:R:90:LYS:O	2.13	0.49
25:Z:28:THR:HG23	25:Z:37:TYR:HE1	1.77	0.49
2:X:157:U:H2'	2:X:158:G:H8	1.76	0.49
15:N:6:GLY:C	35:N:201:EPE:H72	2.38	0.49
2:X:94:A:H2'	2:X:95:A:O4'	2.13	0.49
2:X:425:G:H1	2:X:441:C:H42	1.59	0.49
2:X:1498:U:O2'	2:X:1499:U:H5	1.94	0.49
2:X:2362:A:OP2	13:L:17:ARG:HG2	2.12	0.49
2:X:2446:U:H2'	2:X:2447:C:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:12:U:OP2	3:Y:68:A:O2'	2.28	0.49
11:J:43:THR:HG22	11:J:46:GLN:CD	2.38	0.49
2:X:12:U:H2'	2:X:12:U:O2	2.12	0.49
2:X:266:A:H2'	2:X:267:G:O4'	2.13	0.49
2:X:2627:A:O2'	2:X:2628:C:H5'	2.13	0.49
3:Y:76:A:C2	3:Y:96:G:C4	3.01	0.49
10:I:57:LEU:HD11	27:3:12:LYS:CA	2.43	0.49
13:L:29:PRO:HD2	13:L:88:GLY:HA2	1.95	0.49
18:Q:17:SER:HA	18:Q:20:MET:HE2	1.94	0.49
2:X:267:G:C2'	2:X:268:A:H5''	2.42	0.48
2:X:945:A:O2'	2:X:946:A:H5'	2.13	0.48
2:X:1487:G:C2	2:X:1597:U:O2	2.65	0.48
2:X:1597:U:O3'	2:X:1767:G:N2	2.46	0.48
9:H:30:ARG:HD3	9:H:32:THR:O	2.13	0.48
2:X:654:C:H42	2:X:662:G:H1	1.60	0.48
2:X:1304:G:H5''	25:Z:20:PHE:CE2	2.48	0.48
2:X:1973:U:H2'	2:X:1974:C:C6	2.48	0.48
8:G:79:SER:OG	8:G:81:HIS:HB2	2.12	0.48
12:K:14:LYS:O	12:K:18:ARG:HG3	2.12	0.48
12:K:74:GLU:O	12:K:76:GLU:N	2.46	0.48
17:P:64:MET:HE2	17:P:69:LEU:HD21	1.95	0.48
2:X:767:A:H2'	2:X:768:A:H8	1.78	0.48
2:X:1815:C:H2'	2:X:1816:A:O4'	2.13	0.48
2:X:1932:C:O2'	2:X:1956:G:N7	2.44	0.48
10:I:19:VAL:HG21	10:I:30:THR:HG23	1.95	0.48
18:Q:50:VAL:O	18:Q:82:LEU:HD23	2.13	0.48
2:X:514:G:C2'	2:X:515:G:H5'	2.43	0.48
2:X:538:G:OP2	33:X:3494:SPD:H91	2.14	0.48
2:X:719:G:OP1	5:C:76:GLY:HA3	2.13	0.48
2:X:2842:G:H2'	2:X:2843:A:H5''	1.95	0.48
2:X:278:A:H2'	2:X:279:A:C8	2.47	0.48
2:X:331:G:O2'	2:X:332:A:O5'	2.31	0.48
2:X:676:A:N3	2:X:2442:G:O2'	2.40	0.48
2:X:810:A:H2'	2:X:811:C:C6	2.49	0.48
2:X:1560:A:H4'	32:X:3004:MPD:H12	1.95	0.48
2:X:1770:C:O2'	2:X:1771:A:OP2	2.30	0.48
2:X:1806:U:C5	2:X:1811:A:N7	2.81	0.48
2:X:2257:G:O3'	22:U:32:ASN:HB3	2.13	0.48
4:B:8:ARG:HH21	4:B:54:GLU:CD	2.21	0.48
4:B:118:VAL:HG23	4:B:180:VAL:HG23	1.94	0.48
5:C:148:GLN:HB2	5:C:186:ILE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:66:ASN:O	15:N:70:ARG:HG2	2.14	0.48
22:U:29:TRP:CG	22:U:30:ASN:N	2.81	0.48
1:A:79:ASP:HB3	1:A:93:LEU:O	2.13	0.48
2:X:994:A:H5''	3:Y:85:A:H61	1.76	0.48
2:X:1540:U:H1'	2:X:1625:U:H4'	1.94	0.48
2:X:1699:A:H1'	4:B:127:PHE:CE1	2.48	0.48
2:X:2646:U:H5''	4:B:165:LYS:HA	1.95	0.48
4:B:67:LYS:HD2	4:B:68:TYR:CE1	2.48	0.48
9:H:102:VAL:O	9:H:121:VAL:HA	2.13	0.48
10:I:70:ASN:O	10:I:72:LYS:N	2.45	0.48
21:T:80:LYS:HB2	21:T:84:LYS:C	2.38	0.48
2:X:683:G:N2	2:X:697:U:C6	2.81	0.48
2:X:719:G:H1'	5:C:74:ARG:NE	2.28	0.48
2:X:998:G:C5	2:X:999:U:C5	3.02	0.48
2:X:2357:G:O3'	21:T:52:LYS:HE3	2.13	0.48
2:X:317:G:H2'	2:X:318:A:O4'	2.13	0.48
2:X:514:G:H2'	2:X:515:G:H5'	1.94	0.48
2:X:1494:G:C8	2:X:1495:C:C5	2.99	0.48
2:X:187:C:H2'	2:X:188:C:C6	2.49	0.48
2:X:888:G:N2	2:X:980:U:C2	2.82	0.48
2:X:1440:A:O2'	2:X:1514:A:O2'	2.13	0.48
2:X:1522:G:H2'	2:X:1523:G:H8	1.78	0.48
3:Y:65:G:O6	3:Y:105:G:N2	2.44	0.48
3:Y:90:C:H2'	3:Y:91:C:C6	2.49	0.48
3:Y:103:A:H2'	3:Y:104:C:O4'	2.13	0.48
4:B:95:ASP:C	4:B:97:ASP:H	2.22	0.48
5:C:140:LYS:HA	5:C:142:VAL:HG12	1.95	0.48
19:R:75:THR:HB	19:R:76:ASN:ND2	2.29	0.48
21:T:29:LEU:H	21:T:29:LEU:HD12	1.79	0.48
24:W:12:VAL:HG12	24:W:20:ARG:HG2	1.96	0.48
2:X:226:A:O2'	2:X:466:C:O2	2.32	0.48
2:X:731:U:H5	2:X:833:A:H61	1.58	0.48
2:X:987:U:OP1	10:I:33:ARG:HB3	2.14	0.48
2:X:1088:C:H5'	2:X:1089:C:OP1	2.13	0.48
9:H:12:ASP:CG	9:H:85:VAL:HG13	2.39	0.48
12:K:6:LEU:HA	12:K:13:ARG:HD3	1.96	0.48
12:K:51:GLY:HA2	12:K:86:PHE:CE2	2.49	0.48
15:N:76:TYR:CE2	15:N:80:MET:HE3	2.49	0.48
20:S:22:ARG:NE	20:S:87:THR:HG23	2.29	0.48
2:X:606:G:H22	2:X:621:A:H2	1.61	0.47
3:Y:1:U:O2'	3:Y:2:C:OP2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:84:VAL:HG23	7:E:134:GLU:H	1.78	0.47
23:V:63:GLU:HA	23:V:66:LYS:NZ	2.28	0.47
25:Z:8:THR:HG22	25:Z:12:ARG:HB3	1.96	0.47
2:X:24:G:H2'	2:X:25:U:H6	1.79	0.47
2:X:660:A:N3	2:X:660:A:O4'	2.47	0.47
2:X:665:G:H4'	2:X:666:A:C5'	2.44	0.47
2:X:1700:C:H2'	2:X:1701:U:C6	2.49	0.47
2:X:1700:C:H2'	2:X:1701:U:H6	1.78	0.47
15:N:58:ARG:HA	15:N:61:TRP:CD1	2.48	0.47
1:A:223:SER:OG	2:X:1853:C:H5''	2.15	0.47
2:X:3:U:H2'	2:X:4:U:H6	1.78	0.47
2:X:2856:U:H2'	2:X:2857:A:H8	1.79	0.47
9:H:13:ASN:OD1	9:H:96:THR:N	2.42	0.47
15:N:66:ASN:OD1	15:N:70:ARG:NH1	2.47	0.47
18:Q:55:ILE:HD11	18:Q:76:ARG:NE	2.29	0.47
2:X:294:G:C2	2:X:295:G:C8	3.02	0.47
2:X:437:A:O2'	2:X:456:G:OP1	2.25	0.47
2:X:706:U:O2'	10:I:13:ARG:HA	2.14	0.47
2:X:841:C:H2'	2:X:842:U:C6	2.49	0.47
2:X:1259:U:H2'	2:X:1260:C:C6	2.49	0.47
2:X:2712:G:OP1	14:M:51:LYS:NZ	2.48	0.47
20:S:136:ASN:O	20:S:138:PRO:HD3	2.14	0.47
2:X:39:C:O2'	2:X:658:A:N1	2.42	0.47
2:X:1488:A:H61	2:X:1595:C:N4	2.11	0.47
2:X:1963:A:OP2	2:X:1988:C:N4	2.48	0.47
2:X:2675:G:H2'	2:X:2676:U:C6	2.50	0.47
8:G:94:ARG:HA	8:G:98:PRO:HB3	1.96	0.47
2:X:566:U:H2'	2:X:567:G:N7	2.28	0.47
2:X:829:U:C5	2:X:837:G:C5	3.03	0.47
2:X:1515:G:HO2'	2:X:1516:C:P	2.37	0.47
2:X:1575:A:N3	2:X:1576:A:H5'	2.30	0.47
2:X:2856:U:H2'	2:X:2857:A:C8	2.50	0.47
3:Y:21:G:H22	3:Y:58:G:H22	1.62	0.47
2:X:79:U:O2'	2:X:389:A:H8	1.97	0.47
2:X:627:C:H5	35:N:201:EPE:H102	1.77	0.47
2:X:1336:G:H5''	2:X:1337:A:OP1	2.15	0.47
2:X:1474:C:H2'	2:X:1475:A:C8	2.48	0.47
2:X:1478:A:H61	2:X:1605:A:H62	1.61	0.47
2:X:1511:C:H5'	2:X:1512:U:OP1	2.14	0.47
2:X:1575:A:H2'	2:X:1576:A:C5'	2.45	0.47
2:X:2289:U:H2'	2:X:2290:C:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:2642:U:C2	25:Z:4:PRO:HA	2.49	0.47
3:Y:6:U:H3	3:Y:109:C:H42	1.63	0.47
13:L:30:ARG:HD2	13:L:45:ILE:CD1	2.44	0.47
17:P:6:VAL:HG22	17:P:104:THR:HG23	1.97	0.47
18:Q:51:ALA:HB3	18:Q:81:THR:O	2.15	0.47
19:R:72:ASP:N	19:R:73:PRO:HD2	2.29	0.47
20:S:26:LYS:HE3	20:S:26:LYS:HB2	1.68	0.47
21:T:83:ASP:OD1	21:T:84:LYS:N	2.42	0.47
24:W:15:ARG:HD3	24:W:53:LEU:HD23	1.97	0.47
2:X:1885:G:O2'	2:X:1886:A:O5'	2.28	0.47
2:X:2519:U:H2'	2:X:2520:U:C6	2.49	0.47
2:X:2882:A:C6	2:X:2883:U:C4	3.02	0.47
12:K:22:THR:OG1	12:K:67:ARG:HB2	2.15	0.47
12:K:27:SER:C	12:K:29:ARG:H	2.22	0.47
2:X:909:G:C6	2:X:910:C:N4	2.82	0.47
8:G:25:THR:HB	8:G:28:ARG:HG3	1.95	0.47
10:I:12:SER:OG	10:I:13:ARG:HG3	2.15	0.47
15:N:78:ARG:CB	15:N:78:ARG:HH11	2.28	0.47
15:N:93:LYS:CA	15:N:96:SER:HB3	2.45	0.47
2:X:58:G:N2	2:X:70:G:C4	2.83	0.47
2:X:523:A:H2'	2:X:524:A:C8	2.50	0.47
2:X:1331:C:H5''	12:K:69:VAL:HG13	1.96	0.47
2:X:1379:A:C6	2:X:1382:C:N3	2.83	0.47
2:X:1820:G:O2'	2:X:1927:A:N1	2.43	0.47
2:X:2688:G:H2'	2:X:2689:A:C8	2.49	0.47
2:X:2783:U:H3'	28:4:19:ARG:O	2.15	0.47
20:S:95:ASN:OD1	20:S:96:MET:N	2.48	0.47
2:X:233:U:O2'	2:X:234:C:H5'	2.15	0.46
2:X:379:C:C2	2:X:380:U:C5	3.03	0.46
2:X:1015:C:O2'	2:X:1027:A:N3	2.44	0.46
2:X:1211:G:H2'	2:X:1212:U:H6	1.80	0.46
2:X:1357:G:C2	2:X:1366:U:H5'	2.51	0.46
2:X:1510:U:H3	2:X:1571:G:H22	1.62	0.46
2:X:1514:A:H61	2:X:1567:A:H1'	1.80	0.46
2:X:2903:A:H5''	2:X:2904:U:H5'	1.97	0.46
3:Y:68:A:C2	3:Y:103:A:N1	2.83	0.46
13:L:45:ILE:HG22	13:L:51:VAL:O	2.15	0.46
19:R:32:ARG:HB3	19:R:64:HIS:HA	1.98	0.46
2:X:1528:G:H1	2:X:1547:C:H42	1.62	0.46
2:X:1876:G:H2'	2:X:1877:G:C8	2.51	0.46
2:X:2026:C:H5''	2:X:2750:C:O2'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:33:ASN:HB2	4:B:105:VAL:CG2	2.45	0.46
20:S:27:VAL:HG12	20:S:28:PRO:O	2.14	0.46
1:A:11:ASN:OD1	1:A:14:ARG:NH1	2.48	0.46
1:A:247:MET:HB2	1:A:247:MET:HE3	1.53	0.46
2:X:868:A:H2'	2:X:869:G:C8	2.50	0.46
2:X:1036:C:H2'	2:X:1037:A:H8	1.81	0.46
2:X:1651:C:H4'	2:X:1652:A:O5'	2.15	0.46
2:X:1869:G:C2	2:X:1928:A:C2	3.04	0.46
2:X:2011:U:H2'	2:X:2012:G:C8	2.51	0.46
2:X:2338:A:H3'	2:X:2339:U:H5	1.81	0.46
3:Y:63:U:O2'	3:Y:64:A:H5'	2.15	0.46
4:B:53:PHE:CG	4:B:54:GLU:N	2.81	0.46
5:C:110:LEU:HA	5:C:110:LEU:HD23	1.51	0.46
8:G:49:VAL:O	8:G:51:THR:HG22	2.15	0.46
35:N:201:EPE:H82	35:N:201:EPE:H51	1.61	0.46
19:R:86:VAL:CB	19:R:90:LYS:HG3	2.46	0.46
2:X:2:A:H4'	2:X:3:U:H5'	1.98	0.46
2:X:659:A:O2'	2:X:660:A:H4'	2.15	0.46
2:X:1151:G:H2'	2:X:1152:U:H6	1.81	0.46
2:X:1395:G:C6	2:X:1408:G:N7	2.84	0.46
2:X:2912:A:H4'	2:X:2913:G:O4'	2.16	0.46
3:Y:21:G:N2	3:Y:58:G:H22	2.13	0.46
4:B:106:SER:O	4:B:109:THR:HG23	2.15	0.46
17:P:24:ILE:HD12	17:P:24:ILE:HA	1.80	0.46
24:W:37:VAL:HG11	24:W:43:ILE:HG12	1.96	0.46
25:Z:39:LEU:O	25:Z:41:HIS:ND1	2.48	0.46
2:X:38:A:H1'	5:C:48:THR:O	2.16	0.46
2:X:257:G:N7	27:3:5:LYS:HE3	2.31	0.46
2:X:515:G:H1	26:2:38:LYS:NZ	2.14	0.46
2:X:579:U:H2'	2:X:580:C:C6	2.50	0.46
2:X:955:A:C2	11:J:15:PRO:HG3	2.51	0.46
2:X:1848:A:H2'	2:X:1849:G:C8	2.50	0.46
2:X:2078:A:C2	2:X:2079:G:O6	2.69	0.46
10:I:47:ARG:HE	10:I:47:ARG:HB2	1.55	0.46
14:M:34:ILE:CD1	14:M:43:GLN:HG3	2.45	0.46
1:A:153:GLN:HB3	2:X:1845:U:C4	2.51	0.46
2:X:291:G:H2'	2:X:292:U:C6	2.51	0.46
2:X:1016:G:O5'	2:X:1016:G:H8	1.99	0.46
2:X:2670:G:OP2	33:X:3493:SPD:H72	2.15	0.46
5:C:103:LYS:HA	5:C:106:ARG:HE	1.80	0.46
24:W:10:ARG:HG3	24:W:10:ARG:NH1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:684:U:H2'	2:X:685:C:H6	1.80	0.46
2:X:1093:C:H3'	2:X:1094:A:H8	1.80	0.46
2:X:1539:A:H2'	2:X:1540:U:C5	2.51	0.46
2:X:1609:U:H2'	2:X:1610:G:C8	2.50	0.46
4:B:133:ARG:HH11	4:B:171:GLY:N	2.13	0.46
5:C:51:VAL:CG1	5:C:91:GLY:HA3	2.44	0.46
9:H:6:THR:O	9:H:21:THR:HG23	2.15	0.46
18:Q:16:SER:HB2	18:Q:26:THR:OG1	2.16	0.46
2:X:195:C:O2'	2:X:847:A:N3	2.46	0.46
2:X:305:A:H62	2:X:410:G:N2	2.14	0.46
2:X:402:C:H2'	2:X:403:U:O4'	2.16	0.46
2:X:527:G:OP2	19:R:43:LYS:N	2.37	0.46
2:X:1065:A:H62	2:X:1185:U:H3	1.63	0.46
2:X:1494:G:N7	2:X:1495:C:H5	2.13	0.46
2:X:2126:C:H2'	2:X:2127:G:C8	2.50	0.46
2:X:2670:G:H2'	2:X:2671:A:C8	2.51	0.46
2:X:2749:G:H2'	2:X:2750:C:C6	2.50	0.46
5:C:179:GLN:O	5:C:182:ASN:N	2.43	0.46
10:I:21:ARG:HD3	10:I:21:ARG:HA	1.56	0.46
15:N:61:TRP:O	15:N:65:ILE:HD12	2.14	0.46
15:N:89:ASP:OD2	16:O:51:PRO:HG3	2.15	0.46
24:W:17:GLU:O	24:W:20:ARG:HB2	2.16	0.46
24:W:40:ASN:HB2	24:W:43:ILE:HB	1.98	0.46
2:X:32:C:O2'	2:X:33:U:H5'	2.16	0.46
2:X:811:C:C2'	2:X:812:U:H5'	2.46	0.46
2:X:1810:A:C2	2:X:2614:A:C4	3.03	0.46
2:X:1848:A:H2'	2:X:1849:G:H8	1.79	0.46
2:X:2287:C:H2'	2:X:2288:C:H6	1.81	0.46
2:X:2646:U:O2'	4:B:169:MET:HE2	2.16	0.46
2:X:2807:G:N7	32:X:3006:MPD:H13	2.31	0.46
9:H:90:ASP:O	9:H:91:LYS:HB2	2.16	0.46
11:J:40:SER:HB3	11:J:127:VAL:CG1	2.45	0.46
15:N:83:LEU:CD2	15:N:113:ALA:HB2	2.46	0.46
24:W:50:VAL:HB	24:W:53:LEU:CD1	2.46	0.46
2:X:496:G:P	2:X:1286:G:H22	2.38	0.45
2:X:1490:G:N3	2:X:1490:G:H2'	2.31	0.45
2:X:1518:G:C4	2:X:1519:U:C5	3.04	0.45
2:X:1700:C:C2	2:X:1701:U:C5	3.03	0.45
2:X:2338:A:H3'	2:X:2339:U:C5	2.51	0.45
2:X:2619:G:C6	2:X:2620:U:C4	3.04	0.45
1:A:78:VAL:HG12	1:A:79:ASP:N	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:340:C:H2'	2:X:341:G:O4'	2.16	0.45
2:X:1506:C:C4	2:X:1507:A:C6	3.05	0.45
2:X:1609:U:H2'	2:X:1610:G:H8	1.81	0.45
7:E:133:VAL:HG21	7:E:141:VAL:HA	1.98	0.45
15:N:105:ALA:HB1	16:O:40:PHE:HZ	1.81	0.45
16:O:14:VAL:HG12	16:O:20:ILE:HG21	1.98	0.45
23:V:18:ILE:O	23:V:22:LYS:HG3	2.17	0.45
2:X:434:G:C8	2:X:436:A:C8	3.05	0.45
2:X:1150:A:C8	2:X:1151:G:C8	3.03	0.45
2:X:1410:A:H2'	2:X:1411:G:O4'	2.15	0.45
2:X:1793:C:H2'	2:X:1794:C:C6	2.49	0.45
2:X:2776:A:O2'	7:E:63:THR:HG22	2.16	0.45
3:Y:21:G:N1	3:Y:22:G:O6	2.50	0.45
11:J:137:LEU:CB	20:S:77:TYR:OH	2.63	0.45
27:3:25:SER:C	27:3:26:ARG:HD3	2.41	0.45
2:X:59:U:H2'	2:X:74:U:H5	1.82	0.45
2:X:650:U:N3	2:X:666:A:C2	2.79	0.45
2:X:801:A:H2'	2:X:802:G:O4'	2.16	0.45
2:X:840:C:H2'	2:X:841:C:H6	1.81	0.45
2:X:1505:G:C8	2:X:1506:C:C5	3.05	0.45
2:X:2319:U:H2'	2:X:2320:C:H6	1.80	0.45
2:X:2361:U:O2'	2:X:2362:A:OP1	2.34	0.45
3:Y:4:G:C2	3:Y:112:G:C2	3.04	0.45
1:A:91:ILE:HG22	1:A:105:ILE:HA	1.99	0.45
2:X:734:A:H2'	2:X:735:C:C6	2.51	0.45
2:X:2804:G:H5''	2:X:2805:A:H5'	1.97	0.45
4:B:33:ASN:N	4:B:33:ASN:OD1	2.49	0.45
9:H:13:ASN:ND2	9:H:96:THR:H	2.15	0.45
17:P:72:LYS:HD3	17:P:108:SER:HB2	1.98	0.45
21:T:46:TYR:HD1	21:T:48:GLN:HE21	1.64	0.45
24:W:19:GLN:O	24:W:23:VAL:HG23	2.16	0.45
2:X:65:A:H1'	2:X:502:C:N4	2.32	0.45
2:X:683:G:C4	2:X:696:G:C2	3.05	0.45
2:X:784:A:H1'	2:X:785:C:H5	1.81	0.45
2:X:1301:U:OP1	25:Z:13:LYS:NZ	2.44	0.45
2:X:1575:A:H2'	2:X:1576:A:H5'	1.99	0.45
2:X:2831:G:H2'	2:X:2832:A:O4'	2.17	0.45
5:C:39:LEU:O	5:C:39:LEU:HD12	2.16	0.45
6:D:28:VAL:HA	6:D:29:PRO:HD3	1.82	0.45
12:K:23:SER:HA	12:K:26:ILE:HB	1.99	0.45
1:A:129:ALA:HA	1:A:191:THR:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:319:G:N2	2:X:320:U:O3'	2.49	0.45
2:X:1992:C:H5''	2:X:1993:A:H2'	1.99	0.45
2:X:2718:C:C4	2:X:2746:G:N2	2.85	0.45
3:Y:57:G:H3'	3:Y:58:G:C8	2.51	0.45
4:B:147:PHE:O	4:B:148:HIS:ND1	2.50	0.45
9:H:87:ILE:HD11	9:H:91:LYS:HA	1.99	0.45
2:X:201:C:H2'	2:X:202:A:H5''	1.98	0.45
2:X:1268:C:H2'	2:X:1269:A:C8	2.52	0.45
2:X:2318:U:O2'	2:X:2401:C:O2	2.35	0.45
2:X:2774:G:H2'	2:X:2775:A:C8	2.52	0.45
5:C:70:THR:HG22	5:C:72:ARG:HG3	1.99	0.45
15:N:92:ARG:O	15:N:94:MET:N	2.50	0.45
16:O:2:PHE:HE2	16:O:4:ILE:HD11	1.81	0.45
23:V:31:GLN:HB3	23:V:37:LEU:HG	1.99	0.45
2:X:327:G:O2'	2:X:328:G:H8	1.98	0.45
2:X:511:G:N2	2:X:729:G:H1'	2.32	0.45
2:X:529:A:H5''	19:R:45:GLN:CB	2.47	0.45
2:X:1065:A:C8	2:X:1065:A:C3'	3.00	0.45
2:X:2779:C:H3'	2:X:2780:A:H8	1.81	0.45
33:X:3495:SPD:H52	33:X:3495:SPD:H81	1.83	0.45
9:H:51:VAL:HG12	9:H:94:ARG:NH2	2.29	0.45
10:I:72:LYS:C	10:I:74:TYR:H	2.23	0.45
10:I:84:LYS:HG2	10:I:89:THR:HG22	1.99	0.45
11:J:115:ARG:CZ	11:J:131:PHE:HD2	2.30	0.45
16:O:20:ILE:CG2	16:O:97:ILE:HD11	2.47	0.45
21:T:71:ILE:HG12	21:T:72:ASP:N	2.32	0.45
2:X:901:G:H2'	2:X:902:A:C8	2.52	0.45
2:X:2811:U:H2'	2:X:2812:U:H6	1.81	0.45
2:X:2818:A:H2'	2:X:2819:C:O4'	2.17	0.45
4:B:116:ILE:HD12	4:B:211:ILE:CG2	2.47	0.45
5:C:149:PRO:HA	5:C:169:ASN:O	2.16	0.45
10:I:60:ARG:C	10:I:61:LEU:HG	2.42	0.45
1:A:91:ILE:HA	1:A:106:ALA:H	1.81	0.44
2:X:1854:U:H2'	2:X:1855:G:O4'	2.16	0.44
5:C:39:LEU:O	5:C:42:ALA:HB3	2.17	0.44
10:I:82:LEU:H	10:I:84:LYS:HE3	1.83	0.44
24:W:9:THR:HG21	24:W:55:THR:HG23	1.99	0.44
27:3:24:ARG:HG2	27:3:24:ARG:NH1	2.31	0.44
2:X:523:A:H2'	2:X:524:A:O4'	2.16	0.44
2:X:1257:G:OP1	15:N:19:LYS:HE2	2.17	0.44
2:X:1651:C:H5''	2:X:1652:A:H5'	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1979:A:C6	2:X:1980:A:N1	2.86	0.44
2:X:2004:A:N6	2:X:2005:A:C6	2.85	0.44
2:X:2572:G:H2'	2:X:2573:U:O4'	2.17	0.44
2:X:2903:A:C5'	2:X:2904:U:H5'	2.47	0.44
5:C:7:LEU:HD21	5:C:126:VAL:H	1.81	0.44
8:G:63:ILE:HD12	8:G:63:ILE:HA	1.77	0.44
2:X:59:U:O2'	2:X:73:A:H2'	2.18	0.44
2:X:249:C:H4'	2:X:431:C:O2'	2.18	0.44
2:X:624:C:OP1	15:N:33:LYS:HG3	2.18	0.44
2:X:1038:C:H1'	16:O:10:LYS:HE3	1.99	0.44
2:X:1208:A:H2'	2:X:1209:U:C6	2.53	0.44
2:X:1212:U:H2'	2:X:1213:C:O4'	2.18	0.44
2:X:1295:C:H1'	5:C:83:TRP:HA	1.99	0.44
2:X:1365:G:H2'	2:X:1367:C:C5	2.52	0.44
2:X:1377:U:H4'	2:X:1378:U:OP2	2.17	0.44
2:X:1986:G:C6	2:X:1987:A:C5	3.06	0.44
2:X:2125:U:H2'	2:X:2126:C:O4'	2.17	0.44
3:Y:3:U:H2'	3:Y:4:G:C8	2.53	0.44
7:E:30:LYS:H	7:E:35:ARG:CB	2.30	0.44
17:P:40:ASN:HD22	17:P:40:ASN:H	1.64	0.44
18:Q:3:ALA:HB1	18:Q:41:ALA:HB2	1.97	0.44
2:X:51:G:O2'	2:X:118:A:N6	2.50	0.44
2:X:591:A:H4'	2:X:592:A:C5'	2.40	0.44
2:X:614:U:C4	2:X:618:A:C4	3.06	0.44
2:X:963:A:H4'	3:Y:94:U:O2	2.18	0.44
2:X:2642:U:N1	25:Z:4:PRO:HA	2.33	0.44
2:X:2817:A:C2	2:X:2827:A:C2	3.06	0.44
4:B:22:LEU:N	9:H:72:ASN:O	2.45	0.44
5:C:57:VAL:C	5:C:59:GLY:H	2.25	0.44
5:C:148:GLN:N	5:C:148:GLN:OE1	2.49	0.44
12:K:109:ARG:HD3	12:K:112:ASP:OD1	2.17	0.44
13:L:54:ALA:HB1	13:L:76:VAL:HG23	1.99	0.44
22:U:29:TRP:CG	22:U:30:ASN:H	2.36	0.44
2:X:15:G:O2'	25:Z:18:THR:HG21	2.17	0.44
2:X:810:A:H2'	2:X:811:C:H6	1.82	0.44
2:X:1424:A:H5'	2:X:1512:U:H1'	1.99	0.44
2:X:1463:A:H3'	2:X:1464:U:H5''	1.98	0.44
2:X:1478:A:H61	2:X:1605:A:N6	2.16	0.44
2:X:1561:G:C8	2:X:1562:C:C6	3.06	0.44
2:X:1701:U:H2'	2:X:1702:C:H6	1.83	0.44
2:X:2449:C:H6	2:X:2449:C:H2'	1.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:2871:A:H2'	2:X:2872:G:C8	2.52	0.44
7:E:63:THR:OG1	7:E:64:ASN:N	2.50	0.44
11:J:39:THR:CG2	11:J:99:PRO:HD2	2.47	0.44
11:J:43:THR:HG22	11:J:46:GLN:OE1	2.18	0.44
19:R:77:GLU:HA	19:R:78:PRO:HD3	1.83	0.44
2:X:218:G:C4'	2:X:219:A:H4'	2.48	0.44
2:X:906:A:H2'	2:X:907:G:O4'	2.17	0.44
2:X:1091:G:H2'	2:X:1154:G:N1	2.32	0.44
2:X:1515:G:N2	2:X:1516:C:C2	2.86	0.44
2:X:2670:G:C2	2:X:2799:C:C2	3.06	0.44
2:X:2724:G:H2'	2:X:2725:U:O4'	2.17	0.44
8:G:38:ARG:HA	8:G:119:GLN:NE2	2.32	0.44
9:H:102:VAL:HG13	9:H:106:LEU:HD12	1.99	0.44
17:P:10:ILE:HD13	17:P:10:ILE:HA	1.78	0.44
20:S:78:GLN:HB2	20:S:87:THR:O	2.17	0.44
26:2:15:LYS:O	26:2:16:VAL:HB	2.17	0.44
27:3:53:SER:O	27:3:54:ASP:C	2.61	0.44
2:X:424:C:N4	2:X:425:G:O6	2.50	0.44
2:X:658:A:H3'	2:X:659:A:H5''	1.99	0.44
2:X:675:G:N2	2:X:677:A:H3'	2.33	0.44
2:X:818:U:O2	2:X:823:G:O2'	2.31	0.44
2:X:840:C:H2'	2:X:841:C:C6	2.52	0.44
2:X:868:A:C6	2:X:869:G:C6	3.06	0.44
2:X:908:A:O4'	3:Y:96:G:N2	2.43	0.44
2:X:994:A:H2'	2:X:995:U:O4'	2.17	0.44
2:X:2734:C:O3'	12:K:64:LYS:HG3	2.17	0.44
2:X:2859:G:H21	12:K:98:GLY:HA3	1.83	0.44
5:C:146:LEU:HD22	5:C:146:LEU:HA	1.82	0.44
1:A:144:ILE:HB	1:A:154:ILE:HB	2.00	0.44
2:X:31:C:C4	2:X:32:C:C5	3.06	0.44
2:X:799:U:H4'	2:X:1310:A:H61	1.81	0.44
2:X:1468:G:H2'	2:X:1469:G:O4'	2.17	0.44
2:X:1677:G:C6	2:X:1679:A:C4	3.06	0.44
2:X:2757:U:H2'	2:X:2758:G:C8	2.53	0.44
2:X:2768:A:H2'	2:X:2769:G:O4'	2.18	0.44
4:B:59:TYR:C	4:B:61:LYS:N	2.76	0.44
5:C:96:SER:O	5:C:98:ALA:N	2.50	0.44
14:M:94:VAL:CG1	14:M:99:LEU:HD21	2.48	0.44
20:S:127:ASN:HA	20:S:160:LYS:O	2.16	0.44
2:X:168:A:H3'	2:X:169:G:H5'	1.99	0.44
2:X:534:G:OP2	33:X:3497:SPD:H22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:660:A:H1'	2:X:661:U:O5'	2.17	0.44
2:X:1039:C:OP1	8:G:1:MET:HE2	2.18	0.44
2:X:1492:G:O2'	2:X:1574:G:N3	2.51	0.44
2:X:2848:G:C2	2:X:2849:A:N7	2.86	0.44
5:C:22:ALA:O	5:C:111:ARG:HD3	2.18	0.44
8:G:58:ILE:HD12	8:G:58:ILE:HA	1.67	0.44
9:H:10:VAL:HA	9:H:84:CYS:O	2.18	0.44
13:L:73:ALA:HB2	13:L:103:GLY:O	2.18	0.44
14:M:50:ILE:HD12	14:M:50:ILE:HG23	1.63	0.44
20:S:46:VAL:O	20:S:50:LYS:HG3	2.17	0.44
24:W:3:LYS:HG2	24:W:38:GLU:HA	1.99	0.44
24:W:15:ARG:NH1	24:W:15:ARG:HB3	2.33	0.44
2:X:396:G:H2'	2:X:397:U:H5'	1.99	0.43
2:X:615:A:H2'	2:X:615:A:N3	2.33	0.43
2:X:1751:G:N7	32:X:3010:MPD:H11	2.33	0.43
2:X:2079:G:H4'	4:B:156:MET:O	2.18	0.43
2:X:2089:A:H8	31:X:3003:62B:N1	2.15	0.43
2:X:2218:G:H2'	2:X:2219:C:C6	2.53	0.43
2:X:2269:G:H2'	2:X:2270:U:O4'	2.18	0.43
5:C:57:VAL:O	5:C:59:GLY:N	2.44	0.43
15:N:33:LYS:O	15:N:37:GLN:HG3	2.18	0.43
2:X:17:G:P	25:Z:11:THR:HG22	2.58	0.43
2:X:328:G:N2	2:X:399:U:O2	2.45	0.43
2:X:410:G:H21	2:X:411:A:H62	1.65	0.43
2:X:1351:C:OP1	2:X:1352:C:OP2	2.35	0.43
2:X:1629:U:H2'	2:X:1630:A:H5''	2.00	0.43
2:X:2298:G:H5'	21:T:28:ARG:HD3	2.00	0.43
2:X:2360:A:H5'	2:X:2362:A:H1'	2.00	0.43
16:O:12:ILE:HD13	16:O:12:ILE:HA	1.54	0.43
17:P:19:LEU:HD23	17:P:19:LEU:HA	1.87	0.43
2:X:767:A:H2'	2:X:768:A:C8	2.52	0.43
2:X:2617:A:H2'	2:X:2618:C:C6	2.54	0.43
4:B:198:LYS:HE3	4:B:198:LYS:HB2	1.89	0.43
5:C:49:HIS:O	5:C:49:HIS:ND1	2.46	0.43
12:K:38:LYS:HB3	12:K:41:ARG:NH2	2.34	0.43
14:M:57:VAL:HG12	14:M:58:SER:N	2.33	0.43
2:X:32:C:N4	2:X:33:U:O4	2.52	0.43
2:X:327:G:H2'	2:X:327:G:N3	2.33	0.43
2:X:509:G:N2	2:X:513:G:C5	2.86	0.43
2:X:1054:A:N3	2:X:1197:C:H1'	2.33	0.43
2:X:1072:A:N6	2:X:1169:G:H2'	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1527:A:H2	2:X:1549:C:N3	2.16	0.43
2:X:2098:A:H2'	2:X:2099:G:C8	2.53	0.43
2:X:2344:C:H2'	2:X:2345:A:O4'	2.18	0.43
2:X:2660:A:H2'	2:X:2661:A:O4'	2.18	0.43
3:Y:81:A:H61	3:Y:90:C:H42	1.66	0.43
6:D:101:ASP:C	6:D:103:LEU:H	2.24	0.43
9:H:117:LEU:O	9:H:117:LEU:HD23	2.18	0.43
17:P:72:LYS:HB2	17:P:108:SER:HB2	1.99	0.43
19:R:12:ILE:H	19:R:67:ASN:HA	1.83	0.43
1:A:13:ARG:HA	1:A:16:MET:HG3	2.00	0.43
2:X:291:G:H2'	2:X:292:U:H6	1.84	0.43
2:X:327:G:O2'	2:X:328:G:O5'	2.33	0.43
2:X:896:U:H2'	2:X:897:A:C8	2.54	0.43
2:X:1035:C:H2'	2:X:1036:C:H6	1.84	0.43
2:X:1042:C:P	15:N:92:ARG:HH22	2.42	0.43
2:X:1185:U:H2'	8:G:66:THR:HG22	2.00	0.43
2:X:1304:G:OP2	25:Z:16:ARG:NH1	2.52	0.43
2:X:1885:G:H1'	2:X:1911:A:N6	2.32	0.43
2:X:2883:U:H2'	2:X:2884:G:C8	2.54	0.43
3:Y:74:G:H1	3:Y:97:A:N6	2.15	0.43
4:B:140:PRO:HG2	4:B:145:SER:CB	2.47	0.43
10:I:70:ASN:C	10:I:72:LYS:N	2.76	0.43
12:K:8:ARG:NH1	12:K:16:MET:SD	2.91	0.43
13:L:14:ARG:O	13:L:18:VAL:HG23	2.19	0.43
15:N:116:ALA:C	15:N:117:LEU:HG	2.43	0.43
1:A:106:ALA:HA	1:A:107:PRO:HD3	1.77	0.43
2:X:142:G:H5'	2:X:143:U:OP2	2.18	0.43
2:X:150:A:C6	2:X:151:U:C4	3.06	0.43
2:X:642:U:O2'	2:X:643:G:H5'	2.19	0.43
2:X:691:A:H2	2:X:2376:G:H21	1.66	0.43
2:X:1229:G:OP1	10:I:31:SER:HA	2.18	0.43
2:X:1526:G:N7	2:X:1527:A:N1	2.67	0.43
2:X:1565:U:H2'	2:X:1566:G:O4'	2.18	0.43
3:Y:3:U:O2'	3:Y:25:A:N3	2.50	0.43
3:Y:49:G:C6	3:Y:50:A:C6	3.07	0.43
8:G:40:LYS:HB3	8:G:40:LYS:HE2	1.82	0.43
11:J:98:LYS:HA	11:J:99:PRO:HD2	1.70	0.43
19:R:25:ALA:HB3	19:R:34:VAL:HG23	1.99	0.43
2:X:114:C:H2'	2:X:115:C:H6	1.82	0.43
2:X:224:A:O4'	2:X:236:A:H1'	2.18	0.43
2:X:683:G:C5	2:X:696:G:N1	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1000:G:C4'	11:J:83:MET:HE1	2.48	0.43
2:X:1356:G:C5	2:X:1357:G:C6	3.07	0.43
2:X:1397:G:C6	2:X:1398:G:H1'	2.54	0.43
2:X:1683:U:C2'	2:X:1684:A:H5''	2.47	0.43
2:X:2283:G:H2'	2:X:2284:U:O4'	2.18	0.43
2:X:2514:G:H2'	2:X:2515:A:C8	2.54	0.43
2:X:2652:G:H2'	2:X:2653:C:C6	2.53	0.43
2:X:2712:G:O6	32:X:3005:MPD:O4	2.34	0.43
5:C:117:LYS:HD3	5:C:117:LYS:HA	1.80	0.43
6:D:130:LEU:HD13	6:D:130:LEU:HA	1.68	0.43
10:I:19:VAL:HG22	10:I:27:ASN:HB3	2.01	0.43
18:Q:14:GLU:OE1	18:Q:14:GLU:N	2.39	0.43
2:X:974:U:H2'	2:X:975:U:O4'	2.19	0.43
2:X:1361:G:H1'	2:X:1660:A:N6	2.34	0.43
2:X:1975:G:H1	2:X:1985:C:H42	1.65	0.43
2:X:2820:U:H1'	2:X:2824:G:N2	2.34	0.43
7:E:65:HIS:HA	7:E:68:THR:OG1	2.18	0.43
10:I:19:VAL:CG1	10:I:30:THR:HG23	2.49	0.43
11:J:37:THR:HG21	11:J:130:LYS:HE3	2.01	0.43
12:K:44:VAL:O	12:K:48:ILE:HG23	2.18	0.43
15:N:70:ARG:HD2	15:N:70:ARG:HA	1.81	0.43
15:N:92:ARG:HG2	15:N:92:ARG:H	1.72	0.43
2:X:312:A:N3	2:X:312:A:H2'	2.33	0.43
2:X:691:A:H3'	2:X:692:G:H8	1.84	0.43
2:X:903:G:N3	2:X:2295:A:H2'	2.34	0.43
2:X:1723:A:O5'	2:X:1723:A:H8	2.02	0.43
2:X:2801:C:H2'	2:X:2802:A:O4'	2.19	0.43
5:C:74:ARG:C	5:C:75:GLN:HG2	2.43	0.43
5:C:136:THR:HG22	5:C:140:LYS:HZ2	1.81	0.43
10:I:110:LYS:HA	10:I:129:SER:CB	2.49	0.43
15:N:31:LEU:HD23	15:N:31:LEU:N	2.34	0.43
16:O:8:GLY:C	16:O:10:LYS:H	2.26	0.43
21:T:80:LYS:HB2	21:T:84:LYS:O	2.19	0.43
2:X:53:A:H2'	2:X:54:G:O4'	2.19	0.43
2:X:192:G:O6	2:X:208:G:O2'	2.28	0.43
2:X:784:A:H8	2:X:784:A:H5''	1.84	0.43
2:X:1373:U:H2'	2:X:1374:G:O4'	2.17	0.43
2:X:1561:G:H8	2:X:1562:C:C6	2.36	0.43
2:X:2000:G:H2'	2:X:2001:C:C6	2.54	0.43
2:X:2314:A:C6	2:X:2316:G:C5	3.07	0.43
2:X:2446:U:O4	27:3:28:PHE:CD1	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:2775:A:H1'	7:E:67:THR:CG2	2.38	0.43
7:E:60:GLU:O	7:E:63:THR:HG23	2.18	0.43
8:G:30:SER:HA	8:G:106:ILE:HG12	2.01	0.43
9:H:25:LEU:HA	9:H:25:LEU:HD23	1.67	0.43
2:X:514:G:OP2	26:2:38:LYS:HE3	2.19	0.42
2:X:631:U:H1'	5:C:90:PHE:CD1	2.53	0.42
2:X:862:C:O2'	2:X:884:U:H5''	2.19	0.42
2:X:1599:G:H2'	2:X:1599:G:N3	2.34	0.42
2:X:2783:U:H5''	28:4:19:ARG:HA	2.00	0.42
2:X:2794:C:H41	32:X:3008:MPD:C1	2.32	0.42
33:X:3497:SPD:HN11	33:X:3497:SPD:H51	1.84	0.42
3:Y:68:A:N1	3:Y:103:A:N1	2.66	0.42
14:M:106:ARG:HA	14:M:106:ARG:NE	2.34	0.42
19:R:71:LEU:CB	19:R:73:PRO:HD2	2.49	0.42
23:V:10:THR:C	23:V:12:SER:H	2.18	0.42
24:W:8:LEU:O	24:W:32:ASN:N	2.42	0.42
28:4:25:VAL:N	28:4:34:GLN:O	2.52	0.42
1:A:20:ASP:O	1:A:22:ALA:N	2.47	0.42
2:X:183:A:OP2	2:X:183:A:H3'	2.20	0.42
2:X:428:G:N2	2:X:429:C:H1'	2.34	0.42
2:X:1490:G:C5	2:X:1509:G:N2	2.87	0.42
2:X:1521:A:N7	2:X:1561:G:N1	2.68	0.42
2:X:1528:G:C8	2:X:1529:U:C4	3.07	0.42
2:X:1732:U:O2	2:X:1744:A:H5'	2.19	0.42
2:X:1771:A:O2'	2:X:1772:G:O5'	2.36	0.42
2:X:2848:G:N3	2:X:2849:A:C8	2.87	0.42
3:Y:111:A:H2'	3:Y:112:G:O4'	2.18	0.42
8:G:99:GLU:O	8:G:103:GLU:HB2	2.18	0.42
15:N:60:LEU:O	15:N:61:TRP:C	2.62	0.42
15:N:95:LEU:HD12	15:N:95:LEU:HA	1.75	0.42
20:S:108:LEU:HB3	20:S:109:VAL:H	1.57	0.42
2:X:774:G:H5''	2:X:775:A:H5''	2.02	0.42
2:X:868:A:H2'	2:X:869:G:H8	1.84	0.42
2:X:1039:C:C4	8:G:1:MET:HA	2.54	0.42
2:X:1512:U:H2'	2:X:1513:A:H8	1.84	0.42
2:X:1735:C:O2	2:X:1740:G:N2	2.48	0.42
2:X:2092:C:H1'	2:X:2476:U:H3	1.83	0.42
2:X:2518:U:O2	2:X:2518:U:H2'	2.19	0.42
3:Y:21:G:N2	3:Y:58:G:N2	2.66	0.42
7:E:157:TYR:C	7:E:159:GLY:H	2.28	0.42
8:G:136:GLN:N	8:G:136:GLN:CD	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:63:VAL:HB	9:H:106:LEU:CD1	2.50	0.42
16:O:74:PHE:CE1	16:O:83:LYS:HB2	2.52	0.42
20:S:105:PRO:CD	20:S:124:PRO:HA	2.50	0.42
24:W:15:ARG:HB3	24:W:15:ARG:HH11	1.84	0.42
2:X:563:G:H4'	17:P:18:ARG:NE	2.34	0.42
2:X:684:U:H2'	2:X:685:C:C6	2.54	0.42
2:X:874:A:N7	2:X:2274:A:O2'	2.52	0.42
2:X:1491:C:H4'	2:X:1593:G:H5''	2.02	0.42
2:X:1962:G:H1'	2:X:1991:G:N2	2.35	0.42
2:X:2482:G:H2'	2:X:2483:C:C6	2.55	0.42
5:C:102:PRO:HD2	5:C:105:MET:HE2	2.01	0.42
8:G:59:ASN:OD1	8:G:129:ALA:HB2	2.18	0.42
23:V:46:VAL:O	23:V:50:ILE:HG13	2.19	0.42
2:X:92:G:H2'	2:X:93:U:C6	2.55	0.42
2:X:537:A:H2'	2:X:538:G:O4'	2.20	0.42
2:X:738:U:H1'	2:X:1391:A:H1'	2.00	0.42
2:X:2000:G:H2'	2:X:2001:C:H6	1.85	0.42
8:G:39:GLY:C	8:G:41:ASN:N	2.72	0.42
9:H:14:SER:O	9:H:52:VAL:HG22	2.19	0.42
9:H:24:VAL:HG12	9:H:33:ALA:HB2	2.01	0.42
9:H:87:ILE:HG12	9:H:88:ARG:N	2.32	0.42
10:I:19:VAL:CG2	10:I:27:ASN:HB3	2.49	0.42
21:T:82:ARG:HG2	21:T:83:ASP:N	2.34	0.42
2:X:924:G:N2	2:X:925:G:N7	2.67	0.42
2:X:2747:U:H2'	2:X:2748:A:H8	1.83	0.42
3:Y:46:A:H2'	3:Y:47:C:O4'	2.19	0.42
5:C:123:LEU:O	5:C:188:ASN:HA	2.19	0.42
17:P:72:LYS:N	17:P:106:VAL:O	2.46	0.42
19:R:7:ASP:N	19:R:23:VAL:HG13	2.35	0.42
2:X:152:C:C2'	2:X:153:G:H5'	2.50	0.42
2:X:443:U:H2'	2:X:444:C:C6	2.54	0.42
2:X:672:A:H4'	2:X:673:G:H5'	2.02	0.42
2:X:690:U:H5''	2:X:691:A:OP2	2.20	0.42
2:X:879:U:C2	2:X:880:A:C8	3.08	0.42
2:X:1595:C:C2	2:X:1596:G:C8	3.07	0.42
2:X:1881:A:C8	2:X:1882:G:C8	3.07	0.42
2:X:1905:G:H2'	2:X:1906:C:O4'	2.18	0.42
2:X:2398:G:H2'	2:X:2399:G:O4'	2.20	0.42
2:X:2580:G:H5''	2:X:2581:U:OP2	2.20	0.42
3:Y:92:G:O5'	3:Y:92:G:H8	2.02	0.42
4:B:26:THR:HG21	4:B:201:VAL:CG1	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:158:LYS:O	7:E:160:LYS:N	2.52	0.42
9:H:33:ALA:HB1	9:H:37:ASP:HB3	2.00	0.42
10:I:33:ARG:O	10:I:33:ARG:HG3	2.16	0.42
18:Q:63:LYS:N	18:Q:70:GLY:O	2.52	0.42
21:T:46:TYR:CD1	21:T:48:GLN:NE2	2.88	0.42
27:3:44:LEU:HD23	27:3:45:ARG:H	1.85	0.42
1:A:157:SER:HB3	2:X:1846:A:H5'	2.01	0.42
2:X:727:G:H5'	26:2:27:ASN:ND2	2.35	0.42
2:X:1059:A:O2'	2:X:1060:U:H5'	2.20	0.42
2:X:1168:C:H2'	2:X:1169:G:O4'	2.18	0.42
2:X:1217:U:H6	2:X:1217:U:H2'	1.63	0.42
2:X:1612:C:O2'	2:X:1613:G:H5''	2.18	0.42
2:X:2466:A:O2'	2:X:2627:A:OP1	2.32	0.42
2:X:2679:U:H2'	2:X:2680:U:O4'	2.19	0.42
2:X:2681:A:N1	2:X:2692:A:H5''	2.34	0.42
3:Y:4:G:N2	3:Y:111:A:N7	2.60	0.42
5:C:163:VAL:HG13	5:C:164:GLU:N	2.35	0.42
6:D:34:ILE:HA	6:D:148:LYS:HA	2.02	0.42
8:G:42:LYS:HB2	8:G:44:THR:HG23	2.00	0.42
8:G:46:THR:HB	15:N:64:ARG:HH21	1.85	0.42
12:K:47:LEU:HD23	12:K:47:LEU:HA	1.89	0.42
13:L:44:ILE:HB	13:L:54:ALA:HB2	2.02	0.42
15:N:65:ILE:HG21	15:N:80:MET:CE	2.50	0.42
23:V:28:LEU:HD11	23:V:42:ARG:HG2	2.01	0.42
23:V:38:GLU:H	23:V:38:GLU:HG3	1.52	0.42
2:X:1064:A:C2	2:X:1185:U:C2	3.08	0.42
2:X:1682:C:H4'	2:X:2737:C:O2	2.20	0.42
2:X:1734:A:H62	2:X:1741:G:H21	1.67	0.42
2:X:1805:U:H3'	2:X:1811:A:N6	2.35	0.42
2:X:2065:G:H2'	2:X:2066:G:O4'	2.20	0.42
4:B:122:SER:O	4:B:123:LYS:C	2.63	0.42
5:C:34:PHE:HB2	10:I:1:MET:HE3	2.01	0.42
6:D:114:PHE:CB	6:D:120:LYS:HA	2.49	0.42
21:T:88:SER:HB2	21:T:90:TYR:CE1	2.54	0.42
27:3:54:ASP:HB3	27:3:55:MET:H	1.48	0.42
1:A:17:THR:HG23	1:A:204:ASN:HD22	1.84	0.42
2:X:674:C:H4'	2:X:695:C:O2	2.20	0.42
2:X:956:A:C5	11:J:11:ARG:HD2	2.55	0.42
2:X:1504:U:O2'	2:X:1505:G:O5'	2.37	0.42
2:X:1724:U:N3	2:X:1791:G:OP2	2.52	0.42
2:X:1770:C:O2'	2:X:1771:A:H5'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1770:C:H1'	2:X:1771:A:H5'	2.02	0.42
2:X:1805:U:N3	2:X:1811:A:C8	2.88	0.42
2:X:1857:C:O5'	2:X:1857:C:H6	2.03	0.42
2:X:2343:U:H2'	2:X:2344:C:C6	2.55	0.42
2:X:2757:U:H2'	2:X:2758:G:H8	1.84	0.42
33:X:3497:SPD:H52	33:X:3497:SPD:H81	1.82	0.42
4:B:16:PHE:H	14:M:14:GLN:NE2	2.17	0.42
5:C:19:LEU:HA	5:C:19:LEU:HD23	1.85	0.42
2:X:329:A:N3	2:X:329:A:H2'	2.35	0.41
2:X:629:A:N6	2:X:1289:A:H2	2.08	0.41
2:X:817:G:O2'	2:X:818:U:H5'	2.20	0.41
2:X:877:G:H2'	2:X:878:C:C6	2.55	0.41
2:X:1731:G:N3	2:X:1746:G:N2	2.68	0.41
2:X:2649:U:H5'	4:B:172:ARG:HG3	2.01	0.41
2:X:2758:G:OP1	4:B:182:ASN:ND2	2.34	0.41
24:W:17:GLU:O	24:W:21:LYS:HG3	2.19	0.41
1:A:71:LYS:O	1:A:96:TYR:OH	2.30	0.41
2:X:169:G:H2'	2:X:169:G:N3	2.34	0.41
2:X:332:A:H61	2:X:394:U:H3	1.68	0.41
2:X:1573:A:C2	2:X:1592:A:C8	3.08	0.41
2:X:1967:U:C4	2:X:1991:G:H4'	2.55	0.41
2:X:2257:G:H2'	2:X:2258:U:C6	2.55	0.41
2:X:2424:G:C6	2:X:2425:U:C4	3.08	0.41
4:B:118:VAL:HB	4:B:201:VAL:HG23	2.00	0.41
8:G:36:ILE:HD13	8:G:36:ILE:N	2.35	0.41
10:I:36:LYS:NZ	10:I:42:SER:O	2.53	0.41
18:Q:67:ARG:HD2	18:Q:68:TYR:CE1	2.55	0.41
2:X:70:G:N2	2:X:71:A:N1	2.68	0.41
2:X:510:U:C2	2:X:833:A:C6	3.08	0.41
2:X:1288:G:N7	10:I:18:ARG:NH2	2.64	0.41
2:X:1423:C:H2'	2:X:1424:A:C8	2.56	0.41
2:X:2431:C:H2'	2:X:2432:G:O4'	2.19	0.41
5:C:133:ALA:C	5:C:135:LYS:H	2.28	0.41
5:C:136:THR:O	5:C:140:LYS:HD2	2.21	0.41
8:G:38:ARG:NH1	8:G:111:PRO:HG3	2.35	0.41
8:G:69:LYS:C	8:G:71:THR:N	2.75	0.41
14:M:61:PHE:O	14:M:75:THR:HA	2.20	0.41
15:N:83:LEU:HD23	15:N:83:LEU:HA	1.90	0.41
20:S:107:GLN:HA	20:S:138:PRO:HG2	2.01	0.41
23:V:45:THR:HA	23:V:48:LYS:HD2	2.01	0.41
2:X:59:U:H1'	2:X:73:A:C4	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:187:C:C2	2:X:188:C:C5	3.07	0.41
2:X:375:A:C5	2:X:378:C:C4	3.08	0.41
2:X:984:G:O6	33:X:3495:SPD:H32	2.21	0.41
2:X:1091:G:H4'	2:X:1092:A:O5'	2.20	0.41
2:X:1835:U:H2'	2:X:1836:A:C5'	2.50	0.41
2:X:2333:U:OP2	2:X:2334:G:N1	2.53	0.41
2:X:2489:U:H2'	2:X:2490:C:O4'	2.21	0.41
2:X:2714:U:H2'	2:X:2715:G:O4'	2.21	0.41
2:X:2774:G:N2	2:X:2775:A:N6	2.68	0.41
2:X:2851:G:OP2	4:B:65:SER:HB2	2.21	0.41
2:X:2886:G:C2	2:X:2888:A:H1'	2.56	0.41
4:B:13:THR:O	4:B:25:VAL:HG12	2.20	0.41
4:B:178:VAL:HG12	4:B:202:PRO:HG3	2.01	0.41
5:C:78:ILE:HD13	5:C:78:ILE:H	1.85	0.41
5:C:103:LYS:HA	5:C:106:ARG:CD	2.50	0.41
9:H:91:LYS:HD2	9:H:111:PHE:CE1	2.55	0.41
12:K:17:LEU:HD23	12:K:17:LEU:HA	1.85	0.41
15:N:9:VAL:H	15:N:9:VAL:HG22	1.57	0.41
2:X:152:C:H2'	2:X:153:G:H5'	2.02	0.41
2:X:426:G:C6	2:X:427:A:C5	3.08	0.41
2:X:529:A:H3'	2:X:530:C:C6	2.56	0.41
2:X:627:C:H5	35:N:201:EPE:C10	2.33	0.41
2:X:1151:G:H2'	2:X:1152:U:C6	2.54	0.41
2:X:1508:C:O2'	2:X:1509:G:P	2.78	0.41
2:X:1550:G:H8	2:X:1550:G:H3'	1.85	0.41
2:X:1979:A:OP1	9:H:42:THR:OG1	2.29	0.41
2:X:2803:A:C6	2:X:2809:G:H1'	2.55	0.41
2:X:2856:U:C2	2:X:2857:A:N7	2.89	0.41
3:Y:90:C:H2'	3:Y:91:C:H6	1.84	0.41
8:G:102:ILE:HB	8:G:125:VAL:HG11	2.02	0.41
12:K:20:LEU:HB3	12:K:40:VAL:HG21	2.02	0.41
1:A:85:PRO:HB3	2:X:1614:A:H2'	2.03	0.41
2:X:626:G:P	35:N:201:EPE:H62	2.61	0.41
2:X:796:A:C6	2:X:834:A:C5	3.09	0.41
2:X:1241:A:C6	2:X:1242:A:C6	3.08	0.41
2:X:1271:G:H2'	2:X:1272:U:H6	1.86	0.41
2:X:1325:U:C2	2:X:1364:C:O2	2.74	0.41
2:X:1326:C:H2'	2:X:1327:C:H6	1.86	0.41
2:X:1441:C:H5'	2:X:1514:A:O2'	2.21	0.41
11:J:39:THR:HG22	11:J:98:LYS:HA	2.02	0.41
11:J:57:TYR:HE1	11:J:113:VAL:HG13	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:1:MET:HB3	17:P:2:GLU:H	1.59	0.41
1:A:252:LYS:HA	1:A:253:PRO:HD3	1.84	0.41
2:X:24:G:H2'	2:X:25:U:C6	2.56	0.41
2:X:156:A:H61	2:X:172:U:H3	1.69	0.41
2:X:228:A:C6	2:X:229:A:H1'	2.56	0.41
2:X:968:A:C2'	2:X:969:A:H5'	2.51	0.41
2:X:974:U:O2'	24:W:25:ALA:O	2.23	0.41
2:X:1065:A:H3'	2:X:1065:A:H8	1.83	0.41
2:X:1089:C:H4'	2:X:1090:A:H5''	2.03	0.41
2:X:1526:G:N7	2:X:1527:A:C6	2.88	0.41
2:X:1548:U:H5''	2:X:1549:C:OP2	2.20	0.41
2:X:1982:U:H5	2:X:2584:G:N2	2.18	0.41
2:X:2097:G:C6	2:X:2098:A:C5	3.08	0.41
2:X:2342:U:H2'	2:X:2343:U:C6	2.56	0.41
2:X:2607:U:C5	2:X:2608:G:C6	3.09	0.41
4:B:133:ARG:NH1	4:B:171:GLY:N	2.69	0.41
13:L:73:ALA:HB1	13:L:107:ALA:CB	2.48	0.41
14:M:34:ILE:O	14:M:40:GLU:HA	2.20	0.41
16:O:78:ARG:HD3	16:O:79:ARG:NH2	2.36	0.41
2:X:608:C:H2'	2:X:609:U:O4'	2.21	0.41
2:X:970:U:H6	2:X:970:U:H2'	1.75	0.41
2:X:1352:C:H42	2:X:1374:G:H1	1.69	0.41
2:X:1550:G:H3'	2:X:1550:G:C8	2.56	0.41
2:X:2000:G:C6	2:X:2001:C:C4	3.08	0.41
2:X:2819:C:N4	2:X:2824:G:H1	2.17	0.41
2:X:2837:U:O2	2:X:2856:U:H1'	2.21	0.41
15:N:35:ALA:O	15:N:39:VAL:HG23	2.21	0.41
17:P:13:ALA:HA	17:P:14:PRO:HD3	1.87	0.41
17:P:29:ALA:O	17:P:33:ILE:HG13	2.20	0.41
17:P:69:LEU:HD23	17:P:69:LEU:HA	1.82	0.41
2:X:56:A:C6	2:X:57:C:C4	3.09	0.41
2:X:124:A:C6	26:2:11:ARG:HD3	2.56	0.41
2:X:394:U:H2'	2:X:395:U:H6	1.86	0.41
2:X:1392:G:C5	2:X:1393:C:C5	3.09	0.41
2:X:1476:G:H2'	2:X:1477:U:C6	2.55	0.41
2:X:1699:A:C8	2:X:1700:C:C5	3.09	0.41
2:X:1871:U:C2	2:X:1872:G:C8	3.09	0.41
2:X:1994:C:C4	2:X:1995:G:C5	3.09	0.41
2:X:2075:G:O4'	2:X:2843:A:C6	2.74	0.41
2:X:2532:G:O2'	2:X:2533:U:H5'	2.21	0.41
3:Y:57:G:H3'	3:Y:58:G:H8	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:141:MET:HG3	4:B:148:HIS:CE1	2.55	0.41
8:G:12:ILE:HG12	8:G:13:GLU:N	2.33	0.41
11:J:55:THR:CG2	11:J:64:VAL:HG11	2.50	0.41
12:K:18:ARG:HB2	12:K:67:ARG:HD3	2.03	0.41
13:L:102:HIS:C	13:L:104:ARG:H	2.29	0.41
16:O:70:LYS:HD2	16:O:87:GLY:HA3	2.03	0.41
20:S:34:TYR:CD1	20:S:95:ASN:HB2	2.56	0.41
21:T:70:LYS:HE3	21:T:70:LYS:HB2	1.75	0.41
2:X:666:A:N3	2:X:666:A:O4'	2.53	0.41
2:X:1252:A:H2'	2:X:1253:G:O4'	2.21	0.41
2:X:1482:U:H2'	2:X:1483:A:H8	1.86	0.41
2:X:2306:G:C6	2:X:2307:G:C5	3.08	0.41
2:X:2437:G:H2'	2:X:2438:A:O4'	2.21	0.41
3:Y:100:A:O2'	3:Y:101:G:H5'	2.20	0.41
8:G:33:VAL:HG11	8:G:106:ILE:HD13	2.03	0.41
17:P:3:ALA:HB3	17:P:58:ALA:HB2	2.01	0.41
17:P:80:PRO:O	17:P:100:THR:OG1	2.28	0.41
20:S:17:ASP:O	20:S:20:GLN:HB2	2.20	0.41
21:T:51:THR:HB	21:T:54:TYR:CE1	2.56	0.41
27:3:20:GLY:O	27:3:45:ARG:HA	2.21	0.41
2:X:5:A:C2	2:X:2918:A:C2	3.09	0.40
2:X:250:G:H4'	2:X:432:G:C5	2.56	0.40
2:X:804:G:C2'	2:X:805:G:H5'	2.51	0.40
2:X:1228:A:H2'	2:X:1229:G:O4'	2.21	0.40
2:X:1486:C:N3	2:X:1487:G:C6	2.89	0.40
2:X:1515:G:O2'	2:X:1516:C:P	2.78	0.40
2:X:2500:U:OP1	2:X:2502:C:N4	2.55	0.40
2:X:2850:G:OP2	4:B:86:ARG:NH2	2.51	0.40
2:X:2914:A:H2'	2:X:2915:C:O4'	2.21	0.40
4:B:121:VAL:H	4:B:121:VAL:HG12	1.52	0.40
10:I:84:LYS:HD3	10:I:89:THR:HG21	2.03	0.40
12:K:29:ARG:HH12	12:K:118:ILE:HG21	1.86	0.40
12:K:38:LYS:HB3	12:K:41:ARG:HH21	1.86	0.40
17:P:20:VAL:HG21	17:P:43:SER:HB2	2.03	0.40
20:S:45:GLU:OE1	20:S:85:GLN:NE2	2.54	0.40
1:A:43:ARG:NH1	2:X:736:C:H1'	2.36	0.40
1:A:142:HIS:CE1	1:A:143:ASN:HB2	2.56	0.40
2:X:49:A:C8	2:X:51:G:N2	2.89	0.40
2:X:260:A:C2'	2:X:261:C:H5'	2.51	0.40
2:X:320:U:H6	2:X:320:U:O5'	2.03	0.40
2:X:630:G:OP1	10:I:21:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:710:C:H2'	2:X:711:G:H8	1.86	0.40
2:X:843:G:H2'	2:X:844:G:C8	2.57	0.40
2:X:942:C:H2'	2:X:943:C:H5'	2.03	0.40
2:X:2382:C:H1'	21:T:47:ARG:NH1	2.37	0.40
2:X:2402:G:N2	2:X:2405:A:OP2	2.45	0.40
7:E:136:ILE:H	7:E:136:ILE:HG13	1.62	0.40
7:E:154:PRO:HG3	7:E:162:ILE:O	2.20	0.40
8:G:33:VAL:HA	8:G:36:ILE:HG12	2.04	0.40
9:H:35:ILE:HD13	9:H:62:ILE:HG22	2.02	0.40
9:H:107:ARG:HB2	9:H:107:ARG:HH11	1.86	0.40
1:A:11:ASN:O	1:A:14:ARG:HB3	2.21	0.40
2:X:24:G:O2'	17:P:78:GLU:O	2.40	0.40
2:X:51:G:O2'	2:X:118:A:C6	2.73	0.40
2:X:659:A:C2	2:X:661:U:OP1	2.75	0.40
2:X:897:A:H2'	2:X:898:U:C6	2.56	0.40
2:X:1875:A:C8	2:X:1875:A:H3'	2.57	0.40
2:X:2338:A:H2'	2:X:2338:A:N3	2.36	0.40
2:X:2406:G:H2'	2:X:2407:A:C8	2.56	0.40
2:X:2419:A:H5''	27:3:26:ARG:NH1	2.37	0.40
14:M:99:LEU:O	14:M:102:LEU:HD22	2.21	0.40
20:S:65:VAL:HG12	20:S:66:GLY:N	2.36	0.40
2:X:516:A:C2	2:X:517:A:C4	3.09	0.40
2:X:561:C:C2'	2:X:562:C:H5'	2.52	0.40
2:X:577:A:H2'	15:N:28:LYS:HE3	2.03	0.40
2:X:1209:U:H2'	2:X:1210:U:C6	2.57	0.40
2:X:1332:C:H4'	12:K:67:ARG:CZ	2.51	0.40
2:X:1484:G:O2'	2:X:1485:G:H5'	2.21	0.40
2:X:1599:G:C5	2:X:1600:A:C5	3.10	0.40
2:X:1841:G:C6	2:X:1842:A:C6	3.09	0.40
2:X:1876:G:H2'	2:X:1877:G:H8	1.87	0.40
2:X:2413:U:O2	21:T:49:ARG:HD3	2.22	0.40
2:X:2446:U:H2'	2:X:2447:C:H6	1.86	0.40
2:X:2656:A:C2	2:X:2914:A:C8	3.10	0.40
2:X:2810:A:H2'	2:X:2811:U:C6	2.56	0.40
4:B:6:LEU:HD23	4:B:6:LEU:HA	1.86	0.40
8:G:20:ASP:HA	8:G:58:ILE:HG22	2.03	0.40
12:K:34:GLU:HA	12:K:117:VAL:HG21	2.02	0.40
14:M:15:LEU:HD23	14:M:15:LEU:HA	1.89	0.40
18:Q:3:ALA:HB1	18:Q:41:ALA:CB	2.51	0.40
1:A:54:HIS:NE2	2:X:1850:G:OP1	2.55	0.40
2:X:64:A:O3'	18:Q:70:GLY:HA3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:146:U:H2'	2:X:147:G:O4'	2.22	0.40
2:X:189:G:H2'	2:X:190:G:H8	1.86	0.40
2:X:494:U:H4'	2:X:495:A:OP2	2.20	0.40
2:X:739:U:H1'	2:X:1416:U:O2	2.21	0.40
2:X:870:C:H2'	2:X:871:U:O4'	2.20	0.40
2:X:2255:G:H2'	2:X:2256:U:C6	2.57	0.40
3:Y:23:U:O2'	3:Y:24:C:OP2	2.35	0.40
4:B:156:MET:HB3	4:B:157:ALA:H	1.63	0.40
5:C:51:VAL:HG11	5:C:91:GLY:HA3	2.04	0.40
12:K:51:GLY:HA2	12:K:86:PHE:CZ	2.56	0.40
15:N:62:ILE:HG23	15:N:76:TYR:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	267/277 (96%)	222 (83%)	27 (10%)	18 (7%)	1	11
4	B	213/220 (97%)	187 (88%)	17 (8%)	9 (4%)	2	19
5	C	197/207 (95%)	155 (79%)	31 (16%)	11 (6%)	1	14
6	D	163/179 (91%)	131 (80%)	17 (10%)	15 (9%)	0	6
7	E	155/178 (87%)	120 (77%)	26 (17%)	9 (6%)	1	13
8	G	143/145 (99%)	131 (92%)	8 (6%)	4 (3%)	4	26
9	H	120/122 (98%)	102 (85%)	16 (13%)	2 (2%)	7	35
10	I	129/140 (92%)	91 (70%)	25 (19%)	13 (10%)	0	5
11	J	136/144 (94%)	110 (81%)	15 (11%)	11 (8%)	1	8
12	K	117/122 (96%)	101 (86%)	9 (8%)	7 (6%)	1	13
13	L	107/119 (90%)	86 (80%)	16 (15%)	5 (5%)	2	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	M	108/116 (93%)	85 (79%)	18 (17%)	5 (5%)	2	17
15	N	114/118 (97%)	108 (95%)	6 (5%)	0	100	100
16	O	100/102 (98%)	90 (90%)	5 (5%)	5 (5%)	1	16
17	P	110/117 (94%)	101 (92%)	8 (7%)	1 (1%)	14	47
18	Q	88/91 (97%)	74 (84%)	9 (10%)	5 (6%)	1	14
19	R	100/105 (95%)	71 (71%)	17 (17%)	12 (12%)	0	4
20	S	165/217 (76%)	121 (73%)	23 (14%)	21 (13%)	0	3
21	T	73/94 (78%)	63 (86%)	10 (14%)	0	100	100
22	U	40/62 (64%)	32 (80%)	6 (15%)	2 (5%)	1	16
23	V	63/69 (91%)	55 (87%)	5 (8%)	3 (5%)	2	16
24	W	55/59 (93%)	51 (93%)	3 (6%)	1 (2%)	6	34
25	Z	41/58 (71%)	36 (88%)	4 (10%)	1 (2%)	4	29
26	2	41/45 (91%)	39 (95%)	1 (2%)	1 (2%)	4	29
27	3	58/66 (88%)	42 (72%)	9 (16%)	7 (12%)	0	4
28	4	34/37 (92%)	26 (76%)	8 (24%)	0	100	100
All	All	2937/3209 (92%)	2430 (83%)	339 (12%)	168 (6%)	1	14

All (168) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	35	LYS
1	A	36	PRO
1	A	51	VAL
1	A	78	VAL
1	A	192	ILE
4	B	53	PHE
4	B	96	VAL
4	B	99	TYR
4	B	204	PRO
5	C	15	GLY
5	C	128	ALA
5	C	158	ASN
5	C	166	SER
5	C	175	VAL
6	D	44	VAL
6	D	84	PRO

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Mol	Chain	Res	Type
6	D	104	ILE
6	D	108	LEU
6	D	137	ILE
7	E	50	ILE
7	E	55	PRO
8	G	2	ARG
10	I	30	THR
10	I	46	VAL
10	I	48	PRO
10	I	77	VAL
11	J	4	PRO
11	J	61	GLY
11	J	135	GLU
12	K	75	ASP
12	K	77	THR
13	L	63	ILE
13	L	92	ILE
14	M	36	GLU
16	O	50	ALA
17	P	71	VAL
19	R	25	ALA
19	R	101	ILE
20	S	34	TYR
20	S	109	VAL
20	S	150	ILE
22	U	40	VAL
23	V	3	ALA
23	V	11	THR
27	3	54	ASP
1	A	25	THR
1	A	79	ASP
1	A	126	VAL
1	A	170	LYS
1	A	224	VAL
5	C	97	TYR
5	C	144	SER
5	C	191	SER
6	D	74	ILE
6	D	131	GLY
7	E	35	ARG
9	H	25	LEU
10	I	71	ARG

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Mol	Chain	Res	Type
10	I	101	VAL
10	I	110	LYS
10	I	126	HIS
11	J	10	ARG
11	J	99	PRO
12	K	28	GLU
12	K	76	GLU
13	L	91	GLU
14	M	55	GLY
18	Q	50	VAL
18	Q	66	GLY
18	Q	83	LYS
18	Q	90	PHE
19	R	74	LYS
20	S	81	PRO
20	S	98	GLU
20	S	110	GLY
20	S	130	VAL
20	S	131	THR
20	S	167	ILE
1	A	245	SER
4	B	58	ALA
6	D	75	ALA
6	D	109	PRO
7	E	51	GLU
7	E	107	VAL
7	E	128	ASN
7	E	153	PRO
8	G	40	LYS
8	G	89	THR
10	I	13	ARG
10	I	62	PRO
10	I	87	ASP
11	J	133	LYS
11	J	136	GLU
12	K	6	LEU
14	M	5	LYS
14	M	89	LYS
16	O	52	THR
20	S	12	LYS
20	S	88	HIS
20	S	132	ALA

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Mol	Chain	Res	Type
20	S	142	GLU
22	U	44	PRO
24	W	32	ASN
25	Z	22	ILE
26	2	16	VAL
27	3	28	PHE
27	3	34	ALA
27	3	46	LYS
1	A	39	LYS
1	A	110	LEU
1	A	135	ILE
4	B	60	LYS
4	B	176	ASN
6	D	60	ILE
6	D	89	VAL
6	D	119	LYS
6	D	126	GLY
8	G	130	GLU
9	H	64	ARG
10	I	79	LEU
11	J	9	TYR
11	J	60	ARG
12	K	68	ASN
12	K	71	ILE
14	M	108	LYS
16	O	7	THR
19	R	58	GLU
19	R	67	ASN
19	R	76	ASN
19	R	88	GLY
20	S	13	GLN
20	S	129	GLU
20	S	138	PRO
27	3	47	ALA
1	A	37	LEU
1	A	252	LYS
11	J	89	ALA
13	L	65	THR
16	O	99	LYS
18	Q	86	SER
20	S	38	ASN
27	3	29	THR

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Mol	Chain	Res	Type
27	3	45	ARG
5	C	27	GLU
5	C	171	PRO
6	D	115	GLN
7	E	36	THR
11	J	7	VAL
19	R	6	GLY
19	R	65	VAL
19	R	77	GLU
20	S	124	PRO
1	A	85	PRO
6	D	65	PRO
13	L	93	VAL
20	S	114	GLY
4	B	152	GLY
20	S	133	THR
23	V	6	ILE
10	I	55	LEU
16	O	30	GLY
19	R	78	PRO
19	R	81	VAL
4	B	124	GLY
5	C	61	GLY
7	E	90	VAL
20	S	74	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	112/224 (50%)	96 (86%)	16 (14%)	3	18
4	B	150/177 (85%)	118 (79%)	32 (21%)	1	7
5	C	106/169 (63%)	76 (72%)	30 (28%)	0	3
6	D	15/158 (10%)	12 (80%)	3 (20%)	1	8
7	E	51/156 (33%)	38 (74%)	13 (26%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	G	106/123 (86%)	84 (79%)	22 (21%)	1	7
9	H	91/100 (91%)	71 (78%)	20 (22%)	1	6
10	I	56/108 (52%)	33 (59%)	23 (41%)	0	0
11	J	90/119 (76%)	77 (86%)	13 (14%)	3	18
12	K	91/102 (89%)	74 (81%)	17 (19%)	1	9
13	L	40/95 (42%)	30 (75%)	10 (25%)	0	4
14	M	75/102 (74%)	50 (67%)	25 (33%)	0	2
15	N	91/98 (93%)	70 (77%)	21 (23%)	1	5
16	O	71/86 (83%)	57 (80%)	14 (20%)	1	8
17	P	89/94 (95%)	75 (84%)	14 (16%)	2	15
18	Q	41/82 (50%)	35 (85%)	6 (15%)	3	17
19	R	44/90 (49%)	24 (54%)	20 (46%)	0	0
20	S	88/190 (46%)	70 (80%)	18 (20%)	1	7
21	T	53/75 (71%)	39 (74%)	14 (26%)	0	3
22	U	8/52 (15%)	8 (100%)	0	100	100
23	V	47/62 (76%)	36 (77%)	11 (23%)	1	5
24	W	50/53 (94%)	38 (76%)	12 (24%)	1	5
25	Z	38/51 (74%)	28 (74%)	10 (26%)	0	4
26	2	35/40 (88%)	27 (77%)	8 (23%)	1	6
27	3	33/57 (58%)	26 (79%)	7 (21%)	1	7
28	4	2/35 (6%)	1 (50%)	1 (50%)	0	0
All	All	1673/2698 (62%)	1293 (77%)	380 (23%)	1	6

All (380) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	15	ASN
1	A	17	THR
1	A	46	GLN
1	A	53	HIS
1	A	78	VAL
1	A	90	ASN
1	A	96	TYR
1	A	128	ASN

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Mol	Chain	Res	Type
1	A	141	VAL
1	A	144	ILE
1	A	181	VAL
1	A	204	ASN
1	A	205	VAL
1	A	219	THR
1	A	243	ARG
4	B	13	THR
4	B	26	THR
4	B	29	GLU
4	B	32	GLU
4	B	33	ASN
4	B	43	VAL
4	B	62	ASP
4	B	104	GLU
4	B	107	VAL
4	B	115	VAL
4	B	116	ILE
4	B	118	VAL
4	B	121	VAL
4	B	156	MET
4	B	158	SER
4	B	159	ASP
4	B	167	GLN
4	B	168	LYS
4	B	169	MET
4	B	173	MET
4	B	177	THR
4	B	180	VAL
4	B	192	ASN
4	B	193	LYS
4	B	195	ILE
4	B	198	LYS
4	B	200	ASN
4	B	205	LYS
4	B	208	LEU
4	B	210	GLU
4	B	213	THR
4	B	215	ILE
5	C	6	VAL
5	C	8	LYS
5	C	10	ASP

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Mol	Chain	Res	Type
5	C	17	ILE
5	C	31	SER
5	C	39	LEU
5	C	41	ARG
5	C	43	SER
5	C	49	HIS
5	C	57	VAL
5	C	67	GLN
5	C	68	LYS
5	C	77	THR
5	C	78	ILE
5	C	79	ARG
5	C	88	ILE
5	C	105	MET
5	C	108	LEU
5	C	115	SER
5	C	125	VAL
5	C	136	THR
5	C	144	SER
5	C	145	THR
5	C	146	LEU
5	C	148	GLN
5	C	155	VAL
5	C	164	GLU
5	C	165	LEU
5	C	183	VAL
5	C	186	ILE
6	D	26	MET
6	D	105	SER
6	D	130	LEU
7	E	23	HIS
7	E	24	VAL
7	E	25	THR
7	E	63	THR
7	E	65	HIS
7	E	68	THR
7	E	75	MET
7	E	83	TYR
7	E	84	VAL
7	E	115	ILE
7	E	133	VAL
7	E	136	ILE

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Mol	Chain	Res	Type
7	E	141	VAL
8	G	1	MET
8	G	6	MET
8	G	12	ILE
8	G	18	VAL
8	G	19	ILE
8	G	24	GLN
8	G	29	LEU
8	G	32	GLU
8	G	36	ILE
8	G	41	ASN
8	G	42	LYS
8	G	43	VAL
8	G	44	THR
8	G	46	THR
8	G	51	THR
8	G	58	ILE
8	G	69	LYS
8	G	101	LEU
8	G	102	ILE
8	G	114	ARG
8	G	125	VAL
8	G	143	LEU
9	H	8	LEU
9	H	19	VAL
9	H	21	THR
9	H	23	LYS
9	H	24	VAL
9	H	39	ILE
9	H	47	THR
9	H	56	ASP
9	H	57	VAL
9	H	61	VAL
9	H	63	VAL
9	H	67	SER
9	H	69	VAL
9	H	86	ILE
9	H	90	ASP
9	H	96	THR
9	H	107	ARG
9	H	112	MET
9	H	119	PRO

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Mol	Chain	Res	Type
9	H	122	LEU
10	I	3	LEU
10	I	7	LYS
10	I	19	VAL
10	I	21	ARG
10	I	23	VAL
10	I	25	THR
10	I	31	SER
10	I	36	LYS
10	I	38	GLN
10	I	47	ARG
10	I	50	PHE
10	I	51	GLU
10	I	54	GLN
10	I	55	LEU
10	I	57	LEU
10	I	61	LEU
10	I	70	ASN
10	I	76	ILE
10	I	82	LEU
10	I	84	LYS
10	I	89	THR
10	I	107	SER
10	I	112	LEU
11	J	16	LYS
11	J	17	THR
11	J	27	VAL
11	J	35	GLN
11	J	37	THR
11	J	64	VAL
11	J	72	THR
11	J	75	THR
11	J	91	GLU
11	J	96	VAL
11	J	109	VAL
11	J	120	LEU
11	J	134	ARG
12	K	6	LEU
12	K	25	ILE
12	K	27	SER
12	K	32	THR
12	K	33	THR

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Mol	Chain	Res	Type
12	K	36	ARG
12	K	42	SER
12	K	55	ASP
12	K	65	THR
12	K	66	LEU
12	K	88	GLU
12	K	94	THR
12	K	97	GLN
12	K	101	THR
12	K	109	ARG
12	K	110	ARG
12	K	119	ILE
13	L	11	ARG
13	L	17	ARG
13	L	31	LEU
13	L	33	VAL
13	L	36	SER
13	L	45	ILE
13	L	52	THR
13	L	53	LEU
13	L	96	ARG
13	L	110	GLU
14	M	7	ILE
14	M	10	VAL
14	M	11	THR
14	M	14	GLN
14	M	17	THR
14	M	21	SER
14	M	27	THR
14	M	34	ILE
14	M	48	VAL
14	M	49	VAL
14	M	52	ARG
14	M	53	ARG
14	M	57	VAL
14	M	58	SER
14	M	60	THR
14	M	63	VAL
14	M	70	VAL
14	M	74	ARG
14	M	75	THR
14	M	80	THR

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Mol	Chain	Res	Type
14	M	82	LYS
14	M	83	ILE
14	M	100	TYR
14	M	102	LEU
14	M	106	ARG
15	N	9	VAL
15	N	30	THR
15	N	41	LYS
15	N	48	ARG
15	N	54	LYS
15	N	55	ARG
15	N	58	ARG
15	N	63	THR
15	N	65	ILE
15	N	73	GLU
15	N	74	MET
15	N	75	SER
15	N	78	ARG
15	N	79	LEU
15	N	84	LYS
15	N	92	ARG
15	N	98	ILE
15	N	108	GLN
15	N	112	LYS
15	N	115	ASP
15	N	117	LEU
16	O	1	MET
16	O	10	LYS
16	O	12	ILE
16	O	16	GLU
16	O	25	LEU
16	O	34	THR
16	O	48	VAL
16	O	69	LYS
16	O	71	ILE
16	O	72	THR
16	O	78	ARG
16	O	84	ARG
16	O	94	LYS
16	O	97	ILE
17	P	10	ILE
17	P	17	VAL

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Mol	Chain	Res	Type
17	P	24	ILE
17	P	37	LYS
17	P	38	LEU
17	P	40	ASN
17	P	59	GLU
17	P	65	ASN
17	P	66	THR
17	P	83	LYS
17	P	86	ARG
17	P	109	ASP
17	P	111	LYS
17	P	112	GLU
18	Q	5	ASP
18	Q	49	LYS
18	Q	72	THR
18	Q	76	ARG
18	Q	80	VAL
18	Q	87	ILE
19	R	3	ILE
19	R	4	LYS
19	R	9	VAL
19	R	11	VAL
19	R	23	VAL
19	R	24	ILE
19	R	32	ARG
19	R	33	VAL
19	R	34	VAL
19	R	36	GLU
19	R	39	ASN
19	R	43	LYS
19	R	56	ILE
19	R	59	THR
19	R	68	VAL
19	R	70	LEU
19	R	72	ASP
19	R	80	ARG
19	R	81	VAL
19	R	91	VAL
20	S	14	THR
20	S	18	LEU
20	S	22	ARG
20	S	30	VAL

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Mol	Chain	Res	Type
20	S	31	VAL
20	S	41	VAL
20	S	43	VAL
20	S	46	VAL
20	S	52	ILE
20	S	55	VAL
20	S	69	THR
20	S	85	GLN
20	S	101	THR
20	S	113	VAL
20	S	133	THR
20	S	155	THR
20	S	159	VAL
20	S	161	VAL
21	T	26	SER
21	T	27	LYS
21	T	28	ARG
21	T	29	LEU
21	T	39	VAL
21	T	40	THR
21	T	51	THR
21	T	57	GLU
21	T	61	ARG
21	T	78	GLU
21	T	80	LYS
21	T	82	ARG
21	T	87	VAL
21	T	88	SER
23	V	19	LYS
23	V	20	SER
23	V	23	GLU
23	V	29	ARG
23	V	30	PHE
23	V	34	THR
23	V	38	GLU
23	V	40	THR
23	V	43	ILE
23	V	56	VAL
23	V	62	ILE
24	W	12	VAL
24	W	15	ARG
24	W	17	GLU

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Mol	Chain	Res	Type
24	W	18	THR
24	W	33	SER
24	W	40	ASN
24	W	44	ARG
24	W	50	VAL
24	W	53	LEU
24	W	54	VAL
24	W	56	VAL
24	W	58	GLU
25	Z	3	VAL
25	Z	5	LYS
25	Z	7	ARG
25	Z	15	LYS
25	Z	22	ILE
25	Z	24	VAL
25	Z	37	TYR
25	Z	38	LYS
25	Z	39	LEU
25	Z	43	VAL
26	2	5	THR
26	2	12	LYS
26	2	20	ARG
26	2	22	ARG
26	2	25	THR
26	2	26	LYS
26	2	30	LYS
26	2	41	LYS
27	3	6	THR
27	3	14	VAL
27	3	24	ARG
27	3	29	THR
27	3	49	LEU
27	3	55	MET
27	3	58	VAL
28	4	11	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	90	ASN
1	A	197	ASN

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Mol	Chain	Res	Type
4	B	148	HIS
8	G	41	ASN
10	I	70	ASN
12	K	79	GLN
13	L	43	GLN
13	L	48	ASN
14	M	14	GLN
14	M	31	HIS
15	N	81	ASN
15	N	108	GLN
16	O	63	ASN
17	P	40	ASN
19	R	64	HIS
20	S	10	GLN
22	U	20	HIS
22	U	30	ASN
22	U	32	ASN
26	2	7	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	X	2685/2923 (91%)	652 (24%)	36 (1%)
3	Y	113/114 (99%)	18 (15%)	0
All	All	2798/3037 (92%)	670 (23%)	36 (1%)

All (670) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	X	8	U
2	X	15	G
2	X	17	G
2	X	34	U
2	X	38	A
2	X	39	C
2	X	51	G
2	X	52	A
2	X	60	U
2	X	61	A
2	X	64	A
2	X	66	C

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Mol	Chain	Res	Type
2	X	70	G
2	X	71	A
2	X	75	G
2	X	80	G
2	X	90	A
2	X	91	A
2	X	95	A
2	X	96	G
2	X	101	G
2	X	111	U
2	X	117	A
2	X	118	A
2	X	119	U
2	X	124	A
2	X	131	G
2	X	133	A
2	X	139	U
2	X	140	A
2	X	152	C
2	X	154	A
2	X	156	A
2	X	157	U
2	X	164	A
2	X	165	C
2	X	166	A
2	X	167	U
2	X	169	G
2	X	170	C
2	X	171	A
2	X	172	U
2	X	173	A
2	X	176	A
2	X	177	G
2	X	178	A
2	X	179	A
2	X	180	G
2	X	183	A
2	X	184	C
2	X	185	A
2	X	199	A
2	X	202	A
2	X	219	A

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Mol	Chain	Res	Type
2	X	225	A
2	X	227	G
2	X	233	U
2	X	235	G
2	X	236	A
2	X	248	G
2	X	251	G
2	X	255	G
2	X	268	A
2	X	284	C
2	X	285	U
2	X	286	U
2	X	287	G
2	X	288	C
2	X	289	U
2	X	290	U
2	X	291	G
2	X	293	U
2	X	298	U
2	X	300	G
2	X	301	U
2	X	303	G
2	X	310	C
2	X	311	U
2	X	313	U
2	X	319	G
2	X	320	U
2	X	321	U
2	X	322	A
2	X	328	G
2	X	329	A
2	X	330	C
2	X	332	A
2	X	338	G
2	X	344	U
2	X	353	A
2	X	354	A
2	X	359	A
2	X	364	A
2	X	365	A
2	X	372	A
2	X	373	A

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Mol	Chain	Res	Type
2	X	374	U
2	X	375	A
2	X	377	U
2	X	389	A
2	X	392	U
2	X	394	U
2	X	403	U
2	X	404	U
2	X	405	G
2	X	410	G
2	X	413	C
2	X	415	U
2	X	416	G
2	X	417	A
2	X	418	G
2	X	426	G
2	X	432	G
2	X	434	G
2	X	444	C
2	X	445	G
2	X	447	A
2	X	449	U
2	X	450	C
2	X	451	U
2	X	452	G
2	X	457	G
2	X	458	A
2	X	474	A
2	X	486	G
2	X	497	U
2	X	501	C
2	X	502	C
2	X	503	A
2	X	504	G
2	X	506	A
2	X	526	A
2	X	527	G
2	X	528	C
2	X	539	G
2	X	543	G
2	X	549	U
2	X	550	A

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Mol	Chain	Res	Type
2	X	553	A
2	X	554	C
2	X	555	C
2	X	566	U
2	X	567	G
2	X	572	C
2	X	573	A
2	X	575	G
2	X	576	U
2	X	577	A
2	X	578	G
2	X	583	A
2	X	590	U
2	X	592	A
2	X	593	U
2	X	594	G
2	X	606	G
2	X	614	U
2	X	615	A
2	X	616	G
2	X	618	A
2	X	628	G
2	X	629	A
2	X	630	G
2	X	635	G
2	X	646	A
2	X	647	G
2	X	657	U
2	X	658	A
2	X	659	A
2	X	660	A
2	X	661	U
2	X	666	A
2	X	673	G
2	X	682	A
2	X	683	G
2	X	690	U
2	X	691	A
2	X	692	G
2	X	698	U
2	X	699	U
2	X	702	U

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Mol	Chain	Res	Type
2	X	713	A
2	X	716	C
2	X	722	A
2	X	727	G
2	X	731	U
2	X	737	C
2	X	740	G
2	X	746	G
2	X	765	U
2	X	766	G
2	X	771	G
2	X	774	G
2	X	775	A
2	X	783	G
2	X	784	A
2	X	792	U
2	X	793	G
2	X	802	G
2	X	813	G
2	X	820	G
2	X	823	G
2	X	827	A
2	X	829	U
2	X	836	C
2	X	837	G
2	X	838	A
2	X	850	G
2	X	851	C
2	X	856	U
2	X	857	C
2	X	864	A
2	X	866	A
2	X	872	U
2	X	873	U
2	X	883	C
2	X	887	A
2	X	890	G
2	X	891	A
2	X	892	U
2	X	904	G
2	X	921	C
2	X	923	A

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Mol	Chain	Res	Type
2	X	924	G
2	X	940	U
2	X	942	C
2	X	943	C
2	X	944	G
2	X	947	U
2	X	948	U
2	X	955	A
2	X	969	A
2	X	970	U
2	X	971	U
2	X	972	A
2	X	977	A
2	X	985	A
2	X	989	A
2	X	990	G
2	X	1001	A
2	X	1005	G
2	X	1017	A
2	X	1018	A
2	X	1027	A
2	X	1034	A
2	X	1039	C
2	X	1040	A
2	X	1041	G
2	X	1043	U
2	X	1052	A
2	X	1053	A
2	X	1056	U
2	X	1057	A
2	X	1066	G
2	X	1067	U
2	X	1069	G
2	X	1070	A
2	X	1077	U
2	X	1078	G
2	X	1083	G
2	X	1086	G
2	X	1087	C
2	X	1089	C
2	X	1090	A
2	X	1091	G

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Mol	Chain	Res	Type
2	X	1092	A
2	X	1093	C
2	X	1145	U
2	X	1146	C
2	X	1147	A
2	X	1150	A
2	X	1151	G
2	X	1155	A
2	X	1156	G
2	X	1157	U
2	X	1175	G
2	X	1176	U
2	X	1177	A
2	X	1178	C
2	X	1179	C
2	X	1180	G
2	X	1186	A
2	X	1187	A
2	X	1195	A
2	X	1200	A
2	X	1215	U
2	X	1218	G
2	X	1220	A
2	X	1221	C
2	X	1250	G
2	X	1256	U
2	X	1258	A
2	X	1262	U
2	X	1274	G
2	X	1278	G
2	X	1291	A
2	X	1293	U
2	X	1294	G
2	X	1300	G
2	X	1309	G
2	X	1310	A
2	X	1311	A
2	X	1312	A
2	X	1313	G
2	X	1317	G
2	X	1337	A
2	X	1338	U

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Mol	Chain	Res	Type
2	X	1340	G
2	X	1345	A
2	X	1349	U
2	X	1350	U
2	X	1366	U
2	X	1389	U
2	X	1396	A
2	X	1402	A
2	X	1405	G
2	X	1415	A
2	X	1416	U
2	X	1422	A
2	X	1433	U
2	X	1447	A
2	X	1453	G
2	X	1454	U
2	X	1460	U
2	X	1461	C
2	X	1462	G
2	X	1463	A
2	X	1464	U
2	X	1465	G
2	X	1466	G
2	X	1467	G
2	X	1471	A
2	X	1472	C
2	X	1481	A
2	X	1489	A
2	X	1490	G
2	X	1491	C
2	X	1492	G
2	X	1494	G
2	X	1495	C
2	X	1496	G
2	X	1497	A
2	X	1498	U
2	X	1499	U
2	X	1503	U
2	X	1504	U
2	X	1505	G
2	X	1508	C
2	X	1509	G

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Mol	Chain	Res	Type
2	X	1510	U
2	X	1511	C
2	X	1512	U
2	X	1513	A
2	X	1514	A
2	X	1515	G
2	X	1516	C
2	X	1519	U
2	X	1522	G
2	X	1527	A
2	X	1528	G
2	X	1529	U
2	X	1541	C
2	X	1542	C
2	X	1543	G
2	X	1544	G
2	X	1547	C
2	X	1548	U
2	X	1549	C
2	X	1550	G
2	X	1551	U
2	X	1556	G
2	X	1557	C
2	X	1559	G
2	X	1561	G
2	X	1568	U
2	X	1569	G
2	X	1573	A
2	X	1575	A
2	X	1576	A
2	X	1577	G
2	X	1592	A
2	X	1593	G
2	X	1594	U
2	X	1599	G
2	X	1605	A
2	X	1606	C
2	X	1607	A
2	X	1613	G
2	X	1616	A
2	X	1625	U
2	X	1628	A

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Mol	Chain	Res	Type
2	X	1629	U
2	X	1630	A
2	X	1631	G
2	X	1632	A
2	X	1636	U
2	X	1637	A
2	X	1638	G
2	X	1639	G
2	X	1652	A
2	X	1653	A
2	X	1654	A
2	X	1662	A
2	X	1678	A
2	X	1684	A
2	X	1690	A
2	X	1691	G
2	X	1692	C
2	X	1695	G
2	X	1718	G
2	X	1732	U
2	X	1740	G
2	X	1744	A
2	X	1746	G
2	X	1748	G
2	X	1756	U
2	X	1757	U
2	X	1758	A
2	X	1760	G
2	X	1761	G
2	X	1763	U
2	X	1764	A
2	X	1765	A
2	X	1766	C
2	X	1768	C
2	X	1770	C
2	X	1771	A
2	X	1772	G
2	X	1783	G
2	X	1785	G
2	X	1790	G
2	X	1791	G
2	X	1800	A

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Mol	Chain	Res	Type
2	X	1824	C
2	X	1826	G
2	X	1827	C
2	X	1835	U
2	X	1836	A
2	X	1837	A
2	X	1843	U
2	X	1846	A
2	X	1847	U
2	X	1856	A
2	X	1860	C
2	X	1865	C
2	X	1875	A
2	X	1876	G
2	X	1885	G
2	X	1886	A
2	X	1893	A
2	X	1902	G
2	X	1908	A
2	X	1911	A
2	X	1912	A
2	X	1918	G
2	X	1926	A
2	X	1929	C
2	X	1930	G
2	X	1932	C
2	X	1933	G
2	X	1953	U
2	X	1955	A
2	X	1956	G
2	X	1963	A
2	X	1964	A
2	X	1965	A
2	X	1967	U
2	X	1982	U
2	X	1991	G
2	X	1994	C
2	X	1997	A
2	X	1998	A
2	X	1999	G
2	X	2009	U
2	X	2019	G

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Mol	Chain	Res	Type
2	X	2020	U
2	X	2024	A
2	X	2031	G
2	X	2043	U
2	X	2045	A
2	X	2047	A
2	X	2048	G
2	X	2050	A
2	X	2057	A
2	X	2058	A
2	X	2059	G
2	X	2060	A
2	X	2062	G
2	X	2063	C
2	X	2068	U
2	X	2070	C
2	X	2078	A
2	X	2079	G
2	X	2081	A
2	X	2082	C
2	X	2083	G
2	X	2087	A
2	X	2088	G
2	X	2089	A
2	X	2096	G
2	X	2107	G
2	X	2118	U
2	X	2119	U
2	X	2125	U
2	X	2225	A
2	X	2228	C
2	X	2230	G
2	X	2231	C
2	X	2233	C
2	X	2234	C
2	X	2237	U
2	X	2238	U
2	X	2239	A
2	X	2240	U
2	X	2241	C
2	X	2244	G
2	X	2245	G

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Mol	Chain	Res	Type
2	X	2246	U
2	X	2248	G
2	X	2252	A
2	X	2265	G
2	X	2266	G
2	X	2270	U
2	X	2278	G
2	X	2293	A
2	X	2295	A
2	X	2300	A
2	X	2306	G
2	X	2310	C
2	X	2314	A
2	X	2332	U
2	X	2333	U
2	X	2334	G
2	X	2347	A
2	X	2348	G
2	X	2352	G
2	X	2354	A
2	X	2361	U
2	X	2362	A
2	X	2372	G
2	X	2374	C
2	X	2377	C
2	X	2379	A
2	X	2385	A
2	X	2388	A
2	X	2398	G
2	X	2399	G
2	X	2406	G
2	X	2409	G
2	X	2410	G
2	X	2412	C
2	X	2417	U
2	X	2429	U
2	X	2432	G
2	X	2433	C
2	X	2434	A
2	X	2441	G
2	X	2450	U
2	X	2452	A

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Mol	Chain	Res	Type
2	X	2456	G
2	X	2457	A
2	X	2458	U
2	X	2468	C
2	X	2472	G
2	X	2473	G
2	X	2474	G
2	X	2475	A
2	X	2492	C
2	X	2497	G
2	X	2500	U
2	X	2501	U
2	X	2503	A
2	X	2505	A
2	X	2514	G
2	X	2526	C
2	X	2529	G
2	X	2530	A
2	X	2532	G
2	X	2545	A
2	X	2546	U
2	X	2547	C
2	X	2556	G
2	X	2561	C
2	X	2565	C
2	X	2575	G
2	X	2581	U
2	X	2591	A
2	X	2593	A
2	X	2594	G
2	X	2600	C
2	X	2603	G
2	X	2609	G
2	X	2612	U
2	X	2613	C
2	X	2629	A
2	X	2630	G
2	X	2636	U
2	X	2638	C
2	X	2640	U
2	X	2641	A
2	X	2642	U

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Mol	Chain	Res	Type
2	X	2648	G
2	X	2652	G
2	X	2656	A
2	X	2657	G
2	X	2661	A
2	X	2663	U
2	X	2681	A
2	X	2682	G
2	X	2690	G
2	X	2698	A
2	X	2708	C
2	X	2712	G
2	X	2715	G
2	X	2716	U
2	X	2717	A
2	X	2741	G
2	X	2745	G
2	X	2748	A
2	X	2753	U
2	X	2760	A
2	X	2766	U
2	X	2771	G
2	X	2775	A
2	X	2778	G
2	X	2779	C
2	X	2784	A
2	X	2791	A
2	X	2792	A
2	X	2805	A
2	X	2806	U
2	X	2817	A
2	X	2818	A
2	X	2819	C
2	X	2820	U
2	X	2821	U
2	X	2824	G
2	X	2826	U
2	X	2827	A
2	X	2832	A
2	X	2840	A
2	X	2843	A
2	X	2851	G

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Mol	Chain	Res	Type
2	X	2865	G
2	X	2877	G
2	X	2887	G
2	X	2892	G
2	X	2894	C
2	X	2899	A
2	X	2900	C
2	X	2906	G
2	X	2913	G
2	X	2920	U
3	Y	10	U
3	Y	23	U
3	Y	24	C
3	Y	28	C
3	Y	38	U
3	Y	39	G
3	Y	41	C
3	Y	42	G
3	Y	43	A
3	Y	44	A
3	Y	47	C
3	Y	53	U
3	Y	59	U
3	Y	83	U
3	Y	87	G
3	Y	88	U
3	Y	106	U
3	Y	114	C

All (36) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	X	38	A
2	X	90	A
2	X	165	C
2	X	285	U
2	X	364	A
2	X	416	G
2	X	502	C
2	X	525	A
2	X	614	U
2	X	630	G

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Mol	Chain	Res	Type
2	X	657	U
2	X	660	A
2	X	890	G
2	X	970	U
2	X	1028	G
2	X	1091	G
2	X	1149	U
2	X	1177	A
2	X	1303	A
2	X	1310	A
2	X	1369	G
2	X	1490	G
2	X	1503	U
2	X	1510	U
2	X	1521	A
2	X	1568	U
2	X	1576	A
2	X	1636	U
2	X	1885	G
2	X	1901	C
2	X	2062	G
2	X	2239	A
2	X	2378	G
2	X	2457	A
2	X	2474	G
2	X	2611	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 538 ligands modelled in this entry, 514 are monoatomic - leaving 24 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
32	MPD	X	3004	-	7,7,7	1.04	1 (14%)	9,10,10	0.75	0
32	MPD	X	3009	-	7,7,7	0.55	0	9,10,10	0.35	0
34	EOH	X	3500	-	2,2,2	0.63	0	1,1,1	0.51	0
33	SPD	Y	213	-	9,9,9	0.19	0	8,8,8	0.14	0
35	EPE	N	201	-	15,15,15	1.17	1 (6%)	19,20,20	1.52	3 (15%)
32	MPD	X	3005	-	7,7,7	0.91	0	9,10,10	0.70	0
32	MPD	X	3011	-	7,7,7	1.17	1 (14%)	9,10,10	0.49	0
32	MPD	Q	101	-	7,7,7	0.66	0	9,10,10	0.28	0
32	MPD	X	3007	-	7,7,7	0.35	0	9,10,10	0.43	0
32	MPD	Z	101	-	7,7,7	0.55	0	9,10,10	0.26	0
31	62B	X	3003	-	37,38,38	1.00	2 (5%)	56,60,60	3.22	18 (32%)
33	SPD	X	3492	-	9,9,9	0.40	0	8,8,8	0.42	0
33	SPD	X	3498	-	9,9,9	0.37	0	8,8,8	0.64	0
32	MPD	X	3008	-	7,7,7	1.07	1 (14%)	9,10,10	0.71	0
32	MPD	X	3006	-	7,7,7	0.90	1 (14%)	9,10,10	0.61	0
33	SPD	X	3495	-	9,9,9	0.23	0	8,8,8	0.37	0
33	SPD	X	3497	-	9,9,9	0.11	0	8,8,8	0.34	0
32	MPD	X	3010	-	7,7,7	0.87	0	9,10,10	0.45	0
33	SPD	X	3496	-	9,9,9	0.26	0	8,8,8	0.21	0
34	EOH	S	301	-	2,2,2	0.73	0	1,1,1	0.29	0
32	MPD	J	201	-	7,7,7	1.20	1 (14%)	9,10,10	0.73	0
33	SPD	X	3494	-	9,9,9	0.21	0	8,8,8	0.32	0
34	EOH	X	3499	-	2,2,2	0.63	0	1,1,1	0.49	0
33	SPD	X	3493	-	9,9,9	0.33	0	8,8,8	0.55	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
32	MPD	X	3004	-	-	5/5/5/5	-
32	MPD	X	3009	-	-	4/5/5/5	-
33	SPD	Y	213	-	-	2/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	EPE	N	201	-	-	5/9/19/19	0/1/1/1
32	MPD	X	3005	-	-	4/5/5/5	-
32	MPD	X	3011	-	-	3/5/5/5	-
32	MPD	Q	101	-	-	1/5/5/5	-
32	MPD	X	3007	-	-	0/5/5/5	-
32	MPD	Z	101	-	-	0/5/5/5	-
31	62B	X	3003	-	-	2/12/86/86	0/4/4/4
33	SPD	X	3492	-	-	4/7/7/7	-
33	SPD	X	3498	-	-	2/7/7/7	-
32	MPD	X	3008	-	-	3/5/5/5	-
32	MPD	X	3006	-	-	1/5/5/5	-
33	SPD	X	3495	-	-	5/7/7/7	-
33	SPD	X	3497	-	-	4/7/7/7	-
32	MPD	X	3010	-	-	0/5/5/5	-
33	SPD	X	3496	-	-	1/7/7/7	-
32	MPD	J	201	-	-	1/5/5/5	-
33	SPD	X	3494	-	-	3/7/7/7	-
33	SPD	X	3493	-	-	1/7/7/7	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	X	3003	62B	C10-C11	3.90	1.60	1.56
35	N	201	EPE	C10-S	-3.88	1.72	1.77
31	X	3003	62B	C13-C12	-3.45	1.49	1.55
32	J	201	MPD	C3-C2	2.61	1.61	1.54
32	X	3011	MPD	C3-C2	2.44	1.61	1.54
32	X	3004	MPD	C3-C2	2.39	1.61	1.54
32	X	3008	MPD	C3-C2	2.37	1.61	1.54
32	X	3006	MPD	C3-C2	2.08	1.60	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	X	3003	62B	C18-C12-C11	10.92	115.64	108.16
31	X	3003	62B	C15-C5-C14	-8.14	100.50	108.81
31	X	3003	62B	C6-C5-C14	7.40	117.16	112.13
31	X	3003	62B	C24-C25-C26	-7.23	103.25	111.53
31	X	3003	62B	C13-C12-C19	-6.14	98.31	110.83
31	X	3003	62B	C12-C13-C14	-5.74	112.67	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	X	3003	62B	C13-C14-C5	-5.34	110.55	116.28
31	X	3003	62B	C1-C9-C8	-5.11	98.45	110.13
31	X	3003	62B	C13-C12-C11	4.99	117.24	112.63
31	X	3003	62B	C28-C23-S1	-4.72	103.18	111.27
31	X	3003	62B	C9-C10-C11	4.52	116.68	112.46
35	N	201	EPE	C10-C9-N1	-4.11	96.79	112.36
31	X	3003	62B	C12-C11-C10	4.04	118.69	114.75
35	N	201	EPE	O3S-S-C10	-3.62	98.92	106.00
31	X	3003	62B	C8-C9-C10	3.49	116.37	111.74
31	X	3003	62B	C2-C3-C4	-3.09	105.25	108.53
31	X	3003	62B	C17-C10-C11	-2.87	109.89	112.20
31	X	3003	62B	C7-C6-C5	-2.64	108.62	111.57
31	X	3003	62B	C27-C26-C25	-2.38	107.86	110.25
31	X	3003	62B	C1-C9-C4	2.36	106.90	102.53
35	N	201	EPE	O2S-S-C10	2.22	110.08	106.73

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	X	3004	MPD	C2-C3-C4-O4
32	X	3004	MPD	C2-C3-C4-C5
35	N	201	EPE	N4-C7-C8-O8
33	X	3495	SPD	N6-C7-C8-C9
33	X	3498	SPD	C8-C7-N6-C5
35	N	201	EPE	S-C10-C9-N1
33	X	3497	SPD	N1-C2-C3-C4
33	X	3495	SPD	C8-C7-N6-C5
33	Y	213	SPD	C2-C3-C4-C5
35	N	201	EPE	C8-C7-N4-C5
35	N	201	EPE	C10-C9-N1-C6
33	X	3495	SPD	N1-C2-C3-C4
32	X	3004	MPD	O2-C2-C3-C4
32	X	3004	MPD	C1-C2-C3-C4
32	X	3004	MPD	CM-C2-C3-C4
32	X	3008	MPD	C1-C2-C3-C4
32	X	3008	MPD	CM-C2-C3-C4
32	X	3011	MPD	C1-C2-C3-C4
32	X	3011	MPD	CM-C2-C3-C4
33	X	3492	SPD	C4-C5-N6-C7
31	X	3003	62B	C21-C22-S1-C23
32	X	3006	MPD	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
32	X	3009	MPD	C2-C3-C4-C5
32	X	3011	MPD	C2-C3-C4-C5
32	J	201	MPD	C2-C3-C4-C5
32	Q	101	MPD	C2-C3-C4-C5
33	X	3492	SPD	N1-C2-C3-C4
33	X	3496	SPD	N1-C2-C3-C4
33	X	3498	SPD	N1-C2-C3-C4
33	Y	213	SPD	C4-C5-N6-C7
35	N	201	EPE	C10-C9-N1-C2
33	X	3497	SPD	C2-C3-C4-C5
33	X	3495	SPD	C7-C8-C9-N10
33	X	3497	SPD	N6-C7-C8-C9
33	X	3495	SPD	C2-C3-C4-C5
33	X	3497	SPD	C8-C7-N6-C5
33	X	3494	SPD	N1-C2-C3-C4
33	X	3492	SPD	C3-C4-C5-N6
33	X	3492	SPD	N6-C7-C8-C9
33	X	3493	SPD	N1-C2-C3-C4
32	X	3005	MPD	O2-C2-C3-C4
32	X	3008	MPD	O2-C2-C3-C4
32	X	3005	MPD	C2-C3-C4-O4
32	X	3009	MPD	C2-C3-C4-O4
32	X	3005	MPD	C1-C2-C3-C4
32	X	3005	MPD	CM-C2-C3-C4
32	X	3009	MPD	C1-C2-C3-C4
32	X	3009	MPD	CM-C2-C3-C4
33	X	3494	SPD	C2-C3-C4-C5
33	X	3494	SPD	C8-C7-N6-C5
31	X	3003	62B	C11-C12-C19-C20

There are no ring outliers.

14 monomers are involved in 36 short contacts:

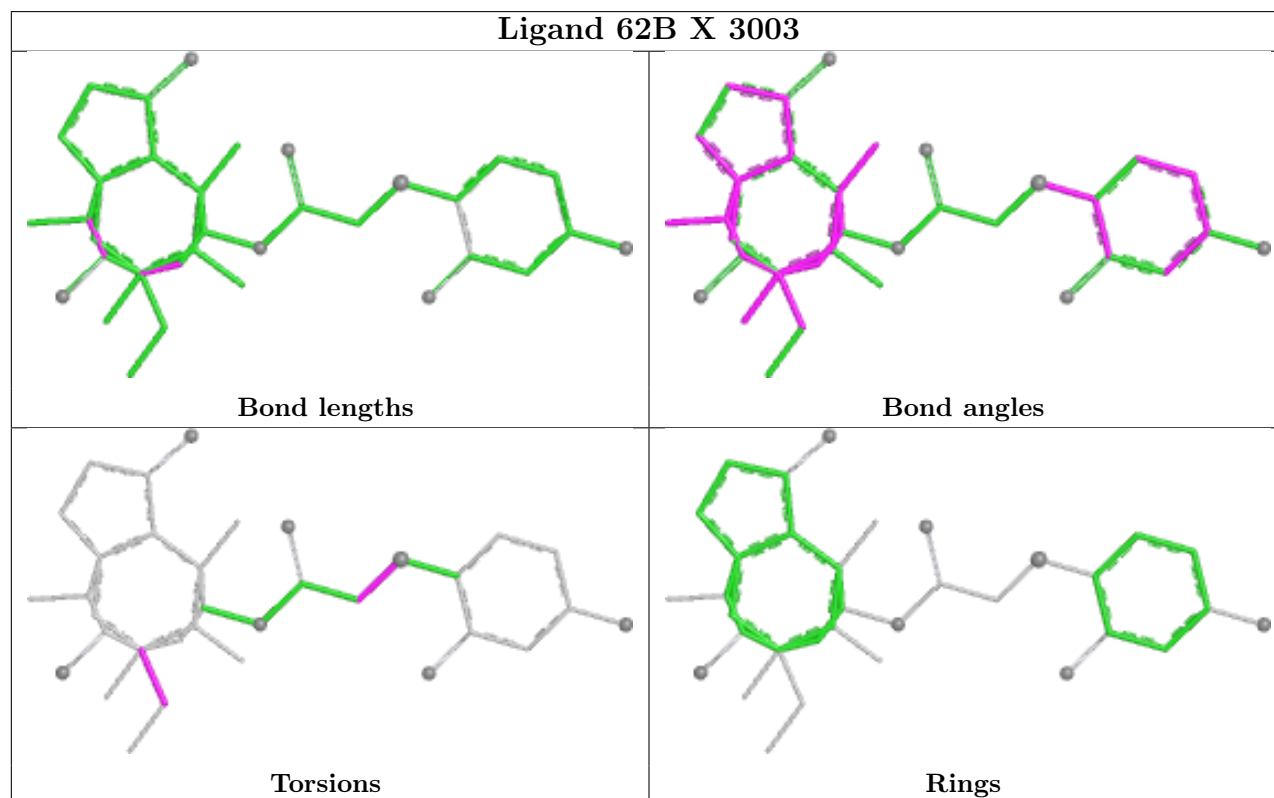
Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	X	3004	MPD	2	0
33	Y	213	SPD	1	0
35	N	201	EPE	17	0
32	X	3005	MPD	1	0
31	X	3003	62B	1	0
33	X	3498	SPD	1	0
32	X	3008	MPD	1	0
32	X	3006	MPD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	X	3495	SPD	2	0
33	X	3497	SPD	3	0
32	X	3010	MPD	1	0
32	J	201	MPD	1	0
33	X	3494	SPD	1	0
33	X	3493	SPD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	269/277 (97%)	0.72	27 (10%) 12 8	92, 138, 160, 172	0
2	X	2705/2923 (92%)	-0.16	90 (3%) 49 27	53, 101, 188, 280	0
3	Y	114/114 (100%)	-0.21	3 (2%) 57 32	76, 125, 175, 180	0
4	B	215/220 (97%)	0.21	6 (2%) 55 30	62, 81, 99, 116	0
5	C	199/207 (96%)	0.03	5 (2%) 58 33	64, 96, 113, 138	0
6	D	165/179 (92%)	0.68	19 (11%) 9 7	166, 193, 231, 239	0
7	E	157/178 (88%)	0.84	23 (14%) 6 5	133, 172, 206, 212	0
8	G	145/145 (100%)	0.01	6 (4%) 41 22	64, 79, 91, 96	0
9	H	122/122 (100%)	-0.21	2 (1%) 70 42	84, 102, 123, 128	0
10	I	131/140 (93%)	0.84	21 (16%) 5 4	58, 116, 136, 142	0
11	J	138/144 (95%)	0.34	9 (6%) 25 15	77, 103, 135, 152	0
12	K	119/122 (97%)	0.49	10 (8%) 17 11	67, 84, 108, 141	0
13	L	109/119 (91%)	0.45	12 (11%) 10 7	121, 130, 157, 189	0
14	M	110/116 (94%)	0.13	6 (5%) 30 17	85, 99, 132, 156	0
15	N	116/118 (98%)	0.35	8 (6%) 23 14	54, 70, 90, 96	0
16	O	102/102 (100%)	-0.21	1 (0%) 79 54	54, 88, 103, 109	0
17	P	112/117 (95%)	0.32	5 (4%) 38 20	64, 75, 114, 139	0
18	Q	90/91 (98%)	0.63	7 (7%) 19 12	98, 122, 138, 170	0
19	R	102/105 (97%)	1.24	26 (25%) 1 2	98, 121, 189, 206	0
20	S	167/217 (76%)	0.09	2 (1%) 76 49	87, 109, 199, 218	0
21	T	75/94 (79%)	0.34	7 (9%) 14 9	85, 97, 115, 129	0
22	U	42/62 (67%)	1.81	21 (50%) 0 1	160, 172, 203, 213	0
23	V	65/69 (94%)	0.61	6 (9%) 14 9	134, 145, 159, 163	0
24	W	57/59 (96%)	-0.09	1 (1%) 67 40	63, 77, 99, 101	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Z	43/58 (74%)	0.14	0 100 100	54, 76, 131, 136	0
26	2	43/45 (95%)	0.18	1 (2%) 61 34	83, 92, 102, 105	0
27	3	60/66 (90%)	0.85	5 (8%) 17 11	80, 89, 105, 109	0
28	4	36/37 (97%)	3.29	26 (72%) 0 0	159, 164, 174, 178	0
All	All	5808/6246 (92%)	0.15	355 (6%) 27 15	53, 103, 190, 280	0

All (355) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
28	4	36	GLN	10.7
28	4	2	LYS	7.6
18	Q	71	TYR	5.6
4	B	173	MET	5.5
1	A	53	HIS	5.5
22	U	13	SER	5.5
28	4	3	VAL	5.4
28	4	23	VAL	5.4
2	X	938	G	5.4
6	D	122	PHE	5.4
28	4	22	LYS	5.3
13	L	4	LYS	5.3
12	K	7	GLY	5.3
12	K	4	ARG	5.2
19	R	32	ARG	5.2
8	G	90	ALA	5.2
2	X	2409	G	5.0
2	X	758	G	4.9
28	4	12	GLU	4.9
7	E	170	ARG	4.9
19	R	35	VAL	4.8
7	E	88	GLU	4.8
28	4	5	PRO	4.7
2	X	1632	A	4.6
2	X	440	C	4.6
2	X	553	A	4.6
19	R	3	ILE	4.5
1	A	94	VAL	4.5
19	R	83	TYR	4.4
19	R	31	ASP	4.4
6	D	68	THR	4.3
2	X	1844	G	4.3

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Mol	Chain	Res	Type	RSRZ
28	4	35	ARG	4.3
2	X	2629	A	4.3
2	X	1452	C	4.3
28	4	1	MET	4.2
2	X	2240	U	4.2
2	X	875	G	4.2
2	X	1526	G	4.1
2	X	34	U	4.1
7	E	164	TYR	4.1
2	X	1550	G	4.1
1	A	154	ILE	4.1
2	X	989	A	4.0
28	4	30	PRO	4.0
11	J	27	VAL	4.0
10	I	118	ASP	4.0
2	X	2503	A	3.9
18	Q	28	ASP	3.9
2	X	2277	G	3.9
28	4	7	VAL	3.9
2	X	2408	C	3.9
4	B	134	HIS	3.9
13	L	5	ILE	3.9
6	D	64	LYS	3.9
19	R	91	VAL	3.8
28	4	24	MET	3.8
6	D	162	THR	3.8
2	X	2723	U	3.7
15	N	25	PHE	3.7
5	C	173	VAL	3.7
2	X	764	C	3.7
22	U	14	THR	3.6
12	K	68	ASN	3.6
19	R	67	ASN	3.6
2	X	988	C	3.6
2	X	420	A	3.6
6	D	5	LYS	3.6
17	P	71	VAL	3.5
20	S	140	ALA	3.5
18	Q	38	VAL	3.5
6	D	83	MET	3.5
5	C	165	LEU	3.5
2	X	33	U	3.5

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Mol	Chain	Res	Type	RSRZ
21	T	64	ASP	3.5
4	B	135	GLY	3.5
6	D	158	THR	3.5
11	J	25	ASN	3.5
14	M	4	HIS	3.5
2	X	1147	A	3.4
10	I	60	ARG	3.4
13	L	64	ALA	3.4
19	R	70	LEU	3.4
4	B	172	ARG	3.3
21	T	65	ASP	3.3
28	4	28	GLU	3.3
28	4	8	LYS	3.3
2	X	2006	C	3.3
14	M	5	LYS	3.3
19	R	36	GLU	3.3
5	C	176	THR	3.2
2	X	2760	A	3.2
28	4	33	LYS	3.2
2	X	1841	G	3.2
28	4	25	VAL	3.2
1	A	218	PRO	3.2
2	X	1635	A	3.2
2	X	2502	C	3.2
6	D	146	VAL	3.2
10	I	42	SER	3.2
6	D	69	LYS	3.2
2	X	1148	C	3.1
2	X	2722	U	3.1
28	4	34	GLN	3.1
7	E	156	PRO	3.1
6	D	66	LEU	3.1
10	I	45	GLY	3.1
23	V	47	ARG	3.1
2	X	1516	C	3.1
17	P	9	THR	3.1
19	R	81	VAL	3.0
21	T	61	ARG	3.0
28	4	4	ARG	3.0
1	A	42	GLY	3.0
2	X	757	G	3.0
1	A	25	THR	3.0

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Mol	Chain	Res	Type	RSRZ
19	R	68	VAL	3.0
2	X	1150	A	3.0
1	A	44	ASN	3.0
10	I	61	LEU	3.0
2	X	1146	C	3.0
17	P	102	HIS	3.0
10	I	52	GLY	3.0
12	K	35	ALA	3.0
2	X	2823	G	3.0
28	4	29	ASN	3.0
2	X	910	C	3.0
19	R	13	ALA	3.0
6	D	84	PRO	2.9
10	I	51	GLU	2.9
7	E	53	VAL	2.9
10	I	33	ARG	2.9
2	X	2635	G	2.9
10	I	10	GLU	2.9
7	E	171	ARG	2.9
19	R	69	GLN	2.9
7	E	165	GLN	2.9
7	E	166	GLY	2.9
13	L	3	SER	2.9
2	X	439	U	2.9
28	4	26	ILE	2.9
8	G	8	ASN	2.9
7	E	57	ASP	2.8
1	A	51	VAL	2.8
2	X	941	A	2.8
18	Q	5	ASP	2.8
22	U	54	LEU	2.8
13	L	32	ASN	2.8
1	A	54	HIS	2.8
1	A	182	ARG	2.8
2	X	1574	G	2.8
1	A	37	LEU	2.8
7	E	55	PRO	2.8
13	L	8	ASN	2.8
22	U	34	GLN	2.8
2	X	2702	A	2.8
19	R	16	ASP	2.8
2	X	1674	U	2.8

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Mol	Chain	Res	Type	RSRZ
2	X	2853	U	2.8
2	X	924	G	2.8
2	X	1900	G	2.8
2	X	372	A	2.8
2	X	1964	A	2.8
20	S	65	VAL	2.7
2	X	2127	G	2.7
10	I	59	ARG	2.7
2	X	419	U	2.7
28	4	6	SER	2.7
7	E	168	TYR	2.7
13	L	56	ALA	2.7
2	X	129	C	2.7
22	U	52	ARG	2.7
15	N	28	LYS	2.7
22	U	44	PRO	2.7
28	4	9	PRO	2.7
8	G	92	GLU	2.7
18	Q	60	PRO	2.7
22	U	16	ASN	2.7
12	K	69	VAL	2.7
6	D	63	GLN	2.7
10	I	54	GLN	2.7
14	M	110	ALA	2.7
1	A	264	LYS	2.7
22	U	48	TRP	2.6
12	K	5	LYS	2.6
21	T	25	GLU	2.6
2	X	2217	G	2.6
1	A	38	PRO	2.6
2	X	1907	U	2.6
1	A	250	TRP	2.6
1	A	45	ASN	2.6
2	X	1865	C	2.6
15	N	6	GLY	2.6
2	X	1060	U	2.6
1	A	41	ALA	2.6
2	X	2634	G	2.6
12	K	11	ASP	2.6
7	E	116	LYS	2.6
7	E	87	LEU	2.6
11	J	19	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	238	ARG	2.5
22	U	28	ARG	2.5
22	U	33	LEU	2.5
19	R	93	ILE	2.5
23	V	43	ILE	2.5
22	U	37	ARG	2.5
24	W	10	ARG	2.5
2	X	2671	A	2.5
28	4	14	CYS	2.5
2	X	1785	G	2.5
2	X	421	C	2.5
19	R	49	GLN	2.5
10	I	84	LYS	2.5
2	X	1908	A	2.5
1	A	11	ASN	2.5
1	A	92	ALA	2.5
1	A	13	ARG	2.5
2	X	1008	C	2.5
2	X	1490	G	2.5
22	U	51	ALA	2.5
22	U	42	GLY	2.5
4	B	168	LYS	2.4
22	U	45	LYS	2.4
14	M	96	ARG	2.4
22	U	17	ARG	2.4
21	T	75	VAL	2.4
7	E	167	GLU	2.4
13	L	91	GLU	2.4
19	R	58	GLU	2.4
22	U	30	ASN	2.4
12	K	10	SER	2.4
28	4	31	LYS	2.4
13	L	95	ASP	2.4
15	N	117	LEU	2.4
2	X	2545	A	2.4
2	X	1797	G	2.4
7	E	148	ILE	2.4
7	E	162	ILE	2.4
18	Q	42	VAL	2.4
19	R	11	VAL	2.4
1	A	43	ARG	2.4
2	X	1551	U	2.3

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Mol	Chain	Res	Type	RSRZ
19	R	64	HIS	2.3
6	D	31	ILE	2.3
10	I	38	GLN	2.3
13	L	53	LEU	2.3
15	N	27	SER	2.3
19	R	104	ASN	2.3
5	C	125	VAL	2.3
2	X	1454	U	2.3
2	X	954	A	2.3
10	I	48	PRO	2.3
23	V	2	LYS	2.3
23	V	54	LYS	2.3
15	N	65	ILE	2.3
23	V	61	GLU	2.3
27	3	40	GLN	2.3
2	X	311	U	2.3
3	Y	6	U	2.3
3	Y	30	U	2.3
17	P	43	SER	2.3
7	E	48	ASN	2.3
11	J	18	THR	2.3
19	R	48	THR	2.3
2	X	1843	U	2.3
2	X	2238	U	2.3
22	U	53	ALA	2.3
7	E	60	GLU	2.3
27	3	54	ASP	2.3
28	4	20	LYS	2.2
6	D	26	MET	2.2
2	X	944	G	2.2
2	X	1877	G	2.2
10	I	28	GLY	2.2
1	A	212	ARG	2.2
26	2	16	VAL	2.2
8	G	11	ASN	2.2
10	I	87	ASP	2.2
2	X	1446	U	2.2
6	D	47	SER	2.2
19	R	9	VAL	2.2
19	R	33	VAL	2.2
9	H	36	GLY	2.2
19	R	14	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	X	2703	C	2.2
27	3	11	ALA	2.2
19	R	51	ASN	2.2
22	U	41	ASP	2.2
2	X	1395	G	2.2
2	X	1643	C	2.2
7	E	115	ILE	2.2
8	G	91	GLY	2.2
1	A	202	LEU	2.2
10	I	40	ALA	2.1
12	K	110	ARG	2.1
12	K	70	GLU	2.1
19	R	84	LYS	2.1
11	J	28	THR	2.1
2	X	511	G	2.1
2	X	2504	C	2.1
10	I	63	LYS	2.1
14	M	76	PHE	2.1
10	I	62	PRO	2.1
11	J	62	GLY	2.1
2	X	2009	U	2.1
1	A	144	ILE	2.1
1	A	78	VAL	2.1
4	B	81	ASP	2.1
23	V	66	LYS	2.1
7	E	161	GLY	2.1
2	X	802	G	2.1
21	T	28	ARG	2.1
1	A	128	ASN	2.1
5	C	201	LYS	2.1
6	D	148	LYS	2.1
7	E	90	VAL	2.1
7	E	54	ARG	2.1
28	4	10	ILE	2.1
11	J	16	LYS	2.1
22	U	35	LYS	2.1
2	X	32	C	2.1
2	X	1549	C	2.1
2	X	1934	G	2.1
2	X	2744	G	2.1
3	Y	39	G	2.1
9	H	37	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
11	J	23	GLY	2.1
14	M	25	GLY	2.1
22	U	15	GLY	2.1
6	D	29	PRO	2.1
6	D	80	ARG	2.1
11	J	14	ARG	2.1
1	A	105	ILE	2.1
2	X	60	U	2.1
2	X	1149	U	2.1
2	X	1488	A	2.0
6	D	92	ARG	2.0
18	Q	2	GLU	2.0
22	U	46	LYS	2.0
27	3	52	LYS	2.0
15	N	68	ALA	2.0
13	L	21	ASN	2.0
2	X	877	G	2.0
2	X	2342	U	2.0
10	I	36	LYS	2.0
13	L	68	THR	2.0
8	G	87	SER	2.0
27	3	25	SER	2.0
7	E	131	VAL	2.0
16	O	11	GLN	2.0
10	I	47	ARG	2.0
2	X	1719	C	2.0
15	N	115	ASP	2.0
21	T	68	PHE	2.0
17	P	17	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
30	MG	X	3435	1/1	0.06	0.29	153,153,153,153	0
30	MG	X	3228	1/1	0.18	0.24	150,150,150,150	0
33	SPD	X	3492	10/10	0.26	0.36	105,105,105,105	0
30	MG	X	3387	1/1	0.35	0.24	175,175,175,175	0
30	MG	X	3327	1/1	0.37	0.46	126,126,126,126	0
30	MG	X	3445	1/1	0.39	0.39	104,104,104,104	0
30	MG	X	3351	1/1	0.40	0.47	116,116,116,116	0
30	MG	X	3349	1/1	0.41	0.58	127,127,127,127	0
30	MG	X	3433	1/1	0.42	0.30	124,124,124,124	0
30	MG	X	3283	1/1	0.43	0.19	129,129,129,129	0
30	MG	X	3340	1/1	0.46	0.20	84,84,84,84	0
30	MG	X	3450	1/1	0.47	0.32	132,132,132,132	0
30	MG	X	3474	1/1	0.47	0.20	106,106,106,106	0
30	MG	X	3260	1/1	0.47	0.25	123,123,123,123	0
30	MG	Y	210	1/1	0.48	0.35	105,105,105,105	0
30	MG	Y	205	1/1	0.49	0.43	94,94,94,94	0
30	MG	A	304	1/1	0.51	0.53	105,105,105,105	0
30	MG	X	3310	1/1	0.52	0.30	129,129,129,129	0
30	MG	X	3253	1/1	0.54	0.34	112,112,112,112	0
30	MG	X	3337	1/1	0.56	0.37	89,89,89,89	0
30	MG	X	3252	1/1	0.57	0.40	114,114,114,114	0
30	MG	X	3259	1/1	0.57	0.26	122,122,122,122	0
30	MG	X	3385	1/1	0.57	0.45	88,88,88,88	0
29	MN	X	3460	1/1	0.58	0.28	182,182,182,182	0
30	MG	G	201	1/1	0.58	0.27	89,89,89,89	0
30	MG	X	3002	1/1	0.58	0.62	100,100,100,100	0
30	MG	X	3394	1/1	0.59	0.20	98,98,98,98	0
30	MG	X	3293	1/1	0.61	0.31	117,117,117,117	0
30	MG	X	3165	1/1	0.63	0.41	84,84,84,84	0
30	MG	Y	203	1/1	0.63	0.13	96,96,96,96	0
30	MG	X	3339	1/1	0.63	0.26	108,108,108,108	0
32	MPD	X	3010	8/8	0.64	0.20	113,113,113,113	0
30	MG	X	3290	1/1	0.64	0.26	98,98,98,98	0
30	MG	X	3295	1/1	0.65	0.32	100,100,100,100	0
30	MG	X	3244	1/1	0.65	0.34	109,109,109,109	0
30	MG	X	3345	1/1	0.66	0.10	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3382	1/1	0.66	0.38	126,126,126,126	0
30	MG	X	3417	1/1	0.67	0.50	82,82,82,82	0
30	MG	X	3406	1/1	0.67	0.27	71,71,71,71	0
30	MG	X	3333	1/1	0.68	0.39	97,97,97,97	0
30	MG	X	3272	1/1	0.68	0.22	104,104,104,104	0
32	MPD	Q	101	8/8	0.68	0.14	137,137,137,137	0
30	MG	X	3299	1/1	0.68	0.22	149,149,149,149	0
33	SPD	X	3497	10/10	0.68	0.15	96,96,96,96	0
30	MG	X	3438	1/1	0.69	0.17	84,84,84,84	0
30	MG	X	3341	1/1	0.69	0.15	96,96,96,96	0
30	MG	X	3396	1/1	0.69	0.23	108,108,108,108	0
30	MG	X	3344	1/1	0.69	0.33	91,91,91,91	0
30	MG	X	3386	1/1	0.70	0.25	88,88,88,88	0
30	MG	X	3308	1/1	0.71	0.18	77,77,77,77	0
30	MG	X	3250	1/1	0.71	0.64	89,89,89,89	0
30	MG	X	3488	1/1	0.71	0.42	100,100,100,100	0
29	MN	X	3146	1/1	0.71	0.10	122,122,122,122	0
30	MG	X	3292	1/1	0.71	0.33	89,89,89,89	0
30	MG	Y	206	1/1	0.71	0.32	104,104,104,104	0
30	MG	X	3305	1/1	0.72	0.27	123,123,123,123	0
30	MG	X	3342	1/1	0.72	0.52	80,80,80,80	0
29	MN	X	3324	1/1	0.72	0.10	164,164,164,164	0
30	MG	X	3265	1/1	0.72	0.57	96,96,96,96	0
32	MPD	J	201	8/8	0.72	0.34	125,125,125,125	0
30	MG	X	3490	1/1	0.72	0.18	100,100,100,100	0
30	MG	X	3347	1/1	0.72	0.41	108,108,108,108	0
30	MG	X	3226	1/1	0.72	0.36	102,102,102,102	0
30	MG	X	3269	1/1	0.73	0.15	132,132,132,132	0
30	MG	X	3393	1/1	0.73	0.24	104,104,104,104	0
30	MG	X	3384	1/1	0.73	0.22	102,102,102,102	0
30	MG	X	3309	1/1	0.74	0.29	105,105,105,105	0
29	MN	X	3316	1/1	0.74	0.14	173,173,173,173	0
30	MG	X	3304	1/1	0.74	0.23	117,117,117,117	0
30	MG	X	3391	1/1	0.75	0.34	107,107,107,107	0
30	MG	X	3362	1/1	0.75	0.24	114,114,114,114	0
29	MN	Y	208	1/1	0.75	0.09	164,164,164,164	0
29	MN	X	3210	1/1	0.76	0.13	201,201,201,201	0
30	MG	X	3277	1/1	0.76	0.39	97,97,97,97	0
30	MG	X	3398	1/1	0.76	0.33	99,99,99,99	0
30	MG	X	3358	1/1	0.76	0.47	88,88,88,88	0
30	MG	X	3294	1/1	0.76	0.24	108,108,108,108	0
30	MG	X	3424	1/1	0.76	0.52	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3363	1/1	0.76	0.23	82,82,82,82	0
30	MG	X	3336	1/1	0.76	0.24	99,99,99,99	0
30	MG	X	3370	1/1	0.77	0.44	113,113,113,113	0
30	MG	X	3291	1/1	0.77	0.41	86,86,86,86	0
30	MG	X	3268	1/1	0.77	0.24	62,62,62,62	0
29	MN	X	3466	1/1	0.77	0.15	155,155,155,155	0
30	MG	X	3334	1/1	0.78	0.25	89,89,89,89	0
30	MG	X	3428	1/1	0.78	0.08	105,105,105,105	0
30	MG	A	303	1/1	0.78	0.93	94,94,94,94	0
30	MG	X	3331	1/1	0.78	0.38	86,86,86,86	0
29	MN	X	3326	1/1	0.78	0.11	145,145,145,145	0
33	SPD	X	3498	10/10	0.78	0.39	93,93,93,93	0
30	MG	X	3303	1/1	0.79	0.18	101,101,101,101	0
30	MG	X	3280	1/1	0.79	0.20	159,159,159,159	0
30	MG	X	3255	1/1	0.79	0.17	94,94,94,94	0
30	MG	X	3400	1/1	0.79	0.19	90,90,90,90	0
30	MG	Y	207	1/1	0.79	0.26	78,78,78,78	0
30	MG	A	302	1/1	0.79	0.22	92,92,92,92	0
30	MG	Y	211	1/1	0.79	0.28	115,115,115,115	0
30	MG	X	3287	1/1	0.80	0.44	102,102,102,102	0
30	MG	X	3412	1/1	0.80	0.28	106,106,106,106	0
30	MG	X	3123	1/1	0.80	0.16	69,69,69,69	0
32	MPD	X	3008	8/8	0.80	0.18	94,94,94,94	0
30	MG	X	3449	1/1	0.80	0.16	86,86,86,86	0
30	MG	X	3205	1/1	0.81	0.11	98,98,98,98	0
30	MG	Y	209	1/1	0.81	0.14	153,153,153,153	0
30	MG	X	3377	1/1	0.81	0.23	121,121,121,121	0
30	MG	X	3335	1/1	0.81	0.23	61,61,61,61	0
29	MN	X	3461	1/1	0.81	0.17	149,149,149,149	0
30	MG	X	3227	1/1	0.81	0.39	95,95,95,95	0
30	MG	X	3482	1/1	0.81	0.24	90,90,90,90	0
30	MG	X	3350	1/1	0.81	0.24	100,100,100,100	0
29	MN	X	3209	1/1	0.81	0.07	150,150,150,150	0
30	MG	X	3288	1/1	0.81	0.28	81,81,81,81	0
29	MN	X	3203	1/1	0.81	0.07	145,145,145,145	0
30	MG	X	3273	1/1	0.81	0.27	124,124,124,124	0
34	EOH	X	3499	3/3	0.81	0.30	80,80,80,80	0
30	MG	X	3229	1/1	0.82	0.35	98,98,98,98	0
32	MPD	X	3009	8/8	0.82	0.33	129,129,129,129	0
30	MG	X	3328	1/1	0.82	0.29	103,103,103,103	0
30	MG	X	3274	1/1	0.82	0.16	99,99,99,99	0
30	MG	X	3352	1/1	0.82	0.86	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MN	X	3237	1/1	0.82	0.07	167,167,167,167	0
33	SPD	X	3494	10/10	0.82	0.18	87,87,87,87	0
30	MG	X	3429	1/1	0.82	0.16	102,102,102,102	0
30	MG	X	3361	1/1	0.82	0.18	86,86,86,86	0
29	MN	X	3447	1/1	0.82	0.08	128,128,128,128	0
29	MN	X	3320	1/1	0.83	0.17	107,107,107,107	0
30	MG	X	3356	1/1	0.83	0.12	83,83,83,83	0
29	MN	X	3468	1/1	0.83	0.10	104,104,104,104	0
30	MG	X	3487	1/1	0.83	0.38	109,109,109,109	0
30	MG	X	3419	1/1	0.83	0.18	107,107,107,107	0
30	MG	X	3443	1/1	0.83	0.23	118,118,118,118	0
30	MG	X	3359	1/1	0.83	0.56	91,91,91,91	0
29	MN	X	3231	1/1	0.83	0.17	161,161,161,161	0
34	EOH	X	3500	3/3	0.83	0.64	99,99,99,99	0
30	MG	X	3141	1/1	0.84	0.20	85,85,85,85	0
32	MPD	X	3007	8/8	0.84	0.13	132,132,132,132	0
30	MG	X	3420	1/1	0.84	0.38	75,75,75,75	0
29	MN	X	3471	1/1	0.84	0.25	130,130,130,130	0
30	MG	X	3302	1/1	0.84	0.12	100,100,100,100	0
30	MG	X	3196	1/1	0.84	0.22	89,89,89,89	0
30	MG	X	3354	1/1	0.84	0.14	75,75,75,75	0
30	MG	X	3238	1/1	0.84	0.26	85,85,85,85	0
29	MN	X	3478	1/1	0.84	0.06	132,132,132,132	0
33	SPD	X	3496	10/10	0.84	0.34	102,102,102,102	0
30	MG	X	3408	1/1	0.84	0.30	97,97,97,97	0
30	MG	X	3410	1/1	0.84	0.18	95,95,95,95	0
30	MG	X	3249	1/1	0.84	0.27	109,109,109,109	0
29	MN	X	3479	1/1	0.84	0.14	171,171,171,171	0
34	EOH	S	301	3/3	0.84	0.56	90,90,90,90	0
30	MG	X	3285	1/1	0.85	0.29	75,75,75,75	0
29	MN	X	3120	1/1	0.85	0.19	166,166,166,166	0
29	MN	X	3425	1/1	0.85	0.17	101,101,101,101	0
30	MG	X	3233	1/1	0.85	0.14	68,68,68,68	0
29	MN	X	3446	1/1	0.85	0.14	142,142,142,142	0
29	MN	X	3175	1/1	0.85	0.13	122,122,122,122	0
30	MG	X	3306	1/1	0.85	0.26	95,95,95,95	0
30	MG	I	201	1/1	0.85	0.73	80,80,80,80	0
30	MG	X	3489	1/1	0.85	0.27	62,62,62,62	0
30	MG	X	3087	1/1	0.85	0.24	55,55,55,55	0
29	MN	R	201	1/1	0.85	0.13	123,123,123,123	0
30	MG	X	3348	1/1	0.86	0.28	72,72,72,72	0
30	MG	X	3329	1/1	0.86	0.28	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MN	X	3263	1/1	0.86	0.10	166,166,166,166	0
30	MG	X	3444	1/1	0.86	0.14	100,100,100,100	0
32	MPD	Z	101	8/8	0.86	0.19	145,145,145,145	0
30	MG	X	3413	1/1	0.86	0.34	90,90,90,90	0
30	MG	X	3144	1/1	0.86	0.28	71,71,71,71	0
33	SPD	X	3495	10/10	0.86	0.16	83,83,83,83	0
30	MG	X	3366	1/1	0.86	0.28	99,99,99,99	0
29	MN	X	3480	1/1	0.86	0.10	175,175,175,175	0
30	MG	X	3373	1/1	0.86	0.24	97,97,97,97	0
33	SPD	Y	213	10/10	0.86	0.36	101,101,101,101	0
29	MN	X	3235	1/1	0.86	0.10	155,155,155,155	0
29	MN	X	3380	1/1	0.86	0.11	151,151,151,151	0
29	MN	X	3182	1/1	0.86	0.08	133,133,133,133	0
30	MG	X	3130	1/1	0.87	0.27	72,72,72,72	0
30	MG	X	3411	1/1	0.87	0.21	82,82,82,82	0
30	MG	X	3485	1/1	0.87	0.23	102,102,102,102	0
29	MN	X	3202	1/1	0.87	0.18	173,173,173,173	0
30	MG	X	3378	1/1	0.87	0.22	83,83,83,83	0
29	MN	X	3225	1/1	0.87	0.15	157,157,157,157	0
30	MG	X	3213	1/1	0.87	0.35	86,86,86,86	0
30	MG	X	3224	1/1	0.87	0.33	66,66,66,66	0
30	MG	X	3236	1/1	0.87	0.31	88,88,88,88	0
30	MG	X	3372	1/1	0.87	0.18	78,78,78,78	0
30	MG	X	3451	1/1	0.87	0.23	115,115,115,115	0
32	MPD	X	3006	8/8	0.88	0.44	82,82,82,82	0
30	MG	X	3414	1/1	0.88	0.27	89,89,89,89	0
30	MG	X	3300	1/1	0.88	0.30	94,94,94,94	0
30	MG	X	3286	1/1	0.88	0.33	77,77,77,77	0
30	MG	X	3246	1/1	0.88	0.23	72,72,72,72	0
30	MG	X	3365	1/1	0.88	0.14	76,76,76,76	0
29	MN	X	3194	1/1	0.88	0.09	138,138,138,138	0
30	MG	X	3142	1/1	0.88	0.19	72,72,72,72	0
29	MN	X	3437	1/1	0.88	0.07	153,153,153,153	0
30	MG	X	3434	1/1	0.88	0.29	64,64,64,64	0
29	MN	X	3155	1/1	0.88	0.32	110,110,110,110	0
29	MN	X	3094	1/1	0.88	0.09	124,124,124,124	0
30	MG	X	3440	1/1	0.88	0.14	79,79,79,79	0
29	MN	X	3325	1/1	0.88	0.07	187,187,187,187	0
29	MN	X	3114	1/1	0.88	0.10	122,122,122,122	0
30	MG	X	3383	1/1	0.88	0.12	75,75,75,75	0
29	MN	X	3183	1/1	0.88	0.06	125,125,125,125	0
30	MG	X	3343	1/1	0.88	0.23	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	C	301	1/1	0.89	0.46	64,64,64,64	0
30	MG	X	3371	1/1	0.89	0.25	88,88,88,88	0
29	MN	X	3321	1/1	0.89	0.05	159,159,159,159	0
30	MG	J	202	1/1	0.89	0.15	92,92,92,92	0
32	MPD	X	3005	8/8	0.89	0.20	78,78,78,78	0
29	MN	X	3322	1/1	0.89	0.12	137,137,137,137	0
30	MG	X	3281	1/1	0.89	0.22	113,113,113,113	0
29	MN	X	3186	1/1	0.89	0.12	143,143,143,143	0
30	MG	X	3473	1/1	0.89	0.21	82,82,82,82	0
29	MN	X	3150	1/1	0.89	0.07	110,110,110,110	0
30	MG	X	3415	1/1	0.89	0.43	81,81,81,81	0
29	MN	X	3469	1/1	0.89	0.08	140,140,140,140	0
30	MG	X	3357	1/1	0.89	0.23	95,95,95,95	0
29	MN	X	3197	1/1	0.89	0.12	138,138,138,138	0
29	MN	X	3119	1/1	0.89	0.09	140,140,140,140	0
30	MG	X	3266	1/1	0.89	0.28	90,90,90,90	0
29	MN	X	3404	1/1	0.89	0.11	131,131,131,131	0
29	MN	X	3019	1/1	0.89	0.20	109,109,109,109	0
29	MN	X	3133	1/1	0.89	0.10	133,133,133,133	0
29	MN	X	3317	1/1	0.89	0.07	137,137,137,137	0
30	MG	X	3367	1/1	0.89	0.42	83,83,83,83	0
30	MG	X	3369	1/1	0.89	0.33	70,70,70,70	0
29	MN	X	3044	1/1	0.89	0.13	116,116,116,116	0
35	EPE	N	201	15/15	0.89	0.17	73,73,73,73	0
30	MG	X	3278	1/1	0.90	0.26	82,82,82,82	0
30	MG	X	3381	1/1	0.90	0.42	97,97,97,97	0
29	MN	X	3462	1/1	0.90	0.08	152,152,152,152	0
29	MN	X	3025	1/1	0.90	0.10	128,128,128,128	0
30	MG	X	3282	1/1	0.90	0.08	85,85,85,85	0
29	MN	X	3124	1/1	0.90	0.07	147,147,147,147	0
30	MG	X	3261	1/1	0.90	0.13	91,91,91,91	0
29	MN	X	3312	1/1	0.90	0.07	115,115,115,115	0
30	MG	X	3242	1/1	0.90	0.18	65,65,65,65	0
30	MG	X	3267	1/1	0.90	0.16	72,72,72,72	0
30	MG	X	3289	1/1	0.90	0.16	110,110,110,110	0
30	MG	X	3346	1/1	0.90	0.20	68,68,68,68	0
30	MG	X	3397	1/1	0.90	0.15	78,78,78,78	0
29	MN	X	3101	1/1	0.90	0.23	131,131,131,131	0
29	MN	X	3173	1/1	0.90	0.07	129,129,129,129	0
30	MG	X	3441	1/1	0.90	0.27	96,96,96,96	0
29	MN	X	3458	1/1	0.90	0.12	127,127,127,127	0
30	MG	Y	212	1/1	0.90	0.29	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3129	1/1	0.90	0.18	79,79,79,79	0
29	MN	X	3379	1/1	0.90	0.07	158,158,158,158	0
29	MN	X	3208	1/1	0.90	0.13	141,141,141,141	0
29	MN	T	101	1/1	0.91	0.13	121,121,121,121	0
30	MG	X	3256	1/1	0.91	0.21	69,69,69,69	0
30	MG	X	3218	1/1	0.91	0.42	75,75,75,75	0
30	MG	X	3221	1/1	0.91	0.20	89,89,89,89	0
29	MN	X	3459	1/1	0.91	0.10	161,161,161,161	0
30	MG	P	201	1/1	0.91	0.16	63,63,63,63	0
29	MN	X	3211	1/1	0.91	0.12	144,144,144,144	0
29	MN	X	3223	1/1	0.91	0.07	119,119,119,119	0
29	MN	X	3058	1/1	0.91	0.13	101,101,101,101	0
29	MN	X	3463	1/1	0.91	0.09	134,134,134,134	0
30	MG	X	3232	1/1	0.91	0.13	74,74,74,74	0
29	MN	X	3153	1/1	0.91	0.10	123,123,123,123	0
29	MN	A	301	1/1	0.91	0.10	138,138,138,138	0
30	MG	X	3483	1/1	0.91	0.21	91,91,91,91	0
29	MN	X	3162	1/1	0.91	0.08	118,118,118,118	0
30	MG	X	3276	1/1	0.91	0.28	67,67,67,67	0
29	MN	X	3199	1/1	0.91	0.12	143,143,143,143	0
29	MN	X	3166	1/1	0.91	0.11	92,92,92,92	0
29	MN	X	3168	1/1	0.91	0.16	115,115,115,115	0
30	MG	X	3247	1/1	0.91	0.28	85,85,85,85	0
29	MN	X	3046	1/1	0.91	0.15	91,91,91,91	0
30	MG	X	3180	1/1	0.91	0.25	78,78,78,78	0
29	MN	X	3147	1/1	0.91	0.07	119,119,119,119	0
30	MG	X	3355	1/1	0.91	0.50	91,91,91,91	0
29	MN	X	3148	1/1	0.91	0.17	144,144,144,144	0
30	MG	X	3388	1/1	0.91	0.23	85,85,85,85	0
29	MN	X	3422	1/1	0.92	0.07	154,154,154,154	0
30	MG	X	3222	1/1	0.92	0.13	80,80,80,80	0
30	MG	X	3307	1/1	0.92	0.14	71,71,71,71	0
29	MN	X	3158	1/1	0.92	0.09	117,117,117,117	0
29	MN	X	3314	1/1	0.92	0.09	147,147,147,147	0
30	MG	X	3476	1/1	0.92	0.17	64,64,64,64	0
30	MG	X	3477	1/1	0.92	0.08	80,80,80,80	0
30	MG	X	3143	1/1	0.92	0.23	59,59,59,59	0
30	MG	X	3423	1/1	0.92	0.20	79,79,79,79	0
29	MN	X	3181	1/1	0.92	0.08	142,142,142,142	0
30	MG	X	3426	1/1	0.92	0.14	104,104,104,104	0
32	MPD	X	3011	8/8	0.92	0.24	75,75,75,75	0
29	MN	X	3159	1/1	0.92	0.10	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3368	1/1	0.92	0.26	87,87,87,87	0
30	MG	X	3230	1/1	0.92	0.11	80,80,80,80	0
30	MG	X	3491	1/1	0.92	0.17	86,86,86,86	0
33	SPD	X	3493	10/10	0.92	0.23	83,83,83,83	0
30	MG	X	3504	1/1	0.92	0.20	74,74,74,74	0
29	MN	X	3470	1/1	0.92	0.17	148,148,148,148	0
30	MG	Y	204	1/1	0.92	0.19	78,78,78,78	0
30	MG	X	3332	1/1	0.92	0.13	81,81,81,81	0
30	MG	X	3297	1/1	0.92	0.14	81,81,81,81	0
29	MN	X	3360	1/1	0.92	0.06	146,146,146,146	0
29	MN	X	3319	1/1	0.92	0.04	158,158,158,158	0
30	MG	X	3212	1/1	0.92	0.21	78,78,78,78	0
29	MN	X	3154	1/1	0.92	0.11	124,124,124,124	0
29	MN	X	3311	1/1	0.92	0.09	124,124,124,124	0
30	MG	G	202	1/1	0.93	0.22	77,77,77,77	0
29	MN	X	3071	1/1	0.93	0.11	98,98,98,98	0
29	MN	X	3102	1/1	0.93	0.14	124,124,124,124	0
30	MG	X	3475	1/1	0.93	0.28	93,93,93,93	0
30	MG	X	3375	1/1	0.93	0.15	76,76,76,76	0
29	MN	X	3184	1/1	0.93	0.05	128,128,128,128	0
29	MN	X	3157	1/1	0.93	0.10	108,108,108,108	0
29	MN	X	3192	1/1	0.93	0.08	138,138,138,138	0
29	MN	Z	102	1/1	0.93	0.15	112,112,112,112	0
29	MN	X	3135	1/1	0.93	0.07	115,115,115,115	0
29	MN	X	3195	1/1	0.93	0.17	139,139,139,139	0
29	MN	X	3454	1/1	0.93	0.11	126,126,126,126	0
29	MN	X	3139	1/1	0.93	0.18	117,117,117,117	0
29	MN	X	3198	1/1	0.93	0.08	125,125,125,125	0
29	MN	X	3111	1/1	0.93	0.11	130,130,130,130	0
29	MN	X	3163	1/1	0.93	0.06	124,124,124,124	0
29	MN	X	3112	1/1	0.93	0.10	124,124,124,124	0
30	MG	X	3298	1/1	0.93	0.30	95,95,95,95	0
30	MG	X	3364	1/1	0.93	0.21	83,83,83,83	0
29	MN	X	3072	1/1	0.93	0.08	123,123,123,123	0
29	MN	X	3323	1/1	0.93	0.11	141,141,141,141	0
29	MN	X	3149	1/1	0.93	0.07	109,109,109,109	0
29	MN	X	3174	1/1	0.93	0.06	121,121,121,121	0
29	MN	X	3073	1/1	0.93	0.09	95,95,95,95	0
29	MN	X	3176	1/1	0.93	0.12	128,128,128,128	0
29	MN	X	3045	1/1	0.93	0.17	96,96,96,96	0
29	MN	X	3140	1/1	0.94	0.06	105,105,105,105	0
30	MG	X	3207	1/1	0.94	0.15	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MN	X	3315	1/1	0.94	0.07	104,104,104,104	0
30	MG	X	3395	1/1	0.94	0.06	79,79,79,79	0
30	MG	X	3254	1/1	0.94	0.12	66,66,66,66	0
30	MG	X	3448	1/1	0.94	0.21	72,72,72,72	0
29	MN	X	3115	1/1	0.94	0.12	116,116,116,116	0
29	MN	X	3439	1/1	0.94	0.33	94,94,94,94	0
30	MG	M	201	1/1	0.94	0.12	68,68,68,68	0
30	MG	X	3258	1/1	0.94	0.07	80,80,80,80	0
32	MPD	X	3004	8/8	0.94	0.29	135,135,135,135	0
29	MN	X	3160	1/1	0.94	0.06	100,100,100,100	0
29	MN	X	3100	1/1	0.94	0.05	96,96,96,96	0
29	MN	X	3185	1/1	0.94	0.05	101,101,101,101	0
29	MN	X	3070	1/1	0.94	0.21	129,129,129,129	0
29	MN	X	3187	1/1	0.94	0.10	137,137,137,137	0
29	MN	X	3191	1/1	0.94	0.06	138,138,138,138	0
29	MN	X	3024	1/1	0.94	0.07	120,120,120,120	0
30	MG	X	3484	1/1	0.94	0.14	77,77,77,77	0
29	MN	X	3131	1/1	0.94	0.08	126,126,126,126	0
30	MG	X	3486	1/1	0.94	0.45	90,90,90,90	0
30	MG	X	3301	1/1	0.94	0.13	72,72,72,72	0
29	MN	X	3001	1/1	0.94	0.27	97,97,97,97	0
29	MN	X	3464	1/1	0.94	0.09	149,149,149,149	0
29	MN	X	3262	1/1	0.94	0.05	143,143,143,143	0
29	MN	X	3134	1/1	0.94	0.18	121,121,121,121	0
30	MG	X	3241	1/1	0.94	0.27	78,78,78,78	0
29	MN	X	3067	1/1	0.94	0.17	104,104,104,104	0
29	MN	X	3402	1/1	0.94	0.06	108,108,108,108	0
30	MG	X	3353	1/1	0.94	0.15	79,79,79,79	0
29	MN	X	3069	1/1	0.94	0.10	103,103,103,103	0
29	MN	X	3472	1/1	0.94	0.17	110,110,110,110	0
29	MN	X	3405	1/1	0.94	0.09	103,103,103,103	0
29	MN	X	3177	1/1	0.95	0.08	125,125,125,125	0
29	MN	X	3178	1/1	0.95	0.05	126,126,126,126	0
29	MN	X	3465	1/1	0.95	0.16	117,117,117,117	0
30	MG	X	3167	1/1	0.95	0.07	62,62,62,62	0
30	MG	X	3430	1/1	0.95	0.10	74,74,74,74	0
30	MG	X	3432	1/1	0.95	0.12	71,71,71,71	0
29	MN	X	3065	1/1	0.95	0.14	97,97,97,97	0
29	MN	X	3078	1/1	0.95	0.10	111,111,111,111	0
30	MG	C	302	1/1	0.95	0.09	78,78,78,78	0
29	MN	X	3151	1/1	0.95	0.11	97,97,97,97	0
29	MN	X	3116	1/1	0.95	0.10	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MN	X	3401	1/1	0.95	0.05	104,104,104,104	0
29	MN	X	3080	1/1	0.95	0.14	78,78,78,78	0
29	MN	X	3081	1/1	0.95	0.15	109,109,109,109	0
30	MG	O	201	1/1	0.95	0.19	51,51,51,51	0
29	MN	X	3121	1/1	0.95	0.07	104,104,104,104	0
30	MG	X	3389	1/1	0.95	0.44	94,94,94,94	0
29	MN	X	3418	1/1	0.95	0.05	124,124,124,124	0
29	MN	Y	202	1/1	0.95	0.05	105,105,105,105	0
29	MN	X	3264	1/1	0.95	0.04	117,117,117,117	0
29	MN	X	3084	1/1	0.95	0.13	123,123,123,123	0
29	MN	X	3436	1/1	0.95	0.11	119,119,119,119	0
29	MN	X	3125	1/1	0.95	0.08	123,123,123,123	0
29	MN	X	3090	1/1	0.95	0.09	97,97,97,97	0
30	MG	X	3399	1/1	0.95	0.19	79,79,79,79	0
29	MN	X	3034	1/1	0.95	0.11	77,77,77,77	0
29	MN	X	3097	1/1	0.95	0.10	109,109,109,109	0
30	MG	X	3279	1/1	0.95	0.29	67,67,67,67	0
29	MN	X	3453	1/1	0.95	0.06	126,126,126,126	0
29	MN	X	3068	1/1	0.95	0.21	94,94,94,94	0
30	MG	X	3239	1/1	0.95	0.31	91,91,91,91	0
29	MN	X	3049	1/1	0.95	0.13	93,93,93,93	0
29	MN	X	3037	1/1	0.95	0.05	90,90,90,90	0
29	MN	X	3059	1/1	0.95	0.14	111,111,111,111	0
30	MG	X	3416	1/1	0.95	0.20	90,90,90,90	0
30	MG	X	3138	1/1	0.95	0.14	72,72,72,72	0
29	MN	X	3060	1/1	0.95	0.07	90,90,90,90	0
30	MG	X	3338	1/1	0.95	0.11	82,82,82,82	0
29	MN	X	3113	1/1	0.95	0.12	96,96,96,96	0
29	MN	X	3164	1/1	0.96	0.06	111,111,111,111	0
29	MN	X	3096	1/1	0.96	0.15	100,100,100,100	0
29	MN	X	3051	1/1	0.96	0.05	97,97,97,97	0
29	MN	X	3374	1/1	0.96	0.06	104,104,104,104	0
29	MN	X	3376	1/1	0.96	0.04	119,119,119,119	0
29	MN	X	3206	1/1	0.96	0.14	95,95,95,95	0
30	MG	Y	201	1/1	0.96	0.23	66,66,66,66	0
30	MG	X	3240	1/1	0.96	0.26	78,78,78,78	0
29	MN	X	3171	1/1	0.96	0.06	114,114,114,114	0
29	MN	X	3392	1/1	0.96	0.06	89,89,89,89	0
29	MN	X	3054	1/1	0.96	0.11	97,97,97,97	0
30	MG	X	3296	1/1	0.96	0.12	45,45,45,45	0
29	MN	X	3056	1/1	0.96	0.15	88,88,88,88	0
29	MN	X	3057	1/1	0.96	0.07	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3248	1/1	0.96	0.17	69,69,69,69	0
29	MN	X	3216	1/1	0.96	0.07	94,94,94,94	0
29	MN	X	3219	1/1	0.96	0.09	85,85,85,85	0
29	MN	X	3421	1/1	0.96	0.13	111,111,111,111	0
29	MN	X	3105	1/1	0.96	0.07	97,97,97,97	0
29	MN	X	3110	1/1	0.96	0.13	117,117,117,117	0
29	MN	X	3043	1/1	0.96	0.10	81,81,81,81	0
29	MN	X	3234	1/1	0.96	0.06	144,144,144,144	0
29	MN	X	3179	1/1	0.96	0.04	106,106,106,106	0
29	MN	X	3076	1/1	0.96	0.07	90,90,90,90	0
29	MN	X	3077	1/1	0.96	0.12	100,100,100,100	0
31	62B	X	3003	35/35	0.96	0.13	65,65,65,65	0
29	MN	X	3452	1/1	0.96	0.04	120,120,120,120	0
29	MN	X	3013	1/1	0.96	0.06	70,70,70,70	0
29	MN	X	3036	1/1	0.96	0.08	86,86,86,86	0
29	MN	X	3457	1/1	0.96	0.11	135,135,135,135	0
30	MG	X	3442	1/1	0.96	0.14	71,71,71,71	0
29	MN	X	3061	1/1	0.96	0.07	92,92,92,92	0
29	MN	X	3117	1/1	0.96	0.06	107,107,107,107	0
30	MG	X	3271	1/1	0.96	0.15	92,92,92,92	0
29	MN	X	3082	1/1	0.96	0.07	112,112,112,112	0
29	MN	X	3188	1/1	0.96	0.12	114,114,114,114	0
29	MN	X	3189	1/1	0.96	0.06	154,154,154,154	0
30	MG	X	3214	1/1	0.96	0.22	86,86,86,86	0
29	MN	X	3027	1/1	0.96	0.13	68,68,68,68	0
29	MN	X	3318	1/1	0.96	0.04	128,128,128,128	0
29	MN	X	3089	1/1	0.96	0.09	113,113,113,113	0
30	MG	X	3390	1/1	0.96	0.15	63,63,63,63	0
29	MN	X	3193	1/1	0.96	0.05	110,110,110,110	0
30	MG	X	3481	1/1	0.96	0.10	82,82,82,82	0
29	MN	X	3122	1/1	0.96	0.09	99,99,99,99	0
29	MN	X	3042	1/1	0.96	0.13	74,74,74,74	0
29	MN	X	3050	1/1	0.96	0.14	98,98,98,98	0
30	MG	X	3284	1/1	0.96	0.09	72,72,72,72	0
29	MN	X	3128	1/1	0.96	0.07	93,93,93,93	0
29	MN	X	3190	1/1	0.97	0.06	124,124,124,124	0
29	MN	X	3092	1/1	0.97	0.09	90,90,90,90	0
29	MN	X	3093	1/1	0.97	0.09	81,81,81,81	0
29	MN	X	3243	1/1	0.97	0.09	114,114,114,114	0
29	MN	X	3467	1/1	0.97	0.17	72,72,72,72	0
29	MN	X	3245	1/1	0.97	0.03	129,129,129,129	0
29	MN	X	3257	1/1	0.97	0.10	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MN	X	3170	1/1	0.97	0.07	104,104,104,104	0
29	MN	X	3403	1/1	0.97	0.10	114,114,114,114	0
29	MN	X	3038	1/1	0.97	0.04	106,106,106,106	0
29	MN	X	3095	1/1	0.97	0.04	79,79,79,79	0
29	MN	X	3407	1/1	0.97	0.14	83,83,83,83	0
29	MN	X	3409	1/1	0.97	0.04	87,87,87,87	0
29	MN	X	3052	1/1	0.97	0.11	90,90,90,90	0
30	MG	X	3275	1/1	0.97	0.07	71,71,71,71	0
29	MN	X	3053	1/1	0.97	0.14	58,58,58,58	0
29	MN	X	3313	1/1	0.97	0.13	117,117,117,117	0
29	MN	X	3098	1/1	0.97	0.03	92,92,92,92	0
29	MN	X	3200	1/1	0.97	0.08	123,123,123,123	0
29	MN	X	3099	1/1	0.97	0.08	82,82,82,82	0
29	MN	X	3020	1/1	0.97	0.07	107,107,107,107	0
29	MN	X	3055	1/1	0.97	0.09	86,86,86,86	0
29	MN	X	3088	1/1	0.97	0.07	101,101,101,101	0
29	MN	X	3103	1/1	0.97	0.08	85,85,85,85	0
29	MN	X	3012	1/1	0.97	0.16	79,79,79,79	0
29	MN	X	3108	1/1	0.97	0.08	89,89,89,89	0
29	MN	X	3455	1/1	0.97	0.05	116,116,116,116	0
30	MG	X	3137	1/1	0.97	0.28	63,63,63,63	0
29	MN	X	3456	1/1	0.97	0.07	113,113,113,113	0
29	MN	X	3132	1/1	0.97	0.04	104,104,104,104	0
29	MN	X	3161	1/1	0.97	0.06	93,93,93,93	0
29	MN	X	3109	1/1	0.97	0.09	92,92,92,92	0
29	MN	X	3033	1/1	0.97	0.14	78,78,78,78	0
29	MN	X	3330	1/1	0.97	0.06	104,104,104,104	0
29	MN	X	3091	1/1	0.97	0.04	92,92,92,92	0
29	MN	X	3014	1/1	0.98	0.05	53,53,53,53	0
29	MN	X	3035	1/1	0.98	0.06	74,74,74,74	0
29	MN	X	3502	1/1	0.98	0.10	88,88,88,88	0
29	MN	X	3503	1/1	0.98	0.03	68,68,68,68	0
29	MN	X	3017	1/1	0.98	0.11	92,92,92,92	0
29	MN	X	3026	1/1	0.98	0.12	66,66,66,66	0
29	MN	X	3022	1/1	0.98	0.03	92,92,92,92	0
29	MN	X	3127	1/1	0.98	0.03	94,94,94,94	0
29	MN	X	3039	1/1	0.98	0.09	79,79,79,79	0
29	MN	X	3074	1/1	0.98	0.15	113,113,113,113	0
29	MN	X	3169	1/1	0.98	0.08	107,107,107,107	0
29	MN	X	3040	1/1	0.98	0.09	81,81,81,81	0
29	MN	X	3041	1/1	0.98	0.06	77,77,77,77	0
29	MN	X	3172	1/1	0.98	0.03	114,114,114,114	0

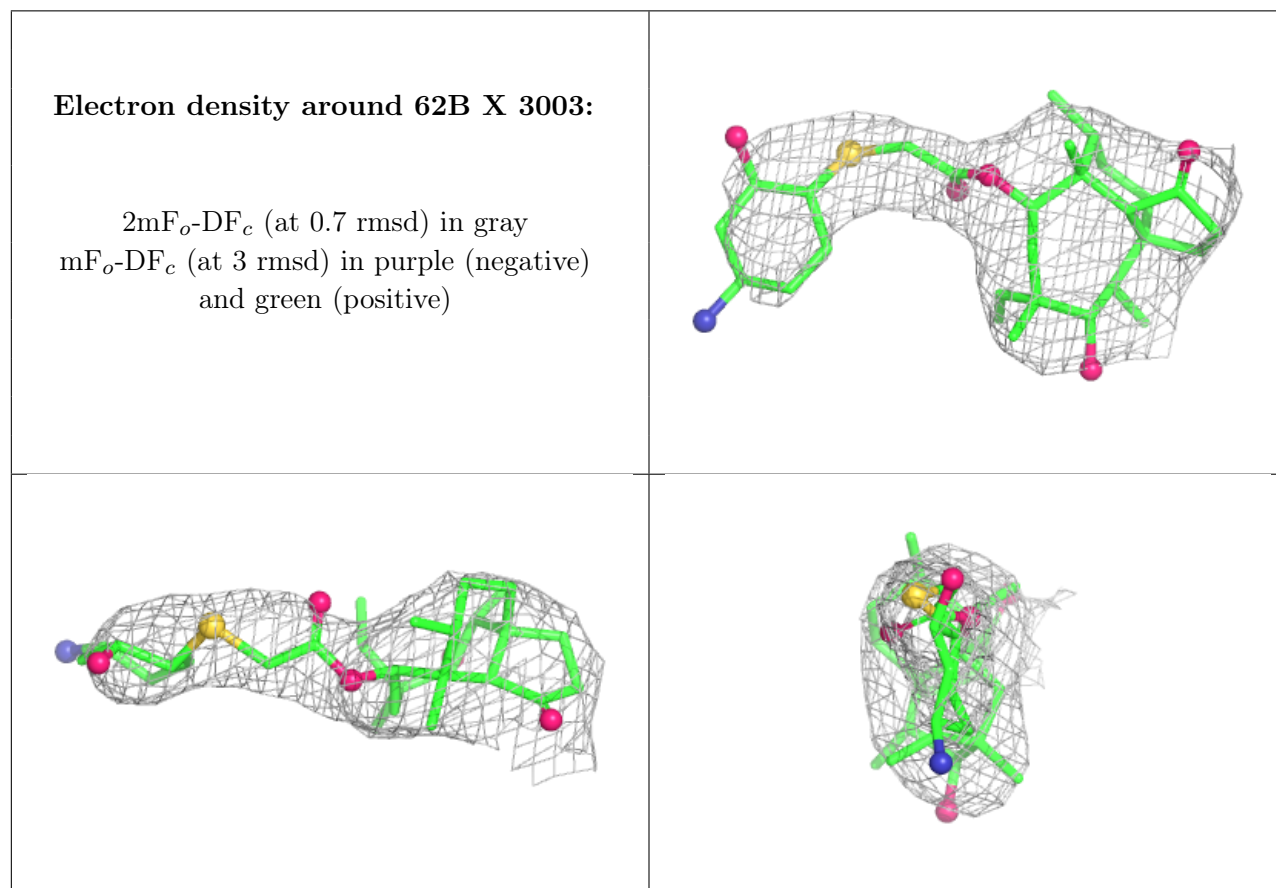
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MN	X	3028	1/1	0.98	0.21	53,53,53,53	0
29	MN	X	3104	1/1	0.98	0.04	94,94,94,94	0
29	MN	X	3079	1/1	0.98	0.08	58,58,58,58	0
29	MN	X	3107	1/1	0.98	0.10	73,73,73,73	0
29	MN	X	3215	1/1	0.98	0.03	87,87,87,87	0
29	MN	X	3029	1/1	0.98	0.09	69,69,69,69	0
29	MN	X	3030	1/1	0.98	0.18	69,69,69,69	0
29	MN	X	3220	1/1	0.98	0.04	103,103,103,103	0
29	MN	X	3031	1/1	0.98	0.09	68,68,68,68	0
29	MN	X	3023	1/1	0.98	0.11	92,92,92,92	0
29	MN	X	3086	1/1	0.98	0.12	92,92,92,92	0
29	MN	X	3062	1/1	0.98	0.05	87,87,87,87	0
30	MG	X	3427	1/1	0.98	0.14	59,59,59,59	0
30	MG	X	3501	1/1	0.98	0.12	64,64,64,64	0
29	MN	X	3152	1/1	0.98	0.10	75,75,75,75	0
29	MN	X	3063	1/1	0.98	0.12	70,70,70,70	0
29	MN	X	3064	1/1	0.98	0.07	84,84,84,84	0
30	MG	X	3431	1/1	0.98	0.10	55,55,55,55	0
29	MN	X	3047	1/1	0.98	0.04	70,70,70,70	0
29	MN	X	3156	1/1	0.98	0.07	77,77,77,77	0
29	MN	X	3066	1/1	0.98	0.07	80,80,80,80	0
29	MN	X	3048	1/1	0.98	0.11	93,93,93,93	0
29	MN	X	3032	1/1	0.99	0.08	64,64,64,64	0
29	MN	X	3126	1/1	0.99	0.02	74,74,74,74	0
29	MN	X	3145	1/1	0.99	0.05	69,69,69,69	0
29	MN	X	3083	1/1	0.99	0.08	73,73,73,73	0
29	MN	X	3118	1/1	0.99	0.06	65,65,65,65	0
29	MN	X	3015	1/1	0.99	0.04	80,80,80,80	0
29	MN	X	3251	1/1	0.99	0.04	81,81,81,81	0
29	MN	X	3021	1/1	0.99	0.04	91,91,91,91	0
29	MN	X	3106	1/1	0.99	0.04	100,100,100,100	0
29	MN	X	3217	1/1	0.99	0.04	86,86,86,86	0
30	MG	X	3204	1/1	0.99	0.05	100,100,100,100	0
29	MN	X	3075	1/1	0.99	0.08	71,71,71,71	0
29	MN	X	3270	1/1	0.99	0.04	110,110,110,110	0
29	MN	X	3016	1/1	0.99	0.02	75,75,75,75	0
29	MN	X	3201	1/1	0.99	0.05	88,88,88,88	0
29	MN	X	3136	1/1	0.99	0.12	55,55,55,55	0
29	MN	X	3018	1/1	1.00	0.04	86,86,86,86	0
29	MN	X	3085	1/1	1.00	0.07	59,59,59,59	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.