



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 10:26 AM GMT

PDB ID : 3OTO
Title : Crystal Structure of the 30S ribosomal subunit from a KsgA mutant of *Thermus thermophilus* (HB8)
Authors : Demirci, H.; Murphy IV, F.; Belardinelli, R.; Kelley, A.C.; Ramakrishnan, V.; Gregory, S.T.; Dahlberg, A.E.; Jorgl, G.
Deposited on : 2010-09-13
Resolution : 3.69 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

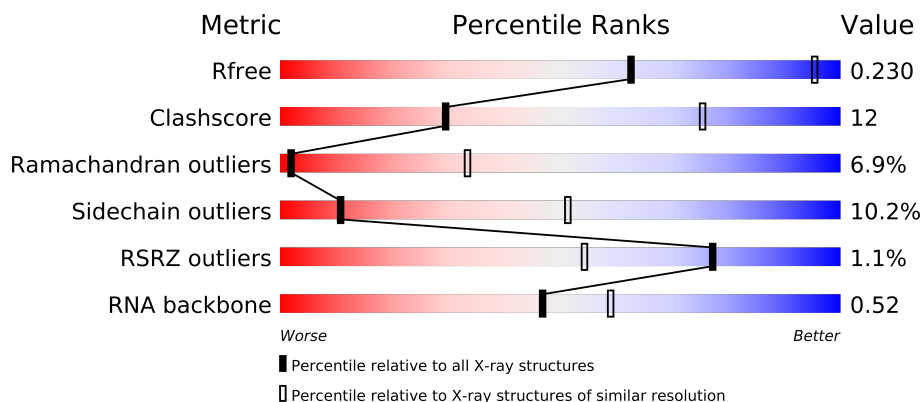
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.69 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.









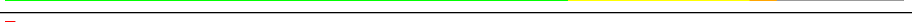

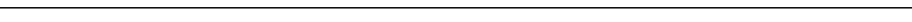
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1098 (4.00-3.40)
Clashscore	79885	1009 (3.94-3.46)
Ramachandran outliers	78287	1016 (3.98-3.42)
Sidechain outliers	78261	1014 (3.98-3.42)
RSRZ outliers	66119	1099 (4.00-3.40)
RNA backbone	1838	1008 (4.52-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1522	
2	B	256	
3	C	239	
4	D	209	
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	135	

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Mol	Chain	Length	Quality of chain
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 51775 atoms, of which 0 are hydrogen and 0 are deuterium.

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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1513	Total	C	N	O	P	0	0	0
			32511	14472	6016	10511	1512			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	0	0
			1873	1195	335	338	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

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

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

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

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	S	0	0	0
			1011	639	198	174				

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

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

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	115	Total	C	N	O	S	0	0	0
			921	569	190	160	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

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

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	73	Total	C	N	O	0	0	0
			597	380	118	99			

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

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

- 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
			762	469	162	129	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	41	VAL	ILE	SEE REMARK 999	UNP P80380

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

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

- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	B	1	Total	Mg	0	0
			1	1		
23	A	91	Total	Mg	0	0
			91	91		
23	D	1	Total	Mg	0	0
			1	1		
23	M	1	Total	Mg	0	0
			1	1		

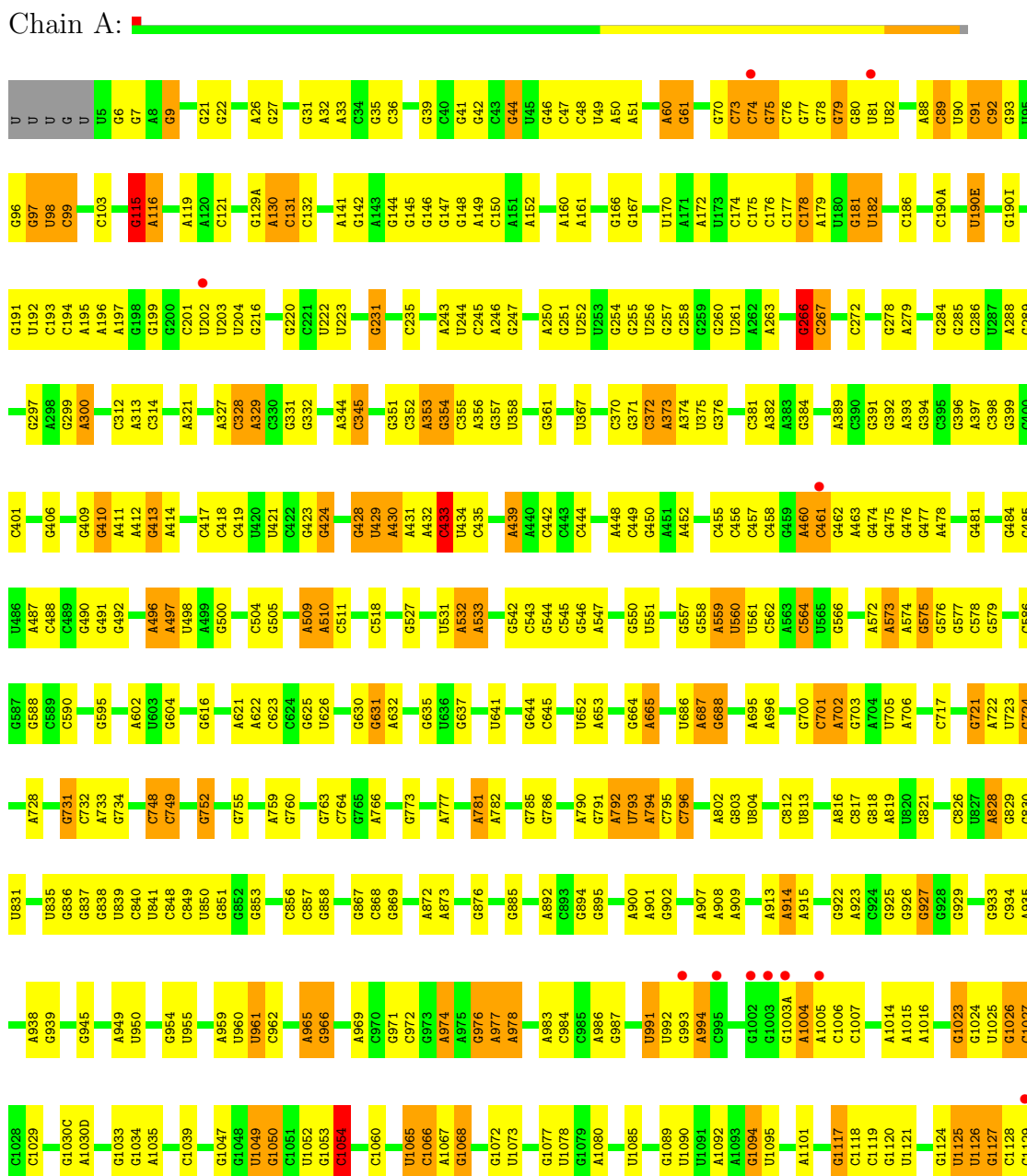
- Molecule 24 is POTASSIUM ION (three-letter code: K) (formula: K).

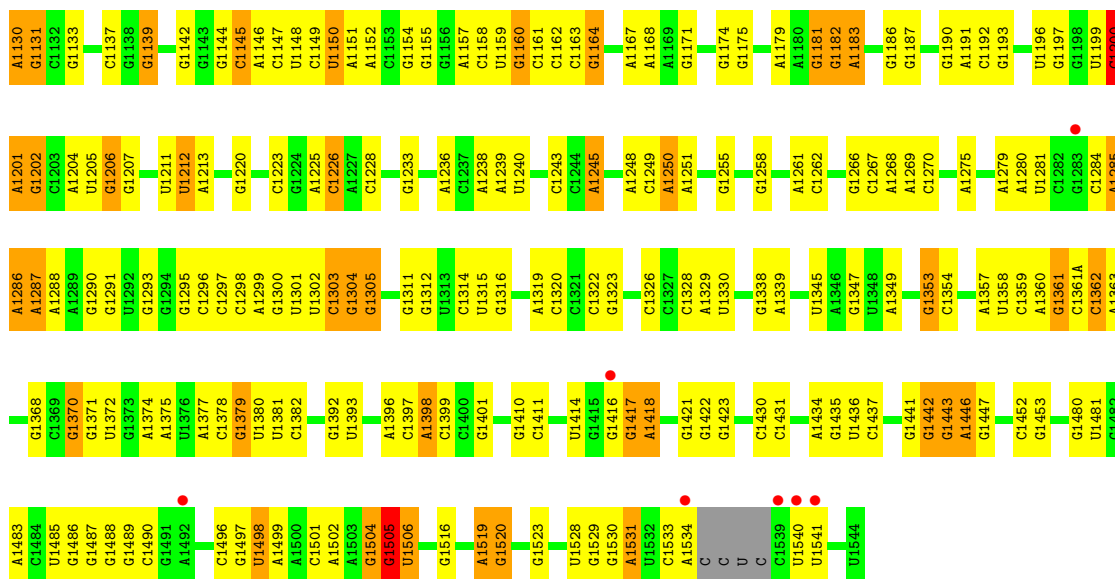
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	41	Total	K	0	0
			41	41		
24	E	1	Total	K	0	0
			1	1		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

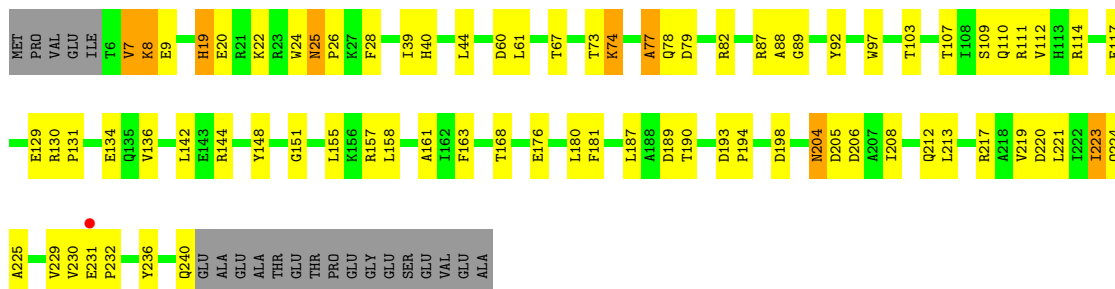
• Molecule 1: 16S rRNA





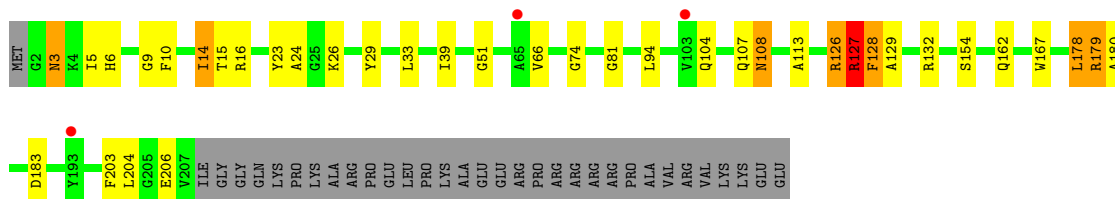
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain B:



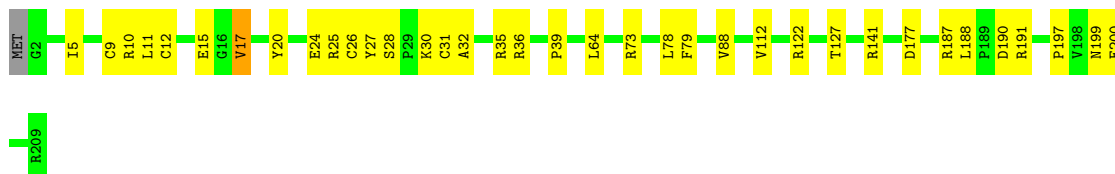
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain C:



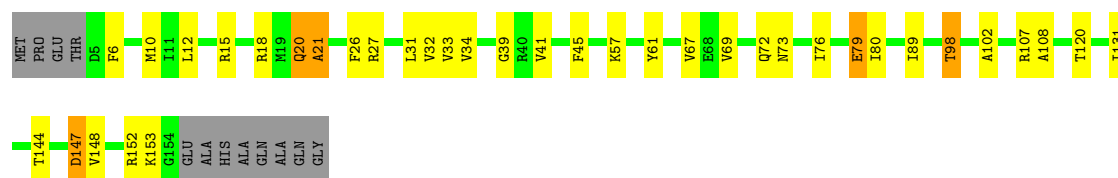
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain D:



• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain E: 



- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain F: 



- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain G: 



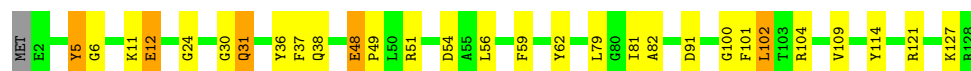
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain H: 



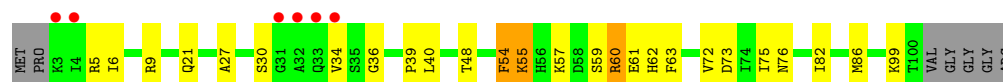
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain I: 



- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain J: 



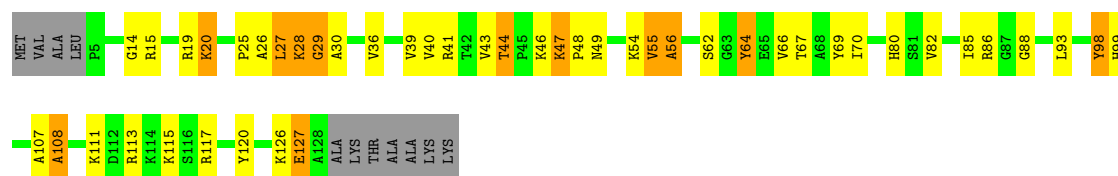
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain K: 



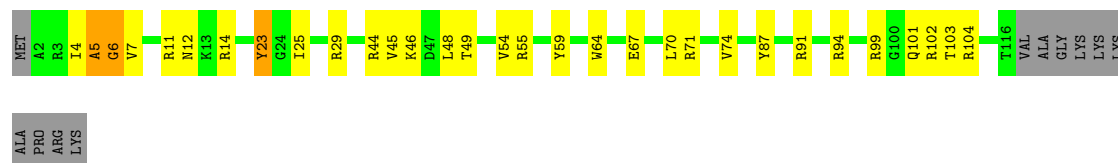
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain L:



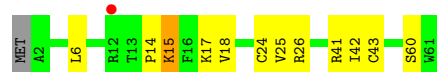
- Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain M:



- Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain N:



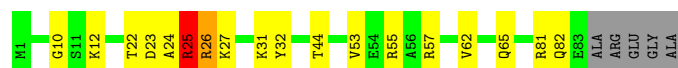
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain O:



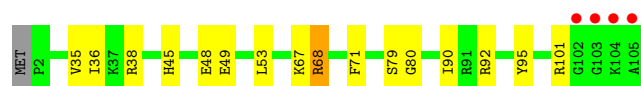
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain P:



- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain Q:



- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain R:

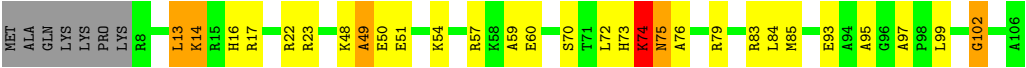


- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain S:



● Molecule 20: 30S RIBOSOMAL PROTEIN S20



● Molecule 21: 30S RIBOSOMAL PROTEIN THX



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	402.09Å 402.09Å 173.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.84 – 3.69 29.84 – 3.69	Depositor EDS
% Data completeness (in resolution range)	92.7 (29.84-3.69) 97.8 (29.84-3.69)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 3.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.173 , 0.231 0.175 , 0.230	Depositor DCC
R_{free} test set	7425 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	112.1	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 57.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 148377 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	51775	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.45	0/36390	0.81	19/56793 (0.0%)
2	B	0.32	0/1908	0.49	0/2577
3	C	0.25	0/1636	0.44	0/2205
4	D	0.31	0/1733	0.47	0/2318
5	E	0.39	0/1162	0.58	0/1564
6	F	0.29	0/856	0.47	0/1154
7	G	0.26	0/1276	0.44	0/1709
8	H	0.42	0/1136	0.59	0/1527
9	I	0.28	0/1029	0.46	0/1378
10	J	0.27	0/805	0.47	0/1082
11	K	0.32	0/900	0.50	0/1213
12	L	0.34	0/986	0.55	0/1320
13	M	0.27	0/931	0.49	0/1248
14	N	0.26	0/501	0.46	0/664
15	O	0.33	0/745	0.51	0/992
16	P	0.33	0/716	0.52	0/963
17	Q	0.39	0/870	0.59	0/1159
18	R	0.30	0/603	0.50	0/799
19	S	0.23	0/661	0.45	0/890
20	T	0.31	0/764	0.50	0/1006
21	U	0.28	0/212	0.51	0/277
All	All	0.41	0/55820	0.73	19/82838 (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
1	A	1	0

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1505	G	C4-N9-C1'	8.15	137.09	126.50
1	A	1505	G	C6-C5-N7	-6.83	126.30	130.40
1	A	1505	G	C8-N9-C1'	-6.33	118.77	127.00
1	A	1505	G	N7-C8-N9	6.30	116.25	113.10
1	A	235	C	C6-N1-C2	5.81	122.62	120.30
1	A	1505	G	C8-N9-C4	-5.71	104.11	106.40
1	A	266	G	C2-N3-C4	-5.58	109.11	111.90
1	A	433	C	C5-C6-N1	5.50	123.75	121.00
1	A	1200	C	C2-N1-C1'	5.49	124.84	118.80
1	A	586	C	C6-N1-C2	5.47	122.49	120.30
1	A	115	G	C4-N9-C1'	5.42	133.55	126.50
1	A	1054	C	N1-C2-O2	5.40	122.14	118.90
1	A	1523	G	C5-C6-N1	-5.22	108.89	111.50
1	A	1054	C	C2-N1-C1'	5.18	124.50	118.80
1	A	853	G	C4-N9-C1'	5.17	133.23	126.50
1	A	115	G	C8-N9-C1'	-5.09	120.38	127.00
1	A	1505	G	N3-C4-C5	-5.09	126.06	128.60
1	A	115	G	N3-C4-N9	5.05	129.03	126.00
1	A	1505	G	N3-C4-N9	5.01	129.01	126.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	410	G	C3'

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32511	0	0	433	0
2	B	1873	0	0	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1612	0	0	14	0
4	D	1703	0	0	12	0
5	E	1146	0	0	14	0
6	F	843	0	0	4	0
7	G	1257	0	0	15	0
8	H	1116	0	0	12	0
9	I	1011	0	0	9	0
10	J	792	0	0	5	0
11	K	885	0	0	7	0
12	L	970	0	0	24	0
13	M	921	0	0	12	0
14	N	492	0	0	4	0
15	O	734	0	0	9	0
16	P	700	0	0	3	0
17	Q	857	0	0	8	0
18	R	597	0	0	4	0
19	S	647	0	0	4	0
20	T	762	0	0	14	0
21	U	208	0	0	2	0
22	D	1	0	0	0	0
22	N	1	0	0	0	0
23	A	91	0	0	0	0
23	B	1	0	0	0	0
23	D	1	0	0	0	0
23	M	1	0	0	0	0
24	A	41	0	0	0	0
24	E	1	0	0	0	0
All	All	51775	0	0	605	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (605) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:79:G:C2	1:A:80:G:N7	2.51	0.79
1:A:80:G:C2	1:A:81:U:C4	2.73	0.76
1:A:1361:G:C6	1:A:1361(A):C:N4	2.55	0.76
1:A:75:G:C2	1:A:76:C:C4	2.78	0.72
1:A:77:G:N1	1:A:92:C:N4	2.40	0.70
1:A:475:G:C2	1:A:476:G:C5	2.80	0.70
1:A:92:C:C5	1:A:93:G:N7	2.61	0.69
1:A:1489:G:C2	1:A:1490:C:C2	2.83	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:432:A:O2'	1:A:433:C:C6	2.48	0.66
1:A:836:G:C6	1:A:851:G:C6	2.83	0.65
1:A:945:G:O6	1:A:1236:A:N1	2.29	0.65
1:A:1442:G:C6	1:A:1446:A:N6	2.65	0.65
1:A:75:G:N2	1:A:76:C:N3	2.45	0.65
1:A:1374:A:C4	1:A:1375:A:C8	2.85	0.64
1:A:1443:G:C4'	1:A:1446:A:O5'	2.46	0.63
11:K:53:SER:O	11:K:55:LYS:N	2.32	0.63
1:A:1250:A:C2	1:A:1287:A:N1	2.67	0.63
1:A:130:A:OP2	1:A:190(E):U:O2'	2.17	0.63
1:A:1240:U:OP1	7:G:119:ARG:NH2	2.32	0.62
1:A:977:A:C8	1:A:1223:C:C4	2.88	0.62
1:A:1359:C:O2'	1:A:1361:G:N7	2.33	0.61
1:A:152:A:N6	1:A:170:U:C2	2.68	0.61
1:A:602:A:C2	1:A:637:G:C2	2.88	0.61
1:A:504:C:C2	1:A:542:G:N2	2.69	0.61
1:A:1148:U:C4	1:A:1149:C:N3	2.69	0.61
1:A:1316:G:N2	1:A:1319:A:OP2	2.34	0.61
1:A:965:A:O2'	1:A:966:G:OP2	2.18	0.61
1:A:721:G:N1	1:A:733:A:C2	2.69	0.61
1:A:1250:A:N1	1:A:1287:A:C2	2.68	0.60
1:A:260:G:C5	1:A:261:U:C5	2.89	0.60
12:L:25:PRO:C	12:L:27:LEU:N	2.54	0.60
20:T:13:LEU:O	20:T:16:HIS:N	2.33	0.60
1:A:1126:U:OP1	1:A:1126:U:C6	2.54	0.60
1:A:279:A:OP2	17:Q:95:TYR:OH	2.19	0.60
1:A:1381:U:C5	1:A:1382:C:C5	2.89	0.60
1:A:1250:A:C2	1:A:1287:A:C6	2.90	0.60
1:A:70:G:C5	1:A:73:C:C4	2.90	0.60
1:A:991:U:C5	1:A:1212:U:C2	2.90	0.60
1:A:103:C:OP1	20:T:17:ARG:NH1	2.35	0.60
1:A:722:A:N6	1:A:724:G:C2	2.70	0.60
1:A:781:A:C5	1:A:802:A:C2	2.90	0.60
15:O:17:ARG:NH1	15:O:17:ARG:CG	2.63	0.59
1:A:1436:U:C5	1:A:1437:C:C4	2.90	0.59
9:I:5:TYR:CD2	9:I:6:GLY:N	2.70	0.59
1:A:721:G:C6	1:A:733:A:C2	2.91	0.59
1:A:103:C:O2'	1:A:172:A:N1	2.35	0.59
1:A:243:A:C2	1:A:246:A:C8	2.91	0.59
1:A:73:C:N3	1:A:97:G:N2	2.50	0.59
1:A:261:U:O2	1:A:263:A:C8	2.55	0.59
3:C:23:TYR:CG	3:C:24:ALA:N	2.71	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:500:G:C5	1:A:546:G:N2	2.71	0.59
1:A:1326:C:OP2	21:U:6:ARG:NE	2.36	0.58
1:A:355:C:C4	1:A:356:A:N7	2.71	0.58
1:A:532:A:O2'	1:A:533:A:OP1	2.21	0.58
1:A:60:A:C4'	1:A:61:G:O5'	2.51	0.58
1:A:688:G:C4	1:A:700:G:N2	2.71	0.58
1:A:974:A:OP2	14:N:41:ARG:NH1	2.35	0.58
3:C:126:ARG:O	3:C:127:ARG:CB	2.52	0.58
1:A:96:G:C6	1:A:97:G:C2	2.92	0.58
1:A:908:A:C2	1:A:909:A:C4	2.92	0.58
1:A:1399:C:O2	1:A:1401:G:C5	2.57	0.58
1:A:88:A:C5	1:A:89:C:C5	2.92	0.57
19:S:5:LEU:O	19:S:6:LYS:CB	2.52	0.57
1:A:1072:G:C5	1:A:1073:U:C4	2.92	0.57
7:G:51:GLN:O	7:G:53:LYS:N	2.37	0.57
1:A:89:C:O2	1:A:89:C:C2'	2.53	0.57
1:A:357:G:C2	1:A:358:U:C5	2.93	0.57
1:A:1015:A:C6	1:A:1016:A:C6	2.93	0.57
1:A:1505:G:O2'	1:A:1506:U:OP2	2.22	0.57
1:A:77:G:C2	1:A:93:G:C2	2.92	0.56
1:A:98:U:C4	1:A:99:C:N4	2.72	0.56
1:A:255:G:N2	1:A:272:C:C2	2.73	0.56
1:A:835:U:OP1	18:R:64:ARG:NH2	2.38	0.56
1:A:376:G:C4	1:A:389:A:C2	2.93	0.56
1:A:463:A:C4	1:A:474:G:C8	2.93	0.56
12:L:27:LEU:C	12:L:29:GLY:N	2.58	0.56
1:A:922:G:N2	1:A:1396:A:C4	2.74	0.56
5:E:57:LYS:O	5:E:61:TYR:CD2	2.59	0.56
1:A:974:A:C8	1:A:974:A:OP1	2.59	0.56
1:A:1434:A:N6	1:A:1435:G:C2	2.73	0.56
17:Q:67:LYS:O	17:Q:68:ARG:CB	2.53	0.56
1:A:922:G:N2	1:A:1396:A:C5	2.74	0.55
1:A:97:G:OP2	1:A:97:G:C8	2.59	0.55
1:A:1124:G:N7	1:A:1145:C:O2'	2.40	0.55
1:A:1085:U:C6	1:A:1094:G:N1	2.75	0.55
1:A:705:U:C5	1:A:706:A:N7	2.75	0.55
1:A:193:C:O2	1:A:194:C:C6	2.60	0.55
9:I:36:TYR:CE2	9:I:37:PHE:CE2	2.95	0.55
1:A:254:G:OP1	17:Q:67:LYS:O	2.24	0.55
1:A:79:G:N2	1:A:91:C:N3	2.54	0.55
1:A:696:A:N3	1:A:786:G:O2'	2.39	0.55
1:A:434:U:C4	1:A:435:C:C4	2.95	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:L:27:LEU:O	12:L:29:GLY:N	2.40	0.55
3:C:203:PHE:CD1	3:C:204:LEU:N	2.75	0.54
1:A:1065:U:C1'	1:A:1066:C:OP2	2.55	0.54
1:A:9:G:C2	1:A:26:A:C2	2.95	0.54
1:A:491:G:N3	1:A:492:G:C8	2.75	0.54
1:A:328:C:O2	1:A:328:C:C2'	2.56	0.54
1:A:665:A:C2	1:A:732:C:C2	2.96	0.54
2:B:103:THR:N	2:B:176:GLU:OE1	2.41	0.54
1:A:80:G:N2	1:A:81:U:C4	2.75	0.54
12:L:28:LYS:O	12:L:30:ALA:N	2.40	0.54
1:A:1174:G:C2	1:A:1175:G:C5	2.96	0.54
1:A:80:G:N2	1:A:81:U:N3	2.56	0.54
1:A:60:A:OP1	1:A:331:G:N1	2.41	0.53
1:A:542:G:OP1	4:D:10:ARG:NH2	2.41	0.53
1:A:558:G:OP2	1:A:559:A:O2'	2.27	0.53
1:A:278:G:C6	17:Q:95:TYR:CD2	2.96	0.53
1:A:409:G:C5	1:A:410:G:N7	2.77	0.53
1:A:75:G:N2	1:A:76:C:C4	2.76	0.53
1:A:1399:C:C2	1:A:1401:G:C5	2.96	0.53
10:J:48:THR:OG1	10:J:62:HIS:NE2	2.42	0.53
1:A:376:G:N3	1:A:389:A:C2	2.77	0.52
13:M:5:ALA:O	13:M:6:GLY:C	2.47	0.52
1:A:1516:G:N2	1:A:1520:G:C4	2.77	0.52
1:A:97:G:C5	1:A:98:U:O4	2.62	0.52
1:A:1416:G:O6	1:A:1417:G:N2	2.42	0.52
1:A:595:G:C5	1:A:641:U:C5	2.97	0.52
1:A:260:G:C4	1:A:261:U:C5	2.97	0.52
1:A:781:A:C4	1:A:802:A:C2	2.97	0.52
1:A:457:C:C2	1:A:458:C:C5	2.98	0.52
1:A:300:A:O5'	1:A:300:A:C8	2.62	0.52
1:A:509:A:O2'	1:A:510:A:C8	2.63	0.52
1:A:949:A:C2	1:A:1233:G:N3	2.78	0.52
1:A:1077:G:N2	1:A:1080:A:OP2	2.42	0.52
14:N:14:PRO:O	14:N:15:LYS:CB	2.58	0.52
7:G:137:LYS:O	7:G:141:VAL:N	2.43	0.52
1:A:976:G:N2	1:A:1363:A:C4	2.78	0.52
1:A:263:A:OP2	20:T:79:ARG:NH1	2.43	0.51
1:A:328:C:C1'	1:A:329:A:OP2	2.58	0.51
4:D:79:PHE:C	4:D:79:PHE:CD2	2.83	0.51
1:A:79:G:N2	1:A:91:C:C2	2.79	0.51
12:L:28:LYS:C	12:L:30:ALA:N	2.64	0.51
1:A:595:G:C6	1:A:641:U:C5	2.98	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1345:U:C2	1:A:1377:A:C2	2.98	0.51
14:N:24:CYS:SG	14:N:43:CYS:SG	3.08	0.51
1:A:73:C:C2	1:A:97:G:N2	2.79	0.51
1:A:1225:A:C5'	1:A:1226:C:OP2	2.58	0.51
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.43	0.51
1:A:1133:G:C2	1:A:1142:G:C2	2.98	0.51
1:A:97:G:C5	1:A:98:U:C4	2.99	0.51
1:A:1261:A:N7	1:A:1262:C:C5	2.79	0.51
1:A:544:G:C5	1:A:545:C:C5	2.99	0.51
1:A:119:A:C8	1:A:288:A:C2	2.98	0.51
1:A:391:G:C6	1:A:392:G:C5	2.99	0.51
1:A:1488:G:C2	1:A:1489:G:C5	2.99	0.51
5:E:79:GLU:O	8:H:104:ARG:CZ	2.59	0.51
1:A:255:G:C2	1:A:272:C:C2	2.99	0.51
1:A:409:G:N2	1:A:433:C:N3	2.59	0.51
1:A:1349:A:C2	1:A:1374:A:C4	2.98	0.51
1:A:1158:C:N4	1:A:1160:G:C5	2.79	0.51
20:T:48:LYS:O	20:T:50:GLU:N	2.44	0.51
7:G:3:ARG:O	7:G:4:ARG:CB	2.59	0.51
1:A:393:A:C2	1:A:394:G:C8	2.99	0.51
1:A:1442:G:C5	1:A:1446:A:N6	2.79	0.50
1:A:978:A:O2'	1:A:1322:C:N3	2.44	0.50
1:A:622:A:C8	1:A:623:C:C5	2.99	0.50
1:A:1501:C:C4	1:A:1504:G:C4	2.98	0.50
1:A:257:G:C4	1:A:258:G:C8	2.99	0.50
5:E:33:VAL:CG1	5:E:34:VAL:N	2.74	0.50
1:A:978:A:C2	1:A:1319:A:C4	2.99	0.50
1:A:1505:G:O2'	1:A:1506:U:P	2.69	0.50
1:A:1480:G:C6	1:A:1481:U:C4	2.99	0.50
1:A:266:G:C5'	1:A:267:C:C5	2.94	0.50
1:A:959:A:O2'	1:A:984:C:O2'	2.29	0.50
13:M:87:TYR:N	19:S:73:GLU:O	2.45	0.50
4:D:200:GLU:OE1	4:D:200:GLU:N	2.45	0.50
1:A:1501:C:N4	1:A:1504:G:N3	2.59	0.50
13:M:12:ASN:N	13:M:45:VAL:CG1	2.74	0.50
1:A:1150:U:O4	1:A:1151:A:N6	2.44	0.50
1:A:929:G:OP1	1:A:1533:C:N4	2.45	0.50
1:A:1266:G:N2	1:A:1269:A:OP2	2.45	0.50
1:A:1287:A:C6	1:A:1288:A:C6	3.00	0.50
9:I:5:TYR:CD2	9:I:5:TYR:C	2.85	0.50
1:A:559:A:C1'	1:A:560:U:OP2	2.60	0.50
6:F:24:GLU:O	6:F:28:ARG:N	2.44	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:7:VAL:O	2:B:8:LYS:CB	2.59	0.50
1:A:49:U:C2	1:A:361:G:N2	2.80	0.50
8:H:82:HIS:CD2	8:H:138:TRP:NE1	2.79	0.50
1:A:1345:U:O2	1:A:1377:A:C6	2.65	0.50
1:A:1261:A:C8	1:A:1262:C:C5	3.00	0.50
1:A:1204:A:C6	1:A:1205:U:O2	2.65	0.50
1:A:792:A:C2	1:A:793:U:C4	3.00	0.50
1:A:1117:G:C5'	1:A:1118:C:OP2	2.60	0.49
1:A:1285:A:C4'	1:A:1286:A:O5'	2.60	0.49
1:A:490:G:C2	1:A:491:G:C8	3.01	0.49
1:A:1034:G:C2	1:A:1035:A:C5	3.01	0.49
2:B:107:THR:C	2:B:109:SER:N	2.66	0.49
1:A:1239:A:C4	1:A:1298:C:N4	2.80	0.49
1:A:89:C:O2	1:A:90:U:O2	2.31	0.49
20:T:72:LEU:O	20:T:74:LYS:N	2.46	0.49
6:F:62:TRP:C	6:F:63:TYR:CD2	2.85	0.49
1:A:1049:U:C4'	1:A:1050:G:OP2	2.60	0.49
12:L:26:ALA:O	12:L:27:LEU:O	2.30	0.49
1:A:448:A:C4	1:A:487:A:N1	2.81	0.49
1:A:1186:G:C2	1:A:1187:G:N9	2.81	0.49
1:A:1130:A:N1	1:A:1146:A:N3	2.60	0.49
1:A:652:U:C2	1:A:752:G:N2	2.81	0.49
1:A:474:G:N3	1:A:475:G:C8	2.80	0.49
1:A:166:G:C2	1:A:167:G:N7	2.81	0.49
2:B:204:ASN:ND2	2:B:206:ASP:N	2.61	0.49
1:A:977:A:C8	1:A:1223:C:N3	2.81	0.49
1:A:1303:C:N4	1:A:1304:G:C6	2.81	0.49
1:A:644:G:C5	1:A:645:C:C5	3.01	0.49
5:E:152:ARG:CZ	8:H:44:PHE:CE1	2.95	0.49
1:A:73:C:O2'	1:A:75:G:N7	2.46	0.49
1:A:748:C:C4'	1:A:749:C:O5'	2.60	0.49
20:T:75:ASN:N	20:T:75:ASN:OD1	2.46	0.48
1:A:1392:G:C4	1:A:1393:U:C5	3.01	0.48
1:A:1200:C:O2	1:A:1200:C:C2'	2.60	0.48
1:A:790:A:C6	1:A:791:G:O6	2.65	0.48
1:A:487:A:C6	1:A:488:C:O2	2.66	0.48
1:A:1164:G:C8	1:A:1164:G:OP2	2.66	0.48
1:A:602:A:N1	1:A:637:G:C6	2.82	0.48
1:A:1434:A:N7	1:A:1435:G:C5	2.82	0.48
1:A:965:A:C1'	1:A:966:G:OP2	2.62	0.48
1:A:96:G:O6	1:A:97:G:C2	2.66	0.48
1:A:146:G:N3	1:A:147:G:C8	2.81	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1488:G:N2	1:A:1489:G:C4	2.81	0.48
1:A:1124:G:O2'	1:A:1145:C:N4	2.46	0.48
1:A:266:G:C1'	1:A:267:C:OP2	2.62	0.48
1:A:1497:G:C5	1:A:1498:U:C4	3.02	0.48
1:A:474:G:C2	1:A:475:G:C8	3.02	0.48
1:A:46:G:C2	1:A:396:G:C2	3.01	0.48
1:A:439:A:C4	1:A:497:A:C2	3.01	0.48
1:A:795:C:C5'	1:A:796:C:OP2	2.61	0.48
5:E:102:ALA:CA	5:E:120:THR:OG1	2.61	0.48
1:A:1024:G:C6	1:A:1025:U:O4	2.67	0.48
1:A:1125:U:O2'	1:A:1126:U:P	2.72	0.48
1:A:448:A:C2	1:A:449:C:C4	3.01	0.48
1:A:1130:A:OP1	1:A:1131:G:N7	2.47	0.48
1:A:790:A:N1	1:A:791:G:C6	2.82	0.48
2:B:73:THR:O	2:B:74:LYS:C	2.51	0.48
6:F:15:ASP:CG	6:F:16:GLN:N	2.68	0.48
6:F:16:GLN:O	6:F:20:ALA:N	2.47	0.48
1:A:444:C:N4	1:A:490:G:N1	2.62	0.47
1:A:1202:G:C4	14:N:42:ILE:CD1	2.97	0.47
1:A:986:A:C6	1:A:1220:G:N1	2.82	0.47
2:B:205:ASP:C	2:B:205:ASP:OD1	2.52	0.47
5:E:20:GLN:O	5:E:21:ALA:O	2.32	0.47
1:A:1126:U:N3	1:A:1127:G:C2	2.83	0.47
1:A:1486:G:C6	1:A:1487:G:N1	2.82	0.47
1:A:965:A:C2'	1:A:966:G:OP2	2.63	0.47
1:A:141:A:C1'	1:A:182:U:O2	2.62	0.47
1:A:1026:G:C2'	1:A:1026:G:N3	2.76	0.47
2:B:134:GLU:C	2:B:136:VAL:N	2.68	0.47
1:A:1089:G:C5	1:A:1090:U:C5	3.02	0.47
1:A:504:C:C2	1:A:542:G:C2	3.03	0.47
18:R:59:SER:O	18:R:60:GLY:C	2.53	0.47
12:L:115:LYS:O	12:L:117:ARG:N	2.48	0.47
8:H:102:ARG:N	8:H:102:ARG:CD	2.78	0.47
1:A:1485:U:O2	1:A:1485:U:C2'	2.61	0.47
5:E:39:GLY:O	5:E:69:VAL:N	2.47	0.47
1:A:500:G:C6	1:A:546:G:C2	3.03	0.47
4:D:25:ARG:C	4:D:27:TYR:N	2.67	0.47
1:A:1487:G:C4	1:A:1488:G:C8	3.03	0.47
1:A:1200:C:OP1	1:A:1201:A:O2'	2.33	0.47
1:A:892:A:C2	1:A:907:A:C4	3.02	0.47
1:A:1245:A:N1	1:A:1293:G:C2	2.83	0.47
1:A:838:G:N2	1:A:849:C:C2	2.82	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:327:A:O2'	1:A:328:C:O4'	2.33	0.47
1:A:625:G:C2	1:A:626:U:C2	3.02	0.47
1:A:144:G:C4	1:A:179:A:C2	3.02	0.47
4:D:177:ASP:C	4:D:177:ASP:OD1	2.52	0.47
19:S:80:TYR:O	19:S:81:ARG:C	2.53	0.47
1:A:949:A:C4	1:A:1233:G:N2	2.83	0.47
1:A:181:G:C1'	1:A:182:U:OP2	2.63	0.47
1:A:1068:G:OP2	1:A:1068:G:C8	2.68	0.47
15:O:9:GLN:O	15:O:13:GLN:N	2.48	0.47
1:A:191:G:C6	1:A:192:U:C4	3.03	0.47
1:A:413:G:N2	1:A:429:U:OP2	2.48	0.46
1:A:1167:A:C6	1:A:1168:A:C6	3.03	0.46
12:L:47:LYS:CB	12:L:48:PRO:CD	2.93	0.46
1:A:460:A:C2	1:A:462:G:C8	3.03	0.46
1:A:1007:C:C2	1:A:1023:G:N2	2.82	0.46
1:A:564:C:OP1	12:L:15:ARG:NE	2.47	0.46
1:A:986:A:C2	1:A:1220:G:C2	3.02	0.46
1:A:578:C:O2'	1:A:728:A:N3	2.48	0.46
1:A:76:C:N4	1:A:93:G:N1	2.63	0.46
1:A:21:G:C2	1:A:22:G:C6	3.04	0.46
12:L:86:ARG:NH2	12:L:99:HIS:CD2	2.84	0.46
4:D:32:ALA:O	4:D:36:ARG:N	2.49	0.46
1:A:1228:C:N4	13:M:104:ARG:O	2.48	0.46
4:D:190:ASP:O	4:D:191:ARG:C	2.53	0.46
1:A:1516:G:N2	1:A:1519:A:OP2	2.48	0.46
9:I:11:LYS:O	9:I:12:GLU:CB	2.64	0.46
1:A:1360:A:C2'	1:A:1361:G:O5'	2.64	0.46
20:T:74:LYS:C	20:T:76:ALA:N	2.69	0.46
1:A:1186:G:C2	1:A:1187:G:C4	3.04	0.46
12:L:113:ARG:NH2	12:L:120:TYR:CE1	2.84	0.46
1:A:900:A:N1	1:A:901:A:C2	2.84	0.46
1:A:1295:G:N1	1:A:1296:C:C2	2.84	0.46
9:I:30:GLY:O	9:I:31:GLN:O	2.33	0.46
1:A:1328:C:C2	1:A:1329:A:C8	3.04	0.46
1:A:172:A:N7	1:A:174:C:C4	2.83	0.46
1:A:994:A:N3	1:A:994:A:C2'	2.79	0.46
1:A:803:G:C6	1:A:804:U:N3	2.84	0.46
1:A:1353:G:C4	1:A:1354:C:C5	3.03	0.46
1:A:686:U:C2	1:A:687:A:N7	2.84	0.46
12:L:98:TYR:N	12:L:98:TYR:CD1	2.84	0.46
15:O:76:GLU:O	15:O:79:ARG:N	2.49	0.46
1:A:475:G:N1	1:A:476:G:C6	2.84	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:92:TYR:CE2	2:B:151:GLY:CA	2.99	0.46
1:A:590:C:OP1	8:H:30:ARG:N	2.49	0.46
3:C:113:ALA:N	3:C:183:ASP:OD1	2.49	0.46
18:R:36:ASN:ND2	18:R:39:VAL:CG1	2.79	0.46
2:B:144:ARG:NH1	2:B:148:TYR:CE1	2.84	0.46
1:A:1120:G:C6	1:A:1121:U:C4	3.04	0.46
1:A:1299:A:N7	1:A:1301:U:O2	2.48	0.46
3:C:23:TYR:CD2	3:C:24:ALA:N	2.84	0.45
1:A:428:G:C5	1:A:430:A:C6	3.04	0.45
1:A:867:G:C2	1:A:868:C:C6	3.04	0.45
1:A:1314:C:N4	19:S:4:SER:OG	2.48	0.45
1:A:409:G:OP1	4:D:24:GLU:O	2.34	0.45
1:A:705:U:C5	1:A:706:A:C5	3.04	0.45
1:A:1181:G:C6	1:A:1182:G:N1	2.84	0.45
1:A:147:G:C2	1:A:148:G:C8	3.04	0.45
1:A:1030(C):G:C6	1:A:1030(D):A:C6	3.04	0.45
12:L:55:VAL:CG1	12:L:56:ALA:N	2.79	0.45
1:A:92:C:C5	1:A:93:G:C8	3.04	0.45
1:A:867:G:C2	1:A:868:C:C5	3.05	0.45
1:A:894:G:C6	1:A:895:G:C5	3.04	0.45
12:L:69:TYR:CD2	12:L:70:ILE:N	2.85	0.45
1:A:1125:U:C2	10:J:5:ARG:NH2	2.85	0.45
15:O:87:ILE:CG2	15:O:88:ARG:N	2.80	0.45
1:A:491:G:C2	1:A:492:G:C5	3.05	0.45
1:A:401:C:O2'	1:A:621:A:N3	2.49	0.45
1:A:491:G:C2	1:A:492:G:C8	3.05	0.45
1:A:550:G:C5	1:A:551:U:C5	3.04	0.45
1:A:77:G:N1	1:A:93:G:C2	2.84	0.45
1:A:76:C:N3	1:A:93:G:N2	2.65	0.45
1:A:792:A:C8	1:A:792:A:OP2	2.69	0.45
2:B:97:TRP:CH2	2:B:176:GLU:OE2	2.70	0.45
1:A:1201:A:C1'	1:A:1202:G:OP2	2.65	0.45
1:A:430:A:C5	1:A:431:A:C8	3.04	0.45
1:A:78:G:C2	1:A:92:C:N3	2.85	0.45
1:A:91:C:C2'	1:A:92:C:O5'	2.65	0.45
1:A:1147:C:O2'	9:I:5:TYR:OH	2.34	0.45
1:A:88:A:C5	1:A:89:C:C6	3.05	0.45
1:A:830:G:C6	1:A:831:U:C4	3.04	0.45
15:O:6:GLU:OE1	15:O:6:GLU:N	2.50	0.45
2:B:193:ASP:OD1	2:B:193:ASP:C	2.56	0.45
3:C:107:GLN:O	3:C:108:ASN:CB	2.65	0.45
20:T:75:ASN:O	20:T:76:ALA:C	2.55	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:986:A:C6	1:A:987:G:C6	3.04	0.44
1:A:763:G:N2	1:A:764:C:C2	2.85	0.44
1:A:1304:G:C6	1:A:1305:G:N1	2.85	0.44
1:A:115:G:O2'	1:A:116:A:OP2	2.35	0.44
1:A:1157:A:C4	1:A:1181:G:N2	2.85	0.44
1:A:1144:G:C2	1:A:1146:A:N6	2.86	0.44
1:A:496:A:C4'	1:A:497:A:OP1	2.65	0.44
17:Q:79:SER:OG	17:Q:80:GLY:N	2.51	0.44
1:A:370:C:C4	1:A:371:G:N7	2.85	0.44
9:I:100:GLY:O	9:I:102:LEU:N	2.50	0.44
1:A:1004:A:N6	1:A:1035:A:C5	2.85	0.44
1:A:954:G:C6	1:A:955:U:N3	2.86	0.44
1:A:177:C:C2	1:A:178:C:C5	3.05	0.44
3:C:14:ILE:O	3:C:16:ARG:N	2.50	0.44
1:A:131:C:O2	1:A:231:G:N2	2.50	0.44
1:A:1486:G:C6	1:A:1487:G:C6	3.05	0.44
1:A:327:A:C2	1:A:329:A:C4	3.06	0.44
1:A:372:C:C1'	1:A:373:A:OP2	2.65	0.44
12:L:43:VAL:CG1	12:L:44:THR:N	2.80	0.44
4:D:11:LEU:O	4:D:12:CYS:C	2.56	0.44
8:H:19:VAL:O	8:H:19:VAL:CG2	2.66	0.44
2:B:87:ARG:O	2:B:88:ALA:CB	2.66	0.44
1:A:1361(A):C:O2	1:A:1362:C:C6	2.71	0.44
1:A:1163:C:N4	1:A:1174:G:C2	2.85	0.44
1:A:456:C:C2	1:A:477:G:N2	2.85	0.44
1:A:35:G:C6	1:A:36:C:N4	2.86	0.44
11:K:125:PHE:N	11:K:125:PHE:CD1	2.85	0.44
7:G:62:PHE:CD2	7:G:62:PHE:C	2.91	0.44
1:A:1128:C:C4	1:A:1139:G:C6	3.04	0.44
7:G:137:LYS:O	7:G:138:LYS:C	2.55	0.44
12:L:20:LYS:CD	12:L:20:LYS:N	2.81	0.44
1:A:1191:A:OP1	3:C:3:ASN:OD1	2.35	0.44
1:A:1358:U:O2'	1:A:1359:C:O4'	2.36	0.44
1:A:1487:G:C2'	1:A:1488:G:C5'	2.96	0.44
1:A:1014:A:N7	1:A:1015:A:N6	2.66	0.44
1:A:181:G:C4'	1:A:182:U:OP2	2.66	0.44
1:A:477:G:C2	1:A:478:A:C5	3.05	0.44
1:A:1371:G:C5	1:A:1372:U:C5	3.06	0.44
5:E:15:ARG:NH1	5:E:26:PHE:CE2	2.86	0.44
1:A:374:A:C6	1:A:375:U:C4	3.06	0.44
1:A:284:G:C4	1:A:285:G:C8	3.06	0.44
1:A:616:G:N3	1:A:625:G:C2	2.85	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:G:18:TYR:OH	7:G:58:PRO:C	2.57	0.43
13:M:70:LEU:C	13:M:70:LEU:CD2	2.87	0.43
1:A:664:G:OP1	18:R:64:ARG:NH1	2.51	0.43
1:A:544:G:C6	1:A:545:C:C4	3.07	0.43
3:C:3:ASN:N	3:C:3:ASN:OD1	2.51	0.43
10:J:54:PHE:O	10:J:55:LYS:O	2.36	0.43
1:A:491:G:C4	1:A:492:G:C8	3.05	0.43
1:A:1418:A:C4	1:A:1483:A:C6	3.06	0.43
1:A:299:G:C6	1:A:300:A:C6	3.07	0.43
1:A:1158:C:N3	1:A:1181:G:N2	2.66	0.43
1:A:142:G:N3	1:A:196:A:C2	2.87	0.43
1:A:97:G:O2'	1:A:98:U:O4'	2.36	0.43
1:A:792:A:C6	1:A:794:A:N6	2.86	0.43
12:L:117:ARG:O	12:L:120:TYR:N	2.51	0.43
1:A:284:G:N3	1:A:285:G:C8	2.86	0.43
1:A:826:C:O2	8:H:15:ASN:ND2	2.52	0.43
7:G:60:LYS:O	7:G:61:VAL:C	2.57	0.43
16:P:65:GLN:CA	16:P:65:GLN:NE2	2.81	0.43
2:B:77:ALA:O	2:B:79:ASP:N	2.51	0.43
1:A:96:G:O6	1:A:97:G:N1	2.52	0.43
1:A:1357:A:C4	1:A:1358:U:C5	3.07	0.43
1:A:1361(A):C:O2	1:A:1362:C:C5	2.71	0.43
1:A:1417:G:O2'	1:A:1483:A:N6	2.52	0.43
1:A:1255:G:C6	1:A:1279:A:N7	2.86	0.43
1:A:89:C:N3	1:A:90:U:O2	2.51	0.43
20:T:49:ALA:O	20:T:50:GLU:C	2.57	0.43
1:A:146:G:C2	1:A:147:G:C8	3.07	0.43
1:A:353:A:C2'	1:A:354:G:OP2	2.66	0.43
12:L:107:ALA:O	12:L:108:ALA:C	2.57	0.43
16:P:23:ASP:OD1	16:P:24:ALA:N	2.52	0.43
1:A:75:G:C2	1:A:96:G:N1	2.87	0.43
1:A:1250:A:C6	1:A:1251:A:N1	2.87	0.43
1:A:1118:C:C2	1:A:1179:A:C2	3.07	0.43
2:B:25:ASN:C	2:B:25:ASN:ND2	2.72	0.43
1:A:695:A:OP2	11:K:53:SER:N	2.51	0.43
1:A:595:G:C6	1:A:641:U:C6	3.07	0.43
2:B:107:THR:O	2:B:110:GLN:N	2.51	0.43
1:A:166:G:C2	1:A:167:G:C5	3.06	0.43
7:G:61:VAL:O	7:G:65:ALA:CB	2.67	0.43
3:C:6:HIS:O	3:C:9:GLY:N	2.52	0.43
1:A:285:G:C2	1:A:286:G:C8	3.07	0.43
17:Q:48:GLU:O	17:Q:49:GLU:C	2.55	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:70:G:N7	1:A:73:C:C4	2.87	0.43
1:A:509:A:N3	1:A:543:C:O2'	2.52	0.43
1:A:191:G:O2'	20:T:102:GLY:O	2.37	0.43
12:L:39:VAL:CG1	12:L:40:VAL:N	2.82	0.43
1:A:41:G:C2	1:A:42:G:C5	3.07	0.43
1:A:381:C:C4	1:A:382:A:C5	3.07	0.43
11:K:22:HIS:CD2	11:K:22:HIS:O	2.72	0.43
10:J:59:SER:O	10:J:60:ARG:CB	2.67	0.43
1:A:1125:U:O2'	1:A:1126:U:OP1	2.36	0.42
1:A:89:C:C2	1:A:90:U:O2	2.71	0.42
1:A:1092:A:C4	1:A:1183:A:C6	3.07	0.42
1:A:461:C:C4'	1:A:462:G:OP2	2.67	0.42
1:A:175:C:C4	1:A:176:C:C5	3.06	0.42
1:A:1379:G:C6	1:A:1380:U:C4	3.07	0.42
1:A:345:C:C6	1:A:345:C:OP2	2.72	0.42
1:A:409:G:N1	1:A:433:C:N4	2.67	0.42
1:A:645:C:O2	1:A:645:C:C2'	2.65	0.42
11:K:56:GLY:O	11:K:57:THR:C	2.56	0.42
1:A:190(A):C:C2	1:A:190(I):G:N2	2.87	0.42
1:A:222:U:C2	1:A:223:U:C5	3.07	0.42
1:A:1148:U:N3	1:A:1149:C:C2	2.87	0.42
20:T:13:LEU:O	20:T:14:LYS:C	2.58	0.42
1:A:448:A:C4	1:A:487:A:C2	3.08	0.42
1:A:1119:C:O2	1:A:1155:G:C2	2.73	0.42
1:A:313:A:C6	1:A:314:C:N4	2.88	0.42
1:A:922:G:O2'	1:A:1398:A:N1	2.52	0.42
1:A:622:A:C8	1:A:623:C:C6	3.08	0.42
1:A:160:A:N6	1:A:161:A:C2	2.87	0.42
1:A:44:G:N3	1:A:399:G:C2	2.87	0.42
1:A:1290:G:C6	1:A:1291:G:C6	3.07	0.42
15:O:78:TYR:CZ	15:O:82:ILE:CD1	3.02	0.42
1:A:77:G:C6	1:A:92:C:N4	2.87	0.42
1:A:1157:A:C4	1:A:1181:G:C2	3.07	0.42
1:A:962:C:O2	1:A:1201:A:C2	2.73	0.42
1:A:1026:G:N2	1:A:1027:C:C6	2.87	0.42
1:A:1330:U:OP1	13:M:23:TYR:O	2.38	0.42
12:L:62:SER:C	12:L:64:TYR:N	2.73	0.42
1:A:858:G:O6	1:A:869:G:C8	2.73	0.42
1:A:1250:A:C2	1:A:1287:A:C2	3.07	0.42
1:A:560:U:C5'	1:A:566:G:N2	2.82	0.42
7:G:137:LYS:O	7:G:140:ASP:N	2.52	0.42
13:M:45:VAL:CG1	13:M:46:LYS:N	2.82	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1118:C:C1'	1:A:1179:A:C4	3.02	0.42
2:B:20:GLU:O	2:B:40:HIS:CD2	2.72	0.42
13:M:54:VAL:O	13:M:55:ARG:C	2.58	0.42
15:O:21:ASP:OD1	15:O:24:SER:CB	2.68	0.42
1:A:1357:A:C6	1:A:1358:U:O4	2.72	0.42
1:A:1072:G:C6	1:A:1073:U:C4	3.07	0.42
1:A:1182:G:C1'	1:A:1183:A:OP2	2.68	0.42
13:M:23:TYR:CD1	13:M:71:ARG:NH2	2.87	0.42
2:B:230:VAL:CG1	2:B:231:GLU:N	2.83	0.42
7:G:21:VAL:C	7:G:23:VAL:N	2.72	0.42
1:A:938:A:C6	1:A:939:G:C5	3.08	0.42
1:A:1487:G:C5	1:A:1488:G:C8	3.08	0.42
1:A:1154:G:N3	1:A:1155:G:C8	2.88	0.42
17:Q:90:ILE:C	17:Q:92:ARG:N	2.72	0.42
1:A:1125:U:C3'	1:A:1126:U:C5	3.03	0.42
12:L:69:TYR:C	12:L:69:TYR:CD2	2.93	0.42
3:C:10:PHE:C	3:C:10:PHE:CD2	2.92	0.42
1:A:417:C:C5	1:A:418:C:C5	3.08	0.42
1:A:978:A:OP1	1:A:978:A:C8	2.73	0.41
7:G:43:PHE:CD2	7:G:44:TYR:CE2	3.08	0.41
4:D:31:CYS:SG	4:D:31:CYS:O	2.78	0.41
15:O:45:VAL:CG2	15:O:46:HIS:N	2.83	0.41
1:A:602:A:N3	1:A:637:G:C2	2.87	0.41
1:A:1392:G:C5	1:A:1393:U:C5	3.08	0.41
1:A:1540:U:C5	1:A:1541:U:C2	3.07	0.41
1:A:6:G:N1	5:E:98:THR:OG1	2.53	0.41
1:A:837:G:C2	1:A:850:U:O2	2.73	0.41
2:B:219:VAL:O	2:B:220:ASP:C	2.59	0.41
1:A:1422:G:C2	1:A:1423:G:C8	3.07	0.41
1:A:88:A:C4	1:A:89:C:C6	3.08	0.41
9:I:100:GLY:C	9:I:102:LEU:N	2.74	0.41
13:M:23:TYR:O	13:M:25:ILE:N	2.53	0.41
1:A:27:G:C6	1:A:557:G:C2	3.08	0.41
1:A:914:A:C2	1:A:915:A:C8	3.08	0.41
1:A:1410:G:N2	1:A:1411:C:C2	2.88	0.41
2:B:223:ILE:C	2:B:225:ALA:N	2.73	0.41
3:C:23:TYR:CZ	3:C:24:ALA:O	2.74	0.41
13:M:4:ILE:O	13:M:5:ALA:O	2.38	0.41
11:K:56:GLY:O	11:K:57:THR:O	2.38	0.41
1:A:1410:G:N2	1:A:1411:C:O2	2.54	0.41
3:C:178:LEU:O	3:C:180:ALA:N	2.54	0.41
1:A:573:A:C6	1:A:574:A:N1	2.88	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1250:A:C2	1:A:1251:A:C2	3.09	0.41
12:L:46:LYS:O	12:L:47:LYS:C	2.59	0.41
8:H:11:THR:O	8:H:15:ASN:N	2.53	0.41
2:B:19:HIS:CE1	2:B:189:ASP:OD1	2.73	0.41
8:H:25:ASP:OD1	8:H:25:ASP:N	2.53	0.41
7:G:120:ILE:O	7:G:121:ALA:C	2.56	0.41
1:A:393:A:C4	1:A:394:G:C8	3.08	0.41
1:A:1421:G:N2	1:A:1480:G:C4	2.89	0.41
1:A:428:G:C1'	1:A:429:U:OP2	2.68	0.41
1:A:575:G:C6	1:A:821:G:N7	2.89	0.41
1:A:423:G:N2	1:A:424:G:C8	2.89	0.41
5:E:107:ARG:O	5:E:108:ALA:C	2.57	0.41
2:B:212:GLN:O	2:B:213:LEU:C	2.58	0.41
1:A:70:G:C6	1:A:73:C:N3	2.89	0.41
1:A:695:A:C6	1:A:696:A:C6	3.08	0.41
1:A:1126:U:C2'	1:A:1126:U:O2	2.68	0.41
2:B:97:TRP:CH2	2:B:176:GLU:CD	2.94	0.41
1:A:933:G:OP2	7:G:3:ARG:O	2.39	0.41
1:A:1370:G:C2	1:A:1371:G:C8	3.09	0.41
1:A:1267:C:C5	1:A:1268:A:C5	3.09	0.41
17:Q:45:HIS:N	17:Q:71:PHE:O	2.54	0.41
5:E:72:GLN:O	5:E:73:ASN:CB	2.68	0.41
20:T:59:ALA:O	20:T:60:GLU:C	2.59	0.41
8:H:112:LEU:N	8:H:112:LEU:CD2	2.84	0.41
1:A:1315:U:C2	1:A:1323:G:N2	2.89	0.41
1:A:74:C:C3'	1:A:75:G:C5'	2.99	0.41
1:A:1374:A:C5	1:A:1375:A:N7	2.89	0.41
1:A:376:G:C2	1:A:389:A:C2	3.09	0.41
10:J:63:PHE:N	10:J:63:PHE:CD1	2.89	0.41
12:L:54:LYS:CD	12:L:54:LYS:N	2.84	0.41
9:I:48:GLU:N	9:I:49:PRO:CD	2.84	0.41
1:A:604:G:C6	1:A:635:G:C6	3.08	0.41
1:A:474:G:C4	1:A:475:G:C8	3.09	0.41
1:A:475:G:C2	1:A:476:G:N7	2.88	0.41
1:A:60:A:OP1	1:A:331:G:N2	2.54	0.41
1:A:922:G:C2	1:A:1396:A:C6	3.09	0.41
1:A:922:G:C6	1:A:923:A:C6	3.08	0.41
1:A:297:G:N2	1:A:300:A:OP2	2.53	0.41
2:B:109:SER:O	2:B:112:VAL:N	2.53	0.41
1:A:1030(C):G:C6	1:A:1030(D):A:N6	2.89	0.41
1:A:186:C:O2'	20:T:85:MET:SD	2.78	0.41
2:B:22:LYS:C	2:B:24:TRP:N	2.73	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:180:LEU:O	2:B:181:PHE:CB	2.68	0.41
13:M:29:ARG:NH2	13:M:64:TRP:CD1	2.89	0.41
5:E:144:THR:O	5:E:148:VAL:CG2	2.68	0.41
1:A:1206:G:C6	1:A:1207:G:C6	3.09	0.41
1:A:1054:C:C3'	1:A:1054:C:O2	2.69	0.41
1:A:828:A:C2'	1:A:829:G:O5'	2.69	0.41
1:A:463:A:C5	1:A:474:G:C8	3.09	0.41
15:O:9:GLN:O	15:O:11:VAL:N	2.53	0.41
1:A:1430:C:C2	1:A:1431:C:C5	3.09	0.41
1:A:450:G:C8	1:A:481:G:C6	3.09	0.41
1:A:1003(A):G:N2	1:A:1039:C:C4	2.89	0.41
4:D:28:SER:O	4:D:30:LYS:N	2.54	0.41
1:A:532:A:N3	1:A:532:A:C2'	2.84	0.40
1:A:1261:A:N6	1:A:1275:A:C8	2.89	0.40
8:H:2:LEU:O	8:H:3:THR:C	2.59	0.40
1:A:961:U:C2	1:A:983:A:C6	3.09	0.40
1:A:1284:C:C2	1:A:1285:A:N7	2.89	0.40
12:L:107:ALA:O	12:L:108:ALA:O	2.38	0.40
2:B:25:ASN:O	2:B:28:PHE:N	2.54	0.40
1:A:701:C:C4'	1:A:702:A:OP2	2.69	0.40
1:A:1029:C:N3	1:A:1033:G:N2	2.69	0.40
16:P:25:ARG:O	16:P:26:ARG:C	2.59	0.40
5:E:147:ASP:OD2	5:E:147:ASP:N	2.55	0.40
1:A:1174:G:N2	1:A:1175:G:C4	2.89	0.40
1:A:1034:G:N1	1:A:1035:A:C6	2.89	0.40
1:A:1204:A:C6	1:A:1205:U:C2	3.09	0.40
1:A:1118:C:O2	1:A:1179:A:C6	2.74	0.40
1:A:448:A:C2	1:A:449:C:C2	3.10	0.40
1:A:146:G:C2	1:A:177:C:N3	2.89	0.40
1:A:1119:C:O2	1:A:1155:G:N2	2.54	0.40
1:A:1243:C:OP2	21:U:10:ARG:NH2	2.54	0.40
2:B:114:ARG:O	2:B:117:GLU:N	2.54	0.40
11:K:111:ASP:OD2	11:K:111:ASP:O	2.38	0.40
1:A:149:A:N3	1:A:150:C:C6	2.89	0.40
1:A:1014:A:N7	1:A:1015:A:C6	2.89	0.40
1:A:255:G:C6	1:A:256:U:O4	2.74	0.40
1:A:1052:U:N3	1:A:1200:C:C4	2.90	0.40
4:D:20:TYR:CD2	4:D:27:TYR:CE1	3.09	0.40
1:A:1371:G:C4	1:A:1372:U:C5	3.09	0.40
3:C:128:PHE:CD2	3:C:129:ALA:N	2.89	0.40
20:T:22:ARG:O	20:T:23:ARG:C	2.60	0.40
1:A:731:G:OP1	1:A:766:A:C1'	2.69	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1124:G:N3	1:A:1127:G:N2	2.69	0.40
1:A:299:G:C5	1:A:300:A:C6	3.09	0.40
1:A:448:A:N1	1:A:449:C:C4	2.90	0.40
1:A:1199:U:C5'	1:A:1200:C:OP2	2.70	0.40
5:E:15:ARG:NH1	5:E:26:PHE:CZ	2.89	0.40
7:G:23:VAL:O	7:G:27:ILE:N	2.55	0.40
1:A:630:G:C3'	1:A:631:G:C8	3.04	0.40
1:A:925:G:C2	1:A:927:G:C8	3.10	0.40
1:A:1531:A:O5'	1:A:1531:A:C8	2.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	233/256 (91%)	168 (72%)	45 (19%)	20 (9%)	1	25
3	C	204/239 (85%)	152 (74%)	37 (18%)	15 (7%)	2	31
4	D	206/209 (99%)	168 (82%)	32 (16%)	6 (3%)	7	60
5	E	148/162 (91%)	119 (80%)	26 (18%)	3 (2%)	11	68
6	F	99/101 (98%)	80 (81%)	17 (17%)	2 (2%)	11	68
7	G	153/156 (98%)	105 (69%)	34 (22%)	14 (9%)	1	24
8	H	136/138 (99%)	115 (85%)	15 (11%)	6 (4%)	4	48
9	I	125/128 (98%)	86 (69%)	28 (22%)	11 (9%)	1	25
10	J	96/105 (91%)	60 (62%)	22 (23%)	14 (15%)	0	10
11	K	117/129 (91%)	85 (73%)	22 (19%)	10 (8%)	1	26
12	L	122/135 (90%)	87 (71%)	22 (18%)	13 (11%)	1	17
13	M	113/126 (90%)	91 (80%)	16 (14%)	6 (5%)	3	42
14	N	58/61 (95%)	40 (69%)	13 (22%)	5 (9%)	1	25
15	O	86/89 (97%)	70 (81%)	13 (15%)	3 (4%)	6	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	P	81/88 (92%)	63 (78%)	11 (14%)	7 (9%)	1	25
17	Q	102/105 (97%)	86 (84%)	14 (14%)	2 (2%)	11	68
18	R	71/88 (81%)	53 (75%)	14 (20%)	4 (6%)	3	40
19	S	78/93 (84%)	47 (60%)	19 (24%)	12 (15%)	0	8
20	T	97/106 (92%)	60 (62%)	28 (29%)	9 (9%)	1	23
21	U	22/27 (82%)	17 (77%)	5 (23%)	0	100	100
All	All	2347/2541 (92%)	1752 (75%)	433 (18%)	162 (7%)	2	33

All (162) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	7	VAL
2	B	8	LYS
3	C	15	THR
3	C	29	TYR
3	C	127	ARG
7	G	4	ARG
8	H	91	ARG
9	I	12	GLU
9	I	31	GLN
9	I	82	ALA
9	I	127	LYS
10	J	30	SER
10	J	55	LYS
10	J	60	ARG
11	K	127	LYS
11	K	128	ALA
12	L	27	LEU
12	L	41	ARG
12	L	47	LYS
12	L	56	ALA
12	L	108	ALA
12	L	126	LYS
13	M	49	THR
14	N	15	LYS
16	P	31	LYS
17	Q	68	ARG
19	S	6	LYS
19	S	9	VAL
20	T	49	ALA

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Mol	Chain	Res	Type
20	T	97	ALA
20	T	99	LEU
2	B	9	GLU
2	B	74	LYS
2	B	78	GLN
2	B	89	GLY
2	B	161	ALA
2	B	229	VAL
3	C	5	ILE
3	C	179	ARG
4	D	5	ILE
4	D	88	VAL
5	E	21	ALA
6	F	44	GLY
7	G	17	VAL
7	G	59	LEU
7	G	155	ARG
8	H	74	PRO
8	H	75	ARG
9	I	54	ASP
9	I	101	PHE
10	J	34	VAL
10	J	61	GLU
10	J	72	VAL
11	K	54	ARG
11	K	117	ASN
11	K	126	ARG
12	L	14	GLY
12	L	28	LYS
12	L	29	GLY
12	L	127	GLU
13	M	5	ALA
13	M	6	GLY
14	N	17	LYS
14	N	60	SER
16	P	10	GLY
16	P	25	ARG
16	P	27	LYS
16	P	82	GLN
18	R	19	LYS
19	S	8	GLY
19	S	25	LYS

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Mol	Chain	Res	Type
19	S	27	GLU
20	T	95	ALA
2	B	77	ALA
2	B	129	GLU
3	C	51	GLY
3	C	74	GLY
3	C	94	LEU
3	C	206	GLU
5	E	27	ARG
5	E	153	LYS
6	F	39	LYS
7	G	78	ARG
7	G	113	GLU
7	G	128	ALA
9	I	38	GLN
10	J	27	ALA
10	J	40	LEU
10	J	73	ASP
10	J	86	MET
11	K	44	SER
11	K	50	TYR
11	K	118	GLY
12	L	80	HIS
13	M	7	VAL
13	M	23	TYR
13	M	67	GLU
15	O	49	ASP
16	P	26	ARG
17	Q	101	ARG
18	R	17	SER
18	R	54	ARG
19	S	4	SER
19	S	30	LEU
19	S	47	HIS
19	S	65	ASN
20	T	14	LYS
20	T	70	SER
20	T	93	GLU
20	T	102	GLY
2	B	131	PRO
2	B	155	LEU
2	B	198	ASP

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Mol	Chain	Res	Type
3	C	39	ILE
3	C	108	ASN
3	C	154	SER
3	C	178	LEU
4	D	35	ARG
7	G	130	GLY
8	H	3	THR
9	I	51	ARG
11	K	57	THR
14	N	18	VAL
14	N	25	VAL
15	O	84	LYS
20	T	74	LYS
2	B	221	LEU
2	B	224	GLN
2	B	232	PRO
3	C	81	GLY
7	G	40	ALA
8	H	105	ARG
9	I	24	GLY
9	I	56	LEU
12	L	55	VAL
15	O	5	LYS
16	P	12	LYS
18	R	87	ARG
19	S	42	PRO
2	B	19	HIS
7	G	25	ALA
7	G	51	GLN
7	G	61	VAL
8	H	73	ASP
9	I	81	ILE
10	J	39	PRO
2	B	26	PRO
7	G	55	GLY
11	K	47	VAL
2	B	130	ARG
2	B	194	PRO
3	C	66	VAL
4	D	39	PRO
10	J	76	ASN
4	D	197	PRO

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Mol	Chain	Res	Type
12	L	88	GLY
19	S	51	VAL
10	J	36	GLY
10	J	82	ILE
4	D	17	VAL
7	G	57	GLU
19	S	54	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	194/220 (88%)	173 (89%)	21 (11%)	9	48
3	C	160/188 (85%)	148 (92%)	12 (8%)	19	67
4	D	180/181 (99%)	166 (92%)	14 (8%)	18	65
5	E	115/123 (94%)	98 (85%)	17 (15%)	4	30
6	F	90/90 (100%)	81 (90%)	9 (10%)	11	52
7	G	126/127 (99%)	116 (92%)	10 (8%)	18	65
8	H	119/119 (100%)	104 (87%)	15 (13%)	7	39
9	I	98/99 (99%)	87 (89%)	11 (11%)	9	45
10	J	87/92 (95%)	80 (92%)	7 (8%)	17	64
11	K	90/99 (91%)	80 (89%)	10 (11%)	9	46
12	L	104/111 (94%)	90 (86%)	14 (14%)	6	35
13	M	93/101 (92%)	81 (87%)	12 (13%)	6	38
14	N	49/50 (98%)	47 (96%)	2 (4%)	41	85
15	O	79/80 (99%)	69 (87%)	10 (13%)	6	38
16	P	72/74 (97%)	63 (88%)	9 (12%)	7	40
17	Q	96/97 (99%)	92 (96%)	4 (4%)	40	84
18	R	64/77 (83%)	57 (89%)	7 (11%)	9	47
19	S	71/80 (89%)	64 (90%)	7 (10%)	11	53
20	T	76/82 (93%)	67 (88%)	9 (12%)	8	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	U	19/22 (86%)	17 (90%)	2 (10%)	10	49
All	All	1982/2112 (94%)	1780 (90%)	202 (10%)	11	51

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	25	ASN
2	B	39	ILE
2	B	44	LEU
2	B	60	ASP
2	B	61	LEU
2	B	67	THR
2	B	82	ARG
2	B	111	ARG
2	B	142	LEU
2	B	157	ARG
2	B	158	LEU
2	B	163	PHE
2	B	168	THR
2	B	187	LEU
2	B	190	THR
2	B	204	ASN
2	B	208	ILE
2	B	217	ARG
2	B	223	ILE
2	B	236	TYR
2	B	240	GLN
3	C	3	ASN
3	C	14	ILE
3	C	26	LYS
3	C	33	LEU
3	C	104	GLN
3	C	126	ARG
3	C	127	ARG
3	C	128	PHE
3	C	132	ARG
3	C	162	GLN
3	C	167	TRP
3	C	179	ARG
4	D	9	CYS
4	D	15	GLU
4	D	17	VAL

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Mol	Chain	Res	Type
4	D	26	CYS
4	D	64	LEU
4	D	73	ARG
4	D	78	LEU
4	D	112	VAL
4	D	122	ARG
4	D	127	THR
4	D	141	ARG
4	D	187	ARG
4	D	188	LEU
4	D	199	ASN
5	E	6	PHE
5	E	10	MET
5	E	12	LEU
5	E	18	ARG
5	E	20	GLN
5	E	31	LEU
5	E	32	VAL
5	E	41	VAL
5	E	45	PHE
5	E	67	VAL
5	E	76	ILE
5	E	79	GLU
5	E	80	ILE
5	E	89	ILE
5	E	98	THR
5	E	131	ILE
5	E	147	ASP
6	F	9	VAL
6	F	10	LEU
6	F	15	ASP
6	F	18	GLN
6	F	23	LYS
6	F	45	LEU
6	F	74	ASP
6	F	77	ARG
6	F	100	ASN
7	G	8	GLU
7	G	12	LEU
7	G	16	LEU
7	G	24	THR
7	G	37	ASN

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Mol	Chain	Res	Type
7	G	41	ARG
7	G	62	PHE
7	G	66	VAL
7	G	114	ARG
7	G	153	HIS
8	H	3	THR
8	H	18	ARG
8	H	19	VAL
8	H	26	VAL
8	H	39	LEU
8	H	59	LEU
8	H	63	LEU
8	H	84	ARG
8	H	85	ARG
8	H	88	LYS
8	H	91	ARG
8	H	102	ARG
8	H	112	LEU
8	H	113	SER
8	H	133	LEU
9	I	5	TYR
9	I	48	GLU
9	I	59	PHE
9	I	62	TYR
9	I	79	LEU
9	I	91	ASP
9	I	102	LEU
9	I	104	ARG
9	I	109	VAL
9	I	114	TYR
9	I	121	ARG
10	J	6	ILE
10	J	9	ARG
10	J	21	GLN
10	J	54	PHE
10	J	57	LYS
10	J	75	ILE
10	J	99	LYS
11	K	11	LYS
11	K	18	ARG
11	K	25	TYR
11	K	29	ILE

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Mol	Chain	Res	Type
11	K	75	TYR
11	K	98	LEU
11	K	105	VAL
11	K	116	HIS
11	K	120	ARG
11	K	126	ARG
12	L	19	ARG
12	L	20	LYS
12	L	36	VAL
12	L	44	THR
12	L	49	ASN
12	L	64	TYR
12	L	66	VAL
12	L	67	THR
12	L	82	VAL
12	L	85	ILE
12	L	93	LEU
12	L	98	TYR
12	L	111	LYS
12	L	127	GLU
13	M	11	ARG
13	M	14	ARG
13	M	44	ARG
13	M	48	LEU
13	M	59	TYR
13	M	74	VAL
13	M	91	ARG
13	M	94	ARG
13	M	99	ARG
13	M	101	GLN
13	M	102	ARG
13	M	103	THR
14	N	6	LEU
14	N	26	ARG
15	O	5	LYS
15	O	11	VAL
15	O	17	ARG
15	O	31	LEU
15	O	36	ILE
15	O	40	SER
15	O	70	LEU
15	O	71	GLN

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Mol	Chain	Res	Type
15	O	79	ARG
15	O	81	LEU
16	P	22	THR
16	P	25	ARG
16	P	32	TYR
16	P	44	THR
16	P	53	VAL
16	P	55	ARG
16	P	57	ARG
16	P	62	VAL
16	P	81	ARG
17	Q	35	VAL
17	Q	36	ILE
17	Q	38	ARG
17	Q	53	LEU
18	R	29	PHE
18	R	31	LEU
18	R	38	GLU
18	R	42	ARG
18	R	47	THR
18	R	54	ARG
18	R	56	THR
19	S	12	ASP
19	S	15	LEU
19	S	18	LYS
19	S	25	LYS
19	S	32	LYS
19	S	37	ARG
19	S	43	GLU
20	T	13	LEU
20	T	51	GLU
20	T	54	LYS
20	T	57	ARG
20	T	73	HIS
20	T	74	LYS
20	T	75	ASN
20	T	83	ARG
20	T	84	LEU
21	U	9	ARG
21	U	22	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1511/1522 (99%)	281 (18%)	35 (2%)

All (281) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	9	G
1	A	31	G
1	A	32	A
1	A	33	A
1	A	39	G
1	A	44	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	60	A
1	A	61	G
1	A	73	C
1	A	74	C
1	A	75	G
1	A	79	G
1	A	82	U
1	A	89	C
1	A	91	C
1	A	92	C
1	A	97	G
1	A	98	U
1	A	99	C
1	A	116	A
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	132	C
1	A	145	G
1	A	178	C
1	A	182	U
1	A	190(E)	U
1	A	195	A
1	A	197	A

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Mol	Chain	Res	Type
1	A	199	G
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	231	G
1	A	244	U
1	A	245	C
1	A	247	G
1	A	251	G
1	A	252	U
1	A	266	G
1	A	267	C
1	A	289	G
1	A	300	A
1	A	312	C
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	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	373	A
1	A	384	G
1	A	397	A
1	A	398	C
1	A	406	G
1	A	410	G
1	A	411	A
1	A	412	A
1	A	413	G
1	A	414	A
1	A	419	C
1	A	421	U
1	A	424	G

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Mol	Chain	Res	Type
1	A	429	U
1	A	430	A
1	A	433	C
1	A	439	A
1	A	442	C
1	A	452	A
1	A	455	C
1	A	460	A
1	A	461	C
1	A	485	G
1	A	497	A
1	A	498	U
1	A	505	G
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	527	G
1	A	531	U
1	A	532	A
1	A	533	A
1	A	547	A
1	A	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	564	C
1	A	572	A
1	A	573	A
1	A	575	G
1	A	576	G
1	A	577	G
1	A	579	G
1	A	588	G
1	A	631	G
1	A	632	A
1	A	653	A
1	A	665	A
1	A	687	A
1	A	688	G
1	A	702	A
1	A	703	G

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Mol	Chain	Res	Type
1	A	717	C
1	A	721	G
1	A	723	U
1	A	724	G
1	A	731	G
1	A	734	G
1	A	749	C
1	A	752	G
1	A	755	G
1	A	759	A
1	A	760	G
1	A	773	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	796	C
1	A	813	U
1	A	816	A
1	A	817	C
1	A	818	G
1	A	819	A
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	856	C
1	A	857	C
1	A	872	A
1	A	873	A
1	A	876	G
1	A	885	G
1	A	902	G
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A

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Mol	Chain	Res	Type
1	A	950	U
1	A	960	U
1	A	961	U
1	A	966	G
1	A	969	A
1	A	971	G
1	A	972	C
1	A	974	A
1	A	976	G
1	A	977	A
1	A	978	A
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1005	A
1	A	1006	C
1	A	1023	G
1	A	1026	G
1	A	1027	C
1	A	1047	G
1	A	1050	G
1	A	1053	G
1	A	1054	C
1	A	1060	C
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1078	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1117	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1137	C
1	A	1139	G
1	A	1145	C

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Mol	Chain	Res	Type
1	A	1150	U
1	A	1152	A
1	A	1159	U
1	A	1160	G
1	A	1161	C
1	A	1162	C
1	A	1164	G
1	A	1171	G
1	A	1181	G
1	A	1183	A
1	A	1190	G
1	A	1192	C
1	A	1193	G
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1206	G
1	A	1211	U
1	A	1212	U
1	A	1213	A
1	A	1226	C
1	A	1238	A
1	A	1245	A
1	A	1248	A
1	A	1249	C
1	A	1250	A
1	A	1258	G
1	A	1270	C
1	A	1280	A
1	A	1281	U
1	A	1286	A
1	A	1287	A
1	A	1297	C
1	A	1300	G
1	A	1302	U
1	A	1303	C
1	A	1304	G
1	A	1305	G
1	A	1311	G
1	A	1312	G

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Mol	Chain	Res	Type
1	A	1320	C
1	A	1338	G
1	A	1339	A
1	A	1347	G
1	A	1353	G
1	A	1361	G
1	A	1362	C
1	A	1368	G
1	A	1370	G
1	A	1378	C
1	A	1379	G
1	A	1397	C
1	A	1398	A
1	A	1414	U
1	A	1417	G
1	A	1418	A
1	A	1441	G
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1447	G
1	A	1452	C
1	A	1453	G
1	A	1496	C
1	A	1499	A
1	A	1502	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1519	A
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1534	A

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	60	A
1	A	115	G
1	A	129(A)	G

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Mol	Chain	Res	Type
1	A	181	G
1	A	250	A
1	A	251	G
1	A	266	G
1	A	328	C
1	A	372	C
1	A	410	G
1	A	428	G
1	A	429	U
1	A	484	G
1	A	496	A
1	A	559	A
1	A	560	U
1	A	687	A
1	A	701	C
1	A	748	C
1	A	812	C
1	A	913	A
1	A	960	U
1	A	965	A
1	A	1004	A
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1182	G
1	A	1201	A
1	A	1285	A
1	A	1443	G
1	A	1498	U
1	A	1504	G
1	A	1505	G
1	A	1528	U

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 138 ligands modelled in this entry, 138 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1513/1522 (99%)	-0.31	18 (1%) 75 52	50, 108, 253, 361	0
2	B	235/256 (91%)	-0.29	1 (0%) 90 78	65, 115, 197, 256	0
3	C	206/239 (86%)	-0.08	3 (1%) 70 46	116, 170, 237, 271	0
4	D	208/209 (99%)	-0.19	0 100 100	63, 111, 160, 175	0
5	E	150/162 (92%)	-0.30	0 100 100	51, 78, 114, 154	0
6	F	101/101 (100%)	-0.29	0 100 100	87, 129, 155, 177	0
7	G	155/156 (99%)	-0.14	2 (1%) 74 50	99, 152, 220, 233	0
8	H	138/138 (100%)	-0.37	0 100 100	41, 72, 104, 137	0
9	I	127/128 (99%)	-0.10	0 100 100	78, 171, 216, 224	0
10	J	98/105 (93%)	0.29	6 (6%) 21 14	122, 178, 274, 291	0
11	K	119/129 (92%)	-0.19	1 (0%) 83 63	62, 106, 146, 183	0
12	L	124/135 (91%)	-0.18	0 100 100	48, 107, 143, 174	0
13	M	115/126 (91%)	-0.15	0 100 100	96, 136, 170, 180	0
14	N	60/61 (98%)	0.17	1 (1%) 67 44	125, 157, 213, 229	0
15	O	88/89 (98%)	-0.30	0 100 100	54, 95, 133, 171	0
16	P	83/88 (94%)	-0.32	0 100 100	69, 99, 137, 199	0
17	Q	104/105 (99%)	-0.16	4 (3%) 38 25	54, 83, 125, 223	0
18	R	73/88 (82%)	-0.29	0 100 100	65, 99, 164, 209	0
19	S	80/93 (86%)	0.13	0 100 100	149, 183, 219, 231	0
20	T	99/106 (93%)	-0.32	1 (1%) 79 57	76, 107, 165, 190	0
21	U	24/27 (88%)	0.65	3 (12%) 5 5	121, 141, 162, 171	0
All	All	3900/4063 (95%)	-0.23	40 (1%) 77 57	41, 116, 222, 361	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	K	128	ALA	7.7
1	A	1541	U	6.7
17	Q	104	LYS	5.9
1	A	1540	U	5.7
10	J	33	GLN	5.6
1	A	1003(A)	G	5.0
17	Q	103	GLY	4.8
1	A	1129	C	4.2
1	A	74	C	4.2
1	A	1003	G	3.8
1	A	1492	A	3.6
1	A	993	G	3.5
20	T	106	ALA	3.5
10	J	32	ALA	3.3
1	A	202	U	3.2
21	U	25	LYS	3.2
17	Q	102	GLY	3.1
1	A	1005	A	3.1
3	C	193	TYR	3.0
17	Q	105	ALA	3.0
10	J	34	VAL	2.9
1	A	1539	C	2.8
21	U	18	TYR	2.8
3	C	65	ALA	2.8
2	B	231	GLU	2.6
1	A	1002	G	2.5
1	A	461	C	2.4
7	G	154	TYR	2.3
10	J	3	LYS	2.3
10	J	4	ILE	2.3
3	C	103	VAL	2.3
7	G	5	ARG	2.3
14	N	12	ARG	2.3
1	A	1534	A	2.2
1	A	1416	G	2.2
21	U	22	ARG	2.2
1	A	81	U	2.2
1	A	995	C	2.2
1	A	1283	G	2.0
10	J	31	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
23	MG	A	1610	1/1	0.28	-	47,47,47,47	0
24	K	A	1647	1/1	0.18	-	85,85,85,85	0
23	MG	A	1613	1/1	0.17	-	39,39,39,39	0
23	MG	A	1620	1/1	0.89	-	92,92,92,92	0
24	K	A	1633	1/1	0.20	-	135,135,135,135	0
24	K	A	1648	1/1	0.24	-	63,63,63,63	0
24	K	A	1658	1/1	0.66	-	107,107,107,107	0
23	MG	A	1582	1/1	0.82	-	83,83,83,83	0
23	MG	A	1576	1/1	0.50	-	78,78,78,78	0
23	MG	A	1627	1/1	0.49	-	39,39,39,39	0
24	K	A	1665	1/1	0.32	-	79,79,79,79	0
24	K	A	1666	1/1	0.55	-	74,74,74,74	0
23	MG	A	1614	1/1	0.15	-	56,56,56,56	0
23	MG	A	1617	1/1	0.30	-	78,78,78,78	0
23	MG	A	1621	1/1	0.10	-	58,58,58,58	0
23	MG	A	1571	1/1	0.41	-	67,67,67,67	0
24	K	A	1660	1/1	0.20	-	126,126,126,126	0
23	MG	A	1572	1/1	0.36	-	35,35,35,35	0
24	K	A	1637	1/1	0.43	-	129,129,129,129	0
23	MG	A	1623	1/1	0.35	-	77,77,77,77	0
23	MG	A	1545	1/1	0.21	-	75,75,75,75	0
23	MG	A	1605	1/1	1.18	-	56,56,56,56	0
23	MG	A	1601	1/1	0.27	-	78,78,78,78	0
23	MG	A	1565	1/1	0.39	-	87,87,87,87	0
23	MG	A	1597	1/1	0.24	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	MG	A	1585	1/1	0.25	-	78,78,78,78	0
24	K	A	1662	1/1	0.29	-	92,92,92,92	0
23	MG	M	127	1/1	0.43	-	76,76,76,76	0
23	MG	A	1594	1/1	0.13	-	46,46,46,46	0
23	MG	A	1629	1/1	0.42	-	61,61,61,61	0
24	K	A	1635	1/1	0.57	-	149,149,149,149	0
23	MG	A	1625	1/1	0.23	-	93,93,93,93	0
23	MG	A	1558	1/1	0.43	-	81,81,81,81	0
23	MG	A	1588	1/1	0.21	-	59,59,59,59	0
23	MG	A	1567	1/1	0.20	-	70,70,70,70	0
23	MG	A	1561	1/1	0.12	-	59,59,59,59	0
23	MG	A	1579	1/1	0.23	-	29,29,29,29	0
23	MG	A	1546	1/1	0.78	-	76,76,76,76	0
23	MG	A	1548	1/1	1.02	-	81,81,81,81	0
23	MG	A	1619	1/1	0.40	-	91,91,91,91	0
24	K	A	1631	1/1	0.38	-	110,110,110,110	0
23	MG	A	1563	1/1	0.24	-	20,20,20,20	0
23	MG	A	1616	1/1	0.39	-	49,49,49,49	0
24	K	A	1671	1/1	0.47	-	79,79,79,79	0
24	K	A	1636	1/1	0.67	-	116,116,116,116	0
24	K	A	1640	1/1	0.49	-	108,108,108,108	0
23	MG	A	1554	1/1	0.61	-	59,59,59,59	0
23	MG	A	1622	1/1	0.55	-	87,87,87,87	0
24	K	A	1649	1/1	0.26	-	75,75,75,75	0
23	MG	A	1609	1/1	0.71	-	96,96,96,96	0
23	MG	A	1607	1/1	0.55	-	65,65,65,65	0
23	MG	A	1628	1/1	0.39	-	65,65,65,65	0
23	MG	A	86	1/1	0.21	-	59,59,59,59	0
23	MG	A	1569	1/1	0.20	-	59,59,59,59	0
24	K	A	1632	1/1	0.17	-	102,102,102,102	0
23	MG	A	1556	1/1	0.43	-	93,93,93,93	0
24	K	E	163	1/1	0.34	-	115,115,115,115	0
24	K	A	1670	1/1	0.34	-	107,107,107,107	0
24	K	A	1644	1/1	0.47	-	55,55,55,55	0
23	MG	A	1559	1/1	0.84	-	53,53,53,53	0
23	MG	A	1611	1/1	0.17	-	56,56,56,56	0
24	K	A	1657	1/1	0.55	-	83,83,83,83	0
23	MG	A	1564	1/1	0.33	-	59,59,59,59	0
24	K	A	1653	1/1	0.14	-	98,98,98,98	0
23	MG	A	1603	1/1	0.49	-	100,100,100,100	0
23	MG	A	1573	1/1	0.37	-	70,70,70,70	0
23	MG	B	257	1/1	0.37	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	MG	A	1547	1/1	0.48	-	86,86,86,86	0
24	K	A	1645	1/1	0.33	-	75,75,75,75	0
23	MG	D	211	1/1	0.14	-	73,73,73,73	0
23	MG	A	1581	1/1	0.47	-	68,68,68,68	0
23	MG	A	1599	1/1	0.64	-	65,65,65,65	0
23	MG	A	1552	1/1	0.20	-	80,80,80,80	0
23	MG	A	1586	1/1	0.30	-	48,48,48,48	0
24	K	A	1661	1/1	0.14	-	79,79,79,79	0
23	MG	A	1555	1/1	0.26	-	95,95,95,95	0
24	K	A	1638	1/1	0.40	-	143,143,143,143	0
23	MG	A	1590	1/1	0.32	-	39,39,39,39	0
23	MG	A	1560	1/1	0.47	-	89,89,89,89	0
23	MG	A	1618	1/1	0.45	-	64,64,64,64	0
23	MG	A	1553	1/1	0.65	-	94,94,94,94	0
23	MG	A	1574	1/1	0.90	-	68,68,68,68	0
24	K	A	1667	1/1	0.37	-	80,80,80,80	0
24	K	A	1669	1/1	0.47	-	98,98,98,98	0
23	MG	A	1608	1/1	0.36	-	72,72,72,72	0
24	K	A	1654	1/1	0.35	-	85,85,85,85	0
23	MG	A	1551	1/1	0.56	-	50,50,50,50	0
23	MG	A	1602	1/1	0.45	-	63,63,63,63	0
23	MG	A	94	1/1	0.30	-	66,66,66,66	0
23	MG	A	1589	1/1	0.23	-	79,79,79,79	0
24	K	A	1656	1/1	0.40	-	105,105,105,105	0
23	MG	A	85	1/1	0.36	-	35,35,35,35	0
23	MG	A	1570	1/1	0.71	-	34,34,34,34	0
24	K	A	1639	1/1	0.65	-	81,81,81,81	0
23	MG	A	1593	1/1	0.56	-	87,87,87,87	0
23	MG	A	1578	1/1	0.51	-	50,50,50,50	0
23	MG	A	1549	1/1	0.51	-	59,59,59,59	0
23	MG	A	1557	1/1	0.84	-	90,90,90,90	0
24	K	A	1659	1/1	0.31	-	76,76,76,76	0
23	MG	A	1562	1/1	0.72	-	54,54,54,54	0
24	K	A	1642	1/1	0.41	-	94,94,94,94	0
23	MG	A	1630	1/1	0.30	-	41,41,41,41	0
23	MG	A	1584	1/1	0.55	-	52,52,52,52	0
23	MG	A	1615	1/1	0.20	-	55,55,55,55	0
23	MG	A	1587	1/1	0.40	-	37,37,37,37	0
24	K	A	1651	1/1	0.43	-	138,138,138,138	0
24	K	A	1663	1/1	0.54	-	99,99,99,99	0
22	ZN	N	141	1/1	0.07	-	150,150,150,150	0
23	MG	A	1575	1/1	0.58	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	K	A	1646	1/1	0.54	-	82,82,82,82	0
23	MG	A	1612	1/1	0.23	-	81,81,81,81	0
23	MG	A	100	1/1	0.22	-	126,126,126,126	0
23	MG	A	1606	1/1	0.35	-	65,65,65,65	0
23	MG	A	1577	1/1	0.59	-	63,63,63,63	0
23	MG	A	1580	1/1	0.40	-	79,79,79,79	0
23	MG	A	1583	1/1	0.39	-	67,67,67,67	0
23	MG	A	1626	1/1	0.13	-	62,62,62,62	0
24	K	A	1634	1/1	0.21	-	134,134,134,134	0
23	MG	A	1550	1/1	0.21	-	52,52,52,52	0
24	K	A	1652	1/1	0.21	-	100,100,100,100	0
23	MG	A	1596	1/1	1.22	-	54,54,54,54	0
23	MG	A	1624	1/1	0.09	-	38,38,38,38	0
23	MG	A	1604	1/1	0.19	-	52,52,52,52	0
24	K	A	1664	1/1	0.22	-	111,111,111,111	0
23	MG	A	1591	1/1	0.34	-	82,82,82,82	0
24	K	A	1668	1/1	0.45	-	95,95,95,95	0
23	MG	A	1568	1/1	0.12	-	17,17,17,17	0
23	MG	A	1566	1/1	0.41	-	90,90,90,90	0
23	MG	A	71	1/1	0.87	-	74,74,74,74	0
24	K	A	1650	1/1	0.12	-	86,86,86,86	0
24	K	A	1643	1/1	0.29	-	122,122,122,122	0
22	ZN	D	210	1/1	0.32	-	85,85,85,85	0
24	K	A	1655	1/1	0.47	-	102,102,102,102	0
23	MG	A	1600	1/1	0.62	-	72,72,72,72	0
23	MG	A	1595	1/1	0.18	-	33,33,33,33	0
24	K	A	1641	1/1	0.69	-	97,97,97,97	0
23	MG	A	1592	1/1	0.35	-	63,63,63,63	0
23	MG	A	1598	1/1	0.66	-	73,73,73,73	0

6.5 Other polymers ⓘ

There are no such residues in this entry.