



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 05:35 PM GMT

PDB ID : 4BPP
Title : The crystal structure of the eukaryotic 40S ribosomal subunit in complex with eIF1 and eIF1A - Complex 4
Authors : Weisser, M.; Voigts-Hoffmann, F.; Rabl, J.; Leibundgut, M.; Ban, N.
Deposited on : 2013-05-27
Resolution : 3.70 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>

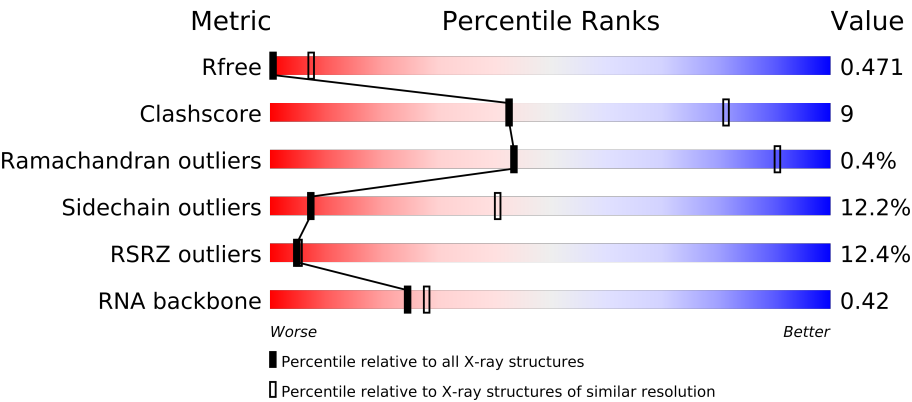
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.70 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	0	211	
2	1	68	
3	2	208	
4	3	197	
5	4	265	
6	5	119	
7	6	81	
8	7	162	
9	8	143	
10	9	189	
11	A	1753	
12	B	241	

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Mol	Chain	Length	Quality of chain
13	C	243	
14	D	181	
15	E	296	
16	F	101	
17	G	200	
18	H	130	
19	I	145	
20	J	120	
21	K	151	
22	L	142	
23	M	155	
24	N	55	
25	O	153	
26	P	149	
27	Q	157	
28	R	343	
29	S	144	
30	T	155	
31	U	126	
32	V	130	
33	W	259	
34	X	80	
35	Y	293	
36	Z	97	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
38	MG	A	5003	-	X
38	MG	A	5008	-	X
38	MG	A	5019	-	X
38	MG	A	5023	-	X
38	MG	A	5026	-	X
38	MG	A	5034	-	X
38	MG	A	5035	-	X
38	MG	A	5053	-	X
38	MG	A	5070	-	X
38	MG	A	5071	-	X
38	MG	A	5078	-	X

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 78902 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 protein called TRANSLATION INITIATION FACTOR EIF-1A FAMILY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	99	Total	C	N	O	S	0	0	0
			817	517	142	152	6			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	-17	MET	-	EXPRESSION TAG	UNP I7MK25
0	-16	GLY	-	EXPRESSION TAG	UNP I7MK25
0	-15	SER	-	EXPRESSION TAG	UNP I7MK25
0	-14	SER	-	EXPRESSION TAG	UNP I7MK25
0	-13	HIS	-	EXPRESSION TAG	UNP I7MK25
0	-12	HIS	-	EXPRESSION TAG	UNP I7MK25
0	-11	HIS	-	EXPRESSION TAG	UNP I7MK25
0	-10	HIS	-	EXPRESSION TAG	UNP I7MK25
0	-9	HIS	-	EXPRESSION TAG	UNP I7MK25
0	-8	HIS	-	EXPRESSION TAG	UNP I7MK25
0	-7	GLU	-	EXPRESSION TAG	UNP I7MK25
0	-6	ASN	-	EXPRESSION TAG	UNP I7MK25
0	-5	LEU	-	EXPRESSION TAG	UNP I7MK25
0	-4	TYR	-	EXPRESSION TAG	UNP I7MK25
0	-3	PHE	-	EXPRESSION TAG	UNP I7MK25
0	-2	GLN	-	EXPRESSION TAG	UNP I7MK25
0	-1	SER	-	EXPRESSION TAG	UNP I7MK25
0	0	ASN	-	EXPRESSION TAG	UNP I7MK25
0	1	ALA	-	EXPRESSION TAG	UNP I7MK25

- Molecule 2 is a protein called 40S RIBOSOMAL PROTEIN RPS28E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1	66	Total	C	N	O	S	0	0	0
			511	308	103	96	4			

- Molecule 3 is a protein called 40S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2	207	Total	C	N	O	S	0	0	0
			1693	1057	336	296	4			

- Molecule 4 is a protein called 40S RIBOSOMAL PROTEIN RPS7E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3	196	Total	C	N	O	S	0	0	0
			1629	1048	286	294	1			

- Molecule 5 is a protein called 40S RIBOSOMAL PROTEIN S3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4	221	Total	C	N	O	S	0	0	0
			1775	1121	319	331	4			

- Molecule 6 is a protein called 40S RIBOSOMAL PROTEIN RPS26E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	5	100	Total	C	N	O	S	0	0	0
			812	496	172	138	6			

- Molecule 7 is a protein called 40S RIBOSOMAL PROTEIN S27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	6	80	Total	C	N	O	S	0	0	0
			632	398	110	116	8			

- Molecule 8 is a protein called 40S RIBOSOMAL PROTEIN RPS10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	7	101	Total	C	N	O	S	0	0	0
			833	546	139	146	2			

- Molecule 9 is a protein called 40S RIBOSOMAL PROTEIN RPS25E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	8	79	Total	C	N	O	S	0	0	0
			615	388	112	113	2			

- Molecule 10 is a protein called 40S RIBOSOMAL PROTEIN RPS31E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	9	93	Total	C	N	O	S	0	0	0
			751	477	143	126	5			

- Molecule 11 is a RNA chain called 18S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	A	1717	Total	C	N	O	P	0	0	0
			36629	16385	6539	11988	1717			

- Molecule 12 is a protein called 40S RIBOSOMAL PROTEIN SA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	B	201	Total	C	N	O	S	0	0	0
			1619	1023	285	301	10			

- Molecule 13 is a protein called 40S RIBOSOMAL PROTEIN RPS3E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	C	228	Total	C	N	O	S	0	0	0
			1811	1167	318	318	8			

- Molecule 14 is a protein called 40S RIBOSOMAL PROTEIN RPS9E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	D	180	Total	C	N	O	S	0	0	0
			1478	932	287	254	5			

- Molecule 15 is a protein called 40S RIBOSOMAL PROTEIN RPS2E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	E	229	Total	C	N	O	S	0	0	0
			1818	1171	321	323	3			

- Molecule 16 is a protein called EIF1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	F	89	Total	C	N	O	S	0	0	0
			736	465	131	137	3			

- Molecule 17 is a protein called 40S RIBOSOMAL PROTEIN RPS5E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	G	192	Total	C	N	O	S	0	0	0
			1520	961	281	270	8			

- Molecule 18 is a protein called 40S RIBOSOMAL PROTEIN RPS22E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	H	129	Total	C	N	O	S	0	0	0
			1040	671	184	180	5			

- Molecule 19 is a protein called 40S RIBOSOMAL PROTEIN RPS16E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	I	143	Total	C	N	O	S	0	0	0
			1135	715	217	198	5			

- Molecule 20 is a protein called 40S RIBOSOMAL PROTEIN RPS20E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	J	108	Total	C	N	O	S	0	0	0
			859	539	154	160	6			

- Molecule 21 is a protein called 40S RIBOSOMAL PROTEIN RPS14E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	K	140	Total	C	N	O	S	0	0	0
			1063	654	206	197	6			

- Molecule 22 is a protein called 40S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	L	140	Total	C	N	O	S	0	0	0
			1086	685	217	179	5			

- Molecule 23 is a protein called 40S RIBOSOMAL PROTEIN RPS18E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	M	153	Total	C	N	O	S	0	0	0
			1231	775	236	215	5			

- Molecule 24 is a protein called 40S RIBOSOMAL PROTEIN RPS29E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	N	54	Total	C	N	O	S	0	0	0
			454	283	92	73	6			

- Molecule 25 is a protein called 40S RIBOSOMAL PROTEIN RPS13E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	O	152	Total	C	N	O	S	0	0	0
			1229	790	233	202	4			

- Molecule 26 is a protein called 40S RIBOSOMAL PROTEIN S24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	P	148	Total	C	N	O	S	0	0	0
			1197	763	221	213				

- Molecule 27 is a protein called 40S RIBOSOMAL PROTEIN RPS11E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Q	156	Total	C	N	O	S	0	0	0
			1267	813	234	216	4			

- Molecule 28 is a protein called 40S RIBOSOMAL PROTEIN RACK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	R	338	Total	C	N	O	S	0	0	0
			2682	1711	462	501	8			

- Molecule 29 is a protein called 40S RIBOSOMAL PROTEIN RPS15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	S	128	Total	C	N	O	S	0	0	0
			1010	648	178	180	4			

- Molecule 30 is a protein called 40S RIBOSOMAL PROTEIN RPS19E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	T	154	Total	C	N	O	S	0	0	0
			1242	785	234	221	2			

- Molecule 31 is a protein called 40S RIBOSOMAL PROTEIN RPS12E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	U	124	Total	C	N	O	S	0	0	0
			952	599	166	182	5			

- Molecule 32 is a protein called 40S RIBOSOMAL PROTEIN RPS17E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	V	119	Total	C	N	O	S	0	0	0
			968	613	180	173	2			

- Molecule 33 is a protein called 40S RIBOSOMAL PROTEIN RPS4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	W	259	Total	C	N	O	S	0	0	0
			2079	1322	383	370	4			

- Molecule 34 is a protein called 40S RIBOSOMAL PROTEIN RPS30E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	X	74	Total	C	N	O	S	0	0	0
			599	376	124	96	3			

- Molecule 35 is a protein called 40S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	Y	228	Total	C	N	O	S	0	0	0
			1826	1157	340	318	11			

- Molecule 36 is a protein called 40S RIBOSOMAL PROTEIN RPS21E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	Z	97	Total	C	N	O	S	0	0	0
			747	458	139	146	4			

- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	9	1	Total	Zn	0	0
			1	1		
37	N	1	Total	Zn	0	0
			1	1		
37	6	1	Total	Zn	0	0
			1	1		

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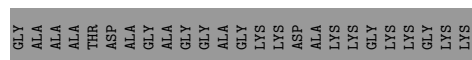
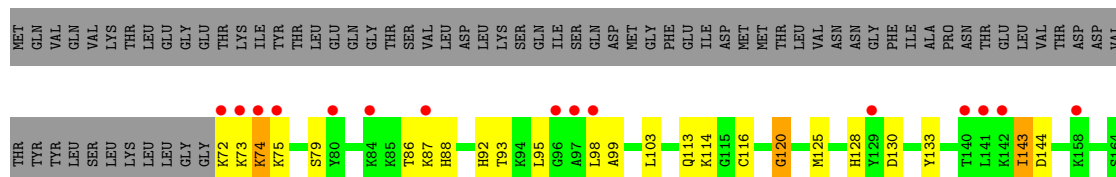
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	5	1	Total	Zn	0	0
			1	1		

- Molecule 38 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	A	79	Total	Mg	0	0
			79	79		

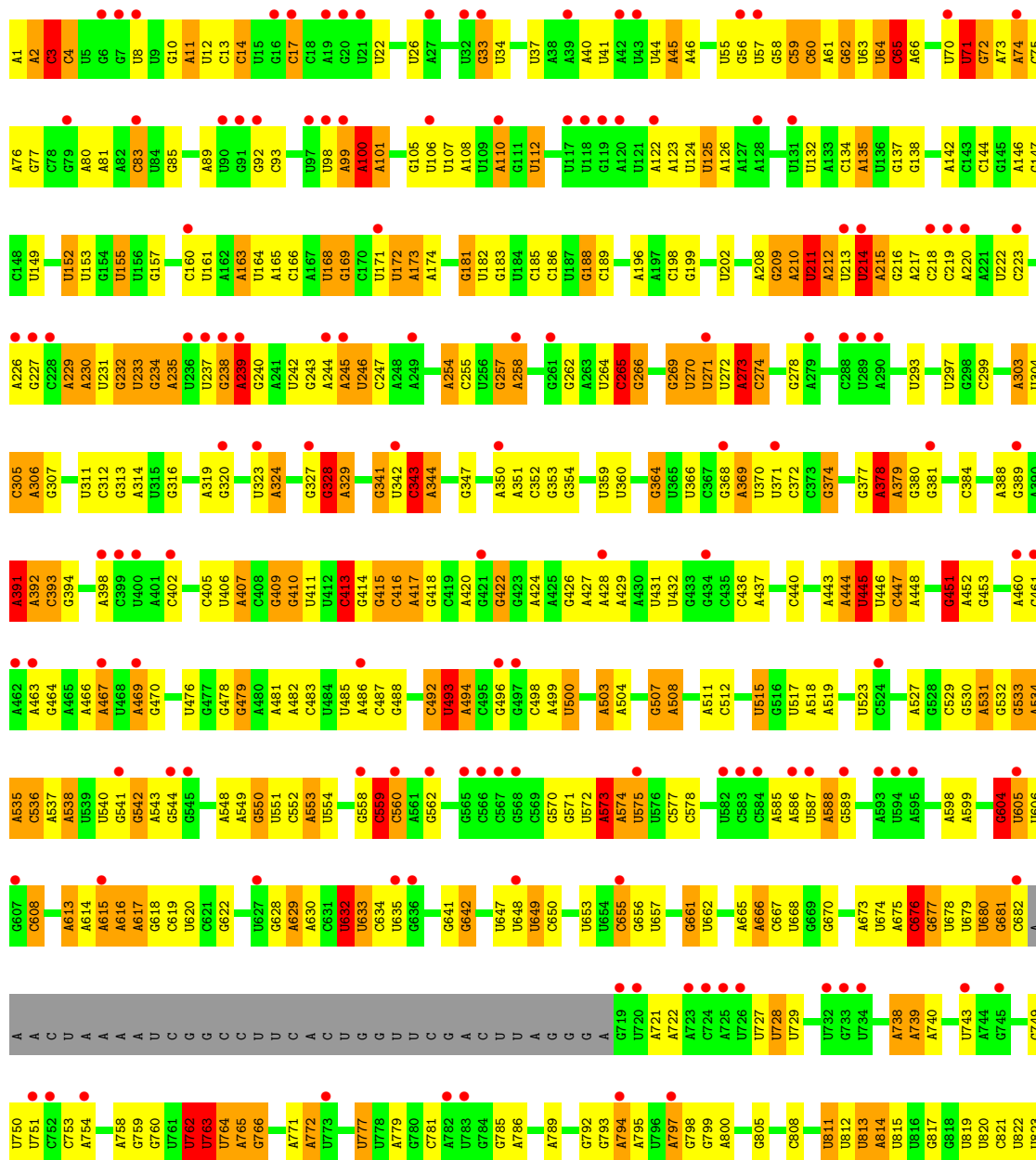
- Molecule 39 is water.

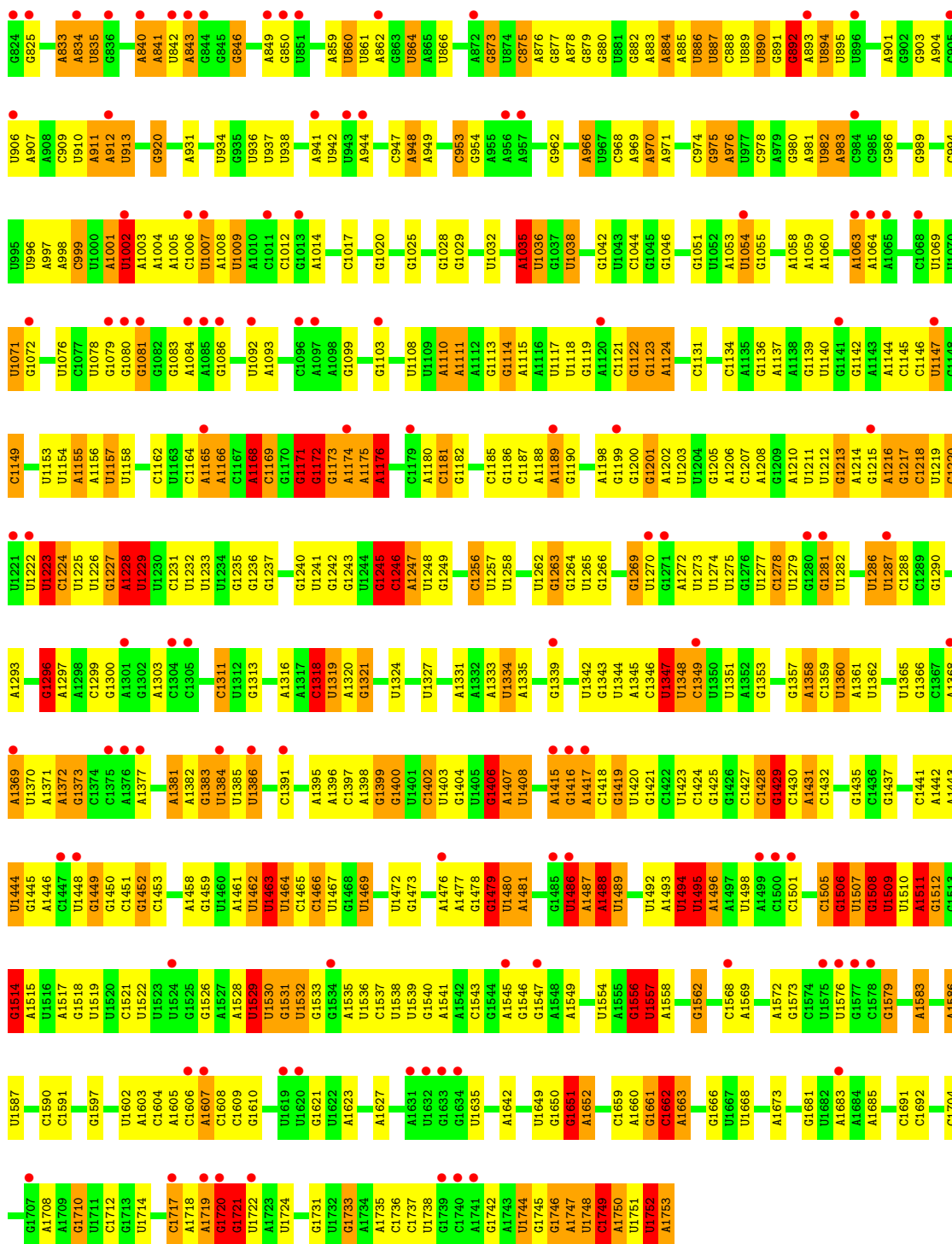
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	A	474	Total	O	0	0
			474	474		

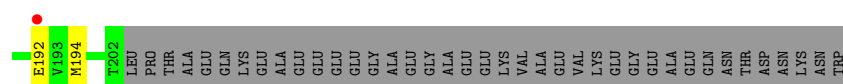


• Molecule 11: 18S RRNA

Chain A:

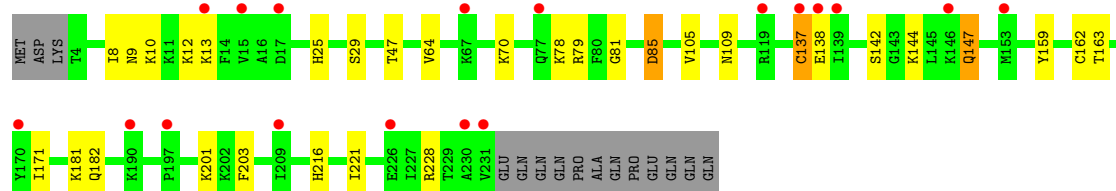






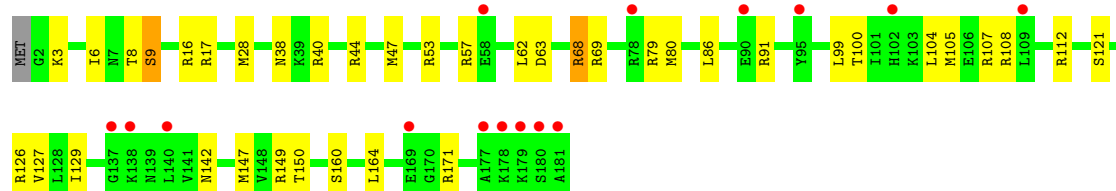
• Molecule 13: 40S RIBOSOMAL PROTEIN RPS3E

Chain C:



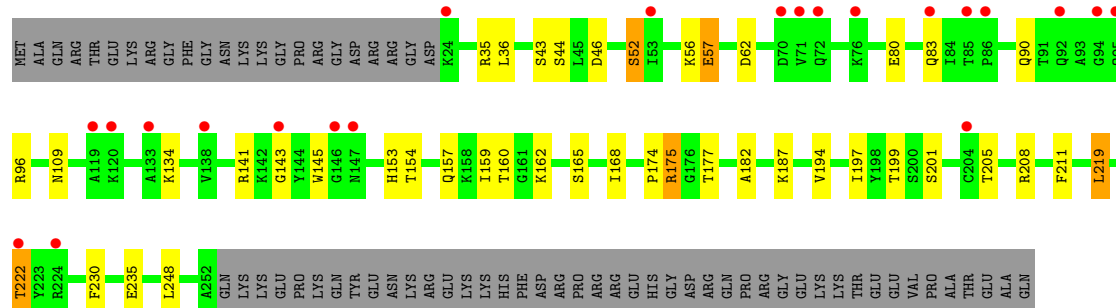
• Molecule 14: 40S RIBOSOMAL PROTEIN RPS9E

Chain D:



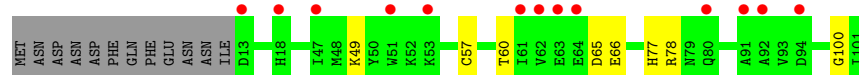
• Molecule 15: 40S RIBOSOMAL PROTEIN RPS2E

Chain E:



• Molecule 16: EIF1

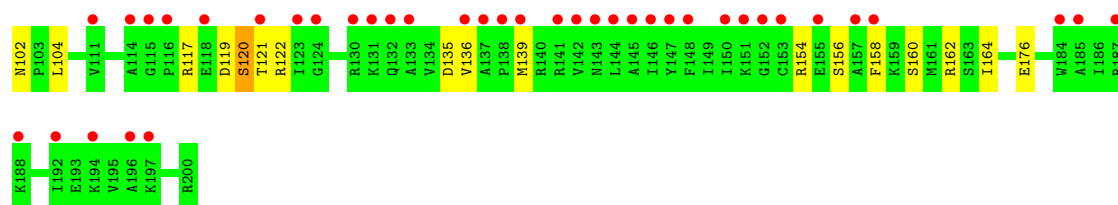
Chain F:



• Molecule 17: 40S RIBOSOMAL PROTEIN RPS5E

Chain G:





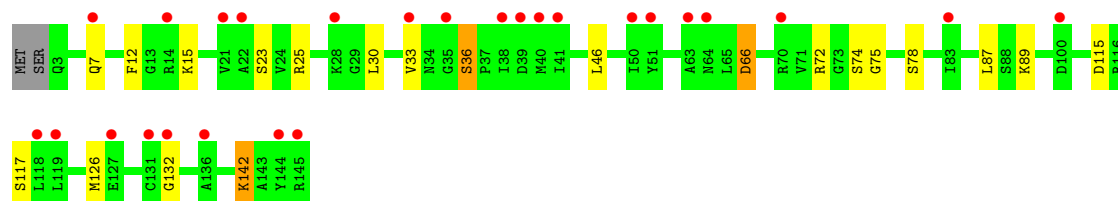
- Molecule 18: 40S RIBOSOMAL PROTEIN RPS22E

Chain H:



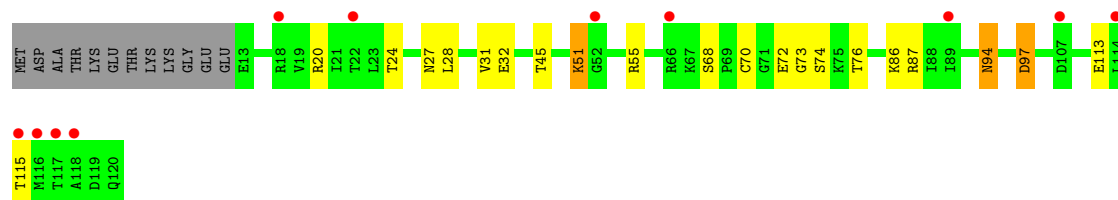
- Molecule 19: 40S RIBOSOMAL PROTEIN RPS16E

Chain I:



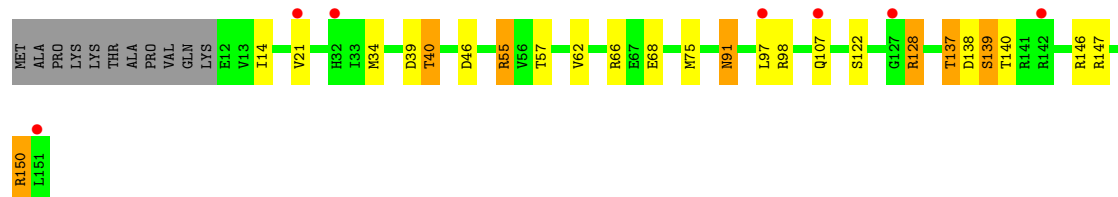
- Molecule 20: 40S RIBOSOMAL PROTEIN RPS20E

Chain J:



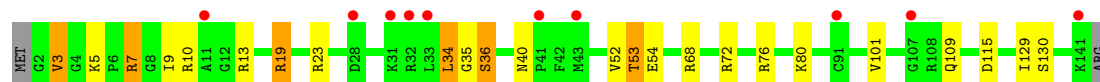
- Molecule 21: 40S RIBOSOMAL PROTEIN RPS14E

Chain K:



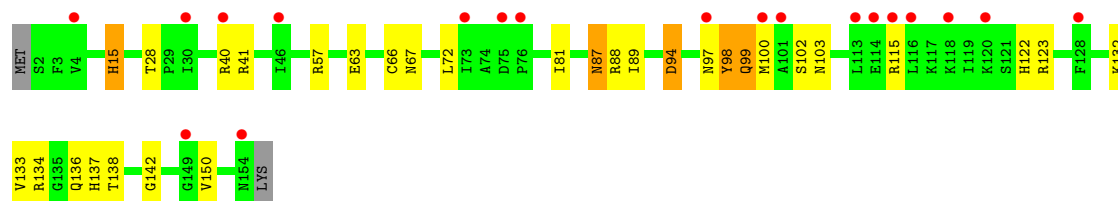
- Molecule 22: 40S RIBOSOMAL PROTEIN S12

Chain L:



- Molecule 23: 40S RIBOSOMAL PROTEIN RPS18E

Chain M: 



- Molecule 24: 40S RIBOSOMAL PROTEIN RPS29E

Chain N: 



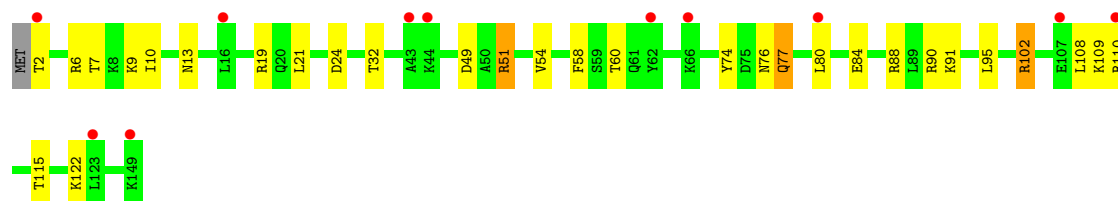
- Molecule 25: 40S RIBOSOMAL PROTEIN RPS13E

Chain O: 



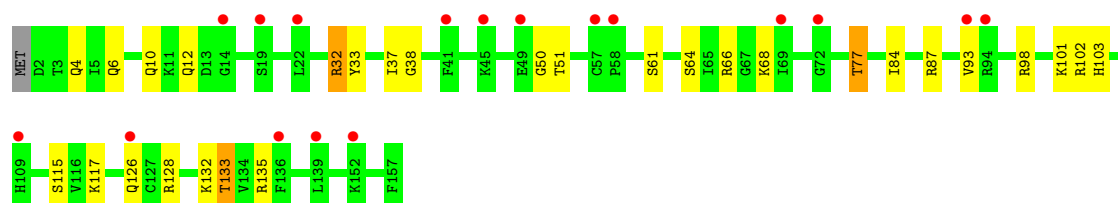
- Molecule 26: 40S RIBOSOMAL PROTEIN S24

Chain P: 



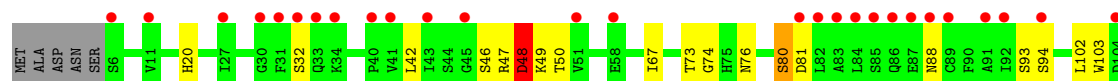
- Molecule 27: 40S RIBOSOMAL PROTEIN RPS11E

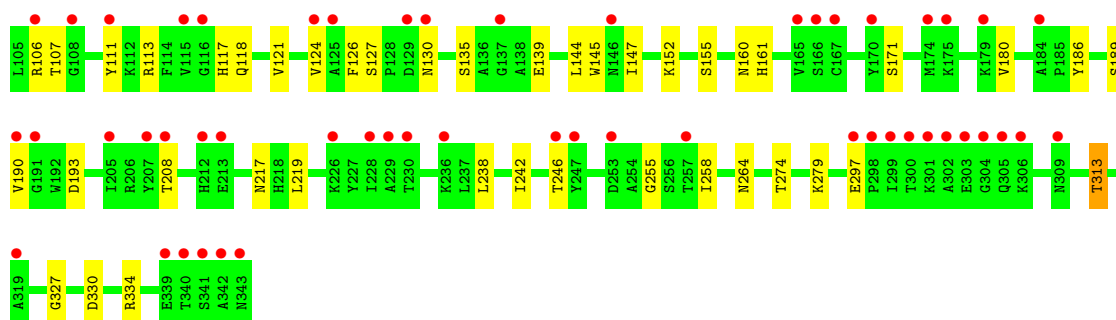
Chain Q: 



- Molecule 28: 40S RIBOSOMAL PROTEIN RACK1

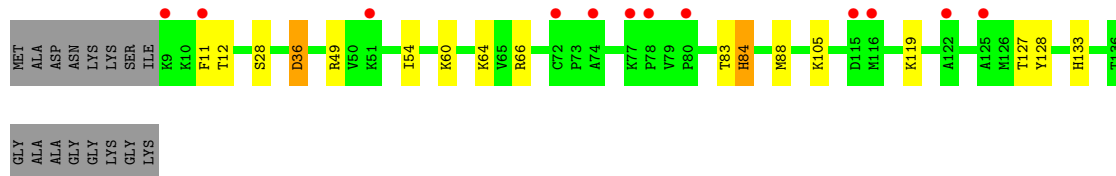
Chain R: 





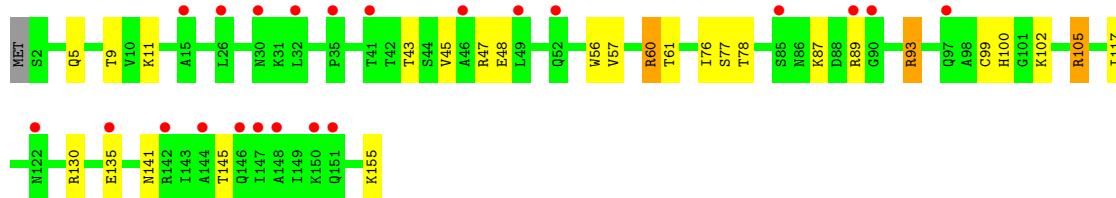
• Molecule 29: 40S RIBOSOMAL PROTEIN RPS15E

Chain S:



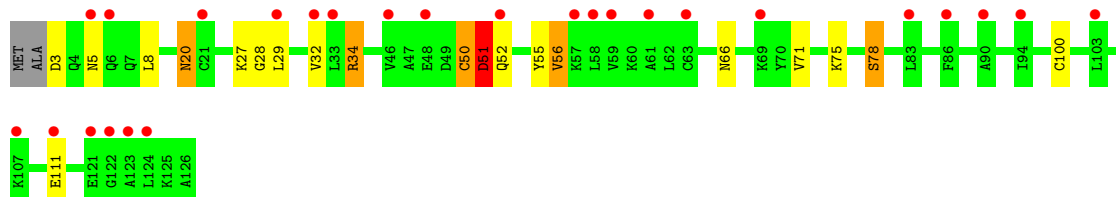
• Molecule 30: 40S RIBOSOMAL PROTEIN RPS19E

Chain T:



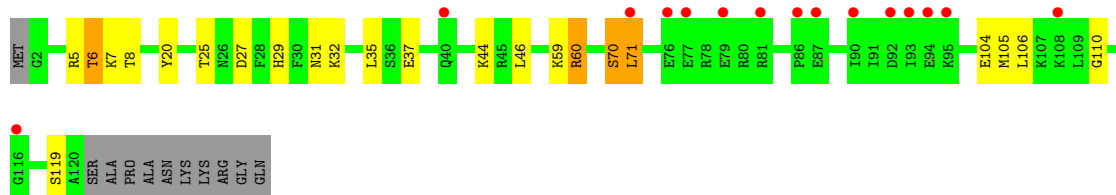
• Molecule 31: 40S RIBOSOMAL PROTEIN RPS12E

Chain U:



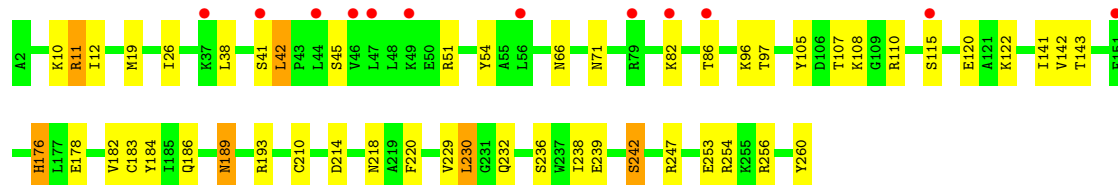
• Molecule 32: 40S RIBOSOMAL PROTEIN RPS17E

Chain V:



• Molecule 33: 40S RIBOSOMAL PROTEIN RPS4E

Chain W:



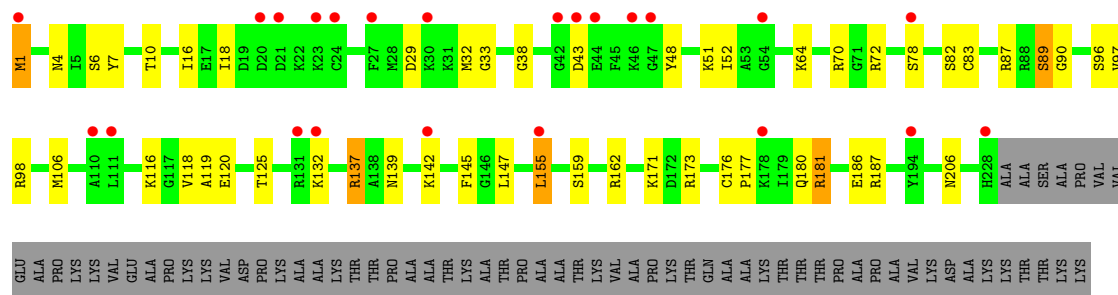
- Molecule 34: 40S RIBOSOMAL PROTEIN RPS30E

Chain X:



- Molecule 35: 40S RIBOSOMAL PROTEIN S6

Chain Y:



- Molecule 36: 40S RIBOSOMAL PROTEIN RPS21E

Chain Z:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	209.99Å 471.55Å 298.54Å 90.00° 91.02° 90.00°	Depositor
Resolution (Å)	49.75 – 3.70 49.75 – 3.70	Depositor EDS
% Data completeness (in resolution range)	91.0 (49.75-3.70) 86.3 (49.75-3.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 3.67Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.202 , 0.229 0.470 , 0.471	Depositor DCC
R_{free} test set	5341 reflections (0.97%)	DCC
Wilson B-factor (Å ²)	97.6	Xtriage
Anisotropy	0.570	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 96.3	EDS
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 607573 reflections	Xtriage
F_o, F_c correlation	0.59	EDS
Total number of atoms	78902	wwPDB-VP
Average B, all atoms (Å ²)	170.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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: ZN, MG

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	0	0.31	0/827	0.57	0/1103
2	1	0.28	0/510	0.65	0/677
3	2	0.32	0/1717	0.61	0/2288
4	3	0.32	0/1656	0.60	0/2223
5	4	0.54	4/1801 (0.2%)	0.70	2/2417 (0.1%)
6	5	0.35	0/823	0.67	0/1100
7	6	0.32	0/640	0.55	0/855
8	7	0.30	0/853	0.56	0/1148
9	8	0.31	0/620	0.62	0/831
10	9	0.31	0/764	0.67	1/1007 (0.1%)
11	A	0.44	1/40993 (0.0%)	1.12	219/63880 (0.3%)
12	B	0.29	0/1652	0.58	0/2240
13	C	0.31	0/1846	0.58	1/2479 (0.0%)
14	D	0.33	0/1501	0.65	0/2003
15	E	0.35	0/1864	0.62	0/2521
16	F	0.30	0/751	0.60	0/1010
17	G	0.31	0/1546	0.62	1/2079 (0.0%)
18	H	0.36	0/1058	0.73	1/1421 (0.1%)
19	I	0.31	0/1151	0.61	0/1540
20	J	0.37	1/868 (0.1%)	0.63	0/1168
21	K	0.33	0/1078	0.70	0/1452
22	L	0.34	0/1103	0.64	0/1471
23	M	0.28	0/1252	0.60	0/1680
24	N	0.34	0/465	0.63	0/619
25	O	0.32	0/1253	0.62	0/1677
26	P	0.31	0/1215	0.60	0/1626
27	Q	0.33	0/1290	0.65	0/1731
28	R	0.29	0/2750	0.60	0/3726
29	S	0.27	0/1028	0.54	0/1374
30	T	0.33	0/1264	0.57	0/1698
31	U	0.30	0/961	0.58	0/1288
32	V	0.30	0/981	0.57	0/1311

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	W	0.34	0/2119	0.62	0/2849
34	X	0.28	0/612	0.54	0/812
35	Y	0.31	0/1852	0.55	0/2462
36	Z	0.33	0/755	0.61	0/1013
All	All	0.39	6/83419 (0.0%)	0.92	225/120779 (0.2%)

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
4	3	0	1
5	4	0	2
7	6	0	1
9	8	0	1
17	G	0	1
18	H	0	2
20	J	0	1
21	K	0	1
25	O	0	1
29	S	0	2
31	U	0	2
32	V	0	1
33	W	0	1
All	All	0	17

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	4	31	TRP	NE1-CE2	-10.69	1.23	1.37
5	4	31	TRP	CD1-NE1	8.48	1.52	1.38
11	A	1586	A	O3'-P	7.60	1.70	1.61
5	4	31	TRP	CD2-CE2	7.60	1.50	1.41
5	4	31	TRP	CG-CD2	6.46	1.54	1.43
20	J	70	CYS	CB-SG	-5.20	1.73	1.81

All (225) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	515	U	N1-C2-O2	12.24	131.37	122.80
11	A	1296	G	N3-C2-N2	-11.41	111.91	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	447	C	C2-N1-C1'	9.34	129.08	118.80
11	A	573	A	C6-N1-C2	9.27	124.16	118.60
11	A	493	U	O4'-C1'-N1	9.11	115.48	108.20
11	A	559	C	O5'-P-OP1	8.96	121.45	110.70
11	A	763	U	C2-N1-C1'	8.91	128.39	117.70
11	A	1134	C	OP2-P-O3'	8.80	124.55	105.20
11	A	1296	G	N1-C2-N2	8.74	124.07	116.20
11	A	393	C	C2-N1-C1'	8.41	128.05	118.80
11	A	445	U	C2-N1-C1'	8.35	127.72	117.70
11	A	1263	G	N3-C2-N2	-8.29	114.09	119.90
11	A	1529	U	C2-N1-C1'	8.25	127.60	117.70
11	A	604	G	C4-N9-C1'	8.18	137.13	126.50
11	A	1229	U	C2-N1-C1'	7.95	127.24	117.70
11	A	1009	U	C4-C5-C6	7.92	124.45	119.70
11	A	763	U	N1-C2-O2	7.87	128.31	122.80
11	A	1225	U	N1-C2-O2	7.82	128.27	122.80
11	A	393	C	C5-C6-N1	7.76	124.88	121.00
11	A	445	U	N1-C2-O2	7.75	128.22	122.80
11	A	391	A	P-O3'-C3'	7.69	128.93	119.70
11	A	559	C	C2-N1-C1'	7.57	127.13	118.80
11	A	445	U	N3-C2-O2	-7.53	116.93	122.20
11	A	270	U	C2-N1-C1'	7.52	126.73	117.70
11	A	887	U	C5-C6-N1	7.48	126.44	122.70
11	A	559	C	N1-C2-O2	7.48	123.39	118.90
11	A	1256	C	OP1-P-O3'	7.39	121.46	105.20
11	A	1752	U	O4'-C1'-N1	7.36	114.09	108.20
11	A	270	U	N1-C2-O2	7.32	127.92	122.80
11	A	573	A	N1-C2-N3	-7.32	125.64	129.30
11	A	777	U	C2-N1-C1'	7.30	126.47	117.70
11	A	515	U	C2-N3-C4	7.11	131.27	127.00
11	A	523	U	C2-N3-C4	-7.02	122.79	127.00
11	A	1009	U	C5-C6-N1	-6.94	119.23	122.70
11	A	152	U	N3-C2-O2	-6.90	117.37	122.20
11	A	763	U	N3-C2-O2	-6.87	117.39	122.20
11	A	1246	C	P-O3'-C3'	6.86	127.93	119.70
11	A	1263	G	N1-C2-N3	6.81	127.98	123.90
11	A	1752	U	N3-C2-O2	-6.79	117.45	122.20
11	A	1303	A	OP2-P-O3'	6.76	120.08	105.20
10	9	120	GLY	N-CA-C	6.72	129.91	113.10
11	A	447	C	C6-N1-C1'	-6.72	112.73	120.80
11	A	1038	U	C5-C6-N1	6.69	126.04	122.70
11	A	447	C	C5-C6-N1	6.68	124.34	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	271	U	OP1-P-O3'	6.68	119.89	105.20
11	A	887	U	O5'-P-OP1	6.64	118.67	110.70
11	A	493	U	N1-C1'-C2'	6.61	122.59	114.00
11	A	1149	C	C5-C6-N1	6.60	124.30	121.00
11	A	887	U	C2-N1-C1'	6.56	125.57	117.70
11	A	515	U	N1-C2-N3	-6.55	110.97	114.90
11	A	559	C	C6-N1-C1'	-6.55	112.94	120.80
11	A	393	C	C6-N1-C1'	-6.54	112.95	120.80
11	A	71	U	C2-N1-C1'	6.54	125.54	117.70
11	A	515	U	N3-C2-O2	-6.48	117.66	122.20
11	A	1263	G	N9-C4-C5	6.47	107.99	105.40
11	A	728	U	C2-N1-C1'	6.46	125.45	117.70
11	A	152	U	C2-N1-C1'	6.46	125.45	117.70
11	A	1168	A	P-O3'-C3'	6.42	127.41	119.70
11	A	1296	G	N3-C4-N9	-6.40	122.16	126.00
11	A	1225	U	C2-N1-C1'	6.38	125.36	117.70
11	A	604	G	C8-N9-C1'	-6.38	118.70	127.00
11	A	515	U	C2-N1-C1'	6.38	125.36	117.70
11	A	447	C	N1-C2-O2	6.38	122.73	118.90
11	A	1508	G	O4'-C1'-N9	6.36	113.29	108.20
11	A	523	U	C5-C4-O4	-6.35	122.09	125.90
11	A	1721	G	C8-N9-C4	-6.33	103.87	106.40
11	A	328	G	P-O3'-C3'	6.30	127.26	119.70
11	A	1721	G	N7-C8-N9	6.29	116.25	113.10
11	A	762	U	C2-N1-C1'	6.28	125.24	117.70
11	A	777	U	N1-C2-O2	6.25	127.17	122.80
11	A	1263	G	C8-N9-C4	-6.24	103.91	106.40
11	A	1744	U	OP1-P-O3'	6.19	118.83	105.20
11	A	271	U	C2-N1-C1'	6.16	125.09	117.70
11	A	1408	U	C2-N1-C1'	6.14	125.06	117.70
11	A	100	A	P-O3'-C3'	6.12	127.04	119.70
11	A	374	G	C6-C5-N7	-6.10	126.74	130.40
11	A	1529	U	N1-C2-O2	6.08	127.05	122.80
11	A	3	C	N1-C2-O2	6.05	122.53	118.90
11	A	1207	C	C2-N1-C1'	6.04	125.45	118.80
11	A	1263	G	N3-C4-N9	-6.04	122.38	126.00
11	A	763	U	C6-N1-C1'	-6.04	112.75	121.20
11	A	1386	U	C2-N1-C1'	6.03	124.94	117.70
11	A	371	U	C2-N1-C1'	6.00	124.89	117.70
11	A	860	U	C5-C6-N1	5.99	125.70	122.70
11	A	833	A	P-O3'-C3'	5.99	126.88	119.70
11	A	1278	C	P-O3'-C3'	5.98	126.87	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1662	C	C6-N1-C2	-5.97	117.91	120.30
11	A	813	U	O5'-P-OP1	5.97	117.86	110.70
5	4	31	TRP	CD2-CE2-CZ2	-5.96	115.15	122.30
11	A	270	U	N3-C2-O2	-5.95	118.03	122.20
11	A	1035	A	C2-N3-C4	5.93	113.57	110.60
11	A	604	G	N7-C8-N9	5.93	116.06	113.10
11	A	413	C	C2-N1-C1'	5.89	125.28	118.80
11	A	1429	G	N3-C4-C5	-5.89	125.66	128.60
11	A	1506	G	P-O3'-C3'	5.89	126.76	119.70
11	A	1229	U	C6-N1-C1'	-5.86	113.00	121.20
11	A	762	U	N1-C2-O2	5.85	126.90	122.80
11	A	271	U	P-O3'-C3'	5.83	126.70	119.70
11	A	666	A	N7-C8-N9	5.83	116.72	113.80
11	A	1749	C	C2-N1-C1'	5.82	125.20	118.80
11	A	661	G	C4-N9-C1'	5.81	134.05	126.50
11	A	1172	G	P-O3'-C3'	5.76	126.62	119.70
11	A	676	C	P-O3'-C3'	5.76	126.61	119.70
11	A	661	G	C8-N9-C1'	-5.76	119.51	127.00
11	A	573	A	OP1-P-O3'	5.72	117.79	105.20
11	A	65	C	C5-C6-N1	5.72	123.86	121.00
11	A	559	C	C5-C6-N1	5.72	123.86	121.00
11	A	1176	A	C8-N9-C4	-5.72	103.51	105.80
11	A	364	G	C4-N9-C1'	5.71	133.92	126.50
11	A	892	G	C8-N9-C4	5.70	108.68	106.40
11	A	1347	U	P-O3'-C3'	5.69	126.53	119.70
11	A	211	U	O4'-C1'-N1	5.69	112.75	108.20
11	A	1511	A	N1-C6-N6	5.68	122.01	118.60
13	C	81	GLY	N-CA-C	-5.67	98.93	113.10
11	A	447	C	C6-N1-C2	-5.66	118.03	120.30
11	A	515	U	C5-C6-N1	5.66	125.53	122.70
11	A	152	U	O4'-C1'-N1	5.66	112.73	108.20
11	A	777	U	N3-C2-O2	-5.66	118.24	122.20
11	A	1278	C	N3-C2-O2	-5.65	117.94	121.90
11	A	1466	C	C2-N1-C1'	5.65	125.01	118.80
11	A	1532	U	N3-C2-O2	-5.63	118.26	122.20
11	A	860	U	C2-N1-C1'	5.62	124.45	117.70
11	A	604	G	C8-N9-C4	-5.61	104.16	106.40
11	A	1207	C	N1-C2-O2	5.61	122.27	118.90
11	A	1263	G	C2-N3-C4	-5.61	109.09	111.90
11	A	343	C	C2-N1-C1'	5.61	124.97	118.80
11	A	163	A	P-O3'-C3'	5.60	126.42	119.70
11	A	617	A	O4'-C1'-N9	5.59	112.67	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1176	A	N7-C8-N9	5.59	116.59	113.80
11	A	632	U	P-O3'-C3'	5.58	126.40	119.70
11	A	1662	C	C5-C6-N1	5.58	123.79	121.00
11	A	1744	U	P-O3'-C3'	5.57	126.38	119.70
11	A	1171	G	C2-N3-C4	5.56	114.68	111.90
11	A	1494	U	P-O3'-C3'	5.54	126.35	119.70
11	A	152	U	N1-C2-O2	5.51	126.66	122.80
17	G	74	HIS	N-CA-C	-5.51	96.14	111.00
11	A	573	A	P-O3'-C3'	5.50	126.29	119.70
11	A	1529	U	N3-C2-O2	-5.49	118.36	122.20
11	A	168	U	P-O3'-C3'	5.48	126.28	119.70
11	A	1463	U	P-O3'-C3'	5.48	126.27	119.70
11	A	3	C	P-O3'-C3'	5.45	126.24	119.70
11	A	34	U	C2-N1-C1'	5.45	124.24	117.70
18	H	55	ASP	N-CA-C	-5.44	96.32	111.00
11	A	1229	U	N1-C2-O2	5.43	126.60	122.80
11	A	762	U	N3-C2-O2	-5.43	118.40	122.20
11	A	1431	A	P-O3'-C3'	5.42	126.20	119.70
11	A	306	A	O4'-C1'-N9	5.42	112.53	108.20
11	A	1529	U	C6-N1-C1'	-5.40	113.64	121.20
11	A	1557	U	P-O3'-C3'	5.40	126.18	119.70
11	A	833	A	OP1-P-O3'	5.38	117.03	105.20
11	A	1054	U	P-O3'-C3'	5.38	126.15	119.70
11	A	445	U	C6-N1-C1'	-5.37	113.69	121.20
11	A	169	G	N3-C4-N9	5.36	129.22	126.00
11	A	1744	U	C2-N1-C1'	5.36	124.13	117.70
11	A	632	U	C2-N1-C1'	5.35	124.12	117.70
11	A	1281	G	C4-N9-C1'	5.35	133.45	126.50
11	A	1495	U	P-O3'-C3'	5.35	126.11	119.70
11	A	573	A	C5-C6-N1	-5.33	115.03	117.70
11	A	152	U	C6-N1-C2	-5.32	117.81	121.00
11	A	575	U	C2-N1-C1'	5.32	124.08	117.70
11	A	1749	C	C6-N1-C2	-5.31	118.17	120.30
11	A	1228	A	P-O3'-C3'	5.30	126.07	119.70
11	A	347	G	C4-N9-C1'	5.30	133.39	126.50
11	A	1651	G	P-O3'-C3'	5.30	126.06	119.70
11	A	99	A	P-O3'-C3'	5.28	126.04	119.70
11	A	273	A	P-O3'-C3'	5.28	126.03	119.70
11	A	214	U	OP1-P-O3'	5.27	116.80	105.20
11	A	1556	G	P-O3'-C3'	5.27	126.03	119.70
11	A	1429	G	C2-N3-C4	5.26	114.53	111.90
11	A	1369	A	C2-N3-C4	5.25	113.23	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	793	G	N3-C4-C5	5.25	131.22	128.60
11	A	1278	C	OP1-P-O3'	5.24	116.74	105.20
11	A	239	A	C4-N9-C1'	5.24	135.74	126.30
11	A	1002	U	P-O3'-C3'	5.24	125.98	119.70
11	A	1334	U	C2-N1-C1'	5.23	123.98	117.70
11	A	1488	A	P-O3'-C3'	5.23	125.98	119.70
5	4	31	TRP	CE2-CD2-CG	-5.21	103.13	107.30
11	A	777	U	C5-C6-N1	5.21	125.30	122.70
11	A	1223	U	P-O3'-C3'	5.21	125.95	119.70
11	A	1514	G	O4'-C1'-N9	5.21	112.36	108.20
11	A	1318	C	P-O3'-C3'	5.20	125.94	119.70
11	A	271	U	C6-N1-C1'	-5.19	113.94	121.20
11	A	270	U	C6-N1-C1'	-5.18	113.94	121.20
11	A	341	G	C4-N9-C1'	5.18	133.24	126.50
11	A	953	C	C2-N1-C1'	5.17	124.49	118.80
11	A	1245	G	C4-N9-C1'	5.17	133.22	126.50
11	A	1508	G	N3-C4-C5	-5.17	126.02	128.60
11	A	3	C	C2-N1-C1'	5.17	124.48	118.80
11	A	188	G	C4-N9-C1'	5.16	133.21	126.50
11	A	371	U	C6-N1-C1'	-5.16	113.98	121.20
11	A	1278	C	C6-N1-C2	-5.16	118.24	120.30
11	A	413	C	P-O3'-C3'	5.16	125.89	119.70
11	A	1009	U	N1-C2-N3	5.16	117.99	114.90
11	A	1486	U	P-O3'-C3'	5.16	125.89	119.70
11	A	1554	U	N1-C2-O2	-5.15	119.19	122.80
11	A	1662	C	C2-N1-C1'	5.15	124.46	118.80
11	A	1720	G	C8-N9-C4	-5.15	104.34	106.40
11	A	887	U	C6-N1-C1'	-5.14	114.01	121.20
11	A	892	G	N3-C4-C5	5.13	131.17	128.60
11	A	1223	U	C3'-C2'-C1'	5.13	105.60	101.50
11	A	378	A	C8-N9-C4	-5.12	103.75	105.80
11	A	890	U	P-O3'-C3'	5.12	125.84	119.70
11	A	1122	G	P-O3'-C3'	5.11	125.83	119.70
11	A	451	G	C4-N9-C1'	5.10	133.13	126.50
11	A	1509	U	P-O3'-C3'	5.10	125.82	119.70
11	A	265	C	C2-N1-C1'	5.09	124.40	118.80
11	A	1149	C	C2-N1-C1'	5.09	124.40	118.80
11	A	1406	G	P-O3'-C3'	5.09	125.81	119.70
11	A	83	C	C2-N1-C1'	5.09	124.40	118.80
11	A	422	G	N7-C8-N9	5.08	115.64	113.10
11	A	1463	U	N1-C2-O2	5.07	126.35	122.80
11	A	886	U	C5-C6-N1	5.07	125.23	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1225	U	C6-N1-C1'	-5.07	114.10	121.20
11	A	1256	C	P-O3'-C3'	5.06	125.77	119.70
11	A	666	A	C8-N9-C4	-5.05	103.78	105.80
11	A	1009	U	O4'-C1'-N1	5.04	112.23	108.20
11	A	214	U	P-O3'-C3'	5.04	125.75	119.70
11	A	1529	U	C5-C6-N1	5.04	125.22	122.70
11	A	1463	U	N3-C2-O2	-5.03	118.68	122.20
11	A	1054	U	C2-N1-C1'	5.02	123.72	117.70
11	A	1296	G	N9-C4-C5	5.02	107.41	105.40
11	A	1122	G	N9-C1'-C2'	-5.01	106.49	112.00
11	A	1508	G	C2-N3-C4	5.01	114.40	111.90
11	A	1479	G	C4-N9-C1'	5.01	133.01	126.50
11	A	1402	C	C3'-C2'-C1'	5.00	105.50	101.50

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	3	131	LEU	Peptide
5	4	238	TYR	Peptide
5	4	71	THR	Peptide
7	6	65	THR	Peptide
9	8	99	ASN	Peptide
17	G	73	PHE	Peptide
18	H	58	SER	Peptide
18	H	66	ILE	Peptide
20	J	72	GLU	Peptide
21	K	137	THR	Peptide
25	O	15	GLY	Peptide
29	S	105	LYS	Peptide
29	S	133	HIS	Peptide
31	U	51	ASP	Peptide
31	U	66	ASN	Peptide
32	V	70	SER	Mainchain
33	W	242	SER	Peptide

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	0	817	0	0	10	0
2	1	511	0	0	4	0
3	2	1693	0	0	25	0
4	3	1629	0	0	17	0
5	4	1775	0	0	15	0
6	5	812	0	0	11	0
7	6	632	0	0	4	0
8	7	833	0	0	11	0
9	8	615	0	0	4	0
10	9	751	0	0	18	0
11	A	36629	0	0	432	0
12	B	1619	0	0	8	0
13	C	1811	0	0	18	0
14	D	1478	0	0	8	0
15	E	1818	0	0	16	0
16	F	736	0	0	2	0
17	G	1520	0	0	12	0
18	H	1040	0	0	8	0
19	I	1135	0	0	7	0
20	J	859	0	0	10	0
21	K	1063	0	0	13	0
22	L	1086	0	0	11	0
23	M	1231	0	0	16	0
24	N	454	0	0	16	0
25	O	1229	0	0	10	0
26	P	1197	0	0	14	0
27	Q	1267	0	0	12	0
28	R	2682	0	0	21	0
29	S	1010	0	0	6	0
30	T	1242	0	0	16	0
31	U	952	0	0	10	0
32	V	968	0	0	12	0
33	W	2079	0	0	16	0
34	X	599	0	0	4	0
35	Y	1826	0	0	24	0
36	Z	747	0	0	6	0
37	5	1	0	0	0	0
37	6	1	0	0	0	0
37	9	1	0	0	0	0
37	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	A	79	0	0	0	0
39	A	474	0	0	49	0
All	All	78902	0	0	640	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 9.

All (640) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:A:1377:A:OP2	17:G:54:LYS:NZ	1.65	1.29
11:A:1214:A:OP1	29:S:64:LYS:NZ	1.71	1.23
9:8:81:ARG:NH2	11:A:1505:C:OP2	1.73	1.20
15:E:141:ARG:NH1	36:Z:25:ASP:OD2	1.76	1.15
36:Z:45:SER:O	36:Z:74:ARG:NH1	1.81	1.14
11:A:1400:G:OP2	39:A:8216:HOH:O	1.74	1.05
11:A:391:A:O2'	11:A:392:A:OP2	1.80	0.98
11:A:416:C:O2'	11:A:417:A:OP2	1.82	0.97
11:A:1318:C:OP2	20:J:51:LYS:NZ	1.98	0.96
10:9:73:LYS:NZ	11:A:1157:U:OP1	1.98	0.96
10:9:87:LYS:NZ	11:A:1187:C:OP2	2.00	0.95
11:A:273:A:O2'	11:A:274:C:OP2	1.84	0.95
28:R:118:GLN:N	28:R:139:GLU:OE2	2.00	0.94
11:A:947:C:OP2	25:O:7:LYS:NZ	2.00	0.94
15:E:80:GLU:OE2	15:E:187:LYS:NZ	1.99	0.93
11:A:81:A:OP2	39:A:7767:HOH:O	1.85	0.93
11:A:1486:U:O2'	11:A:1487:A:OP2	1.85	0.93
11:A:229:A:O2'	11:A:230:A:OP2	1.86	0.92
11:A:604:G:O2'	11:A:605:U:OP2	1.88	0.91
11:A:1494:U:O2'	11:A:1495:U:OP2	1.87	0.91
11:A:1311:C:O2'	11:A:1313:G:N7	2.05	0.90
11:A:989:G:N7	39:A:7205:HOH:O	2.06	0.89
6:5:7:ASN:ND2	11:A:1750:A:OP1	2.06	0.88
11:A:1428:C:OP1	39:A:8116:HOH:O	1.92	0.88
11:A:4:C:O2'	14:D:17:ARG:NH2	2.07	0.88
11:A:108:A:O2'	27:Q:66:ARG:NH1	2.07	0.88
11:A:676:C:O2'	11:A:677:G:OP2	1.91	0.86
11:A:1506:G:O2'	11:A:1507:U:OP2	1.94	0.86
11:A:789:A:OP1	39:A:7828:HOH:O	1.93	0.86
6:5:97:ARG:O	11:A:1750:A:O2'	1.94	0.86
28:R:47:ARG:O	28:R:49:LYS:N	2.09	0.86
11:A:1450:G:OP1	30:T:60:ARG:NH1	2.08	0.86
11:A:1452:G:O6	30:T:11:LYS:NZ	2.09	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:A:413:C:OP2	35:Y:87:ARG:NH2	2.08	0.84
11:A:467:A:OP2	14:D:126:ARG:NH2	2.10	0.84
11:A:1226:U:OP1	31:U:34:ARG:NH1	2.11	0.84
11:A:1001:A:O2'	11:A:1002:U:OP2	1.96	0.84
11:A:1185:C:N4	39:A:8148:HOH:O	2.11	0.83
11:A:986:G:OP1	39:A:7879:HOH:O	1.95	0.83
11:A:1399:G:OP1	39:A:8216:HOH:O	1.97	0.82
11:A:1319:U:OP2	20:J:20:ARG:NH2	2.14	0.81
11:A:920:G:OP2	39:A:7043:HOH:O	1.98	0.81
11:A:406:U:O2	11:A:409:G:N2	2.14	0.80
11:A:846:G:OP2	25:O:123:ARG:NH1	2.14	0.80
11:A:11:A:OP1	39:A:7094:HOH:O	1.98	0.80
3:2:2:GLY:N	11:A:384:C:OP1	2.15	0.80
11:A:1473:G:OP1	30:T:102:LYS:NZ	2.14	0.80
11:A:613:A:OP1	39:A:7988:HOH:O	2.00	0.80
5:4:222:LYS:NZ	11:A:864:U:OP2	2.15	0.79
1:0:103:LYS:NZ	1:0:110:GLU:O	2.16	0.79
11:A:1556:G:N2	11:A:1583:A:OP2	2.14	0.79
11:A:1428:C:O2'	11:A:1429:G:OP1	2.00	0.79
10:9:92:HIS:CE1	11:A:1201:G:OP2	2.36	0.78
11:A:1508:G:O2'	11:A:1509:U:OP2	2.00	0.78
11:A:608:C:OP1	39:A:7253:HOH:O	2.01	0.78
11:A:265:C:OP1	35:Y:180:GLN:NE2	2.16	0.78
23:M:94:ASP:OD2	23:M:98:TYR:OH	2.02	0.78
11:A:1155:A:N3	11:A:1182:G:O2'	2.17	0.78
11:A:1211:U:O2	11:A:1218:C:N4	2.17	0.78
11:A:1154:U:O2'	11:A:1156:A:N7	2.17	0.78
8:7:6:LYS:NZ	31:U:27:LYS:NZ	2.32	0.78
23:M:89:ILE:O	23:M:97:ASN:ND2	2.17	0.78
21:K:34:MET:SD	21:K:98:ARG:NH1	2.58	0.77
11:A:215:A:N6	11:A:811:U:O4	2.18	0.77
11:A:269:G:O6	11:A:273:A:N6	2.18	0.77
11:A:3:C:O2'	11:A:4:C:OP1	2.02	0.77
11:A:10:G:O6	11:A:1117:U:N3	2.18	0.77
3:2:145:ARG:NH1	11:A:183:G:O6	2.18	0.76
28:R:46:SER:OG	28:R:48:ASP:OD1	2.02	0.75
11:A:904:A:OP1	11:A:994:C:O2'	2.04	0.75
11:A:1441:C:O2	11:A:1543:C:O2'	2.05	0.75
27:Q:77:THR:O	27:Q:77:THR:OG1	2.04	0.75
11:A:1245:G:O2'	11:A:1246:C:OP2	2.05	0.75
11:A:1720:G:O2'	11:A:1721:G:OP2	2.04	0.75
11:A:647:U:O2'	11:A:649:U:OP2	2.05	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:A:589:G:OP2	39:A:7366:HOH:O	2.04	0.75
19:I:66:ASP:N	19:I:66:ASP:OD1	2.17	0.74
4:3:113:ARG:NH2	11:A:633:U:OP1	2.21	0.74
11:A:1535:A:OP1	30:T:87:LYS:NZ	2.21	0.74
11:A:246:U:OP2	27:Q:33:TYR:OH	2.05	0.74
11:A:840:A:OP2	25:O:66:ARG:NH2	2.22	0.73
11:A:1518:G:OP2	23:M:134:ARG:NH1	2.21	0.73
11:A:608:C:OP1	39:A:7252:HOH:O	2.06	0.73
11:A:508:A:OP1	39:A:7814:HOH:O	2.04	0.73
11:A:1274:U:O4	39:A:7943:HOH:O	2.07	0.73
11:A:232:G:O2'	11:A:233:U:OP2	2.06	0.73
11:A:1335:A:N3	30:T:5:GLN:NE2	2.36	0.73
11:A:1005:A:OP2	39:A:7044:HOH:O	2.06	0.72
11:A:70:U:OP1	35:Y:171:LYS:NZ	2.22	0.72
11:A:765:A:C6	26:P:19:ARG:NH1	2.57	0.72
11:A:1651:G:O2'	11:A:1652:A:OP2	2.06	0.72
23:M:40:ARG:NH2	30:T:48:GLU:OE1	2.23	0.71
11:A:209:G:O2'	11:A:210:A:OP2	2.07	0.71
11:A:1362:U:OP1	32:V:59:LYS:NZ	2.24	0.71
11:A:353:G:OP1	39:A:7605:HOH:O	2.08	0.71
6:5:37:LYS:NZ	11:A:911:A:OP2	2.23	0.71
2:1:43:ARG:NH2	2:1:59:GLU:O	2.23	0.71
11:A:1360:U:O2'	11:A:1361:A:OP2	2.08	0.70
11:A:1168:A:O2'	11:A:1169:C:OP2	2.10	0.70
27:Q:32:ARG:NH1	27:Q:50:GLY:O	2.24	0.70
11:A:1171:G:OP1	24:N:40:ARG:NH2	2.24	0.70
13:C:10:LYS:NZ	20:J:113:GLU:OE2	2.25	0.70
11:A:1449:G:OP1	30:T:43:THR:OG1	2.08	0.70
11:A:1661:G:O2'	11:A:1662:C:OP2	2.10	0.70
11:A:1531:G:N7	39:A:8229:HOH:O	2.25	0.69
11:A:1176:A:OP1	11:A:1427:C:N4	2.26	0.69
10:9:72:LYS:NZ	11:A:1243:G:OP1	2.25	0.69
11:A:444:A:O2'	11:A:445:U:OP1	2.11	0.69
11:A:1708:A:N6	39:A:7701:HOH:O	2.26	0.69
3:2:31:ARG:NH2	11:A:324:A:OP1	2.26	0.69
3:2:150:ARG:NH2	11:A:181:G:OP1	2.25	0.69
11:A:234:G:O2'	11:A:235:A:O4'	2.11	0.69
11:A:92:G:OP1	33:W:10:LYS:NZ	2.26	0.69
13:C:9:ASN:O	13:C:13:LYS:N	2.26	0.68
10:9:92:HIS:NE2	11:A:1201:G:N7	2.41	0.68
5:4:220:LYS:NZ	11:A:864:U:OP1	2.26	0.68
7:6:65:THR:O	7:6:67:GLY:N	2.27	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:A:71:U:O2'	11:A:72:G:OP2	2.12	0.68
11:A:1446:A:O2'	11:A:1512:G:OP1	2.11	0.68
11:A:1576:U:OP1	19:I:132:GLY:N	2.27	0.68
1:0:43:ASN:ND2	1:0:43:ASN:O	2.27	0.68
5:4:210:ILE:O	11:A:1036:U:O2'	2.12	0.68
11:A:1449:G:OP2	30:T:47:ARG:NH1	2.28	0.67
11:A:1480:U:O2'	11:A:1481:A:O5'	2.12	0.67
6:5:34:LYS:NZ	11:A:1746:G:N7	2.43	0.67
3:2:82:ARG:NH1	11:A:254:A:OP1	2.28	0.67
7:6:47:ASN:N	7:6:47:ASN:OD1	2.28	0.67
11:A:1469:U:OP1	30:T:78:THR:OG1	2.12	0.67
3:2:10:LYS:NZ	11:A:328:G:O2'	2.28	0.67
11:A:550:G:OP1	34:X:59:SER:OG	2.13	0.67
11:A:573:A:N6	13:C:147:GLN:OE1	2.28	0.67
11:A:969:A:OP2	39:A:7204:HOH:O	2.12	0.67
9:8:99:ASN:O	9:8:102:GLN:N	2.27	0.67
11:A:1265:U:O2'	12:B:106:ASN:OD1	2.13	0.66
11:A:1145:C:OP1	23:M:132:LYS:NZ	2.28	0.66
10:9:92:HIS:CE1	11:A:1201:G:C8	2.84	0.66
11:A:901:A:N7	39:A:7559:HOH:O	2.28	0.66
11:A:573:A:N1	13:C:147:GLN:OE1	2.28	0.66
3:2:153:ARG:NH1	11:A:189:C:O2	2.28	0.66
11:A:60:C:O2	11:A:266:G:O2'	2.14	0.66
27:Q:4:GLN:NE2	27:Q:10:GLN:O	2.29	0.66
11:A:1173:G:O5'	39:A:8020:HOH:O	2.13	0.66
11:A:864:U:O2	21:K:137:THR:N	2.29	0.66
6:5:32:LYS:NZ	11:A:910:U:O2	2.29	0.66
11:A:1479:G:N7	39:A:8084:HOH:O	2.29	0.65
11:A:1514:G:O2'	11:A:1541:A:N6	2.30	0.65
11:A:1712:C:O2	11:A:1733:G:N2	2.29	0.65
11:A:760:G:N7	26:P:9:LYS:NZ	2.44	0.65
11:A:605:U:OP2	22:L:5:LYS:NZ	2.30	0.65
11:A:535:A:O2'	11:A:536:C:O5'	2.14	0.65
8:7:74:GLU:OE1	8:7:77:LYS:NZ	2.30	0.64
17:G:101:ARG:NH2	17:G:176:GLU:OE1	2.30	0.64
11:A:1357:G:OP1	32:V:32:LYS:NZ	2.30	0.64
11:A:100:A:OP1	11:A:299:C:N4	2.30	0.64
14:D:53:ARG:NH2	15:E:175:ARG:O	2.31	0.64
3:2:97:GLU:O	3:2:101:THR:OG1	2.14	0.64
11:A:999:C:N4	39:A:7716:HOH:O	2.31	0.64
11:A:533:G:N2	39:A:7640:HOH:O	2.29	0.64
11:A:553:A:C2	13:C:181:LYS:NZ	2.66	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
35:Y:89:SER:OG	35:Y:90:GLY:N	2.30	0.64
11:A:1282:U:O3'	11:A:1373:G:O2'	2.17	0.63
11:A:1263:G:N2	11:A:1296:G:N2	2.46	0.63
11:A:1568:C:OP2	24:N:18:LYS:NZ	2.31	0.63
11:A:1147:U:OP2	23:M:137:HIS:CE1	2.52	0.63
11:A:1164:C:O3'	19:I:142:LYS:NZ	2.32	0.63
28:R:102:LEU:O	28:R:111:TYR:N	2.32	0.63
28:R:93:SER:OG	28:R:103:TRP:NE1	2.32	0.63
11:A:1145:C:OP2	23:M:142:GLY:N	2.32	0.63
5:4:172:ARG:O	5:4:176:THR:OG1	2.17	0.63
11:A:1217:G:O2'	11:A:1218:C:OP2	2.16	0.63
11:A:754:A:O2'	14:D:9:SER:OG	2.17	0.63
11:A:1118:U:O2'	15:E:90:GLN:O	2.17	0.62
1:0:62:GLY:N	11:A:560:C:OP1	2.31	0.62
11:A:1164:C:OP2	11:A:1165:A:O2'	2.17	0.62
13:C:216:HIS:O	32:V:20:TYR:OH	2.18	0.62
22:L:13:ARG:NH2	27:Q:101:LYS:O	2.32	0.62
3:2:12:ARG:NH1	11:A:101:A:OP2	2.33	0.62
11:A:1071:U:OP1	18:H:71:LYS:NZ	2.33	0.62
11:A:379:A:OP1	11:A:415:G:O2'	2.18	0.62
11:A:411:U:OP1	35:Y:96:SER:OG	2.18	0.62
11:A:1223:U:O2'	11:A:1224:C:O4'	2.17	0.62
11:A:1286:U:O2'	11:A:1287:U:OP2	2.18	0.62
15:E:143:GLY:N	15:E:154:THR:O	2.33	0.61
4:3:144:ARG:O	18:H:42:GLN:NE2	2.32	0.61
28:R:217:ASN:ND2	28:R:258:ILE:O	2.32	0.61
4:3:110:SER:OG	11:A:794:A:OP1	2.18	0.61
33:W:182:VAL:O	33:W:230:LEU:N	2.33	0.61
11:A:642:G:N2	11:A:667:C:O2	2.33	0.61
11:A:986:G:OP1	39:A:7877:HOH:O	2.16	0.61
11:A:2:A:O2'	11:A:3:C:OP2	2.18	0.61
11:A:519:A:OP1	26:P:91:LYS:NZ	2.34	0.61
28:R:171:SER:OG	28:R:186:TYR:O	2.19	0.61
4:3:115:ARG:NH1	11:A:632:U:C4	2.69	0.61
11:A:144:C:O4'	35:Y:132:LYS:NZ	2.34	0.61
11:A:1752:U:O2'	11:A:1753:A:O5'	2.19	0.61
11:A:680:U:O2'	11:A:681:G:OP1	2.18	0.61
11:A:1710:G:O6	39:A:7703:HOH:O	2.13	0.60
21:K:139:SER:OG	21:K:140:THR:O	2.20	0.60
28:R:47:ARG:NH1	32:V:27:ASP:OD2	2.34	0.60
11:A:1556:G:O2'	11:A:1557:U:OP1	2.20	0.60
11:A:585:A:OP2	34:X:44:ARG:NH2	2.33	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:A:378:A:OP2	11:A:378:A:C8	2.55	0.60
11:A:515:U:O2'	26:P:58:PHE:O	2.19	0.60
4:3:192:PHE:CG	7:6:21:ARG:NH1	2.70	0.60
26:P:32:THR:OG1	26:P:60:THR:OG1	2.19	0.60
33:W:189:ASN:OD1	33:W:189:ASN:N	2.34	0.59
11:A:1488:A:OP1	20:J:86:LYS:NZ	2.36	0.59
11:A:1419:G:OP1	39:A:8037:HOH:O	2.17	0.59
22:L:34:LEU:O	22:L:36:SER:N	2.36	0.59
11:A:469:A:N6	39:A:7637:HOH:O	2.34	0.59
11:A:146:A:O2'	35:Y:4:ASN:OD1	2.20	0.59
11:A:59:C:N4	11:A:62:G:OP1	2.35	0.59
11:A:243:G:O2'	27:Q:38:GLY:O	2.20	0.59
32:V:6:THR:OG1	32:V:7:LYS:N	2.36	0.59
4:3:117:ARG:NH1	11:A:834:A:C5	2.71	0.59
31:U:50:CYS:SG	31:U:51:ASP:N	2.76	0.59
23:M:87:ASN:OD1	23:M:99:GLN:NE2	2.36	0.59
11:A:1156:A:O2'	11:A:1181:C:O2'	2.20	0.59
11:A:615:A:O2'	11:A:1078:U:O2'	2.21	0.59
6:5:4:LYS:NZ	11:A:1747:A:OP1	2.35	0.59
11:A:879:G:N2	21:K:68:GLU:OE1	2.35	0.58
11:A:912:A:O2'	11:A:913:U:OP1	2.21	0.58
5:4:57:ARG:NH1	11:A:873:G:OP1	2.36	0.58
16:F:57:CYS:SG	16:F:77:HIS:NE2	2.76	0.58
11:A:45:A:N1	11:A:424:A:O2'	2.36	0.58
11:A:1353:G:OP1	20:J:87:ARG:NH2	2.37	0.58
8:7:29:GLU:OE2	24:N:7:ARG:NH1	2.36	0.58
11:A:1186:G:OP1	11:A:1218:C:O2'	2.21	0.58
4:3:5:LYS:NZ	4:3:37:LEU:O	2.37	0.58
11:A:1347:U:O2'	11:A:1348:U:OP2	2.20	0.58
11:A:409:G:O2'	11:A:410:G:O5'	2.21	0.58
11:A:911:A:N6	39:A:7031:HOH:O	2.35	0.58
12:B:62:ALA:O	36:Z:64:LYS:NZ	2.37	0.58
28:R:81:ASP:N	28:R:94:SER:OG	2.37	0.57
11:A:420:A:N3	11:A:432:U:O2'	2.37	0.57
11:A:1313:G:O2'	28:R:74:GLY:O	2.22	0.57
26:P:13:ASN:ND2	33:W:54:TYR:O	2.37	0.57
34:X:53:ASP:OD1	34:X:53:ASP:N	2.37	0.57
11:A:299:C:OP2	27:Q:102:ARG:NH1	2.38	0.57
11:A:1419:G:OP1	39:A:8040:HOH:O	2.17	0.57
11:A:1166:A:OP2	20:J:73:GLY:CA	2.52	0.57
11:A:1463:U:O2'	11:A:1464:U:O5'	2.21	0.57
11:A:1189:A:N6	24:N:3:ASN:OD1	2.38	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
28:R:144:LEU:O	28:R:152:LYS:N	2.38	0.57
28:R:297:GLU:N	28:R:297:GLU:OE1	2.38	0.56
8:7:16:LEU:O	8:7:20:GLY:N	2.37	0.56
28:R:193:ASP:N	28:R:193:ASP:OD1	2.38	0.56
17:G:117:ARG:O	17:G:136:VAL:N	2.38	0.56
15:E:174:PRO:O	15:E:177:THR:OG1	2.23	0.56
39:A:7476:HOH:O	26:P:90:ARG:NH2	2.38	0.56
6:5:5:ARG:NH2	11:A:1748:U:OP2	2.38	0.56
22:L:68:ARG:NH2	22:L:115:ASP:OD2	2.38	0.56
11:A:573:A:O2'	11:A:574:A:OP1	2.22	0.56
23:M:102:SER:OG	23:M:103:ASN:N	2.36	0.56
13:C:228:ARG:NH1	28:R:242:ILE:O	2.39	0.56
11:A:1562:G:N7	39:A:8102:HOH:O	2.33	0.56
11:A:517:U:O2'	11:A:519:A:N7	2.38	0.56
35:Y:29:ASP:OD1	35:Y:70:ARG:NH2	2.38	0.56
26:P:76:ASN:OD1	26:P:77:GLN:N	2.39	0.56
5:4:35:ARG:O	5:4:101:THR:OG1	2.24	0.56
11:A:1383:G:O2'	11:A:1384:U:OP1	2.22	0.56
11:A:1213:G:O2'	29:S:84:HIS:N	2.39	0.56
11:A:797:A:N6	11:A:835:U:N3	2.54	0.55
11:A:1452:G:O4'	11:A:1452:G:OP2	2.24	0.55
32:V:25:THR:O	32:V:31:ASN:ND2	2.40	0.55
11:A:1158:U:O4	11:A:1172:G:N2	2.39	0.55
11:A:765:A:C5	26:P:19:ARG:NH1	2.74	0.55
11:A:1081:G:O2'	11:A:1111:A:N1	2.39	0.55
5:4:122:THR:N	5:4:146:THR:OG1	2.39	0.55
11:A:738:A:O2'	11:A:739:A:OP1	2.24	0.55
11:A:1517:A:OP1	23:M:133:VAL:N	2.39	0.55
21:K:128:ARG:CG	21:K:128:ARG:NH1	2.70	0.55
11:A:1223:U:O2'	11:A:1224:C:O5'	2.25	0.55
11:A:470:G:N2	11:A:503:A:N1	2.55	0.55
11:A:493:U:O2	11:A:493:U:O2'	2.25	0.55
11:A:1514:G:N2	11:A:1541:A:OP1	2.40	0.55
11:A:398:A:O2'	11:A:1642:A:N3	2.39	0.55
11:A:1206:A:OP2	11:A:1217:G:O2'	2.25	0.55
11:A:1190:G:C4	11:A:1415:A:C6	2.95	0.55
5:4:238:TYR:O	5:4:240:HIS:N	2.39	0.55
11:A:70:U:OP1	35:Y:173:ARG:NH2	2.40	0.54
15:E:219:LEU:O	15:E:222:THR:OG1	2.25	0.54
12:B:85:PHE:O	12:B:89:THR:OG1	2.26	0.54
5:4:95:ASP:O	5:4:98:ASN:ND2	2.40	0.54
11:A:840:A:O2'	11:A:841:A:O5'	2.26	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:3:120:THR:OG1	11:A:633:U:OP2	2.25	0.54
11:A:622:G:N1	11:A:948:A:OP2	2.40	0.54
8:7:3:HIS:CE1	11:A:1229:U:C4	2.96	0.54
8:7:6:LYS:NZ	31:U:20:ASN:ND2	2.55	0.54
12:B:192:GLU:N	12:B:192:GLU:OE1	2.41	0.54
11:A:1246:C:O2'	11:A:1247:A:OP1	2.26	0.54
11:A:1121:C:C4'	11:A:1608:C:OP2	2.56	0.54
15:E:35:ARG:NH1	15:E:248:LEU:O	2.41	0.54
4:3:161:ASP:OD1	4:3:161:ASP:N	2.41	0.54
11:A:172:U:C4'	11:A:173:A:OP2	2.57	0.53
11:A:533:G:N2	39:A:7636:HOH:O	2.41	0.53
36:Z:41:SER:OG	36:Z:42:ASN:N	2.39	0.53
11:A:17:C:O2'	11:A:1110:A:N1	2.42	0.53
11:A:885:A:N3	11:A:975:G:O2'	2.41	0.53
31:U:75:LYS:O	31:U:78:SER:OG	2.26	0.53
11:A:1051:G:O6	39:A:7667:HOH:O	2.16	0.53
33:W:254:ARG:NH1	33:W:260:TYR:CG	2.76	0.53
11:A:416:C:O2'	11:A:417:A:P	2.66	0.53
11:A:1176:A:N3	24:N:9:HIS:NE2	2.57	0.53
35:Y:162:ARG:NH1	35:Y:176:CYS:SG	2.82	0.53
11:A:573:A:C6	13:C:147:GLN:OE1	2.62	0.52
28:R:80:SER:OG	28:R:121:VAL:O	2.27	0.52
18:H:23:LYS:NZ	36:Z:34:TRP:O	2.41	0.52
11:A:1428:C:OP1	39:A:8119:HOH:O	2.19	0.52
11:A:934:U:OP1	11:A:1044:C:O2'	2.28	0.52
11:A:1201:G:C6	11:A:1227:G:C6	2.98	0.52
10:9:88:HIS:NE2	11:A:1220:C:OP2	2.42	0.52
21:K:39:ASP:OD1	21:K:40:THR:N	2.43	0.52
2:1:21:ARG:NH2	17:G:122:ARG:NH1	2.57	0.52
11:A:1372:A:OP1	32:V:60:ARG:NH1	2.43	0.52
11:A:242:U:C2	11:A:244:A:OP2	2.63	0.52
3:2:25:ARG:NH2	11:A:377:G:OP2	2.42	0.52
11:A:1450:G:P	30:T:60:ARG:NH1	2.83	0.52
11:A:1119:G:O2'	11:A:1607:A:N1	2.43	0.52
11:A:537:A:OP2	11:A:538:A:OP2	2.28	0.52
11:A:641:G:N2	11:A:668:U:O2	2.43	0.51
11:A:531:A:N3	39:A:7637:HOH:O	2.35	0.51
15:E:141:ARG:NH1	15:E:230:PHE:CZ	2.79	0.51
3:2:24:LYS:NZ	11:A:1683:A:OP1	2.44	0.51
28:R:155:SER:OG	28:R:160:ASN:ND2	2.43	0.51
12:B:145:ASP:O	12:B:148:SER:OG	2.28	0.51
1:0:97:ASP:O	1:0:101:ASN:ND2	2.43	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:A:954:G:N1	11:A:1001:A:O2'	2.43	0.51
30:T:57:VAL:O	30:T:61:THR:OG1	2.28	0.51
11:A:98:U:O2'	11:A:101:A:N3	2.44	0.51
11:A:1213:G:C4	29:S:84:HIS:CD2	2.99	0.51
8:7:3:HIS:CD2	11:A:1229:U:C2	2.99	0.51
11:A:1568:C:P	24:N:18:LYS:NZ	2.84	0.51
11:A:1751:U:O2'	11:A:1753:A:N6	2.44	0.51
11:A:894:U:N3	21:K:55:ARG:NH2	2.58	0.51
15:E:145:TRP:O	18:H:98:GLN:NE2	2.44	0.51
11:A:1691:C:N4	39:A:7957:HOH:O	2.44	0.50
9:8:49:ASN:O	9:8:52:SER:OG	2.29	0.50
11:A:112:U:O2'	11:A:324:A:N3	2.44	0.50
1:0:22:LYS:CB	10:9:74:LYS:NZ	2.74	0.50
11:A:1185:C:O2'	11:A:1216:A:C2	2.64	0.50
11:A:976:A:N6	11:A:982:U:OP2	2.45	0.50
11:A:1173:G:OP2	39:A:8021:HOH:O	2.19	0.50
9:8:78:SER:OG	23:M:57:ARG:NH2	2.44	0.50
11:A:1501:C:OP2	17:G:86:LYS:NZ	2.45	0.50
5:4:72:LEU:O	5:4:79:SER:OG	2.30	0.50
11:A:1147:U:OP2	23:M:137:HIS:NE2	2.44	0.50
11:A:772:A:O2'	33:W:108:LYS:NZ	2.45	0.50
14:D:38:ASN:ND2	14:D:40:ARG:NH1	2.60	0.50
11:A:343:C:O2'	11:A:344:A:OP2	2.30	0.49
31:U:28:GLY:O	31:U:32:VAL:N	2.44	0.49
17:G:21:GLU:OE1	17:G:102:ASN:ND2	2.45	0.49
10:9:130:ASP:OD1	10:9:130:ASP:N	2.46	0.49
11:A:135:A:O2'	35:Y:187:ARG:NH1	2.44	0.49
12:B:147:ASP:OD2	12:B:162:ARG:NH2	2.45	0.49
20:J:32:GLU:OE1	20:J:55:ARG:NH2	2.45	0.49
11:A:1108:U:OP1	11:A:1621:G:O2'	2.30	0.49
11:A:884:A:OP2	21:K:66:ARG:N	2.46	0.49
11:A:238:G:O2'	11:A:239:A:P	2.70	0.49
39:A:8103:HOH:O	30:T:93:ARG:NH1	2.46	0.49
11:A:316:G:OP1	27:Q:133:THR:OG1	2.30	0.49
28:R:330:ASP:OD2	28:R:334:ARG:NH2	2.46	0.49
11:A:1406:G:O2'	11:A:1407:A:OP2	2.30	0.49
11:A:1262:U:OP1	15:E:96:ARG:NH1	2.45	0.49
31:U:55:TYR:CG	31:U:56:VAL:N	2.80	0.49
11:A:1488:A:O2'	11:A:1489:U:O5'	2.31	0.49
11:A:588:A:OP1	14:D:40:ARG:NH1	2.45	0.49
25:O:4:MET:SD	25:O:126:ARG:NH1	2.85	0.49
23:M:15:HIS:NE2	23:M:66:CYS:SG	2.86	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
19:I:74:SER:OG	19:I:75:GLY:N	2.45	0.48
11:A:978:C:O2'	11:A:980:G:N7	2.46	0.48
11:A:558:G:N1	11:A:574:A:OP2	2.47	0.48
11:A:1569:A:C8	24:N:13:TYR:CD2	3.00	0.48
11:A:892:G:O2'	11:A:893:A:C8	2.66	0.48
11:A:238:G:O2'	11:A:238:G:N3	2.46	0.48
11:A:1321:G:O2'	11:A:1349:C:N3	2.46	0.48
28:R:135:SER:OG	28:R:145:TRP:NE1	2.47	0.48
21:K:91:ASN:N	21:K:91:ASN:OD1	2.47	0.48
35:Y:155:LEU:O	35:Y:159:SER:OG	2.32	0.48
15:E:62:ASP:OD1	15:E:134:LYS:NZ	2.46	0.48
11:A:451:G:OP1	26:P:102:ARG:NH2	2.47	0.48
16:F:78:ARG:NH1	16:F:100:GLY:CA	2.76	0.48
11:A:1287:U:OP1	11:A:1300:G:N2	2.47	0.48
11:A:1464:U:OP2	11:A:1465:C:C5	2.67	0.48
31:U:52:GLN:O	31:U:55:TYR:CD1	2.66	0.48
11:A:1059:A:N3	11:A:1115:A:O2'	2.47	0.48
11:A:1246:C:OP2	11:A:1399:G:OP2	2.31	0.48
4:3:197:LYS:N	11:A:1029:G:OP1	2.46	0.48
11:A:1391:C:OP1	24:N:53:LYS:NZ	2.47	0.48
10:9:92:HIS:NE2	11:A:1201:G:C5	2.82	0.48
11:A:372:C:O2'	11:A:739:A:N1	2.46	0.48
11:A:629:A:OP1	39:A:7830:HOH:O	2.18	0.48
11:A:1246:C:O2'	11:A:1247:A:P	2.72	0.47
11:A:894:U:C4	21:K:55:ARG:NH2	2.82	0.47
8:7:93:LYS:O	13:C:70:LYS:NZ	2.47	0.47
13:C:85:ASP:OD1	13:C:85:ASP:N	2.45	0.47
11:A:407:A:O2'	11:A:409:G:O6	2.32	0.47
28:R:255:GLY:N	28:R:279:LYS:NZ	2.62	0.47
5:4:149:THR:O	5:4:151:ALA:N	2.47	0.47
11:A:478:G:O2'	11:A:494:A:N6	2.47	0.47
35:Y:38:GLY:N	35:Y:48:TYR:O	2.47	0.47
11:A:1506:G:O2'	11:A:1507:U:P	2.73	0.47
11:A:1509:U:OP2	11:A:1509:U:C4'	2.62	0.47
11:A:1007:U:O2'	11:A:1009:U:C5	2.67	0.47
6:5:43:ASP:OD2	6:5:50:LYS:NZ	2.48	0.47
21:K:147:ARG:NH1	21:K:150:ARG:NH2	2.61	0.47
11:A:507:G:O2'	11:A:508:A:OP2	2.33	0.47
11:A:235:A:O2'	11:A:814:A:OP2	2.33	0.47
11:A:1190:G:C5	11:A:1415:A:C2	3.02	0.47
11:A:1537:C:OP1	23:M:41:ARG:NH1	2.48	0.47
1:0:111:ASN:OD1	1:0:111:ASN:N	2.47	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:3:70:TYR:OH	4:3:129:ASP:OD1	2.32	0.47
3:2:22:ARG:NH2	11:A:293:U:OP1	2.47	0.47
10:9:92:HIS:CE1	11:A:1201:G:N7	2.83	0.47
18:H:70:ASN:N	18:H:130:TYR:O	2.48	0.47
11:A:74:A:O2'	35:Y:177:PRO:O	2.32	0.47
10:9:99:ALA:O	10:9:113:GLN:NE2	2.48	0.47
32:V:106:LEU:O	32:V:110:GLY:N	2.47	0.47
24:N:16:ASP:CG	24:N:26:ARG:NH1	2.68	0.47
10:9:88:HIS:CE1	11:A:1217:G:N2	2.83	0.47
12:B:35:HIS:NE2	32:V:104:GLU:OE1	2.48	0.47
35:Y:116:LYS:NZ	35:Y:125:THR:OG1	2.48	0.46
5:4:111:ASP:N	5:4:111:ASP:OD1	2.48	0.46
11:A:573:A:N1	13:C:147:GLN:CD	2.68	0.46
11:A:316:G:OP1	27:Q:133:THR:N	2.48	0.46
35:Y:48:TYR:OH	35:Y:119:ALA:O	2.33	0.46
11:A:327:G:C4	11:A:329:A:C8	3.03	0.46
11:A:63:U:C5'	11:A:64:U:OP2	2.64	0.46
11:A:1214:A:O2'	11:A:1216:A:OP2	2.33	0.46
11:A:982:U:C4'	11:A:983:A:OP2	2.63	0.46
11:A:1462:U:C4'	11:A:1463:U:OP2	2.63	0.46
11:A:369:A:OP2	11:A:370:U:OP2	2.33	0.46
11:A:1476:A:N1	11:A:1521:C:O2'	2.48	0.46
11:A:1494:U:O2'	11:A:1495:U:P	2.73	0.46
32:V:70:SER:O	32:V:71:LEU:C	2.53	0.46
4:3:165:GLU:N	4:3:165:GLU:OE1	2.49	0.46
29:S:36:ASP:N	29:S:36:ASP:OD1	2.47	0.46
11:A:33:G:C5	11:A:467:A:N6	2.83	0.46
11:A:500:U:OP1	34:X:28:ARG:NH2	2.49	0.46
27:Q:68:LYS:O	27:Q:126:GLN:N	2.49	0.46
11:A:1472:U:OP2	30:T:105:ARG:NH2	2.49	0.46
13:C:144:LYS:NZ	13:C:182:GLN:O	2.49	0.46
11:A:493:U:C4'	11:A:494:A:OP2	2.63	0.45
11:A:1416:G:O2'	11:A:1417:A:OP1	2.33	0.45
35:Y:1:MET:N	35:Y:18:ILE:O	2.48	0.45
11:A:110:A:C6	11:A:245:A:C5	3.04	0.45
11:A:1053:A:C4	11:A:1063:A:N6	2.85	0.45
11:A:1486:U:O2'	13:C:9:ASN:CA	2.65	0.45
11:A:1420:U:OP2	39:A:8036:HOH:O	2.21	0.45
3:2:64:ARG:NE	3:2:181:GLY:O	2.48	0.45
11:A:1324:U:OP1	19:I:25:ARG:NH1	2.50	0.45
11:A:893:A:C5	11:A:894:U:C4	3.04	0.45
11:A:1240:G:N7	39:A:8007:HOH:O	2.36	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:6:5:LEU:N	18:H:24:GLN:NE2	2.65	0.45
11:A:879:G:C6	11:A:880:G:C6	3.04	0.45
17:G:119:ASP:OD1	17:G:120:SER:N	2.50	0.45
10:9:116:CYS:O	10:9:120:GLY:N	2.49	0.45
3:2:24:LYS:O	11:A:391:A:C8	2.70	0.45
11:A:1480:U:O2'	11:A:1481:A:C8	2.70	0.45
17:G:47:THR:OG1	17:G:65:GLU:OE1	2.35	0.45
31:U:5:ASN:O	31:U:8:LEU:N	2.49	0.45
17:G:70:THR:O	17:G:154:ARG:NH2	2.49	0.45
11:A:1444:U:O2'	17:G:77:ASN:OD1	2.35	0.45
28:R:313:THR:N	28:R:327:GLY:O	2.50	0.45
11:A:630:A:OP2	39:A:7827:HOH:O	2.20	0.45
11:A:297:U:O4	39:A:7336:HOH:O	2.21	0.45
11:A:1486:U:O2'	11:A:1487:A:P	2.74	0.45
11:A:409:G:O2'	11:A:410:G:O4'	2.35	0.45
11:A:615:A:C5'	11:A:616:A:OP2	2.65	0.45
11:A:1228:A:O2'	11:A:1229:U:OP1	2.35	0.45
11:A:56:G:O5'	26:P:109:LYS:NZ	2.50	0.45
11:A:446:U:O4'	33:W:66:ASN:ND2	2.49	0.45
33:W:120:GLU:N	33:W:120:GLU:OE1	2.50	0.45
11:A:878:A:O2'	11:A:894:U:O2'	2.35	0.44
26:P:49:ASP:OD1	26:P:51:ARG:NE	2.50	0.44
24:N:39:ARG:CG	24:N:39:ARG:NH1	2.80	0.44
6:5:72:LYS:NZ	11:A:909:C:OP1	2.50	0.44
2:1:53:ASP:OD1	17:G:32:TYR:OH	2.35	0.44
33:W:42:LEU:O	33:W:86:THR:OG1	2.35	0.44
11:A:1514:G:O2'	11:A:1515:A:C8	2.71	0.44
4:3:141:ILE:O	18:H:52:VAL:N	2.50	0.44
11:A:1123:G:C4'	11:A:1124:A:OP2	2.65	0.44
11:A:14:C:O2'	11:A:613:A:N1	2.50	0.44
11:A:234:G:O2'	11:A:235:A:P	2.76	0.44
20:J:27:ASN:OD1	20:J:28:LEU:N	2.50	0.44
6:5:7:ASN:N	11:A:1749:C:O2	2.50	0.44
3:2:64:ARG:NH2	11:A:323:U:OP1	2.50	0.44
11:A:214:U:OP2	11:A:214:U:C6	2.70	0.44
11:A:93:C:O2	11:A:417:A:O2'	2.35	0.44
11:A:1495:U:C4'	11:A:1496:A:OP2	2.65	0.44
11:A:416:C:N3	11:A:420:A:N6	2.66	0.44
3:2:111:GLU:OE2	3:2:171:ARG:NH2	2.51	0.44
11:A:1269:G:N2	11:A:1272:A:OP2	2.51	0.44
3:2:185:ARG:NH2	11:A:202:U:O2	2.50	0.44
11:A:1358:A:OP1	32:V:29:HIS:NE2	2.51	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:74:ASP:N	1:0:74:ASP:OD1	2.51	0.44
15:E:52:SER:OG	36:Z:30:ARG:NH2	2.50	0.44
11:A:1165:A:C4'	11:A:1166:A:OP2	2.65	0.44
8:7:3:HIS:CE1	11:A:1229:U:N3	2.86	0.44
11:A:105:G:O2'	11:A:779:A:N1	2.50	0.44
11:A:4:C:OP2	15:E:201:SER:OG	2.35	0.43
11:A:1569:A:C5	24:N:13:TYR:CE2	3.06	0.43
11:A:1084:A:O2'	11:A:1704:C:O2'	2.36	0.43
11:A:1275:U:O4	39:A:7939:HOH:O	2.21	0.43
35:Y:33:GLY:N	35:Y:52:ILE:O	2.51	0.43
33:W:239:GLU:CD	33:W:239:GLU:N	2.72	0.43
11:A:1180:A:OP2	39:A:8039:HOH:O	2.21	0.43
22:L:53:THR:N	22:L:72:ARG:O	2.51	0.43
11:A:762:U:C5	26:P:6:ARG:NH1	2.86	0.43
11:A:1171:G:C5'	24:N:39:ARG:NH1	2.81	0.43
11:A:740:A:O2'	33:W:12:ILE:O	2.36	0.43
11:A:479:G:N1	11:A:492:C:O2	2.51	0.43
11:A:605:U:OP1	22:L:19:ARG:NH2	2.51	0.43
33:W:105:TYR:N	33:W:184:TYR:OH	2.52	0.43
13:C:137:CYS:SG	13:C:138:GLU:N	2.91	0.43
22:L:7:ARG:NH1	22:L:7:ARG:CG	2.81	0.43
24:N:16:ASP:OD1	24:N:26:ARG:NH1	2.52	0.43
11:A:64:U:O2'	11:A:65:C:O5'	2.37	0.43
11:A:763:U:C5	11:A:763:U:OP2	2.72	0.43
11:A:841:A:O2'	11:A:843:A:OP1	2.36	0.43
11:A:534:A:OP1	11:A:534:A:C5	2.72	0.43
11:A:57:U:O2'	11:A:443:A:N3	2.52	0.43
11:A:1299:C:OP1	13:C:159:TYR:OH	2.36	0.43
11:A:3:C:O2'	15:E:182:ALA:N	2.51	0.43
11:A:620:U:O2'	25:O:115:TYR:OH	2.36	0.43
11:A:931:A:P	25:O:96:LYS:NZ	2.92	0.43
35:Y:137:ARG:NH1	35:Y:181:ARG:NE	2.67	0.43
11:A:606:U:OP2	22:L:5:LYS:NZ	2.52	0.43
11:A:1721:G:C3'	11:A:1721:G:C8	3.02	0.43
11:A:1423:U:OP1	24:N:9:HIS:ND1	2.51	0.43
11:A:1174:A:OP1	11:A:1175:A:OP2	2.36	0.43
20:J:97:ASP:N	20:J:97:ASP:OD1	2.51	0.43
23:M:63:GLU:O	23:M:67:ASN:ND2	2.52	0.43
12:B:79:GLN:NE2	12:B:95:SER:O	2.52	0.43
4:3:5:LYS:O	4:3:42:LEU:N	2.52	0.43
19:I:115:ASP:OD1	19:I:117:SER:N	2.52	0.43
1:0:63:ARG:NH1	11:A:559:C:OP2	2.52	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:A:1496:A:N1	11:A:1579:G:N2	2.67	0.43
11:A:303:A:C2	11:A:305:C:C2	3.06	0.43
11:A:1357:G:O2'	11:A:1381:A:N6	2.52	0.42
8:7:83:SER:OG	31:U:111:GLU:OE2	2.36	0.42
3:2:166:GLN:OE1	3:2:173:LEU:N	2.51	0.42
11:A:655:C:O4'	11:A:655:C:OP2	2.37	0.42
11:A:534:A:O2'	11:A:537:A:N1	2.53	0.42
8:7:19:ASP:OD2	13:C:78:LYS:NZ	2.52	0.42
11:A:1505:C:C4'	11:A:1511:A:N6	2.82	0.42
11:A:1661:G:C2'	11:A:1662:C:OP2	2.67	0.42
3:2:11:ARG:O	27:Q:132:LYS:NZ	2.52	0.42
11:A:463:A:O2'	14:D:9:SER:OG	2.37	0.42
20:J:94:ASN:ND2	20:J:97:ASP:OD2	2.53	0.42
33:W:71:ASN:OD1	33:W:96:LYS:NZ	2.53	0.42
14:D:62:LEU:CD1	14:D:68:ARG:NH1	2.83	0.42
11:A:970:A:O2'	11:A:1738:U:O2	2.38	0.42
23:M:122:HIS:CE1	29:S:128:TYR:OH	2.73	0.42
5:4:90:VAL:CG1	5:4:226:ARG:NH1	2.83	0.42
11:A:33:G:C4	11:A:467:A:C6	3.08	0.42
11:A:954:G:OP1	25:O:111:LYS:NZ	2.53	0.42
11:A:125:U:OP2	11:A:125:U:C4'	2.68	0.42
35:Y:142:LYS:O	35:Y:147:LEU:N	2.53	0.42
4:3:178:THR:O	4:3:179:THR:OG1	2.37	0.42
11:A:866:U:O2	11:A:966:A:O2'	2.38	0.42
11:A:1752:U:O2'	11:A:1753:A:P	2.77	0.42
11:A:138:G:N2	11:A:166:C:O2	2.53	0.42
3:2:84:THR:OG1	3:2:85:LYS:N	2.52	0.42
2:1:20:SER:O	11:A:1591:C:C6	2.72	0.42
11:A:1651:G:C5	11:A:1673:A:N6	2.88	0.42
11:A:562:G:N7	22:L:68:ARG:NH1	2.67	0.42
11:A:1032:U:N3	11:A:1035:A:N6	2.68	0.42
3:2:5:ARG:NH2	11:A:323:U:O2'	2.53	0.42
11:A:1358:A:C5	11:A:1382:A:C6	3.07	0.42
11:A:211:U:C4'	11:A:212:A:OP2	2.68	0.42
1:0:26:VAL:O	1:0:94:TYR:OH	2.38	0.42
17:G:66:ARG:CG	17:G:66:ARG:NH1	2.82	0.42
11:A:1602:U:O2'	11:A:1717:C:O2'	2.38	0.41
11:A:1742:G:N7	21:K:146:ARG:NH2	2.68	0.41
11:A:81:A:O2'	11:A:142:A:O2'	2.38	0.41
11:A:1147:U:O4'	11:A:1168:A:N6	2.52	0.41
33:W:193:ARG:NH1	33:W:220:PHE:CE1	2.88	0.41
11:A:542:G:O2'	11:A:549:A:N1	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:A:1208:A:N6	11:A:1217:G:O6	2.52	0.41
11:A:1651:G:C2'	11:A:1652:A:OP2	2.68	0.41
11:A:1662:C:O2'	11:A:1663:A:OP1	2.39	0.41
11:A:764:U:C5	11:A:766:G:C2	3.08	0.41
11:A:875:C:N4	11:A:892:G:C4	2.88	0.41
30:T:99:CYS:SG	30:T:100:HIS:N	2.92	0.41
11:A:366:U:OP1	22:L:23:ARG:NH2	2.54	0.41
11:A:1086:G:O2'	11:A:1103:G:O6	2.37	0.41
5:4:74:ASP:OD1	5:4:74:ASP:N	2.54	0.41
11:A:1153:U:N3	11:A:1157:U:C5	2.89	0.41
11:A:538:A:N1	11:A:587:U:O2'	2.53	0.41
26:P:74:TYR:CE1	26:P:84:GLU:OE2	2.73	0.41
10:9:75:LYS:NZ	11:A:1418:C:OP2	2.54	0.41
10:9:128:HIS:ND1	11:A:1222:U:O2'	2.54	0.41
4:3:146:ASP:OD1	4:3:148:THR:OG1	2.39	0.41
33:W:176:HIS:CD2	33:W:178:GLU:OE2	2.73	0.41
11:A:89:A:C6	11:A:389:G:C6	3.09	0.41
11:A:1650:G:C6	11:A:1651:G:N1	2.88	0.41
11:A:464:G:O2'	11:A:753:C:O2	2.38	0.41
11:A:1476:A:C2	11:A:1522:U:O4'	2.74	0.41
6:5:82:HIS:ND1	11:A:1719:A:N1	2.68	0.41
11:A:1144:A:O2'	11:A:1515:A:O2'	2.39	0.41
33:W:11:ARG:N	33:W:26:ILE:O	2.54	0.41
19:I:36:SER:OG	30:T:11:LYS:O	2.39	0.41
11:A:410:G:OP1	35:Y:72:ARG:NH1	2.53	0.41
11:A:912:A:O2'	11:A:913:U:P	2.79	0.41
22:L:54:GLU:OE1	22:L:72:ARG:NH1	2.53	0.41
11:A:763:U:C6	11:A:763:U:OP2	2.74	0.41
5:4:148:LYS:NZ	5:4:152:GLY:C	2.75	0.41
3:2:204:GLN:O	3:2:208:LYS:N	2.54	0.41
11:A:137:G:OP2	35:Y:139:ASN:ND2	2.54	0.41
25:O:71:GLN:NE2	25:O:79:LYS:NZ	2.69	0.41
11:A:1212:U:O4	29:S:60:LYS:NZ	2.53	0.41
1:0:56:ARG:NH1	1:0:85:ASP:OD2	2.54	0.41
21:K:46:ASP:N	21:K:46:ASP:OD1	2.54	0.41
11:A:155:U:OP2	35:Y:83:CYS:O	2.38	0.41
30:T:141:ASN:O	30:T:145:THR:OG1	2.39	0.41
28:R:127:SER:O	28:R:130:ASN:N	2.54	0.41
11:A:1692:C:N4	39:A:7960:HOH:O	2.54	0.41
11:A:1058:A:C2	11:A:1114:G:N3	2.89	0.40
4:3:72:VAL:O	4:3:75:SER:OG	2.39	0.40
11:A:1569:A:C4	24:N:13:TYR:CE2	3.09	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:9:114:LYS:O	10:9:125:MET:N	2.54	0.40
11:A:1012:C:O2'	18:H:2:VAL:N	2.54	0.40
15:E:153:HIS:N	15:E:153:HIS:ND1	2.69	0.40
25:O:101:ARG:NH1	25:O:145:ALA:CB	2.84	0.40
10:9:133:TYR:OH	11:A:1206:A:N3	2.55	0.40
11:A:1373:G:OP1	32:V:5:ARG:N	2.54	0.40
11:A:1059:A:C6	11:A:1060:A:C6	3.09	0.40
11:A:257:G:C5'	11:A:258:A:OP2	2.70	0.40
11:A:1529:U:C2'	11:A:1530:U:OP2	2.69	0.40
3:2:72:ASN:ND2	11:A:255:C:O4'	2.54	0.40
11:A:1318:C:O2'	11:A:1319:U:OP1	2.39	0.40
11:A:1113:G:C2	11:A:1114:G:C8	3.09	0.40
13:C:147:GLN:CA	13:C:147:GLN:OE1	2.69	0.40
3:2:21:HIS:N	3:2:21:HIS:ND1	2.69	0.40
3:2:140:ASN:N	3:2:140:ASN:ND2	2.70	0.40
11:A:676:C:O2'	11:A:677:G:P	2.79	0.40
25:O:66:ARG:O	25:O:70:GLY:N	2.55	0.40
35:Y:64:LYS:NZ	35:Y:82:SER:OG	2.54	0.40
13:C:25:HIS:CD2	24:N:48:HIS:CE1	3.10	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	
1	0	97/211 (46%)	91 (94%)	6 (6%)	0	100	100
2	1	64/68 (94%)	62 (97%)	2 (3%)	0	100	100
3	2	205/208 (99%)	195 (95%)	10 (5%)	0	100	100
4	3	194/197 (98%)	187 (96%)	7 (4%)	0	100	100
5	4	219/265 (83%)	203 (93%)	13 (6%)	3 (1%)	16	74
6	5	98/119 (82%)	98 (100%)	0	0	100	100
7	6	78/81 (96%)	71 (91%)	6 (8%)	1 (1%)	18	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	7	99/162 (61%)	95 (96%)	4 (4%)	0	100	100
9	8	77/143 (54%)	73 (95%)	4 (5%)	0	100	100
10	9	91/189 (48%)	89 (98%)	1 (1%)	1 (1%)	21	79
12	B	199/241 (83%)	197 (99%)	2 (1%)	0	100	100
13	C	226/243 (93%)	214 (95%)	12 (5%)	0	100	100
14	D	178/181 (98%)	174 (98%)	4 (2%)	0	100	100
15	E	227/296 (77%)	212 (93%)	14 (6%)	1 (0%)	43	90
16	F	87/101 (86%)	82 (94%)	5 (6%)	0	100	100
17	G	190/200 (95%)	178 (94%)	10 (5%)	2 (1%)	21	79
18	H	127/130 (98%)	112 (88%)	14 (11%)	1 (1%)	27	83
19	I	141/145 (97%)	132 (94%)	9 (6%)	0	100	100
20	J	106/120 (88%)	104 (98%)	2 (2%)	0	100	100
21	K	138/151 (91%)	133 (96%)	5 (4%)	0	100	100
22	L	138/142 (97%)	125 (91%)	11 (8%)	2 (1%)	16	74
23	M	151/155 (97%)	138 (91%)	11 (7%)	2 (1%)	18	76
24	N	52/55 (94%)	49 (94%)	3 (6%)	0	100	100
25	O	150/153 (98%)	140 (93%)	9 (6%)	1 (1%)	30	85
26	P	146/149 (98%)	135 (92%)	11 (8%)	0	100	100
27	Q	154/157 (98%)	149 (97%)	5 (3%)	0	100	100
28	R	336/343 (98%)	307 (91%)	27 (8%)	2 (1%)	33	86
29	S	126/144 (88%)	122 (97%)	3 (2%)	1 (1%)	27	83
30	T	152/155 (98%)	144 (95%)	8 (5%)	0	100	100
31	U	122/126 (97%)	112 (92%)	10 (8%)	0	100	100
32	V	117/130 (90%)	115 (98%)	1 (1%)	1 (1%)	25	82
33	W	257/259 (99%)	247 (96%)	10 (4%)	0	100	100
34	X	72/80 (90%)	68 (94%)	4 (6%)	0	100	100
35	Y	226/293 (77%)	215 (95%)	10 (4%)	1 (0%)	43	90
36	Z	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
All	All	5135/5889 (87%)	4861 (95%)	255 (5%)	19 (0%)	43	90

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	L	3	VAL
25	O	152	VAL
28	R	48	ASP
5	4	239	SER
7	6	66	GLY
22	L	35	GLY
32	V	71	LEU
5	4	150	SER
18	H	59	LYS
29	S	54	ILE
35	Y	89	SER
17	G	51	TYR
17	G	158	PHE
5	4	23	ILE
28	R	180	VAL
15	E	57	GLU
10	9	143	ILE
23	M	81	ILE
23	M	150	VAL

5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	90/192 (47%)	83 (92%)	7 (8%)	18	65
2	1	55/57 (96%)	44 (80%)	11 (20%)	2	13
3	2	184/185 (100%)	158 (86%)	26 (14%)	5	33
4	3	182/183 (100%)	153 (84%)	29 (16%)	4	27
5	4	197/225 (88%)	167 (85%)	30 (15%)	4	29
6	5	90/107 (84%)	76 (84%)	14 (16%)	4	27
7	6	71/72 (99%)	60 (84%)	11 (16%)	4	28
8	7	91/136 (67%)	83 (91%)	8 (9%)	14	60
9	8	70/109 (64%)	59 (84%)	11 (16%)	4	27
10	9	81/156 (52%)	72 (89%)	9 (11%)	9	46
12	B	180/211 (85%)	164 (91%)	16 (9%)	14	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	C	196/210 (93%)	178 (91%)	18 (9%)	13	57
14	D	161/162 (99%)	128 (80%)	33 (20%)	2	12
15	E	193/250 (77%)	168 (87%)	25 (13%)	6	37
16	F	80/92 (87%)	76 (95%)	4 (5%)	34	81
17	G	163/169 (96%)	145 (89%)	18 (11%)	9	47
18	H	116/117 (99%)	97 (84%)	19 (16%)	3	24
19	I	120/122 (98%)	105 (88%)	15 (12%)	7	40
20	J	101/111 (91%)	91 (90%)	10 (10%)	11	53
21	K	112/121 (93%)	97 (87%)	15 (13%)	6	36
22	L	112/114 (98%)	96 (86%)	16 (14%)	5	32
23	M	133/135 (98%)	120 (90%)	13 (10%)	12	53
24	N	48/49 (98%)	41 (85%)	7 (15%)	5	31
25	O	135/136 (99%)	118 (87%)	17 (13%)	7	39
26	P	133/134 (99%)	117 (88%)	16 (12%)	7	41
27	Q	140/141 (99%)	122 (87%)	18 (13%)	6	38
28	R	291/295 (99%)	264 (91%)	27 (9%)	13	56
29	S	108/117 (92%)	97 (90%)	11 (10%)	11	51
30	T	133/134 (99%)	120 (90%)	13 (10%)	12	53
31	U	103/104 (99%)	93 (90%)	10 (10%)	12	54
32	V	107/115 (93%)	98 (92%)	9 (8%)	16	62
33	W	226/226 (100%)	194 (86%)	32 (14%)	5	33
34	X	61/67 (91%)	54 (88%)	7 (12%)	8	44
35	Y	197/244 (81%)	177 (90%)	20 (10%)	11	51
36	Z	82/82 (100%)	74 (90%)	8 (10%)	12	53
All	All	4542/5080 (89%)	3989 (88%)	553 (12%)	7	40

All (553) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	25	LEU
1	0	43	ASN
1	0	46	LEU
1	0	61	CYS
1	0	76	VAL

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Mol	Chain	Res	Type
1	0	91	LEU
1	0	97	ASP
2	1	6	THR
2	1	10	ARG
2	1	18	THR
2	1	27	VAL
2	1	32	ILE
2	1	36	GLU
2	1	41	LEU
2	1	45	VAL
2	1	49	CYS
2	1	55	LEU
2	1	58	MET
3	2	18	MET
3	2	21	HIS
3	2	34	SER
3	2	36	THR
3	2	49	ARG
3	2	56	VAL
3	2	67	ARG
3	2	74	SER
3	2	84	THR
3	2	86	ILE
3	2	89	VAL
3	2	101	THR
3	2	103	THR
3	2	108	SER
3	2	136	THR
3	2	137	VAL
3	2	140	ASN
3	2	144	SER
3	2	167	PHE
3	2	173	LEU
3	2	175	CYS
3	2	176	ILE
3	2	177	THR
3	2	179	ARG
3	2	183	SER
3	2	203	LEU
4	3	3	LEU
4	3	7	HIS
4	3	9	LYS

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Mol	Chain	Res	Type
4	3	13	THR
4	3	39	SER
4	3	41	ILE
4	3	52	LYS
4	3	54	ASN
4	3	63	ILE
4	3	88	LEU
4	3	92	VAL
4	3	101	GLU
4	3	102	SER
4	3	109	LYS
4	3	113	ARG
4	3	115	ARG
4	3	116	SER
4	3	117	ARG
4	3	132	LEU
4	3	139	LYS
4	3	142	ARG
4	3	148	THR
4	3	152	ARG
4	3	153	ILE
4	3	161	ASP
4	3	175	LYS
4	3	178	THR
4	3	179	THR
4	3	196	LYS
5	4	28	ARG
5	4	44	SER
5	4	48	THR
5	4	50	VAL
5	4	53	SER
5	4	63	ILE
5	4	70	SER
5	4	71	THR
5	4	74	ASP
5	4	80	ASN
5	4	84	TRP
5	4	91	ILE
5	4	92	ASP
5	4	98	ASN
5	4	109	THR
5	4	110	ARG

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Mol	Chain	Res	Type
5	4	111	ASP
5	4	115	SER
5	4	120	TRP
5	4	127	ARG
5	4	130	CYS
5	4	132	THR
5	4	146	THR
5	4	155	SER
5	4	157	THR
5	4	159	THR
5	4	207	THR
5	4	217	THR
5	4	218	ILE
5	4	230	ASP
6	5	10	ARG
6	5	18	THR
6	5	21	VAL
6	5	23	CYS
6	5	30	VAL
6	5	33	ASP
6	5	37	LYS
6	5	44	MET
6	5	49	SER
6	5	69	LEU
6	5	89	ARG
6	5	90	CYS
6	5	92	GLU
6	5	95	ARG
7	6	9	ILE
7	6	23	ILE
7	6	31	MET
7	6	43	MET
7	6	47	ASN
7	6	54	CYS
7	6	58	SER
7	6	62	CYS
7	6	63	LYS
7	6	77	PHE
7	6	79	ILE
8	7	9	LYS
8	7	16	LEU
8	7	24	LEU

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Mol	Chain	Res	Type
8	7	35	THR
8	7	40	LEU
8	7	47	ARG
8	7	50	LYS
8	7	64	THR
9	8	37	ASP
9	8	39	VAL
9	8	51	GLU
9	8	67	SER
9	8	68	THR
9	8	75	VAL
9	8	76	ASN
9	8	78	SER
9	8	84	MET
9	8	94	GLU
9	8	115	LYS
10	9	74	LYS
10	9	79	SER
10	9	86	THR
10	9	93	THR
10	9	95	LEU
10	9	98	LEU
10	9	103	LEU
10	9	143	ILE
10	9	144	ASP
12	B	16	SER
12	B	17	ASN
12	B	23	ILE
12	B	38	VAL
12	B	54	LYS
12	B	55	LEU
12	B	63	VAL
12	B	89	THR
12	B	105	THR
12	B	110	LEU
12	B	134	SER
12	B	136	VAL
12	B	159	CYS
12	B	164	THR
12	B	169	MET
12	B	194	MET
13	C	8	ILE

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Mol	Chain	Res	Type
13	C	12	LYS
13	C	29	SER
13	C	47	THR
13	C	64	VAL
13	C	79	ARG
13	C	85	ASP
13	C	105	VAL
13	C	109	ASN
13	C	137	CYS
13	C	142	SER
13	C	147	GLN
13	C	162	CYS
13	C	163	THR
13	C	171	ILE
13	C	201	LYS
13	C	203	PHE
13	C	221	ILE
14	D	3	LYS
14	D	6	ILE
14	D	8	THR
14	D	9	SER
14	D	16	ARG
14	D	28	MET
14	D	44	ARG
14	D	47	MET
14	D	57	ARG
14	D	63	ASP
14	D	68	ARG
14	D	69	ARG
14	D	79	ARG
14	D	80	MET
14	D	86	LEU
14	D	91	ARG
14	D	99	LEU
14	D	100	THR
14	D	104	LEU
14	D	105	MET
14	D	107	ARG
14	D	108	ARG
14	D	112	ARG
14	D	121	SER
14	D	127	VAL

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Mol	Chain	Res	Type
14	D	129	ILE
14	D	142	ASN
14	D	147	MET
14	D	149	ARG
14	D	150	THR
14	D	160	SER
14	D	164	LEU
14	D	171	ARG
15	E	36	LEU
15	E	43	SER
15	E	44	SER
15	E	46	ASP
15	E	52	SER
15	E	56	LYS
15	E	57	GLU
15	E	83	GLN
15	E	109	ASN
15	E	157	GLN
15	E	159	ILE
15	E	160	THR
15	E	162	LYS
15	E	165	SER
15	E	168	ILE
15	E	175	ARG
15	E	194	VAL
15	E	197	ILE
15	E	199	THR
15	E	205	THR
15	E	208	ARG
15	E	211	PHE
15	E	219	LEU
15	E	222	THR
15	E	235	GLU
16	F	49	LYS
16	F	60	THR
16	F	65	ASP
16	F	66	GLU
17	G	24	ILE
17	G	28	CYS
17	G	42	VAL
17	G	53	VAL
17	G	63	ILE

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Mol	Chain	Res	Type
17	G	66	ARG
17	G	89	LYS
17	G	99	THR
17	G	101	ARG
17	G	104	LEU
17	G	120	SER
17	G	121	THR
17	G	135	ASP
17	G	139	MET
17	G	156	SER
17	G	160	SER
17	G	162	ARG
17	G	164	ILE
18	H	3	LYS
18	H	11	LEU
18	H	12	LYS
18	H	27	LEU
18	H	28	ARG
18	H	30	VAL
18	H	31	SER
18	H	44	ASN
18	H	47	ILE
18	H	57	ARG
18	H	65	LEU
18	H	66	ILE
18	H	70	ASN
18	H	97	ARG
18	H	101	ASN
18	H	103	VAL
18	H	106	THR
18	H	107	THR
18	H	121	THR
19	I	7	GLN
19	I	12	PHE
19	I	15	LYS
19	I	23	SER
19	I	30	LEU
19	I	33	VAL
19	I	36	SER
19	I	46	LEU
19	I	66	ASP
19	I	72	ARG

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Mol	Chain	Res	Type
19	I	78	SER
19	I	87	LEU
19	I	89	LYS
19	I	126	MET
19	I	142	LYS
20	J	24	THR
20	J	31	VAL
20	J	45	THR
20	J	51	LYS
20	J	68	SER
20	J	74	SER
20	J	76	THR
20	J	94	ASN
20	J	97	ASP
20	J	115	THR
21	K	14	ILE
21	K	21	VAL
21	K	40	THR
21	K	55	ARG
21	K	57	THR
21	K	62	VAL
21	K	75	MET
21	K	91	ASN
21	K	97	LEU
21	K	107	GLN
21	K	122	SER
21	K	128	ARG
21	K	138	ASP
21	K	139	SER
21	K	150	ARG
22	L	3	VAL
22	L	7	ARG
22	L	9	ILE
22	L	10	ARG
22	L	19	ARG
22	L	34	LEU
22	L	36	SER
22	L	40	ASN
22	L	52	VAL
22	L	53	THR
22	L	76	ARG
22	L	80	LYS

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Mol	Chain	Res	Type
22	L	101	VAL
22	L	109	GLN
22	L	129	ILE
22	L	130	SER
23	M	15	HIS
23	M	28	THR
23	M	72	LEU
23	M	87	ASN
23	M	88	ARG
23	M	94	ASP
23	M	98	TYR
23	M	99	GLN
23	M	100	MET
23	M	115	ARG
23	M	123	ARG
23	M	136	GLN
23	M	138	THR
24	N	2	PRO
24	N	3	ASN
24	N	32	LYS
24	N	39	ARG
24	N	40	ARG
24	N	43	ARG
24	N	49	ILE
25	O	3	ARG
25	O	7	LYS
25	O	9	LYS
25	O	11	LYS
25	O	13	ILE
25	O	14	SER
25	O	26	LYS
25	O	34	THR
25	O	48	THR
25	O	59	GLN
25	O	66	ARG
25	O	93	LEU
25	O	104	LEU
25	O	109	LYS
25	O	118	ILE
25	O	126	ARG
25	O	127	LEU
26	P	2	THR

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Mol	Chain	Res	Type
26	P	7	THR
26	P	10	ILE
26	P	21	LEU
26	P	24	ASP
26	P	51	ARG
26	P	54	VAL
26	P	77	GLN
26	P	80	LEU
26	P	88	ARG
26	P	95	LEU
26	P	102	ARG
26	P	108	LEU
26	P	110	ARG
26	P	115	THR
26	P	122	LYS
27	Q	6	GLN
27	Q	12	GLN
27	Q	32	ARG
27	Q	37	ILE
27	Q	51	THR
27	Q	61	SER
27	Q	64	SER
27	Q	77	THR
27	Q	84	ILE
27	Q	87	ARG
27	Q	93	VAL
27	Q	98	ARG
27	Q	103	HIS
27	Q	115	SER
27	Q	117	LYS
27	Q	128	ARG
27	Q	133	THR
27	Q	135	ARG
28	R	20	HIS
28	R	32	SER
28	R	42	LEU
28	R	48	ASP
28	R	50	THR
28	R	67	ILE
28	R	73	THR
28	R	76	ASN
28	R	80	SER

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Mol	Chain	Res	Type
28	R	88	ASN
28	R	106	ARG
28	R	107	THR
28	R	113	ARG
28	R	117	HIS
28	R	124	VAL
28	R	126	PHE
28	R	147	ILE
28	R	161	HIS
28	R	189	SER
28	R	190	VAL
28	R	208	THR
28	R	219	LEU
28	R	238	LEU
28	R	246	THR
28	R	264	ASN
28	R	274	THR
28	R	313	THR
29	S	11	PHE
29	S	12	THR
29	S	28	SER
29	S	36	ASP
29	S	49	ARG
29	S	66	ARG
29	S	83	THR
29	S	84	HIS
29	S	88	MET
29	S	119	LYS
29	S	127	THR
30	T	9	THR
30	T	45	VAL
30	T	56	TRP
30	T	60	ARG
30	T	76	ILE
30	T	77	SER
30	T	89	ARG
30	T	93	ARG
30	T	105	ARG
30	T	117	ILE
30	T	130	ARG
30	T	135	GLU
30	T	155	LYS

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Mol	Chain	Res	Type
31	U	3	ASP
31	U	20	ASN
31	U	29	LEU
31	U	34	ARG
31	U	50	CYS
31	U	51	ASP
31	U	56	VAL
31	U	71	VAL
31	U	78	SER
31	U	100	CYS
32	V	6	THR
32	V	8	THR
32	V	35	LEU
32	V	37	GLU
32	V	44	LYS
32	V	46	LEU
32	V	60	ARG
32	V	105	MET
32	V	119	SER
33	W	11	ARG
33	W	19	MET
33	W	38	LEU
33	W	41	SER
33	W	42	LEU
33	W	45	SER
33	W	51	ARG
33	W	82	LYS
33	W	97	THR
33	W	107	THR
33	W	110	ARG
33	W	115	SER
33	W	122	LYS
33	W	141	ILE
33	W	142	VAL
33	W	143	THR
33	W	176	HIS
33	W	183	CYS
33	W	186	GLN
33	W	189	ASN
33	W	210	CYS
33	W	214	ASP
33	W	218	ASN

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Mol	Chain	Res	Type
33	W	229	VAL
33	W	230	LEU
33	W	232	GLN
33	W	236	SER
33	W	238	ILE
33	W	242	SER
33	W	247	ARG
33	W	253	GLU
33	W	256	ARG
34	X	4	MET
34	X	5	HIS
34	X	8	LEU
34	X	35	SER
34	X	53	ASP
34	X	59	SER
34	X	62	TRP
35	Y	1	MET
35	Y	6	SER
35	Y	7	TYR
35	Y	10	THR
35	Y	16	ILE
35	Y	32	MET
35	Y	43	ASP
35	Y	51	LYS
35	Y	78	SER
35	Y	97	VAL
35	Y	98	ARG
35	Y	106	MET
35	Y	118	VAL
35	Y	120	GLU
35	Y	137	ARG
35	Y	145	PHE
35	Y	155	LEU
35	Y	181	ARG
35	Y	186	GLU
35	Y	206	ASN
36	Z	14	THR
36	Z	17	ILE
36	Z	22	GLU
36	Z	25	ASP
36	Z	31	LYS
36	Z	47	VAL

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Mol	Chain	Res	Type
36	Z	61	THR
36	Z	75	SER

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
11	A	1716/1753 (97%)	647 (37%)	149 (8%)

All (647) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	A	2	A
11	A	3	C
11	A	4	C
11	A	8	U
11	A	11	A
11	A	12	U
11	A	13	C
11	A	14	C
11	A	17	C
11	A	22	U
11	A	26	U
11	A	33	G
11	A	37	U
11	A	40	A
11	A	41	U
11	A	44	U
11	A	45	A
11	A	46	A
11	A	55	U
11	A	58	G
11	A	59	C
11	A	60	C
11	A	62	G
11	A	64	U
11	A	65	C
11	A	66	A
11	A	71	U

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Mol	Chain	Res	Type
11	A	72	G
11	A	73	A
11	A	74	A
11	A	75	C
11	A	76	A
11	A	77	G
11	A	80	A
11	A	83	C
11	A	85	G
11	A	99	A
11	A	100	A
11	A	101	A
11	A	106	U
11	A	107	U
11	A	110	A
11	A	112	U
11	A	122	A
11	A	123	A
11	A	124	U
11	A	125	U
11	A	126	A
11	A	132	U
11	A	134	C
11	A	135	A
11	A	147	G
11	A	149	U
11	A	152	U
11	A	153	U
11	A	155	U
11	A	157	G
11	A	160	C
11	A	161	U
11	A	163	A
11	A	164	U
11	A	165	A
11	A	168	U
11	A	169	G
11	A	171	U
11	A	172	U
11	A	173	A
11	A	174	A
11	A	181	G

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Mol	Chain	Res	Type
11	A	182	U
11	A	185	C
11	A	186	C
11	A	188	G
11	A	196	A
11	A	199	G
11	A	208	A
11	A	209	G
11	A	210	A
11	A	211	U
11	A	212	A
11	A	213	U
11	A	214	U
11	A	215	A
11	A	216	G
11	A	217	A
11	A	218	C
11	A	219	C
11	A	220	A
11	A	222	U
11	A	223	C
11	A	226	A
11	A	227	G
11	A	229	A
11	A	230	A
11	A	231	U
11	A	232	G
11	A	233	U
11	A	234	G
11	A	235	A
11	A	237	U
11	A	238	G
11	A	239	A
11	A	240	G
11	A	246	U
11	A	247	C
11	A	254	A
11	A	258	A
11	A	262	G
11	A	264	U
11	A	265	C
11	A	266	G

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Mol	Chain	Res	Type
11	A	269	G
11	A	270	U
11	A	271	U
11	A	272	U
11	A	273	A
11	A	274	C
11	A	278	G
11	A	303	A
11	A	304	U
11	A	305	C
11	A	306	A
11	A	307	G
11	A	311	U
11	A	312	C
11	A	313	G
11	A	314	A
11	A	319	A
11	A	320	G
11	A	324	A
11	A	329	A
11	A	341	G
11	A	342	U
11	A	343	C
11	A	344	A
11	A	350	A
11	A	351	A
11	A	352	C
11	A	354	G
11	A	359	U
11	A	360	U
11	A	364	G
11	A	368	G
11	A	369	A
11	A	374	G
11	A	378	A
11	A	379	A
11	A	381	G
11	A	388	A
11	A	391	A
11	A	392	A
11	A	393	C
11	A	394	G

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Mol	Chain	Res	Type
11	A	402	C
11	A	405	C
11	A	407	A
11	A	409	G
11	A	410	G
11	A	413	C
11	A	414	G
11	A	415	G
11	A	416	C
11	A	417	A
11	A	418	G
11	A	422	G
11	A	426	G
11	A	428	A
11	A	429	A
11	A	431	U
11	A	436	C
11	A	437	A
11	A	440	C
11	A	444	A
11	A	445	U
11	A	447	C
11	A	448	A
11	A	452	A
11	A	453	G
11	A	460	A
11	A	461	C
11	A	466	A
11	A	467	A
11	A	469	A
11	A	476	U
11	A	479	G
11	A	481	A
11	A	482	A
11	A	483	C
11	A	485	U
11	A	487	C
11	A	488	G
11	A	492	C
11	A	493	U
11	A	494	A
11	A	496	G

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Mol	Chain	Res	Type
11	A	499	A
11	A	500	U
11	A	503	A
11	A	504	A
11	A	508	A
11	A	511	A
11	A	512	C
11	A	518	A
11	A	527	A
11	A	529	C
11	A	530	G
11	A	531	A
11	A	532	G
11	A	533	G
11	A	534	A
11	A	535	A
11	A	536	C
11	A	538	A
11	A	540	U
11	A	541	G
11	A	542	G
11	A	544	G
11	A	548	A
11	A	550	G
11	A	551	U
11	A	552	C
11	A	553	A
11	A	554	U
11	A	559	C
11	A	560	C
11	A	570	G
11	A	571	G
11	A	572	U
11	A	573	A
11	A	574	A
11	A	575	U
11	A	577	C
11	A	578	C
11	A	586	A
11	A	588	A
11	A	598	A
11	A	599	A

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Mol	Chain	Res	Type
11	A	605	U
11	A	608	C
11	A	613	A
11	A	614	A
11	A	615	A
11	A	616	A
11	A	617	A
11	A	618	G
11	A	619	C
11	A	628	G
11	A	629	A
11	A	633	U
11	A	634	C
11	A	635	U
11	A	642	G
11	A	648	U
11	A	649	U
11	A	650	C
11	A	653	U
11	A	655	C
11	A	656	G
11	A	657	U
11	A	661	G
11	A	662	U
11	A	665	A
11	A	666	A
11	A	670	G
11	A	673	A
11	A	674	U
11	A	676	C
11	A	677	G
11	A	678	U
11	A	680	U
11	A	681	G
11	A	682	C
11	A	721	A
11	A	722	A
11	A	727	U
11	A	728	U
11	A	729	U
11	A	739	A
11	A	743	U

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Mol	Chain	Res	Type
11	A	749	G
11	A	750	U
11	A	751	U
11	A	758	A
11	A	759	G
11	A	762	U
11	A	764	U
11	A	765	A
11	A	766	G
11	A	772	A
11	A	777	U
11	A	781	C
11	A	785	G
11	A	786	A
11	A	792	G
11	A	794	A
11	A	795	A
11	A	797	A
11	A	798	G
11	A	799	G
11	A	800	A
11	A	805	G
11	A	808	C
11	A	811	U
11	A	812	U
11	A	813	U
11	A	814	A
11	A	815	U
11	A	817	G
11	A	819	U
11	A	820	U
11	A	821	C
11	A	822	U
11	A	823	U
11	A	825	G
11	A	834	A
11	A	835	U
11	A	840	A
11	A	841	A
11	A	842	U
11	A	843	A
11	A	846	G

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Mol	Chain	Res	Type
11	A	849	A
11	A	850	G
11	A	859	A
11	A	860	U
11	A	861	U
11	A	862	A
11	A	864	U
11	A	873	G
11	A	875	C
11	A	876	A
11	A	877	G
11	A	882	G
11	A	883	A
11	A	884	A
11	A	886	U
11	A	887	U
11	A	888	C
11	A	889	U
11	A	890	U
11	A	891	G
11	A	892	G
11	A	894	U
11	A	895	U
11	A	903	G
11	A	906	U
11	A	907	A
11	A	911	A
11	A	913	U
11	A	920	G
11	A	936	U
11	A	937	U
11	A	938	U
11	A	941	A
11	A	942	U
11	A	944	A
11	A	948	A
11	A	949	A
11	A	953	C
11	A	962	G
11	A	966	A
11	A	968	C
11	A	970	A

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Mol	Chain	Res	Type
11	A	971	A
11	A	974	C
11	A	975	G
11	A	976	A
11	A	981	A
11	A	983	A
11	A	996	U
11	A	997	A
11	A	998	A
11	A	999	C
11	A	1002	U
11	A	1003	A
11	A	1004	A
11	A	1006	C
11	A	1007	U
11	A	1008	A
11	A	1014	A
11	A	1017	C
11	A	1020	G
11	A	1025	G
11	A	1028	G
11	A	1035	A
11	A	1036	U
11	A	1038	U
11	A	1042	G
11	A	1046	G
11	A	1055	G
11	A	1063	A
11	A	1064	A
11	A	1069	U
11	A	1072	G
11	A	1076	U
11	A	1080	G
11	A	1081	G
11	A	1083	G
11	A	1092	U
11	A	1093	A
11	A	1099	G
11	A	1111	A
11	A	1114	G
11	A	1122	G
11	A	1123	G

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Mol	Chain	Res	Type
11	A	1124	A
11	A	1131	C
11	A	1136	G
11	A	1137	A
11	A	1139	G
11	A	1140	U
11	A	1142	G
11	A	1146	C
11	A	1147	U
11	A	1149	C
11	A	1155	A
11	A	1157	U
11	A	1162	C
11	A	1165	A
11	A	1166	A
11	A	1168	A
11	A	1169	C
11	A	1171	G
11	A	1172	G
11	A	1173	G
11	A	1174	A
11	A	1175	A
11	A	1176	A
11	A	1181	C
11	A	1189	A
11	A	1198	A
11	A	1199	G
11	A	1200	G
11	A	1201	G
11	A	1202	A
11	A	1203	U
11	A	1205	G
11	A	1210	A
11	A	1213	G
11	A	1215	G
11	A	1216	A
11	A	1217	G
11	A	1218	C
11	A	1219	U
11	A	1220	C
11	A	1223	U
11	A	1224	C

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Mol	Chain	Res	Type
11	A	1227	G
11	A	1228	A
11	A	1229	U
11	A	1232	U
11	A	1233	U
11	A	1235	G
11	A	1236	G
11	A	1237	G
11	A	1242	G
11	A	1245	G
11	A	1246	C
11	A	1247	A
11	A	1248	U
11	A	1249	G
11	A	1256	C
11	A	1257	U
11	A	1258	U
11	A	1264	G
11	A	1266	G
11	A	1269	G
11	A	1270	U
11	A	1273	U
11	A	1278	C
11	A	1279	U
11	A	1281	G
11	A	1286	U
11	A	1287	U
11	A	1288	C
11	A	1290	G
11	A	1293	A
11	A	1296	G
11	A	1297	A
11	A	1311	C
11	A	1316	A
11	A	1318	C
11	A	1319	U
11	A	1320	A
11	A	1321	G
11	A	1327	U
11	A	1331	A
11	A	1333	A
11	A	1334	U

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Mol	Chain	Res	Type
11	A	1339	G
11	A	1343	G
11	A	1344	U
11	A	1345	A
11	A	1347	U
11	A	1348	U
11	A	1349	C
11	A	1351	U
11	A	1358	A
11	A	1359	C
11	A	1360	U
11	A	1365	U
11	A	1366	G
11	A	1368	A
11	A	1369	A
11	A	1370	U
11	A	1371	A
11	A	1372	A
11	A	1373	G
11	A	1381	A
11	A	1383	G
11	A	1384	U
11	A	1385	U
11	A	1386	U
11	A	1395	A
11	A	1396	A
11	A	1397	C
11	A	1398	A
11	A	1399	G
11	A	1400	G
11	A	1402	C
11	A	1403	U
11	A	1404	G
11	A	1406	G
11	A	1407	A
11	A	1408	U
11	A	1415	A
11	A	1416	G
11	A	1417	A
11	A	1419	G
11	A	1421	G
11	A	1424	C

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Mol	Chain	Res	Type
11	A	1425	G
11	A	1428	C
11	A	1429	G
11	A	1430	C
11	A	1431	A
11	A	1432	C
11	A	1435	G
11	A	1437	G
11	A	1442	A
11	A	1444	U
11	A	1445	G
11	A	1448	U
11	A	1449	G
11	A	1452	G
11	A	1453	C
11	A	1458	A
11	A	1459	G
11	A	1461	A
11	A	1462	U
11	A	1463	U
11	A	1464	U
11	A	1466	C
11	A	1467	U
11	A	1469	U
11	A	1477	A
11	A	1478	G
11	A	1479	G
11	A	1480	U
11	A	1481	A
11	A	1487	A
11	A	1488	A
11	A	1489	U
11	A	1492	U
11	A	1493	A
11	A	1494	U
11	A	1495	U
11	A	1496	A
11	A	1498	U
11	A	1505	C
11	A	1506	G
11	A	1507	U
11	A	1508	G

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Mol	Chain	Res	Type
11	A	1509	U
11	A	1510	U
11	A	1511	A
11	A	1512	G
11	A	1514	G
11	A	1519	U
11	A	1526	G
11	A	1528	A
11	A	1529	U
11	A	1530	U
11	A	1531	G
11	A	1532	U
11	A	1533	G
11	A	1536	U
11	A	1538	U
11	A	1539	U
11	A	1540	G
11	A	1545	A
11	A	1546	G
11	A	1547	G
11	A	1549	A
11	A	1556	G
11	A	1557	U
11	A	1558	A
11	A	1562	G
11	A	1572	A
11	A	1573	G
11	A	1579	G
11	A	1583	A
11	A	1587	U
11	A	1590	C
11	A	1597	G
11	A	1603	A
11	A	1604	C
11	A	1606	C
11	A	1607	A
11	A	1609	C
11	A	1610	G
11	A	1623	A
11	A	1627	A
11	A	1635	U
11	A	1649	U

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Mol	Chain	Res	Type
11	A	1652	A
11	A	1659	C
11	A	1660	A
11	A	1661	G
11	A	1662	C
11	A	1663	A
11	A	1666	G
11	A	1668	U
11	A	1681	G
11	A	1685	A
11	A	1710	G
11	A	1714	U
11	A	1717	C
11	A	1718	A
11	A	1719	A
11	A	1720	G
11	A	1721	G
11	A	1722	U
11	A	1724	U
11	A	1731	G
11	A	1733	G
11	A	1735	A
11	A	1736	C
11	A	1737	C
11	A	1745	G
11	A	1746	G
11	A	1747	A
11	A	1748	U
11	A	1749	C
11	A	1750	A
11	A	1752	U
11	A	1753	A

All (149) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	1	A
11	A	2	A
11	A	3	C
11	A	61	A
11	A	64	U
11	A	65	C

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Mol	Chain	Res	Type
11	A	71	U
11	A	99	A
11	A	100	A
11	A	163	A
11	A	168	U
11	A	171	U
11	A	172	U
11	A	181	G
11	A	198	C
11	A	209	G
11	A	211	U
11	A	213	U
11	A	214	U
11	A	229	A
11	A	232	G
11	A	234	G
11	A	237	U
11	A	238	G
11	A	239	A
11	A	245	A
11	A	257	G
11	A	271	U
11	A	272	U
11	A	273	A
11	A	312	C
11	A	328	G
11	A	341	G
11	A	343	C
11	A	378	A
11	A	380	G
11	A	391	A
11	A	393	C
11	A	409	G
11	A	413	C
11	A	414	G
11	A	427	A
11	A	444	A
11	A	451	G
11	A	486	A
11	A	492	C
11	A	493	U
11	A	498	C

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Mol	Chain	Res	Type
11	A	499	A
11	A	507	G
11	A	534	A
11	A	536	C
11	A	543	A
11	A	550	G
11	A	572	U
11	A	573	A
11	A	604	G
11	A	615	A
11	A	632	U
11	A	665	A
11	A	675	A
11	A	676	C
11	A	679	U
11	A	680	U
11	A	738	A
11	A	763	U
11	A	764	U
11	A	771	A
11	A	794	A
11	A	798	G
11	A	814	A
11	A	833	A
11	A	834	A
11	A	840	A
11	A	882	G
11	A	890	U
11	A	912	A
11	A	941	A
11	A	982	U
11	A	1001	A
11	A	1002	U
11	A	1054	U
11	A	1071	U
11	A	1079	G
11	A	1080	G
11	A	1092	U
11	A	1110	A
11	A	1122	G
11	A	1123	G
11	A	1146	C

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Mol	Chain	Res	Type
11	A	1168	A
11	A	1172	G
11	A	1175	A
11	A	1188	A
11	A	1199	G
11	A	1201	G
11	A	1217	G
11	A	1223	U
11	A	1228	A
11	A	1231	C
11	A	1236	G
11	A	1241	U
11	A	1245	G
11	A	1246	C
11	A	1256	C
11	A	1257	U
11	A	1277	U
11	A	1278	C
11	A	1286	U
11	A	1318	C
11	A	1342	U
11	A	1346	C
11	A	1347	U
11	A	1365	U
11	A	1371	A
11	A	1383	G
11	A	1397	C
11	A	1402	C
11	A	1403	U
11	A	1406	G
11	A	1428	C
11	A	1429	G
11	A	1431	A
11	A	1443	A
11	A	1444	U
11	A	1451	C
11	A	1452	G
11	A	1462	U
11	A	1463	U
11	A	1480	U
11	A	1486	U
11	A	1488	A

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Mol	Chain	Res	Type
11	A	1494	U
11	A	1495	U
11	A	1506	G
11	A	1509	U
11	A	1529	U
11	A	1556	G
11	A	1557	U
11	A	1586	A
11	A	1605	A
11	A	1651	G
11	A	1661	G
11	A	1662	C
11	A	1720	G
11	A	1721	G
11	A	1744	U
11	A	1749	C
11	A	1752	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 83 ligands modelled in this entry, 83 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	0	99/211 (46%)	0.86	7 (7%) 16 11	92, 149, 224, 274	0
2	1	66/68 (97%)	0.80	9 (13%) 4 4	203, 261, 324, 343	0
3	2	207/208 (99%)	0.80	16 (7%) 13 10	71, 144, 216, 259	0
4	3	196/197 (99%)	0.77	21 (10%) 6 7	116, 179, 252, 285	0
5	4	221/265 (83%)	0.66	17 (7%) 13 10	103, 155, 208, 245	0
6	5	100/119 (84%)	0.93	11 (11%) 6 6	86, 134, 219, 240	0
7	6	80/81 (98%)	0.80	5 (6%) 19 13	117, 170, 216, 228	0
8	7	101/162 (62%)	1.02	15 (14%) 3 4	130, 187, 230, 255	0
9	8	79/143 (55%)	1.17	17 (21%) 1 2	252, 277, 348, 437	0
10	9	93/189 (49%)	0.97	15 (16%) 2 3	197, 257, 314, 331	0
11	A	1717/1753 (97%)	1.22	245 (14%) 3 4	79, 137, 297, 532	0
12	B	201/241 (83%)	0.59	10 (4%) 28 18	103, 168, 221, 256	0
13	C	228/243 (93%)	0.72	18 (7%) 13 10	89, 156, 238, 280	0
14	D	180/181 (99%)	0.99	15 (8%) 11 9	86, 115, 180, 234	0
15	E	229/296 (77%)	0.93	22 (9%) 8 8	81, 123, 226, 266	0
16	F	89/101 (88%)	1.01	13 (14%) 3 4	93, 146, 216, 259	0
17	G	192/200 (96%)	1.49	58 (30%) 1 2	198, 256, 315, 346	0
18	H	129/130 (99%)	0.73	4 (3%) 47 29	76, 117, 156, 179	0
19	I	143/145 (98%)	1.08	26 (18%) 2 3	152, 218, 272, 312	0
20	J	108/120 (90%)	0.89	11 (10%) 7 7	89, 145, 231, 248	0
21	K	140/151 (92%)	0.93	7 (5%) 28 18	89, 147, 206, 225	0
22	L	140/142 (98%)	0.94	10 (7%) 16 11	77, 105, 148, 213	0
23	M	153/155 (98%)	0.83	19 (12%) 5 5	198, 260, 333, 366	0
24	N	54/55 (98%)	0.74	1 (1%) 64 41	95, 135, 203, 233	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	O	152/153 (99%)	1.00	22 (14%) 3 4	91, 153, 215, 269	0
26	P	148/149 (99%)	0.79	11 (7%) 14 11	92, 125, 170, 225	0
27	Q	156/157 (99%)	1.01	17 (10%) 6 7	80, 129, 223, 275	0
28	R	338/343 (98%)	1.23	79 (23%) 1 2	172, 250, 315, 352	0
29	S	128/144 (88%)	0.78	12 (9%) 9 8	231, 263, 309, 342	0
30	T	154/155 (99%)	1.04	22 (14%) 3 4	169, 226, 303, 354	0
31	U	124/126 (98%)	1.15	26 (20%) 1 2	210, 259, 325, 375	0
32	V	119/130 (91%)	0.86	15 (12%) 4 5	135, 188, 258, 292	0
33	W	259/259 (100%)	0.75	12 (4%) 31 20	76, 118, 164, 211	0
34	X	74/80 (92%)	0.99	13 (17%) 2 3	84, 141, 259, 292	0
35	Y	228/293 (77%)	0.85	23 (10%) 7 7	99, 163, 225, 282	0
36	Z	97/97 (100%)	1.13	22 (22%) 1 2	106, 143, 197, 210	0
All	All	6922/7642 (90%)	0.99	866 (12%) 5 5	71, 161, 290, 532	0

All (866) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	D	181	ALA	13.8
28	R	125	ALA	11.2
28	R	87	GLU	8.5
14	D	180	SER	8.3
25	O	83	ALA	8.1
28	R	82	LEU	8.0
28	R	170	TYR	7.9
20	J	117	THR	7.5
16	F	13	ASP	6.9
28	R	301	LYS	6.9
20	J	118	ALA	6.6
11	A	719	G	6.5
17	G	146	ILE	6.5
30	T	52	GLN	6.4
11	A	1416	G	6.4
28	R	31	PHE	6.3
28	R	340	THR	6.2
23	M	76	PRO	6.2
16	F	62	VAL	6.2
31	U	59	VAL	6.1
17	G	32	TYR	6.1

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Mol	Chain	Res	Type	RSRZ
17	G	137	ALA	6.1
15	E	24	LYS	6.0
1	0	19	ASN	6.0
32	V	95	LYS	5.8
32	V	94	GLU	5.8
30	T	151	GLN	5.8
28	R	30	GLY	5.7
20	J	116	MET	5.7
31	U	6	GLN	5.7
9	8	57	PRO	5.7
11	A	70	U	5.7
31	U	33	LEU	5.6
17	G	131	LYS	5.6
8	7	71	GLU	5.5
25	O	82	CYS	5.5
4	3	44	GLN	5.4
17	G	55	LYS	5.3
25	O	84	PRO	5.3
28	R	246	THR	5.2
4	3	52	LYS	5.2
17	G	155	GLU	5.2
21	K	151	LEU	5.2
17	G	116	PRO	5.2
35	Y	46	LYS	5.1
28	R	33	GLN	5.1
19	I	21	VAL	5.0
5	4	78	ASN	4.9
17	G	185	ALA	4.9
2	1	47	GLY	4.9
9	8	62	LYS	4.9
7	6	68	LYS	4.9
8	7	98	ASN	4.8
34	X	73	ALA	4.8
2	1	12	MET	4.7
14	D	178	LYS	4.7
9	8	113	GLU	4.7
28	R	253	ASP	4.7
15	E	72	GLN	4.6
7	6	71	ILE	4.6
36	Z	71	GLY	4.6
11	A	648	U	4.5
28	R	302	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
17	G	184	TRP	4.5
17	G	114	ALA	4.5
11	A	1384	U	4.5
28	R	84	LEU	4.5
22	L	32	ARG	4.5
27	Q	19	SER	4.5
11	A	1376	A	4.4
9	8	98	LYS	4.4
28	R	298	PRO	4.4
28	R	83	ALA	4.4
11	A	724	C	4.4
28	R	175	LYS	4.4
9	8	45	ILE	4.4
10	9	84	LYS	4.4
6	5	64	GLN	4.3
6	5	19	ARG	4.3
10	9	97	ALA	4.3
17	G	9	THR	4.3
21	K	21	VAL	4.3
4	3	147	GLY	4.3
31	U	90	ALA	4.2
11	A	682	C	4.2
22	L	33	LEU	4.2
11	A	1215	G	4.2
32	V	77	GLU	4.2
34	X	1	MET	4.2
35	Y	142	LYS	4.2
4	3	194	THR	4.2
17	G	53	VAL	4.2
17	G	153	CYS	4.1
29	S	80	PRO	4.1
29	S	122	ALA	4.1
10	9	73	LYS	4.1
28	R	124	VAL	4.1
28	R	229	ALA	4.1
5	4	77	ASP	4.1
30	T	46	ALA	4.0
17	G	188	LYS	4.0
30	T	135	GLU	4.0
36	Z	16	LEU	4.0
28	R	309	ASN	4.0
5	4	213	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
15	E	147	ASN	4.0
11	A	1576	U	4.0
28	R	305	GLN	3.9
29	S	77	LYS	3.9
17	G	148	PHE	3.9
5	4	21	ARG	3.9
2	1	50	ARG	3.9
10	9	74	LYS	3.9
32	V	87	GLU	3.9
36	Z	15	GLY	3.9
3	2	88	ASP	3.9
15	E	70	ASP	3.9
11	A	289	U	3.9
11	A	1447	C	3.9
17	G	147	TYR	3.8
23	M	73	ILE	3.8
20	J	18	ARG	3.8
30	T	41	THR	3.8
28	R	247	TYR	3.8
25	O	23	ARG	3.8
28	R	343	ASN	3.8
8	7	55	LEU	3.8
16	F	47	ILE	3.8
26	P	110	ARG	3.8
17	G	54	LYS	3.7
28	R	208	THR	3.7
32	V	92	ASP	3.7
11	A	732	U	3.7
31	U	83	LEU	3.7
11	A	119	G	3.7
11	A	824	G	3.7
11	A	236	U	3.7
17	G	118	GLU	3.7
17	G	130	ARG	3.7
1	0	67	LYS	3.7
19	I	41	ILE	3.7
9	8	95	LYS	3.7
28	R	306	LYS	3.7
19	I	132	GLY	3.7
28	R	32	SER	3.7
29	S	116	MET	3.6
11	A	171	U	3.6

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Mol	Chain	Res	Type	RSRZ
29	S	115	ASP	3.6
19	I	51	TYR	3.6
31	U	46	VAL	3.6
15	E	119	ALA	3.6
30	T	150	LYS	3.6
35	Y	43	ASP	3.6
11	A	226	A	3.6
11	A	797	A	3.6
28	R	106	ARG	3.6
1	0	50	CYS	3.6
32	V	116	GLY	3.6
13	C	137	CYS	3.6
9	8	59	LYS	3.6
36	Z	19	ASP	3.6
28	R	300	THR	3.5
30	T	89	ARG	3.5
17	G	115	GLY	3.5
19	I	33	VAL	3.5
3	2	18	MET	3.5
35	Y	1	MET	3.5
11	A	1577	G	3.5
34	X	72	ALA	3.5
34	X	70	MET	3.5
31	U	58	LEU	3.5
25	O	9	LYS	3.5
8	7	56	GLU	3.5
3	2	17	ARG	3.5
11	A	851	U	3.5
1	0	66	LYS	3.5
12	B	174	ILE	3.5
28	R	174	MET	3.5
26	P	107	GLU	3.5
6	5	12	GLN	3.5
28	R	88	ASN	3.5
17	G	150	ILE	3.5
25	O	153	GLN	3.4
8	7	101	SER	3.4
8	7	99	PHE	3.4
15	E	95	GLN	3.4
25	O	8	GLY	3.4
14	D	90	GLU	3.4
11	A	583	C	3.4

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Mol	Chain	Res	Type	RSRZ
9	8	39	VAL	3.4
28	R	228	ILE	3.4
30	T	144	ALA	3.4
22	L	91	CYS	3.4
11	A	17	C	3.4
10	9	80	TYR	3.4
15	E	204	CYS	3.4
23	M	30	ILE	3.4
15	E	133	ALA	3.3
31	U	123	ALA	3.3
3	2	86	ILE	3.3
34	X	66	LYS	3.3
12	B	51	GLN	3.3
36	Z	20	LYS	3.3
11	A	1375	C	3.3
13	C	197	PRO	3.3
19	I	22	ALA	3.3
11	A	844	G	3.3
35	Y	78	SER	3.3
25	O	91	TYR	3.3
29	S	51	LYS	3.3
11	A	834	A	3.3
15	E	85	THR	3.3
33	W	82	LYS	3.3
17	G	136	VAL	3.3
34	X	71	ASP	3.3
35	Y	44	GLU	3.3
11	A	751	U	3.3
23	M	154	ASN	3.3
17	G	132	GLN	3.3
34	X	36	TYR	3.3
14	D	58	GLU	3.2
11	A	1221	U	3.2
17	G	121	THR	3.2
2	1	68	ARG	3.2
11	A	1620	U	3.2
4	3	196	LYS	3.2
11	A	636	G	3.2
17	G	152	GLY	3.2
6	5	66	ILE	3.2
16	F	64	GLU	3.2
10	9	140	THR	3.2

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Mol	Chain	Res	Type	RSRZ
17	G	82	ALA	3.2
18	H	43	LYS	3.2
9	8	64	LEU	3.2
16	F	80	GLN	3.2
33	W	44	LEU	3.2
27	Q	93	VAL	3.2
15	E	120	LYS	3.2
31	U	86	PHE	3.2
3	2	208	LYS	3.2
31	U	63	CYS	3.2
15	E	222	THR	3.2
27	Q	41	PHE	3.2
28	R	339	GLU	3.2
31	U	61	ALA	3.2
4	3	84	LEU	3.2
11	A	1086	G	3.2
14	D	102	HIS	3.2
17	G	24	ILE	3.2
17	G	194	LYS	3.2
11	A	258	A	3.2
17	G	139	MET	3.2
11	A	1054	U	3.2
14	D	95	TYR	3.2
11	A	1501	C	3.2
11	A	1606	C	3.2
11	A	725	A	3.1
11	A	840	A	3.1
11	A	567	C	3.1
29	S	11	PHE	3.1
11	A	1386	U	3.1
11	A	1368	A	3.1
11	A	1417	A	3.1
26	P	44	LYS	3.1
35	Y	131	ARG	3.1
11	A	271	U	3.1
11	A	1006	C	3.1
11	A	733	G	3.1
28	R	236	LYS	3.1
18	H	127	GLY	3.1
25	O	66	ARG	3.1
28	R	226	LYS	3.1
11	A	1007	U	3.1

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Mol	Chain	Res	Type	RSRZ
20	J	52	GLY	3.1
11	A	850	G	3.1
11	A	402	C	3.1
11	A	1740	C	3.1
28	R	40	PRO	3.0
11	A	1377	A	3.0
19	I	28	LYS	3.0
19	I	39	ASP	3.0
29	S	72	CYS	3.0
11	A	460	A	3.0
28	R	45	GLY	3.0
11	A	461	C	3.0
32	V	40	GLN	3.0
15	E	53	ILE	3.0
31	U	124	LEU	3.0
32	V	81	ARG	3.0
19	I	131	CYS	3.0
13	C	119	ARG	3.0
11	A	428	A	3.0
28	R	137	GLY	3.0
36	Z	60	ALA	3.0
23	M	114	GLU	3.0
31	U	32	VAL	3.0
35	Y	228	HIS	3.0
36	Z	96	GLN	3.0
27	Q	94	ARG	3.0
35	Y	27	PHE	3.0
11	A	228	C	3.0
30	T	32	LEU	3.0
23	M	101	ALA	3.0
28	R	230	THR	3.0
28	R	299	ILE	3.0
10	9	141	LEU	3.0
10	9	72	LYS	3.0
14	D	177	ALA	3.0
28	R	191	GLY	3.0
23	M	128	PHE	3.0
35	Y	23	LYS	3.0
15	E	86	PRO	3.0
33	W	56	LEU	3.0
23	M	118	LYS	3.0
30	T	142	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
3	2	82	ARG	2.9
14	D	138	LYS	2.9
4	3	78	ARG	2.9
17	G	56	PHE	2.9
11	A	595	A	2.9
11	A	984	C	2.9
11	A	558	G	2.9
11	A	1633	G	2.9
13	C	170	TYR	2.9
19	I	64	ASN	2.9
12	B	192	GLU	2.9
4	3	48	PHE	2.9
33	W	47	LEU	2.9
29	S	9	LYS	2.9
5	4	128	VAL	2.9
28	R	304	GLY	2.9
11	A	1165	A	2.9
21	K	107	GLN	2.9
28	R	11	VAL	2.9
28	R	91	ALA	2.9
9	8	38	LYS	2.9
25	O	81	GLY	2.9
5	4	198	ASP	2.8
11	A	110	A	2.8
11	A	582	U	2.8
25	O	11	LYS	2.8
19	I	118	LEU	2.8
31	U	21	CYS	2.8
17	G	141	ARG	2.8
11	A	32	U	2.8
11	A	399	C	2.8
11	A	566	C	2.8
11	A	1301	A	2.8
32	V	86	PRO	2.8
3	2	124	HIS	2.8
11	A	1287	U	2.8
1	0	110	GLU	2.8
5	4	25	PRO	2.8
1	0	18	GLU	2.8
1	0	20	GLU	2.8
13	C	138	GLU	2.8
30	T	30	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
11	A	905	C	2.8
11	A	1141	G	2.8
11	A	1339	G	2.8
12	B	124	ARG	2.8
10	9	75	LYS	2.8
11	A	1271	G	2.8
13	C	146	LYS	2.8
7	6	69	VAL	2.8
28	R	165	VAL	2.8
31	U	48	GLU	2.8
11	A	723	A	2.8
19	I	100	ASP	2.8
8	7	100	ILE	2.8
11	A	238	G	2.8
11	A	568	G	2.8
17	G	59	THR	2.8
17	G	143	ASN	2.8
28	R	257	THR	2.8
16	F	94	ASP	2.7
5	4	75	LEU	2.7
11	A	42	A	2.7
11	A	467	A	2.7
11	A	1476	A	2.7
11	A	7	G	2.7
16	F	61	ILE	2.7
36	Z	22	GLU	2.7
31	U	69	LYS	2.7
9	8	102	GLN	2.7
25	O	90	LEU	2.7
28	R	166	SER	2.7
32	V	90	ILE	2.7
11	A	782	A	2.7
13	C	230	ALA	2.7
4	3	45	VAL	2.7
36	Z	95	ILE	2.7
11	A	1534	G	2.7
9	8	42	ALA	2.7
11	A	223	C	2.7
17	G	43	PHE	2.7
11	A	1199	G	2.7
11	A	843	A	2.7
11	A	893	A	2.7

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Mol	Chain	Res	Type	RSRZ
28	R	85	SER	2.7
11	A	743	U	2.7
11	A	1722	U	2.7
11	A	79	G	2.7
35	Y	47	GLY	2.7
32	V	71	LEU	2.7
11	A	131	U	2.7
25	O	75	ARG	2.7
33	W	79	ARG	2.7
11	A	1607	A	2.7
16	F	53	LYS	2.7
11	A	1578	C	2.7
35	Y	42	GLY	2.7
36	Z	67	VAL	2.7
11	A	496	G	2.7
4	3	73	LEU	2.7
11	A	1545	A	2.7
10	9	129	TYR	2.6
11	A	842	U	2.6
16	F	92	ALA	2.6
17	G	133	ALA	2.6
30	T	148	ALA	2.6
35	Y	54	GLY	2.6
11	A	720	U	2.6
19	I	35	GLY	2.6
11	A	1720	G	2.6
11	A	398	A	2.6
11	A	1305	C	2.6
11	A	56	G	2.6
5	4	61	GLU	2.6
11	A	906	U	2.6
17	G	111	VAL	2.6
23	M	75	ASP	2.6
9	8	60	VAL	2.6
35	Y	110	ALA	2.6
36	Z	94	PRO	2.6
5	4	157	THR	2.6
17	G	30	GLN	2.6
19	I	38	ILE	2.6
17	G	60	GLN	2.6
8	7	85	ASP	2.6
2	1	9	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
11	A	635	U	2.6
23	M	120	LYS	2.6
22	L	41	PRO	2.6
28	R	51	VAL	2.6
6	5	92	GLU	2.6
2	1	46	LYS	2.6
11	A	122	A	2.6
11	A	1011	C	2.6
11	A	1568	C	2.6
4	3	47	GLU	2.6
28	R	213	GLU	2.6
11	A	562	G	2.5
20	J	22	THR	2.5
6	5	11	SER	2.5
14	D	179	LYS	2.5
31	U	52	GLN	2.5
35	Y	21	ASP	2.5
28	R	342	ALA	2.5
11	A	43	U	2.5
11	A	1063	A	2.5
26	P	149	LYS	2.5
11	A	118	U	2.5
11	A	594	U	2.5
26	P	16	LEU	2.5
14	D	137	GLY	2.5
28	R	58	GLU	2.5
28	R	92	ILE	2.5
11	A	261	G	2.5
16	F	91	ALA	2.5
35	Y	155	LEU	2.5
23	M	115	ARG	2.5
31	U	57	LYS	2.5
23	M	113	LEU	2.5
30	T	49	LEU	2.5
8	7	74	GLU	2.5
32	V	93	ILE	2.5
11	A	1147	U	2.5
27	Q	14	GLY	2.5
19	I	50	ILE	2.5
11	A	541	G	2.5
36	Z	92	LEU	2.5
11	A	1500	C	2.5

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Mol	Chain	Res	Type	RSRZ
33	W	37	LYS	2.5
30	T	146	GLN	2.5
30	T	85	SER	2.5
25	O	64	GLN	2.5
28	R	86	GLN	2.5
11	A	320	G	2.5
11	A	497	G	2.5
11	A	794	A	2.5
11	A	862	A	2.5
8	7	102	LYS	2.5
11	A	584	C	2.5
19	I	63	ALA	2.5
11	A	39	A	2.5
12	B	55	LEU	2.5
25	O	151	LEU	2.5
11	A	421	G	2.5
11	A	752	C	2.5
28	R	297	GLU	2.5
23	M	46	ILE	2.5
28	R	184	ALA	2.4
34	X	74	ALA	2.4
11	A	1632	U	2.4
17	G	187	ARG	2.4
2	1	51	VAL	2.4
36	Z	93	TYR	2.4
11	A	1120	A	2.4
11	A	288	C	2.4
11	A	783	U	2.4
11	A	836	G	2.4
9	8	97	ALA	2.4
11	A	120	A	2.4
22	L	31	LYS	2.4
15	E	76	LYS	2.4
19	I	136	ALA	2.4
30	T	122	ASN	2.4
11	A	872	A	2.4
11	A	1084	A	2.4
13	C	67	LYS	2.4
34	X	67	LYS	2.4
5	4	131	LYS	2.4
11	A	83	C	2.4
11	A	219	C	2.4

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Mol	Chain	Res	Type	RSRZ
28	R	81	ASP	2.4
32	V	79	GLU	2.4
4	3	31	PRO	2.4
4	3	62	LEU	2.4
8	7	58	ILE	2.4
11	A	1092	U	2.4
11	A	91	G	2.4
11	A	1068	C	2.4
15	E	92	GLN	2.4
33	W	46	VAL	2.4
12	B	183	GLY	2.4
19	I	70	ARG	2.4
6	5	4	LYS	2.4
11	A	220	A	2.4
11	A	486	A	2.4
11	A	593	A	2.4
11	A	734	U	2.4
11	A	1174	A	2.4
17	G	123	ILE	2.4
35	Y	132	LYS	2.4
12	B	120	VAL	2.4
27	Q	22	LEU	2.4
17	G	25	GLN	2.4
28	R	108	GLY	2.4
11	A	371	U	2.4
5	4	222	LYS	2.4
11	A	1085	A	2.4
3	2	22	ARG	2.4
17	G	197	LYS	2.4
31	U	107	LYS	2.4
31	U	122	GLY	2.4
11	A	587	U	2.4
36	Z	74	ARG	2.4
11	A	1499	A	2.4
28	R	115	VAL	2.3
5	4	45	PHE	2.3
10	9	142	LYS	2.3
11	A	565	G	2.3
8	7	13	TYR	2.3
25	O	17	ALA	2.3
28	R	43	ILE	2.3
22	L	43	MET	2.3

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Mol	Chain	Res	Type	RSRZ
11	A	1064	A	2.3
27	Q	45	LYS	2.3
8	7	80	LEU	2.3
11	A	655	C	2.3
11	A	1072	G	2.3
11	A	8	U	2.3
11	A	97	U	2.3
29	S	78	PRO	2.3
36	Z	51	ILE	2.3
11	A	128	A	2.3
11	A	350	A	2.3
11	A	754	A	2.3
19	I	40	MET	2.3
17	G	33	ILE	2.3
29	S	74	ALA	2.3
3	2	135	ARG	2.3
14	D	140	LEU	2.3
11	A	943	U	2.3
15	E	138	VAL	2.3
21	K	142	ARG	2.3
7	6	67	GLY	2.3
14	D	109	LEU	2.3
3	2	19	PRO	2.3
28	R	319	ALA	2.3
11	A	1634	G	2.3
11	A	1619	U	2.3
4	3	65	VAL	2.3
23	M	100	MET	2.3
13	C	226	GLU	2.3
20	J	107	ASP	2.3
35	Y	20	ASP	2.3
17	G	86	LYS	2.3
28	R	6	SER	2.3
15	E	94	GLY	2.3
25	O	18	LEU	2.3
27	Q	126	GLN	2.3
4	3	148	THR	2.3
3	2	54	VAL	2.3
11	A	21	U	2.3
28	R	111	TYR	2.3
11	A	1739	G	2.3
33	W	41	SER	2.3

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Mol	Chain	Res	Type	RSRZ
16	F	51	TRP	2.3
35	Y	111	LEU	2.3
35	Y	24	CYS	2.3
26	P	66	LYS	2.3
27	Q	72	GLY	2.3
32	V	108	LYS	2.3
36	Z	83	LEU	2.3
11	A	589	G	2.3
28	R	212	HIS	2.3
5	4	130	CYS	2.3
2	1	48	ALA	2.3
11	A	27	A	2.3
15	E	83	GLN	2.3
17	G	142	VAL	2.3
11	A	218	C	2.3
11	A	524	C	2.3
11	A	342	U	2.3
11	A	400	U	2.3
28	R	303	GLU	2.3
11	A	389	G	2.3
29	S	125	ALA	2.3
33	W	49	LYS	2.3
11	A	74	A	2.3
28	R	207	TYR	2.3
28	R	341	SER	2.3
36	Z	72	SER	2.3
35	Y	178	LYS	2.3
28	R	116	GLY	2.3
11	A	1281	G	2.2
11	A	1065	A	2.2
13	C	153	MET	2.2
11	A	1524	U	2.2
13	C	190	LYS	2.2
28	R	41	VAL	2.2
20	J	115	THR	2.2
33	W	115	SER	2.2
11	A	92	G	2.2
11	A	745	G	2.2
11	A	1719	A	2.2
11	A	773	U	2.2
28	R	190	VAL	2.2
16	F	63	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
23	M	97	ASN	2.2
11	A	1013	G	2.2
28	R	104	ASP	2.2
19	I	83	ILE	2.2
27	Q	58	PRO	2.2
11	A	117	U	2.2
22	L	141	LYS	2.2
28	R	34	LYS	2.2
10	9	96	GLY	2.2
4	3	57	ALA	2.2
6	5	13	LYS	2.2
11	A	1103	G	2.2
27	Q	152	LYS	2.2
12	B	123	PRO	2.2
34	X	31	PRO	2.2
4	3	190	LYS	2.2
11	A	214	U	2.2
11	A	627	U	2.2
11	A	726	U	2.2
15	E	71	VAL	2.2
21	K	32	HIS	2.2
28	R	146	ASN	2.2
25	O	109	LYS	2.2
7	6	75	CYS	2.2
11	A	825	G	2.2
11	A	1485	G	2.2
11	A	244	A	2.2
11	A	463	A	2.2
28	R	27	ILE	2.2
5	4	57	ARG	2.2
6	5	22	PRO	2.2
17	G	192	ILE	2.2
28	R	205	ILE	2.2
17	G	124	GLY	2.2
28	R	130	ASN	2.2
10	9	98	LEU	2.2
14	D	169	GLU	2.2
27	Q	69	ILE	2.2
30	T	147	ILE	2.2
11	A	1222	U	2.2
15	E	224	ARG	2.2
11	A	560	C	2.2

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Mol	Chain	Res	Type	RSRZ
6	5	27	GLY	2.2
11	A	327	G	2.2
11	A	368	G	2.2
11	A	381	G	2.2
11	A	615	A	2.2
18	H	29	PRO	2.2
11	A	1575	U	2.2
17	G	158	PHE	2.2
26	P	62	TYR	2.2
26	P	123	LEU	2.2
35	Y	30	LYS	2.2
13	C	139	ILE	2.2
11	A	1486	U	2.2
11	A	1547	G	2.2
35	Y	194	TYR	2.2
17	G	61	CYS	2.2
17	G	138	PRO	2.2
19	I	127	GLU	2.2
32	V	76	GLU	2.2
13	C	231	VAL	2.2
17	G	31	ASN	2.2
11	A	19	A	2.2
11	A	57	U	2.2
11	A	1080	G	2.2
11	A	1270	U	2.2
11	A	1683	A	2.2
22	L	11	ALA	2.2
5	4	96	GLY	2.2
20	J	89	ILE	2.2
24	N	4	LYS	2.2
36	Z	52	ALA	2.1
20	J	114	LEU	2.1
11	A	545	G	2.1
11	A	1081	G	2.1
4	3	95	THR	2.1
28	R	179	LYS	2.1
11	A	6	G	2.1
11	A	249	A	2.1
13	C	15	VAL	2.1
13	C	209	ILE	2.1
21	K	97	LEU	2.1
31	U	5	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
31	U	111	GLU	2.1
11	A	90	U	2.1
11	A	237	U	2.1
11	A	245	A	2.1
11	A	849	A	2.1
28	R	129	ASP	2.1
31	U	29	LEU	2.1
33	W	151	PHE	2.1
20	J	66	ARG	2.1
30	T	15	ALA	2.1
11	A	1717	C	2.1
3	2	97	GLU	2.1
3	2	101	THR	2.1
31	U	103	LEU	2.1
11	A	1448	U	2.1
6	5	68	LYS	2.1
11	A	279	A	2.1
11	A	469	A	2.1
11	A	586	A	2.1
11	A	20	G	2.1
11	A	544	G	2.1
17	G	44	VAL	2.1
9	8	114	ASP	2.1
36	Z	44	GLN	2.1
11	A	106	U	2.1
11	A	575	U	2.1
11	A	956	A	2.1
5	4	195	ILE	2.1
11	A	1391	C	2.1
12	B	89	THR	2.1
28	R	94	SER	2.1
33	W	86	THR	2.1
19	I	7	GLN	2.1
30	T	35	PRO	2.1
11	A	239	A	2.1
11	A	957	A	2.1
11	A	1189	A	2.1
11	A	1741	A	2.1
27	Q	57	CYS	2.1
28	R	89	CYS	2.1
28	R	167	CYS	2.1
11	A	33	G	2.1

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Mol	Chain	Res	Type	RSRZ
27	Q	109	HIS	2.1
11	A	1304	C	2.1
10	9	158	LYS	2.1
17	G	151	LYS	2.1
22	L	107	GLY	2.1
25	O	63	PRO	2.1
27	Q	49	GLU	2.1
26	P	80	LEU	2.1
10	9	87	LYS	2.1
11	A	944	A	2.1
11	A	1631	A	2.1
15	E	143	GLY	2.1
21	K	127	GLY	2.1
30	T	90	GLY	2.1
25	O	77	LEU	2.1
30	T	97	GLN	2.1
8	7	70	LYS	2.1
11	A	896	U	2.1
14	D	78	ARG	2.1
31	U	94	ILE	2.1
31	U	121	GLU	2.1
23	M	4	VAL	2.1
27	Q	139	LEU	2.1
11	A	290	A	2.1
11	A	16	G	2.1
16	F	18	HIS	2.1
19	I	145	ARG	2.1
15	E	146	GLY	2.1
34	X	7	THR	2.1
11	A	1179	C	2.1
13	C	77	GLN	2.1
9	8	44	PHE	2.1
27	Q	136	PHE	2.1
36	Z	29	PRO	2.1
11	A	1079	G	2.0
11	A	1707	G	2.0
30	T	26	LEU	2.0
4	3	94	PHE	2.0
11	A	605	U	2.0
11	A	1096	C	2.0
23	M	40	ARG	2.0
34	X	40	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
11	A	912	A	2.0
11	A	941	A	2.0
12	B	153	VAL	2.0
3	2	25	ARG	2.0
17	G	66	ARG	2.0
19	I	14	ARG	2.0
34	X	43	ARG	2.0
4	3	96	ALA	2.0
11	A	213	U	2.0
11	A	323	U	2.0
11	A	1349	C	2.0
25	O	152	VAL	2.0
17	G	157	ALA	2.0
23	M	149	GLY	2.0
26	P	43	ALA	2.0
36	Z	65	THR	2.0
2	1	11	ILE	2.0
3	2	158	ALA	2.0
11	A	99	A	2.0
26	P	2	THR	2.0
3	2	8	LYS	2.0
11	A	227	G	2.0
11	A	434	G	2.0
11	A	1280	G	2.0
17	G	145	ALA	2.0
18	H	10	CYS	2.0
19	I	144	TYR	2.0
11	A	160	C	2.0
9	8	111	VAL	2.0
22	L	28	ASP	2.0
4	3	5	LYS	2.0
11	A	1369	A	2.0
11	A	1415	A	2.0
13	C	13	LYS	2.0
36	Z	43	ASP	2.0
19	I	119	LEU	2.0
11	A	98	U	2.0
11	A	607	G	2.0
11	A	1002	U	2.0
13	C	17	ASP	2.0
25	O	45	LYS	2.0
23	M	116	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
8	7	67	TYR	2.0
17	G	196	ALA	2.0
11	A	462	A	2.0
11	A	1097	A	2.0
17	G	144	LEU	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
38	MG	A	5035	1/1	0.30	27.00	196,196,196,196	0
38	MG	A	5053	1/1	1.24	25.66	256,256,256,256	0
38	MG	A	5071	1/1	0.56	22.97	238,238,238,238	0
38	MG	A	5034	1/1	0.62	7.31	220,220,220,220	0
38	MG	A	5008	1/1	0.46	5.51	170,170,170,170	0
38	MG	A	5019	1/1	0.47	5.26	184,184,184,184	0
38	MG	A	5078	1/1	0.36	3.78	241,241,241,241	0
38	MG	A	5026	1/1	0.41	3.07	208,208,208,208	0
38	MG	A	5070	1/1	0.47	2.91	251,251,251,251	0
38	MG	A	5023	1/1	0.35	2.65	127,127,127,127	0
38	MG	A	5038	1/1	0.38	2.00	191,191,191,191	0
38	MG	A	5054	1/1	0.29	1.61	169,169,169,169	0
38	MG	A	5030	1/1	0.26	1.50	229,229,229,229	0
38	MG	A	5048	1/1	0.39	1.48	222,222,222,222	0
38	MG	A	5077	1/1	0.30	1.22	235,235,235,235	0
38	MG	A	5003	1/1	0.52	0.95	175,175,175,175	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
38	MG	A	5029	1/1	0.30	0.76	217,217,217,217	0
38	MG	A	5028	1/1	0.38	0.71	163,163,163,163	0
38	MG	A	5057	1/1	0.35	0.64	178,178,178,178	0
38	MG	A	5059	1/1	0.32	0.64	205,205,205,205	0
38	MG	A	5066	1/1	0.34	0.21	251,251,251,251	0
38	MG	A	5049	1/1	0.33	0.17	207,207,207,207	0
38	MG	A	5056	1/1	0.37	0.13	238,238,238,238	0
38	MG	A	5041	1/1	0.35	-0.15	162,162,162,162	0
38	MG	A	5039	1/1	0.27	-0.31	120,120,120,120	0
38	MG	A	5075	1/1	0.20	-0.31	239,239,239,239	0
38	MG	A	5006	1/1	0.28	-0.65	159,159,159,159	0
38	MG	A	5022	1/1	0.34	-0.76	108,108,108,108	0
38	MG	A	5073	1/1	0.31	-0.78	221,221,221,221	0
38	MG	A	5031	1/1	0.26	-0.86	218,218,218,218	0
37	ZN	6	500	1/1	0.16	-1.05	173,173,173,173	0
38	MG	A	5012	1/1	0.22	-1.10	118,118,118,118	0
38	MG	A	5013	1/1	0.25	-1.22	218,218,218,218	0
38	MG	A	5002	1/1	0.24	-1.26	111,111,111,111	0
38	MG	A	5044	1/1	0.23	-1.27	134,134,134,134	0
37	ZN	N	500	1/1	0.21	-1.30	132,132,132,132	0
38	MG	A	5047	1/1	0.23	-1.39	128,128,128,128	0
38	MG	A	5058	1/1	0.20	-1.40	227,227,227,227	0
38	MG	A	5040	1/1	0.24	-1.43	161,161,161,161	0
37	ZN	9	500	1/1	0.11	-1.45	278,278,278,278	0
38	MG	A	5024	1/1	0.21	-1.47	144,144,144,144	0
38	MG	A	5069	1/1	0.16	-1.56	199,199,199,199	0
38	MG	A	5065	1/1	0.31	-1.56	146,146,146,146	0
38	MG	A	5017	1/1	0.25	-1.59	192,192,192,192	0
38	MG	A	5052	1/1	0.21	-1.59	218,218,218,218	0
38	MG	A	5043	1/1	0.24	-1.73	197,197,197,197	0
38	MG	A	5050	1/1	0.21	-1.77	123,123,123,123	0
38	MG	A	5068	1/1	0.22	-1.89	169,169,169,169	0
38	MG	A	5036	1/1	0.26	-1.97	199,199,199,199	0
38	MG	A	5072	1/1	0.27	-2.06	146,146,146,146	0
37	ZN	5	500	1/1	0.14	-2.09	117,117,117,117	0
38	MG	A	5042	1/1	0.22	-2.10	177,177,177,177	0
38	MG	A	5062	1/1	0.13	-2.15	213,213,213,213	0
38	MG	A	5037	1/1	0.23	-2.22	178,178,178,178	0
38	MG	A	5076	1/1	0.20	-2.23	201,201,201,201	0
38	MG	A	5021	1/1	0.21	-2.31	189,189,189,189	0
38	MG	A	5005	1/1	0.28	-2.31	123,123,123,123	0
38	MG	A	5060	1/1	0.20	-2.42	148,148,148,148	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
38	MG	A	5067	1/1	0.12	-2.43	220,220,220,220	0
38	MG	A	5020	1/1	0.24	-2.43	199,199,199,199	0
38	MG	A	5074	1/1	0.24	-2.48	198,198,198,198	0
38	MG	A	5001	1/1	0.16	-2.64	159,159,159,159	0
38	MG	A	5009	1/1	0.19	-2.82	110,110,110,110	0
38	MG	A	5004	1/1	0.19	-2.96	167,167,167,167	0
38	MG	A	5007	1/1	0.23	-3.28	142,142,142,142	0
38	MG	A	5014	1/1	0.30	-3.33	206,206,206,206	0
38	MG	A	5016	1/1	0.15	-3.92	191,191,191,191	0
38	MG	A	5033	1/1	0.18	-3.92	122,122,122,122	0
38	MG	A	5018	1/1	0.28	-3.96	104,104,104,104	0
38	MG	A	5015	1/1	0.24	-4.46	118,118,118,118	0
38	MG	A	5046	1/1	0.20	-4.48	148,148,148,148	0
38	MG	A	5032	1/1	0.21	-4.56	174,174,174,174	0
38	MG	A	5000	1/1	0.15	-4.63	107,107,107,107	0
38	MG	A	5063	1/1	0.17	-4.93	141,141,141,141	0
38	MG	A	5025	1/1	0.16	-5.11	105,105,105,105	0
38	MG	A	5011	1/1	0.23	-5.45	187,187,187,187	0
38	MG	A	5064	1/1	0.12	-5.62	186,186,186,186	0
38	MG	A	5051	1/1	0.15	-5.67	162,162,162,162	0
38	MG	A	5010	1/1	0.13	-7.41	201,201,201,201	0
38	MG	A	5061	1/1	0.16	-13.41	132,132,132,132	0
38	MG	A	5027	1/1	0.14	-40.33	162,162,162,162	0
38	MG	A	5055	1/1	0.31	-	152,152,152,152	0
38	MG	A	5045	1/1	0.12	-	197,197,197,197	0

6.5 Other polymers ⓘ

There are no such residues in this entry.