



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:15 PM UTC

PDB ID : 5IWA / pdb_00005iwa
Title : Crystal structure of the 30S ribosomal subunit from *Thermus thermophilus* in complex with the GE81112 peptide antibiotic
Authors : Schedlbauer, A.; Kaminishi, T.; Ochoa-Lizarralde, B.; Chieko, N.; Masahito, K.; Takemoto, C.; Yokoyama, S.; Connell, S.R.; Fucini, P.
Deposited on : 2016-03-22
Resolution : 3.50 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

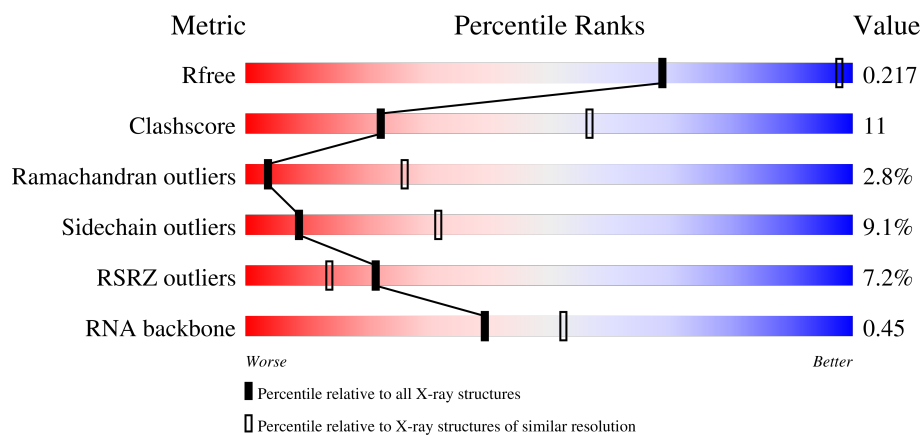
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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.



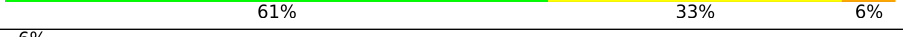
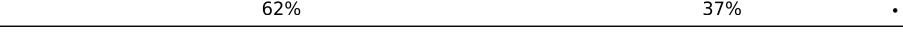
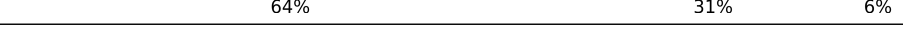
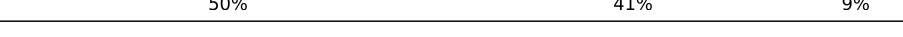
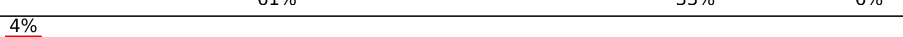
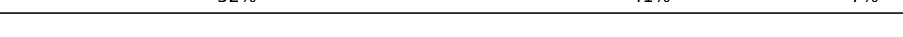
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

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	B	226	4% 59% 36% .
2	C	206	% 63% 33% .
3	D	208	5% 60% 34% ..

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Mol	Chain	Length	Quality of chain
4	E	157	
5	F	101	
6	G	155	
7	H	138	
8	I	127	
9	J	99	
10	K	115	
11	L	124	
12	M	125	
13	N	60	
14	O	88	
15	P	85	
16	Q	104	
17	R	71	
18	S	83	
19	T	103	
20	V	24	
21	A	1509	

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
22	MG	A	3438	-	-	-	X
22	MG	A	3453	-	-	-	X
22	MG	A	3483	-	-	-	X
23	ZN	N	101	-	-	X	-

2 Entry composition [i](#)

There are 24 unique types of molecules in this entry. The entry contains 52089 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 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	225	Total	C	N	O	S	0	0	0
			1837	1171	331	330	5			

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	157	Total	C	N	O	S	0	0	0
			1199	754	228	213	4			

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	127	Total	C	N	O	S	0	0	0
			1010	639	197	174				

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	99	Total	C	N	O	S	0	0	0
			802	504	157	140	1			

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	115	Total	C	N	O	S	0	0	0
			854	531	160	160	3			

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	125	Total	C	N	O	S	0	0	0
			987	611	203	171	2			

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	O	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	85	Total	C	N	O	S	0	0	0
			717	452	144	120	1			

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	Q	104	Total	C	N	O	S	0	0	0
			857	547	160	148	2			

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	R	71	Total	C	N	O	S	0	0	0
			585	373	116	96				

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	S	83	Total	C	N	O	S	0	0	0
			666	424	124	116	2			

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	T	103	Total	C	N	O	S	0	0	0
			797	493	169	133	2			

- Molecule 20 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	V	24	Total	C	N	O	S	0	0	0
			209	128	50	31				

- Molecule 21 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	A	1509	Total	C	N	O	P	0	7	0
			32589	14507	6043	10524	1515			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	A	-	expression tag	GB 55771382
A	2	A	-	expression tag	GB 55771382
A	3	A	-	expression tag	GB 55771382

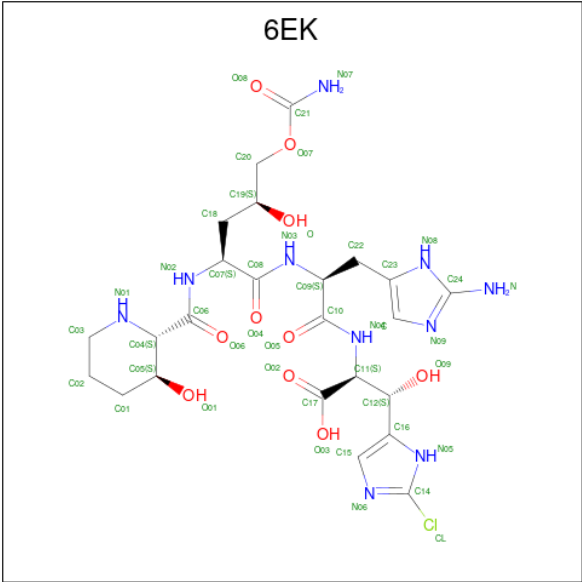
- Molecule 22 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	B	1	Total	Mg	0	0
			1	1		
22	E	1	Total	Mg	0	0
			1	1		
22	H	1	Total	Mg	0	0
			1	1		
22	K	1	Total	Mg	0	0
			1	1		
22	O	1	Total	Mg	0	0
			1	1		
22	S	1	Total	Mg	0	0
			1	1		
22	A	198	Total	Mg	0	0
			198	198		

- Molecule 23 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	D	1	Total	Zn	0	0
			1	1		
23	N	1	Total	Zn	0	0
			1	1		

- Molecule 24 is (2S,3S)-2-([(2S)-3-(2-amino-1H-imidazol-5-yl)-2-([(2S,4S)-5-(carbamoyloxy)-4-hydroxy-2-([(2S,3S)-3-hydroxypiperidin-2-yl]carbonyl]amino)pentanoyl]amino}propanoyl]amino)-3-(2-chloro-1H-imidazol-5-yl)-3-hydroxypropanoic acid (CCD ID: 6EK) (formula: C₂₄H₃₅ClN₁₀O₁₀).

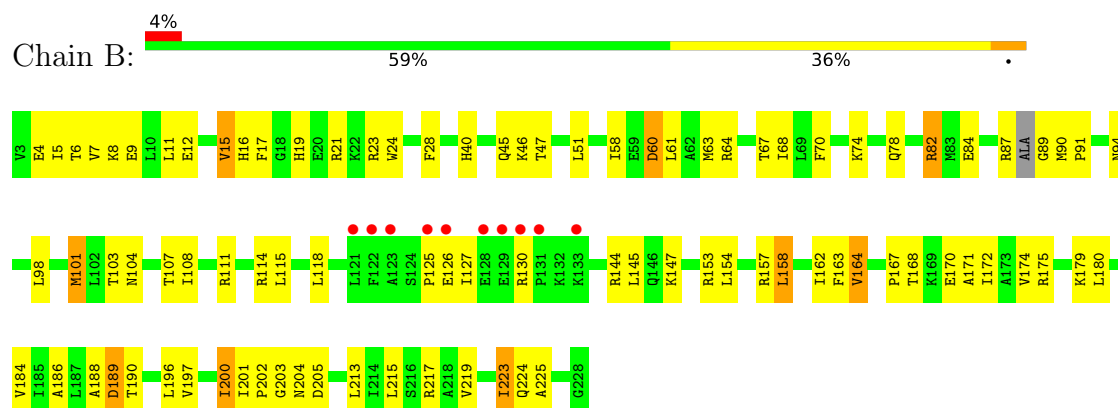


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	M	1	Total	C	Cl	N	O	0	0
			45	24	1	10	10		

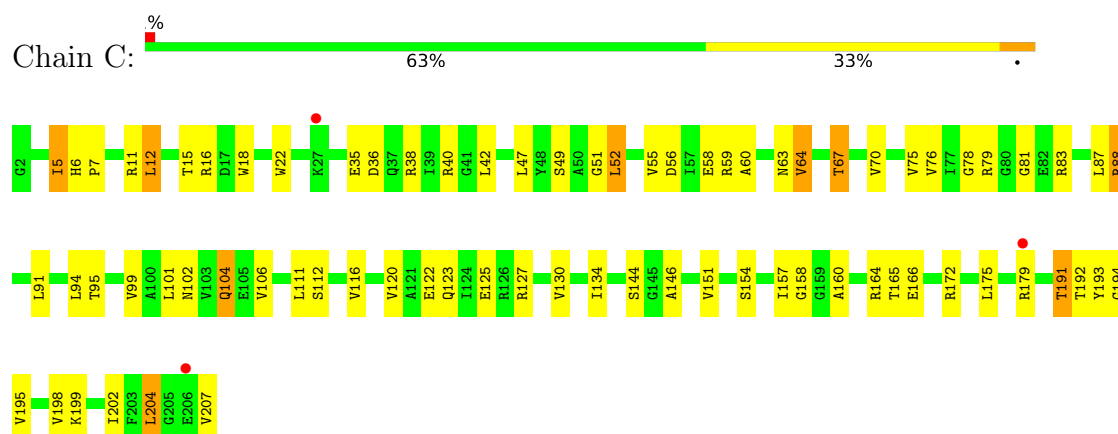
3 Residue-property plots [i](#)

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.

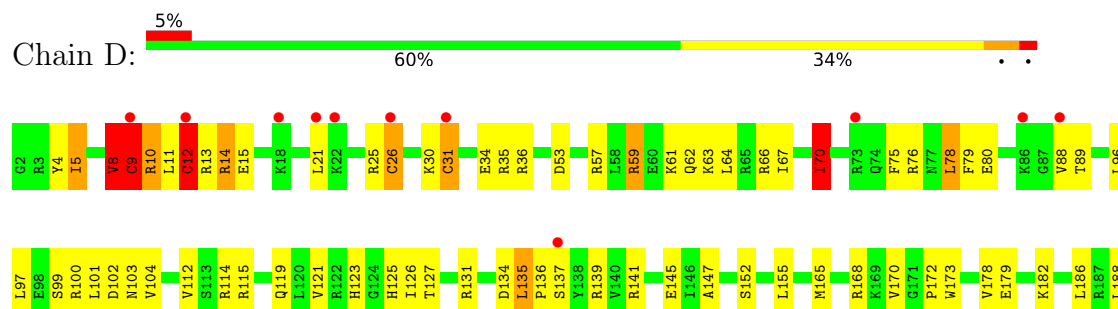
• Molecule 1: 30S ribosomal protein S2

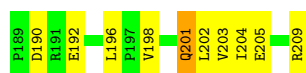


• Molecule 2: 30S ribosomal protein S3

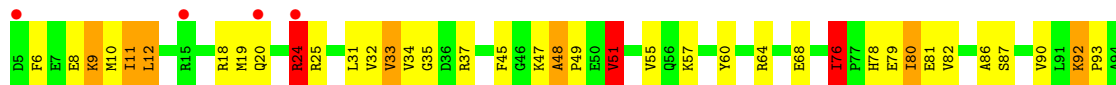


• Molecule 3: 30S ribosomal protein S4





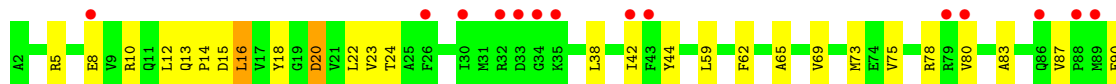
• Molecule 4: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S6



• Molecule 6: 30S ribosomal protein S7

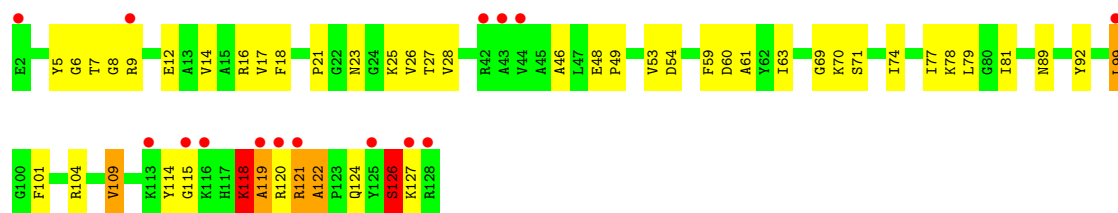


• Molecule 7: 30S ribosomal protein S8

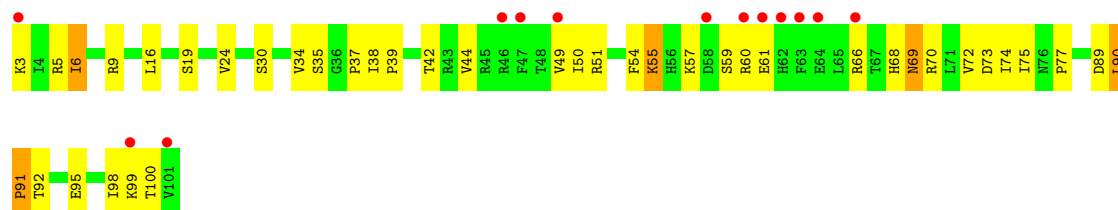


• Molecule 8: 30S ribosomal protein S9

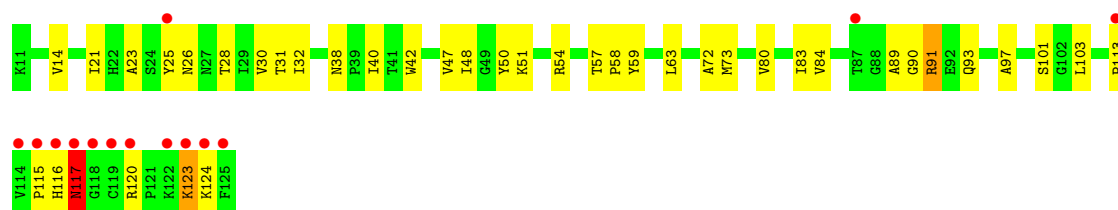




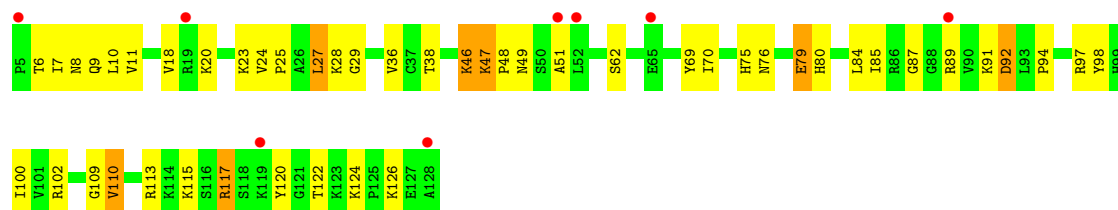
• Molecule 9: 30S ribosomal protein S10



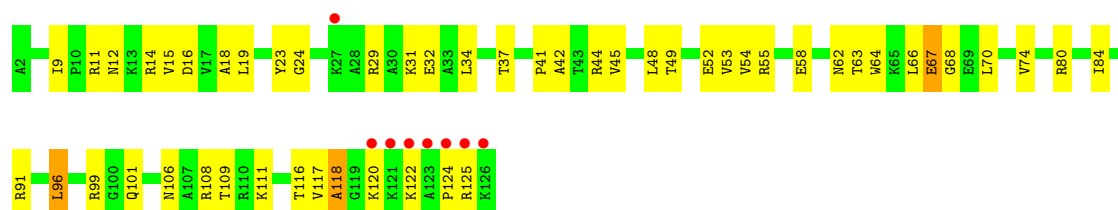
• Molecule 10: 30S ribosomal protein S11



• Molecule 11: 30S ribosomal protein S12



• Molecule 12: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S14 type Z

Chain N:  62% 37%



- Molecule 14: 30S ribosomal protein S15

Chain O:  64% 31% 6%



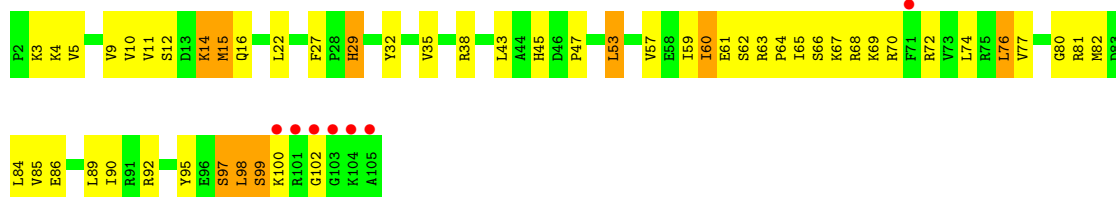
- Molecule 15: 30S ribosomal protein S16

Chain P:  64% 36%



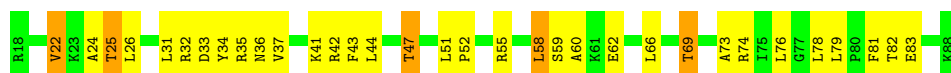
- Molecule 16: 30S ribosomal protein S17

Chain Q:  7% 50% 41% 9%



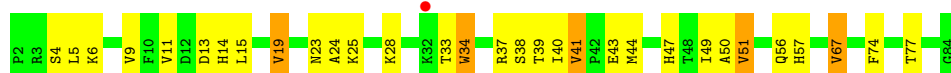
- Molecule 17: 30S ribosomal protein S18

Chain R:  54% 39% 7%



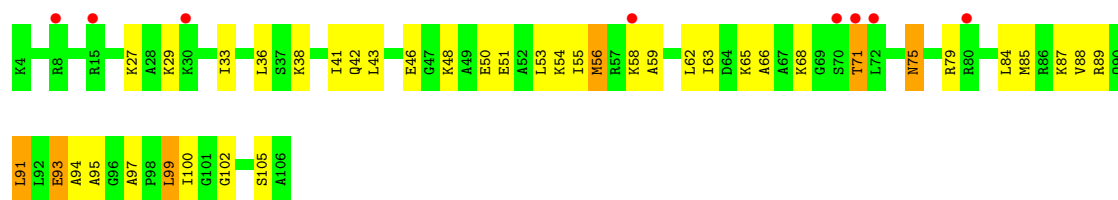
- Molecule 18: 30S ribosomal protein S19

Chain S:  63% 31% 6%

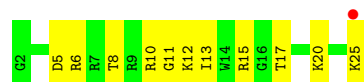


- Molecule 19: 30S ribosomal protein S20

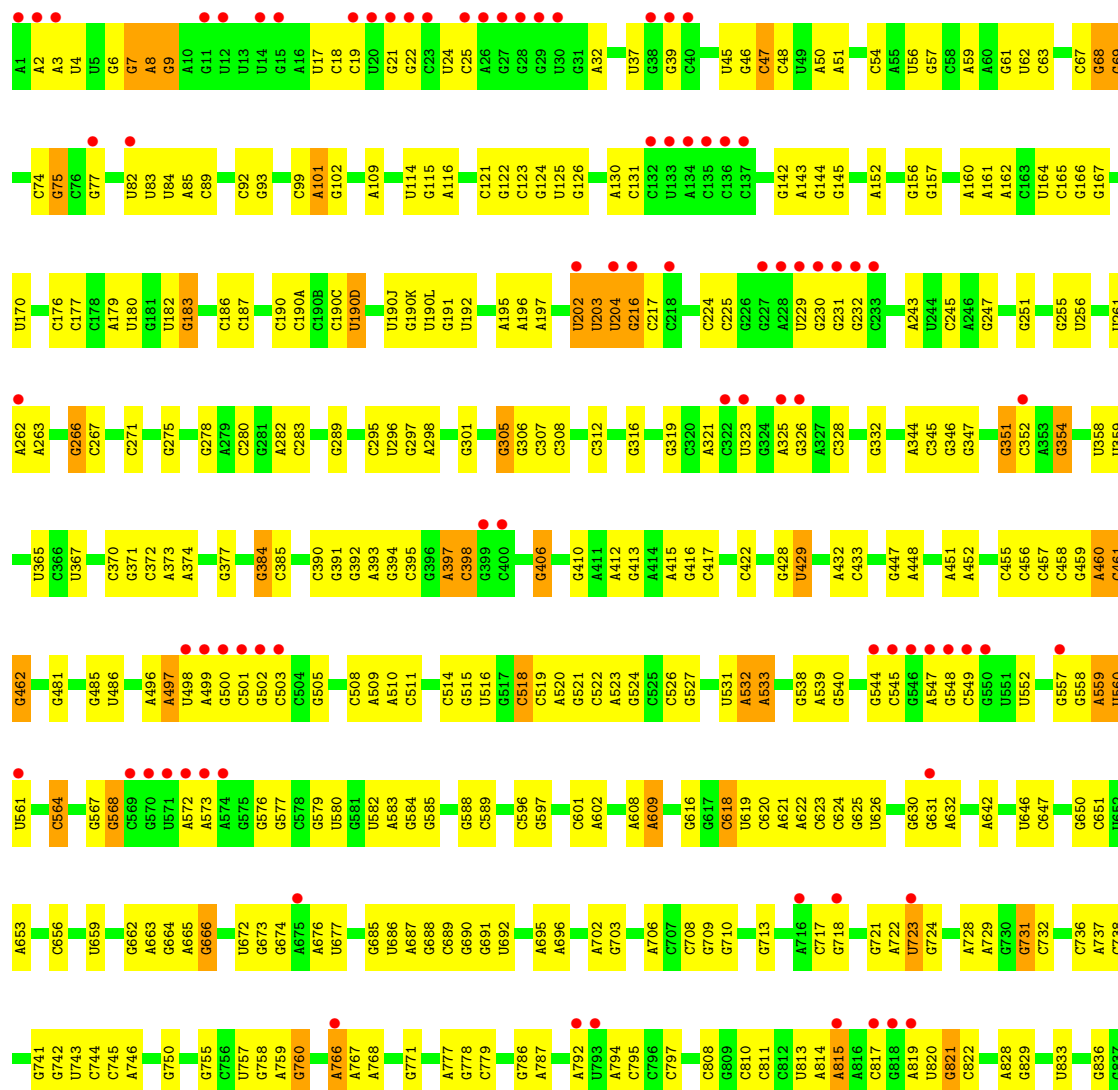
Chain T:  8% 61% 33% 6%

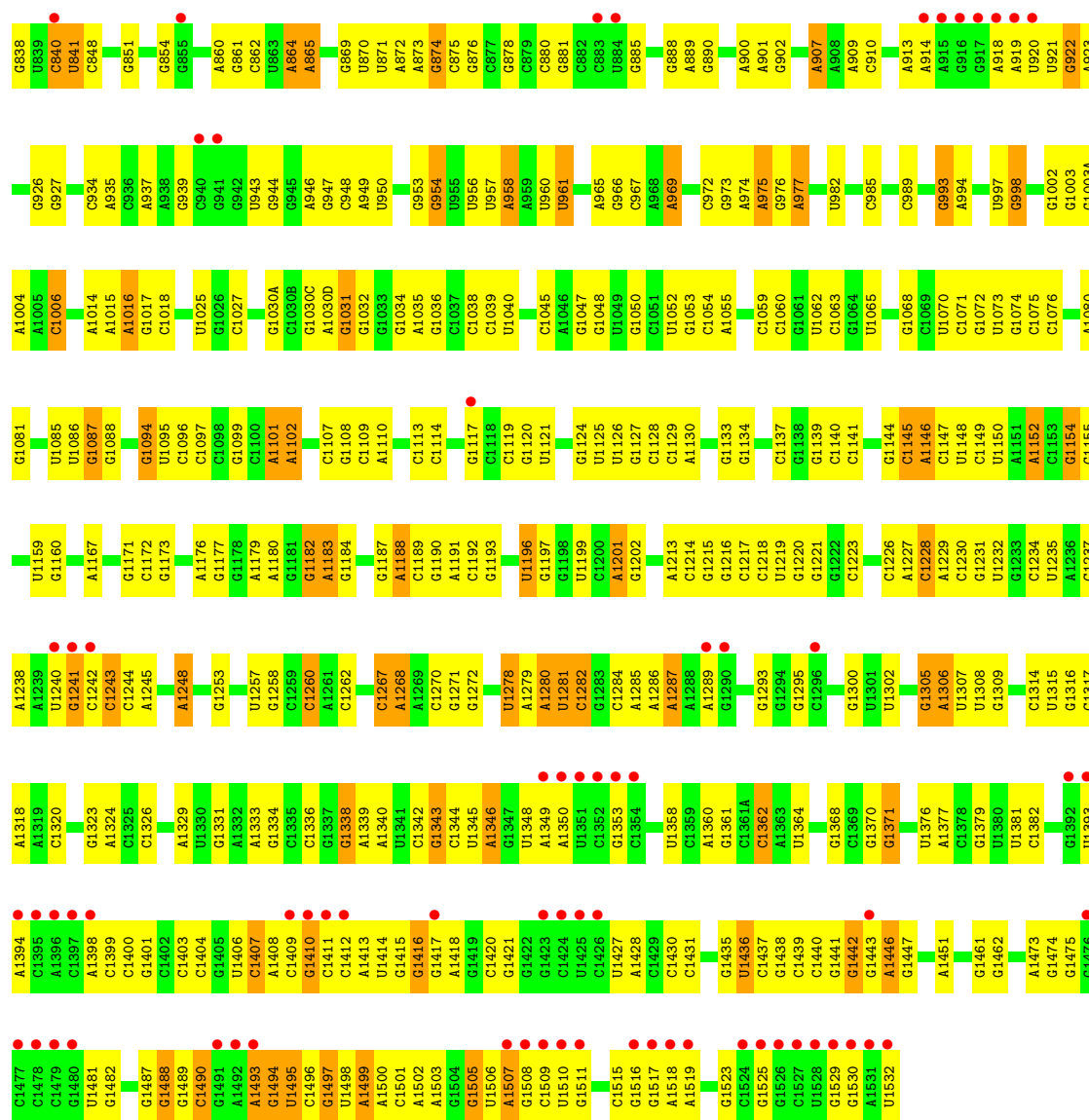


- Molecule 20: 30S ribosomal protein Thx



- Molecule 21: 16S ribosomal RNA





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	413.14Å 413.14Å 173.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.03 – 3.50 80.03 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (80.03-3.50) 99.8 (80.03-3.50)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.7.3 _928	Depositor
R, R_{free}	0.166 , 0.218 0.169 , 0.217	Depositor DCC
R_{free} test set	9369 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	138.9	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 109.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	52089	wwPDB-VP
Average B, all atoms (Å ²)	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 6EK, MG, ZN

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	B	0.64	0/1868	1.06	4/2512 (0.2%)
2	C	0.65	0/1637	1.04	4/2205 (0.2%)
3	D	0.74	0/1733	1.21	11/2318 (0.5%)
4	E	0.87	0/1216	1.34	13/1636 (0.8%)
5	F	0.58	0/856	1.05	2/1154 (0.2%)
6	G	0.57	0/1276	0.96	0/1709
7	H	0.79	0/1136	1.28	12/1527 (0.8%)
8	I	0.60	0/1029	1.09	8/1379 (0.6%)
9	J	0.62	0/815	1.01	2/1095 (0.2%)
10	K	0.63	0/869	1.12	7/1173 (0.6%)
11	L	0.69	0/987	1.13	4/1320 (0.3%)
12	M	0.60	0/998	1.07	3/1336 (0.2%)
13	N	0.61	0/501	1.17	5/664 (0.8%)
14	O	0.63	0/745	1.04	1/992 (0.1%)
15	P	0.69	0/733	1.04	3/984 (0.3%)
16	Q	0.68	0/870	1.14	6/1159 (0.5%)
17	R	0.66	0/590	1.04	0/782
18	S	0.52	0/681	0.95	2/915 (0.2%)
19	T	0.56	0/800	1.08	3/1052 (0.3%)
20	V	0.58	0/213	1.02	1/277 (0.4%)
21	A	0.41	0/36483	0.48	0/56943
All	All	0.51	0/56036	0.74	91/83132 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1
7	H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
11	L	0	1
All	All	0	3

There are no bond length outliers.

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	51	VAL	CB-CA-C	-10.69	103.02	114.35
7	H	71	GLY	CA-C-N	-10.33	109.42	120.47
7	H	71	GLY	C-N-CA	-10.33	109.42	120.47
3	D	31	CYS	N-CA-C	-9.03	97.71	110.35
3	D	9	CYS	N-CA-C	-8.28	93.17	110.80
4	E	127	ASN	CA-C-N	7.91	129.72	119.84
4	E	127	ASN	C-N-CA	7.91	129.72	119.84
3	D	141	ARG	CA-C-N	-7.58	112.19	119.85
3	D	141	ARG	C-N-CA	-7.58	112.19	119.85
7	H	75	ARG	CA-C-N	7.56	129.29	119.84
7	H	75	ARG	C-N-CA	7.56	129.29	119.84
3	D	126	ILE	N-CA-C	7.34	118.38	108.11
13	N	31	ARG	CA-C-N	-7.34	111.53	122.24
13	N	31	ARG	C-N-CA	-7.34	111.53	122.24
7	H	19	VAL	N-CA-C	-7.22	105.79	112.43
10	K	91	ARG	N-CA-C	-6.95	103.64	111.07
20	V	20	LYS	N-CA-C	-6.90	103.69	111.14
3	D	70	ILE	N-CA-C	6.78	123.44	109.34
15	P	84	ALA	N-CA-C	6.72	118.52	108.31
3	D	26	CYS	N-CA-C	-6.58	104.14	111.71
10	K	38	ASN	CA-C-N	6.57	126.52	119.76
10	K	38	ASN	C-N-CA	6.57	126.52	119.76
3	D	88	VAL	CB-CA-C	-6.37	103.08	111.81
19	T	91	LEU	N-CA-C	-6.32	106.78	114.75
4	E	24	ARG	N-CA-C	-6.26	102.10	110.55
11	L	47	LYS	CA-C-N	-6.26	113.47	121.04
11	L	47	LYS	C-N-CA	-6.26	113.47	121.04
7	H	79	VAL	N-CA-C	-6.26	106.43	111.81
3	D	21	LEU	N-CA-C	-6.24	105.50	113.23
1	B	68	ILE	CB-CA-C	-6.19	101.92	110.96
14	O	11	VAL	CB-CA-C	-6.17	103.94	112.02
13	N	35	ARG	N-CA-C	-6.09	102.07	110.35
4	E	76	ILE	CA-C-N	6.04	125.93	119.28
4	E	76	ILE	C-N-CA	6.04	125.93	119.28
3	D	8	VAL	N-CA-C	6.00	117.12	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	158	LEU	CA-C-N	5.93	126.26	119.92
1	B	158	LEU	C-N-CA	5.93	126.26	119.92
7	H	100	ILE	N-CA-C	-5.86	103.21	108.95
7	H	100	ILE	CB-CA-C	-5.84	104.58	110.89
19	T	93	GLU	N-CA-C	-5.80	104.32	111.40
10	K	124	LYS	N-CA-C	-5.78	101.48	110.10
12	M	62	ASN	N-CA-C	5.75	120.31	113.12
11	L	92	ASP	N-CA-C	5.70	119.34	112.38
19	T	97	ALA	N-CA-C	5.70	116.15	109.60
5	F	60	PHE	N-CA-C	5.70	118.24	109.07
15	P	84	ALA	CB-CA-C	-5.69	110.00	116.54
15	P	83	GLU	N-CA-C	5.66	117.44	108.79
16	Q	29	HIS	CA-C-N	5.64	125.35	119.82
16	Q	29	HIS	C-N-CA	5.64	125.35	119.82
4	E	32	VAL	N-CA-C	5.63	116.23	108.12
13	N	33	VAL	N-CA-C	5.61	116.81	108.23
2	C	81	GLY	N-CA-C	-5.57	107.33	115.63
4	E	113	ALA	N-CA-C	-5.56	105.22	111.28
2	C	104	GLN	N-CA-C	5.55	117.45	108.34
7	H	56	LYS	CA-C-N	5.54	126.77	119.84
7	H	56	LYS	C-N-CA	5.54	126.77	119.84
8	I	122	ALA	CA-C-N	5.49	125.39	119.85
8	I	122	ALA	C-N-CA	5.49	125.39	119.85
3	D	12	CYS	CA-CB-SG	5.44	126.92	114.40
8	I	109	VAL	CB-CA-C	-5.44	103.11	111.71
10	K	25	TYR	N-CA-C	-5.44	106.60	113.18
1	B	224	GLN	N-CA-C	-5.43	105.00	111.03
7	H	53	VAL	N-CA-C	5.40	115.56	107.51
10	K	14	VAL	N-CA-C	5.38	114.49	106.85
4	E	92	LYS	CA-C-N	-5.37	115.04	120.31
4	E	92	LYS	C-N-CA	-5.37	115.04	120.31
8	I	126	SER	N-CA-C	5.37	122.23	110.80
16	Q	12	SER	N-CA-C	5.36	117.35	108.13
4	E	157	HIS	N-CA-C	-5.35	103.42	110.43
13	N	31	ARG	N-CA-C	5.35	119.74	111.56
2	C	158	GLY	N-CA-C	-5.34	102.92	112.22
8	I	118	LYS	N-CA-C	5.27	122.03	110.80
2	C	130	VAL	N-CA-C	5.26	115.48	110.53
4	E	48	ALA	CA-C-N	-5.25	114.37	120.04
4	E	48	ALA	C-N-CA	-5.25	114.37	120.04
16	Q	102	GLY	N-CA-C	5.25	117.70	110.56
7	H	84	ARG	N-CA-C	5.23	116.90	108.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	6	ILE	N-CA-C	5.23	115.38	107.80
18	S	34	TRP	N-CA-C	-5.23	107.57	114.31
16	Q	27	PHE	CA-C-N	-5.21	114.37	119.99
16	Q	27	PHE	C-N-CA	-5.21	114.37	119.99
18	S	67	VAL	N-CA-C	5.14	117.02	111.58
5	F	81	ILE	CB-CA-C	-5.12	105.32	112.02
11	L	109	GLY	N-CA-C	-5.12	104.68	112.51
8	I	14	VAL	N-CA-C	5.08	115.30	107.77
8	I	115	GLY	N-CA-C	-5.07	108.32	115.32
12	M	96	LEU	CA-C-N	-5.07	115.01	120.03
12	M	96	LEU	C-N-CA	-5.07	115.01	120.03
9	J	69	ASN	N-CA-C	5.05	116.64	108.41
10	K	40	ILE	CB-CA-C	-5.02	107.44	111.71
8	I	77	ILE	CB-CA-C	-5.01	105.29	111.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	11	LEU	Peptide
7	H	90	GLY	Peptide
11	L	46	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1837	0	1888	57	0
2	C	1613	0	1677	39	0
3	D	1703	0	1764	52	0
4	E	1199	0	1251	50	0
5	F	843	0	857	27	0
6	G	1257	0	1296	31	0
7	H	1116	0	1177	27	0
8	I	1010	0	1037	30	0
9	J	802	0	849	27	0
10	K	854	0	868	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	L	971	0	1057	28	0
12	M	987	0	1050	33	0
13	N	492	0	530	15	0
14	O	734	0	771	21	0
15	P	717	0	738	18	0
16	Q	857	0	928	35	0
17	R	585	0	657	26	0
18	S	666	0	686	20	0
19	T	797	0	907	25	0
20	V	209	0	221	6	0
21	A	32589	0	16447	443	0
22	A	198	0	0	0	0
22	B	1	0	0	0	0
22	E	1	0	0	0	0
22	H	1	0	0	0	0
22	K	1	0	0	0	0
22	O	1	0	0	0	0
22	S	1	0	0	0	0
23	D	1	0	0	0	0
23	N	1	0	0	2	0
24	M	45	0	0	0	0
All	All	52089	0	36656	928	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 11.

All (928) 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)
9:J:61:GLU:OE1	13:N:45:ARG:NH1	2.00	0.93
21:A:664:G:H22	21:A:741:G:H1	1.21	0.88
6:G:94:ARG:NH1	21:A:1377:A:OP2	2.10	0.85
10:K:57:THR:HG22	10:K:59:TYR:H	1.40	0.84
8:I:16:ARG:NH1	21:A:1147:C:O2	2.11	0.84
12:M:11:ARG:HA	12:M:45:VAL:HB	1.60	0.83
9:J:19:SER:HB2	9:J:91:PRO:HG3	1.60	0.83
15:P:28:ARG:NH2	21:A:390:C:O3'	2.16	0.79
1:B:104:ASN:OD1	1:B:107:THR:OG1	2.01	0.78
12:M:37:THR:O	12:M:55:ARG:NH2	2.17	0.78
21:A:975:A:H5'	21:A:975:A:H8	1.48	0.78
4:E:18:ARG:NH2	21:A:1070:U:OP1	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:15:ASP:OD1	6:G:44:TYR:OH	2.02	0.77
19:T:50:GLU:HB2	19:T:99:LEU:HD12	1.67	0.77
13:N:27:CYS:HG	23:N:101:ZN:ZN	0.96	0.77
9:J:3:LYS:HB2	9:J:77:PRO:HG3	1.66	0.76
12:M:14:ARG:NH2	21:A:1295:G:O2'	2.17	0.76
4:E:9:LYS:HG3	4:E:112:LEU:HD11	1.65	0.76
4:E:144:THR:HB	4:E:146:ALA:HB3	1.67	0.76
4:E:78:HIS:HA	7:H:105:ARG:HG3	1.68	0.76
4:E:20:GLN:HG2	4:E:25:ARG:HH21	1.50	0.75
9:J:44:VAL:HG22	9:J:66:ARG:HG2	1.69	0.75
21:A:736:C:H2'	21:A:737:A:C8	2.20	0.75
3:D:103:ASN:OD1	3:D:114:ARG:NH1	2.19	0.75
8:I:9:ARG:NH2	21:A:1119:C:OP2	2.19	0.75
21:A:695:A:H2'	21:A:696:A:C8	2.21	0.75
21:A:1030(A):G:N2	21:A:1030(D):A:OP2	2.19	0.74
21:A:1027:C:H42	21:A:1034:G:H1	1.35	0.74
21:A:1030(C):G:H2'	21:A:1030(D):A:C8	2.22	0.74
21:A:1488:G:H2'	21:A:1489:G:C8	2.24	0.73
8:I:46:ALA:HB2	8:I:74:ILE:HG23	1.71	0.72
21:A:1172:C:H2'	21:A:1173:G:H8	1.53	0.72
2:C:193:TYR:HB3	21:A:532:A:N6	2.05	0.71
8:I:71:SER:HA	8:I:74:ILE:HD12	1.70	0.71
13:N:18:VAL:HG21	21:A:1316:G:H4'	1.73	0.71
11:L:46:LYS:HD3	11:L:94:PRO:HG3	1.73	0.71
21:A:662:G:H2'	21:A:663:A:C8	2.26	0.71
14:O:56:LEU:HA	14:O:59:MET:HE2	1.72	0.71
12:M:49:THR:HB	12:M:52:GLU:HB2	1.73	0.70
14:O:82:ILE:HD13	14:O:88:ARG:HG2	1.73	0.70
21:A:204:U:H4'	21:A:216:G:H5''	1.72	0.70
21:A:946:A:H2'	21:A:947:G:C8	2.26	0.70
1:B:6:THR:HG22	1:B:8:LYS:H	1.57	0.69
6:G:139:GLU:O	6:G:143:ARG:NH1	2.25	0.69
7:H:12:ARG:HD3	7:H:26:VAL:HG22	1.74	0.69
3:D:30:LYS:O	3:D:31:CYS:C	2.35	0.69
4:E:35:GLY:HA3	4:E:112:LEU:HB3	1.74	0.68
10:K:48:ILE:HG13	10:K:63:LEU:HB3	1.74	0.68
21:A:1406:U:H5'	21:A:1407:C:OP2	1.93	0.68
4:E:144:THR:O	4:E:146:ALA:N	2.26	0.68
21:A:1435:G:H2'	21:A:1436:U:C6	2.28	0.68
2:C:35:GLU:OE1	2:C:59:ARG:NH2	2.25	0.68
21:A:1039:C:H2'	21:A:1040:U:H6	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:60:ALA:HB3	2:C:63:ASN:HB2	1.73	0.68
8:I:118:LYS:HB2	8:I:121:ARG:HB3	1.74	0.68
21:A:1442:G:H4'	21:A:1446:A:O4'	1.94	0.68
2:C:64:VAL:HG23	2:C:99:VAL:HA	1.76	0.67
15:P:4:ILE:HB	15:P:66:PRO:HB3	1.75	0.67
17:R:47:THR:HA	17:R:83:GLU:HB2	1.74	0.67
21:A:316:G:OP2	21:A:351:G:O2'	2.12	0.67
11:L:49:ASN:ND2	11:L:92:ASP:OD2	2.27	0.67
8:I:21:PRO:HA	8:I:59:PHE:HA	1.75	0.67
13:N:27:CYS:SG	23:N:101:ZN:ZN	1.82	0.67
2:C:47:LEU:HD22	2:C:76:VAL:HG22	1.76	0.66
21:A:1413:A:H2'	21:A:1414:U:H6	1.59	0.66
8:I:26:VAL:HG22	8:I:61:ALA:HB3	1.78	0.66
3:D:196:LEU:HB2	3:D:198:VAL:HG22	1.78	0.66
21:A:186:C:H2'	21:A:187:C:C6	2.30	0.66
21:A:459:G:O6	21:A:461:C:H5'	1.96	0.66
21:A:662:G:H2'	21:A:663:A:H8	1.60	0.66
12:M:24:GLY:HA3	12:M:66:LEU:HD22	1.78	0.66
1:B:6:THR:HB	1:B:9:GLU:HG3	1.79	0.65
21:A:1343:G:H2'	21:A:1344:C:C6	2.31	0.65
21:A:1518[B]:A:H2'	21:A:1519[B]:A:C8	2.31	0.65
10:K:21:ILE:HB	10:K:84:VAL:HG12	1.79	0.65
19:T:53:LEU:HB2	19:T:100:ILE:HD12	1.77	0.65
6:G:146:GLU:HB3	6:G:149:ARG:HH21	1.61	0.65
14:O:26:GLU:HG3	14:O:81:LEU:HD22	1.78	0.65
21:A:1437:C:H2'	21:A:1438:G:C8	2.32	0.65
9:J:66:ARG:HD2	13:N:57:ARG:HH12	1.62	0.65
8:I:46:ALA:HA	8:I:78:LYS:HB2	1.79	0.64
21:A:1176:A:H2'	21:A:1177:G:C8	2.32	0.64
11:L:117:ARG:HG2	11:L:122:THR:HB	1.78	0.64
21:A:92:C:H2'	21:A:93:G:C8	2.32	0.64
5:F:94:GLN:HG3	17:R:32:ARG:HD3	1.80	0.64
7:H:83:ILE:HG13	7:H:137:VAL:HG13	1.79	0.64
12:M:101:GLN:N	12:M:101:GLN:OE1	2.30	0.64
21:A:757:U:H2'	21:A:758:G:O4'	1.98	0.64
13:N:42:ILE:HG21	21:A:1202:G:C2	2.33	0.63
21:A:1515:C:H2'	21:A:1516[B]:G:C8	2.33	0.63
11:L:115:LYS:O	11:L:117:ARG:N	2.31	0.63
21:A:1415:G:H2'	21:A:1416:G:C8	2.33	0.63
21:A:460:A:O2'	21:A:461:C:H5''	1.98	0.63
21:A:811:C:O2'	21:A:901:A:N1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:864:A:H2'	21:A:865:A:C8	2.32	0.63
3:D:59:ARG:NH2	21:A:544:G:OP1	2.26	0.63
11:L:110:VAL:HG23	11:L:120:TYR:HB3	1.81	0.63
7:H:113:SER:HB2	7:H:134:ILE:HD11	1.80	0.63
21:A:1515:C:H2'	21:A:1516[B]:G:H8	1.62	0.63
6:G:20:ASP:HB3	6:G:23:VAL:HG23	1.81	0.62
16:Q:97:SER:OG	16:Q:98:LEU:N	2.32	0.62
19:T:79:ARG:NH2	21:A:261:U:OP2	2.31	0.62
11:L:89:ARG:HG3	11:L:97:ARG:HG2	1.81	0.62
21:A:7:G:H5'	21:A:298:A:O4'	1.98	0.62
14:O:87:ILE:HG22	14:O:88:ARG:H	1.63	0.62
21:A:45:U:H2'	21:A:46:G:C8	2.34	0.62
3:D:8:VAL:O	3:D:10:ARG:N	2.32	0.62
21:A:1409:C:H2'	21:A:1410:G:C8	2.35	0.62
21:A:677:U:H3	21:A:713:G:H22	1.46	0.62
21:A:838:G:C6	21:A:840:C:H1'	2.34	0.62
21:A:1493:A:O2'	21:A:1494:G:O5'	2.18	0.62
7:H:97:VAL:HG13	7:H:98:LYS:HG3	1.82	0.62
16:Q:86:GLU:O	16:Q:90:ILE:HG13	2.00	0.62
1:B:87:ARG:O	1:B:89:GLY:N	2.33	0.62
3:D:15:GLU:OE2	3:D:66:ARG:NH1	2.33	0.62
8:I:126:SER:HB3	21:A:1232:U:OP1	2.00	0.62
12:M:117:VAL:HG22	12:M:118:ALA:H	1.64	0.62
15:P:32:TYR:HE2	15:P:35:LYS:HB2	1.65	0.62
20:V:8:THR:HB	20:V:11:GLY:H	1.64	0.62
4:E:31:LEU:HD13	4:E:45:PHE:HD1	1.65	0.62
21:A:1149:C:H2'	21:A:1150:U:C6	2.34	0.61
8:I:114:TYR:HE1	9:J:59:SER:HA	1.65	0.61
15:P:9:PHE:CE2	15:P:18:ARG:HD2	2.34	0.61
21:A:1086:U:H3	21:A:1099:G:H22	1.47	0.61
2:C:52:LEU:HB2	2:C:70:VAL:HG22	1.83	0.61
21:A:975:A:H5'	21:A:975:A:C8	2.34	0.61
11:L:79:GLU:O	11:L:80:HIS:ND1	2.33	0.61
19:T:50:GLU:O	19:T:100:ILE:HD11	2.00	0.61
5:F:87:ARG:HD3	21:A:673:G:H5'	1.82	0.61
11:L:69:TYR:OH	21:A:522:C:OP2	2.14	0.61
14:O:36:ILE:HG12	14:O:59:MET:HE3	1.82	0.60
21:A:1039:C:H2'	21:A:1040:U:C6	2.36	0.60
2:C:116:VAL:HG21	2:C:202:ILE:HD11	1.82	0.60
10:K:58:PRO:HB3	10:K:93:GLN:HG3	1.83	0.60
21:A:792[B]:A:O2'	21:A:794[B]:A:N7	2.28	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:1:MET:HB2	5:F:68:PRO:HA	1.84	0.60
10:K:58:PRO:HD3	10:K:89:ALA:HB1	1.82	0.60
21:A:186:C:H2'	21:A:187:C:H6	1.66	0.60
1:B:4:GLU:O	1:B:217:ARG:NH1	2.34	0.60
10:K:31:THR:HG21	21:A:706:A:N3	2.17	0.60
15:P:74:LEU:HD22	15:P:79:VAL:HG21	1.84	0.60
4:E:51:VAL:O	4:E:55:VAL:HG23	2.02	0.60
21:A:1281:U:O2'	21:A:1282:C:OP1	2.18	0.60
15:P:47:ASP:OD1	15:P:47:ASP:N	2.33	0.59
3:D:76:ARG:O	3:D:80:GLU:HG2	2.02	0.59
21:A:397:A:H5'	21:A:398:C:OP1	2.02	0.59
2:C:191:THR:O	2:C:194:GLY:N	2.33	0.59
6:G:10:ARG:HH22	21:A:1346:A:H2'	1.66	0.59
4:E:64:ARG:NH1	21:A:1074:G:OP1	2.35	0.59
2:C:35:GLU:CD	2:C:59:ARG:HH22	2.11	0.59
5:F:22:GLU:HA	5:F:25:ILE:HG22	1.85	0.59
11:L:92:ASP:HB2	21:A:523:A:H61	1.68	0.59
21:A:92:C:H2'	21:A:93:G:H8	1.67	0.59
4:E:76:ILE:HG13	4:E:93:PRO:HB3	1.84	0.59
6:G:38:LEU:O	6:G:42:ILE:HG13	2.03	0.59
11:L:27:LEU:O	11:L:29:GLY:N	2.36	0.59
6:G:65:ALA:HB2	6:G:128:ALA:HB2	1.84	0.58
16:Q:67:LYS:O	16:Q:70:ARG:NH1	2.36	0.58
7:H:9:MET:HG3	7:H:26:VAL:HG11	1.83	0.58
19:T:102:GLY:O	21:A:191:G:O2'	2.19	0.58
7:H:89:PRO:HG2	21:A:878:G:H5'	1.85	0.58
21:A:1413:A:H2	21:A:1487:G:H22	1.50	0.58
13:N:37:PHE:HB3	13:N:39:LEU:HD12	1.85	0.58
16:Q:53:LEU:HD12	16:Q:82:MET:HE1	1.85	0.58
18:S:33:THR:OG1	18:S:34:TRP:N	2.35	0.58
3:D:57:ARG:HH11	3:D:57:ARG:HG2	1.69	0.58
1:B:15:VAL:O	1:B:204:ASN:N	2.34	0.57
4:E:113:ALA:HB3	4:E:115:VAL:HG23	1.85	0.57
18:S:14:HIS:CE1	21:A:1014:A:H4'	2.39	0.57
21:A:922:G:H2'	21:A:923:A:C8	2.39	0.57
15:P:9:PHE:HE2	15:P:18:ARG:HD2	1.69	0.57
16:Q:66:SER:O	16:Q:70:ARG:NH1	2.37	0.57
17:R:34:TYR:HA	17:R:69:THR:HG23	1.85	0.57
9:J:24:VAL:HG21	9:J:37:PRO:HD3	1.86	0.57
8:I:69:GLY:HA3	21:A:1371:G:O3'	2.05	0.57
17:R:26:LEU:HD11	17:R:42:ARG:HD2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:22:LEU:HG	6:G:62:PHE:HE2	1.69	0.57
9:J:54:PHE:HD2	9:J:55:LYS:HG2	1.69	0.57
4:E:126:ARG:HG3	4:E:126:ARG:HH11	1.69	0.57
12:M:54:VAL:O	12:M:58:GLU:HG2	2.04	0.57
21:A:161:A:H2'	21:A:162:A:C8	2.40	0.57
21:A:1415:G:H2'	21:A:1416:G:H8	1.69	0.57
15:P:3:LYS:HD3	21:A:377:G:OP1	2.04	0.57
21:A:900:A:H2'	21:A:901:A:C8	2.40	0.57
21:A:937:A:N6	21:A:1345:U:O4	2.36	0.57
21:A:1113:C:H2'	21:A:1114:C:H6	1.68	0.57
1:B:157:ARG:HD2	1:B:158:LEU:H	1.69	0.56
19:T:42:GLN:HG3	19:T:43:LEU:HD23	1.86	0.56
21:A:305:G:H4'	21:A:306:G:H21	1.70	0.56
4:E:153:LYS:O	4:E:155:GLU:N	2.38	0.56
21:A:1410:G:H1	21:A:1490:C:N4	2.04	0.56
1:B:5:ILE:HD11	1:B:213:LEU:HD21	1.87	0.56
4:E:6:PHE:HB3	4:E:35:GLY:O	2.05	0.56
21:A:384:G:H2'	21:A:385:C:C6	2.40	0.56
1:B:104:ASN:ND2	21:A:1074:G:O4'	2.39	0.56
1:B:21:ARG:HH11	1:B:40:HIS:HE1	1.53	0.56
3:D:125:HIS:ND1	3:D:152:SER:OG	2.26	0.56
21:A:179:A:H2'	21:A:180:U:C6	2.41	0.56
21:A:1427:U:H2'	21:A:1428:A:C8	2.41	0.56
21:A:1016:A:H2'	21:A:1017:G:O4'	2.06	0.56
21:A:1201:A:H4'	21:A:1202:G:H5''	1.88	0.56
2:C:199:LYS:NZ	21:A:1059:C:OP2	2.39	0.56
5:F:48:LEU:HD13	5:F:52:ILE:HG13	1.86	0.56
21:A:625:G:H2'	21:A:626:U:H6	1.70	0.56
21:A:1393:U:HO2'	21:A:1501:C:HO2'	1.53	0.55
21:A:1305:G:N2	21:A:1331:G:H1'	2.22	0.55
9:J:5:ARG:NH2	21:A:1125:U:O3'	2.40	0.55
21:A:394:G:H2'	21:A:395:C:C6	2.42	0.55
21:A:976:G:N2	21:A:1362:C:OP2	2.28	0.55
21:A:1286:A:H2'	21:A:1287:A:H4'	1.89	0.55
21:A:125:U:H2'	21:A:126:G:C8	2.41	0.55
21:A:1062:U:H2'	21:A:1063:C:C6	2.42	0.55
2:C:12:LEU:HD21	2:C:18:TRP:CE2	2.42	0.55
6:G:113:GLU:HB2	6:G:119:ARG:HG2	1.88	0.55
8:I:8:GLY:HA2	8:I:79:LEU:HD23	1.88	0.55
21:A:191:G:H2'	21:A:192:U:O4'	2.06	0.55
21:A:861:G:HO2'	21:A:874:G:HO2'	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1278:U:H5''	21:A:1279:A:H5'	1.89	0.55
9:J:9:ARG:NH2	9:J:95:GLU:OE2	2.39	0.55
14:O:54:ARG:O	14:O:58:MET:HG3	2.07	0.55
5:F:60:PHE:CE1	17:R:78:LEU:HD11	2.41	0.55
13:N:29:ARG:NH2	21:A:974:A:OP1	2.38	0.55
12:M:12:ASN:O	12:M:44:ARG:NH1	2.40	0.54
1:B:70:PHE:CD1	1:B:163:PHE:HB3	2.43	0.54
2:C:91:LEU:O	2:C:95:THR:HG23	2.08	0.54
7:H:29:SER:HB3	7:H:32:LYS:HG3	1.89	0.54
8:I:12:GLU:HB2	21:A:1371:G:OP1	2.07	0.54
5:F:18:GLN:HA	5:F:21:LEU:HD23	1.89	0.54
21:A:183:G:O5'	21:A:183:G:H8	1.91	0.54
21:A:1234:C:H1'	21:A:1364:U:O2	2.07	0.54
21:A:45:U:H2'	21:A:46:G:H8	1.72	0.54
19:T:41:ILE:HG21	19:T:87:LYS:HD2	1.89	0.54
1:B:164:VAL:HG23	1:B:170:GLU:HG3	1.90	0.54
7:H:14:ARG:O	7:H:17:THR:OG1	2.26	0.54
12:M:48:LEU:HD13	12:M:53:VAL:HG22	1.89	0.54
16:Q:76:LEU:HG	16:Q:77:VAL:N	2.23	0.54
15:P:28:ARG:HH21	21:A:390:C:H4'	1.73	0.54
21:A:1172:C:H2'	21:A:1173:G:C8	2.39	0.54
3:D:165:MET:HE1	3:D:168:ARG:HE	1.73	0.53
21:A:166:G:H2'	21:A:167:G:H8	1.73	0.53
3:D:63:LYS:O	3:D:67:ILE:HG13	2.08	0.53
21:A:673:G:H2'	21:A:674:G:C8	2.44	0.53
21:A:1145:C:H1'	21:A:1146:A:C8	2.43	0.53
7:H:17:THR:HA	7:H:65:TYR:OH	2.08	0.53
21:A:1437:C:H2'	21:A:1438:G:H8	1.72	0.53
1:B:4:GLU:HG2	1:B:5:ILE:H	1.73	0.53
9:J:57:LYS:HD3	21:A:972:C:OP2	2.08	0.53
21:A:69:G:H1	21:A:99:C:H42	1.56	0.53
21:A:176:C:H2'	21:A:177:C:C6	2.44	0.53
21:A:1188:A:H5''	21:A:1189:C:OP2	2.08	0.53
5:F:53:ALA:HB2	5:F:86:ARG:HD2	1.91	0.53
21:A:625:G:H2'	21:A:626:U:C6	2.44	0.53
21:A:1148:U:H2'	21:A:1149:C:O4'	2.08	0.53
19:T:89:ARG:NH2	19:T:105:SER:O	2.37	0.53
21:A:1497:G:O2'	21:A:1518[B]:A:H2	1.91	0.53
4:E:139:LEU:HD23	4:E:142:LEU:HD11	1.90	0.53
21:A:622:A:C8	21:A:623:C:C5	2.97	0.53
3:D:25:ARG:HD2	21:A:410:G:OP2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:743:U:H2'	21:A:744:C:C6	2.44	0.53
8:I:114:TYR:CE1	9:J:59:SER:HA	2.44	0.53
16:Q:97:SER:O	16:Q:99:SER:N	2.42	0.53
21:A:518:C:H4'	21:A:519:C:H5''	1.90	0.53
21:A:1229:A:H2'	21:A:1230:C:C6	2.43	0.53
3:D:36:ARG:NH2	21:A:429:U:OP2	2.40	0.52
3:D:61:LYS:HA	3:D:203:VAL:HG22	1.91	0.52
6:G:38:LEU:HD21	21:A:1240:U:H1'	1.91	0.52
6:G:62:PHE:HD1	6:G:124:LEU:HD21	1.73	0.52
21:A:696:A:N3	21:A:786:G:O2'	2.41	0.52
21:A:1031:G:H2'	21:A:1032:G:C8	2.45	0.52
21:A:1126:U:O2	21:A:1281:U:C2	2.63	0.52
12:M:99:ARG:NH2	21:A:1309:G:N7	2.56	0.52
21:A:767:A:H2'	21:A:768:A:H8	1.75	0.52
21:A:1260:C:OP1	21:A:1284:C:H4'	2.09	0.52
21:A:1461:G:H2'	21:A:1462:G:H8	1.74	0.52
17:R:37:VAL:CG2	17:R:78:LEU:HB3	2.40	0.52
18:S:77:THR:O	21:A:958:A:N6	2.43	0.52
21:A:460:A:H5''	21:A:460:A:H8	1.75	0.52
9:J:6:ILE:HB	9:J:72:VAL:HG12	1.90	0.52
21:A:1409:C:H2'	21:A:1410:G:H8	1.74	0.52
21:A:1229:A:H2'	21:A:1230:C:H6	1.75	0.52
2:C:134:ILE:HG23	2:C:151:VAL:HB	1.92	0.52
4:E:107:ARG:HG3	4:E:107:ARG:HH11	1.74	0.52
4:E:144:THR:HB	4:E:147:ASP:H	1.74	0.52
21:A:1487:G:O2'	21:A:1488:G:H5'	2.10	0.52
3:D:8:VAL:O	3:D:9:CYS:C	2.51	0.52
8:I:48:GLU:N	8:I:49:PRO:HD2	2.24	0.52
9:J:57:LYS:HE2	9:J:60:ARG:NH1	2.25	0.52
15:P:74:LEU:O	15:P:79:VAL:HG23	2.09	0.52
20:V:12:LYS:NZ	21:A:1326:C:OP1	2.42	0.52
4:E:86:ALA:CB	21:A:19:C:H5''	2.40	0.52
5:F:89:MET:HE2	17:R:76:LEU:HG	1.92	0.52
9:J:5:ARG:HG3	9:J:73:ASP:OD1	2.10	0.52
17:R:74:ARG:HD3	17:R:81:PHE:HA	1.91	0.52
1:B:28:PHE:CD2	1:B:190:THR:HA	2.45	0.52
21:A:539:A:H2'	21:A:540:G:C8	2.45	0.52
16:Q:10:VAL:HB	16:Q:53:LEU:HA	1.91	0.51
21:A:502:G:H2'	21:A:503:C:O4'	2.10	0.51
21:A:631:G:O2'	21:A:632:A:O4'	2.22	0.51
5:F:54:LYS:HE3	21:A:710:G:H5''	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1125:U:O2'	21:A:1126:U:H2'	2.10	0.51
21:A:1410:G:H1	21:A:1490:C:H42	1.56	0.51
3:D:102:ASP:OD1	3:D:103:ASN:N	2.44	0.51
4:E:82:VAL:HG21	4:E:138:ALA:HA	1.92	0.51
12:M:14:ARG:NE	12:M:42:ALA:HA	2.26	0.51
13:N:4:LYS:HD2	21:A:1047:G:H5''	1.92	0.51
18:S:39:THR:HG22	18:S:40:ILE:H	1.75	0.51
2:C:91:LEU:HB3	2:C:99:VAL:HG21	1.93	0.51
8:I:120:ARG:O	8:I:122:ALA:N	2.43	0.51
21:A:918:A:H2'	21:A:919:A:C8	2.45	0.51
19:T:33:ILE:HD13	19:T:63:ILE:HG12	1.92	0.51
21:A:373:A:O2'	21:A:451:A:N7	2.43	0.51
10:K:120:ARG:NH2	21:A:1525:G:OP1	2.40	0.51
21:A:692:U:H1'	21:A:695:A:N7	2.26	0.51
4:E:92:LYS:HB3	4:E:119:LEU:HB2	1.92	0.51
21:A:358:U:H2'	21:A:359:U:O4'	2.11	0.51
21:A:514:C:H2'	21:A:515:G:C8	2.46	0.51
21:A:731:G:O2'	21:A:732:C:H5'	2.11	0.51
21:A:737:A:H2'	21:A:738:C:C6	2.46	0.51
20:V:5:ASP:O	20:V:11:GLY:HA3	2.11	0.51
21:A:646:U:H2'	21:A:647:C:C6	2.46	0.51
2:C:111:LEU:HD23	2:C:204:LEU:HD21	1.92	0.51
2:C:193:TYR:HB3	21:A:532:A:H61	1.73	0.51
9:J:35:SER:HB3	21:A:1124:G:H5''	1.93	0.51
20:V:6:ARG:NH1	20:V:15:ARG:HH12	2.09	0.51
4:E:106:PRO:O	4:E:110:LEU:HG	2.11	0.50
4:E:144:THR:H	4:E:147:ASP:HB2	1.76	0.50
21:A:1075:C:H2'	21:A:1076:C:H6	1.76	0.50
21:A:1191:A:H2'	21:A:1192:C:C6	2.46	0.50
12:M:84:ILE:HG22	18:S:74:PHE:HE1	1.75	0.50
21:A:631:G:H2'	21:A:632:A:C8	2.46	0.50
3:D:57:ARG:HD3	3:D:202:LEU:HD22	1.92	0.50
3:D:165:MET:CE	3:D:168:ARG:HE	2.24	0.50
8:I:104:ARG:NH2	21:A:1117:G:H5''	2.26	0.50
21:A:262:A:C6	21:A:263:A:C6	2.99	0.50
21:A:1342:C:O2'	21:A:1343:G:H5'	2.11	0.50
18:S:41:VAL:HB	18:S:43:GLU:OE1	2.11	0.50
21:A:1440:C:H2'	21:A:1441:G:O4'	2.11	0.50
5:F:4:TYR:CZ	5:F:72:VAL:HG21	2.46	0.50
7:H:25:ASP:OD1	7:H:60:ARG:HG3	2.11	0.50
21:A:229:U:H2'	21:A:230:G:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:47:LYS:HD3	21:A:1080:A:OP1	2.11	0.50
16:Q:45:HIS:CD2	16:Q:47:PRO:HG3	2.47	0.50
18:S:49:ILE:HG22	18:S:51:VAL:HG12	1.94	0.50
21:A:306:G:H2'	21:A:307:C:H5'	1.92	0.50
21:A:1199:U:O2'	21:A:1202:G:OP1	2.29	0.50
3:D:5:ILE:HG21	21:A:406:G:H5'	1.92	0.50
15:P:55:ARG:O	15:P:58:TYR:HB3	2.11	0.50
21:A:618:C:N4	21:A:621:A:N7	2.59	0.50
3:D:59:ARG:HH12	3:D:62:GLN:HG3	1.77	0.50
3:D:59:ARG:HH22	21:A:544:G:P	2.33	0.50
8:I:89:ASN:HB3	8:I:92:TYR:CD2	2.46	0.50
21:A:455:C:H2'	21:A:456:C:C6	2.47	0.50
21:A:601:C:H2'	21:A:602:A:H8	1.77	0.50
21:A:1145:C:H4'	21:A:1146:A:O5'	2.11	0.50
21:A:1333:A:H2'	21:A:1334:G:O4'	2.11	0.50
3:D:53:ASP:O	3:D:57:ARG:HG2	2.12	0.50
15:P:32:TYR:CE2	15:P:35:LYS:HB2	2.45	0.50
21:A:771:G:N2	21:A:808:C:O2	2.43	0.50
21:A:1096:C:H2'	21:A:1097:C:H6	1.77	0.50
6:G:107:ALA:HA	6:G:110:GLN:HG2	1.94	0.49
14:O:32:LEU:O	14:O:36:ILE:HG13	2.12	0.49
21:A:1498:U:H4'	21:A:1519[B]:A:C2	2.47	0.49
4:E:19:MET:HE1	4:E:24:ARG:NH1	2.26	0.49
16:Q:60:ILE:HG21	16:Q:74:LEU:HD13	1.93	0.49
1:B:189:ASP:HB2	1:B:205:ASP:CG	2.37	0.49
12:M:16:ASP:HB3	12:M:41:PRO:HB3	1.94	0.49
20:V:10:ARG:NH1	21:A:1243:C:OP2	2.45	0.49
21:A:160:A:H1'	21:A:344:A:C5	2.47	0.49
21:A:232:G:H1'	21:A:262:A:N1	2.27	0.49
5:F:53:ALA:CB	5:F:86:ARG:HD2	2.41	0.49
14:O:62:GLN:HE22	21:A:656:C:H4'	1.77	0.49
1:B:74:LYS:NZ	1:B:205:ASP:O	2.35	0.49
4:E:95:ALA:HB1	4:E:96:PRO:HD2	1.95	0.49
3:D:31:CYS:O	3:D:34:GLU:HB2	2.13	0.49
11:L:76:ASN:ND2	11:L:76:ASN:O	2.46	0.49
16:Q:65:ILE:HB	16:Q:69:LYS:HB2	1.94	0.49
19:T:46:GLU:OE1	19:T:48:LYS:NZ	2.44	0.49
21:A:101:A:O2'	21:A:102:G:H5'	2.13	0.49
21:A:1430:C:H2'	21:A:1431:C:H6	1.77	0.49
9:J:51:ARG:HD2	9:J:59:SER:HB2	1.94	0.49
14:O:53:HIS:O	14:O:56:LEU:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1182:G:H4'	21:A:1183:A:H5'	1.95	0.49
10:K:113:PRO:HB3	21:A:676:A:H5''	1.93	0.49
11:L:8:ASN:OD1	21:A:585:G:H4'	2.13	0.49
21:A:1107:C:C4	21:A:1108:G:C8	2.99	0.49
21:A:1120:G:H2'	21:A:1121:U:C6	2.48	0.49
1:B:219:VAL:O	1:B:223:ILE:HG12	2.13	0.49
9:J:42:THR:HG22	9:J:68:HIS:HA	1.95	0.49
16:Q:3:LYS:HD3	16:Q:61:GLU:O	2.13	0.49
21:A:161:A:H2'	21:A:162:A:H8	1.76	0.49
16:Q:53:LEU:HD13	16:Q:85:VAL:HG11	1.94	0.49
21:A:622:A:C8	21:A:623:C:C6	3.01	0.49
3:D:135:LEU:HD11	21:A:619:U:C2	2.47	0.48
21:A:967:C:OP1	21:A:969:A:H5'	2.13	0.48
21:A:1003:G:N2	21:A:1038:C:O2	2.31	0.48
7:H:13:ILE:O	7:H:17:THR:HG23	2.12	0.48
12:M:14:ARG:HE	12:M:42:ALA:HA	1.78	0.48
15:P:8:ARG:HB3	15:P:28:ARG:NH1	2.28	0.48
18:S:28:LYS:HE3	18:S:47:HIS:CD2	2.47	0.48
3:D:201:GLN:HA	3:D:204:ILE:HD12	1.95	0.48
16:Q:60:ILE:HG12	16:Q:61:GLU:N	2.28	0.48
21:A:17:U:H2'	21:A:18:C:C6	2.48	0.48
1:B:51:LEU:HD13	1:B:201:ILE:HG23	1.94	0.48
5:F:69:GLU:O	5:F:72:VAL:HG23	2.13	0.48
17:R:43:PHE:O	17:R:44:LEU:HD23	2.14	0.48
21:A:123:C:OP1	21:A:312:C:H5'	2.13	0.48
21:A:532:A:H3'	21:A:533:A:C5'	2.43	0.48
21:A:1228:C:H2'	21:A:1229:A:H8	1.77	0.48
2:C:111:LEU:HD11	2:C:144:SER:HB2	1.95	0.48
9:J:68:HIS:ND1	21:A:1152:A:OP1	2.47	0.48
21:A:737:A:H2'	21:A:738:C:H6	1.78	0.48
21:A:1128:C:H4'	21:A:1148:U:O2	2.13	0.48
5:F:87:ARG:NH1	21:A:673:G:H5''	2.27	0.48
16:Q:63:ARG:HG3	21:A:130:A:C8	2.48	0.48
20:V:12:LYS:HG3	20:V:17:THR:OG1	2.14	0.48
21:A:1133:G:N2	21:A:1141:C:O2	2.42	0.48
7:H:33:GLU:HG3	7:H:48:TYR:CE2	2.49	0.48
16:Q:32:TYR:CE1	21:A:564:C:H5'	2.49	0.48
21:A:1219:U:H2'	21:A:1220:G:H8	1.77	0.48
3:D:78:LEU:HD13	3:D:96:LEU:HB3	1.96	0.48
4:E:79:GLU:HA	4:E:93:PRO:HD3	1.94	0.48
7:H:15:ASN:HD21	21:A:875:C:H1'	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:25:THR:C	17:R:26:LEU:HD12	2.39	0.48
21:A:1230:C:H2'	21:A:1231:G:H8	1.78	0.48
21:A:1487:G:H2'	21:A:1488:G:O4'	2.13	0.48
7:H:33:GLU:OE2	7:H:50:ARG:NH2	2.46	0.48
10:K:50:TYR:HE1	10:K:54:ARG:HE	1.61	0.48
12:M:116:THR:HA	21:A:1228:C:H4'	1.96	0.48
17:R:58:LEU:HD13	17:R:62:GLU:HB3	1.95	0.48
21:A:124:G:C6	21:A:125:U:N3	2.82	0.48
21:A:583:A:H2'	21:A:584:G:O4'	2.14	0.48
21:A:1234:C:O2'	21:A:1235:U:H5'	2.14	0.48
1:B:111:ARG:HH21	1:B:145:LEU:HD21	1.79	0.48
4:E:57:LYS:HE3	21:A:1073:U:OP2	2.14	0.48
9:J:42:THR:HG21	9:J:68:HIS:ND1	2.29	0.48
1:B:60:ASP:OD1	1:B:61:LEU:N	2.47	0.47
3:D:9:CYS:HA	3:D:12:CYS:HB2	1.95	0.47
6:G:103:TRP:NE1	6:G:137:LYS:HD2	2.29	0.47
11:L:7:ILE:O	11:L:10:LEU:N	2.47	0.47
11:L:7:ILE:HD13	11:L:7:ILE:HA	1.72	0.47
1:B:170:GLU:O	1:B:172:ILE:N	2.47	0.47
3:D:172:PRO:HD2	3:D:173:TRP:CE3	2.49	0.47
7:H:86:ILE:HG21	7:H:133:LEU:HG	1.95	0.47
11:L:47:LYS:HB2	11:L:48:PRO:HD3	1.96	0.47
16:Q:14:LYS:HB3	21:A:275:G:O5'	2.14	0.47
21:A:620:C:H2'	21:A:621:A:O4'	2.14	0.47
21:A:767:A:H2'	21:A:768:A:C8	2.49	0.47
1:B:5:ILE:HG21	1:B:51:LEU:HD23	1.96	0.47
3:D:145:GLU:OE1	3:D:182:LYS:HD3	2.14	0.47
4:E:127:ASN:HA	4:E:128:PRO:HD2	1.56	0.47
7:H:97:VAL:C	7:H:99:GLU:H	2.21	0.47
10:K:31:THR:HG22	10:K:42:TRP:HB2	1.97	0.47
21:A:255:G:H2'	21:A:256:U:C6	2.50	0.47
21:A:1154:G:H2'	21:A:1155:G:C8	2.50	0.47
1:B:90:MET:HB3	1:B:91:PRO:HD2	1.96	0.47
7:H:86:ILE:HD12	7:H:135:CYS:C	2.38	0.47
9:J:42:THR:HG21	9:J:68:HIS:HD1	1.80	0.47
21:A:37:U:O2'	21:A:500:G:H4'	2.15	0.47
21:A:1130:A:N6	21:A:1144:G:H21	2.13	0.47
1:B:11:LEU:HD23	1:B:16:HIS:NE2	2.29	0.47
1:B:21:ARG:NH1	1:B:40:HIS:HE1	2.11	0.47
21:A:880:C:H2'	21:A:881:G:H8	1.79	0.47
21:A:909:A:H2'	21:A:910:C:O4'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:127:THR:HB	3:D:147:ALA:HB3	1.97	0.47
3:D:188:LEU:HD12	3:D:188:LEU:H	1.79	0.47
10:K:97:ALA:O	10:K:101:SER:HB3	2.14	0.47
14:O:83:GLU:C	14:O:85:LEU:H	2.23	0.47
16:Q:81:ARG:HG3	16:Q:84:LEU:HD12	1.97	0.47
21:A:501:C:H2'	21:A:502:G:C8	2.50	0.47
21:A:794[B]:A:H2'	21:A:795:C:C6	2.49	0.47
21:A:190(J):U:H2'	21:A:190(K):G:C8	2.50	0.47
21:A:1403:C:H2'	21:A:1404:C:C6	2.50	0.47
21:A:1510:U:H2'	21:A:1511:G:C8	2.50	0.47
10:K:26:ASN:ND2	21:A:691:G:OP2	2.44	0.47
18:S:11:VAL:HG13	18:S:38:SER:HB3	1.97	0.47
21:A:413:G:N2	21:A:428:G:H1'	2.29	0.47
21:A:1070:U:H2'	21:A:1071:C:C6	2.50	0.47
21:A:1228:C:H2'	21:A:1229:A:C8	2.50	0.47
3:D:127:THR:HA	3:D:131:ARG:O	2.15	0.47
8:I:121:ARG:NH1	8:I:122:ALA:O	2.48	0.47
14:O:11:VAL:HG21	14:O:34:LEU:HD12	1.96	0.47
1:B:125:PRO:O	1:B:127:ILE:N	2.47	0.46
3:D:119:GLN:HG2	3:D:123:HIS:CE1	2.50	0.46
8:I:120:ARG:HG3	21:A:1348:U:H4'	1.96	0.46
10:K:23:ALA:HB2	10:K:28:THR:HG23	1.97	0.46
15:P:28:ARG:HD2	15:P:29:ASP:OD1	2.16	0.46
18:S:50:ALA:HB1	18:S:57:HIS:HB3	1.97	0.46
21:A:1191:A:H2'	21:A:1192:C:H6	1.80	0.46
21:A:1406:U:H3	21:A:1495:U:H3	1.63	0.46
1:B:197:VAL:HG11	1:B:200:ILE:HG13	1.97	0.46
6:G:15:ASP:OD1	6:G:16:LEU:N	2.48	0.46
21:A:1179:A:N6	21:A:1180:A:C6	2.83	0.46
1:B:21:ARG:HH11	1:B:40:HIS:CE1	2.33	0.46
1:B:70:PHE:HD1	1:B:163:PHE:HB3	1.80	0.46
1:B:98:LEU:O	1:B:101:MET:HG3	2.15	0.46
5:F:15:ASP:OD1	5:F:15:ASP:N	2.49	0.46
12:M:45:VAL:O	12:M:48:LEU:HD12	2.15	0.46
21:A:116:A:O5'	21:A:116:A:H8	1.98	0.46
21:A:432:A:C8	21:A:433:C:C5	3.03	0.46
21:A:1342:C:H2'	21:A:1343:G:C8	2.50	0.46
21:A:1404:C:H1'	21:A:1499:A:C2	2.50	0.46
2:C:38:ARG:HD3	2:C:94:LEU:HD11	1.98	0.46
6:G:133:GLY:HA2	6:G:136:LYS:HB2	1.97	0.46
16:Q:4:LYS:HD2	16:Q:5:VAL:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:152:A:N6	21:A:170:U:O2	2.49	0.46
2:C:36:ASP:OD1	2:C:59:ARG:NH1	2.48	0.46
7:H:20:TYR:HA	7:H:65:TYR:CZ	2.51	0.46
13:N:12:ARG:NH2	21:A:994:A:O2'	2.49	0.46
21:A:224:C:H2'	21:A:225:C:C6	2.51	0.46
21:A:544:G:C6	21:A:545:C:C4	3.04	0.46
21:A:1414:U:H2'	21:A:1415:G:C8	2.50	0.46
1:B:164:VAL:HG13	1:B:186:ALA:HB2	1.98	0.46
2:C:75:VAL:O	2:C:83:ARG:HD3	2.16	0.46
4:E:60:TYR:CE1	4:E:64:ARG:HD3	2.51	0.46
19:T:51:GLU:O	19:T:54:LYS:HB3	2.16	0.46
21:A:109:A:C6	21:A:326:G:C6	3.04	0.46
21:A:997:U:H2'	21:A:998:G:O4'	2.16	0.46
21:A:1006:C:H6	21:A:1006:C:O5'	1.98	0.46
1:B:9:GLU:OE1	1:B:217:ARG:NH2	2.48	0.46
2:C:40:ARG:NH1	2:C:55:VAL:O	2.49	0.46
6:G:73:MET:HA	6:G:91:VAL:HG23	1.98	0.46
21:A:59:A:H1'	21:A:354:G:N2	2.30	0.46
3:D:64:LEU:HD23	3:D:75:PHE:HZ	1.80	0.46
14:O:69:TYR:CZ	14:O:73:GLU:HG3	2.50	0.46
21:A:74:C:H2'	21:A:75:G:O4'	2.16	0.46
21:A:447:G:O6	21:A:485:G:O2'	2.33	0.46
4:E:121:LYS:HG3	4:E:122:GLU:O	2.15	0.46
11:L:117:ARG:NH2	21:A:501:C:OP1	2.49	0.46
17:R:24:ALA:C	17:R:26:LEU:H	2.24	0.46
21:A:840:C:H5'	21:A:841:U:OP1	2.15	0.46
21:A:1219:U:H2'	21:A:1220:G:C8	2.51	0.46
6:G:18:TYR:CD2	6:G:59:LEU:HB3	2.51	0.45
11:L:70:ILE:HG12	11:L:100:ILE:HD12	1.98	0.45
21:A:56:U:H2'	21:A:57:G:C8	2.51	0.45
21:A:1052:U:O2'	21:A:1055:A:OP2	2.32	0.45
21:A:1338:G:H2'	21:A:1339:A:C8	2.51	0.45
2:C:56:ASP:HB2	2:C:67:THR:HB	1.98	0.45
4:E:33:VAL:HG11	4:E:109:ILE:HA	1.98	0.45
8:I:18:PHE:CE2	21:A:1130:A:H5'	2.51	0.45
21:A:394:G:H2'	21:A:395:C:H6	1.80	0.45
3:D:79:PHE:CZ	3:D:204:ILE:HA	2.51	0.45
21:A:515:G:H2'	21:A:516:U:O4'	2.16	0.45
5:F:79:LEU:HB3	5:F:88:VAL:HG21	1.97	0.45
7:H:56:LYS:HA	7:H:57:PRO:HD2	1.71	0.45
3:D:10:ARG:HA	3:D:13:ARG:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:48:TRP:CD1	15:P:48:TRP:H	2.34	0.45
21:A:457:C:H2'	21:A:458:C:H6	1.80	0.45
21:A:821:G:H2'	21:A:822:C:H6	1.81	0.45
21:A:821:G:H2'	21:A:822:C:C6	2.51	0.45
21:A:976:G:C8	21:A:1358:U:C2	3.05	0.45
21:A:1360:A:H2'	21:A:1361:G:O4'	2.16	0.45
21:A:1517[B]:G:H3'	21:A:1518[B]:A:C8	2.52	0.45
4:E:121:LYS:NZ	21:A:9:G:OP2	2.23	0.45
6:G:119:ARG:NH2	21:A:1240:U:OP1	2.35	0.45
14:O:57:LEU:N	14:O:57:LEU:HD23	2.31	0.45
21:A:190(C):C:H2'	21:A:190(D):U:O4'	2.17	0.45
21:A:1133:G:H2'	21:A:1134:G:C8	2.52	0.45
12:M:16:ASP:HB2	12:M:31:LYS:HE2	1.99	0.45
13:N:3:ARG:HG2	21:A:1048:G:H5''	1.98	0.45
19:T:38:LYS:HE2	21:A:1439:C:OP1	2.16	0.45
21:A:731:G:OP1	21:A:766:A:H1'	2.17	0.45
21:A:745:C:H2'	21:A:746:A:C8	2.52	0.45
21:A:836:G:C6	21:A:851:G:C6	3.05	0.45
1:B:82:ARG:HB2	1:B:94:ASN:ND2	2.31	0.45
16:Q:89:LEU:HD23	16:Q:89:LEU:HA	1.78	0.45
18:S:23:ASN:C	18:S:25:LYS:H	2.25	0.45
21:A:559:A:H4'	21:A:560:U:H5''	1.99	0.45
21:A:890:G:N2	21:A:907:A:OP2	2.40	0.45
21:A:1499:A:OP2	21:A:1505:G:OP2	2.35	0.45
1:B:19:HIS:HB3	1:B:23:ARG:HH21	1.81	0.45
2:C:78:GLY:HA3	2:C:83:ARG:HB3	1.97	0.45
3:D:201:GLN:O	3:D:205:GLU:HG3	2.17	0.45
4:E:90:VAL:HG12	4:E:121:LYS:O	2.17	0.45
10:K:73:MET:HE2	10:K:103:LEU:HG	1.98	0.45
11:L:113:ARG:HD3	21:A:538:G:OP1	2.17	0.45
17:R:76:LEU:HB3	17:R:78:LEU:HD13	1.99	0.45
19:T:84:LEU:O	19:T:88:VAL:HG23	2.17	0.45
21:A:160:A:O2'	21:A:344:A:N6	2.50	0.45
21:A:373:A:C2	21:A:374:A:C8	3.05	0.45
9:J:54:PHE:CD2	9:J:55:LYS:HG2	2.50	0.45
12:M:15:VAL:HG12	12:M:19:LEU:HD11	1.99	0.45
16:Q:63:ARG:HG2	16:Q:64:PRO:HD2	1.99	0.45
17:R:34:TYR:H	17:R:34:TYR:HD2	1.63	0.45
21:A:21:G:H2'	21:A:22:G:C8	2.52	0.45
21:A:946:A:O2'	21:A:1333:A:N3	2.46	0.45
1:B:104:ASN:HD22	21:A:1074:G:C1'	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:125:GLU:C	2:C:127:ARG:H	2.24	0.44
4:E:8:GLU:HG2	4:E:34:VAL:HG22	1.99	0.44
4:E:80:ILE:HG12	4:E:81:GLU:N	2.32	0.44
8:I:25:LYS:HG2	8:I:60:ASP:OD1	2.17	0.44
9:J:49:VAL:HG12	13:N:41:ARG:HB2	1.99	0.44
17:R:51:LEU:HA	17:R:52:PRO:HD3	1.86	0.44
18:S:41:VAL:HG22	18:S:44:MET:HE3	1.99	0.44
21:A:156:G:C2	21:A:166:G:C2	3.05	0.44
21:A:1101:A:H4'	21:A:1102:A:H5'	1.98	0.44
21:A:1308:U:H2'	21:A:1309:G:C8	2.52	0.44
21:A:1323:G:H2'	21:A:1324:A:C8	2.53	0.44
6:G:12:LEU:HD13	6:G:24:THR:HG22	1.99	0.44
16:Q:62:SER:OG	16:Q:72:ARG:HD3	2.17	0.44
21:A:282:A:H3'	21:A:283:C:H6	1.82	0.44
21:A:1127:G:H5'	21:A:1280:A:O2'	2.17	0.44
21:A:1349:A:C4	21:A:1350:A:C8	3.05	0.44
1:B:171:ALA:HA	1:B:174:VAL:HB	1.99	0.44
19:T:56:MET:HE2	19:T:85:MET:HA	1.99	0.44
21:A:1179:A:H2'	21:A:1180:A:O4'	2.16	0.44
21:A:1349:A:H2'	21:A:1350:A:H8	1.83	0.44
2:C:59:ARG:HG2	2:C:64:VAL:HG12	1.97	0.44
12:M:49:THR:HB	12:M:52:GLU:H	1.82	0.44
19:T:66:ALA:HB1	19:T:71:THR:HB	1.99	0.44
21:A:114:U:H2'	21:A:115:G:C8	2.52	0.44
21:A:757:U:OP1	21:A:822:C:O2'	2.32	0.44
21:A:953:G:H2'	21:A:954:G:O4'	2.16	0.44
21:A:1316:G:N2	21:A:1318:A:H3'	2.32	0.44
1:B:153:ARG:HG3	1:B:154:LEU:HD12	2.00	0.44
1:B:179:LYS:NZ	21:A:1075:C:OP1	2.45	0.44
4:E:11:ILE:HG23	4:E:105:VAL:HG22	2.00	0.44
5:F:60:PHE:C	5:F:61:LEU:HD23	2.43	0.44
6:G:69:VAL:HG12	6:G:100:ALA:HA	1.98	0.44
6:G:78:ARG:HB3	6:G:87:VAL:HG21	1.99	0.44
7:H:103:VAL:HG21	7:H:109:ILE:C	2.43	0.44
13:N:45:ARG:NH2	21:A:1060:C:OP1	2.51	0.44
17:R:59:SER:OG	17:R:60:ALA:N	2.51	0.44
18:S:15:LEU:O	18:S:19:VAL:HG22	2.17	0.44
21:A:948:C:O2'	21:A:949:A:H5'	2.17	0.44
4:E:10:MET:HE2	4:E:10:MET:HB2	1.61	0.44
11:L:6:THR:OG1	11:L:9:GLN:HG3	2.18	0.44
16:Q:3:LYS:HD2	16:Q:60:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:164:ARG:HG2	2:C:164:ARG:HH11	1.82	0.44
2:C:179:ARG:O	2:C:207:VAL:HG23	2.17	0.44
6:G:13:GLN:CD	6:G:14:PRO:HD2	2.43	0.44
21:A:295:C:C4	21:A:296:U:C4	3.06	0.44
21:A:869:G:H4'	21:A:872:A:C8	2.52	0.44
21:A:1110:A:O5'	21:A:1110:A:H8	2.01	0.44
3:D:99:SER:HB3	3:D:139:ARG:HG3	2.00	0.44
5:F:87:ARG:HD3	21:A:673:G:C5'	2.48	0.44
2:C:5:ILE:HD12	2:C:6:HIS:H	1.83	0.44
1:B:108:ILE:HD13	1:B:108:ILE:HA	1.87	0.43
7:H:112:LEU:HD12	7:H:133:LEU:HA	2.00	0.43
9:J:50:ILE:HD11	9:J:57:LYS:HG3	1.99	0.43
21:A:278:G:O4'	21:A:282:A:H1'	2.18	0.43
2:C:157:ILE:HD12	2:C:166:GLU:HG2	2.00	0.43
4:E:160:ALA:O	4:E:161:GLN:HG3	2.18	0.43
5:F:16:GLN:O	5:F:16:GLN:NE2	2.51	0.43
6:G:10:ARG:NH2	21:A:1346:A:H2'	2.30	0.43
21:A:582:U:C2	21:A:760:G:C6	3.06	0.43
3:D:61:LYS:HE2	3:D:61:LYS:HB3	1.81	0.43
5:F:6:VAL:HB	5:F:63:TYR:HB2	2.01	0.43
6:G:62:PHE:CD1	6:G:124:LEU:HD11	2.53	0.43
8:I:28:VAL:HA	8:I:63:ILE:O	2.18	0.43
12:M:67:GLU:HB3	12:M:68:GLY:H	1.45	0.43
16:Q:43:LEU:HD23	16:Q:43:LEU:HA	1.73	0.43
21:A:282:A:H3'	21:A:283:C:C6	2.53	0.43
21:A:325:A:H2'	21:A:326:G:O4'	2.18	0.43
21:A:723:U:O2	21:A:723:U:H2'	2.18	0.43
21:A:1400:C:H4'	21:A:1401:G:OP2	2.18	0.43
1:B:162:ILE:O	1:B:162:ILE:HG13	2.19	0.43
2:C:83:ARG:O	2:C:87:LEU:HG	2.19	0.43
2:C:112:SER:O	2:C:116:VAL:HG23	2.18	0.43
10:K:123:LYS:HD3	21:A:1523:G:OP1	2.18	0.43
18:S:5:LEU:HD23	18:S:5:LEU:HA	1.61	0.43
18:S:6:LYS:NZ	21:A:1314:C:OP1	2.32	0.43
18:S:37:ARG:NH1	21:A:1318:A:H1'	2.34	0.43
19:T:58:LYS:HB2	19:T:58:LYS:HE3	1.85	0.43
21:A:461:C:O2'	21:A:462:G:OP1	2.27	0.43
21:A:993:G:H4'	21:A:994:A:OP2	2.18	0.43
21:A:1508:G:H2'	21:A:1509:C:H6	1.83	0.43
1:B:46:LYS:O	1:B:47:THR:C	2.61	0.43
4:E:20:GLN:HG2	4:E:25:ARG:NH2	2.24	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:87:SER:HB3	4:E:131:ILE:CD1	2.49	0.43
5:F:33:TYR:HD1	5:F:71:ARG:HD2	1.83	0.43
14:O:33:THR:HG23	14:O:63:ARG:NH1	2.33	0.43
14:O:78:TYR:CZ	14:O:82:ILE:HD11	2.52	0.43
16:Q:9:VAL:HG23	16:Q:22:LEU:HB3	2.00	0.43
17:R:33:ASP:OD2	17:R:36:ASN:HB2	2.18	0.43
21:A:373:A:H1'	21:A:481:G:N3	2.33	0.43
21:A:778:G:H2'	21:A:779:C:O4'	2.17	0.43
21:A:1085:U:C2	21:A:1094:G:O6	2.72	0.43
21:A:722:A:N3	21:A:722:A:H3'	2.34	0.43
21:A:743:U:H2'	21:A:744:C:H6	1.82	0.43
2:C:5:ILE:N	21:A:1190:G:OP1	2.52	0.43
3:D:102:ASP:HB3	3:D:136:PRO:HB3	2.00	0.43
3:D:202:LEU:HA	3:D:202:LEU:HD23	1.59	0.43
4:E:11:ILE:HD11	4:E:108:ALA:HB3	1.99	0.43
6:G:73:MET:HB2	6:G:90:GLU:HA	1.99	0.43
10:K:115:PRO:C	10:K:117:ASN:H	2.26	0.43
16:Q:38:ARG:HD3	16:Q:38:ARG:HA	1.84	0.43
21:A:179:A:H2'	21:A:180:U:H6	1.84	0.43
21:A:271:C:O5'	21:A:271:C:H6	2.02	0.43
21:A:505:G:H1	21:A:526:C:H42	1.66	0.43
21:A:567:G:H2'	21:A:568:G:O4'	2.19	0.43
21:A:582:U:H2'	21:A:583:A:C8	2.53	0.43
11:L:7:ILE:HD12	11:L:7:ILE:HG23	1.82	0.43
19:T:59:ALA:O	19:T:63:ILE:HG13	2.18	0.43
21:A:1087:G:H2'	21:A:1088:G:C8	2.54	0.43
21:A:1216:G:H2'	21:A:1217:C:H6	1.83	0.43
21:A:1307:U:H2'	21:A:1308:U:O4'	2.18	0.43
3:D:121:VAL:HG12	3:D:134:ASP:HA	2.00	0.43
5:F:62:TRP:CH2	5:F:64:GLN:HB2	2.54	0.43
7:H:64:LYS:HG2	7:H:79:VAL:HG21	2.01	0.43
19:T:75:ASN:HD22	19:T:75:ASN:H	1.65	0.43
21:A:130:A:H1'	21:A:263:A:O2'	2.19	0.43
21:A:417:C:H6	21:A:417:C:O5'	2.01	0.43
21:A:888:G:O5'	21:A:888:G:H8	2.01	0.43
21:A:1245:A:C2	21:A:1293:G:C2	3.06	0.43
21:A:1306:A:N3	21:A:1306:A:H2'	2.33	0.43
12:M:80:ARG:O	12:M:84:ILE:HG13	2.19	0.43
21:A:685:G:O2'	21:A:686:U:H5'	2.19	0.43
21:A:1018:C:O5'	21:A:1018:C:H6	2.01	0.43
4:E:19:MET:HE1	4:E:24:ARG:HH11	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:33:VAL:HB	4:E:112:LEU:HD12	2.00	0.42
7:H:2:LEU:HD12	7:H:2:LEU:HA	1.79	0.42
7:H:112:LEU:HD12	7:H:112:LEU:HA	1.84	0.42
16:Q:62:SER:HB3	16:Q:72:ARG:HD3	2.01	0.42
19:T:65:LYS:O	19:T:68:LYS:HG2	2.19	0.42
21:A:961:U:OP2	21:A:1223:C:H1'	2.19	0.42
8:I:99:LEU:HB2	8:I:101:PHE:CE2	2.55	0.42
17:R:73:ALA:HB3	17:R:79:LEU:HD12	2.00	0.42
19:T:105:SER:HB3	21:A:190(L):U:H3	1.83	0.42
21:A:432:A:H3'	21:A:433:C:C6	2.54	0.42
21:A:690:G:H2'	21:A:691:G:O4'	2.19	0.42
21:A:1108:G:C5	21:A:1109:C:C5	3.07	0.42
21:A:1237:C:H2'	21:A:1336:C:H5	1.85	0.42
21:A:1271:G:H2'	21:A:1272:G:C8	2.54	0.42
2:C:7:PRO:O	2:C:11:ARG:NH1	2.52	0.42
3:D:14:ARG:HA	3:D:14:ARG:HD3	1.72	0.42
6:G:13:GLN:NE2	6:G:14:PRO:HD2	2.34	0.42
12:M:111:LYS:NZ	21:A:1226:C:O2'	2.51	0.42
16:Q:67:LYS:HB2	21:A:266:G:H3'	2.01	0.42
21:A:608:A:C2'	21:A:609:A:H5'	2.49	0.42
3:D:155:LEU:HA	3:D:155:LEU:HD23	1.80	0.42
6:G:62:PHE:CD1	6:G:124:LEU:HD21	2.53	0.42
12:M:29:ARG:HD2	21:A:1329:A:H5'	2.01	0.42
12:M:34:LEU:HD12	12:M:41:PRO:HB3	2.01	0.42
12:M:52:GLU:HA	12:M:55:ARG:HD3	2.01	0.42
14:O:87:ILE:O	14:O:88:ARG:HG3	2.19	0.42
15:P:49:LEU:HD13	15:P:73:LEU:HD22	2.02	0.42
17:R:55:ARG:HE	17:R:55:ARG:HB2	1.58	0.42
21:A:202:U:H5''	21:A:203:U:OP2	2.19	0.42
21:A:296:U:H2'	21:A:297:G:C8	2.55	0.42
21:A:745:C:H2'	21:A:746:A:H8	1.84	0.42
21:A:1075:C:H2'	21:A:1076:C:C6	2.54	0.42
21:A:1145:C:H5'	21:A:1146:A:OP1	2.20	0.42
21:A:1154:G:H2'	21:A:1155:G:H8	1.83	0.42
21:A:1381:U:H2'	21:A:1382:C:C6	2.54	0.42
21:A:1507:A:C2	21:A:1508:G:C5	3.07	0.42
1:B:60:ASP:OD2	1:B:64:ARG:NH1	2.34	0.42
4:E:11:ILE:HG22	4:E:12:LEU:HD23	2.02	0.42
4:E:79:GLU:OE2	7:H:104:ARG:HA	2.20	0.42
8:I:99:LEU:H	8:I:99:LEU:HD12	1.84	0.42
12:M:24:GLY:CA	12:M:66:LEU:HD22	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:55:ILE:O	19:T:58:LYS:N	2.53	0.42
21:A:164:U:H2'	21:A:165:C:C6	2.54	0.42
21:A:415:A:H2'	21:A:416:G:O4'	2.19	0.42
21:A:545:C:O2'	21:A:549:C:OP1	2.33	0.42
21:A:624:C:H2'	21:A:625:G:H8	1.84	0.42
21:A:977:A:H1'	21:A:982:U:O4	2.20	0.42
1:B:189:ASP:OD2	1:B:204:ASN:HA	2.19	0.42
5:F:2:ARG:HG3	5:F:69:GLU:HB3	2.01	0.42
8:I:70:LYS:HE3	21:A:1248:A:N3	2.34	0.42
14:O:58:MET:HE2	14:O:58:MET:HB3	1.86	0.42
15:P:10:GLY:HA3	15:P:14:ASN:O	2.19	0.42
16:Q:66:SER:H	16:Q:69:LYS:HB2	1.83	0.42
18:S:6:LYS:NZ	21:A:1271:G:H4'	2.34	0.42
21:A:390:C:H2'	21:A:391:G:C8	2.55	0.42
1:B:114:ARG:NH2	1:B:118:LEU:HD21	2.35	0.42
3:D:172:PRO:HD2	3:D:173:TRP:CZ3	2.55	0.42
4:E:48:ALA:HB1	4:E:49:PRO:HD2	2.01	0.42
7:H:114:THR:C	7:H:116:LYS:H	2.28	0.42
11:L:11:VAL:HG13	16:Q:29:HIS:CD2	2.54	0.42
21:A:676:A:H2'	21:A:677:U:H6	1.84	0.42
21:A:1267:C:H5''	21:A:1268:A:OP2	2.19	0.42
3:D:97:LEU:HA	3:D:97:LEU:HD23	1.80	0.42
4:E:11:ILE:HG21	4:E:31:LEU:HD23	2.02	0.42
8:I:17:VAL:HG11	8:I:81:ILE:HA	2.02	0.42
14:O:83:GLU:O	14:O:85:LEU:N	2.52	0.42
21:A:664:G:O2'	21:A:666:G:OP2	2.29	0.42
21:A:880:C:H2'	21:A:881:G:C8	2.55	0.42
21:A:953:G:H5''	21:A:965:A:H61	1.85	0.42
21:A:1308:U:H2'	21:A:1309:G:H8	1.85	0.42
1:B:103:THR:HA	1:B:180:LEU:HD11	2.01	0.42
12:M:9:ILE:HD12	12:M:18:ALA:HB1	2.01	0.42
21:A:509:A:OP2	21:A:510:A:OP2	2.37	0.42
21:A:1243:C:H2'	21:A:1244:C:C6	2.55	0.42
21:A:1406:U:O3'	21:A:1517[A]:G:N2	2.52	0.42
5:F:85:VAL:HG11	5:F:88:VAL:HG23	2.02	0.42
8:I:5:TYR:CG	8:I:6:GLY:N	2.88	0.42
16:Q:92:ARG:O	16:Q:95:TYR:HB2	2.19	0.42
17:R:78:LEU:N	17:R:78:LEU:HD12	2.34	0.42
21:A:306:G:H2'	21:A:307:C:C5'	2.50	0.42
21:A:370:C:H2'	21:A:371:G:C8	2.55	0.42
21:A:499:A:H4'	21:A:500:G:OP1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1068:G:N7	21:A:1094:G:H2'	2.35	0.42
5:F:22:GLU:O	5:F:26:ILE:HG13	2.21	0.41
21:A:67:C:H2'	21:A:68:G:C8	2.55	0.41
21:A:814:A:O2'	21:A:815:A:H3'	2.20	0.41
8:I:118:LYS:O	8:I:119:ALA:CB	2.68	0.41
10:K:116:HIS:CD2	21:A:718:G:C5	3.08	0.41
18:S:51:VAL:O	18:S:57:HIS:HA	2.20	0.41
21:A:190:C:H2'	21:A:190(A):C:H6	1.85	0.41
21:A:1482:G:O5'	21:A:1482:G:H8	2.03	0.41
3:D:100:ARG:O	3:D:104:VAL:HG23	2.21	0.41
11:L:20:LYS:HB3	11:L:20:LYS:HE3	1.91	0.41
12:M:70:LEU:O	12:M:74:VAL:HG22	2.20	0.41
21:A:624:C:H2'	21:A:625:G:C8	2.56	0.41
21:A:860:A:H2'	21:A:861:G:O4'	2.20	0.41
21:A:1278:U:H5'	21:A:1279:A:O4'	2.21	0.41
21:A:1473:A:H2'	21:A:1474:G:C8	2.55	0.41
4:E:11:ILE:HA	4:E:11:ILE:HD13	1.56	0.41
5:F:28:ARG:HA	5:F:31:GLU:HB2	2.02	0.41
6:G:12:LEU:HD23	6:G:12:LEU:HA	1.77	0.41
21:A:1015:A:N3	21:A:1218:C:O2'	2.46	0.41
21:A:1071:C:O2'	21:A:1072:G:H5'	2.20	0.41
21:A:1241:G:H2'	21:A:1242:C:C6	2.54	0.41
21:A:1271:G:H2'	21:A:1272:G:H8	1.85	0.41
21:A:1420:C:H2'	21:A:1421:G:C8	2.55	0.41
1:B:144:ARG:NH1	1:B:144:ARG:HB3	2.35	0.41
8:I:16:ARG:O	8:I:63:ILE:HA	2.20	0.41
11:L:75:HIS:HA	11:L:102:ARG:HH22	1.86	0.41
11:L:84:LEU:HG	11:L:85:ILE:N	2.34	0.41
19:T:29:LYS:O	19:T:33:ILE:HG13	2.20	0.41
21:A:166:G:H2'	21:A:167:G:C8	2.54	0.41
1:B:130:ARG:H	1:B:130:ARG:HG2	1.68	0.41
3:D:173:TRP:O	3:D:186:LEU:HB2	2.21	0.41
9:J:39:PRO:HA	9:J:70:ARG:HD3	2.02	0.41
10:K:51:LYS:HD3	10:K:51:LYS:HA	1.66	0.41
16:Q:62:SER:CB	16:Q:72:ARG:HD3	2.50	0.41
21:A:142:G:O2'	21:A:196:A:N1	2.48	0.41
1:B:19:HIS:HB3	1:B:23:ARG:NH2	2.36	0.41
1:B:84:GLU:HG3	1:B:215:LEU:HB3	2.03	0.41
1:B:223:ILE:HG12	1:B:223:ILE:H	1.60	0.41
10:K:58:PRO:HA	10:K:90:GLY:HA3	2.03	0.41
10:K:103:LEU:HD23	10:K:103:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:64:ARG:O	14:O:68:ARG:HB2	2.21	0.41
17:R:31:LEU:HD22	17:R:66:LEU:HB2	2.03	0.41
17:R:43:PHE:C	17:R:44:LEU:HD23	2.45	0.41
21:A:22:G:H4'	21:A:885:G:C8	2.56	0.41
21:A:47:C:H6	21:A:365:U:H2'	1.86	0.41
21:A:176:C:H2'	21:A:177:C:H6	1.82	0.41
3:D:192:GLU:N	3:D:192:GLU:CD	2.79	0.41
6:G:132:GLY:O	6:G:134:ALA:N	2.53	0.41
11:L:89:ARG:NH1	11:L:91:LYS:HA	2.36	0.41
12:M:29:ARG:HG2	12:M:64:TRP:CZ2	2.55	0.41
12:M:49:THR:CB	12:M:52:GLU:HB2	2.46	0.41
14:O:21:ASP:OD1	21:A:750:G:O2'	2.39	0.41
19:T:89:ARG:C	19:T:91:LEU:H	2.28	0.41
21:A:947:G:H2'	21:A:948:C:C6	2.56	0.41
1:B:15:VAL:HG13	1:B:203:GLY:HA3	2.02	0.41
1:B:51:LEU:HD12	1:B:201:ILE:HG12	2.02	0.41
1:B:144:ARG:O	1:B:147:LYS:HB3	2.20	0.41
2:C:22:TRP:HB3	2:C:59:ARG:HB2	2.02	0.41
2:C:102:ASN:OD1	2:C:102:ASN:N	2.51	0.41
4:E:131:ILE:HD13	4:E:131:ILE:HA	1.94	0.41
9:J:57:LYS:HD2	21:A:973:G:OP1	2.21	0.41
12:M:91:ARG:NH1	12:M:96:LEU:HD12	2.36	0.41
16:Q:43:LEU:HD12	16:Q:68:ARG:HB2	2.03	0.41
17:R:34:TYR:CD2	17:R:34:TYR:N	2.84	0.41
17:R:76:LEU:HA	17:R:76:LEU:HD23	1.89	0.41
21:A:24:U:H2'	21:A:25:C:C6	2.56	0.41
21:A:99:C:H2'	21:A:101:A:C8	2.56	0.41
21:A:122:G:C2	21:A:123:C:C2	3.09	0.41
21:A:142:G:H2'	21:A:143:A:H8	1.86	0.41
21:A:255:G:H2'	21:A:256:U:H6	1.86	0.41
21:A:870:U:H4'	21:A:871:U:H5''	2.03	0.41
2:C:122:GLU:O	2:C:125:GLU:N	2.54	0.41
10:K:32:ILE:HD12	10:K:72:ALA:HB2	2.02	0.41
17:R:22:VAL:O	17:R:26:LEU:HD13	2.21	0.41
18:S:4:SER:HB3	21:A:1314:C:OP2	2.21	0.41
18:S:13:ASP:OD1	18:S:13:ASP:N	2.54	0.41
21:A:861:G:O2'	21:A:874:G:O2'	2.32	0.41
21:A:1489:G:H2'	21:A:1490:C:O4'	2.21	0.41
1:B:188:ALA:O	1:B:202:PRO:HA	2.21	0.40
5:F:62:TRP:HB2	17:R:35:ARG:HH12	1.86	0.40
9:J:9:ARG:HG2	9:J:69:ASN:OD1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:89:ALA:O	10:K:91:ARG:N	2.54	0.40
11:L:25:PRO:HD2	11:L:98:TYR:OH	2.20	0.40
12:M:120:LYS:HA	12:M:120:LYS:HD3	1.61	0.40
19:T:93:GLU:C	19:T:95:ALA:H	2.29	0.40
21:A:229:U:H2'	21:A:230:G:H8	1.85	0.40
21:A:608:A:H2'	21:A:609:A:O4'	2.22	0.40
21:A:630:G:O2'	21:A:631:G:H5'	2.22	0.40
21:A:650:G:O2'	21:A:651:C:H5'	2.21	0.40
21:A:833:U:O2	21:A:854:G:C2	2.74	0.40
21:A:976:G:N7	21:A:1358:U:C2	2.89	0.40
21:A:1035:A:H2'	21:A:1036:G:O4'	2.21	0.40
21:A:1054:C:H5	21:A:1196:U:C6	2.38	0.40
21:A:1096:C:H2'	21:A:1097:C:C6	2.55	0.40
3:D:101:LEU:HA	3:D:101:LEU:HD12	1.78	0.40
3:D:209:ARG:HB2	21:A:8:A:N6	2.36	0.40
21:A:62:U:H2'	21:A:63:C:C6	2.56	0.40
21:A:985:C:C2	21:A:1221:G:N2	2.89	0.40
21:A:1072:G:H2'	21:A:1073:U:O4'	2.21	0.40
1:B:63:MET:HE3	1:B:225:ALA:HB1	2.04	0.40
1:B:167:PRO:HD3	1:B:186:ALA:HB1	2.02	0.40
2:C:70:VAL:HG11	2:C:76:VAL:HG23	2.03	0.40
2:C:88:ARG:HG3	2:C:101:LEU:HB3	2.03	0.40
6:G:103:TRP:CD1	6:G:137:LYS:HD2	2.56	0.40
10:K:63:LEU:HD23	10:K:63:LEU:HA	1.83	0.40
10:K:73:MET:HG2	10:K:103:LEU:HD21	2.02	0.40
11:L:87:GLY:HA3	21:A:552:U:O3'	2.22	0.40
13:N:9:LYS:HB2	13:N:9:LYS:HE3	1.93	0.40
16:Q:15:MET:HE3	16:Q:15:MET:HB2	1.51	0.40
19:T:41:ILE:HD12	19:T:42:GLN:N	2.36	0.40
21:A:392:G:C2	21:A:393:A:C4	3.09	0.40
21:A:557:G:H2'	21:A:558:G:O4'	2.21	0.40
21:A:689:C:H2'	21:A:690:G:O4'	2.20	0.40
21:A:708:C:H2'	21:A:709:G:H8	1.85	0.40
21:A:766:A:C8	21:A:814:A:N6	2.89	0.40
21:A:956:U:H2'	21:A:957:U:O4'	2.22	0.40
21:A:1413:A:H2'	21:A:1414:U:C6	2.48	0.40
2:C:120:VAL:O	2:C:123:GLN:HB2	2.21	0.40
14:O:8:LYS:NZ	21:A:659:U:OP2	2.37	0.40
15:P:33:ILE:HD13	21:A:229:U:H5''	2.03	0.40
21:A:447:G:H2'	21:A:485:G:N2	2.37	0.40
21:A:920:U:H2'	21:A:921:U:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:943:U:C2'	21:A:944:G:H5'	2.51	0.40
21:A:1495:U:C4	21:A:1496:C:N4	2.89	0.40
21:A:1507:A:C2	21:A:1508:G:C4	3.09	0.40
1:B:16:HIS:CE1	1:B:17:PHE:CE1	3.10	0.40
3:D:4:TYR:O	3:D:115:ARG:NH2	2.55	0.40
11:L:11:VAL:HG13	16:Q:29:HIS:HD2	1.86	0.40
13:N:26:ARG:HD2	13:N:47:LEU:HD11	2.03	0.40
21:A:496:A:H4'	21:A:497:A:OP1	2.21	0.40
21:A:501:C:H2'	21:A:502:G:H8	1.86	0.40
21:A:692:U:H5'	21:A:797:C:H5'	2.04	0.40
21:A:742:G:H8	21:A:742:G:O5'	2.04	0.40
21:A:1129:C:H1'	21:A:1130:A:N7	2.36	0.40
21:A:1215:G:C2	21:A:1216:G:C8	3.09	0.40
21:A:1481:U:H2'	21:A:1482:G:O4'	2.21	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	B	221/226 (98%)	184 (83%)	32 (14%)	5 (2%)	5	30
2	C	204/206 (99%)	176 (86%)	23 (11%)	5 (2%)	4	28
3	D	206/208 (99%)	185 (90%)	18 (9%)	3 (2%)	8	37
4	E	155/157 (99%)	132 (85%)	17 (11%)	6 (4%)	2	20
5	F	99/101 (98%)	87 (88%)	12 (12%)	0	100	100
6	G	153/155 (99%)	127 (83%)	22 (14%)	4 (3%)	4	27
7	H	136/138 (99%)	118 (87%)	15 (11%)	3 (2%)	5	30
8	I	125/127 (98%)	102 (82%)	18 (14%)	5 (4%)	2	19
9	J	97/99 (98%)	77 (79%)	14 (14%)	6 (6%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	K	113/115 (98%)	98 (87%)	14 (12%)	1 (1%)	14	47
11	L	122/124 (98%)	104 (85%)	16 (13%)	2 (2%)	7	36
12	M	123/125 (98%)	101 (82%)	16 (13%)	6 (5%)	1	16
13	N	58/60 (97%)	49 (84%)	7 (12%)	2 (3%)	3	23
14	O	86/88 (98%)	69 (80%)	11 (13%)	6 (7%)	1	10
15	P	83/85 (98%)	71 (86%)	11 (13%)	1 (1%)	10	41
16	Q	102/104 (98%)	84 (82%)	11 (11%)	7 (7%)	1	10
17	R	69/71 (97%)	59 (86%)	8 (12%)	2 (3%)	3	26
18	S	81/83 (98%)	69 (85%)	11 (14%)	1 (1%)	10	41
19	T	101/103 (98%)	86 (85%)	13 (13%)	2 (2%)	6	32
20	V	22/24 (92%)	20 (91%)	2 (9%)	0	100	100
All	All	2356/2399 (98%)	1998 (85%)	291 (12%)	67 (3%)	4	26

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	78	GLN
3	D	70	ILE
4	E	146	ALA
4	E	154	GLY
4	E	156	ALA
8	I	121	ARG
9	J	89	ASP
10	K	117	ASN
12	M	67	GLU
16	Q	100	LYS
19	T	99	LEU
1	B	126	GLU
2	C	51	GLY
2	C	160	ALA
3	D	10	ARG
3	D	12	CYS
4	E	37	ARG
4	E	128	PRO
6	G	133	GLY
8	I	119	ALA
8	I	126	SER
8	I	127	LYS

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Mol	Chain	Res	Type
9	J	55	LYS
13	N	36	PHE
14	O	21	ASP
14	O	84	LYS
14	O	86	GLY
14	O	88	ARG
15	P	24	ALA
16	Q	16	GLN
16	Q	99	SER
17	R	41	LYS
1	B	101	MET
7	H	29	SER
7	H	76	PRO
8	I	118	LYS
9	J	90	LEU
9	J	91	PRO
11	L	28	LYS
11	L	51	ALA
12	M	106	ASN
13	N	60	SER
14	O	34	LEU
16	Q	14	LYS
16	Q	98	LEU
2	C	146	ALA
4	E	145	LYS
6	G	83	ALA
9	J	30	SER
9	J	100	THR
12	M	23	TYR
12	M	125	ARG
16	Q	97	SER
17	R	25	THR
18	S	24	ALA
1	B	24	TRP
1	B	82	ARG
2	C	192	THR
7	H	91	ARG
16	Q	80	GLY
19	T	94	ALA
2	C	106	VAL
12	M	118	ALA
14	O	24	SER

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Mol	Chain	Res	Type
6	G	80	VAL
12	M	124	PRO
6	G	111	ARG

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	B	195/195 (100%)	179 (92%)	16 (8%)	10	34
2	C	160/160 (100%)	139 (87%)	21 (13%)	4	20
3	D	180/180 (100%)	161 (89%)	19 (11%)	6	27
4	E	119/119 (100%)	104 (87%)	15 (13%)	4	21
5	F	90/90 (100%)	78 (87%)	12 (13%)	4	20
6	G	126/126 (100%)	119 (94%)	7 (6%)	19	46
7	H	119/119 (100%)	108 (91%)	11 (9%)	8	32
8	I	98/98 (100%)	90 (92%)	8 (8%)	10	34
9	J	89/89 (100%)	80 (90%)	9 (10%)	7	28
10	K	87/87 (100%)	81 (93%)	6 (7%)	14	39
11	L	104/104 (100%)	92 (88%)	12 (12%)	5	24
12	M	98/100 (98%)	93 (95%)	5 (5%)	21	48
13	N	49/49 (100%)	45 (92%)	4 (8%)	10	34
14	O	79/79 (100%)	76 (96%)	3 (4%)	29	55
15	P	73/73 (100%)	66 (90%)	7 (10%)	8	30
16	Q	96/96 (100%)	88 (92%)	8 (8%)	10	34
17	R	62/62 (100%)	57 (92%)	5 (8%)	11	35
18	S	72/72 (100%)	66 (92%)	6 (8%)	10	34
19	T	80/80 (100%)	74 (92%)	6 (8%)	12	37
20	V	19/19 (100%)	17 (90%)	2 (10%)	6	27
All	All	1995/1997 (100%)	1813 (91%)	182 (9%)	9	32

All (182) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	7	VAL
1	B	12	GLU
1	B	15	VAL
1	B	45	GLN
1	B	58	ILE
1	B	60	ASP
1	B	67	THR
1	B	115	LEU
1	B	164	VAL
1	B	168	THR
1	B	175	ARG
1	B	184	VAL
1	B	189	ASP
1	B	196	LEU
1	B	200	ILE
1	B	223	ILE
2	C	5	ILE
2	C	12	LEU
2	C	15	THR
2	C	16	ARG
2	C	42	LEU
2	C	49	SER
2	C	52	LEU
2	C	58	GLU
2	C	64	VAL
2	C	67	THR
2	C	79	ARG
2	C	88	ARG
2	C	104	GLN
2	C	154	SER
2	C	165	THR
2	C	172	ARG
2	C	175	LEU
2	C	191	THR
2	C	195	VAL
2	C	198	VAL
2	C	204	LEU
3	D	5	ILE
3	D	8	VAL
3	D	9	CYS
3	D	12	CYS
3	D	14	ARG

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Mol	Chain	Res	Type
3	D	26	CYS
3	D	35	ARG
3	D	59	ARG
3	D	70	ILE
3	D	78	LEU
3	D	89	THR
3	D	112	VAL
3	D	135	LEU
3	D	137	SER
3	D	170	VAL
3	D	178	VAL
3	D	179	GLU
3	D	190	ASP
3	D	201	GLN
4	E	9	LYS
4	E	11	ILE
4	E	12	LEU
4	E	24	ARG
4	E	33	VAL
4	E	51	VAL
4	E	68	GLU
4	E	76	ILE
4	E	80	ILE
4	E	120	THR
4	E	123	LEU
4	E	144	THR
4	E	147	ASP
4	E	148	VAL
4	E	155	GLU
5	F	2	ARG
5	F	21	LEU
5	F	47	ARG
5	F	61	LEU
5	F	67	MET
5	F	69	GLU
5	F	75	LEU
5	F	79	LEU
5	F	83	ASP
5	F	91	VAL
5	F	96	PRO
5	F	100	ASN
6	G	5	ARG

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Mol	Chain	Res	Type
6	G	8	GLU
6	G	16	LEU
6	G	20	ASP
6	G	75	VAL
6	G	124	LEU
6	G	141	VAL
7	H	23	SER
7	H	30	ARG
7	H	52	ASP
7	H	70	GLN
7	H	84	ARG
7	H	103	VAL
7	H	112	LEU
7	H	114	THR
7	H	115	SER
7	H	118	VAL
7	H	137	VAL
8	I	7	THR
8	I	23	ASN
8	I	27	THR
8	I	53	VAL
8	I	54	ASP
8	I	99	LEU
8	I	109	VAL
8	I	124	GLN
9	J	16	LEU
9	J	34	VAL
9	J	38	ILE
9	J	74	ILE
9	J	75	ILE
9	J	90	LEU
9	J	92	THR
9	J	98	ILE
9	J	99	LYS
10	K	30	VAL
10	K	47	VAL
10	K	80	VAL
10	K	83	ILE
10	K	117	ASN
10	K	123	LYS
11	L	18	VAL
11	L	23	LYS

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Mol	Chain	Res	Type
11	L	24	VAL
11	L	27	LEU
11	L	36	VAL
11	L	38	THR
11	L	62	SER
11	L	79	GLU
11	L	110	VAL
11	L	117	ARG
11	L	124	LYS
11	L	126	LYS
12	M	32	GLU
12	M	63	THR
12	M	108	ARG
12	M	109	THR
12	M	122	LYS
13	N	13	THR
13	N	18	VAL
13	N	22	THR
13	N	58	LYS
14	O	3	ILE
14	O	22	THR
14	O	87	ILE
15	P	2	VAL
15	P	11	SER
15	P	25	ARG
15	P	45	THR
15	P	51	VAL
15	P	62	VAL
15	P	69	THR
16	Q	11	VAL
16	Q	15	MET
16	Q	35	VAL
16	Q	53	LEU
16	Q	57	VAL
16	Q	59	ILE
16	Q	60	ILE
16	Q	76	LEU
17	R	22	VAL
17	R	47	THR
17	R	58	LEU
17	R	69	THR
17	R	82	THR

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Mol	Chain	Res	Type
18	S	9	VAL
18	S	19	VAL
18	S	41	VAL
18	S	51	VAL
18	S	56	GLN
18	S	67	VAL
19	T	27	LYS
19	T	36	LEU
19	T	56	MET
19	T	62	LEU
19	T	71	THR
19	T	75	ASN
20	V	13	ILE
20	V	25	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	16	HIS
1	B	40	HIS
1	B	212	GLN
2	C	37	GLN
4	E	141	GLN
5	F	11	ASN
5	F	13	ASN
5	F	27	GLN
6	G	13	GLN
6	G	110	GLN
9	J	33	GLN
9	J	76	ASN
10	K	99	GLN
10	K	117	ASN
14	O	62	GLN
18	S	14	HIS
18	S	47	HIS
19	T	75	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	A	1501/1509 (99%)	282 (18%)	11 (0%)

All (282) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	A	2	A
21	A	3	A
21	A	4	U
21	A	6	G
21	A	7	G
21	A	8	A
21	A	9	G
21	A	32	A
21	A	39	G
21	A	47	C
21	A	48	C
21	A	50	A
21	A	51	A
21	A	54	C
21	A	61	G
21	A	68	G
21	A	69	G
21	A	75	G
21	A	77	G
21	A	82	U
21	A	83	U
21	A	84	U
21	A	85	A
21	A	89	C
21	A	101	A
21	A	121	C
21	A	131	C
21	A	144	G
21	A	145	G
21	A	157	G
21	A	182	U
21	A	183	G
21	A	190(D)	U
21	A	195	A
21	A	197	A
21	A	202	U
21	A	203	U
21	A	204	U

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Mol	Chain	Res	Type
21	A	216	G
21	A	217	C
21	A	231	G
21	A	243	A
21	A	245	C
21	A	247	G
21	A	251	G
21	A	266	G
21	A	267	C
21	A	280	C
21	A	289	G
21	A	301	G
21	A	305	G
21	A	308	C
21	A	319	G
21	A	321	A
21	A	323	U
21	A	328	C
21	A	332	G
21	A	345	C
21	A	346	G
21	A	347	G
21	A	351	G
21	A	352	C
21	A	354	G
21	A	367	U
21	A	372	C
21	A	384	G
21	A	397	A
21	A	398	C
21	A	406	G
21	A	412	A
21	A	422	C
21	A	429	U
21	A	448	A
21	A	452	A
21	A	460	A
21	A	461	C
21	A	462	G
21	A	486	U
21	A	497	A
21	A	498	U

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Mol	Chain	Res	Type
21	A	508	C
21	A	511	C
21	A	518	C
21	A	520	A
21	A	521	G
21	A	524	G
21	A	527	G
21	A	531	U
21	A	532	A
21	A	533	A
21	A	547	A
21	A	548	G
21	A	559	A
21	A	560	U
21	A	561	U
21	A	564	C
21	A	568	G
21	A	572	A
21	A	573	A
21	A	576	G
21	A	577	G
21	A	579	G
21	A	580	U
21	A	588	G
21	A	589	C
21	A	596	C
21	A	597	G
21	A	609	A
21	A	616	G
21	A	618	C
21	A	642	A
21	A	653	A
21	A	665	A
21	A	666	G
21	A	672	U
21	A	687	A
21	A	688	G
21	A	702	A
21	A	703	G
21	A	717	C
21	A	721	G
21	A	723	U

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Mol	Chain	Res	Type
21	A	724	G
21	A	728	A
21	A	729	A
21	A	731	G
21	A	755	G
21	A	759	A
21	A	760	G
21	A	766	A
21	A	777	A
21	A	787	A
21	A	810	C
21	A	813	U
21	A	815	A
21	A	817	C
21	A	819	A
21	A	820	U
21	A	821	G
21	A	828	A
21	A	829	G
21	A	840	C
21	A	841	U
21	A	848	C
21	A	862	C
21	A	864	A
21	A	865	A
21	A	873	A
21	A	874	G
21	A	876	G
21	A	889	A
21	A	902	G
21	A	907	A
21	A	913	A
21	A	914	A
21	A	922	G
21	A	926	G
21	A	927	G
21	A	934	C
21	A	935	A
21	A	939	G
21	A	950	U
21	A	954	G
21	A	958	A

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Mol	Chain	Res	Type
21	A	960	U
21	A	961	U
21	A	966	G
21	A	969	A
21	A	975	A
21	A	977	A
21	A	989	C
21	A	993	G
21	A	998	G
21	A	1002	G
21	A	1003(A)	G
21	A	1004	A
21	A	1006	C
21	A	1016	A
21	A	1025	U
21	A	1031	G
21	A	1045	C
21	A	1050	G
21	A	1053	G
21	A	1065	U
21	A	1081	G
21	A	1087	G
21	A	1094	G
21	A	1095	U
21	A	1101	A
21	A	1102	A
21	A	1137	C
21	A	1139	G
21	A	1140	C
21	A	1146	A
21	A	1152	A
21	A	1154	G
21	A	1159	U
21	A	1160	G
21	A	1167	A
21	A	1171	G
21	A	1182	G
21	A	1183	A
21	A	1184	G
21	A	1187	G
21	A	1188	A
21	A	1193	G

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Mol	Chain	Res	Type
21	A	1196	U
21	A	1197	G
21	A	1201	A
21	A	1213	A
21	A	1214	C
21	A	1227	A
21	A	1228	C
21	A	1238	A
21	A	1241	G
21	A	1243	C
21	A	1248	A
21	A	1253	G
21	A	1257	U
21	A	1258	G
21	A	1260	C
21	A	1262	C
21	A	1267	C
21	A	1268	A
21	A	1270	C
21	A	1278	U
21	A	1280	A
21	A	1282	C
21	A	1285	A
21	A	1287	A
21	A	1289	A
21	A	1300	G
21	A	1302	U
21	A	1305	G
21	A	1306	A
21	A	1315	U
21	A	1317	C
21	A	1320	C
21	A	1338	G
21	A	1340	A
21	A	1343	G
21	A	1346	A
21	A	1353	G
21	A	1362	C
21	A	1368	G
21	A	1370	G
21	A	1371	G
21	A	1376	U

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Mol	Chain	Res	Type
21	A	1379	G
21	A	1394	A
21	A	1398	A
21	A	1399	C
21	A	1407	C
21	A	1408	A
21	A	1411	C
21	A	1412	C
21	A	1416	G
21	A	1417	G
21	A	1418	A
21	A	1436	U
21	A	1442	G
21	A	1443	G
21	A	1446	A
21	A	1447	G
21	A	1451	A
21	A	1475	G
21	A	1488	G
21	A	1490	C
21	A	1493	A
21	A	1494	G
21	A	1495	U
21	A	1497	G
21	A	1499	A
21	A	1500	A
21	A	1502	A
21	A	1503	A
21	A	1505	G
21	A	1506	U
21	A	1507	A
21	A	1529	G
21	A	1530	G
21	A	1532	U

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	A	83	U
21	A	85	A
21	A	202	U
21	A	372	C

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Mol	Chain	Res	Type
21	A	460	A
21	A	461	C
21	A	531	U
21	A	1145	C
21	A	1281	U
21	A	1410	G
21	A	1417	G

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 207 ligands modelled in this entry, 206 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	6EK	M	201	-	42,47,47	2.74	16 (38%)	48,65,65	2.13	14 (29%)

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
24	6EK	M	201	-	-	12/49/60/60	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	M	201	6EK	C21-N07	6.80	1.45	1.33
24	M	201	6EK	C10-N04	6.68	1.48	1.34
24	M	201	6EK	C08-N03	5.94	1.46	1.34
24	M	201	6EK	C06-N02	5.65	1.46	1.34
24	M	201	6EK	C24-N	5.23	1.46	1.34
24	M	201	6EK	C22-C23	4.86	1.57	1.49
24	M	201	6EK	C11-N04	3.56	1.53	1.45
24	M	201	6EK	O07-C21	3.52	1.40	1.35
24	M	201	6EK	C01-C05	-3.10	1.47	1.52
24	M	201	6EK	C11-C17	2.54	1.56	1.52
24	M	201	6EK	C02-C01	-2.46	1.47	1.53
24	M	201	6EK	C09-C10	-2.38	1.46	1.52
24	M	201	6EK	C12-C16	2.23	1.55	1.50
24	M	201	6EK	O01-C05	-2.16	1.38	1.43
24	M	201	6EK	O02-C17	2.08	1.28	1.22
24	M	201	6EK	O03-C17	-2.02	1.24	1.30

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	M	201	6EK	O07-C21-N07	7.04	119.87	111.11
24	M	201	6EK	O08-C21-N07	-4.50	118.48	125.58
24	M	201	6EK	N08-C24-N09	-4.43	108.34	112.36
24	M	201	6EK	O07-C21-O08	-3.72	119.65	123.08
24	M	201	6EK	C20-O07-C21	3.26	120.84	116.26
24	M	201	6EK	C16-C15-N06	-3.18	108.12	111.46
24	M	201	6EK	C12-C11-N04	2.94	118.15	111.07
24	M	201	6EK	C02-C01-C05	2.65	116.47	111.56
24	M	201	6EK	C04-C06-N02	2.60	121.99	116.39
24	M	201	6EK	C09-C10-N04	2.59	122.15	116.63
24	M	201	6EK	O01-C05-C01	-2.36	104.22	109.99
24	M	201	6EK	O05-C10-N04	-2.30	118.83	122.96
24	M	201	6EK	N-C24-N08	2.15	125.70	122.63
24	M	201	6EK	C07-C08-N03	2.14	121.19	116.63

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	M	201	6EK	N07-C21-O07-C20
24	M	201	6EK	O08-C21-O07-C20

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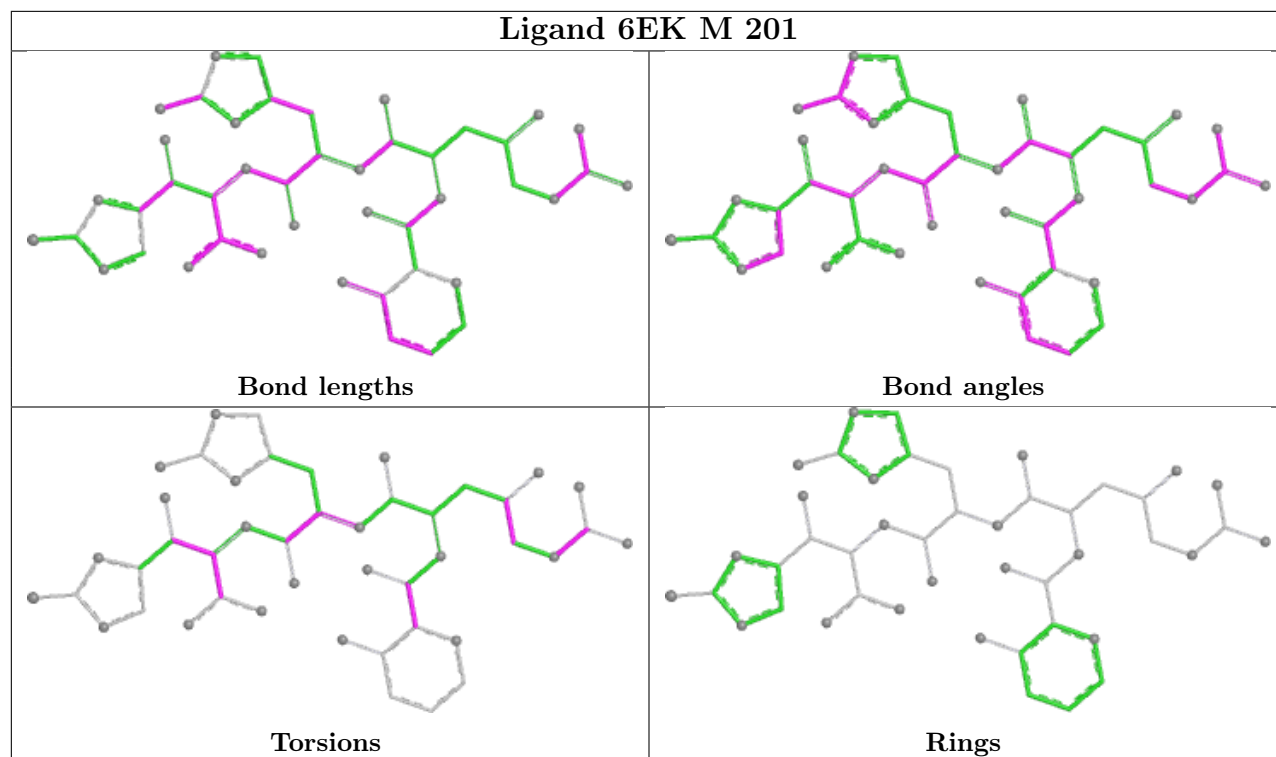
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Mol	Chain	Res	Type	Atoms
24	M	201	6EK	N01-C04-C06-N02
24	M	201	6EK	N04-C11-C12-O09
24	M	201	6EK	C12-C11-C17-O02
24	M	201	6EK	C12-C11-C17-O03
24	M	201	6EK	N03-C09-C10-O05
24	M	201	6EK	N03-C09-C10-N04
24	M	201	6EK	C22-C09-N03-C08
24	M	201	6EK	O-C19-C20-O07
24	M	201	6EK	N01-C04-C06-O06
24	M	201	6EK	C22-C09-C10-O05

There are no ring outliers.

No monomer is involved in short contacts.

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	B	225/226 (99%)	-0.30	10 (4%)	39	21	92, 135, 194, 222	0
2	C	206/206 (100%)	-0.33	3 (1%)	72	47	106, 140, 172, 207	0
3	D	208/208 (100%)	0.15	11 (5%)	32	18	92, 124, 157, 174	0
4	E	157/157 (100%)	-0.04	5 (3%)	50	29	84, 109, 158, 232	0
5	F	101/101 (100%)	-0.31	0	100	100	113, 158, 201, 242	0
6	G	155/155 (100%)	0.57	23 (14%)	5	5	128, 170, 207, 228	0
7	H	138/138 (100%)	-0.26	3 (2%)	62	37	83, 110, 139, 192	0
8	I	127/127 (100%)	0.40	15 (11%)	9	6	110, 166, 204, 217	0
9	J	99/99 (100%)	0.51	13 (13%)	7	6	112, 168, 227, 242	0
10	K	115/115 (100%)	0.26	14 (12%)	8	6	118, 155, 183, 197	0
11	L	124/124 (100%)	0.34	8 (6%)	25	15	96, 133, 163, 224	0
12	M	125/125 (100%)	0.01	8 (6%)	25	15	128, 160, 190, 363	0
13	N	60/60 (100%)	-0.26	0	100	100	113, 134, 162, 175	0
14	O	88/88 (100%)	-0.46	0	100	100	107, 135, 169, 205	0
15	P	85/85 (100%)	-0.10	0	100	100	103, 129, 159, 215	0
16	Q	104/104 (100%)	0.27	7 (6%)	24	15	98, 133, 169, 247	0
17	R	71/71 (100%)	-0.41	0	100	100	106, 137, 201, 218	0
18	S	83/83 (100%)	0.09	1 (1%)	76	52	145, 168, 199, 215	0
19	T	103/103 (100%)	0.20	8 (7%)	19	12	130, 156, 198, 227	0
20	V	24/24 (100%)	0.36	1 (4%)	40	22	136, 149, 173, 177	0
21	A	1509/1509 (100%)	0.03	150 (9%)	13	8	64, 138, 216, 315	7 (0%)
All	All	3907/3908 (99%)	0.02	280 (7%)	21	14	64, 141, 204, 363	7 (0%)

All (280) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	G	33	ASP	8.2
10	K	117	ASN	7.6
21	A	136	C	7.4
6	G	106	GLN	7.0
21	A	793[A]	U	6.6
12	M	124	PRO	6.3
6	G	112	PRO	6.2
16	Q	104	LYS	6.0
21	A	916	G	5.9
21	A	917	G	5.9
3	D	12	CYS	5.8
10	K	124	LYS	5.8
21	A	723	U	5.7
10	K	118	GLY	5.6
8	I	128	ARG	5.6
21	A	134	A	5.4
21	A	400	C	5.4
21	A	1518[A]	A	5.3
6	G	32	ARG	5.1
21	A	1351	U	5.0
10	K	125	PHE	5.0
21	A	135	C	4.9
16	Q	105	ALA	4.8
21	A	228	A	4.8
21	A	1517[A]	G	4.8
1	B	128	GLU	4.8
10	K	114	VAL	4.7
21	A	1289	A	4.7
21	A	1528	U	4.7
16	Q	101	ARG	4.7
21	A	1491	G	4.6
12	M	123	ALA	4.6
21	A	30	U	4.5
21	A	548	G	4.5
10	K	116	HIS	4.4
21	A	39	G	4.4
21	A	1527	C	4.3
21	A	26	A	4.2
9	J	64	GLU	4.2
9	J	58	ASP	4.2
21	A	27	G	4.2
21	A	216	G	4.2
21	A	326	G	4.2

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Mol	Chain	Res	Type	RSRZ
21	A	573	A	4.2
10	K	87	THR	4.1
21	A	20	U	4.1
21	A	227	G	4.1
8	I	121	ARG	4.1
1	B	123	ALA	4.1
21	A	1479	C	4.1
10	K	115	PRO	4.1
21	A	399	G	4.0
9	J	66	ARG	4.0
19	T	70	SER	4.0
21	A	1526	G	4.0
11	L	19	ARG	4.0
21	A	572	A	3.9
21	A	137	C	3.9
21	A	1477	C	3.9
21	A	574	A	3.9
21	A	631	G	3.9
6	G	35	LYS	3.8
3	D	31	CYS	3.8
21	A	1410	G	3.8
12	M	121	LYS	3.7
21	A	29	G	3.7
21	A	1353	G	3.7
4	E	15	ARG	3.7
21	A	1529	G	3.7
12	M	126	LYS	3.7
16	Q	100	LYS	3.7
21	A	132	C	3.6
21	A	28	G	3.6
8	I	127	LYS	3.6
21	A	1478	C	3.6
21	A	1516[A]	G	3.6
1	B	129	GLU	3.6
1	B	130	ARG	3.6
21	A	549	C	3.5
21	A	1411	C	3.5
9	J	60	ARG	3.5
21	A	230	G	3.5
21	A	1525	G	3.5
19	T	71	THR	3.5
21	A	1352	C	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	126	GLU	3.5
21	A	918	A	3.5
21	A	500	G	3.5
21	A	1508	G	3.5
3	D	9	CYS	3.5
21	A	503	C	3.5
21	A	1492	A	3.5
21	A	502	G	3.5
10	K	119	CYS	3.5
21	A	1530	G	3.4
21	A	322	C	3.4
21	A	19	C	3.4
21	A	231	G	3.4
21	A	818	G	3.4
6	G	110	GLN	3.4
16	Q	102	GLY	3.3
21	A	25	C	3.3
21	A	2	A	3.3
1	B	122	PHE	3.3
21	A	545	C	3.3
21	A	82	U	3.3
21	A	229	U	3.3
21	A	1509	C	3.3
21	A	819	A	3.3
21	A	1394	A	3.2
21	A	21	G	3.2
21	A	323	U	3.2
21	A	919	A	3.2
12	M	125	ARG	3.2
21	A	569	C	3.2
8	I	43	ALA	3.2
3	D	73	ARG	3.1
21	A	817	C	3.1
21	A	1493	A	3.1
4	E	155	GLU	3.1
9	J	47	PHE	3.1
21	A	1350	A	3.1
6	G	109	ASN	3.1
16	Q	103	GLY	3.1
21	A	1354	C	3.1
21	A	1397	C	3.1
21	A	1476	G	3.0

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Mol	Chain	Res	Type	RSRZ
10	K	123	LYS	3.0
6	G	115	ARG	3.0
8	I	9	ARG	3.0
11	L	52	LEU	3.0
19	T	8	ARG	3.0
21	A	22	G	3.0
21	A	1511	G	3.0
21	A	1241	G	3.0
3	D	22	LYS	3.0
21	A	40	C	3.0
21	A	940	C	3.0
21	A	1393	U	3.0
4	E	5	ASP	3.0
8	I	115	GLY	2.9
21	A	499	A	2.9
21	A	547	A	2.9
21	A	914	A	2.9
21	A	544	G	2.9
21	A	550	G	2.9
21	A	570	G	2.9
10	K	122	LYS	2.9
21	A	12	U	2.9
21	A	1510	U	2.9
8	I	125	TYR	2.9
21	A	571	U	2.9
12	M	122	LYS	2.9
21	A	1507	A	2.8
21	A	1240	U	2.8
21	A	1426	C	2.8
9	J	46	ARG	2.8
21	A	792[A]	A	2.8
6	G	8	GLU	2.8
11	L	119	LYS	2.8
21	A	941	G	2.8
21	A	262	A	2.8
3	D	26	CYS	2.8
21	A	11	G	2.8
21	A	675	A	2.8
21	A	1531	A	2.8
21	A	233	C	2.7
21	A	1443	G	2.7
21	A	1	A	2.7

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Mol	Chain	Res	Type	RSRZ
21	A	133	U	2.7
8	I	116	LYS	2.7
8	I	119	ALA	2.7
21	A	325	A	2.7
21	A	915	A	2.7
2	C	206	GLU	2.7
21	A	204	U	2.7
9	J	62	HIS	2.7
7	H	54	ASP	2.7
11	L	5	PRO	2.7
21	A	501	C	2.7
21	A	883	C	2.7
21	A	1424	C	2.7
21	A	1524	C	2.7
11	L	65	GLU	2.7
3	D	86	LYS	2.7
21	A	716	A	2.7
21	A	1349	A	2.7
21	A	15	G	2.7
21	A	202	U	2.7
21	A	855	G	2.7
21	A	498	U	2.6
21	A	718	G	2.6
18	S	32	LYS	2.6
9	J	101	VAL	2.6
8	I	113	LYS	2.6
4	E	20	GLN	2.6
10	K	113	PRO	2.6
11	L	128	ALA	2.6
21	A	232	G	2.6
6	G	113	GLU	2.6
6	G	26	PHE	2.6
6	G	42	ILE	2.5
3	D	21	LEU	2.5
6	G	30	ILE	2.5
21	A	3	A	2.5
2	C	179	ARG	2.5
10	K	25	TYR	2.5
9	J	49	VAL	2.5
21	A	14	U	2.5
21	A	1396	A	2.5
6	G	43	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
6	G	86	GLN	2.5
9	J	3	LYS	2.5
11	L	51	ALA	2.5
21	A	1409	C	2.5
21	A	1417	G	2.5
21	A	1423	G	2.5
21	A	884	U	2.5
9	J	99	LYS	2.5
21	A	766	A	2.5
19	T	72	LEU	2.4
21	A	557	G	2.4
8	I	2	GLU	2.4
10	K	120	ARG	2.4
21	A	1412	C	2.4
21	A	1480	G	2.4
3	D	137	SER	2.4
19	T	15	ARG	2.4
6	G	120	ILE	2.4
7	H	18	ARG	2.4
6	G	89	MET	2.4
12	M	120	LYS	2.4
19	T	30	LYS	2.3
8	I	42	ARG	2.3
20	V	25	LYS	2.3
21	A	23	C	2.3
6	G	80	VAL	2.3
4	E	24	ARG	2.3
21	A	77	G	2.3
8	I	120	ARG	2.3
21	A	352	C	2.3
19	T	80	ARG	2.3
21	A	1392	G	2.3
21	A	920	U	2.3
21	A	1532	U	2.3
21	A	815	A	2.3
6	G	105	VAL	2.3
1	B	133	LYS	2.2
1	B	131	PRO	2.2
6	G	88	PRO	2.2
9	J	63	PHE	2.2
16	Q	71	PHE	2.2
21	A	1398	A	2.2

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Mol	Chain	Res	Type	RSRZ
21	A	1242	C	2.2
9	J	61	GLU	2.2
21	A	38	G	2.2
21	A	1117	G	2.2
1	B	125	PRO	2.2
21	A	1519[A]	A	2.2
21	A	1395	C	2.2
8	I	44	VAL	2.2
8	I	99	LEU	2.2
11	L	89	ARG	2.2
19	T	58	LYS	2.2
6	G	34	GLY	2.1
7	H	46	LYS	2.1
21	A	546	G	2.1
21	A	1290	G	2.1
21	A	561	U	2.1
2	C	27	LYS	2.1
3	D	18	LYS	2.1
3	D	88	VAL	2.1
6	G	93	PRO	2.1
21	A	218	C	2.1
6	G	79	ARG	2.1
21	A	1425	U	2.1
12	M	27	LYS	2.1
21	A	840	C	2.0
21	A	1296	C	2.0
1	B	121	LEU	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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
22	MG	A	3495	1/1	0.46	0.28	135,135,135,135	0
22	MG	A	3564	1/1	0.57	0.12	127,127,127,127	0
22	MG	A	3486	1/1	0.58	0.23	121,121,121,121	0
22	MG	A	3543	1/1	0.63	0.24	126,126,126,126	0
22	MG	A	3515	1/1	0.64	0.19	130,130,130,130	0
22	MG	A	3552	1/1	0.66	0.12	118,118,118,118	0
22	MG	A	3483	1/1	0.67	0.40	112,112,112,112	0
22	MG	A	3451	1/1	0.69	0.35	129,129,129,129	0
22	MG	A	3528	1/1	0.69	0.19	125,125,125,125	0
22	MG	A	3529	1/1	0.69	0.32	119,119,119,119	0
22	MG	A	3589	1/1	0.69	0.20	109,109,109,109	0
22	MG	A	3430	1/1	0.70	0.27	133,133,133,133	0
22	MG	A	3562	1/1	0.70	0.28	114,114,114,114	0
22	MG	A	3540	1/1	0.70	0.14	121,121,121,121	0
22	MG	A	3583	1/1	0.70	0.37	113,113,113,113	0
22	MG	A	3438	1/1	0.70	0.48	124,124,124,124	0
22	MG	A	3513	1/1	0.71	0.14	145,145,145,145	0
22	MG	A	3530	1/1	0.72	0.17	113,113,113,113	0
22	MG	A	3587	1/1	0.73	0.14	115,115,115,115	0
22	MG	A	3457	1/1	0.73	0.38	111,111,111,111	0
22	MG	A	3401	1/1	0.74	0.22	137,137,137,137	0
22	MG	A	3554	1/1	0.75	0.18	122,122,122,122	0
22	MG	A	3406	1/1	0.75	0.07	111,111,111,111	0
22	MG	A	3424	1/1	0.75	0.19	133,133,133,133	0
22	MG	A	3576	1/1	0.75	0.27	114,114,114,114	0
22	MG	A	3429	1/1	0.75	0.24	134,134,134,134	0
22	MG	A	3464	1/1	0.75	0.28	108,108,108,108	0
22	MG	S	101	1/1	0.75	0.30	118,118,118,118	0
22	MG	A	3412	1/1	0.76	0.32	122,122,122,122	0
22	MG	A	3474	1/1	0.76	0.23	92,92,92,92	0
22	MG	A	3481	1/1	0.76	0.30	103,103,103,103	0
22	MG	A	3510	1/1	0.77	0.32	101,101,101,101	0
22	MG	A	3550	1/1	0.78	0.34	123,123,123,123	0
22	MG	A	3425	1/1	0.78	0.29	106,106,106,106	0
22	MG	A	3416	1/1	0.78	0.31	125,125,125,125	0
22	MG	A	3465	1/1	0.79	0.24	136,136,136,136	0
22	MG	A	3442	1/1	0.79	0.19	101,101,101,101	0
22	MG	A	3476	1/1	0.79	0.32	111,111,111,111	0
22	MG	A	3427	1/1	0.79	0.22	112,112,112,112	0
22	MG	A	3405	1/1	0.79	0.08	125,125,125,125	0
22	MG	A	3439	1/1	0.79	0.24	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	3477	1/1	0.80	0.66	94,94,94,94	0
22	MG	A	3453	1/1	0.80	0.48	110,110,110,110	0
22	MG	A	3582	1/1	0.81	0.10	111,111,111,111	0
22	MG	A	3531	1/1	0.81	0.59	135,135,135,135	0
22	MG	B	301	1/1	0.81	0.20	131,131,131,131	0
22	MG	O	101	1/1	0.81	0.45	92,92,92,92	0
22	MG	A	3404	1/1	0.82	0.26	105,105,105,105	0
22	MG	A	3432	1/1	0.82	0.21	101,101,101,101	0
22	MG	A	3595	1/1	0.82	0.64	127,127,127,127	0
22	MG	A	3571	1/1	0.83	0.31	108,108,108,108	0
22	MG	A	3573	1/1	0.83	0.42	99,99,99,99	0
22	MG	A	3418	1/1	0.83	0.21	124,124,124,124	0
22	MG	A	3541	1/1	0.83	0.23	108,108,108,108	0
22	MG	A	3435	1/1	0.84	0.43	132,132,132,132	0
22	MG	A	3469	1/1	0.84	0.21	83,83,83,83	0
22	MG	A	3551	1/1	0.84	0.25	94,94,94,94	0
22	MG	A	3512	1/1	0.85	0.21	122,122,122,122	0
22	MG	A	3506	1/1	0.85	0.07	128,128,128,128	0
22	MG	A	3502	1/1	0.85	0.26	100,100,100,100	0
22	MG	A	3594	1/1	0.85	0.20	115,115,115,115	0
22	MG	A	3511	1/1	0.85	0.28	76,76,76,76	0
22	MG	A	3561	1/1	0.86	0.29	98,98,98,98	0
22	MG	A	3407	1/1	0.86	0.19	96,96,96,96	0
22	MG	A	3484	1/1	0.86	0.37	91,91,91,91	0
22	MG	A	3500	1/1	0.86	0.36	108,108,108,108	0
22	MG	A	3598	1/1	0.86	0.70	123,123,123,123	0
22	MG	A	3534	1/1	0.87	0.23	112,112,112,112	0
22	MG	A	3473	1/1	0.87	0.30	89,89,89,89	0
22	MG	A	3485	1/1	0.87	0.58	96,96,96,96	0
22	MG	A	3575	1/1	0.87	0.20	138,138,138,138	0
22	MG	A	3431	1/1	0.87	0.17	111,111,111,111	0
22	MG	A	3426	1/1	0.87	0.15	98,98,98,98	0
22	MG	A	3563	1/1	0.88	0.07	132,132,132,132	0
22	MG	A	3468	1/1	0.88	0.06	128,128,128,128	0
22	MG	A	3440	1/1	0.88	0.15	124,124,124,124	0
22	MG	A	3556	1/1	0.88	0.09	84,84,84,84	0
22	MG	A	3590	1/1	0.88	0.14	111,111,111,111	0
22	MG	A	3538	1/1	0.88	0.27	95,95,95,95	0
22	MG	A	3516	1/1	0.88	0.11	95,95,95,95	0
22	MG	A	3577	1/1	0.88	0.15	88,88,88,88	0
24	6EK	M	201	45/45	0.88	0.18	180,269,292,301	0
22	MG	A	3544	1/1	0.89	0.10	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	3574	1/1	0.89	0.12	100,100,100,100	0
22	MG	A	3501	1/1	0.89	0.34	83,83,83,83	0
22	MG	A	3452	1/1	0.89	0.20	93,93,93,93	0
22	MG	A	3514	1/1	0.89	0.18	104,104,104,104	0
22	MG	A	3578	1/1	0.89	0.22	108,108,108,108	0
22	MG	A	3533	1/1	0.89	0.09	118,118,118,118	0
22	MG	A	3491	1/1	0.89	0.31	104,104,104,104	0
22	MG	A	3479	1/1	0.89	0.24	94,94,94,94	0
22	MG	A	3539	1/1	0.89	0.08	108,108,108,108	0
22	MG	A	3518	1/1	0.89	0.16	115,115,115,115	0
22	MG	A	3526	1/1	0.89	0.13	110,110,110,110	0
22	MG	A	3567	1/1	0.89	0.09	103,103,103,103	0
22	MG	A	3597	1/1	0.89	0.19	128,128,128,128	0
22	MG	A	3569	1/1	0.89	0.11	105,105,105,105	0
22	MG	A	3414	1/1	0.89	0.26	92,92,92,92	0
22	MG	A	3467	1/1	0.90	0.45	85,85,85,85	0
22	MG	A	3527	1/1	0.90	0.28	98,98,98,98	0
22	MG	A	3592	1/1	0.90	0.14	114,114,114,114	0
22	MG	A	3579	1/1	0.90	0.15	94,94,94,94	0
22	MG	A	3456	1/1	0.90	0.23	95,95,95,95	0
22	MG	A	3517	1/1	0.90	0.19	82,82,82,82	0
22	MG	A	3408	1/1	0.90	0.18	108,108,108,108	0
22	MG	A	3588	1/1	0.90	0.11	105,105,105,105	0
22	MG	A	3570	1/1	0.91	0.18	102,102,102,102	0
22	MG	A	3524	1/1	0.91	0.10	85,85,85,85	0
22	MG	A	3411	1/1	0.91	0.32	117,117,117,117	0
22	MG	A	3403	1/1	0.91	0.33	83,83,83,83	0
22	MG	A	3410	1/1	0.91	0.30	76,76,76,76	0
22	MG	A	3449	1/1	0.91	0.21	114,114,114,114	0
22	MG	A	3489	1/1	0.91	0.16	111,111,111,111	0
22	MG	A	3482	1/1	0.91	0.32	92,92,92,92	0
22	MG	A	3532	1/1	0.91	0.06	119,119,119,119	0
22	MG	A	3581	1/1	0.91	0.26	107,107,107,107	0
22	MG	A	3492	1/1	0.91	0.38	97,97,97,97	0
22	MG	A	3585	1/1	0.92	0.23	114,114,114,114	0
22	MG	A	3586	1/1	0.92	0.43	112,112,112,112	0
22	MG	A	3523	1/1	0.92	0.10	85,85,85,85	0
22	MG	A	3422	1/1	0.92	0.19	89,89,89,89	0
22	MG	A	3499	1/1	0.92	0.10	107,107,107,107	0
22	MG	A	3417	1/1	0.92	0.28	85,85,85,85	0
22	MG	A	3448	1/1	0.92	0.22	97,97,97,97	0
22	MG	A	3409	1/1	0.92	0.38	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	3493	1/1	0.92	0.26	92,92,92,92	0
22	MG	A	3507	1/1	0.92	0.34	105,105,105,105	0
22	MG	A	3508	1/1	0.92	0.21	107,107,107,107	0
22	MG	A	3509	1/1	0.92	0.22	100,100,100,100	0
22	MG	A	3450	1/1	0.93	0.29	89,89,89,89	0
22	MG	A	3535	1/1	0.93	0.23	68,68,68,68	0
22	MG	A	3488	1/1	0.93	0.25	115,115,115,115	0
22	MG	A	3494	1/1	0.93	0.32	94,94,94,94	0
22	MG	A	3557	1/1	0.93	0.06	103,103,103,103	0
22	MG	A	3558	1/1	0.93	0.19	108,108,108,108	0
22	MG	A	3433	1/1	0.93	0.12	87,87,87,87	0
22	MG	A	3593	1/1	0.93	0.16	110,110,110,110	0
22	MG	A	3519	1/1	0.93	0.09	103,103,103,103	0
22	MG	A	3522	1/1	0.93	0.24	73,73,73,73	0
22	MG	A	3497	1/1	0.93	0.20	82,82,82,82	0
22	MG	A	3546	1/1	0.93	0.14	110,110,110,110	0
23	ZN	D	301	1/1	0.93	0.37	121,121,121,121	0
22	MG	A	3463	1/1	0.93	0.11	80,80,80,80	0
22	MG	A	3559	1/1	0.94	0.20	104,104,104,104	0
22	MG	A	3441	1/1	0.94	0.33	76,76,76,76	0
22	MG	A	3402	1/1	0.94	0.21	93,93,93,93	0
22	MG	A	3549	1/1	0.94	0.19	116,116,116,116	0
22	MG	A	3445	1/1	0.94	0.13	75,75,75,75	0
22	MG	A	3446	1/1	0.94	0.24	68,68,68,68	0
22	MG	A	3413	1/1	0.94	0.18	94,94,94,94	0
22	MG	A	3454	1/1	0.94	0.15	87,87,87,87	0
22	MG	A	3455	1/1	0.94	0.25	67,67,67,67	0
22	MG	A	3490	1/1	0.94	0.19	118,118,118,118	0
22	MG	A	3521	1/1	0.94	0.32	73,73,73,73	0
22	MG	A	3548	1/1	0.95	0.06	97,97,97,97	0
22	MG	A	3423	1/1	0.95	0.24	75,75,75,75	0
22	MG	A	3568	1/1	0.95	0.16	76,76,76,76	0
22	MG	A	3458	1/1	0.95	0.21	65,65,65,65	0
22	MG	A	3459	1/1	0.95	0.12	83,83,83,83	0
22	MG	A	3475	1/1	0.95	0.21	94,94,94,94	0
22	MG	A	3572	1/1	0.95	0.21	118,118,118,118	0
22	MG	A	3487	1/1	0.95	0.19	84,84,84,84	0
22	MG	A	3591	1/1	0.95	0.06	116,116,116,116	0
22	MG	A	3421	1/1	0.95	0.11	83,83,83,83	0
22	MG	A	3447	1/1	0.95	0.18	72,72,72,72	0
22	MG	A	3437	1/1	0.95	0.22	66,66,66,66	0
22	MG	A	3542	1/1	0.95	0.11	139,139,139,139	0

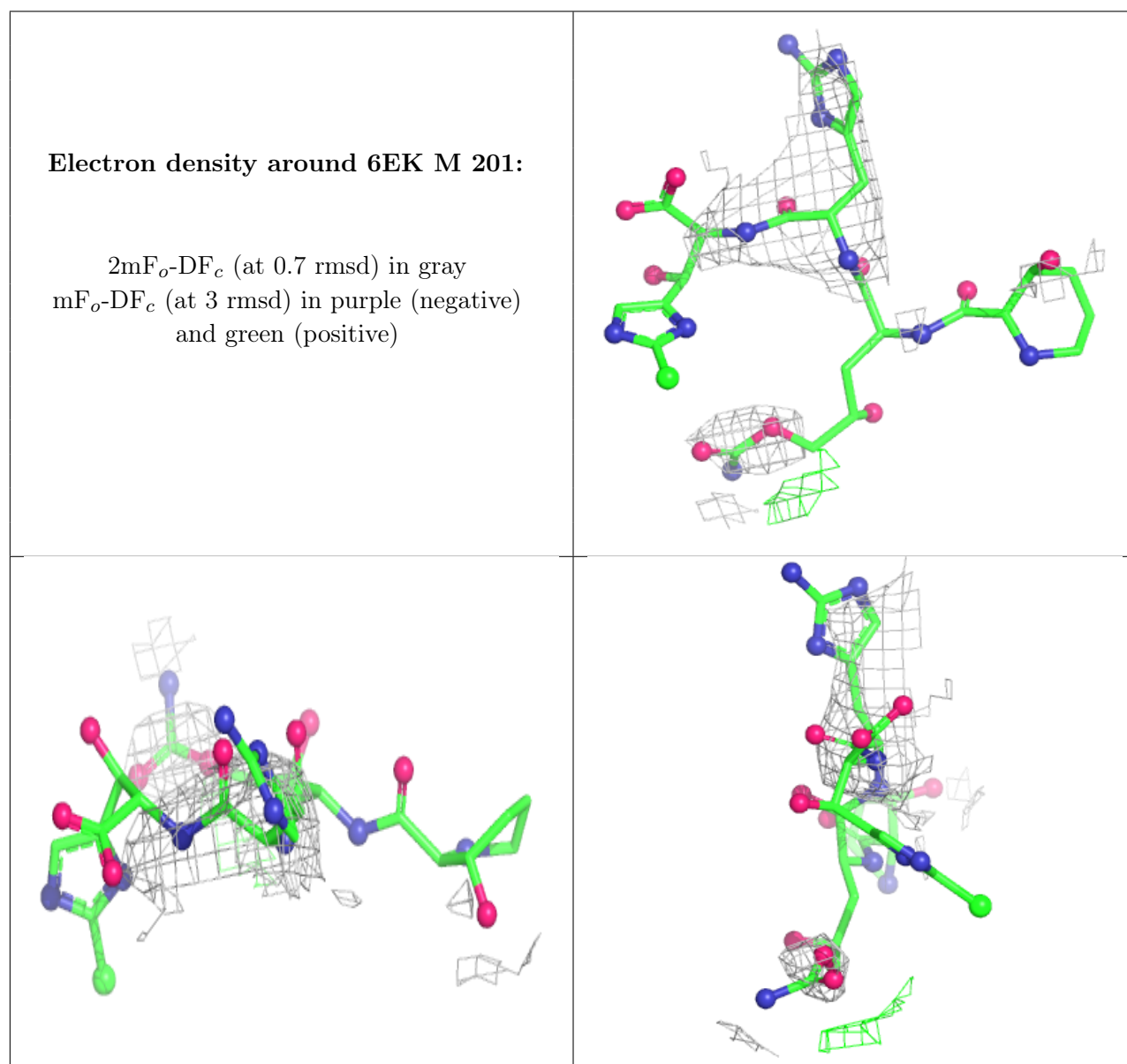
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	3503	1/1	0.95	0.16	101,101,101,101	0
22	MG	H	201	1/1	0.95	0.18	69,69,69,69	0
22	MG	A	3580	1/1	0.95	0.17	91,91,91,91	0
22	MG	A	3444	1/1	0.95	0.11	75,75,75,75	0
22	MG	A	3436	1/1	0.96	0.09	94,94,94,94	0
22	MG	K	201	1/1	0.96	0.21	83,83,83,83	0
22	MG	A	3478	1/1	0.96	0.12	76,76,76,76	0
22	MG	A	3536	1/1	0.96	0.17	93,93,93,93	0
22	MG	A	3537	1/1	0.96	0.13	81,81,81,81	0
22	MG	A	3428	1/1	0.96	0.12	98,98,98,98	0
22	MG	A	3480	1/1	0.96	0.31	68,68,68,68	0
22	MG	A	3460	1/1	0.96	0.42	74,74,74,74	0
22	MG	A	3470	1/1	0.96	0.07	106,106,106,106	0
22	MG	A	3461	1/1	0.96	0.10	89,89,89,89	0
22	MG	E	201	1/1	0.96	0.30	67,67,67,67	0
22	MG	A	3419	1/1	0.96	0.20	81,81,81,81	0
22	MG	A	3596	1/1	0.96	0.25	108,108,108,108	0
22	MG	A	3545	1/1	0.96	0.07	118,118,118,118	0
22	MG	A	3520	1/1	0.96	0.25	71,71,71,71	0
22	MG	A	3565	1/1	0.96	0.16	81,81,81,81	0
22	MG	A	3566	1/1	0.96	0.27	88,88,88,88	0
22	MG	A	3496	1/1	0.97	0.14	98,98,98,98	0
22	MG	A	3553	1/1	0.97	0.11	77,77,77,77	0
22	MG	A	3560	1/1	0.97	0.13	71,71,71,71	0
22	MG	A	3471	1/1	0.97	0.15	70,70,70,70	0
22	MG	A	3525	1/1	0.97	0.13	79,79,79,79	0
22	MG	A	3443	1/1	0.97	0.21	72,72,72,72	0
22	MG	A	3498	1/1	0.98	0.08	78,78,78,78	0
22	MG	A	3584	1/1	0.98	0.10	97,97,97,97	0
22	MG	A	3462	1/1	0.98	0.08	73,73,73,73	0
22	MG	A	3504	1/1	0.98	0.07	98,98,98,98	0
22	MG	A	3547	1/1	0.98	0.04	94,94,94,94	0
22	MG	A	3555	1/1	0.98	0.09	110,110,110,110	0
22	MG	A	3505	1/1	0.98	0.11	122,122,122,122	0
22	MG	A	3420	1/1	0.98	0.15	78,78,78,78	0
22	MG	A	3466	1/1	0.98	0.11	74,74,74,74	0
22	MG	A	3472	1/1	0.99	0.04	94,94,94,94	0
22	MG	A	3434	1/1	0.99	0.07	77,77,77,77	0
22	MG	A	3415	1/1	0.99	0.10	64,64,64,64	0
23	ZN	N	101	1/1	1.00	0.01	144,144,144,144	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.