



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 01:50 pm BST

PDB ID : 6CAS  
Title : Serial Femtosecond X-ray Crystal Structure of 30S ribosomal subunit from *Thermus thermophilus* in complex with N1MS  
Authors : DeMirci, H.  
Deposited on : 2018-01-31  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

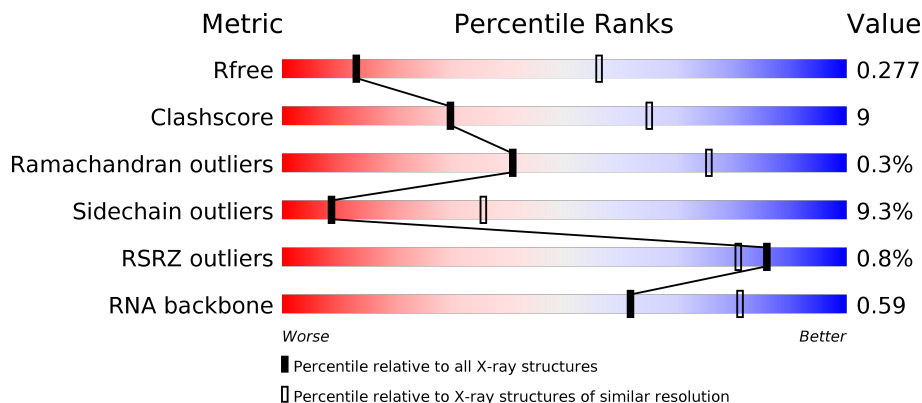
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	1517	
2	B	255	
3	C	238	
4	D	208	

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Mol	Chain	Length	Quality of chain
5	E	161	
6	F	101	
7	G	155	
8	H	138	
9	I	127	
10	J	104	
11	K	128	
12	L	131	
13	M	125	
14	N	60	
15	O	88	
16	P	88	
17	Q	104	
18	R	87	
19	S	92	
20	T	105	
21	U	26	
22	Y	6	
23	W	15	

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
24	MG	A	1601	-	-	-	X
24	MG	A	1625	-	-	-	X
24	MG	A	1677	-	-	-	X
24	MG	A	1680	-	-	-	X
24	MG	A	1696	-	-	-	X

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
24	MG	A	1709	-	-	-	X
24	MG	A	1714	-	-	-	X
24	MG	A	1733	-	-	-	X
24	MG	A	1741	-	-	-	X
24	MG	A	1756	-	-	-	X
24	MG	A	1759	-	-	-	X
24	MG	A	1767	-	-	-	X
24	MG	A	1773	-	-	-	X
24	MG	A	1790	-	-	-	X
24	MG	A	1826	-	-	-	X
24	MG	A	1830	-	-	-	X
24	MG	B	303	-	-	-	X

## 2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 52613 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S Ribosomal RNA rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1512	32507	14477	6012	10506	1512	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	C	U	conflict	GB 55771382

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	234	1900	1213	341	341	5	0	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	206	1612	1016	314	281	1	0	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	150	1146	724	217	201	4	0	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

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

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	98	792	498	156	137	1	0	0	0

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	116	864	537	164	160	3	0	0	0

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	124	972	612	195	163	2	0	0	0

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	118	937	579	193	163	2	0	0	0

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	O	87	729	457	146	124	2	0	0	0

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	P	83	700	443	139	117	1	0	0	0

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	Q	99	823	528	151	142	2	0	0	0

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	R	70	574	367	112	95	0	0	0

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	S	80	647	414	119	112	2	0	0	0

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 22 is a RNA chain called RNA (5'-R(\*UP\*UP\*UP\*UP\*UP\*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Y	6	Total	C	N	O	P	0	0	0
			117	54	12	46	5			

- Molecule 23 is a RNA chain called RNA (5'-R(\*GP\*GP\*GP\*AP\*UP\*UP\*GP\*AP\*AP\*AP\*AP\*UP\*CP\*CP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	15	Total	C	N	O	P	0	0	0
			319	144	60	101	14			

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	P	3	Total	Mg	0	0
			3	3		
24	J	1	Total	Mg	0	0
			1	1		
24	Q	3	Total	Mg	0	0
			3	3		
24	D	4	Total	Mg	0	0
			4	4		
24	E	2	Total	Mg	0	0
			2	2		
24	H	2	Total	Mg	0	0
			2	2		
24	B	3	Total	Mg	0	0
			3	3		
24	I	1	Total	Mg	0	0
			1	1		
24	C	2	Total	Mg	0	0
			2	2		

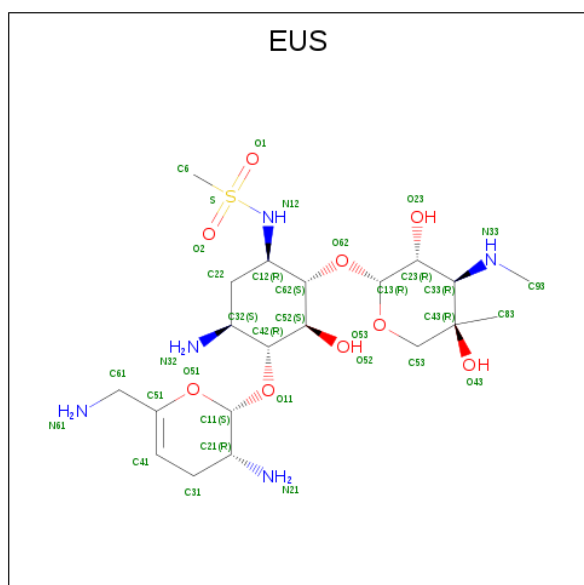
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	274	Total Mg 274 274	0	0
24	L	3	Total Mg 3 3	0	0
24	S	1	Total Mg 1 1	0	0
24	F	1	Total Mg 1 1	0	0

- Molecule 25 is N-[(1R,2S,3S,4R,5S)-5-amino-4-[(2S,3R)-3-amino-6-(aminomethyl)-3,4-dihydro-2H-pyran-2-yl]oxy}-2-[[3-deoxy-4-C-methyl-3-(methylamino)-beta-L-arabinopyranosyl]oxy]-3-hydroxycyclohexyl]methanesulfonamide (three-letter code: EUS) (formula:  $C_{20}H_{39}N_5O_9S$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C N O S 35 20 5 9 1	0	0

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

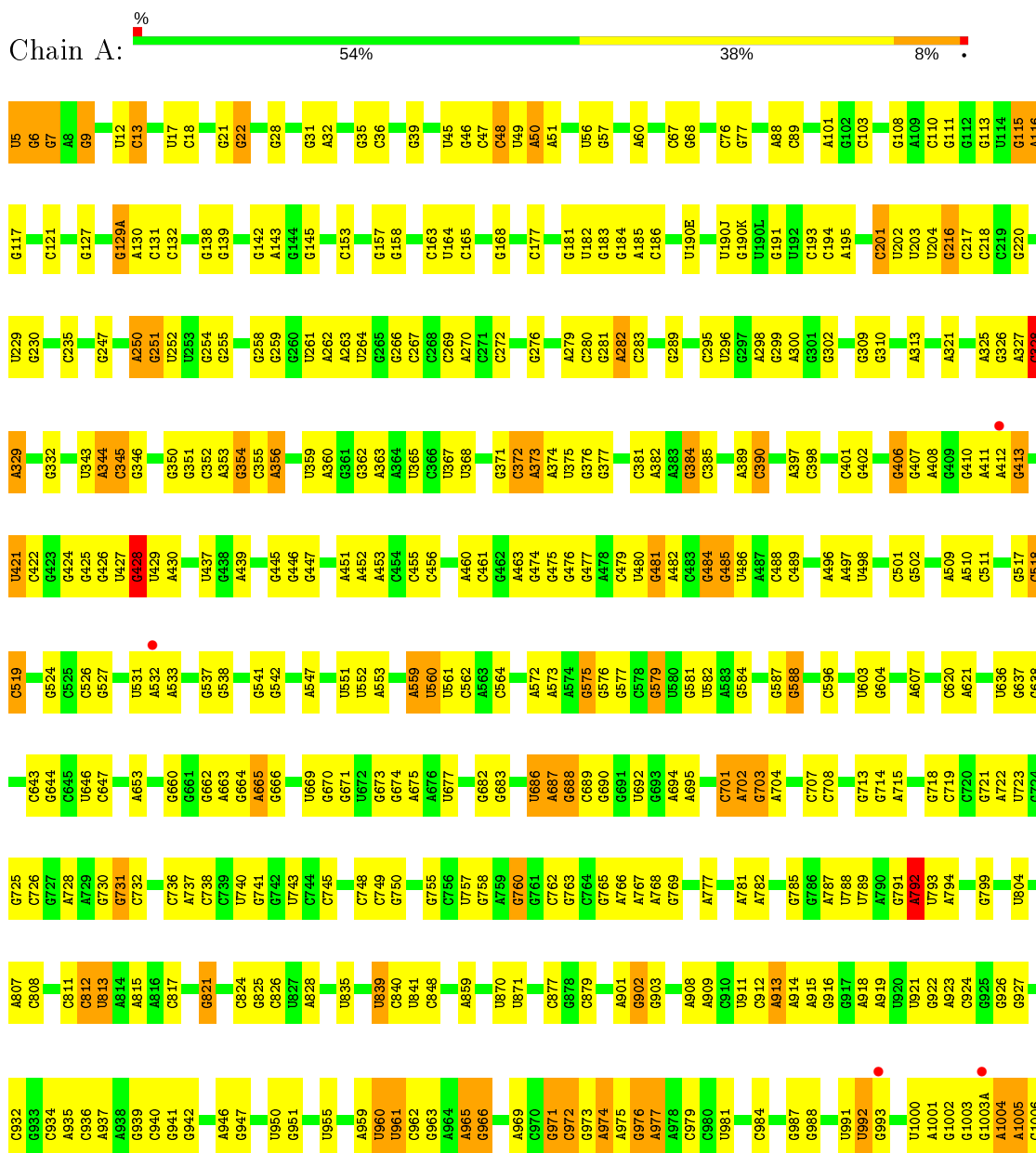
- Molecule 27 is water.

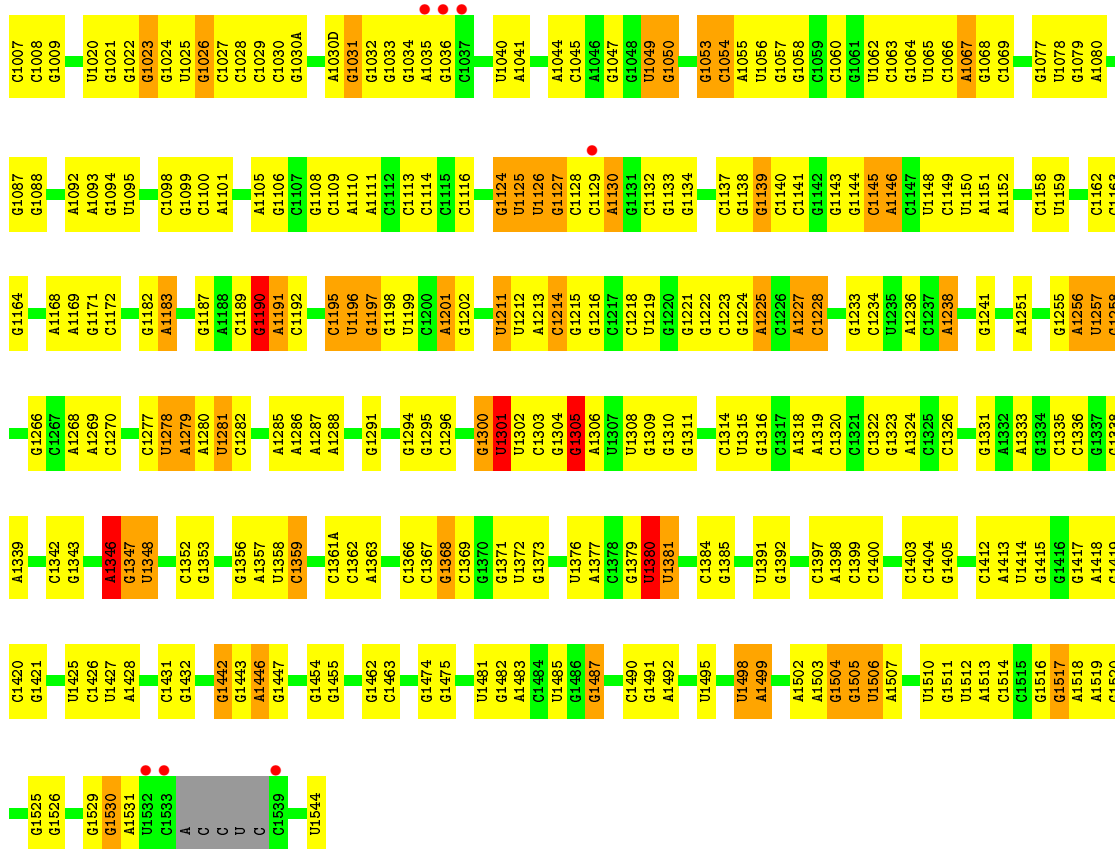
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	A	233	Total 233	O 233	0	0
27	C	1	Total 1	O 1	0	0
27	D	2	Total 2	O 2	0	0
27	E	6	Total 6	O 6	0	0
27	L	1	Total 1	O 1	0	0
27	N	1	Total 1	O 1	0	0
27	T	1	Total 1	O 1	0	0

### 3 Residue-property plots

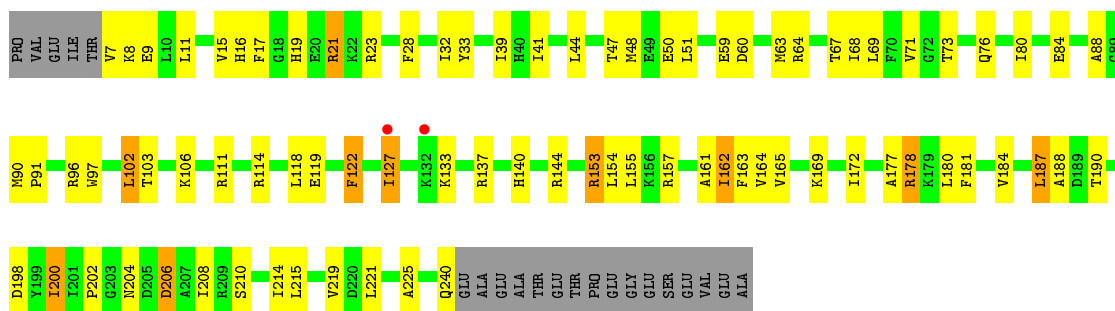
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: 16S Ribosomal RNA rRNA

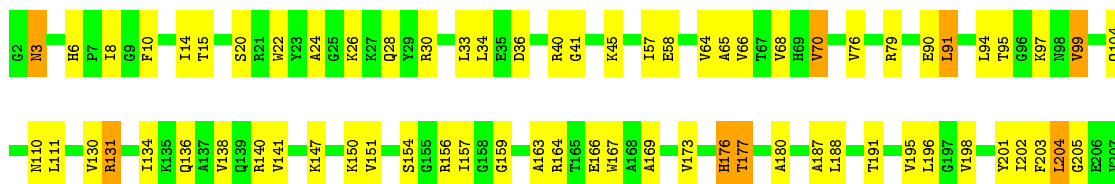




• Molecule 2: 30S ribosomal protein S2

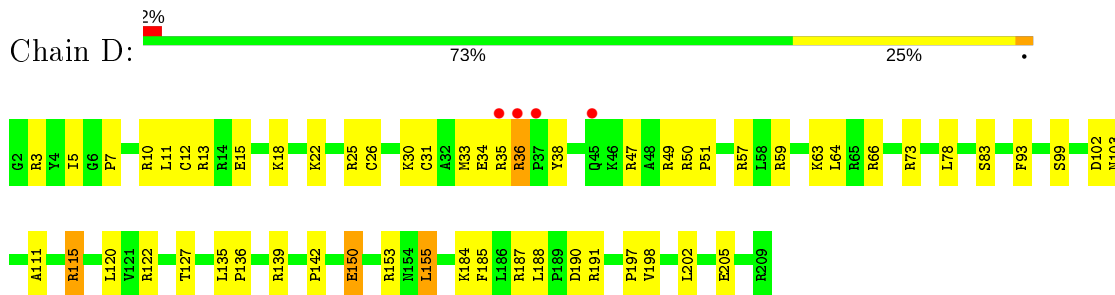


• Molecule 3: 30S ribosomal protein S3

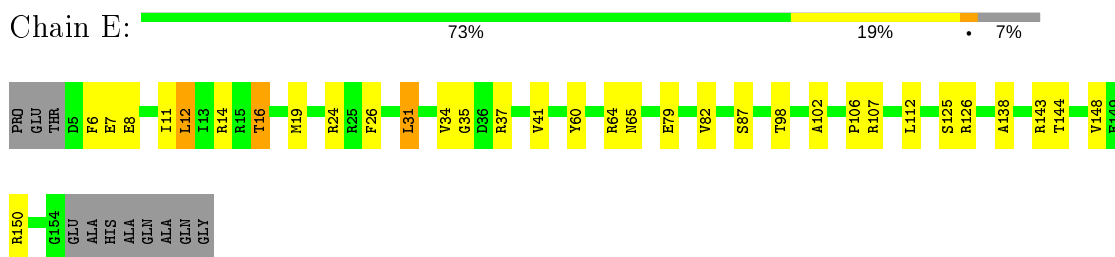


IIE  
GLY  
GLY  
GLN  
LYS  
PRO  
LYS  
ALA  
ARG  
PRO  
GLU  
LEU  
PRO  
LYS  
ALA  
GLU  
GLU  
ARG  
PRO  
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ALA  
VAL  
ARG  
VAL  
LYS  
LYS  
GLU  
GLU

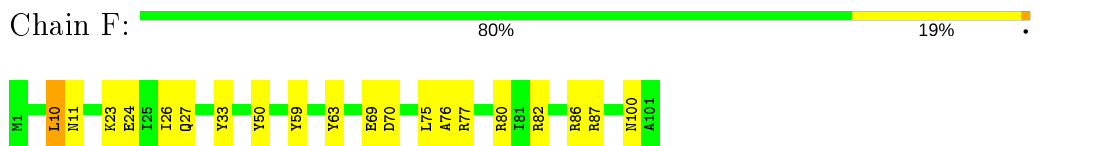
• Molecule 4: 30S ribosomal protein S4



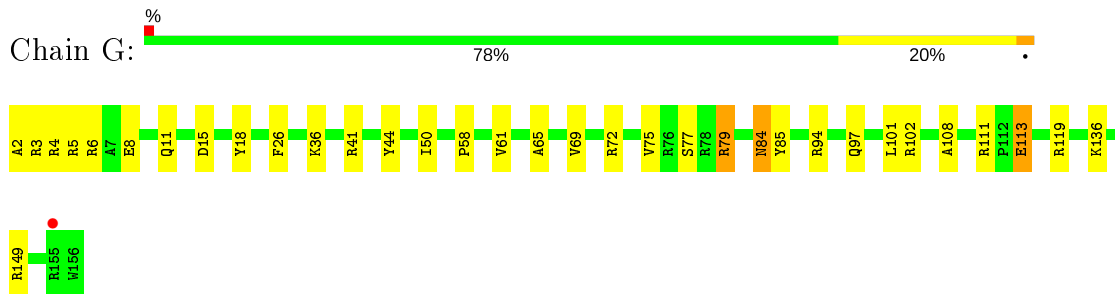
• Molecule 5: 30S ribosomal protein S5



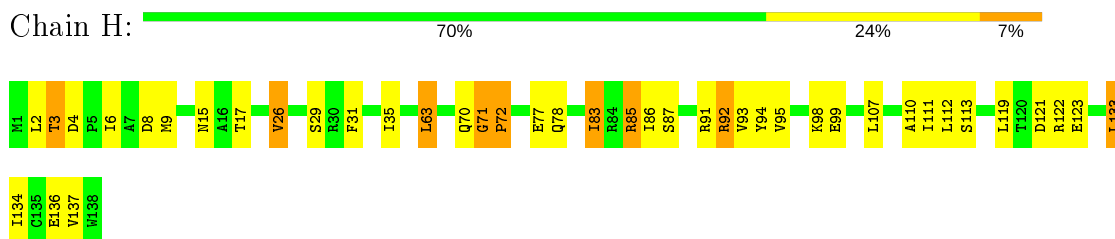
• Molecule 6: 30S ribosomal protein S6



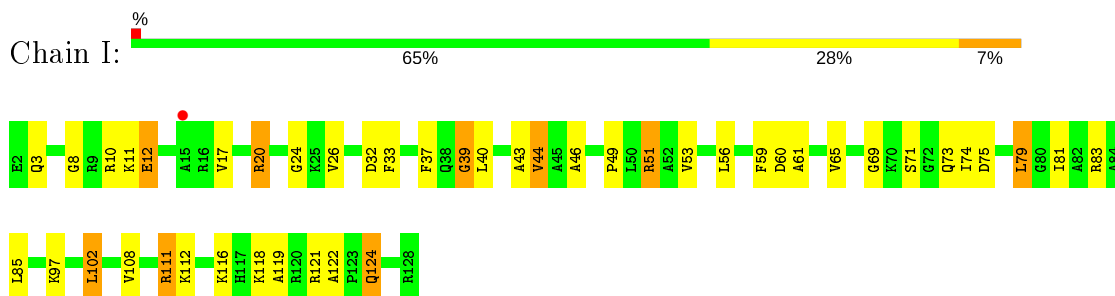
• Molecule 7: 30S ribosomal protein S7



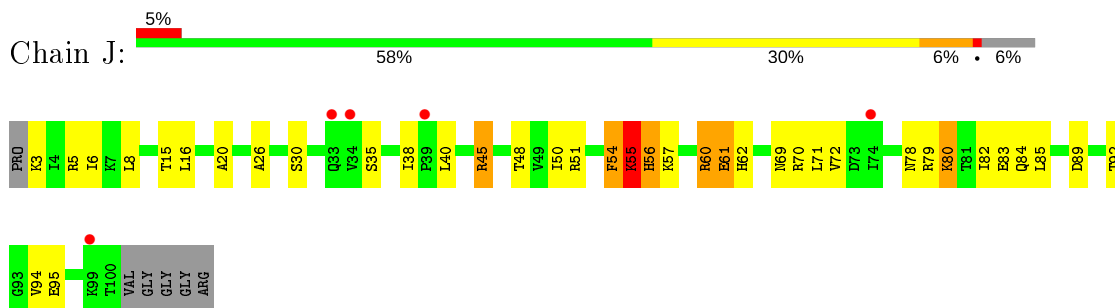
• Molecule 8: 30S ribosomal protein S8



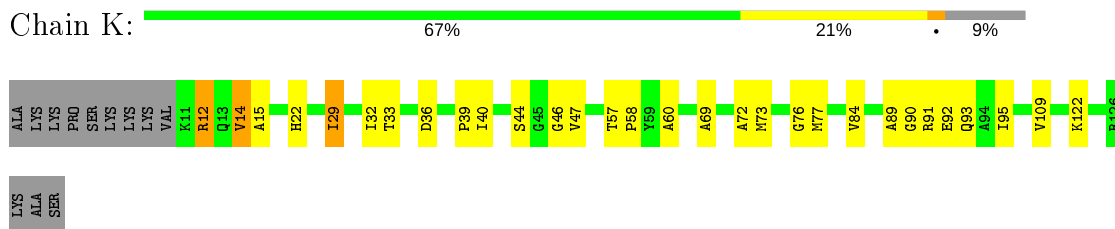
- Molecule 9: 30S ribosomal protein S9



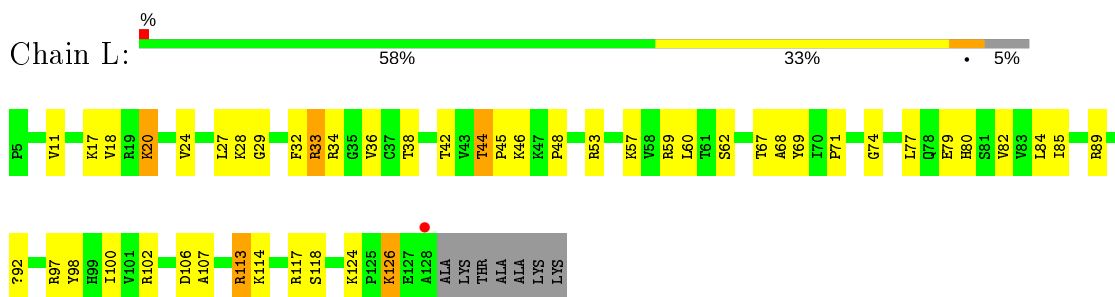
- Molecule 10: 30S ribosomal protein S10



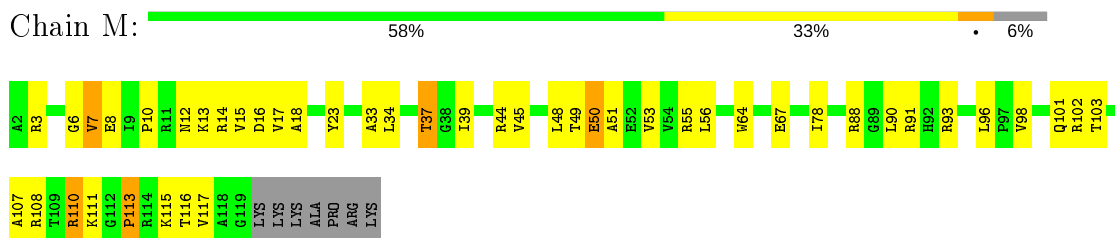
- Molecule 11: 30S ribosomal protein S11



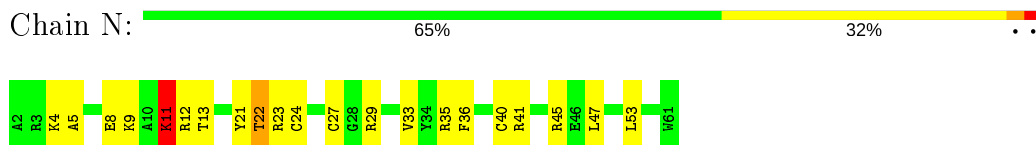
- Molecule 12: 30S ribosomal protein S12



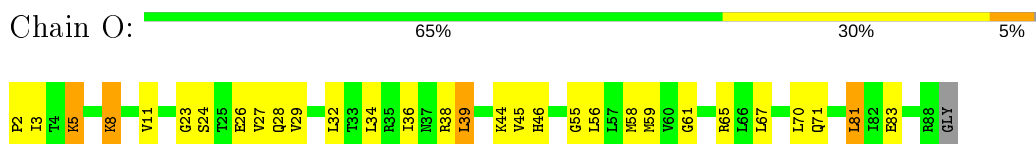
- Molecule 13: 30S ribosomal protein S13



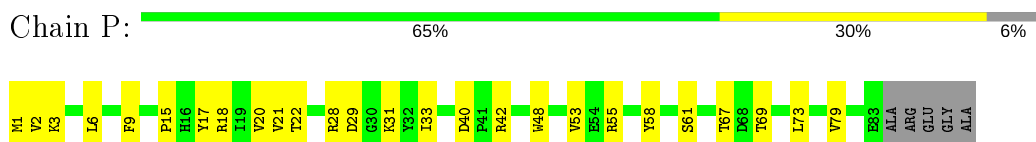
- Molecule 14: 30S ribosomal protein S14 type Z



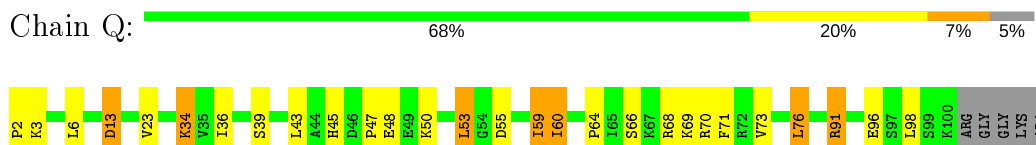
- Molecule 15: 30S ribosomal protein S15



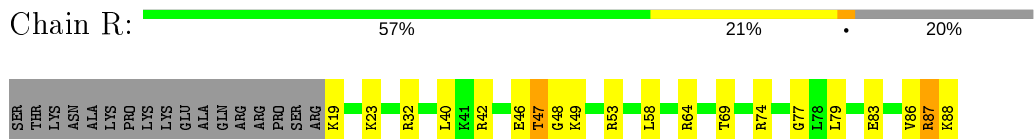
- Molecule 16: 30S ribosomal protein S16



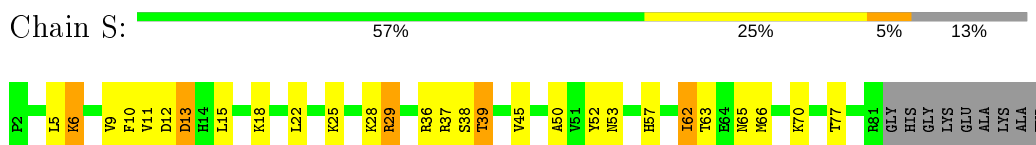
- Molecule 17: 30S ribosomal protein S17



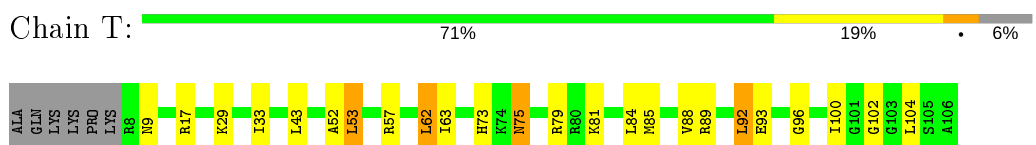
- Molecule 18: 30S ribosomal protein S18



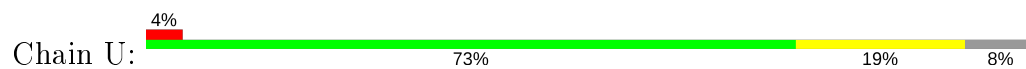
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



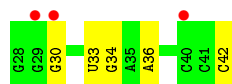
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: RNA (5'-R(\*UP\*UP\*UP\*UP\*UP\*U)-3')



- Molecule 23: RNA (5'-R(\*GP\*GP\*GP\*AP\*UP\*UP\*GP\*AP\*AP\*AP\*AP\*UP\*CP\*CP\*C)-3')





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	402.10Å 402.10Å 175.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.19 – 3.50 39.19 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (39.19-3.50) 98.2 (39.19-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.01 (at 3.48Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, $R_{free}$	0.247 , 0.277 0.247 , 0.277	Depositor DCC
$R_{free}$ test set	1142 reflections (0.65%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	85.3	Xtrriage
Anisotropy	0.043	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 91.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.35$ , $\langle L^2 \rangle = 0.18$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	52613	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.23% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MA6, G7M, 0TD, MG, 2MG, 5MC, UR3, 4OC, M2G, EUS, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.28	0/36040	0.81	18/56243 (0.0%)
2	B	0.27	0/1935	0.44	0/2609
3	C	0.26	0/1636	0.46	0/2205
4	D	0.26	0/1733	0.41	0/2318
5	E	0.28	0/1162	0.48	0/1564
6	F	0.26	0/856	0.43	0/1154
7	G	0.26	0/1276	0.39	0/1709
8	H	0.29	0/1136	0.47	0/1527
9	I	0.28	0/1029	0.49	1/1379 (0.1%)
10	J	0.25	0/805	0.51	0/1082
11	K	0.26	0/879	0.45	0/1187
12	L	0.27	0/977	0.50	0/1306
13	M	0.25	0/947	0.48	0/1270
14	N	0.28	0/501	0.45	0/664
15	O	0.25	0/740	0.41	0/987
16	P	0.26	0/716	0.48	0/963
17	Q	0.37	1/836 (0.1%)	0.47	0/1117
18	R	0.28	0/579	0.44	0/768
19	S	0.26	0/661	0.47	0/890
20	T	0.25	0/765	0.42	0/1007
21	U	0.25	0/212	0.41	0/277
22	Y	0.26	0/128	0.96	0/196
23	W	0.30	0/357	0.84	0/555
All	All	0.28	1/55906 (0.0%)	0.72	19/82977 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
8	H	0	1
10	J	0	2
13	M	0	2
14	N	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	96	GLU	CD-OE2	6.91	1.33	1.25

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	839	U	C2-N1-C1'	6.93	126.02	117.70
1	A	328	C	C2-N1-C1'	6.37	125.80	118.80
1	A	328	C	N1-C2-O2	6.04	122.52	118.90
1	A	1301	U	P-O3'-C3'	5.96	126.86	119.70
1	A	839	U	N1-C2-O2	5.89	126.92	122.80
1	A	1305	G	P-O3'-C3'	5.71	126.56	119.70
1	A	839	U	N3-C2-O2	-5.52	118.33	122.20
1	A	1190	G	P-O3'-C3'	5.48	126.28	119.70
1	A	913	A	P-O3'-C3'	5.32	126.08	119.70
9	I	39	GLY	N-CA-C	-5.31	99.82	113.10
1	A	1201	A	P-O3'-C3'	5.22	125.96	119.70
1	A	1346	A	P-O3'-C3'	5.18	125.91	119.70
1	A	792	A	P-O3'-C3'	5.17	125.90	119.70
1	A	1158	C	N1-C2-O2	5.14	121.98	118.90
1	A	328	C	P-O3'-C3'	5.11	125.83	119.70
1	A	428	G	P-O3'-C3'	5.05	125.76	119.70
1	A	1498	UR3	P-O3'-C3'	5.03	125.73	119.70
1	A	1067	A	P-O3'-C3'	5.02	125.72	119.70
1	A	1380	U	P-O3'-C3'	5.02	125.72	119.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	166	GLU	Peptide
8	H	71	GLY	Peptide
10	J	54	PHE	Peptide

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Mol	Chain	Res	Type	Group
10	J	55	LYS	Peptide
13	M	113	PRO	Peptide
13	M	6	GLY	Peptide
14	N	11	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	A	32507	0	16431	449	0
2	B	1900	0	1951	49	0
3	C	1612	0	1676	46	0
4	D	1703	0	1763	37	0
5	E	1146	0	1207	20	0
6	F	843	0	857	13	0
7	G	1257	0	1296	20	0
8	H	1116	0	1177	29	0
9	I	1010	0	1037	33	0
10	J	792	0	835	28	0
11	K	864	0	881	17	0
12	L	972	0	1057	33	0
13	M	937	0	995	28	0
14	N	492	0	529	19	0
15	O	729	0	768	20	0
16	P	700	0	720	13	0
17	Q	823	0	891	21	0
18	R	574	0	644	18	0
19	S	647	0	673	20	0
20	T	763	0	861	15	0
21	U	208	0	221	3	0
22	Y	117	0	62	1	0
23	W	319	0	164	1	0
24	A	274	0	0	0	0
24	B	3	0	0	0	0
24	C	2	0	0	0	0
24	D	4	0	0	0	0
24	E	2	0	0	0	0
24	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	H	2	0	0	0	0
24	I	1	0	0	0	0
24	J	1	0	0	0	0
24	L	3	0	0	0	0
24	P	3	0	0	0	0
24	Q	3	0	0	0	0
24	S	1	0	0	0	0
25	A	35	0	0	2	0
26	D	1	0	0	0	0
26	N	1	0	0	0	0
27	A	233	0	0	5	0
27	C	1	0	0	0	0
27	D	2	0	0	0	0
27	E	6	0	0	0	0
27	L	1	0	0	0	0
27	N	1	0	0	0	0
27	T	1	0	0	0	0
All	All	52613	0	36696	813	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 9.

All (813) 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)
1:A:664:G:H22	1:A:741:G:H1	1.11	0.96
20:T:100:ILE:HG22	20:T:102:GLY:H	1.39	0.87
1:A:768:A:N6	27:A:1902:HOH:O	2.08	0.85
1:A:532:A:N6	3:C:159:GLY:O	2.11	0.83
13:M:3:ARG:HE	13:M:7:VAL:HG12	1.45	0.81
1:A:298:A:N6	27:A:1903:HOH:O	2.14	0.80
1:A:452:A:N6	1:A:480:U:O2	2.15	0.79
1:A:537:G:OP1	12:L:113:ARG:NH2	2.16	0.78
1:A:407:G:OP1	4:D:115:ARG:NH1	2.17	0.77
1:A:1403:C:O2	1:A:1499:A:N6	2.16	0.77
1:A:542:G:OP1	4:D:10:ARG:NH2	2.17	0.76
1:A:1128:C:O2'	1:A:1130:A:N7	2.18	0.76
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.17	0.76
19:S:12:ASP:H	19:S:38:SER:HB3	1.52	0.75
14:N:8:GLU:HB2	14:N:11:LYS:HE3	1.69	0.75
2:B:114:ARG:HH11	2:B:118:LEU:HD21	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1022:G:N2	1:A:1023:G:N7	2.34	0.74
4:D:15:GLU:OE1	4:D:59:ARG:NH2	2.21	0.73
1:A:1373:G:H5''	7:G:36:LYS:HE3	1.71	0.73
1:A:145:G:H1	1:A:177:C:H42	1.36	0.73
1:A:955:U:H1'	1:A:1227:A:H61	1.53	0.73
1:A:1100:C:OP1	2:B:96:ARG:NH1	2.23	0.72
2:B:162:ILE:HD12	2:B:177:ALA:HB2	1.71	0.71
12:L:33:ARG:HD3	12:L:62:SER:HB3	1.72	0.71
19:S:36:ARG:NH1	19:S:52:TYR:O	2.23	0.71
1:A:677:U:H3	1:A:713:G:H22	1.38	0.70
1:A:1057:G:H5''	3:C:154:SER:HB2	1.74	0.70
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.74	0.70
1:A:1125:U:OP2	1:A:1145:C:N4	2.26	0.69
1:A:501:C:H2'	1:A:502:G:C8	2.28	0.69
1:A:411:A:OP2	4:D:25:ARG:NH2	2.27	0.68
15:O:55:GLY:HA2	15:O:58:MET:HE2	1.75	0.67
2:B:119:GLU:OE1	2:B:153:ARG:NH2	2.27	0.67
1:A:951:G:OP2	13:M:102:ARG:NH2	2.27	0.67
1:A:372:C:H4'	1:A:373:A:O5'	1.93	0.67
3:C:70:VAL:HG21	3:C:76:VAL:HG21	1.75	0.67
1:A:1005:A:N3	1:A:1026:G:N2	2.43	0.67
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.77	0.67
1:A:1454:G:H2'	1:A:1455:G:H8	1.60	0.66
20:T:75:ASN:N	20:T:75:ASN:OD1	2.25	0.66
2:B:68:ILE:HG12	2:B:161:ALA:HB3	1.78	0.66
1:A:538:G:H5''	12:L:114:LYS:HB2	1.77	0.65
1:A:280:C:N3	17:Q:39:SER:OG	2.29	0.65
4:D:64:LEU:HB2	4:D:198:VAL:HG11	1.78	0.65
1:A:811:C:O2'	1:A:901:A:N1	2.29	0.65
1:A:362:G:N2	1:A:365:U:OP2	2.30	0.64
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.29	0.64
1:A:410:G:OP1	4:D:30:LYS:NZ	2.27	0.64
1:A:190(J):U:H2'	1:A:190(K):G:C8	2.32	0.64
16:P:21:VAL:HG12	16:P:33:ILE:HD12	1.80	0.64
12:L:74:GLY:O	12:L:102:ARG:NH1	2.27	0.64
1:A:390:C:O3'	16:P:28:ARG:NH2	2.31	0.64
1:A:976:G:OP2	1:A:1358:U:O2'	2.16	0.64
1:A:1544:U:H4'	22:Y:1:U:H5'	1.79	0.64
1:A:1028:C:H42	1:A:1033:G:H1	1.43	0.64
1:A:1125:U:H3	10:J:5:ARG:HH21	1.44	0.64
10:J:55:LYS:HD2	10:J:56:HIS:H	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:84:ASN:N	7:G:84:ASN:OD1	2.30	0.63
1:A:603:U:H2'	1:A:604:G:C8	2.34	0.63
1:A:1031:G:H2'	1:A:1032:G:H8	1.63	0.63
9:I:112:LYS:HA	9:I:119:ALA:HB2	1.81	0.63
1:A:1502:A:H2	1:A:1505:G:H1	1.46	0.63
1:A:1443:G:H5''	1:A:1446:A:H5'	1.79	0.62
1:A:1413:A:H2	1:A:1487:G:H22	1.47	0.62
1:A:452:A:O2'	1:A:453:A:O4'	2.16	0.62
12:L:38:THR:HB	12:L:57:LYS:HB2	1.81	0.62
18:R:32:ARG:HA	18:R:69:THR:HG21	1.81	0.62
1:A:1196:U:OP1	1:A:1197:G:H5'	2.00	0.62
1:A:1228:C:H4'	13:M:116:THR:HA	1.81	0.62
1:A:603:U:H2'	1:A:604:G:H8	1.64	0.62
1:A:1281:U:H5'	1:A:1282:C:H5	1.65	0.62
1:A:737:A:H2'	1:A:738:C:C6	2.35	0.62
1:A:1020:U:H2'	1:A:1021:G:H8	1.64	0.61
2:B:102:LEU:HD21	2:B:162:ILE:HD11	1.82	0.61
3:C:14:ILE:HG22	3:C:15:THR:HG23	1.81	0.61
11:K:90:GLY:HA2	11:K:93:GLN:HB2	1.81	0.61
10:J:8:LEU:HB2	10:J:70:ARG:HB2	1.82	0.61
1:A:413:G:H2'	1:A:428:G:N2	2.15	0.61
1:A:718:G:O6	18:R:74:ARG:NH1	2.34	0.61
4:D:187:ARG:NH1	4:D:188:LEU:H	1.97	0.61
1:A:31:G:N2	1:A:48:C:OP1	2.32	0.61
18:R:48:GLY:O	18:R:74:ARG:NH2	2.34	0.61
20:T:92:LEU:O	20:T:96:GLY:HA2	2.01	0.60
2:B:63:MET:HB3	2:B:225:ALA:HB1	1.82	0.60
1:A:401:C:H2'	1:A:402:G:C8	2.36	0.60
1:A:671:G:H5'	6:F:77:ARG:HH21	1.66	0.60
1:A:1195:C:H3'	1:A:1196:U:H5''	1.82	0.60
3:C:57:ILE:HG12	3:C:66:VAL:HG22	1.83	0.60
1:A:1031:G:H2'	1:A:1032:G:C8	2.37	0.60
1:A:1291:G:OP1	7:G:41:ARG:NH2	2.32	0.60
1:A:1278:U:H5'	1:A:1279:A:O4'	2.02	0.59
1:A:1213:A:N6	1:A:1215:G:N3	2.50	0.59
13:M:107:ALA:HB3	13:M:111:LYS:HE3	1.83	0.59
1:A:1143:G:H2'	1:A:1144:G:C8	2.38	0.59
1:A:235:C:N4	27:A:1906:HOH:O	2.34	0.59
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.83	0.59
8:H:111:ILE:HG22	8:H:134:ILE:HD12	1.85	0.59
15:O:36:ILE:HD13	15:O:59:MET:HE3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:11:VAL:HG21	17:Q:34:LYS:HG2	1.84	0.59
1:A:1214:C:H3'	1:A:1215:G:H8	1.66	0.59
1:A:1392:G:H21	1:A:1502:A:H8	1.50	0.59
1:A:1134:G:H1	1:A:1140:C:H42	1.50	0.59
1:A:835:U:OP1	18:R:64:ARG:NH2	2.30	0.59
1:A:1004:A:H5''	1:A:1025:U:C4	2.37	0.59
1:A:1139:G:H4'	1:A:1140:C:H5'	1.84	0.59
1:A:1126:U:O4	1:A:1127:G:N2	2.36	0.59
1:A:250:A:H4'	1:A:251:G:O5'	2.02	0.58
1:A:1002:G:H2'	1:A:1003:G:C8	2.39	0.58
1:A:1419:G:N2	1:A:1481:U:O2	2.34	0.58
1:A:1510:U:H2'	1:A:1511:G:C8	2.37	0.58
1:A:427:U:OP1	4:D:13:ARG:NH2	2.36	0.58
1:A:110:C:H2'	1:A:111:G:O4'	2.04	0.58
1:A:923:A:O2'	1:A:1399:C:OP2	2.18	0.58
9:I:97:LYS:HA	9:I:102:LEU:HD11	1.85	0.58
1:A:1391:U:H2'	1:A:1392:G:C8	2.38	0.58
1:A:877:C:O2	8:H:3:THR:HG21	2.04	0.58
15:O:39:LEU:HB3	15:O:56:LEU:HD12	1.85	0.58
18:R:53:ARG:NH1	18:R:58:LEU:O	2.35	0.58
8:H:95:VAL:HB	8:H:99:GLU:HB2	1.86	0.58
1:A:1314:C:C5	19:S:6:LYS:HD3	2.39	0.58
1:A:750:G:N3	15:O:23:GLY:HA3	2.19	0.58
3:C:156:ARG:H	3:C:163:ALA:HA	1.68	0.57
1:A:877:C:HO2'	8:H:3:THR:HG1	1.52	0.57
1:A:1027:C:H42	1:A:1034:G:H1	1.51	0.57
1:A:1064:G:N2	1:A:1190:G:HO2'	2.02	0.57
1:A:299:G:H2'	1:A:300:A:C8	2.39	0.57
14:N:47:LEU:HB3	14:N:53:LEU:HD21	1.86	0.57
1:A:1308:U:OP1	13:M:98:VAL:N	2.37	0.57
1:A:992:U:H3	1:A:1044:A:H62	1.51	0.57
2:B:48:MET:HA	2:B:51:LEU:HB2	1.85	0.57
2:B:97:TRP:HZ2	2:B:102:LEU:HD22	1.70	0.57
8:H:86:ILE:HD11	8:H:136:GLU:HG3	1.86	0.57
9:I:43:ALA:HA	9:I:74:ILE:HD13	1.84	0.57
1:A:103:C:OP1	20:T:17:ARG:NH1	2.38	0.57
1:A:979:C:OP1	1:A:1223:C:N4	2.37	0.57
1:A:932:C:H5''	7:G:3:ARG:HD2	1.86	0.57
2:B:71:VAL:HB	2:B:164:VAL:HG12	1.86	0.57
1:A:6:G:H1	5:E:98:THR:HG1	1.53	0.57
3:C:150:LYS:HB3	3:C:201:TYR:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:U:OP2	1:A:422:C:N4	2.38	0.57
1:A:877:C:O2'	8:H:3:THR:OG1	2.22	0.57
19:S:45:VAL:HA	19:S:62:ILE:HG13	1.86	0.57
5:E:144:THR:O	5:E:148:VAL:HG23	2.05	0.57
8:H:110:ALA:HB3	8:H:121:ASP:HB3	1.86	0.57
7:G:15:ASP:OD1	7:G:44:TYR:OH	2.23	0.56
1:A:1379:G:O6	7:G:2:ALA:N	2.38	0.56
12:L:53:ARG:NH1	12:L:92:0TD:OD2	2.28	0.56
1:A:1047:G:H5''	14:N:4:LYS:HD2	1.86	0.56
7:G:113:GLU:HG3	7:G:119:ARG:HA	1.87	0.56
2:B:178:ARG:HB3	8:H:72:PRO:HG3	1.87	0.56
2:B:32:ILE:HD11	2:B:190:THR:HG23	1.88	0.56
11:K:84:VAL:HG11	11:K:91:ARG:HD3	1.87	0.56
15:O:26:GLU:HA	15:O:81:LEU:HD11	1.87	0.56
8:H:112:LEU:HD23	8:H:133:LEU:HA	1.87	0.56
11:K:12:ARG:HD2	11:K:14:VAL:HG13	1.88	0.56
1:A:1030(A):G:N2	1:A:1030(D):A:OP2	2.39	0.56
1:A:9:G:H5''	5:E:126:ARG:HD3	1.87	0.56
1:A:1266:G:N2	1:A:1269:A:OP2	2.34	0.56
2:B:80:ILE:HD11	2:B:208:ILE:HG23	1.88	0.56
9:I:8:GLY:H	9:I:83:ARG:HH11	1.54	0.56
1:A:1009:G:H1	1:A:1020:U:H3	1.54	0.56
1:A:1111:A:N1	3:C:177:THR:HB	2.20	0.56
14:N:24:CYS:SG	14:N:40:CYS:N	2.77	0.56
1:A:660:G:H1	1:A:745:C:H42	1.54	0.55
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.89	0.55
1:A:216:G:H2'	1:A:217:C:C6	2.41	0.55
1:A:757:U:O2'	1:A:879:C:O2	2.24	0.55
5:E:143:ARG:NE	8:H:77:GLU:OE2	2.37	0.55
13:M:49:THR:HG22	13:M:51:ALA:H	1.70	0.55
1:A:60:A:N6	1:A:110:C:N3	2.51	0.55
4:D:12:CYS:HB3	4:D:33:MET:HG2	1.88	0.55
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.46	0.55
1:A:421:U:H5'	1:A:422:C:C5	2.42	0.55
1:A:475:G:H2'	1:A:476:G:H8	1.72	0.55
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.47	0.55
1:A:673:G:O3'	6:F:87:ARG:NH2	2.40	0.55
2:B:21:ARG:HA	2:B:39:ILE:HA	1.87	0.55
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.89	0.55
20:T:29:LYS:O	20:T:33:ILE:HG12	2.07	0.55
1:A:636:U:H2'	1:A:637:G:C8	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:U:H2'	1:A:552:U:C6	2.42	0.55
1:A:686:U:HO2'	1:A:687:A:H8	1.53	0.55
1:A:579:G:H5'	1:A:728:A:H1'	1.89	0.55
1:A:946:A:H2'	1:A:947:G:C8	2.41	0.55
1:A:411:A:N3	1:A:413:G:O2'	2.33	0.54
1:A:1356:G:H2'	1:A:1357:A:C8	2.41	0.54
1:A:825:G:O2'	8:H:8:ASP:OD1	2.17	0.54
13:M:96:LEU:O	13:M:110:ARG:NH1	2.40	0.54
1:A:1040:U:H2'	1:A:1041:A:C8	2.43	0.54
1:A:908:A:H2'	1:A:909:A:C8	2.43	0.54
1:A:157:G:H2'	1:A:158:G:H8	1.71	0.54
1:A:1367:C:H5'	10:J:60:ARG:HE	1.71	0.54
11:K:109:VAL:HG22	18:R:86:VAL:HG22	1.90	0.54
1:A:1020:U:H2'	1:A:1021:G:C8	2.42	0.54
1:A:113:G:H1'	1:A:354:G:H5'	1.90	0.54
1:A:1291:G:H4'	9:I:39:GLY:HA3	1.88	0.54
15:O:45:VAL:HG23	15:O:46:HIS:HD2	1.72	0.54
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.90	0.53
14:N:22:THR:HB	14:N:33:VAL:HB	1.90	0.53
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.41	0.53
1:A:1412:C:H2'	1:A:1413:A:C8	2.43	0.53
15:O:3:ILE:HD11	15:O:38:ARG:HG3	1.89	0.53
1:A:1505:G:O2'	1:A:1506:U:OP2	2.19	0.53
1:A:527:G7M:H8	1:A:527:G7M:H5''	1.91	0.53
1:A:1124:G:H5'	10:J:35:SER:O	2.09	0.53
10:J:50:ILE:H	10:J:50:ILE:HD12	1.73	0.53
16:P:28:ARG:NH1	16:P:29:ASP:OD1	2.41	0.53
1:A:620:C:H2'	1:A:621:A:O4'	2.08	0.53
10:J:26:ALA:O	10:J:84:GLN:NE2	2.41	0.53
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.73	0.53
1:A:115:G:H4'	1:A:116:A:O5'	2.09	0.53
8:H:31:PHE:O	8:H:35:ILE:HG12	2.09	0.53
1:A:1125:U:H3	10:J:5:ARG:NH2	2.07	0.53
1:A:1145:C:O2'	1:A:1146:A:O5'	2.27	0.53
1:A:1222:G:OP2	1:A:1322:C:N4	2.34	0.53
1:A:666:G:H5'	1:A:726:C:H1'	1.90	0.53
4:D:102:ASP:HB3	4:D:136:PRO:HB3	1.90	0.53
9:I:65:VAL:HG11	9:I:73:GLN:HB3	1.91	0.52
1:A:1077:G:N2	1:A:1080:A:OP2	2.40	0.52
1:A:1318:A:O2'	19:S:37:ARG:HB3	2.09	0.52
1:A:1405:G:N7	25:A:1814:EUS:N33	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:G:O2'	20:T:102:GLY:O	2.15	0.52
1:A:1420:C:H2'	1:A:1421:G:H8	1.75	0.52
1:A:437:U:H5'	4:D:155:LEU:HD21	1.92	0.52
1:A:643:C:H2'	1:A:644:G:H8	1.75	0.52
1:A:924:C:O2'	1:A:1502:A:N6	2.42	0.52
21:U:12:LYS:HG2	21:U:22:ARG:HB3	1.92	0.52
4:D:190:ASP:OD1	4:D:191:ARG:N	2.42	0.52
1:A:1474:G:H2'	1:A:1475:G:C8	2.45	0.52
1:A:1525:G:H2'	1:A:1526:G:H8	1.75	0.52
1:A:501:C:H2'	1:A:502:G:H8	1.74	0.52
1:A:769:G:H4'	1:A:1513:A:H4'	1.92	0.52
1:A:1300:G:H4'	1:A:1301:U:O5'	2.10	0.52
1:A:455:C:H42	1:A:477:G:H1	1.57	0.52
1:A:359:U:H2'	1:A:360:A:C8	2.46	0.51
1:A:45:U:H2'	1:A:46:G:C8	2.45	0.51
2:B:184:VAL:N	2:B:198:ASP:OD2	2.35	0.51
3:C:187:ALA:HB3	3:C:198:VAL:HB	1.92	0.51
1:A:587:G:O2'	1:A:588:G:OP2	2.24	0.51
1:A:1218:C:H2'	1:A:1219:U:C6	2.46	0.51
1:A:229:U:H2'	1:A:230:G:H8	1.76	0.51
20:T:43:LEU:HB2	20:T:52:ALA:HB2	1.92	0.51
10:J:79:ARG:O	10:J:83:GLU:N	2.42	0.51
1:A:1049:U:H4'	1:A:1050:G:O5'	2.11	0.51
2:B:181:PHE:CD2	8:H:70:GLN:HB3	2.46	0.51
10:J:50:ILE:HA	10:J:60:ARG:HB3	1.93	0.51
1:A:1513:A:H2'	1:A:1514:C:C6	2.46	0.51
1:A:456:C:H42	1:A:476:G:H1	1.57	0.51
5:E:148:VAL:HG21	8:H:107:LEU:HD13	1.92	0.51
13:M:90:LEU:HD23	13:M:93:ARG:HD2	1.92	0.51
16:P:6:LEU:HD23	16:P:17:TYR:CG	2.46	0.51
1:A:190(J):U:H2'	1:A:190(K):G:H8	1.72	0.51
1:A:269:C:H2'	1:A:270:A:C8	2.46	0.51
1:A:384:G:H2'	1:A:385:C:C6	2.46	0.51
2:B:97:TRP:CZ2	2:B:102:LEU:HD22	2.46	0.51
3:C:33:LEU:HD21	14:N:53:LEU:HD22	1.92	0.51
7:G:113:GLU:HB2	7:G:119:ARG:HG2	1.93	0.51
1:A:1027:C:N4	1:A:1034:G:H1	2.09	0.50
1:A:1419:G:H1	1:A:1481:U:H3	1.59	0.50
1:A:962:C:H2'	1:A:963:G:C8	2.46	0.50
2:B:76:GLN:NE2	2:B:206:ASP:OD2	2.38	0.50
14:N:12:ARG:HG3	14:N:13:THR:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1490:C:H2'	1:A:1491:G:H8	1.76	0.50
1:A:1504:G:OP1	1:A:1507:A:H4'	2.12	0.50
1:A:662:G:H1	1:A:743:U:H3	1.58	0.50
2:B:59:GLU:HB2	2:B:221:LEU:HD11	1.92	0.50
5:E:60:TYR:OH	5:E:64:ARG:NH2	2.44	0.50
5:E:65:ASN:ND2	5:E:65:ASN:O	2.44	0.50
1:A:1358:U:H5''	14:N:35:ARG:HG3	1.94	0.50
1:A:1454:G:H2'	1:A:1455:G:C8	2.42	0.50
1:A:974:A:H8	1:A:974:A:OP1	1.95	0.50
5:E:82:VAL:HG21	5:E:138:ALA:HA	1.94	0.50
13:M:50:GLU:HA	13:M:53:VAL:HB	1.94	0.50
1:A:1108:G:H5'	3:C:176:HIS:CD2	2.47	0.50
1:A:766:A:H2'	1:A:767:A:O4'	2.11	0.50
8:H:9:MET:HG3	8:H:26:VAL:HG21	1.93	0.50
1:A:1116:C:O2'	9:I:108:VAL:HG21	2.11	0.50
18:R:46:GLU:CD	18:R:46:GLU:H	2.15	0.50
18:R:47:THR:HA	18:R:83:GLU:HB2	1.94	0.50
1:A:1127:G:H1	1:A:1145:C:H42	1.58	0.50
1:A:384:G:H2'	1:A:385:C:H6	1.77	0.50
5:E:102:ALA:O	5:E:107:ARG:NH1	2.43	0.50
4:D:63:LYS:NZ	4:D:197:PRO:O	2.45	0.50
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.44	0.50
4:D:26:CYS:HA	4:D:31:CYS:HB2	1.94	0.50
1:A:987:G:H2'	1:A:988:G:H8	1.77	0.49
12:L:117:ARG:NH2	12:L:124:LYS:HD3	2.27	0.49
12:L:60:LEU:HD11	12:L:85:ILE:HD12	1.93	0.49
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.94	0.49
1:A:707:C:H2'	1:A:708:C:C6	2.47	0.49
1:A:261:U:OP2	20:T:79:ARG:NH2	2.45	0.49
1:A:153:C:H42	1:A:168:G:H1	1.60	0.49
1:A:406:G:H5'	4:D:5:ILE:HG21	1.95	0.49
4:D:102:ASP:OD1	4:D:103:ASN:N	2.45	0.49
1:A:7:G:H5'	1:A:298:A:O4'	2.11	0.49
1:A:662:G:H2'	1:A:663:A:C8	2.47	0.49
3:C:150:LYS:HB2	3:C:173:VAL:HG21	1.94	0.49
1:A:1164:G:H1	1:A:1172:C:H42	1.59	0.49
1:A:1442:G:N1	1:A:1446:A:N7	2.61	0.49
1:A:475:G:H2'	1:A:476:G:C8	2.48	0.49
1:A:674:G:H2'	1:A:675:A:H8	1.78	0.49
10:J:15:THR:HG22	10:J:94:VAL:HB	1.94	0.49
17:Q:6:LEU:HB3	17:Q:23:VAL:HG11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:62:ILE:HD12	19:S:66:MET:HG3	1.93	0.49
1:A:1008:C:N4	1:A:1021:G:H1	2.10	0.49
2:B:17:PHE:HD1	2:B:41:ILE:HD12	1.77	0.49
1:A:826:C:O2	8:H:15:ASN:ND2	2.45	0.49
19:S:18:LYS:O	19:S:22:LEU:HG	2.13	0.49
1:A:1079:G:O3'	5:E:14:ARG:NH2	2.46	0.49
14:N:9:LYS:HD2	14:N:23:ARG:HB2	1.94	0.49
15:O:45:VAL:HG23	15:O:46:HIS:CD2	2.47	0.49
20:T:63:ILE:HG21	20:T:81:LYS:HG3	1.93	0.49
1:A:1338:G:H2'	1:A:1339:A:C8	2.47	0.49
1:A:1404:5MC:H2'	1:A:1405:G:C8	2.47	0.49
1:A:518:C:H4'	1:A:519:C:O5'	2.12	0.49
2:B:240:GLN:OE1	2:B:240:GLN:N	2.45	0.49
5:E:87:SER:OG	5:E:125:SER:O	2.28	0.49
11:K:57:THR:HG23	11:K:60:ALA:H	1.77	0.49
12:L:77:LEU:HD21	12:L:107:ALA:HB2	1.95	0.49
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.47	0.49
17:Q:45:HIS:CD2	17:Q:47:PRO:HG3	2.48	0.49
1:A:1256:A:H4'	1:A:1257:U:O5'	2.13	0.49
1:A:1064:G:H22	1:A:1190:G:HO2'	1.61	0.49
1:A:1342:C:H2'	1:A:1343:G:C8	2.48	0.49
2:B:19:HIS:CE1	2:B:206:ASP:HB2	2.46	0.49
14:N:24:CYS:H	14:N:33:VAL:HG21	1.78	0.49
1:A:1006:C:H2'	1:A:1007:C:H6	1.77	0.48
13:M:91:ARG:HH22	13:M:103:THR:HG21	1.78	0.48
1:A:1257:U:O2'	1:A:1258:G:OP2	2.31	0.48
1:A:1288:A:N3	1:A:1352:C:O2'	2.42	0.48
1:A:908:A:H2'	1:A:909:A:H8	1.77	0.48
16:P:9:PHE:CE2	16:P:18:ARG:HD2	2.48	0.48
1:A:1040:U:H2'	1:A:1041:A:H8	1.78	0.48
1:A:1525:G:H2'	1:A:1526:G:C8	2.48	0.48
1:A:559:A:OP1	5:E:126:ARG:NH1	2.42	0.48
1:A:719:C:O2'	18:R:49:LYS:HB3	2.14	0.48
3:C:64:VAL:HG12	3:C:66:VAL:HG23	1.94	0.48
1:A:1213:A:N1	1:A:1215:G:H1'	2.28	0.48
1:A:787:A:N6	1:A:792:A:O2'	2.46	0.48
1:A:1007:C:H1'	1:A:1023:G:H1	1.78	0.48
1:A:1148:U:H2'	1:A:1149:C:O4'	2.14	0.48
1:A:987:G:H2'	1:A:988:G:C8	2.49	0.48
16:P:15:PRO:HD2	16:P:42:ARG:HD3	1.95	0.48
1:A:1064:G:N2	1:A:1190:G:O2'	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1251:A:N3	1:A:1369:C:O2'	2.45	0.48
1:A:5:U:H4'	1:A:6:G:O5'	2.13	0.48
1:A:974:A:OP2	14:N:41:ARG:NH1	2.46	0.48
1:A:762:C:H2'	1:A:763:G:C8	2.49	0.48
2:B:16:HIS:CE1	2:B:210:SER:HB2	2.49	0.48
4:D:7:PRO:HG2	4:D:10:ARG:HD2	1.95	0.48
1:A:1000:U:H2'	1:A:1001:A:C8	2.49	0.48
3:C:24:ALA:HB1	3:C:28:GLN:HB2	1.95	0.48
1:A:1189:C:P	10:J:51:ARG:HH22	2.36	0.48
1:A:463:A:H2'	1:A:474:G:O4'	2.14	0.48
2:B:15:VAL:HG12	2:B:210:SER:HB3	1.95	0.48
2:B:187:LEU:HD23	2:B:214:ILE:HG21	1.94	0.48
3:C:36:ASP:HB3	3:C:40:ARG:HH12	1.79	0.48
7:G:5:ARG:HG2	7:G:6:ARG:H	1.78	0.48
1:A:1384:C:H2'	1:A:1385:G:C8	2.49	0.48
1:A:1512:U:H2'	1:A:1513:A:C8	2.49	0.48
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.95	0.48
12:L:82:VAL:O	12:L:106:ASP:HB2	2.13	0.48
13:M:15:VAL:HG12	13:M:34:LEU:HD21	1.96	0.48
1:A:13:C:H42	1:A:915:A:N6	2.11	0.47
1:A:193:C:H2'	1:A:194:C:H6	1.79	0.47
1:A:740:U:H2'	1:A:741:G:H8	1.79	0.47
1:A:812:C:H4'	1:A:813:U:O5'	2.13	0.47
3:C:180:ALA:HB1	3:C:205:GLY:O	2.14	0.47
1:A:1427:U:H2'	1:A:1428:A:C8	2.49	0.47
1:A:1495:U:O4	25:A:1814:EUS:N12	2.47	0.47
1:A:21:G:H2'	1:A:22:G:C8	2.49	0.47
1:A:674:G:H2'	1:A:675:A:C8	2.49	0.47
1:A:738:C:H5''	6:F:69:GLU:HB3	1.94	0.47
1:A:807:A:H2'	1:A:808:C:C6	2.49	0.47
13:M:3:ARG:NE	13:M:7:VAL:HG12	2.20	0.47
18:R:40:LEU:HB3	18:R:79:LEU:HD11	1.95	0.47
1:A:481:G:O2'	1:A:482:A:H8	1.97	0.47
3:C:134:ILE:HG23	3:C:151:VAL:HB	1.97	0.47
3:C:6:HIS:CE1	3:C:8:ILE:HB	2.49	0.47
7:G:79:ARG:HA	7:G:84:ASN:HB3	1.96	0.47
1:A:824:C:H2'	1:A:825:G:H8	1.79	0.47
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.97	0.47
9:I:24:GLY:HA2	9:I:59:PHE:O	2.14	0.47
1:A:976:G:H5''	1:A:1358:U:O2'	2.14	0.47
1:A:201:C:H42	1:A:216:G:H1	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:971:G:H4'	1:A:972:C:H5''	1.97	0.47
3:C:26:LYS:HZ2	10:J:45:ARG:HE	1.61	0.47
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.95	0.47
1:A:327:A:HO2'	1:A:328:C:H6	1.63	0.47
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.96	0.47
8:H:92:ARG:HG2	8:H:94:TYR:OH	2.13	0.47
1:A:636:U:H2'	1:A:637:G:H8	1.79	0.47
2:B:28:PHE:CD2	2:B:190:THR:HA	2.50	0.47
1:A:946:A:O2'	1:A:1333:A:N3	2.41	0.47
7:G:18:TYR:OH	7:G:58:PRO:HG2	2.15	0.47
9:I:26:VAL:HG13	9:I:61:ALA:HB3	1.97	0.47
1:A:1516:G:H2'	1:A:1518:MA6:OP2	2.14	0.47
1:A:276:G:O2'	17:Q:68:ARG:NH1	2.48	0.47
1:A:371:G:O2'	1:A:372:C:H5'	2.13	0.47
1:A:376:G:H2'	1:A:377:G:C8	2.49	0.47
1:A:426:G:OP1	4:D:38:TYR:OH	2.33	0.47
2:B:204:ASN:HD22	2:B:204:ASN:H	1.61	0.47
12:L:89:ARG:NH2	12:L:97:ARG:HE	2.12	0.47
15:O:29:VAL:HG11	15:O:67:LEU:HD21	1.96	0.47
1:A:355:C:H5'	1:A:389:A:OP2	2.15	0.47
1:A:560:U:H4'	1:A:561:U:H5''	1.97	0.47
3:C:130:VAL:HG11	3:C:157:ILE:HG23	1.96	0.47
15:O:24:SER:HB2	15:O:27:VAL:HG23	1.96	0.47
17:Q:59:ILE:HG23	17:Q:71:PHE:CD2	2.50	0.47
1:A:1162:C:H2'	1:A:1163:C:C6	2.49	0.47
1:A:309:G:O2'	1:A:607:A:N1	2.48	0.47
1:A:67:C:H2'	1:A:68:G:C8	2.50	0.47
1:A:977:A:O2'	1:A:981:U:N3	2.46	0.47
10:J:80:LYS:H	10:J:80:LYS:HD2	1.80	0.47
1:A:1098:C:H2'	1:A:1099:G:O4'	2.15	0.46
1:A:184:G:H2'	1:A:185:A:H8	1.80	0.46
1:A:401:C:H2'	1:A:402:G:H8	1.78	0.46
1:A:688:G:H2'	1:A:689:C:C6	2.50	0.46
1:A:973:G:H3'	1:A:974:A:H5''	1.97	0.46
17:Q:13:ASP:HB2	17:Q:53:LEU:HD12	1.97	0.46
1:A:1518:MA6:H8	1:A:1518:MA6:O5'	2.15	0.46
1:A:413:G:H2'	1:A:428:G:H22	1.79	0.46
1:A:1368:G:H5''	9:I:112:LYS:HB3	1.97	0.46
1:A:1225:A:N3	1:A:1225:A:H2'	2.30	0.46
1:A:671:G:H5'	6:F:77:ARG:NH2	2.30	0.46
9:I:10:ARG:NH1	9:I:75:ASP:OD2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1053:G:HO2'	1:A:1199:U:H5	1.63	0.46
1:A:701:C:H5''	1:A:703:G:H5'	1.97	0.46
1:A:665:A:H2'	1:A:732:C:O2	2.16	0.46
3:C:30:ARG:HG2	14:N:36:PHE:O	2.15	0.46
5:E:102:ALA:HB1	5:E:106:PRO:HB2	1.97	0.46
6:F:33:TYR:CD1	6:F:75:LEU:HD23	2.51	0.46
10:J:30:SER:HB3	10:J:80:LYS:HB2	1.96	0.46
16:P:53:VAL:HG12	16:P:79:VAL:HG22	1.97	0.46
1:A:1359:C:H1'	1:A:1361(A):C:H41	1.81	0.46
1:A:157:G:H2'	1:A:158:G:C8	2.50	0.46
1:A:646:U:H2'	1:A:647:C:C6	2.50	0.46
1:A:88:A:H2'	1:A:89:C:O4'	2.15	0.46
2:B:114:ARG:NH1	2:B:118:LEU:HD21	2.25	0.46
7:G:26:PHE:HD1	7:G:101:LEU:HD22	1.81	0.46
10:J:40:LEU:HB2	10:J:69:ASN:HB2	1.98	0.46
12:L:36:VAL:HG22	12:L:82:VAL:HG12	1.97	0.46
17:Q:55:ASP:HB3	17:Q:76:LEU:HD21	1.98	0.46
1:A:1392:G:N2	1:A:1502:A:H8	2.14	0.46
1:A:344:A:H5'	1:A:345:C:C5	2.51	0.46
1:A:575:G:O2'	1:A:821:G:H5'	2.16	0.46
1:A:902:G:H2'	1:A:903:G:H8	1.80	0.46
5:E:35:GLY:HA3	5:E:112:LEU:HB3	1.98	0.46
1:A:302:G:H5''	12:L:17:LYS:NZ	2.30	0.46
15:O:11:VAL:HG21	15:O:34:LEU:HD13	1.97	0.46
16:P:40:ASP:HB3	16:P:48:TRP:HB2	1.97	0.46
19:S:28:LYS:HG2	19:S:29:ARG:H	1.80	0.46
1:A:1310:G:H2'	1:A:1311:G:H8	1.81	0.46
1:A:950:U:H2'	1:A:951:G:C8	2.51	0.46
11:K:22:HIS:HB3	11:K:29:ILE:HD13	1.97	0.46
11:K:32:ILE:O	11:K:40:ILE:N	2.41	0.46
12:L:48:PRO:HD2	12:L:92:0TD:H8	1.97	0.46
13:M:23:TYR:CD2	13:M:67:GLU:HA	2.50	0.46
18:R:19:LYS:HB2	18:R:19:LYS:HE3	1.75	0.46
1:A:1029:C:H2'	1:A:1030:C:C6	2.51	0.46
1:A:1062:U:H2'	1:A:1063:C:C6	2.51	0.46
1:A:911:U:H2'	1:A:912:C:C6	2.51	0.46
8:H:83:ILE:HG12	8:H:137:VAL:HG22	1.97	0.46
9:I:53:VAL:HG21	9:I:85:LEU:HD21	1.98	0.46
10:J:16:LEU:O	10:J:20:ALA:N	2.44	0.46
12:L:11:VAL:HG11	17:Q:36:ILE:HG21	1.98	0.46
1:A:1168:A:H2'	1:A:1169:A:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1367:C:H4'	10:J:48:THR:HG21	1.98	0.46
16:P:58:TYR:O	16:P:61:SER:OG	2.24	0.46
1:A:1007:C:O2	1:A:1023:G:N1	2.49	0.46
1:A:17:U:H2'	1:A:18:C:C6	2.50	0.46
11:K:33:THR:HA	11:K:39:PRO:HA	1.98	0.46
1:A:1150:U:O4	1:A:1151:A:N6	2.49	0.45
8:H:63:LEU:H	8:H:63:LEU:HD22	1.81	0.45
3:C:26:LYS:HD3	10:J:45:ARG:HH21	1.81	0.45
1:A:1490:C:H2'	1:A:1491:G:C8	2.50	0.45
1:A:870:U:H4'	1:A:871:U:H5''	1.98	0.45
4:D:99:SER:HB3	4:D:139:ARG:HG3	1.99	0.45
11:K:69:ALA:O	11:K:73:MET:HG2	2.16	0.45
13:M:101:GLN:OE1	13:M:101:GLN:N	2.49	0.45
1:A:1080:A:O3'	5:E:16:THR:OG1	2.32	0.45
1:A:1323:G:H2'	1:A:1324:A:C8	2.52	0.45
1:A:381:C:H2'	1:A:382:A:O4'	2.17	0.45
2:B:102:LEU:HB3	2:B:180:LEU:HD12	1.97	0.45
9:I:116:LYS:HD2	9:I:122:ALA:HA	1.98	0.45
13:M:3:ARG:HA	13:M:8:GLU:O	2.16	0.45
19:S:5:LEU:HD21	19:S:70:LYS:HZ1	1.82	0.45
1:A:1035:A:H2'	1:A:1036:G:C8	2.51	0.45
1:A:936:C:H2'	1:A:937:A:O4'	2.17	0.45
1:A:1111:A:H61	3:C:177:THR:HB	1.82	0.45
8:H:119:LEU:HB3	8:H:123:GLU:HB2	1.98	0.45
10:J:26:ALA:HB1	10:J:84:GLN:HB2	1.97	0.45
1:A:264:U:O2'	17:Q:64:PRO:O	2.31	0.45
1:A:488:C:H2'	1:A:489:C:C6	2.51	0.45
7:G:108:ALA:O	7:G:111:ARG:HB2	2.16	0.45
17:Q:6:LEU:HB2	17:Q:59:ILE:HG22	1.99	0.45
1:A:12:U:H4'	1:A:526:C:O2'	2.16	0.45
1:A:665:A:H3'	1:A:725:G:N2	2.32	0.45
1:A:960:U:H4'	1:A:961:U:C5'	2.47	0.45
2:B:188:ALA:O	2:B:202:PRO:HA	2.16	0.45
2:B:16:HIS:HD2	2:B:204:ASN:HD22	1.63	0.45
2:B:60:ASP:CG	2:B:64:ARG:HH12	2.20	0.45
1:A:1366:C:H2'	1:A:1367:C:C6	2.52	0.45
1:A:229:U:H2'	1:A:230:G:C8	2.52	0.45
1:A:1251:A:H5'	9:I:12:GLU:HG2	1.99	0.45
1:A:1087:G:H2'	1:A:1088:G:C8	2.52	0.45
1:A:258:G:H2'	1:A:259:G:H8	1.82	0.45
1:A:736:C:H2'	1:A:737:A:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.99	0.45
4:D:18:LYS:HB3	4:D:18:LYS:HE2	1.77	0.45
6:F:11:ASN:HD22	6:F:86:ARG:NH2	2.15	0.45
13:M:16:ASP:OD1	13:M:16:ASP:N	2.50	0.45
18:R:87:ARG:HD2	18:R:87:ARG:HA	1.86	0.45
9:I:49:PRO:HB2	9:I:81:ILE:HG22	1.99	0.45
6:F:100:ASN:HA	18:R:23:LYS:HE3	1.99	0.45
1:A:1238:A:OP2	1:A:1335:C:H1'	2.18	0.44
1:A:1425:U:H2'	1:A:1426:C:C6	2.52	0.44
1:A:327:A:O2'	1:A:328:C:O4'	2.33	0.44
1:A:714:G:H2'	1:A:715:A:C8	2.53	0.44
8:H:86:ILE:HD12	8:H:133:LEU:HD22	1.99	0.44
8:H:17:THR:O	8:H:78:GLN:NE2	2.50	0.44
15:O:2:PRO:HB2	15:O:3:ILE:H	1.64	0.44
19:S:13:ASP:OD1	19:S:13:ASP:N	2.50	0.44
19:S:5:LEU:HD12	19:S:9:VAL:HG13	1.98	0.44
2:B:96:ARG:HH21	2:B:169:LYS:HZ1	1.64	0.44
3:C:202:ILE:HG22	3:C:204:LEU:HD23	1.99	0.44
3:C:26:LYS:NZ	10:J:45:ARG:HE	2.15	0.44
1:A:1006:C:H2'	1:A:1007:C:C6	2.52	0.44
1:A:49:U:O2'	1:A:50:A:H2'	2.18	0.44
3:C:147:LYS:HE3	3:C:203:PHE:CE2	2.52	0.44
13:M:13:LYS:O	13:M:45:VAL:HG23	2.17	0.44
14:N:24:CYS:HB3	14:N:29:ARG:HB3	2.00	0.44
15:O:5:LYS:HA	15:O:8:LYS:HB2	1.99	0.44
1:A:1308:U:H2'	1:A:1309:G:C8	2.52	0.44
1:A:1380:U:H1'	1:A:1381:U:OP2	2.18	0.44
5:E:11:ILE:HG22	5:E:12:LEU:HD12	1.98	0.44
1:A:1342:C:O2'	9:I:124:GLN:HB2	2.18	0.44
1:A:1296:C:H5'	13:M:14:ARG:HD2	1.98	0.44
1:A:263:A:OP2	20:T:79:ARG:NH1	2.50	0.44
1:A:310:G:H5''	16:P:31:LYS:HB2	1.98	0.44
1:A:328:C:H4'	1:A:329:A:O5'	2.17	0.44
1:A:824:C:H2'	1:A:825:G:C8	2.52	0.44
1:A:918:A:H2'	1:A:919:A:C8	2.53	0.44
2:B:155:LEU:HA	2:B:155:LEU:HD23	1.79	0.44
2:B:50:GLU:HB3	2:B:200:ILE:O	2.18	0.44
1:A:1442:G:O6	1:A:1446:A:N6	2.43	0.44
1:A:445:G:H2'	1:A:446:G:C8	2.52	0.44
1:A:1233:G:H2'	1:A:1234:C:C6	2.52	0.44
1:A:116:A:H61	1:A:313:A:H1'	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:G:H2'	1:A:36:C:C6	2.52	0.44
12:L:20:LYS:HG3	12:L:20:LYS:H	1.68	0.44
14:N:21:TYR:HE2	14:N:23:ARG:HE	1.64	0.44
1:A:1255:G:OP2	3:C:26:LYS:NZ	2.41	0.44
3:C:41:GLY:O	3:C:45:LYS:HG2	2.18	0.44
3:C:58:GLU:HB2	3:C:65:ALA:HB3	2.00	0.44
1:A:620:C:N1	4:D:135:LEU:HD13	2.32	0.44
16:P:3:LYS:HE2	16:P:3:LYS:HB3	1.88	0.44
1:A:1113:C:H2'	1:A:1114:C:C6	2.53	0.44
1:A:1211:U:H1'	1:A:1213:A:C2	2.53	0.44
1:A:1316:G:N1	1:A:1319:A:OP2	2.48	0.44
1:A:501:C:O3'	12:L:118:SER:OG	2.35	0.44
6:F:76:ALA:O	6:F:80:ARG:HG3	2.17	0.43
19:S:50:ALA:HB1	19:S:57:HIS:HB3	2.00	0.43
1:A:791:G:O6	1:A:792:A:N6	2.50	0.43
3:C:131:ARG:HB2	3:C:131:ARG:HE	1.60	0.43
3:C:110:ASN:O	3:C:141:VAL:HG22	2.19	0.43
7:G:72:ARG:H	7:G:72:ARG:HG2	1.61	0.43
12:L:32:PHE:HB3	12:L:84:LEU:HD11	2.01	0.43
1:A:282:A:H3'	1:A:283:C:C6	2.53	0.43
1:A:299:G:C6	1:A:300:A:C6	3.07	0.43
1:A:541:G:H2'	1:A:542:G:H8	1.84	0.43
1:A:932:C:H5'	7:G:4:ARG:HG3	2.01	0.43
2:B:68:ILE:O	2:B:90:MET:HB3	2.18	0.43
15:O:44:LYS:HB3	15:O:44:LYS:HE3	1.72	0.43
17:Q:43:LEU:HB2	17:Q:68:ARG:O	2.18	0.43
1:A:1003(A):G:H2'	1:A:1004:A:H4'	2.00	0.43
1:A:327:A:O2'	1:A:328:C:H6	2.00	0.43
1:A:445:G:H2'	1:A:446:G:H8	1.82	0.43
1:A:669:U:H2'	1:A:670:G:C8	2.53	0.43
1:A:959:A:HO2'	1:A:984:C:HO2'	1.64	0.43
2:B:133:LYS:O	2:B:137:ARG:HG3	2.18	0.43
3:C:134:ILE:O	3:C:138:VAL:HG23	2.19	0.43
13:M:33:ALA:O	13:M:37:THR:OG1	2.24	0.43
17:Q:59:ILE:HD11	17:Q:73:VAL:HG22	2.00	0.43
1:A:1092:A:N3	1:A:1183:A:N6	2.66	0.43
1:A:1318:A:H4'	19:S:10:PHE:CD2	2.53	0.43
1:A:258:G:H2'	1:A:259:G:C8	2.53	0.43
1:A:401:C:O2'	1:A:621:A:N3	2.46	0.43
1:A:960:U:H1'	1:A:1223:C:H5'	2.00	0.43
3:C:68:VAL:HG12	3:C:70:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1376:U:H2'	1:A:1377:A:C8	2.53	0.43
1:A:142:G:H2'	1:A:143:A:H8	1.83	0.43
1:A:217:C:H2'	1:A:218:C:C6	2.53	0.43
4:D:150:GLU:HA	4:D:153:ARG:HG3	2.00	0.43
4:D:187:ARG:HH22	4:D:188:LEU:HB2	1.84	0.43
12:L:27:LEU:HG	12:L:28:LYS:H	1.84	0.43
13:M:88:ARG:HG3	13:M:98:VAL:HG13	2.00	0.43
1:A:1132:C:H2'	1:A:1133:G:H8	1.84	0.43
1:A:977:A:N7	1:A:1223:C:H2'	2.34	0.43
1:A:452:A:O2'	1:A:453:A:O5'	2.35	0.43
3:C:131:ARG:NH2	3:C:164:ARG:HH22	2.17	0.43
1:A:1198:G:H2'	1:A:1199:U:C6	2.54	0.43
1:A:56:U:H2'	1:A:57:G:C8	2.53	0.43
1:A:673:G:H2'	1:A:674:G:C8	2.53	0.43
1:A:689:C:H2'	1:A:690:G:O4'	2.19	0.43
1:A:939:G:H2'	1:A:940:C:C6	2.53	0.43
1:A:965:A:H4'	1:A:966:M2G:OP1	2.18	0.43
2:B:140:HIS:O	2:B:144:ARG:HG2	2.18	0.43
7:G:94:ARG:O	7:G:97:GLN:HB3	2.18	0.43
20:T:53:LEU:HD22	20:T:53:LEU:HA	1.86	0.43
1:A:164:U:H2'	1:A:165:C:C6	2.54	0.43
1:A:298:A:H2'	1:A:299:G:O4'	2.19	0.43
1:A:637:G:H2'	1:A:638:G:H8	1.84	0.43
2:B:172:ILE:H	2:B:172:ILE:HG13	1.53	0.43
4:D:57:ARG:HG3	4:D:202:LEU:HD13	2.01	0.43
13:M:34:LEU:HD13	13:M:39:ILE:HB	2.01	0.43
17:Q:59:ILE:HD12	17:Q:73:VAL:HA	2.01	0.43
1:A:1366:C:O3'	10:J:60:ARG:NH2	2.45	0.43
1:A:447:G:H1	1:A:485:G:H2'	1.84	0.43
1:A:977:A:N6	27:A:1913:HOH:O	2.52	0.43
2:B:16:HIS:HD2	2:B:204:ASN:ND2	2.17	0.43
2:B:16:HIS:ND1	2:B:210:SER:HB2	2.34	0.43
9:I:37:PHE:HA	9:I:40:LEU:HD12	2.00	0.43
11:K:122:LYS:HE3	11:K:122:LYS:HB2	1.80	0.43
19:S:36:ARG:HG2	19:S:36:ARG:H	1.62	0.43
1:A:479:C:H2'	1:A:480:U:O4'	2.18	0.42
11:K:44:SER:H	11:K:47:VAL:HB	1.84	0.42
1:A:1221:G:O3'	19:S:77:THR:HG21	2.19	0.42
1:A:1414:U:H2'	1:A:1415:G:H8	1.85	0.42
1:A:688:G:O2'	1:A:704:A:N1	2.36	0.42
2:B:47:THR:HA	2:B:202:PRO:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:50:ILE:HD11	7:G:61:VAL:HG11	2.01	0.42
9:I:10:ARG:HG2	9:I:75:ASP:HB2	2.01	0.42
13:M:96:LEU:C	13:M:110:ARG:HG2	2.39	0.42
18:R:86:VAL:O	18:R:87:ARG:HD3	2.19	0.42
19:S:29:ARG:N	19:S:29:ARG:HD2	2.34	0.42
1:A:1003(A):G:C5	1:A:1004:A:H1'	2.54	0.42
1:A:1419:G:H2'	1:A:1420:C:C6	2.55	0.42
1:A:363:A:OP2	12:L:34:ARG:NE	2.53	0.42
1:A:582:U:C2	1:A:760:G:C6	3.07	0.42
1:A:962:C:H2'	1:A:963:G:H8	1.83	0.42
12:L:77:LEU:HD23	12:L:77:LEU:HA	1.86	0.42
1:A:950:U:H2'	1:A:951:G:H8	1.85	0.42
7:G:77:SER:HA	7:G:85:TYR:O	2.20	0.42
9:I:20:ARG:O	9:I:60:ASP:N	2.49	0.42
11:K:15:ALA:HA	11:K:76:GLY:O	2.18	0.42
1:A:1371:G:OP2	9:I:11:LYS:HE2	2.19	0.42
1:A:1105:A:H2'	1:A:1106:G:C8	2.55	0.42
1:A:325:A:H2'	1:A:326:G:O4'	2.20	0.42
1:A:484:G:H4'	1:A:485:G:O5'	2.19	0.42
9:I:51:ARG:HG3	9:I:56:LEU:HD21	2.01	0.42
10:J:55:LYS:HD2	10:J:56:HIS:N	2.32	0.42
1:A:1268:A:N3	1:A:1326:C:O2'	2.47	0.42
1:A:1530:G:H2'	1:A:1531:A:C8	2.55	0.42
1:A:193:C:H2'	1:A:194:C:C6	2.55	0.42
1:A:767:A:H2'	1:A:768:A:O4'	2.20	0.42
4:D:142:PRO:HA	4:D:185:PHE:HD1	1.85	0.42
6:F:23:LYS:O	6:F:27:GLN:HG2	2.20	0.42
6:F:26:ILE:HG21	6:F:63:TYR:HE2	1.85	0.42
9:I:3:GLN:HG3	9:I:20:ARG:HG3	2.01	0.42
11:K:72:ALA:HB1	11:K:77:MET:HG3	2.01	0.42
1:A:1309:G:H5'	13:M:78:ILE:HD11	2.01	0.42
17:Q:3:LYS:HD3	17:Q:60:ILE:HD11	2.01	0.42
18:R:47:THR:HG22	18:R:48:GLY:H	1.85	0.42
4:D:3:ARG:HD3	4:D:3:ARG:HA	1.85	0.42
10:J:82:ILE:HA	10:J:85:LEU:HB2	2.02	0.42
15:O:56:LEU:HA	15:O:59:MET:HE2	2.02	0.42
20:T:89:ARG:HH21	20:T:104:LEU:HB3	1.84	0.42
1:A:1462:G:H2'	1:A:1463:C:C6	2.55	0.42
1:A:375:U:H2'	1:A:376:G:C8	2.55	0.42
9:I:69:GLY:O	9:I:73:GLN:HG3	2.20	0.42
1:A:553:A:O2'	12:L:29:GLY:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:23:GLY:O	15:O:28:GLN:NE2	2.48	0.42
1:A:1197:G:H5''	27:A:1995:HOH:O	2.19	0.42
1:A:1346:A:H4'	1:A:1347:G:O5'	2.20	0.42
1:A:1372:U:H5''	9:I:71:SER:HB3	2.02	0.42
1:A:373:A:H1'	1:A:481:G:H1'	2.01	0.42
8:H:6:ILE:HB	8:H:85:ARG:NH1	2.35	0.42
20:T:88:VAL:O	20:T:92:LEU:HB2	2.20	0.42
1:A:1105:A:H2'	1:A:1106:G:H8	1.84	0.41
1:A:1305:G:N2	1:A:1331:G:H1'	2.35	0.41
3:C:131:ARG:HH22	3:C:164:ARG:HH22	1.67	0.41
6:F:70:ASP:N	6:F:70:ASP:OD1	2.53	0.41
7:G:65:ALA:O	7:G:69:VAL:HG23	2.20	0.41
9:I:51:ARG:HE	9:I:51:ARG:HB2	1.51	0.41
1:A:1057:G:H2'	1:A:1058:G:O4'	2.19	0.41
1:A:1133:G:H1	1:A:1141:C:H42	1.68	0.41
1:A:129(A):G:N2	1:A:190(E):U:H5''	2.36	0.41
1:A:132:C:H5'	1:A:262:A:O2'	2.21	0.41
1:A:1417:G:O2'	1:A:1483:A:N6	2.54	0.41
1:A:356:A:N3	1:A:368:U:O2'	2.37	0.41
3:C:188:LEU:HD11	3:C:195:VAL:HG13	2.01	0.41
4:D:11:LEU:HD13	4:D:66:ARG:HD2	2.02	0.41
13:M:91:ARG:NH2	13:M:103:THR:HG21	2.35	0.41
1:A:6:G:H4'	1:A:298:A:H4'	2.02	0.41
1:A:407:G:H2'	1:A:408:A:C8	2.55	0.41
1:A:424:G:H2'	1:A:425:G:H8	1.85	0.41
4:D:184:LYS:HB2	4:D:184:LYS:HE3	1.86	0.41
15:O:38:ARG:HA	15:O:38:ARG:HD3	1.93	0.41
20:T:33:ILE:HD13	20:T:62:LEU:HB3	2.03	0.41
1:A:1222:G:H5'	19:S:77:THR:HG21	2.01	0.41
1:A:1348:U:OP2	1:A:1373:G:N1	2.49	0.41
1:A:1517:G:N7	1:A:1518:MA6:H103	2.35	0.41
3:C:26:LYS:H	3:C:26:LYS:HG2	1.73	0.41
8:H:87:SER:HA	8:H:93:VAL:HG23	2.02	0.41
1:A:1314:C:H2'	1:A:1315:U:C6	2.55	0.41
1:A:254:G:H5''	17:Q:69:LYS:HD2	2.02	0.41
1:A:424:G:H2'	1:A:425:G:C8	2.56	0.41
2:B:88:ALA:HB2	2:B:219:VAL:HG13	2.03	0.41
3:C:20:SER:OG	3:C:40:ARG:NH2	2.25	0.41
5:E:7:GLU:OE1	5:E:37:ARG:NH2	2.47	0.41
12:L:68:ALA:HB1	12:L:100:ILE:HG13	2.02	0.41
17:Q:48:GLU:HB2	17:Q:50:LYS:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:87:ARG:O	18:R:88:LYS:HB2	2.20	0.41
1:A:1294:G:H2'	1:A:1295:G:H8	1.85	0.41
1:A:940:C:H2'	1:A:941:G:C8	2.55	0.41
2:B:178:ARG:O	8:H:72:PRO:HD3	2.21	0.41
1:A:1187:G:H4'	9:I:111:ARG:NH1	2.35	0.41
12:L:46:LYS:HB2	12:L:92:0TD:CSB	2.51	0.41
13:M:10:PRO:O	13:M:45:VAL:HG11	2.21	0.41
1:A:344:A:H5'	1:A:345:C:H5	1.86	0.41
1:A:768:A:OP1	1:A:804:U:H4'	2.21	0.41
1:A:972:C:H4'	10:J:57:LYS:HD3	2.02	0.41
1:A:1190:G:O3'	3:C:3:ASN:HB2	2.20	0.41
12:L:69:TYR:O	12:L:100:ILE:HB	2.21	0.41
19:S:25:LYS:N	19:S:25:LYS:HD2	2.36	0.41
1:A:186:C:O2'	20:T:85:MET:SD	2.71	0.41
1:A:295:C:H2'	1:A:296:U:O4'	2.20	0.41
1:A:28:G:O2'	1:A:296:U:OP1	2.39	0.41
1:A:765:G:C6	1:A:812:C:C2	3.09	0.41
1:A:788:U:H2'	1:A:789:U:O4'	2.21	0.41
1:A:909:A:N3	1:A:1413:A:O2'	2.50	0.41
4:D:18:LYS:NZ	4:D:26:CYS:O	2.32	0.41
1:A:921:U:O2'	5:E:19:MET:O	2.28	0.41
2:B:181:PHE:HD2	8:H:70:GLN:HB3	1.83	0.41
12:L:44:THR:HA	12:L:45:PRO:HD3	1.92	0.41
16:P:69:THR:O	16:P:73:LEU:HG	2.21	0.41
1:A:1109:C:H2'	1:A:1110:A:O4'	2.20	0.41
1:A:687:A:H4'	1:A:688:G:O5'	2.20	0.41
3:C:136:GLN:O	3:C:140:ARG:HG3	2.21	0.41
4:D:187:ARG:NH2	4:D:188:LEU:HB2	2.36	0.41
9:I:44:VAL:HG12	9:I:51:ARG:HH22	1.86	0.41
9:I:8:GLY:H	9:I:83:ARG:NH1	2.18	0.41
11:K:57:THR:CG2	11:K:60:ALA:H	2.34	0.41
12:L:126:LYS:HB2	12:L:126:LYS:HE2	1.93	0.41
19:S:11:VAL:HG13	19:S:38:SER:HB2	2.02	0.41
1:A:701:C:H4'	1:A:702:A:O5'	2.19	0.41
1:A:730:G:C5	1:A:731:G:H1'	2.55	0.41
3:C:20:SER:HB3	3:C:22:TRP:HE1	1.85	0.41
9:I:8:GLY:HA2	9:I:79:LEU:HD13	2.02	0.41
12:L:69:TYR:O	12:L:71:PRO:HD3	2.20	0.41
19:S:10:PHE:O	19:S:39:THR:OG1	2.32	0.41
1:A:1277:C:O2'	1:A:1279:A:H1'	2.21	0.41
1:A:142:G:H2'	1:A:143:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1399:C:C2	1:A:1502:A:N6	2.89	0.41
1:A:757:U:H2'	1:A:758:G:O4'	2.21	0.41
1:A:76:C:H2'	1:A:77:G:H8	1.86	0.41
12:L:36:VAL:HG13	12:L:82:VAL:HG12	2.02	0.41
16:P:22:THR:HA	16:P:33:ILE:HG13	2.02	0.41
1:A:1030:C:H2'	1:A:1030(A):G:C8	2.56	0.40
1:A:1291:G:H5''	9:I:39:GLY:O	2.21	0.40
1:A:1294:G:H2'	1:A:1295:G:C8	2.56	0.40
1:A:1236:A:O2'	1:A:1304:G:H4'	2.20	0.40
1:A:343:U:O2'	1:A:346:G:O6	2.37	0.40
1:A:581:G:OP1	15:O:61:GLY:HA3	2.21	0.40
1:A:692:U:H2'	1:A:694:A:OP2	2.21	0.40
2:B:215:LEU:HD23	2:B:215:LEU:HA	1.90	0.40
10:J:6:ILE:HB	10:J:72:VAL:HB	2.03	0.40
11:K:92:GLU:HA	11:K:95:ILE:HD12	2.03	0.40
12:L:46:LYS:HD3	12:L:92:0TD:H4	2.04	0.40
13:M:51:ALA:O	13:M:55:ARG:HG3	2.21	0.40
1:A:1216:G:H5''	14:N:5:ALA:HB2	2.04	0.40
1:A:138:G:H2'	1:A:139:G:H8	1.86	0.40
1:A:1418:A:N6	1:A:1482:G:H1'	2.36	0.40
1:A:1420:C:H2'	1:A:1421:G:C8	2.56	0.40
1:A:1498:UR3:O4'	1:A:1519:MA6:H2	2.21	0.40
1:A:620:C:C2	4:D:135:LEU:HD22	2.55	0.40
1:A:688:G:H5'	11:K:46:GLY:C	2.41	0.40
2:B:122:PHE:HA	2:B:127:ILE:HG23	2.03	0.40
5:E:8:GLU:HB3	5:E:34:VAL:HG22	2.04	0.40
14:N:21:TYR:CD2	14:N:23:ARG:HG2	2.56	0.40
1:A:721:G:OP2	18:R:53:ARG:HG3	2.21	0.40
21:U:13:ILE:HG22	21:U:22:ARG:CZ	2.51	0.40
1:A:1030(D):A:H8	1:A:1030(D):A:O5'	2.04	0.40
1:A:1054:C:H2'	23:W:34:G:H5'	2.02	0.40
1:A:1431:C:H2'	1:A:1432:G:O4'	2.22	0.40
2:B:90:MET:HA	2:B:91:PRO:HD3	1.96	0.40
3:C:79:ARG:HG3	3:C:79:ARG:H	1.69	0.40
4:D:57:ARG:HE	4:D:205:GLU:HB3	1.85	0.40
1:A:1257:U:O2'	1:A:1258:G:P	2.80	0.40
1:A:427:U:OP2	4:D:36:ARG:NH2	2.51	0.40
1:A:474:G:H2'	1:A:475:G:C8	2.57	0.40
1:A:682:G:H2'	1:A:683:G:H8	1.87	0.40
1:A:722:A:H3'	1:A:722:A:N3	2.36	0.40
1:A:902:G:H2'	1:A:903:G:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:32:ASP:OD1	9:I:33:PHE:N	2.54	0.40
11:K:58:PRO:HD3	11:K:89:ALA:HB1	2.03	0.40
15:O:5:LYS:HD3	15:O:5:LYS:H	1.87	0.40
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.57	0.40
21:U:12:LYS:HB3	21:U:22:ARG:HD2	2.03	0.40
1:A:1056:U:H5'	3:C:163:ALA:HB2	2.03	0.40
1:A:1162:C:H2'	1:A:1163:C:H6	1.85	0.40
1:A:1190:G:HO2'	1:A:1191:A:P	2.39	0.40
1:A:1069:C:O2'	1:A:1192:C:H1'	2.22	0.40
1:A:255:G:C2	1:A:272:C:C2	3.10	0.40
1:A:939:G:H5''	7:G:102:ARG:NH2	2.37	0.40
4:D:50:ARG:HA	4:D:51:PRO:HD3	1.96	0.40
4:D:78:LEU:HB3	4:D:93:PHE:HE1	1.86	0.40
8:H:121:ASP:OD1	8:H:122:ARG:N	2.54	0.40
9:I:17:VAL:HG11	9:I:81:ILE:HA	2.02	0.40
13:M:56:LEU:HD23	13:M:56:LEU:HA	1.91	0.40
1:A:127:G:O2'	17:Q:2:PRO:O	2.40	0.40
1:A:584:G:H5'	17:Q:91:ARG:HH22	1.86	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	
2	B	232/255 (91%)	219 (94%)	13 (6%)	0	100	100
3	C	204/238 (86%)	186 (91%)	18 (9%)	0	100	100
4	D	206/208 (99%)	201 (98%)	5 (2%)	0	100	100
5	E	148/161 (92%)	144 (97%)	4 (3%)	0	100	100
6	F	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
7	G	153/155 (99%)	148 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	136/138 (99%)	131 (96%)	3 (2%)	2 (2%)	10	45
9	I	125/127 (98%)	115 (92%)	10 (8%)	0	100	100
10	J	96/104 (92%)	82 (85%)	11 (12%)	3 (3%)	4	30
11	K	114/128 (89%)	108 (95%)	6 (5%)	0	100	100
12	L	121/131 (92%)	111 (92%)	10 (8%)	0	100	100
13	M	116/125 (93%)	102 (88%)	13 (11%)	1 (1%)	17	56
14	N	58/60 (97%)	50 (86%)	8 (14%)	0	100	100
15	O	85/88 (97%)	83 (98%)	2 (2%)	0	100	100
16	P	81/88 (92%)	78 (96%)	3 (4%)	0	100	100
17	Q	97/104 (93%)	91 (94%)	6 (6%)	0	100	100
18	R	68/87 (78%)	65 (96%)	3 (4%)	0	100	100
19	S	78/92 (85%)	74 (95%)	4 (5%)	0	100	100
20	T	97/105 (92%)	86 (89%)	11 (11%)	0	100	100
21	U	22/26 (85%)	22 (100%)	0	0	100	100
All	All	2336/2521 (93%)	2192 (94%)	138 (6%)	6 (0%)	41	75

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	55	LYS
10	J	56	HIS
8	H	71	GLY
8	H	72	PRO
13	M	113	PRO
10	J	54	PHE

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/219 (92%)	175 (87%)	27 (13%)	4	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	160/187 (86%)	141 (88%)	19 (12%)	5	25
4	D	180/180 (100%)	168 (93%)	12 (7%)	16	48
5	E	115/122 (94%)	106 (92%)	9 (8%)	12	42
6	F	90/90 (100%)	87 (97%)	3 (3%)	38	68
7	G	126/126 (100%)	118 (94%)	8 (6%)	18	51
8	H	119/119 (100%)	108 (91%)	11 (9%)	9	36
9	I	98/98 (100%)	88 (90%)	10 (10%)	7	32
10	J	87/91 (96%)	75 (86%)	12 (14%)	3	20
11	K	88/98 (90%)	84 (96%)	4 (4%)	27	61
12	L	103/107 (96%)	92 (89%)	11 (11%)	6	30
13	M	94/100 (94%)	82 (87%)	12 (13%)	4	22
14	N	49/49 (100%)	47 (96%)	2 (4%)	30	63
15	O	79/79 (100%)	70 (89%)	9 (11%)	5	26
16	P	72/74 (97%)	67 (93%)	5 (7%)	15	47
17	Q	94/96 (98%)	86 (92%)	8 (8%)	10	39
18	R	61/76 (80%)	58 (95%)	3 (5%)	25	59
19	S	71/79 (90%)	62 (87%)	9 (13%)	4	22
20	T	76/81 (94%)	67 (88%)	9 (12%)	5	25
21	U	19/21 (90%)	17 (90%)	2 (10%)	7	31
All	All	1983/2092 (95%)	1798 (91%)	185 (9%)	9	35

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	VAL
2	B	8	LYS
2	B	9	GLU
2	B	11	LEU
2	B	21	ARG
2	B	23	ARG
2	B	33	TYR
2	B	44	LEU
2	B	67	THR
2	B	69	LEU
2	B	73	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	102	LEU
2	B	103	THR
2	B	106	LYS
2	B	111	ARG
2	B	122	PHE
2	B	127	ILE
2	B	153	ARG
2	B	154	LEU
2	B	157	ARG
2	B	162	ILE
2	B	163	PHE
2	B	165	VAL
2	B	178	ARG
2	B	187	LEU
2	B	200	ILE
2	B	206	ASP
3	C	3	ASN
3	C	10	PHE
3	C	34	LEU
3	C	70	VAL
3	C	90	GLU
3	C	91	LEU
3	C	94	LEU
3	C	95	THR
3	C	97	LYS
3	C	99	VAL
3	C	104	GLN
3	C	111	LEU
3	C	131	ARG
3	C	167	TRP
3	C	176	HIS
3	C	177	THR
3	C	191	THR
3	C	196	LEU
3	C	204	LEU
4	D	34	GLU
4	D	35	ARG
4	D	36	ARG
4	D	47	ARG
4	D	49	ARG
4	D	73	ARG
4	D	83	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	D	115	ARG
4	D	122	ARG
4	D	127	THR
4	D	150	GLU
4	D	155	LEU
5	E	6	PHE
5	E	12	LEU
5	E	16	THR
5	E	24	ARG
5	E	26	PHE
5	E	31	LEU
5	E	41	VAL
5	E	79	GLU
5	E	150	ARG
6	F	10	LEU
6	F	24	GLU
6	F	82	ARG
7	G	8	GLU
7	G	11	GLN
7	G	75	VAL
7	G	79	ARG
7	G	84	ASN
7	G	113	GLU
7	G	136	LYS
7	G	149	ARG
8	H	2	LEU
8	H	3	THR
8	H	26	VAL
8	H	29	SER
8	H	63	LEU
8	H	83	ILE
8	H	85	ARG
8	H	91	ARG
8	H	92	ARG
8	H	98	LYS
8	H	133	LEU
9	I	12	GLU
9	I	20	ARG
9	I	44	VAL
9	I	51	ARG
9	I	79	LEU
9	I	102	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	I	111	ARG
9	I	118	LYS
9	I	121	ARG
9	I	124	GLN
10	J	3	LYS
10	J	38	ILE
10	J	45	ARG
10	J	55	LYS
10	J	60	ARG
10	J	61	GLU
10	J	62	HIS
10	J	71	LEU
10	J	78	ASN
10	J	80	LYS
10	J	89	ASP
10	J	95	GLU
11	K	12	ARG
11	K	14	VAL
11	K	29	ILE
11	K	36	ASP
12	L	18	VAL
12	L	20	LYS
12	L	33	ARG
12	L	42	THR
12	L	44	THR
12	L	59	ARG
12	L	67	THR
12	L	79	GLU
12	L	80	HIS
12	L	113	ARG
12	L	126	LYS
13	M	7	VAL
13	M	12	ASN
13	M	17	VAL
13	M	37	THR
13	M	44	ARG
13	M	48	LEU
13	M	50	GLU
13	M	64	TRP
13	M	108	ARG
13	M	110	ARG
13	M	115	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
13	M	117	VAL
14	N	11	LYS
14	N	22	THR
15	O	5	LYS
15	O	8	LYS
15	O	32	LEU
15	O	39	LEU
15	O	65	ARG
15	O	70	LEU
15	O	71	GLN
15	O	81	LEU
15	O	83	GLU
16	P	1	MET
16	P	2	VAL
16	P	20	VAL
16	P	55	ARG
16	P	67	THR
17	Q	13	ASP
17	Q	34	LYS
17	Q	53	LEU
17	Q	59	ILE
17	Q	60	ILE
17	Q	76	LEU
17	Q	91	ARG
17	Q	98	LEU
18	R	42	ARG
18	R	47	THR
18	R	87	ARG
19	S	6	LYS
19	S	13	ASP
19	S	15	LEU
19	S	29	ARG
19	S	39	THR
19	S	53	ASN
19	S	62	ILE
19	S	63	THR
19	S	65	ASN
20	T	9	ASN
20	T	53	LEU
20	T	57	ARG
20	T	62	LEU
20	T	73	HIS

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Mol	Chain	Res	Type
20	T	75	ASN
20	T	84	LEU
20	T	92	LEU
20	T	93	GLU
21	U	6	ARG
21	U	25	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	16	HIS
2	B	204	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1508/1517 (99%)	238 (15%)	46 (3%)
22	Y	5/6 (83%)	2 (40%)	0
23	W	14/15 (93%)	4 (28%)	0
All	All	1527/1538 (99%)	244 (15%)	46 (3%)

All (244) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	9	G
1	A	13	C
1	A	22	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	101	A
1	A	108	G
1	A	116	A
1	A	117	G
1	A	121	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	163	C
1	A	182	U
1	A	183	G
1	A	195	A
1	A	201	C
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	220	G
1	A	247	G
1	A	251	G
1	A	252	U
1	A	266	G
1	A	267	C
1	A	279	A
1	A	282	A
1	A	289	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	344	A
1	A	345	C
1	A	350	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	356	A
1	A	367	U
1	A	372	C
1	A	373	A
1	A	374	A
1	A	384	G
1	A	390	C
1	A	397	A
1	A	398	C
1	A	406	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	412	A
1	A	413	G
1	A	421	U
1	A	429	U
1	A	430	A
1	A	439	A
1	A	451	A
1	A	460	A
1	A	461	C
1	A	481	G
1	A	485	G
1	A	486	U
1	A	497	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	517	G
1	A	518	C
1	A	519	C
1	A	524	G
1	A	531	U
1	A	533	A
1	A	547	A
1	A	559	A
1	A	560	U
1	A	562	C
1	A	564	C
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	588	G
1	A	596	C
1	A	653	A
1	A	665	A
1	A	686	U
1	A	687	A
1	A	688	G
1	A	695	A
1	A	701	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	702	A
1	A	703	G
1	A	723	U
1	A	731	G
1	A	749	C
1	A	755	G
1	A	760	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	785	G
1	A	792	A
1	A	793	U
1	A	794	A
1	A	799	G
1	A	812	C
1	A	813	U
1	A	815	A
1	A	817	C
1	A	821	G
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	859	A
1	A	902	G
1	A	914	A
1	A	916	G
1	A	922	G
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	942	G
1	A	960	U
1	A	961	U
1	A	966	M2G
1	A	969	A
1	A	971	G
1	A	972	C
1	A	974	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	975	A
1	A	976	G
1	A	977	A
1	A	991	U
1	A	992	U
1	A	993	G
1	A	1004	A
1	A	1005	A
1	A	1023	G
1	A	1024	G
1	A	1026	G
1	A	1031	G
1	A	1045	C
1	A	1050	G
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1078	U
1	A	1093	A
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1146	A
1	A	1152	A
1	A	1159	U
1	A	1171	G
1	A	1183	A
1	A	1191	A
1	A	1195	C
1	A	1196	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1197	G
1	A	1201	A
1	A	1202	G
1	A	1211	U
1	A	1212	U
1	A	1214	C
1	A	1224	G
1	A	1225	A
1	A	1227	A
1	A	1228	C
1	A	1238	A
1	A	1241	G
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1270	C
1	A	1278	U
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1286	A
1	A	1287	A
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1306	A
1	A	1320	C
1	A	1336	C
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1353	G
1	A	1359	C
1	A	1362	C
1	A	1363	A
1	A	1368	G
1	A	1381	U
1	A	1397	C
1	A	1398	A
1	A	1400	5MC
1	A	1442	G
1	A	1446	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1447	G
1	A	1485	U
1	A	1487	G
1	A	1492	A
1	A	1499	A
1	A	1503	A
1	A	1504	G
1	A	1506	U
1	A	1517	G
1	A	1520	G
1	A	1529	G
1	A	1530	G
22	Y	5	U
22	Y	6	U
23	W	30	G
23	W	33	U
23	W	36	A
23	W	42	C

All (46) RNA pucker outliers are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	5	U
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	204	U
1	A	250	A
1	A	251	G
1	A	281	G
1	A	328	C
1	A	372	C
1	A	428	G
1	A	429	U
1	A	484	G
1	A	485	G
1	A	496	A
1	A	509	A
1	A	518	C
1	A	559	A
1	A	575	G
1	A	687	A

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Mol	Chain	Res	Type
1	A	701	C
1	A	748	C
1	A	792	A
1	A	812	C
1	A	913	A
1	A	960	U
1	A	965	A
1	A	992	U
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1126	U
1	A	1145	C
1	A	1182	G
1	A	1190	G
1	A	1201	A
1	A	1256	A
1	A	1257	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1305	G
1	A	1346	A
1	A	1347	G
1	A	1380	U
1	A	1505	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	A	1541	1,24	17,21,22	1.01	2 (11%)	20,30,33	3.08	6 (30%)
1	MA6	A	1519	1	19,26,27	1.26	2 (10%)	18,38,41	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5MC	A	1407	1	15,22,23	1.04	1 (6%)	19,32,35	1.09	1 (5%)
1	2MG	A	1207	1	19,26,27	2.40	4 (21%)	21,38,41	1.99	3 (14%)
1	PSU	A	516	1,24	17,21,22	1.05	2 (11%)	20,30,33	3.13	6 (30%)
1	MA6	A	1518	1	19,26,27	1.09	1 (5%)	18,38,41	0.72	0
1	4OC	A	1402	1,24	16,23,24	0.92	2 (12%)	17,32,35	0.75	0
1	5MC	A	1404	1	15,22,23	0.95	1 (6%)	19,32,35	1.15	2 (10%)
1	5MC	A	1400	1	15,22,23	1.04	1 (6%)	19,32,35	1.04	2 (10%)
1	G7M	A	527	1,24	20,26,27	1.67	3 (15%)	20,39,42	1.84	6 (30%)
1	UR3	A	1498	1	14,22,23	0.99	1 (7%)	15,32,35	1.03	0
1	M2G	A	966	1	20,27,28	2.01	4 (20%)	22,40,43	2.43	5 (22%)
1	5MC	A	967	1	15,22,23	0.98	0	19,32,35	1.00	1 (5%)
1	PSU	A	1540	1	17,21,22	1.06	1 (5%)	20,30,33	3.15	6 (30%)
12	0TD	L	92	12	4,9,10	0.87	0	3,11,13	1.90	1 (33%)

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
1	PSU	A	1541	1,24	-	1/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	3/7/29/30	0/3/3/3
1	5MC	A	1407	1	-	0/5/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
1	PSU	A	516	1,24	-	0/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	0/7/29/30	0/3/3/3
1	4OC	A	1402	1,24	-	2/9/29/30	0/2/2/2
1	5MC	A	1404	1	-	0/5/25/26	0/2/2/2
1	5MC	A	1400	1	-	2/5/25/26	0/2/2/2
1	G7M	A	527	1,24	-	2/3/25/26	0/3/3/3
1	UR3	A	1498	1	-	0/5/25/26	0/2/2/2
1	M2G	A	966	1	-	3/7/29/30	0/3/3/3
1	5MC	A	967	1	-	1/5/25/26	0/2/2/2
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
12	0TD	L	92	12	-	1/3/12/14	-

All (25) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1207	2MG	C2-N2	7.44	1.40	1.34
1	A	1207	2MG	C6-N1	5.98	1.43	1.33
1	A	966	M2G	C6-N1	5.93	1.43	1.33
1	A	527	G7M	C2-N2	4.83	1.43	1.33
1	A	966	M2G	C2-N2	4.07	1.41	1.34
1	A	966	M2G	C2-N1	3.57	1.40	1.34
1	A	966	M2G	C4-N3	3.41	1.41	1.35
1	A	1519	MA6	C6-N1	3.40	1.38	1.33
1	A	527	G7M	C4-N3	3.21	1.40	1.35
1	A	1540	PSU	C4-N3	3.11	1.38	1.33
1	A	516	PSU	C4-N3	3.06	1.38	1.33
1	A	1541	PSU	C4-N3	3.01	1.38	1.33
1	A	527	G7M	C6-N1	2.95	1.38	1.33
1	A	1518	MA6	C6-N1	2.86	1.37	1.33
1	A	1207	2MG	C4-N3	2.72	1.39	1.35
1	A	1498	UR3	C6-N1	2.50	1.38	1.35
1	A	1400	5MC	C5-C4	2.50	1.45	1.41
1	A	1519	MA6	C2-N1	2.35	1.38	1.33
1	A	1207	2MG	C2-N1	2.29	1.41	1.34
1	A	1407	5MC	C2-N3	2.26	1.42	1.38
1	A	1404	5MC	C5-C4	2.22	1.44	1.41
1	A	1402	4OC	C5-C4	2.09	1.44	1.39
1	A	516	PSU	O4'-C1'	-2.09	1.41	1.44
1	A	1402	4OC	C2-N3	2.02	1.42	1.38
1	A	1541	PSU	O4'-C1'	-2.01	1.41	1.44

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1540	PSU	N1-C2-N3	-10.73	119.90	128.43
1	A	516	PSU	N1-C2-N3	-10.68	119.94	128.43
1	A	1541	PSU	N1-C2-N3	-10.55	120.04	128.43
1	A	966	M2G	C5-C6-N1	-8.03	112.45	123.43
1	A	1207	2MG	C5-C6-N1	-7.47	113.21	123.43
1	A	966	M2G	C6-N1-C2	5.99	123.31	116.18
1	A	516	PSU	C4-N3-C2	5.88	120.11	115.14
1	A	1540	PSU	C4-N3-C2	5.53	119.81	115.14
1	A	1541	PSU	C4-N3-C2	5.31	119.63	115.14
1	A	516	PSU	C5-C4-N3	-4.39	119.71	125.36
1	A	1540	PSU	C5-C4-N3	-4.17	119.99	125.36
1	A	527	G7M	C2-N3-C4	4.17	120.11	115.36
1	A	1541	PSU	C5-C4-N3	-4.04	120.15	125.36
1	A	1207	2MG	C6-N1-C2	3.78	121.95	115.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	G7M	N3-C2-N1	-3.72	122.26	127.22
1	A	1541	PSU	C5-C6-N1	-3.53	120.11	124.44
1	A	527	G7M	C6-C5-C4	-3.47	117.49	120.80
1	A	1541	PSU	C6-N1-C2	3.31	120.81	115.36
1	A	1540	PSU	C5-C6-N1	-3.29	120.39	124.44
1	A	1540	PSU	C6-N1-C2	3.22	120.67	115.36
1	A	516	PSU	C5-C6-N1	-3.16	120.56	124.44
1	A	516	PSU	C6-N1-C2	3.08	120.44	115.36
1	A	527	G7M	C5-C6-N1	-2.92	119.43	123.43
1	A	966	M2G	N3-C2-N2	2.92	120.14	117.18
1	A	1404	5MC	N4-C4-N3	-2.81	113.06	117.03
12	L	92	0TD	CSB-SB-CB	-2.65	96.64	101.85
1	A	527	G7M	C6-N1-C2	2.65	120.14	115.93
1	A	1407	5MC	C2-N3-C4	2.44	118.96	116.02
1	A	1400	5MC	N4-C4-N3	-2.41	113.62	117.03
1	A	1404	5MC	C2-N3-C4	2.34	118.84	116.02
1	A	1540	PSU	C5-C1'-C2'	-2.33	111.16	115.32
1	A	527	G7M	C1'-N9-C4	-2.29	122.61	126.64
1	A	967	5MC	C2-N3-C4	2.28	118.76	116.02
1	A	1400	5MC	C2-N3-C4	2.25	118.74	116.02
1	A	966	M2G	N1-C2-N2	-2.13	115.04	117.19
1	A	1541	PSU	O4'-C1'-C2'	2.08	108.03	104.66
1	A	1207	2MG	C4-C5-N7	2.06	111.55	109.40
1	A	516	PSU	O4'-C1'-C2'	2.04	107.96	104.66
1	A	966	M2G	C2-N3-C4	-2.02	112.98	115.28

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1519	MA6	C3'-C4'-C5'-O5'
1	A	966	M2G	C4'-C5'-O5'-P
12	L	92	0TD	CG-CB-SB-CSB
1	A	1519	MA6	O4'-C4'-C5'-O5'
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	527	G7M	C3'-C4'-C5'-O5'
1	A	966	M2G	O4'-C4'-C5'-O5'
1	A	1519	MA6	C5-C6-N6-C9
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	527	G7M	O4'-C4'-C5'-O5'
1	A	966	M2G	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	967	5MC	O4'-C4'-C5'-O5'
1	A	1541	PSU	O4'-C1'-C5-C4
1	A	1402	4OC	C3'-C4'-C5'-O5'

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1519	MA6	1	0
1	A	1518	MA6	3	0
1	A	1404	5MC	1	0
1	A	527	G7M	1	0
1	A	1498	UR3	1	0
1	A	966	M2G	1	0
12	L	92	0TD	4	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 303 ligands modelled in this entry, 302 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
25	EUS	A	1814	-	32,37,37	1.89	5 (15%)	34,56,56	1.47	4 (11%)

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
25	EUS	A	1814	-	-	3/14/70/70	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1814	EUS	O1-S	5.79	1.53	1.43
25	A	1814	EUS	O2-S	5.66	1.53	1.43
25	A	1814	EUS	C31-C41	-4.70	1.40	1.50
25	A	1814	EUS	C61-C51	-3.72	1.40	1.48
25	A	1814	EUS	S-N12	2.10	1.66	1.62

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1814	EUS	O2-S-O1	-6.33	109.75	118.85
25	A	1814	EUS	C93-N33-C33	-2.61	110.59	114.38
25	A	1814	EUS	O1-S-N12	2.33	110.79	107.23
25	A	1814	EUS	C13-O62-C62	-2.18	112.56	117.96

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	1814	EUS	C23-C33-N33-C93
25	A	1814	EUS	C12-N12-S-C6
25	A	1814	EUS	C12-N12-S-O1

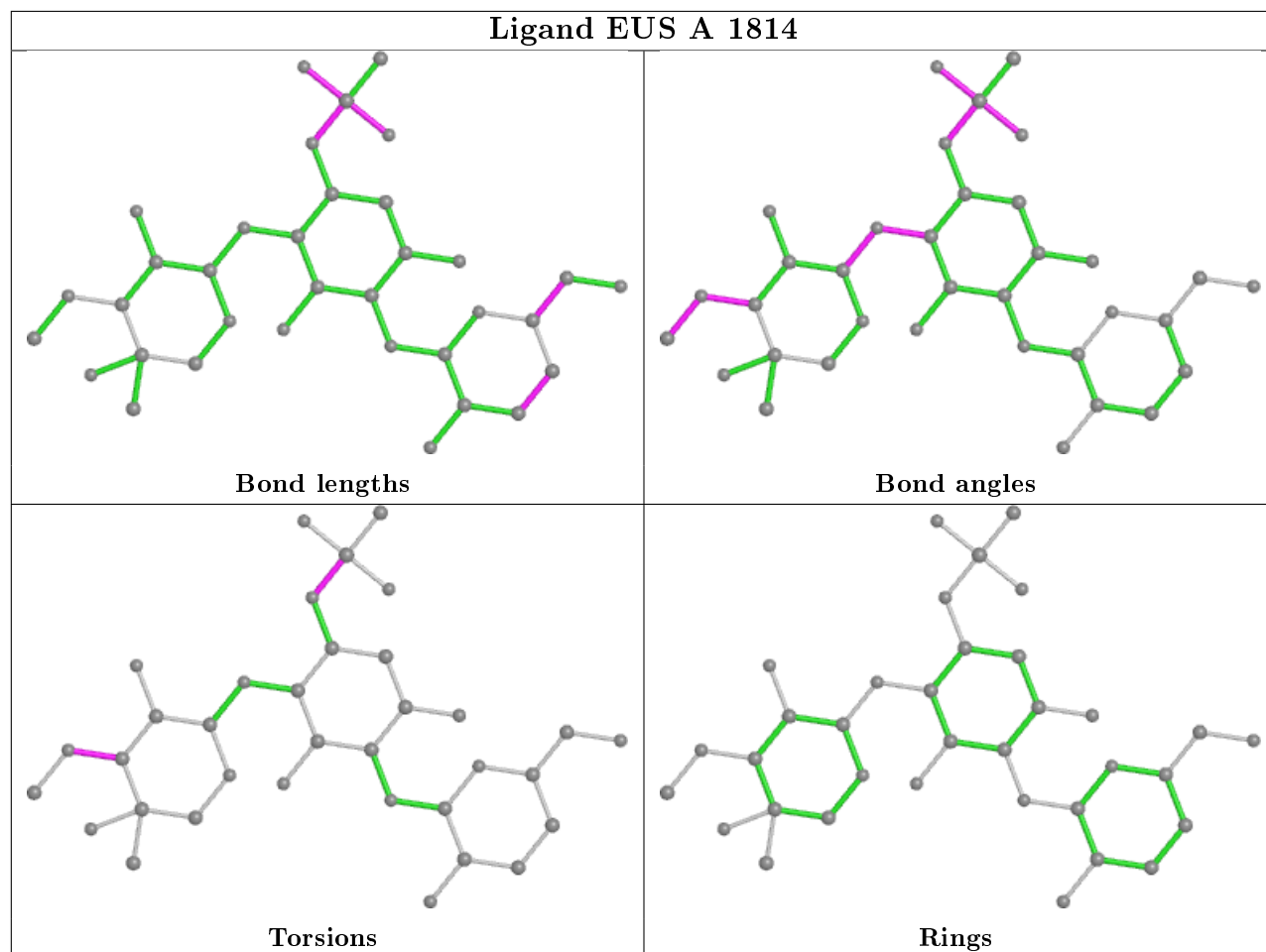
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	1814	EUS	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1498/1517 (98%)	-0.27	11 (0%) 87 83	51, 89, 179, 277	0
2	B	234/255 (91%)	-0.37	2 (0%) 84 79	68, 105, 180, 221	0
3	C	206/238 (86%)	-0.25	0 100 100	94, 131, 172, 199	0
4	D	208/208 (100%)	-0.28	4 (1%) 66 61	61, 105, 161, 180	0
5	E	150/161 (93%)	-0.52	0 100 100	44, 65, 102, 153	0
6	F	101/101 (100%)	-0.59	0 100 100	58, 98, 130, 156	0
7	G	155/155 (100%)	-0.32	1 (0%) 89 86	70, 107, 172, 208	0
8	H	138/138 (100%)	-0.70	0 100 100	32, 58, 81, 139	0
9	I	127/127 (100%)	-0.16	1 (0%) 86 81	92, 130, 170, 212	0
10	J	98/104 (94%)	0.22	5 (5%) 28 25	100, 152, 202, 232	0
11	K	116/128 (90%)	-0.39	0 100 100	48, 81, 126, 148	0
12	L	123/131 (93%)	-0.41	1 (0%) 86 81	55, 91, 133, 181	0
13	M	118/125 (94%)	-0.38	0 100 100	70, 106, 145, 230	0
14	N	60/60 (100%)	-0.30	0 100 100	89, 106, 152, 182	0
15	O	87/88 (98%)	-0.42	0 100 100	49, 72, 116, 163	0
16	P	83/88 (94%)	-0.60	0 100 100	53, 78, 113, 173	0
17	Q	99/104 (95%)	-0.56	0 100 100	37, 63, 103, 148	0
18	R	70/87 (80%)	-0.39	0 100 100	50, 82, 133, 190	0
19	S	80/92 (86%)	-0.05	0 100 100	87, 131, 194, 240	0
20	T	99/105 (94%)	-0.39	0 100 100	64, 84, 140, 188	0
21	U	24/26 (92%)	0.17	1 (4%) 36 32	97, 117, 154, 171	0
22	Y	6/6 (100%)	1.09	1 (16%) 1 2	94, 119, 165, 194	0
23	W	15/15 (100%)	1.27	3 (20%) 1 1	103, 145, 178, 190	0
All	All	3895/4059 (95%)	-0.31	30 (0%) 86 81	32, 95, 171, 277	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1129	C	7.6
1	A	1533	C	5.2
4	D	45	GLN	4.1
1	A	1539	C	4.0
22	Y	6	U	3.8
4	D	37	PRO	3.6
1	A	412	A	3.4
1	A	532	A	3.1
21	U	18	TYR	3.1
12	L	128	ALA	3.0
1	A	1035	A	3.0
10	J	33	GLN	3.0
4	D	35	ARG	2.9
23	W	29	G	2.8
4	D	36	ARG	2.7
9	I	15	ALA	2.7
10	J	99	LYS	2.6
10	J	34	VAL	2.6
7	G	155	ARG	2.6
23	W	30	G	2.5
10	J	74	ILE	2.5
2	B	127	ILE	2.3
1	A	1037	C	2.3
23	W	40	C	2.2
1	A	1036	G	2.2
1	A	1532	U	2.2
1	A	1003(A)	G	2.1
2	B	132	LYS	2.0
1	A	993	G	2.0
10	J	39	PRO	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	PSU	A	1540	20/21	0.83	0.57	265,273,277,281	0
1	2MG	A	1207	24/25	0.92	0.17	123,130,141,143	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	PSU	A	1541	20/21	0.92	0.31	196,209,234,234	0
1	MA6	A	1519	24/25	0.93	0.27	66,75,82,84	0
1	PSU	A	516	20/21	0.94	0.14	100,107,109,110	0
12	0TD	L	92	10/11	0.94	0.19	105,124,130,130	0
1	5MC	A	1400	21/22	0.95	0.18	68,74,77,80	0
1	5MC	A	1407	21/22	0.95	0.21	74,79,86,95	0
1	MA6	A	1518	24/25	0.95	0.23	71,85,95,97	0
1	G7M	A	527	24/25	0.96	0.18	72,74,82,84	0
1	M2G	A	966	25/26	0.96	0.17	88,95,100,103	0
1	5MC	A	967	21/22	0.96	0.15	72,74,78,82	0
1	5MC	A	1404	21/22	0.96	0.17	66,68,71,72	0
1	4OC	A	1402	22/23	0.96	0.18	70,73,78,82	0
1	UR3	A	1498	21/22	0.97	0.20	66,69,72,79	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
24	MG	A	1812	1/1	0.37	0.29	487,487,487,487	0
24	MG	A	1714	1/1	0.45	0.53	191,191,191,191	0
24	MG	A	1676	1/1	0.51	0.13	116,116,116,116	0
24	MG	A	1875	1/1	0.53	0.19	106,106,106,106	0
24	MG	A	1696	1/1	0.55	0.53	96,96,96,96	0
24	MG	A	1709	1/1	0.60	0.52	75,75,75,75	0
24	MG	A	1677	1/1	0.61	0.59	135,135,135,135	0
24	MG	A	1692	1/1	0.62	0.29	127,127,127,127	0
24	MG	A	1679	1/1	0.64	0.21	38,38,38,38	0
24	MG	A	1773	1/1	0.67	0.58	85,85,85,85	0
24	MG	D	304	1/1	0.69	0.26	97,97,97,97	0
24	MG	A	1826	1/1	0.70	0.43	111,111,111,111	0
24	MG	A	1790	1/1	0.70	0.77	117,117,117,117	0
24	MG	A	1794	1/1	0.72	0.39	172,172,172,172	0
24	MG	A	1857	1/1	0.72	0.20	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
24	MG	A	1759	1/1	0.73	0.59	50,50,50,50	0
24	MG	A	1820	1/1	0.73	0.17	45,45,45,45	0
24	MG	A	1861	1/1	0.73	0.21	97,97,97,97	0
24	MG	A	1767	1/1	0.74	0.76	51,51,51,51	0
24	MG	A	1780	1/1	0.74	0.19	91,91,91,91	0
24	MG	A	1830	1/1	0.74	0.64	108,108,108,108	0
24	MG	A	1822	1/1	0.75	0.24	75,75,75,75	0
24	MG	A	1661	1/1	0.76	0.26	113,113,113,113	0
24	MG	A	1717	1/1	0.76	0.27	61,61,61,61	0
24	MG	S	101	1/1	0.76	0.17	54,54,54,54	0
24	MG	A	1786	1/1	0.77	0.20	75,75,75,75	0
24	MG	A	1741	1/1	0.77	0.46	47,47,47,47	0
24	MG	A	1680	1/1	0.78	0.72	57,57,57,57	0
24	MG	A	1667	1/1	0.78	0.36	72,72,72,72	0
24	MG	L	201	1/1	0.78	0.12	89,89,89,89	0
24	MG	B	303	1/1	0.78	0.61	121,121,121,121	0
24	MG	A	1760	1/1	0.78	0.25	60,60,60,60	0
24	MG	A	1793	1/1	0.78	0.23	163,163,163,163	0
24	MG	A	1865	1/1	0.78	0.14	71,71,71,71	0
24	MG	A	1756	1/1	0.79	0.69	46,46,46,46	0
24	MG	A	1665	1/1	0.79	0.17	76,76,76,76	0
24	MG	A	1625	1/1	0.79	0.57	54,54,54,54	0
24	MG	A	1601	1/1	0.80	0.78	142,142,142,142	0
24	MG	A	1853	1/1	0.80	0.34	80,80,80,80	0
24	MG	A	1639	1/1	0.80	0.11	77,77,77,77	0
24	MG	A	1633	1/1	0.80	0.32	34,34,34,34	0
24	MG	A	1795	1/1	0.80	0.24	104,104,104,104	0
24	MG	A	1733	1/1	0.80	0.43	59,59,59,59	0
24	MG	A	1684	1/1	0.80	0.33	83,83,83,83	0
24	MG	A	1613	1/1	0.81	0.21	115,115,115,115	0
24	MG	A	1808	1/1	0.81	0.64	59,59,59,59	0
24	MG	B	302	1/1	0.81	0.06	51,51,51,51	0
24	MG	A	1745	1/1	0.81	0.25	37,37,37,37	0
24	MG	C	302	1/1	0.82	0.20	60,60,60,60	0
24	MG	Q	201	1/1	0.82	0.11	28,28,28,28	0
24	MG	A	1743	1/1	0.82	0.37	73,73,73,73	0
24	MG	A	1711	1/1	0.82	0.19	52,52,52,52	0
24	MG	A	1646	1/1	0.83	0.41	64,64,64,64	0
24	MG	A	1796	1/1	0.83	0.21	48,48,48,48	0
24	MG	A	1650	1/1	0.83	0.32	47,47,47,47	0
24	MG	A	1705	1/1	0.83	0.42	40,40,40,40	0
24	MG	A	1616	1/1	0.83	0.24	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
24	MG	A	1675	1/1	0.83	0.38	72,72,72,72	0
24	MG	A	1851	1/1	0.83	0.34	66,66,66,66	0
24	MG	A	1664	1/1	0.84	0.46	80,80,80,80	0
24	MG	A	1817	1/1	0.84	0.48	52,52,52,52	0
24	MG	A	1669	1/1	0.84	0.43	171,171,171,171	0
24	MG	A	1804	1/1	0.84	0.62	64,64,64,64	0
24	MG	A	1634	1/1	0.84	0.26	106,106,106,106	0
24	MG	A	1803	1/1	0.84	0.32	24,24,24,24	0
24	MG	A	1693	1/1	0.84	0.14	97,97,97,97	0
24	MG	A	1792	1/1	0.84	0.21	114,114,114,114	0
24	MG	A	1612	1/1	0.85	0.12	131,131,131,131	0
24	MG	P	103	1/1	0.85	0.15	42,42,42,42	0
24	MG	A	1769	1/1	0.85	0.22	19,19,19,19	0
24	MG	D	302	1/1	0.85	0.21	60,60,60,60	0
24	MG	A	1776	1/1	0.85	0.30	49,49,49,49	0
24	MG	A	1784	1/1	0.85	0.28	66,66,66,66	0
24	MG	A	1729	1/1	0.85	0.35	51,51,51,51	0
24	MG	A	1716	1/1	0.86	0.39	29,29,29,29	0
24	MG	A	1668	1/1	0.86	0.25	37,37,37,37	0
24	MG	A	1863	1/1	0.86	0.28	38,38,38,38	0
24	MG	A	1775	1/1	0.86	0.87	77,77,77,77	0
24	MG	A	1721	1/1	0.86	0.27	119,119,119,119	0
24	MG	A	1659	1/1	0.86	0.29	23,23,23,23	0
24	MG	A	1670	1/1	0.86	0.45	58,58,58,58	0
24	MG	A	1854	1/1	0.86	0.42	87,87,87,87	0
24	MG	A	1719	1/1	0.86	0.27	39,39,39,39	0
24	MG	A	1811	1/1	0.86	0.31	74,74,74,74	0
24	MG	A	1658	1/1	0.87	0.27	32,32,32,32	0
24	MG	A	1797	1/1	0.87	0.35	44,44,44,44	0
24	MG	A	1859	1/1	0.87	0.29	100,100,100,100	0
24	MG	A	1832	1/1	0.87	0.24	14,14,14,14	0
24	MG	A	1610	1/1	0.87	0.22	55,55,55,55	0
24	MG	A	1617	1/1	0.88	0.59	89,89,89,89	0
24	MG	A	1778	1/1	0.88	0.10	47,47,47,47	0
24	MG	A	1708	1/1	0.88	0.37	58,58,58,58	0
24	MG	P	101	1/1	0.88	0.25	31,31,31,31	0
24	MG	A	1783	1/1	0.88	0.40	41,41,41,41	0
24	MG	A	1815	1/1	0.88	0.22	65,65,65,65	0
24	MG	I	201	1/1	0.88	0.13	59,59,59,59	0
24	MG	A	1727	1/1	0.88	0.73	60,60,60,60	0
24	MG	A	1873	1/1	0.88	0.31	93,93,93,93	0
24	MG	A	1685	1/1	0.88	0.36	282,282,282,282	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	1723	1/1	0.88	0.27	32,32,32,32	0
24	MG	A	1844	1/1	0.88	0.24	27,27,27,27	0
24	MG	A	1662	1/1	0.88	0.15	108,108,108,108	0
24	MG	A	1615	1/1	0.88	0.10	34,34,34,34	0
24	MG	A	1757	1/1	0.88	0.24	38,38,38,38	0
24	MG	A	1847	1/1	0.88	0.29	29,29,29,29	0
24	MG	A	1690	1/1	0.88	0.20	78,78,78,78	0
24	MG	A	1623	1/1	0.88	0.23	13,13,13,13	0
24	MG	A	1837	1/1	0.88	0.36	23,23,23,23	0
24	MG	A	1732	1/1	0.88	0.47	52,52,52,52	0
24	MG	A	1838	1/1	0.88	0.43	52,52,52,52	0
24	MG	A	1715	1/1	0.88	0.37	81,81,81,81	0
24	MG	A	1687	1/1	0.88	0.23	54,54,54,54	0
24	MG	A	1736	1/1	0.89	0.19	38,38,38,38	0
24	MG	A	1651	1/1	0.89	0.17	70,70,70,70	0
24	MG	A	1855	1/1	0.89	0.38	40,40,40,40	0
24	MG	A	1726	1/1	0.89	0.26	40,40,40,40	0
24	MG	A	1718	1/1	0.89	0.33	72,72,72,72	0
24	MG	A	1762	1/1	0.89	0.26	24,24,24,24	0
24	MG	A	1699	1/1	0.89	0.17	44,44,44,44	0
24	MG	A	1798	1/1	0.89	0.33	30,30,30,30	0
24	MG	A	1698	1/1	0.89	0.18	134,134,134,134	0
24	MG	A	1771	1/1	0.89	0.23	32,32,32,32	0
24	MG	A	1738	1/1	0.89	0.18	41,41,41,41	0
24	MG	A	1686	1/1	0.90	0.28	22,22,22,22	0
24	MG	A	1748	1/1	0.90	0.39	55,55,55,55	0
24	MG	A	1739	1/1	0.90	0.13	12,12,12,12	0
24	MG	A	1652	1/1	0.90	0.09	69,69,69,69	0
24	MG	A	1766	1/1	0.90	0.15	41,41,41,41	0
24	MG	A	1764	1/1	0.90	0.25	48,48,48,48	0
24	MG	A	1770	1/1	0.90	0.28	57,57,57,57	0
24	MG	A	1606	1/1	0.90	0.16	32,32,32,32	0
24	MG	A	1843	1/1	0.90	0.35	42,42,42,42	0
24	MG	A	1805	1/1	0.90	0.17	64,64,64,64	0
24	MG	A	1806	1/1	0.90	0.36	56,56,56,56	0
24	MG	A	1829	1/1	0.91	0.25	32,32,32,32	0
24	MG	A	1724	1/1	0.91	0.17	14,14,14,14	0
24	MG	A	1813	1/1	0.91	0.28	36,36,36,36	0
24	MG	A	1655	1/1	0.91	0.35	44,44,44,44	0
24	MG	A	1840	1/1	0.91	0.18	15,15,15,15	0
24	MG	A	1810	1/1	0.91	0.21	78,78,78,78	0
24	MG	A	1626	1/1	0.91	0.21	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	1860	1/1	0.91	0.14	95,95,95,95	0
24	MG	A	1713	1/1	0.91	0.37	37,37,37,37	0
24	MG	A	1636	1/1	0.91	0.23	51,51,51,51	0
24	MG	A	1849	1/1	0.91	0.18	19,19,19,19	0
24	MG	A	1645	1/1	0.91	0.32	36,36,36,36	0
24	MG	F	201	1/1	0.91	0.19	75,75,75,75	0
24	MG	A	1842	1/1	0.91	0.27	75,75,75,75	0
24	MG	A	1654	1/1	0.91	0.40	35,35,35,35	0
24	MG	A	1614	1/1	0.91	0.20	117,117,117,117	0
24	MG	A	1824	1/1	0.91	0.25	30,30,30,30	0
24	MG	A	1845	1/1	0.92	0.17	22,22,22,22	0
24	MG	A	1774	1/1	0.92	0.23	51,51,51,51	0
24	MG	A	1768	1/1	0.92	0.12	40,40,40,40	0
24	MG	A	1627	1/1	0.92	0.23	49,49,49,49	0
24	MG	A	1691	1/1	0.92	0.27	35,35,35,35	0
24	MG	A	1750	1/1	0.92	0.35	41,41,41,41	0
24	MG	P	102	1/1	0.92	0.28	12,12,12,12	0
24	MG	A	1828	1/1	0.92	0.26	27,27,27,27	0
24	MG	A	1642	1/1	0.92	0.25	95,95,95,95	0
24	MG	A	1871	1/1	0.92	0.12	57,57,57,57	0
24	MG	A	1644	1/1	0.92	0.23	58,58,58,58	0
24	MG	A	1782	1/1	0.92	0.25	26,26,26,26	0
24	MG	E	202	1/1	0.92	0.39	112,112,112,112	0
24	MG	A	1836	1/1	0.92	0.31	25,25,25,25	0
24	MG	J	201	1/1	0.93	0.20	34,34,34,34	0
24	MG	A	1720	1/1	0.93	0.26	44,44,44,44	0
24	MG	A	1781	1/1	0.93	0.20	80,80,80,80	0
24	MG	A	1850	1/1	0.93	0.18	19,19,19,19	0
25	EUS	A	1814	35/35	0.93	0.27	75,82,108,110	0
24	MG	A	1635	1/1	0.93	0.18	78,78,78,78	0
24	MG	A	1867	1/1	0.93	0.14	49,49,49,49	0
24	MG	A	1833	1/1	0.93	0.35	48,48,48,48	0
24	MG	A	1603	1/1	0.93	0.14	77,77,77,77	0
24	MG	A	1697	1/1	0.93	0.24	36,36,36,36	0
24	MG	A	1631	1/1	0.93	0.27	100,100,100,100	0
24	MG	A	1725	1/1	0.93	0.15	12,12,12,12	0
24	MG	A	1746	1/1	0.93	0.21	52,52,52,52	0
24	MG	A	1611	1/1	0.93	0.11	93,93,93,93	0
24	MG	A	1779	1/1	0.93	0.32	45,45,45,45	0
24	MG	A	1761	1/1	0.93	0.35	90,90,90,90	0
24	MG	A	1809	1/1	0.93	0.22	102,102,102,102	0
26	ZN	N	101	1/1	0.94	0.15	149,149,149,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
24	MG	A	1666	1/1	0.94	0.18	78,78,78,78	0
24	MG	A	1673	1/1	0.94	0.21	33,33,33,33	0
24	MG	A	1604	1/1	0.94	0.20	27,27,27,27	0
24	MG	A	1648	1/1	0.94	0.20	36,36,36,36	0
24	MG	A	1758	1/1	0.94	0.20	0,0,0,0	0
24	MG	D	303	1/1	0.94	0.06	57,57,57,57	0
24	MG	A	1628	1/1	0.94	0.21	83,83,83,83	0
24	MG	A	1869	1/1	0.94	0.15	35,35,35,35	0
24	MG	A	1712	1/1	0.94	0.10	46,46,46,46	0
24	MG	A	1649	1/1	0.94	0.19	88,88,88,88	0
24	MG	A	1821	1/1	0.94	0.10	46,46,46,46	0
24	MG	A	1751	1/1	0.94	0.13	29,29,29,29	0
24	MG	A	1852	1/1	0.94	0.28	45,45,45,45	0
24	MG	A	1866	1/1	0.94	0.14	34,34,34,34	0
24	MG	A	1695	1/1	0.94	0.18	111,111,111,111	0
24	MG	Q	202	1/1	0.94	0.19	14,14,14,14	0
24	MG	A	1700	1/1	0.94	0.19	151,151,151,151	0
24	MG	A	1731	1/1	0.94	0.27	56,56,56,56	0
24	MG	A	1825	1/1	0.94	0.20	73,73,73,73	0
24	MG	A	1728	1/1	0.94	0.14	27,27,27,27	0
24	MG	A	1682	1/1	0.94	0.17	103,103,103,103	0
24	MG	A	1607	1/1	0.94	0.15	94,94,94,94	0
24	MG	A	1609	1/1	0.94	0.21	49,49,49,49	0
24	MG	A	1703	1/1	0.94	0.30	66,66,66,66	0
24	MG	A	1660	1/1	0.94	0.14	39,39,39,39	0
24	MG	A	1802	1/1	0.94	0.14	43,43,43,43	0
24	MG	A	1621	1/1	0.94	0.63	72,72,72,72	0
24	MG	A	1710	1/1	0.95	0.76	37,37,37,37	0
24	MG	A	1674	1/1	0.95	0.18	22,22,22,22	0
24	MG	A	1785	1/1	0.95	0.19	37,37,37,37	0
24	MG	A	1862	1/1	0.95	0.28	21,21,21,21	0
24	MG	A	1602	1/1	0.95	0.14	52,52,52,52	0
24	MG	A	1789	1/1	0.95	0.18	65,65,65,65	0
24	MG	A	1818	1/1	0.95	0.22	16,16,16,16	0
24	MG	A	1683	1/1	0.95	0.11	71,71,71,71	0
24	MG	A	1647	1/1	0.95	0.09	93,93,93,93	0
24	MG	A	1672	1/1	0.95	0.11	60,60,60,60	0
24	MG	A	1754	1/1	0.95	0.11	32,32,32,32	0
24	MG	A	1701	1/1	0.95	0.18	64,64,64,64	0
24	MG	A	1735	1/1	0.95	0.15	41,41,41,41	0
24	MG	A	1870	1/1	0.95	0.24	8,8,8,8	0
24	MG	A	1747	1/1	0.95	0.17	38,38,38,38	0

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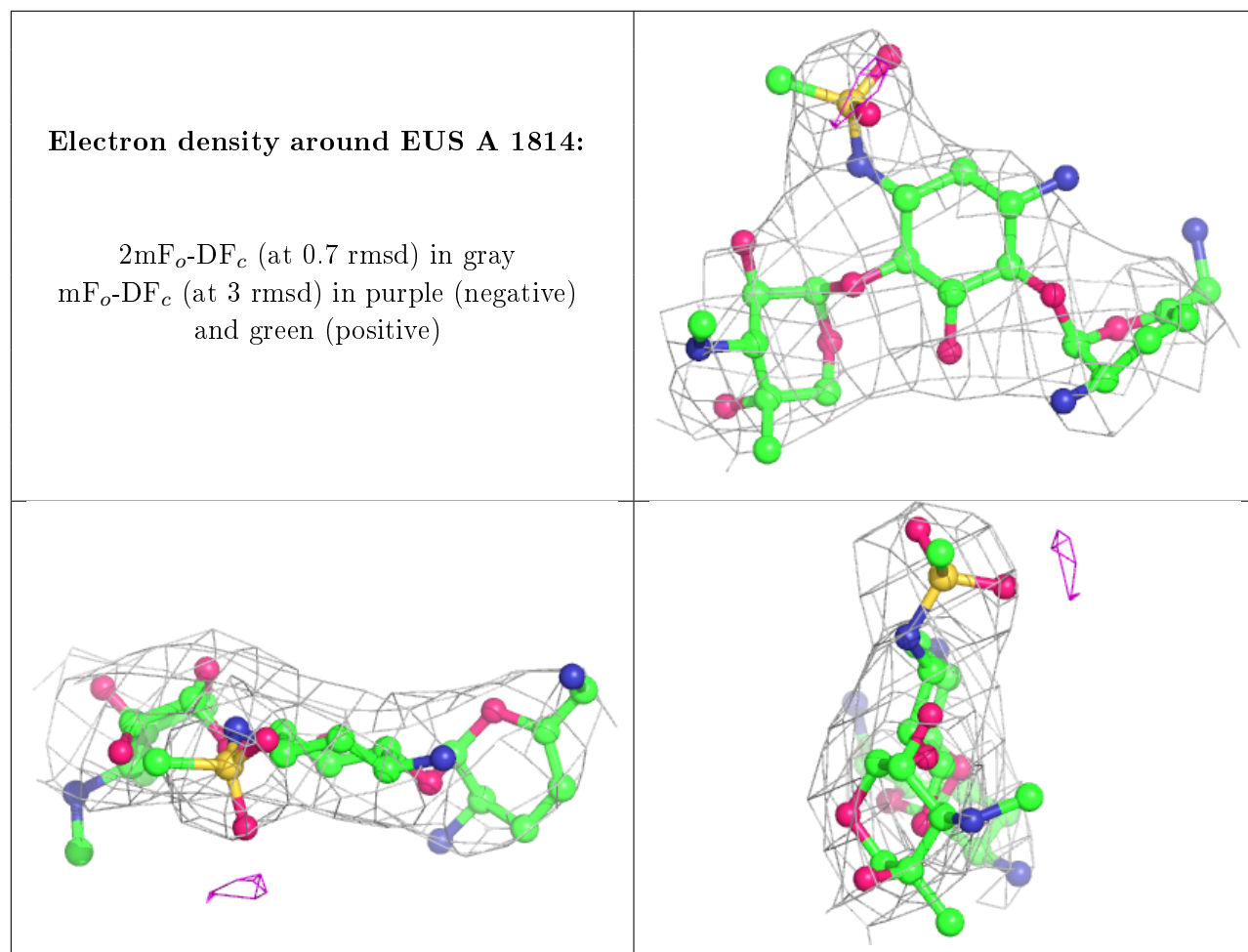
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
24	MG	A	1688	1/1	0.95	0.41	29,29,29,29	0
24	MG	A	1641	1/1	0.95	0.16	90,90,90,90	0
24	MG	A	1753	1/1	0.95	0.22	42,42,42,42	0
24	MG	A	1678	1/1	0.95	0.13	37,37,37,37	0
24	MG	A	1629	1/1	0.95	0.15	17,17,17,17	0
24	MG	B	301	1/1	0.95	0.34	23,23,23,23	0
24	MG	A	1630	1/1	0.95	0.20	92,92,92,92	0
24	MG	A	1839	1/1	0.95	0.14	18,18,18,18	0
24	MG	A	1834	1/1	0.95	0.27	19,19,19,19	0
24	MG	A	1749	1/1	0.96	0.10	42,42,42,42	0
24	MG	A	1637	1/1	0.96	0.22	24,24,24,24	0
24	MG	A	1868	1/1	0.96	0.23	32,32,32,32	0
24	MG	A	1722	1/1	0.96	0.13	25,25,25,25	0
24	MG	A	1752	1/1	0.96	0.26	26,26,26,26	0
24	MG	A	1787	1/1	0.96	0.24	26,26,26,26	0
24	MG	A	1689	1/1	0.96	0.20	51,51,51,51	0
24	MG	D	305	1/1	0.96	0.16	20,20,20,20	0
24	MG	A	1640	1/1	0.96	0.15	46,46,46,46	0
24	MG	A	1744	1/1	0.96	0.12	10,10,10,10	0
24	MG	A	1846	1/1	0.96	0.17	27,27,27,27	0
24	MG	A	1765	1/1	0.96	0.17	26,26,26,26	0
24	MG	L	203	1/1	0.96	0.18	37,37,37,37	0
24	MG	A	1638	1/1	0.96	0.17	56,56,56,56	0
24	MG	A	1704	1/1	0.96	0.09	71,71,71,71	0
24	MG	H	202	1/1	0.96	0.17	14,14,14,14	0
24	MG	A	1605	1/1	0.96	0.18	113,113,113,113	0
24	MG	A	1618	1/1	0.96	0.10	48,48,48,48	0
24	MG	A	1841	1/1	0.96	0.18	27,27,27,27	0
24	MG	A	1632	1/1	0.96	0.11	39,39,39,39	0
24	MG	A	1772	1/1	0.96	0.15	19,19,19,19	0
24	MG	A	1619	1/1	0.96	0.14	71,71,71,71	0
24	MG	A	1737	1/1	0.96	0.09	71,71,71,71	0
24	MG	A	1624	1/1	0.96	0.10	29,29,29,29	0
24	MG	A	1874	1/1	0.96	0.15	65,65,65,65	0
24	MG	A	1694	1/1	0.96	0.09	10,10,10,10	0
24	MG	A	1707	1/1	0.96	0.14	90,90,90,90	0
24	MG	A	1848	1/1	0.96	0.19	41,41,41,41	0
24	MG	A	1864	1/1	0.96	0.13	24,24,24,24	0
24	MG	A	1872	1/1	0.96	0.21	75,75,75,75	0
24	MG	Q	203	1/1	0.96	0.20	47,47,47,47	0
24	MG	A	1730	1/1	0.96	0.12	32,32,32,32	0
24	MG	A	1742	1/1	0.96	0.11	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	1823	1/1	0.97	0.15	8,8,8,8	0
24	MG	A	1740	1/1	0.97	0.08	21,21,21,21	0
24	MG	A	1663	1/1	0.97	0.22	93,93,93,93	0
24	MG	A	1622	1/1	0.97	0.19	4,4,4,4	0
24	MG	A	1671	1/1	0.97	0.12	104,104,104,104	0
24	MG	A	1800	1/1	0.97	0.09	23,23,23,23	0
24	MG	H	201	1/1	0.97	0.10	10,10,10,10	0
24	MG	A	1807	1/1	0.97	0.25	6,6,6,6	0
24	MG	A	1801	1/1	0.97	0.12	23,23,23,23	0
24	MG	A	1643	1/1	0.97	0.18	22,22,22,22	0
24	MG	A	1656	1/1	0.97	0.11	65,65,65,65	0
24	MG	A	1653	1/1	0.97	0.18	40,40,40,40	0
24	MG	A	1620	1/1	0.97	0.10	47,47,47,47	0
24	MG	A	1816	1/1	0.97	0.10	53,53,53,53	0
24	MG	A	1657	1/1	0.97	0.40	40,40,40,40	0
24	MG	A	1856	1/1	0.97	0.20	43,43,43,43	0
24	MG	C	301	1/1	0.97	0.18	68,68,68,68	0
24	MG	A	1777	1/1	0.97	0.08	17,17,17,17	0
24	MG	A	1835	1/1	0.97	0.28	9,9,9,9	0
24	MG	A	1608	1/1	0.97	0.08	34,34,34,34	0
24	MG	A	1706	1/1	0.97	0.31	163,163,163,163	0
24	MG	L	202	1/1	0.98	0.20	32,32,32,32	0
24	MG	A	1681	1/1	0.98	0.12	52,52,52,52	0
24	MG	A	1763	1/1	0.98	0.11	10,10,10,10	0
24	MG	A	1702	1/1	0.98	0.27	84,84,84,84	0
24	MG	A	1831	1/1	0.98	0.17	8,8,8,8	0
24	MG	A	1858	1/1	0.98	0.18	34,34,34,34	0
24	MG	E	201	1/1	0.98	0.51	116,116,116,116	0
24	MG	A	1734	1/1	0.98	0.14	39,39,39,39	0
24	MG	A	1827	1/1	0.98	0.11	86,86,86,86	0
24	MG	A	1819	1/1	0.98	0.08	17,17,17,17	0
24	MG	A	1791	1/1	0.98	0.12	93,93,93,93	0
26	ZN	D	301	1/1	0.98	0.21	82,82,82,82	0
24	MG	A	1755	1/1	0.99	0.11	18,18,18,18	0
24	MG	A	1788	1/1	0.99	0.52	103,103,103,103	0
24	MG	A	1799	1/1	0.99	0.16	39,39,39,39	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.