



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 03:27 AM GMT

PDB ID : 3F1G
Title : Crystal structure of a translation termination complex formed with release factor RF2. This file contains the 30S subunit, RF2, two tRNA, and mRNA molecules of the second 70S ribosome. The entire crystal structure contains two 70S ribosomes as described in remark 400.
Authors : Korostelev, A.; Asahara, H.; Lancaster, L.; Laurberg, M.; Hirschi, A.; Noller, H.F.
Deposited on : 2008-10-27
Resolution : 3.00 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>

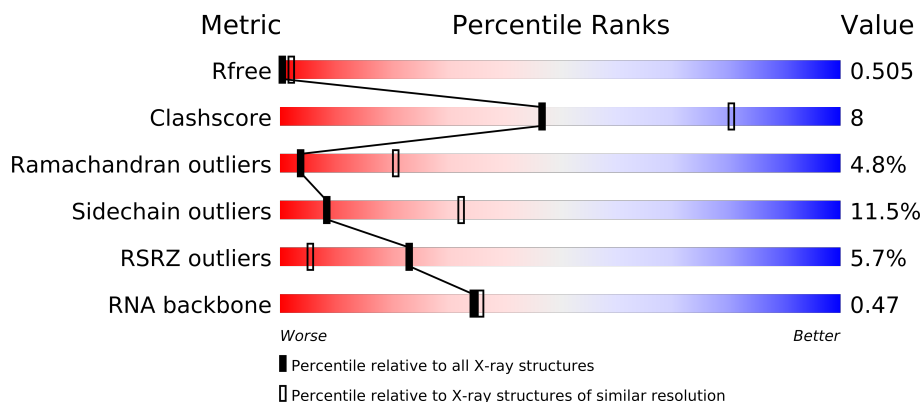
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.00 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	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)
RNA backbone	1838	1070 (3.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	1525	
2	Y	77	
2	Z	77	
3	V	27	
4	B	256	
5	C	239	
6	D	209	
7	E	162	
8	F	101	
9	G	156	
10	H	138	
11	I	128	

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Mol	Chain	Length	Quality of chain
12	J	105	
13	K	129	
14	L	134	
15	M	126	
16	N	61	
17	O	89	
18	P	88	
19	Q	105	
20	R	88	
21	S	93	
22	T	106	
23	U	27	
24	X	378	

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 58018 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a RNA chain called 16S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1504	Total	C	N	O	P	0	0	0
			32332	14391	5994	10444	1503			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	466	G	C	CONFLICT	GB 155076

- Molecule 2 is a RNA chain called P and E-site tRNA(fMet).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Z	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
2	Y	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	V	10	Total	C	N	O	P	0	0	0
			214	98	44	63	9			

- Molecule 4 is a protein called 30S ribosomal protein S2.

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

- Molecule 5 is a protein called 30S ribosomal protein S3.

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

- Molecule 6 is a protein called 30S ribosomal protein S4.

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

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 8 is a protein called 30S ribosomal protein S6.

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

- Molecule 9 is a protein called 30S ribosomal protein S7.

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

- Molecule 10 is a protein called 30S ribosomal protein S8.

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

- Molecule 11 is a protein called 30S ribosomal protein S9.

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

- Molecule 12 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

- Molecule 13 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	114	Total	C	N	O	S	0	0	0
			842	522	159	158	3			

- Molecule 14 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	L	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	2	ALA	-	INSERTION	UNP P61941
L	3	LEU	-	INSERTION	UNP P61941

- Molecule 15 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

- Molecule 16 is a protein called 30S ribosomal protein S14.

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

- Molecule 17 is a protein called 30S ribosomal protein S15.

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

- Molecule 18 is a protein called 30S ribosomal protein S16.

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

- Molecule 19 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			

- Molecule 20 is a protein called 30S ribosomal protein S18.

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

- Molecule 21 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	78	Total	C	N	O	S	0	0	0
			629	403	114	110	2			

- Molecule 22 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 23 is a protein called 30S ribosomal protein Thx.

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

- Molecule 24 is a protein called Bacterial peptide chain release factor 2 (RF-2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	362	Total	C	N	O	S	0	0	0
			2876	1794	518	556	8			

- Molecule 25 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 26 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

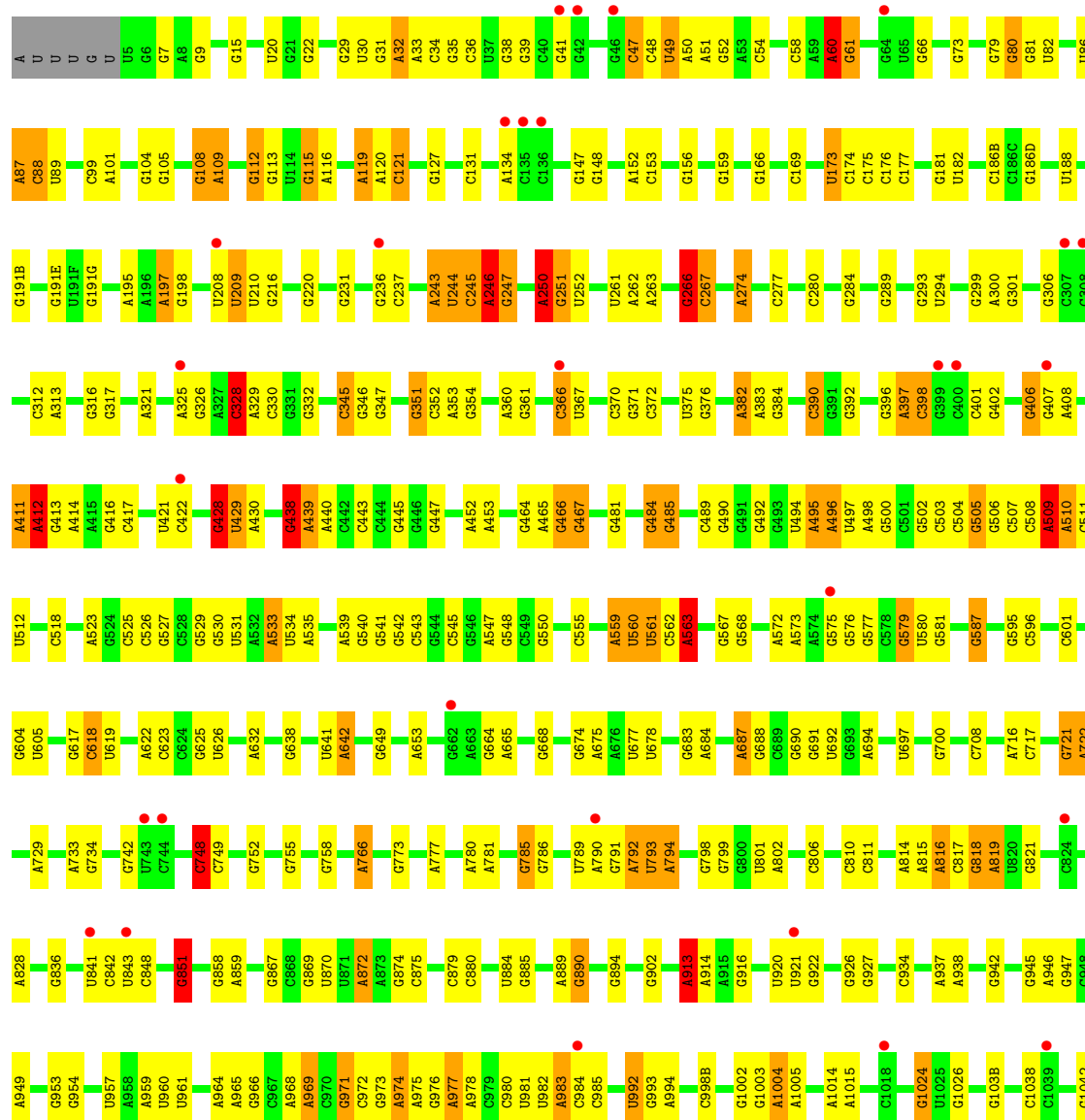
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	G	2	Total 2	Mg 2	0	0
26	Q	1	Total 1	Mg 1	0	0
26	K	3	Total 3	Mg 3	0	0
26	H	2	Total 2	Mg 2	0	0
26	B	2	Total 2	Mg 2	0	0
26	C	1	Total 1	Mg 1	0	0
26	Z	15	Total 15	Mg 15	0	0
26	A	222	Total 222	Mg 222	0	0
26	T	1	Total 1	Mg 1	0	0
26	O	1	Total 1	Mg 1	0	0
26	Y	13	Total 13	Mg 13	0	0
26	L	1	Total 1	Mg 1	0	0
26	S	1	Total 1	Mg 1	0	0
26	F	5	Total 5	Mg 5	0	0

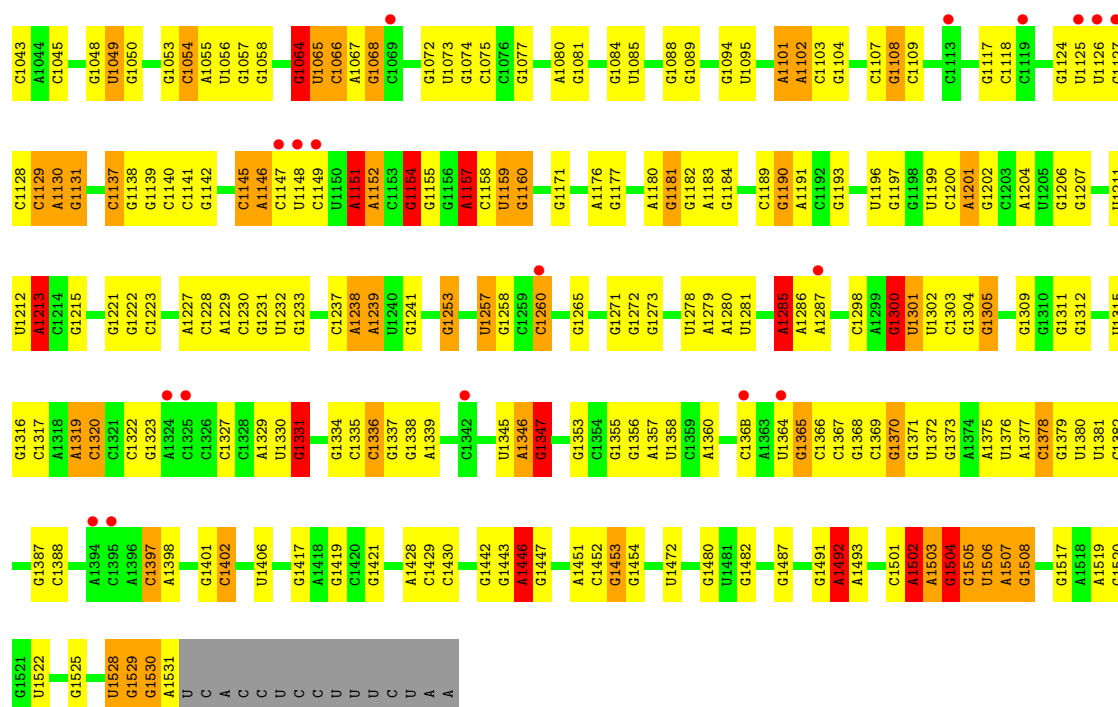
3 Residue-property plots

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

• Molecule 1: 16S RRNA

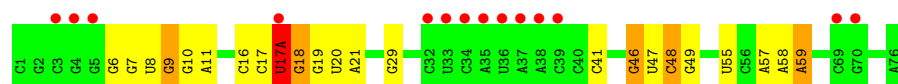
Chain A: 





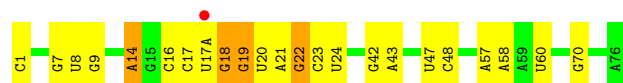
• Molecule 2: P and E-site tRNA(fMet)

Chain Z:



• Molecule 2: P and E-site tRNA(fMet)

Chain Y:



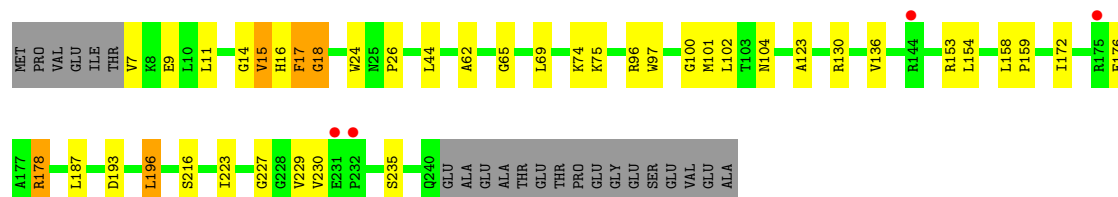
• Molecule 3: mRNA

Chain V:

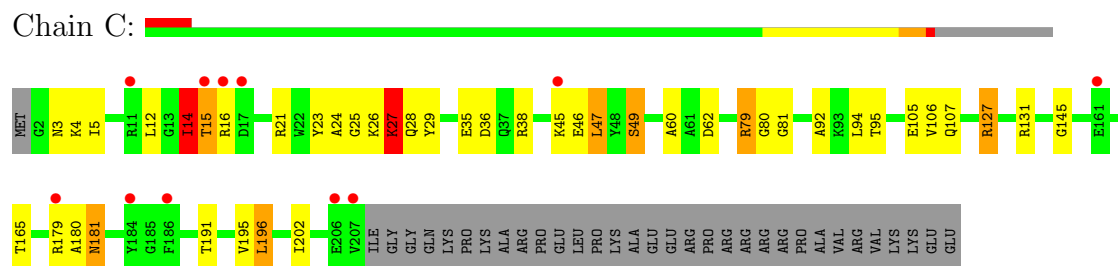


• Molecule 4: 30S ribosomal protein S2

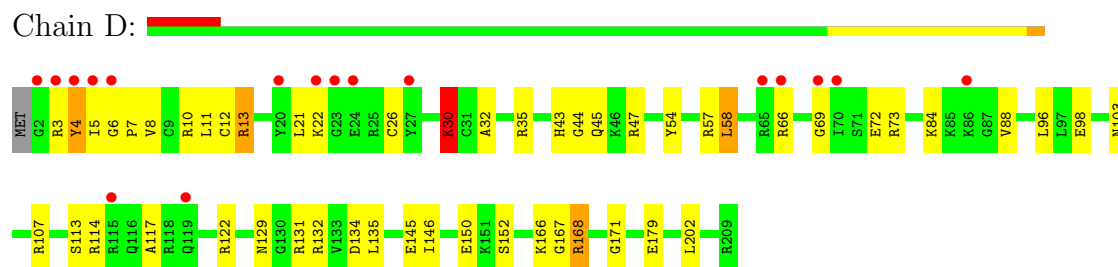
Chain B:



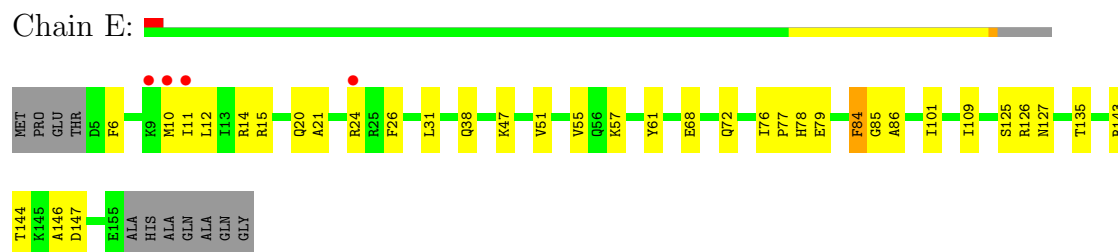
- Molecule 5: 30S ribosomal protein S3



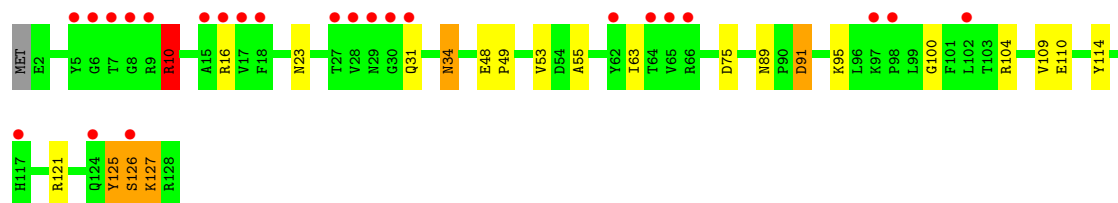
- Molecule 6: 30S ribosomal protein S4



- Molecule 7: 30S ribosomal protein S5

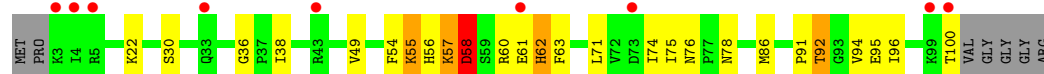


Chain I:



- Molecule 12: 30S ribosomal protein S10

Chain J:



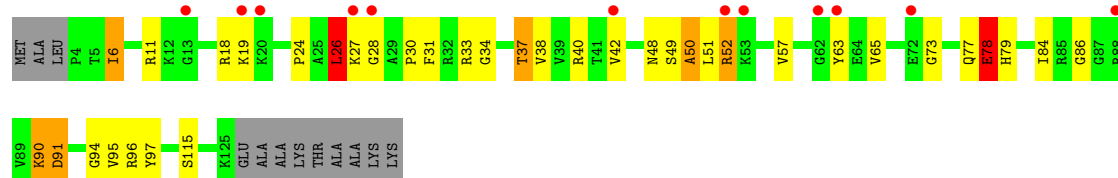
- Molecule 13: 30S ribosomal protein S11

Chain K:



- Molecule 14: 30S ribosomal protein S12

Chain L:



- Molecule 15: 30S ribosomal protein S13

Chain M:



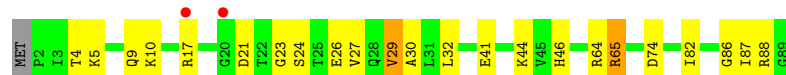
- Molecule 16: 30S ribosomal protein S14

Chain N:



- Molecule 17: 30S ribosomal protein S15

Chain O:



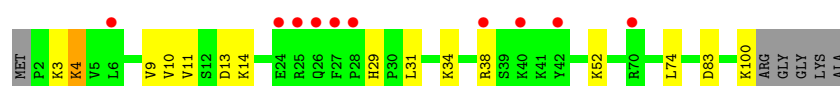
- Molecule 18: 30S ribosomal protein S16

Chain P:



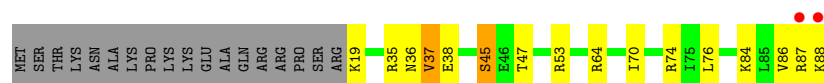
- Molecule 19: 30S ribosomal protein S17

Chain Q:



- Molecule 20: 30S ribosomal protein S18

Chain R:



- Molecule 21: 30S ribosomal protein S19

Chain S:



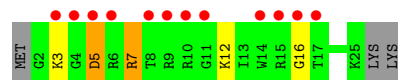
- Molecule 22: 30S ribosomal protein S20

Chain T:



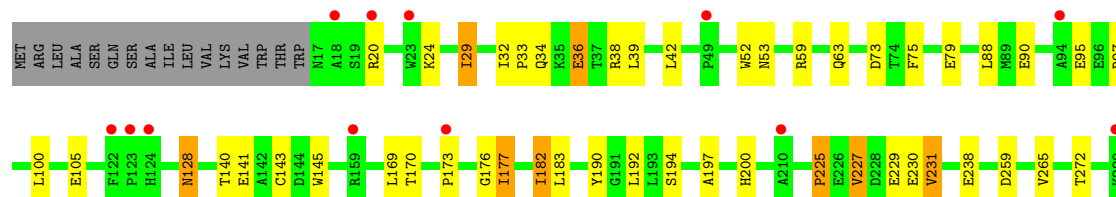
- Molecule 23: 30S ribosomal protein Thx

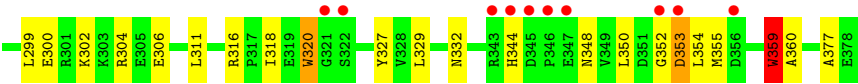
Chain U:



- Molecule 24: Bacterial peptide chain release factor 2 (RF-2)

Chain X:





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.24Å 456.78Å 618.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.95 – 3.00 50.99 – 2.99	Depositor EDS
% Data completeness (in resolution range)	97.3 (49.95-3.00) 97.2 (50.99-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.280 , 0.316 0.498 , 0.505	Depositor DCC
R_{free} test set	10573 reflections (0.92%)	DCC
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.11 , 15.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 1158087 reflections	Xtriage
F_o, F_c correlation	0.57	EDS
Total number of atoms	58018	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.24% 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	A	0.55	1/36194 (0.0%)	1.10	110/56493 (0.2%)
2	Y	0.54	0/1832	1.03	2/2855 (0.1%)
2	Z	0.45	0/1832	0.94	1/2855 (0.0%)
3	V	0.64	0/241	1.30	1/374 (0.3%)
4	B	0.27	0/1935	0.47	0/2609
5	C	0.28	0/1636	0.46	0/2205
6	D	0.30	0/1733	0.49	0/2318
7	E	0.29	0/1171	0.50	0/1576
8	F	0.30	0/856	0.49	0/1154
9	G	0.28	0/1276	0.46	0/1709
10	H	0.29	0/1136	0.50	0/1527
11	I	0.26	0/1029	0.45	0/1378
12	J	0.27	0/807	0.48	0/1085
13	K	0.38	0/856	0.53	0/1157
14	L	0.33	0/972	0.57	0/1301
15	M	0.25	0/943	0.49	0/1265
16	N	0.30	0/501	0.47	0/664
17	O	0.32	0/745	0.48	0/992
18	P	0.27	0/716	0.47	0/963
19	Q	0.30	0/836	0.48	0/1117
20	R	0.32	0/579	0.50	0/768
21	S	0.25	0/642	0.46	0/865
22	T	0.27	0/764	0.47	0/1006
23	U	0.25	0/212	0.45	0/277
24	X	0.27	0/2926	0.48	0/3953
All	All	0.47	1/62370 (0.0%)	0.94	114/92466 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	G	C3'-O3'	5.06	1.49	1.42

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1492	A	C3'-C2'-C1'	-9.32	94.04	101.50
1	A	1151	A	C1'-O4'-C4'	-9.25	102.50	109.90
1	A	115	G	P-O3'-C3'	8.75	130.21	119.70
1	A	328	C	C1'-O4'-C4'	-8.70	102.94	109.90
1	A	173	U	P-O3'-C3'	8.63	130.06	119.70
1	A	328	C	P-O3'-C3'	8.28	129.64	119.70
1	A	913	A	P-O3'-C3'	8.27	129.62	119.70
1	A	1064	G	P-O3'-C3'	8.19	129.53	119.70
1	A	412	A	C1'-O4'-C4'	-7.96	103.53	109.90
1	A	1049	U	P-O3'-C3'	7.85	129.12	119.70
1	A	1502	A	P-O3'-C3'	7.84	129.11	119.70
1	A	509	A	C3'-C2'-C1'	-7.83	95.24	101.50
1	A	1504	G	P-O3'-C3'	7.59	128.81	119.70
1	A	1528	U	P-O3'-C3'	7.57	128.79	119.70
1	A	971	G	C1'-O4'-C4'	-7.56	103.86	109.90
3	V	21	A	P-O3'-C3'	7.49	128.69	119.70
1	A	366	C	P-O3'-C3'	7.40	128.58	119.70
1	A	793	U	C1'-O4'-C4'	-7.35	104.02	109.90
1	A	890	G	C3'-C2'-C1'	-7.33	95.64	101.50
1	A	60	A	P-O3'-C3'	7.24	128.38	119.70
1	A	108	G	C4'-C3'-C2'	-7.19	95.41	102.60
1	A	250	A	P-O3'-C3'	7.11	128.23	119.70
1	A	484	G	P-O3'-C3'	7.10	128.22	119.70
1	A	748	C	P-O3'-C3'	6.95	128.04	119.70
1	A	559	A	C1'-O4'-C4'	-6.88	104.39	109.90
1	A	428	G	P-O3'-C3'	6.86	127.93	119.70
1	A	879	C	C4'-C3'-C2'	-6.78	95.82	102.60
1	A	1257	U	C1'-O4'-C4'	-6.76	104.49	109.90
1	A	1522	U	C4'-C3'-C2'	-6.73	95.87	102.60
1	A	466	G	C3'-C2'-C1'	-6.69	96.15	101.50
2	Y	70	G	C3'-C2'-C1'	-6.67	96.16	101.50
1	A	351	G	P-O3'-C3'	6.67	127.70	119.70
1	A	799	G	C4'-C3'-C2'	-6.67	95.93	102.60
1	A	1285	A	P-O3'-C3'	6.63	127.66	119.70
1	A	872	A	C1'-O4'-C4'	-6.62	104.60	109.90
1	A	1101	A	P-O3'-C3'	6.61	127.63	119.70
1	A	1502	A	C1'-O4'-C4'	-6.60	104.62	109.90
1	A	438	G	P-O3'-C3'	6.52	127.52	119.70
1	A	274	A	O4'-C1'-N9	6.49	113.39	108.20
1	A	266	G	P-O3'-C3'	6.44	127.43	119.70
1	A	1129	C	P-O3'-C3'	6.43	127.42	119.70
1	A	872	A	O4'-C1'-N9	6.43	113.34	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	A	P-O3'-C3'	6.34	127.31	119.70
1	A	1300	G	P-O3'-C3'	6.32	127.29	119.70
1	A	793	U	O4'-C1'-N1	6.27	113.21	108.20
1	A	618	C	C1'-O4'-C4'	-6.25	104.90	109.90
1	A	108	G	O4'-C1'-N9	6.18	113.14	108.20
1	A	786	G	C4'-C3'-C2'	-6.17	96.43	102.60
1	A	1472	U	C4'-C3'-C2'	-6.12	96.48	102.60
1	A	1159	U	C1'-O4'-C4'	-6.07	105.04	109.90
1	A	773	G	C4'-C3'-C2'	-6.03	96.57	102.60
1	A	851	G	C4'-C3'-C2'	-6.01	96.59	102.60
1	A	1331	G	C3'-C2'-C1'	5.98	106.28	101.50
1	A	1257	U	O4'-C1'-N1	5.95	112.96	108.20
1	A	1446	A	C3'-C2'-C1'	-5.95	96.74	101.50
1	A	729	A	C4'-C3'-C2'	-5.94	96.66	102.60
1	A	115	G	O4'-C1'-N9	-5.91	103.47	108.20
1	A	1002	G	C3'-C2'-C1'	-5.88	96.80	101.50
1	A	1154	G	C4'-C3'-C2'	-5.83	96.77	102.60
1	A	103(B)	G	C3'-C2'-C1'	-5.81	96.85	101.50
1	A	1201	A	P-O3'-C3'	5.81	126.67	119.70
1	A	412	A	O4'-C1'-N9	5.76	112.81	108.20
1	A	1145	C	P-O3'-C3'	5.69	126.53	119.70
1	A	721	G	P-O3'-C3'	5.65	126.48	119.70
1	A	243	A	P-O3'-C3'	5.64	126.47	119.70
1	A	209	U	C3'-C2'-C1'	5.64	106.01	101.50
1	A	1157	A	P-O3'-C3'	5.63	126.46	119.70
1	A	121	C	N1-C2-O2	5.63	122.28	118.90
1	A	687	A	P-O3'-C3'	5.61	126.44	119.70
2	Y	1	C	C3'-C2'-C1'	-5.59	97.03	101.50
1	A	722	A	C3'-C2'-C1'	5.53	105.92	101.50
1	A	649	G	O4'-C1'-N9	5.53	112.62	108.20
1	A	971	G	O4'-C1'-N9	5.52	112.62	108.20
1	A	87	A	P-O3'-C3'	5.50	126.30	119.70
1	A	371	G	C4'-C3'-C2'	-5.48	97.12	102.60
1	A	495	A	C3'-C2'-C1'	-5.45	97.14	101.50
1	A	880	C	C6-N1-C2	5.45	122.48	120.30
1	A	274	A	C1'-O4'-C4'	-5.44	105.55	109.90
1	A	159	G	C4'-C3'-C2'	-5.44	97.16	102.60
1	A	108	G	C1'-O4'-C4'	-5.39	105.58	109.90
1	A	1137	C	C3'-C2'-C1'	5.39	105.81	101.50
1	A	119	A	P-O3'-C3'	5.38	126.15	119.70
1	A	7	G	C1'-O4'-C4'	-5.37	105.61	109.90
1	A	563	A	C1'-O4'-C4'	-5.35	105.62	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	G	C4-C5-N7	-5.33	108.67	110.80
1	A	1530	G	O4'-C1'-N9	5.33	112.46	108.20
1	A	299	G	C5-C6-N1	-5.32	108.84	111.50
1	A	721	G	C3'-C2'-C1'	5.32	105.75	101.50
1	A	587	G	C3'-C2'-C1'	5.31	105.75	101.50
1	A	1347	G	C1'-O4'-C4'	-5.31	105.65	109.90
1	A	700	G	C4'-C3'-C2'	-5.29	97.31	102.60
1	A	277	C	O4'-C1'-N1	5.26	112.41	108.20
1	A	1213	A	C3'-C2'-C1'	5.25	105.70	101.50
1	A	345	C	C4'-C3'-C2'	-5.23	97.37	102.60
1	A	1211	U	C1'-O4'-C4'	-5.21	105.73	109.90
1	A	785	G	C4'-C3'-C2'	-5.20	97.40	102.60
1	A	191(B)	G	C4'-C3'-C2'	-5.19	97.41	102.60
1	A	533	A	P-O3'-C3'	5.18	125.92	119.70
1	A	789	U	C4'-C3'-C2'	-5.16	97.44	102.60
1	A	112	G	C4'-C3'-C2'	-5.15	97.45	102.60
1	A	280	C	C3'-C2'-C1'	-5.14	97.39	101.50
2	Z	17(A)	U	P-O3'-C3'	5.13	125.85	119.70
1	A	1346	A	C3'-C2'-C1'	-5.12	97.40	101.50
1	A	543	C	C4'-C3'-C2'	-5.12	97.48	102.60
1	A	806	C	C4'-C3'-C2'	-5.12	97.48	102.60
1	A	810	C	C4'-C3'-C2'	-5.12	97.48	102.60
1	A	1492	A	C4'-C3'-C2'	-5.08	97.52	102.60
1	A	1189	C	C1'-O4'-C4'	-5.05	105.86	109.90
1	A	1054	C	O4'-C1'-N1	5.04	112.24	108.20
1	A	1048	G	C4'-C3'-C2'	-5.04	97.56	102.60
1	A	697	U	C4'-C3'-C2'	-5.03	97.57	102.60
1	A	992	U	C3'-C2'-C1'	5.03	105.52	101.50
1	A	1189	C	C4'-C3'-C2'	-5.02	97.58	102.60
1	A	1406	U	C4'-C3'-C2'	-5.00	97.60	102.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32332	0	0	264	0
2	Y	1640	0	0	6	0
2	Z	1640	0	0	7	0
3	V	214	0	0	2	0
4	B	1900	0	0	13	0
5	C	1612	0	0	10	0
6	D	1703	0	0	17	0
7	E	1155	0	0	9	0
8	F	843	0	0	2	0
9	G	1257	0	0	11	0
10	H	1116	0	0	8	0
11	I	1011	0	0	6	0
12	J	794	0	0	9	0
13	K	842	0	0	6	0
14	L	956	0	0	19	0
15	M	933	0	0	9	0
16	N	492	0	0	7	0
17	O	734	0	0	8	0
18	P	700	0	0	5	0
19	Q	823	0	0	4	0
20	R	574	0	0	2	0
21	S	629	0	0	5	0
22	T	762	0	0	8	0
23	U	208	0	0	2	0
24	X	2876	0	0	17	0
25	D	1	0	0	0	0
25	N	1	0	0	0	0
26	A	222	0	0	0	0
26	B	2	0	0	0	0
26	C	1	0	0	0	0
26	F	5	0	0	0	0
26	G	2	0	0	0	0
26	H	2	0	0	0	0
26	K	3	0	0	0	0
26	L	1	0	0	0	0
26	O	1	0	0	0	0
26	Q	1	0	0	0	0
26	S	1	0	0	0	0
26	T	1	0	0	0	0
26	Y	13	0	0	0	0
26	Z	15	0	0	0	0
All	All	58018	0	0	425	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 8.

All (425) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1492:A:C6	24:X:320:TRP:CH2	2.71	0.78
1:A:1492:A:C5	24:X:320:TRP:CH2	2.76	0.74
10:H:102:ARG:N	10:H:102:ARG:NE	2.38	0.71
8:F:87:ARG:NH1	8:F:87:ARG:CG	2.56	0.68
16:N:45:ARG:O	16:N:49:HIS:CD2	2.48	0.67
1:A:1442:G:N7	1:A:1446:A:C2	2.64	0.66
5:C:14:ILE:CG1	5:C:15:THR:N	2.63	0.62
22:T:69:GLY:O	22:T:73:HIS:CD2	2.52	0.62
1:A:1378:C:C5	1:A:1379:G:C8	2.88	0.61
1:A:1077:G:N2	1:A:1080:A:OP2	2.33	0.61
1:A:328:C:O2	1:A:328:C:C2'	2.49	0.61
1:A:1004:A:C8	1:A:1026:G:C6	2.89	0.61
1:A:1381:U:C5	1:A:1382:C:C4	2.88	0.60
1:A:618:C:N3	1:A:622:A:N6	2.50	0.60
7:E:84:PHE:O	7:E:86:ALA:N	2.35	0.60
1:A:965:A:C2	1:A:969:A:C2	2.91	0.59
6:D:103:ASN:OD1	6:D:114:ARG:NH2	2.35	0.59
1:A:785:G:N2	1:A:798:G:C4	2.71	0.59
16:N:24:CYS:CB	16:N:27:CYS:SG	2.91	0.58
1:A:974:A:OP1	1:A:974:A:C8	2.57	0.58
6:D:4:TYR:O	6:D:6:GLY:N	2.37	0.58
4:B:15:VAL:C	4:B:16:HIS:CG	2.77	0.58
1:A:81:G:OP2	1:A:82:U:C5	2.56	0.58
1:A:1231:G:C4	1:A:1232:U:C5	2.92	0.58
10:H:50:ARG:NH1	10:H:50:ARG:CG	2.67	0.58
6:D:11:LEU:C	6:D:13:ARG:N	2.55	0.57
7:E:57:LYS:O	7:E:61:TYR:CD2	2.58	0.57
22:T:100:ILE:O	22:T:102:GLY:N	2.38	0.57
12:J:55:LYS:O	12:J:56:HIS:CG	2.57	0.56
21:S:79:THR:O	21:S:80:TYR:CB	2.53	0.56
1:A:1151:A:O2'	1:A:1152:A:C8	2.58	0.56
9:G:57:GLU:N	9:G:57:GLU:CD	2.59	0.56
6:D:43:HIS:O	6:D:45:GLN:N	2.38	0.56
1:A:1127:G:N2	1:A:1146:A:N6	2.52	0.56
20:R:35:ARG:O	20:R:37:VAL:N	2.38	0.56
1:A:1309:G:C6	1:A:1329:A:C2	2.94	0.55
11:I:125:TYR:CD2	11:I:126:SER:N	2.74	0.55
1:A:1265:G:C2	1:A:1271:G:C2	2.95	0.55
1:A:370:C:C2	1:A:392:G:C2	2.95	0.55
1:A:1239:A:C4	1:A:1298:C:N4	2.75	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1492:A:N6	24:X:320:TRP:CH2	2.75	0.55
1:A:1221:G:OP1	1:A:1320:C:N4	2.40	0.55
1:A:560:U:O2'	1:A:561:U:OP2	2.25	0.55
1:A:523:A:N6	14:L:52:ARG:NH1	2.54	0.54
1:A:1507:A:C2	1:A:1508:G:C4	2.95	0.54
1:A:244:U:C6	1:A:894:G:N2	2.75	0.54
1:A:1501:C:N4	1:A:1504:G:C2	2.75	0.54
1:A:186(D):G:C6	1:A:191(E):G:N1	2.75	0.54
1:A:1057:G:C4	1:A:1204:A:C2	2.95	0.54
1:A:1147:C:O2	11:I:16:ARG:NH2	2.41	0.54
1:A:530:G:N2	1:A:1492:A:N6	2.56	0.54
1:A:464:G:N2	1:A:467:G:N7	2.56	0.54
15:M:67:GLU:CG	15:M:68:GLY:N	2.71	0.54
1:A:112:G:C2	1:A:113:G:C8	2.96	0.53
1:A:250:A:C4'	1:A:251:G:O5'	2.56	0.53
6:D:30:LYS:C	6:D:32:ALA:N	2.62	0.53
17:O:74:ASP:C	17:O:74:ASP:OD2	2.47	0.53
19:Q:3:LYS:O	19:Q:4:LYS:C	2.48	0.53
1:A:1238:A:C2	1:A:1241:G:N3	2.77	0.53
1:A:973:G:OP1	12:J:57:LYS:NZ	2.42	0.52
1:A:81:G:N7	1:A:82:U:C4	2.77	0.52
22:T:71:THR:CG2	22:T:72:LEU:N	2.73	0.52
24:X:128:ASN:N	24:X:128:ASN:OD1	2.40	0.52
14:L:52:ARG:NH1	14:L:91:ASP:OD2	2.42	0.52
1:A:1502:A:O2'	1:A:1503:A:O5'	2.28	0.52
1:A:668:G:O2'	17:O:46:HIS:CD2	2.63	0.52
1:A:1206:G:C6	1:A:1207:G:C5	2.98	0.52
1:A:1365:G:C5	1:A:1366:C:C5	2.98	0.52
1:A:1417:G:C6	1:A:1482:G:C6	2.98	0.52
1:A:1160:G:C6	1:A:1181:G:O6	2.63	0.52
1:A:60:A:C4'	1:A:61:G:O5'	2.57	0.52
1:A:792:A:N3	1:A:794:A:C5	2.78	0.51
6:D:167:GLY:O	6:D:168:ARG:C	2.48	0.51
1:A:147:G:C2	1:A:176:C:N3	2.77	0.51
1:A:965:A:C2	1:A:969:A:N1	2.79	0.51
1:A:505:G:C6	1:A:535:A:C2	2.99	0.51
14:L:49:SER:O	14:L:50:ALA:CB	2.58	0.51
1:A:1397:C:OP2	3:V:23:A:N6	2.44	0.51
1:A:1300:G:O2'	1:A:1301:U:P	2.69	0.51
1:A:1442:G:C8	1:A:1442:G:C3'	2.94	0.51
1:A:236:G:C6	1:A:237:C:C4	2.99	0.51
1:A:1084:G:C5	1:A:1085:U:C4	2.99	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
24:X:145:TRP:CZ3	24:X:200:HIS:O	2.64	0.51
1:A:691:G:O6	13:K:55:LYS:NZ	2.44	0.51
1:A:913:A:OP2	14:L:90:LYS:NZ	2.43	0.51
1:A:949:A:C2	1:A:1233:G:N3	2.79	0.51
1:A:81:G:N7	1:A:82:U:N3	2.59	0.51
14:L:33:ARG:CG	14:L:34:GLY:N	2.73	0.50
1:A:506:G:C6	1:A:507:C:C4	2.99	0.50
1:A:1305:G:N2	1:A:1331:G:C2'	2.74	0.50
24:X:190:TYR:CE1	24:X:225:PRO:CD	2.94	0.50
1:A:38:G:C2	1:A:397:A:C2	2.98	0.50
1:A:112:G:C2	1:A:330:C:N4	2.79	0.50
1:A:792:A:C4	1:A:794:A:C6	3.00	0.50
5:C:79:ARG:N	5:C:79:ARG:CD	2.74	0.50
4:B:17:PHE:N	4:B:17:PHE:CD2	2.78	0.50
4:B:178:ARG:NH2	10:H:68:ARG:NH2	2.60	0.50
1:A:836:G:C6	1:A:851:G:C6	2.99	0.50
1:A:262:A:C6	1:A:263:A:C6	3.00	0.50
1:A:503:C:OP2	14:L:115:SER:OG	2.30	0.50
24:X:29:ILE:O	24:X:33:PRO:CD	2.59	0.50
12:J:94:VAL:CG1	12:J:95:GLU:N	2.74	0.49
14:L:77:GLN:O	14:L:79:HIS:N	2.45	0.49
1:A:443:C:C2	1:A:492:G:C2	3.00	0.49
13:K:15:ALA:O	13:K:78:GLN:N	2.45	0.49
1:A:581:G:O6	1:A:758:G:C8	2.66	0.49
1:A:617:G:C2	1:A:618:C:C5	3.00	0.49
2:Y:23:C:C2	2:Y:24:U:C5	3.00	0.49
1:A:642:A:N3	10:H:113:SER:OG	2.45	0.49
1:A:411:A:C3'	1:A:411:A:C8	2.96	0.49
17:O:87:ILE:CG2	17:O:88:ARG:N	2.75	0.49
1:A:625:G:C6	1:A:626:U:C4	3.01	0.49
2:Z:9:G:C5	2:Z:46:G:N1	2.81	0.49
1:A:1260:C:C6	1:A:1260:C:C3'	2.94	0.49
1:A:748:C:C6	1:A:748:C:OP2	2.66	0.49
1:A:47:C:O2	1:A:49:U:C5	2.65	0.49
1:A:375:U:C4	1:A:376:G:N7	2.80	0.49
4:B:100:GLY:O	4:B:101:MET:C	2.51	0.49
1:A:1492:A:C5	24:X:320:TRP:CZ2	3.01	0.48
1:A:766:A:C5	1:A:814:A:C2	3.01	0.48
19:Q:29:HIS:ND1	19:Q:31:LEU:N	2.61	0.48
7:E:20:GLN:O	7:E:21:ALA:C	2.51	0.48
22:T:100:ILE:CG2	22:T:101:GLY:N	2.76	0.48
1:A:1305:G:O2'	1:A:1331:G:N2	2.47	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
19:Q:13:ASP:OD1	19:Q:13:ASP:N	2.47	0.48
1:A:407:G:C6	1:A:408:A:N6	2.81	0.48
1:A:325:A:C6	1:A:326:G:C2	3.01	0.48
10:H:91:ARG:CG	10:H:91:ARG:NH1	2.75	0.48
14:L:24:PRO:C	14:L:26:LEU:N	2.67	0.48
5:C:195:VAL:CG1	5:C:196:LEU:N	2.76	0.48
1:A:563:A:C8	1:A:567:G:O4'	2.67	0.48
1:A:1065:U:OP2	1:A:1190:G:N2	2.47	0.48
21:S:80:TYR:O	21:S:80:TYR:CG	2.67	0.48
24:X:190:TYR:O	24:X:194:SER:N	2.46	0.48
1:A:1451:A:C8	1:A:1453:G:O6	2.67	0.48
1:A:1074:G:C2	1:A:1102:A:C2	3.02	0.47
1:A:1003:G:N2	1:A:1038:C:C2	2.82	0.47
1:A:382:A:C2	1:A:383:A:C4	3.02	0.47
12:J:38:ILE:N	12:J:71:LEU:O	2.47	0.47
1:A:86:U:C2'	1:A:87:A:C8	2.98	0.47
1:A:109:A:C6	1:A:326:G:C6	3.02	0.47
1:A:1253:G:N1	1:A:1285:A:N6	2.63	0.47
24:X:302:LYS:O	24:X:306:GLU:N	2.47	0.47
1:A:396:G:O2'	1:A:398:C:OP1	2.32	0.47
9:G:135:VAL:O	9:G:139:GLU:N	2.48	0.47
24:X:176:GLY:O	24:X:177:ILE:CB	2.62	0.47
1:A:1357:A:C5	1:A:1358:U:C4	3.03	0.47
1:A:412:A:N3	6:D:35:ARG:NH2	2.61	0.47
1:A:1316:G:N1	1:A:1319:A:OP2	2.47	0.47
1:A:1074:G:C2	1:A:1075:C:C2	3.02	0.47
1:A:1231:G:C5	1:A:1232:U:C5	3.03	0.47
14:L:78:GLU:O	14:L:79:HIS:CG	2.67	0.47
1:A:529:G:O6	14:L:48:ASN:ND2	2.47	0.47
1:A:922:G:O2'	1:A:1398:A:N1	2.48	0.47
1:A:1311:G:N2	1:A:1327:C:C2	2.82	0.47
24:X:182:ILE:CG1	24:X:183:LEU:N	2.77	0.47
9:G:58:PRO:O	9:G:62:PHE:N	2.48	0.47
2:Z:55:U:C2	2:Z:57:A:OP2	2.68	0.47
14:L:26:LEU:C	14:L:28:GLY:N	2.68	0.47
11:I:10:ARG:NH1	11:I:75:ASP:OD2	2.48	0.47
2:Z:11:A:C8	2:Z:11:A:O5'	2.67	0.47
1:A:1379:G:C6	1:A:1380:U:C4	3.03	0.46
1:A:1157:A:C6	1:A:1180:A:C6	3.03	0.46
16:N:21:TYR:OH	16:N:23:ARG:NH2	2.48	0.46
1:A:1338:G:C6	1:A:1339:A:C6	3.02	0.46
1:A:1206:G:O6	1:A:1207:G:C6	2.69	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1154:G:C2	1:A:1155:G:C8	3.04	0.46
1:A:957:U:O2	1:A:959:A:C8	2.69	0.46
1:A:261:U:C5	22:T:79:ARG:NH1	2.83	0.46
2:Z:8:U:O2	2:Z:21:A:C2	2.68	0.46
12:J:62:HIS:O	12:J:62:HIS:CD2	2.68	0.46
14:L:78:GLU:O	14:L:79:HIS:CD2	2.68	0.46
9:G:105:VAL:O	9:G:106:GLN:C	2.54	0.46
11:I:114:TYR:CE1	12:J:60:ARG:N	2.84	0.46
16:N:40:CYS:SG	16:N:43:CYS:SG	3.14	0.46
14:L:96:ARG:C	14:L:97:TYR:CD1	2.89	0.46
2:Z:29:G:N2	2:Z:41:C:N3	2.63	0.46
4:B:11:LEU:O	4:B:16:HIS:CE1	2.68	0.46
6:D:11:LEU:O	6:D:12:CYS:C	2.52	0.46
14:L:30:PRO:O	14:L:31:PHE:CD2	2.69	0.46
1:A:1355:G:C6	1:A:1368:G:C6	3.04	0.46
1:A:438:G:O2'	1:A:494:U:O4	2.34	0.46
14:L:26:LEU:O	14:L:28:GLY:N	2.49	0.45
1:A:542:G:OP1	6:D:10:ARG:NH2	2.49	0.45
16:N:27:CYS:SG	16:N:40:CYS:SG	3.14	0.45
1:A:937:A:C2	1:A:1379:G:C6	3.05	0.45
1:A:1356:G:C2'	1:A:1357:A:C8	2.99	0.45
1:A:1176:A:C6	1:A:1177:G:C6	3.04	0.45
1:A:575:G:C6	1:A:821:G:N7	2.84	0.45
1:A:1375:A:C5	1:A:1376:U:C4	3.04	0.45
22:T:9:ASN:O	22:T:10:LEU:C	2.55	0.45
1:A:579:G:C4	1:A:580:U:C5	3.05	0.45
18:P:80:PHE:CD1	18:P:80:PHE:N	2.84	0.45
1:A:1057:G:C5	1:A:1204:A:C2	3.04	0.45
1:A:29:G:N2	1:A:555:C:C2	2.84	0.45
2:Z:48:C:N3	2:Z:59:A:C8	2.84	0.45
1:A:875:C:O2'	10:H:14:ARG:NH1	2.49	0.45
1:A:1505:G:C5'	1:A:1505:G:C8	3.00	0.45
1:A:1336:C:O4'	1:A:1337:G:C2	2.69	0.45
1:A:134:A:N6	18:P:25:ARG:NH1	2.64	0.45
1:A:148:G:C2	1:A:175:C:N3	2.84	0.45
1:A:35:G:C2	1:A:550:G:C2	3.04	0.45
9:G:40:ALA:O	9:G:44:TYR:CD1	2.70	0.45
1:A:312:C:N4	1:A:313:A:N6	2.64	0.45
1:A:1004:A:N7	1:A:1026:G:C5	2.84	0.45
1:A:974:A:OP2	16:N:41:ARG:NH1	2.50	0.45
4:B:62:ALA:O	4:B:65:GLY:N	2.49	0.45
1:A:1347:G:N2	1:A:1373:G:C2'	2.80	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:100:GLY:N	4:B:176:GLU:OE2	2.48	0.45
6:D:150:GLU:C	6:D:152:SER:N	2.70	0.45
1:A:692:U:O2'	1:A:694:A:N7	2.49	0.45
1:A:266:G:O2'	1:A:267:C:OP2	2.34	0.45
1:A:1501:C:N3	1:A:1504:G:C6	2.85	0.45
1:A:506:G:C5	1:A:507:C:C5	3.05	0.45
1:A:683:G:C2	1:A:708:C:N3	2.85	0.45
1:A:622:A:C8	1:A:623:C:C6	3.05	0.45
1:A:1387:G:C6	1:A:1388:C:N4	2.85	0.45
5:C:23:TYR:CD2	5:C:24:ALA:N	2.85	0.45
15:M:106:ASN:N	15:M:106:ASN:OD1	2.49	0.45
1:A:1064:G:O4'	1:A:1066:C:C6	2.70	0.44
1:A:964:A:OP1	1:A:1199:U:OP1	2.36	0.44
15:M:103:THR:C	15:M:105:THR:N	2.70	0.44
1:A:983:A:C3'	1:A:983:A:N3	2.80	0.44
1:A:1421:G:C2	1:A:1480:G:C2	3.05	0.44
1:A:1330:U:O3'	15:M:23:TYR:CE2	2.70	0.44
1:A:1130:A:C2	1:A:1146:A:C4	3.06	0.44
1:A:1505:G:C5'	1:A:1506:U:OP1	2.66	0.44
21:S:33:THR:OG1	21:S:34:TRP:N	2.50	0.44
23:U:5:ASP:O	23:U:7:ARG:N	2.50	0.44
5:C:25:GLY:O	5:C:27:LYS:N	2.50	0.44
7:E:78:HIS:CE1	7:E:143:ARG:N	2.86	0.44
1:A:15:G:O4'	7:E:24:ARG:NH2	2.49	0.44
1:A:619:U:N3	6:D:134:ASP:OD2	2.51	0.44
1:A:177:C:OP1	22:T:65:LYS:NZ	2.51	0.44
6:D:54:TYR:O	6:D:58:LEU:N	2.50	0.44
1:A:1128:C:O2'	1:A:1130:A:N7	2.51	0.44
1:A:985:C:C2	1:A:1221:G:C2	3.05	0.44
1:A:49:U:C2	1:A:361:G:N2	2.86	0.44
1:A:1068:G:N2	1:A:1191:A:N3	2.66	0.44
1:A:1074:G:C4	1:A:1102:A:C2	3.06	0.44
5:C:46:GLU:O	5:C:47:LEU:CB	2.65	0.44
1:A:1370:G:C2	1:A:1371:G:C8	3.06	0.44
4:B:24:TRP:CZ3	4:B:26:PRO:CA	3.00	0.44
10:H:104:ARG:NH1	10:H:138:TRP:CZ3	2.85	0.44
9:G:154:TYR:O	9:G:156:TRP:CD1	2.70	0.44
1:A:81:G:C5	1:A:82:U:C2	3.06	0.44
1:A:1074:G:N3	1:A:1102:A:C2	2.86	0.44
1:A:38:G:N1	1:A:397:A:C2	2.86	0.44
22:T:15:ARG:O	22:T:19:SER:N	2.51	0.44
1:A:1309:G:C2	1:A:1329:A:N3	2.86	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:D:30:LYS:O	6:D:30:LYS:CG	2.65	0.44
1:A:949:A:N1	1:A:1233:G:C4	2.85	0.44
16:N:27:CYS:SG	16:N:29:ARG:CB	3.06	0.44
1:A:1088:G:C6	1:A:1089:G:N7	2.85	0.44
1:A:1503:A:O2'	1:A:1504:G:O5'	2.35	0.44
1:A:502:G:C6	1:A:503:C:C4	3.06	0.44
1:A:1042:G:C2	1:A:1043:C:C2	3.06	0.44
13:K:66:LEU:O	13:K:67:ASP:C	2.57	0.44
1:A:664:G:N2	1:A:742:G:C2	2.86	0.44
1:A:1057:G:C6	1:A:1058:G:C4	3.06	0.43
1:A:1072:G:C5	1:A:1073:U:C4	3.05	0.43
1:A:439:A:C4	1:A:496:A:C2	3.05	0.43
1:A:186(B):C:N4	1:A:191(G):G:N1	2.66	0.43
15:M:4:ILE:C	15:M:6:GLY:N	2.71	0.43
1:A:52:G:C6	1:A:360:A:C2	3.06	0.43
7:E:146:ALA:O	7:E:147:ASP:C	2.56	0.43
1:A:41:G:C6	1:A:402:G:C6	3.06	0.43
6:D:22:LYS:CB	6:D:26:CYS:SG	3.06	0.43
1:A:250:A:O4'	1:A:252:U:C6	2.71	0.43
1:A:601:C:C2	1:A:638:G:N2	2.86	0.43
17:O:21:ASP:OD1	17:O:24:SER:CB	2.66	0.43
1:A:1130:A:N7	1:A:1131:G:N7	2.66	0.43
14:L:30:PRO:O	14:L:31:PHE:CG	2.71	0.43
10:H:36:LEU:O	10:H:40:ALA:N	2.51	0.43
1:A:197:A:N1	1:A:220:G:O2'	2.50	0.43
2:Y:19:G:C2	2:Y:57:A:N3	2.87	0.43
4:B:178:ARG:NH1	4:B:196:LEU:O	2.51	0.43
1:A:814:A:N7	1:A:816:A:C4	2.87	0.43
8:F:38:GLU:O	8:F:39:LYS:C	2.57	0.43
12:J:75:ILE:CG1	12:J:76:ASN:N	2.82	0.43
1:A:1005:A:N6	1:A:1024:G:O2'	2.51	0.43
1:A:88:C:C2'	1:A:89:U:C6	3.01	0.43
12:J:57:LYS:O	12:J:58:ASP:CB	2.66	0.43
1:A:104:G:C6	1:A:105:G:N7	2.87	0.43
1:A:998(B):C:O2	1:A:1042:G:N2	2.51	0.43
9:G:26:PHE:CD2	9:G:62:PHE:CE1	3.07	0.43
1:A:525:C:N4	1:A:526:C:N4	2.67	0.43
1:A:416:G:C6	1:A:417:C:N3	2.86	0.43
9:G:15:ASP:OD2	9:G:16:LEU:N	2.51	0.43
1:A:540:G:C6	1:A:541:G:C5	3.07	0.43
1:A:1014:A:C2'	1:A:1015:A:C8	3.01	0.43
19:Q:83:ASP:OD1	19:Q:83:ASP:N	2.51	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1371:G:C6	1:A:1372:U:C4	3.07	0.43
1:A:781:A:C5	1:A:802:A:C2	3.07	0.43
1:A:818:G:C3'	1:A:819:A:C5'	2.97	0.43
1:A:872:A:C2	1:A:874:G:C6	3.07	0.43
1:A:946:A:C2	1:A:947:G:C5	3.06	0.43
1:A:1141:C:C2	1:A:1142:G:C8	3.06	0.43
5:C:180:ALA:O	5:C:181:ASN:O	2.36	0.43
1:A:489:C:C2	1:A:490:G:C8	3.07	0.42
1:A:35:G:C6	1:A:36:C:N4	2.87	0.42
9:G:85:TYR:CE1	9:G:154:TYR:CE1	3.07	0.42
1:A:953:G:C6	1:A:954:G:C5	3.07	0.42
6:D:98:GLU:OE1	6:D:107:ARG:NE	2.52	0.42
1:A:245:C:C2	1:A:284:G:C2	3.07	0.42
1:A:401:C:C3'	1:A:401:C:C6	3.02	0.42
1:A:790:A:C6	1:A:791:G:C6	3.07	0.42
1:A:504:C:O4'	1:A:510:A:C2	2.72	0.42
1:A:1088:G:C5	1:A:1089:G:N7	2.88	0.42
15:M:94:ARG:NH2	21:S:80:TYR:CE2	2.87	0.42
1:A:1128:C:O2'	1:A:1130:A:C5	2.72	0.42
1:A:959:A:C2	1:A:1222:G:O4'	2.72	0.42
9:G:153:HIS:CD2	9:G:154:TYR:CZ	3.07	0.42
5:C:92:ALA:C	5:C:94:LEU:N	2.73	0.42
2:Y:18:G:C4	2:Y:58:A:C2	3.07	0.42
18:P:82:GLN:NE2	18:P:82:GLN:N	2.66	0.42
1:A:428:G:C4'	1:A:429:U:O5'	2.66	0.42
1:A:690:G:C6	1:A:691:G:N1	2.87	0.42
1:A:325:A:N6	1:A:326:G:N1	2.67	0.42
1:A:920:U:C2'	1:A:921:U:C6	3.03	0.42
13:K:105:VAL:O	13:K:106:LYS:C	2.57	0.42
1:A:33:A:C2'	1:A:34:C:C6	3.02	0.42
1:A:370:C:N3	1:A:392:G:C2	2.88	0.42
1:A:1102:A:C6	1:A:1103:C:N4	2.88	0.42
1:A:198:G:C6	1:A:220:G:C2	3.08	0.42
1:A:32:A:C2	1:A:33:A:C4	3.07	0.42
11:I:48:GLU:N	11:I:49:PRO:CD	2.82	0.42
24:X:32:ILE:O	24:X:36:GLU:N	2.52	0.42
1:A:390:C:O3'	18:P:28:ARG:NH2	2.53	0.42
1:A:1379:G:C6	1:A:1380:U:O4	2.72	0.42
17:O:29:VAL:O	17:O:30:ALA:C	2.57	0.42
1:A:246:A:C4'	1:A:247:G:OP1	2.68	0.42
2:Y:14:A:C6	2:Y:22:G:C5	3.08	0.42
1:A:1453:G:N2	1:A:1454:G:C4	2.88	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1148:U:C5	1:A:1149:C:C4	3.08	0.42
23:U:12:LYS:O	23:U:16:GLY:N	2.53	0.42
1:A:293:G:C6	1:A:294:U:C4	3.07	0.42
1:A:1237:C:O4'	1:A:1334:G:N2	2.53	0.42
1:A:1300:G:O2'	1:A:1303:C:N4	2.53	0.42
1:A:266:G:C3'	1:A:266:G:C8	3.03	0.42
1:A:406:G:C4	1:A:495:A:C5	3.08	0.42
1:A:674:G:N2	1:A:717:C:O2	2.52	0.42
1:A:316:G:C2	1:A:317:G:N7	2.88	0.42
7:E:84:PHE:CD2	7:E:84:PHE:C	2.93	0.42
1:A:464:G:N2	1:A:467:G:C8	2.88	0.42
1:A:858:G:O6	1:A:869:G:C8	2.72	0.42
13:K:34:ASP:OD2	13:K:34:ASP:C	2.57	0.42
1:A:73:G:C2	1:A:99:C:O2	2.72	0.42
1:A:506:G:C5	1:A:507:C:C4	3.08	0.42
1:A:1304:G:C6	1:A:1305:G:N1	2.88	0.42
1:A:156:G:C2	1:A:166:G:C2	3.08	0.42
1:A:677:U:C4	1:A:678:U:C4	3.08	0.42
4:B:7:VAL:C	4:B:9:GLU:N	2.72	0.42
1:A:977:A:C8	1:A:1223:C:N3	2.88	0.42
1:A:147:G:N2	1:A:176:C:C2	2.88	0.41
12:J:49:VAL:O	12:J:60:ARG:CB	2.68	0.41
1:A:1073:U:O2	4:B:104:ASN:ND2	2.52	0.41
1:A:66:G:C6	1:A:104:G:C2	3.08	0.41
1:A:152:A:C8	1:A:153:C:C5	3.08	0.41
2:Z:17(A):U:O2'	2:Z:18:G:P	2.78	0.41
2:Y:42:G:C4	2:Y:43:A:C8	3.08	0.41
17:O:9:GLN:O	17:O:10:LYS:C	2.57	0.41
1:A:1401:G:C6	1:A:1402:C:C2	3.08	0.41
24:X:229:GLU:CG	24:X:230:GLU:N	2.83	0.41
1:A:80:G:C2'	1:A:81:G:C8	3.03	0.41
13:K:78:GLN:O	13:K:104:GLN:N	2.53	0.41
5:C:105:GLU:CG	5:C:106:VAL:N	2.83	0.41
1:A:937:A:C2	1:A:1379:G:O6	2.73	0.41
7:E:126:ARG:O	7:E:127:ASN:C	2.59	0.41
6:D:129:ASN:OD1	6:D:145:GLU:N	2.53	0.41
1:A:447:G:C2'	1:A:485:G:N2	2.84	0.41
1:A:1378:C:C5	1:A:1379:G:N9	2.89	0.41
1:A:82:U:O2	1:A:86:U:C5	2.73	0.41
1:A:1130:A:N3	1:A:1146:A:C2	2.88	0.41
18:P:58:TYR:O	18:P:61:SER:N	2.54	0.41
1:A:1272:G:C4	1:A:1273:G:C8	3.09	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:C:35:GLU:O	5:C:36:ASP:C	2.58	0.41
11:I:91:ASP:N	11:I:91:ASP:OD1	2.52	0.41
1:A:1229:A:C2	1:A:1230:C:C4	3.09	0.41
15:M:73:GLU:O	15:M:77:ASN:N	2.54	0.41
1:A:300:A:C3'	1:A:300:A:C8	3.03	0.41
15:M:13:LYS:O	15:M:14:ARG:C	2.58	0.41
3:V:24:A:C2	7:E:15:ARG:NH1	2.88	0.41
1:A:604:G:C5	1:A:605:U:C5	3.08	0.41
21:S:16:LEU:O	21:S:20:LEU:N	2.54	0.41
1:A:1088:G:C4	1:A:1089:G:C8	3.08	0.41
2:Y:21:A:O2'	2:Y:22:G:C8	2.74	0.41
1:A:236:G:C5	1:A:237:C:C5	3.09	0.41
1:A:815:A:C2	1:A:1529:G:C4	3.09	0.41
1:A:766:A:C4	1:A:814:A:C2	3.09	0.41
1:A:1367:C:N3	1:A:1368:G:N7	2.69	0.41
6:D:113:SER:O	6:D:117:ALA:N	2.54	0.41
1:A:1108:G:C5	1:A:1109:C:C5	3.09	0.41
1:A:1107:C:C4	1:A:1108:G:C8	3.09	0.41
1:A:509:A:C8	1:A:509:A:C3'	3.04	0.41
24:X:355:MET:O	24:X:359:TRP:CE3	2.74	0.41
1:A:1369:C:O2'	1:A:1370:G:O4'	2.38	0.41
1:A:20:U:C2	1:A:916:G:N2	2.88	0.41
1:A:937:A:C5	1:A:938:A:N7	2.88	0.40
1:A:1309:G:OP2	15:M:99:ARG:NH1	2.54	0.40
1:A:445:G:C6	1:A:490:G:C6	3.09	0.40
1:A:1345:U:C2	1:A:1377:A:C6	3.09	0.40
1:A:79:G:N2	1:A:80:G:C4	2.89	0.40
1:A:1221:G:C4	1:A:1222:G:C8	3.09	0.40
4:B:17:PHE:O	4:B:18:GLY:O	2.39	0.40
1:A:1157:A:C6	1:A:1180:A:C5	3.08	0.40
17:O:29:VAL:O	17:O:32:LEU:N	2.53	0.40
1:A:156:G:C6	1:A:166:G:C6	3.09	0.40
14:L:6:ILE:CD1	14:L:6:ILE:N	2.84	0.40
1:A:780:A:C2	1:A:801:U:C5	3.09	0.40
17:O:64:ARG:O	17:O:65:ARG:C	2.60	0.40
1:A:1130:A:C2	1:A:1146:A:C5	3.09	0.40
24:X:352:GLY:O	24:X:354:LEU:N	2.54	0.40
4:B:223:ILE:O	4:B:227:GLY:N	2.55	0.40
1:A:539:A:C6	1:A:540:G:C6	3.10	0.40
1:A:1213:A:C5	1:A:1215:G:C4	3.10	0.40
1:A:675:A:N1	1:A:716:A:C2	2.90	0.40
1:A:1315:U:O2'	1:A:1360:A:O2'	2.39	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:L:57:VAL:N	14:L:65:VAL:O	2.54	0.40
24:X:259:ASP:O	24:X:259:ASP:OD1	2.39	0.40
9:G:113:GLU:CD	9:G:113:GLU:N	2.75	0.40
1:A:1428:A:C6	1:A:1429:C:C4	3.10	0.40
1:A:683:G:C6	1:A:684:A:C6	3.09	0.40
14:L:37:THR:CG2	14:L:38:VAL:N	2.84	0.40
20:R:70:ILE:O	20:R:74:ARG:CG	2.69	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	
4	B	232/256 (91%)	174 (75%)	48 (21%)	10 (4%)	4	23
5	C	204/239 (85%)	138 (68%)	52 (26%)	14 (7%)	2	9
6	D	206/209 (99%)	169 (82%)	26 (13%)	11 (5%)	3	18
7	E	149/162 (92%)	117 (78%)	26 (17%)	6 (4%)	5	25
8	F	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	22	70
9	G	153/156 (98%)	125 (82%)	27 (18%)	1 (1%)	30	78
10	H	136/138 (99%)	112 (82%)	18 (13%)	6 (4%)	4	22
11	I	125/128 (98%)	93 (74%)	23 (18%)	9 (7%)	2	8
12	J	96/105 (91%)	77 (80%)	13 (14%)	6 (6%)	2	12
13	K	112/129 (87%)	94 (84%)	12 (11%)	6 (5%)	3	17
14	L	120/134 (90%)	87 (72%)	22 (18%)	11 (9%)	1	5
15	M	115/126 (91%)	91 (79%)	20 (17%)	4 (4%)	6	30
16	N	58/61 (95%)	46 (79%)	11 (19%)	1 (2%)	14	54
17	O	86/89 (97%)	69 (80%)	14 (16%)	3 (4%)	6	30
18	P	81/88 (92%)	60 (74%)	18 (22%)	3 (4%)	5	28
19	Q	97/105 (92%)	79 (81%)	16 (16%)	2 (2%)	11	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	R	68/88 (77%)	46 (68%)	17 (25%)	5 (7%)	2	8
21	S	76/93 (82%)	50 (66%)	18 (24%)	8 (10%)	1	3
22	T	97/106 (92%)	72 (74%)	18 (19%)	7 (7%)	2	8
23	U	22/27 (82%)	12 (54%)	8 (36%)	2 (9%)	1	5
24	X	360/378 (95%)	288 (80%)	58 (16%)	14 (4%)	5	26
All	All	2692/2918 (92%)	2086 (78%)	476 (18%)	130 (5%)	4	20

All (130) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	C	45	LYS
5	C	47	LEU
5	C	181	ASN
6	D	5	ILE
6	D	44	GLY
7	E	85	GLY
12	J	30	SER
12	J	58	ASP
13	K	106	LYS
14	L	50	ALA
15	M	101	GLN
20	R	86	VAL
21	S	80	TYR
22	T	99	LEU
23	U	7	ARG
24	X	177	ILE
24	X	225	PRO
24	X	231	VAL
24	X	318	ILE
24	X	359	TRP
4	B	14	GLY
4	B	18	GLY
4	B	235	SER
5	C	4	LYS
5	C	60	ALA
5	C	81	GLY
6	D	3	ARG
6	D	7	PRO
6	D	88	VAL
6	D	168	ARG

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Mol	Chain	Res	Type
6	D	171	GLY
7	E	38	GLN
9	G	7	ALA
10	H	2	LEU
11	I	100	GLY
11	I	127	LYS
12	J	92	THR
13	K	117	ASN
13	K	118	GLY
14	L	94	GLY
18	P	78	GLY
21	S	11	VAL
21	S	24	ALA
21	S	26	GLY
21	S	31	ILE
24	X	173	PRO
24	X	197	ALA
24	X	353	ASP
24	X	360	ALA
24	X	377	ALA
4	B	123	ALA
4	B	136	VAL
4	B	216	SER
5	C	14	ILE
5	C	15	THR
5	C	26	LYS
5	C	27	LYS
5	C	49	SER
5	C	80	GLY
5	C	127	ARG
6	D	30	LYS
6	D	69	GLY
7	E	77	PRO
10	H	91	ARG
10	H	99	GLU
11	I	10	ARG
11	I	31	GLN
11	I	34	ASN
12	J	57	LYS
13	K	105	VAL
14	L	11	ARG
14	L	26	LEU

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Mol	Chain	Res	Type
14	L	27	LYS
14	L	78	GLU
17	O	86	GLY
18	P	34	GLU
20	R	36	ASN
20	R	45	SER
21	S	6	LYS
21	S	29	ARG
22	T	98	PRO
23	U	3	LYS
24	X	332	ASN
6	D	84	LYS
7	E	6	PHE
7	E	125	SER
10	H	3	THR
11	I	55	ALA
11	I	89	ASN
12	J	36	GLY
12	J	91	PRO
14	L	18	ARG
14	L	63	TYR
15	M	104	ARG
15	M	117	VAL
17	O	23	GLY
19	Q	4	LYS
19	Q	34	LYS
20	R	64	ARG
22	T	97	ALA
24	X	95	GLU
24	X	320	TRP
4	B	130	ARG
4	B	158	LEU
4	B	230	VAL
6	D	47	ARG
8	F	81	ILE
11	I	126	SER
13	K	89	ALA
15	M	106	ASN
16	N	16	PHE
18	P	54	GLU
22	T	71	THR
22	T	95	ALA

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Mol	Chain	Res	Type
22	T	101	GLY
4	B	159	PRO
5	C	145	GLY
7	E	109	ILE
10	H	98	LYS
11	I	53	VAL
13	K	49	GLY
14	L	73	GLY
14	L	95	VAL
22	T	100	ILE
10	H	51	VAL
14	L	86	GLY
17	O	29	VAL
20	R	37	VAL
21	S	9	VAL
24	X	227	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	
4	B	202/220 (92%)	185 (92%)	17 (8%)	16	51
5	C	160/188 (85%)	138 (86%)	22 (14%)	5	24
6	D	180/181 (99%)	161 (89%)	19 (11%)	10	36
7	E	116/123 (94%)	99 (85%)	17 (15%)	4	21
8	F	90/90 (100%)	81 (90%)	9 (10%)	11	39
9	G	126/127 (99%)	119 (94%)	7 (6%)	30	72
10	H	119/119 (100%)	106 (89%)	13 (11%)	9	35
11	I	98/99 (99%)	86 (88%)	12 (12%)	7	29
12	J	88/92 (96%)	75 (85%)	13 (15%)	4	21
13	K	86/99 (87%)	74 (86%)	12 (14%)	5	23
14	L	103/110 (94%)	91 (88%)	12 (12%)	8	31
15	M	94/101 (93%)	85 (90%)	9 (10%)	12	43
16	N	49/50 (98%)	44 (90%)	5 (10%)	11	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	O	79/80 (99%)	70 (89%)	9 (11%)	8	33
18	P	72/74 (97%)	66 (92%)	6 (8%)	16	52
19	Q	94/97 (97%)	86 (92%)	8 (8%)	15	51
20	R	61/77 (79%)	52 (85%)	9 (15%)	4	21
21	S	69/80 (86%)	58 (84%)	11 (16%)	4	17
22	T	76/82 (93%)	68 (90%)	8 (10%)	10	37
23	U	19/22 (86%)	18 (95%)	1 (5%)	32	74
24	X	305/319 (96%)	260 (85%)	45 (15%)	4	21
All	All	2286/2430 (94%)	2022 (88%)	264 (12%)	8	32

All (264) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	15	VAL
4	B	17	PHE
4	B	44	LEU
4	B	69	LEU
4	B	74	LYS
4	B	75	LYS
4	B	96	ARG
4	B	97	TRP
4	B	102	LEU
4	B	153	ARG
4	B	154	LEU
4	B	172	ILE
4	B	178	ARG
4	B	187	LEU
4	B	193	ASP
4	B	196	LEU
4	B	229	VAL
5	C	3	ASN
5	C	5	ILE
5	C	12	LEU
5	C	14	ILE
5	C	16	ARG
5	C	21	ARG
5	C	27	LYS
5	C	28	GLN
5	C	29	TYR

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Mol	Chain	Res	Type
5	C	38	ARG
5	C	49	SER
5	C	62	ASP
5	C	79	ARG
5	C	95	THR
5	C	107	GLN
5	C	127	ARG
5	C	131	ARG
5	C	165	THR
5	C	179	ARG
5	C	191	THR
5	C	196	LEU
5	C	202	ILE
6	D	4	TYR
6	D	8	VAL
6	D	13	ARG
6	D	21	LEU
6	D	30	LYS
6	D	57	ARG
6	D	58	LEU
6	D	66	ARG
6	D	72	GLU
6	D	73	ARG
6	D	96	LEU
6	D	122	ARG
6	D	131	ARG
6	D	132	ARG
6	D	135	LEU
6	D	146	ILE
6	D	166	LYS
6	D	179	GLU
6	D	202	LEU
7	E	10	MET
7	E	11	ILE
7	E	12	LEU
7	E	14	ARG
7	E	26	PHE
7	E	31	LEU
7	E	47	LYS
7	E	51	VAL
7	E	55	VAL
7	E	68	GLU

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Mol	Chain	Res	Type
7	E	72	GLN
7	E	76	ILE
7	E	79	GLU
7	E	84	PHE
7	E	101	ILE
7	E	135	THR
7	E	144	THR
8	F	16	GLN
8	F	17	SER
8	F	21	LEU
8	F	27	GLN
8	F	46	ARG
8	F	52	ILE
8	F	64	GLN
8	F	86	ARG
8	F	100	ASN
9	G	5	ARG
9	G	13	GLN
9	G	24	THR
9	G	66	VAL
9	G	80	VAL
9	G	113	GLU
9	G	153	HIS
10	H	1	MET
10	H	25	ASP
10	H	26	VAL
10	H	50	ARG
10	H	51	VAL
10	H	75	ARG
10	H	91	ARG
10	H	99	GLU
10	H	102	ARG
10	H	111	ILE
10	H	120	THR
10	H	136	GLU
10	H	137	VAL
11	I	10	ARG
11	I	23	ASN
11	I	34	ASN
11	I	63	ILE
11	I	91	ASP
11	I	95	LYS

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Mol	Chain	Res	Type
11	I	104	ARG
11	I	109	VAL
11	I	110	GLU
11	I	121	ARG
11	I	125	TYR
11	I	127	LYS
12	J	22	LYS
12	J	54	PHE
12	J	55	LYS
12	J	58	ASP
12	J	61	GLU
12	J	62	HIS
12	J	63	PHE
12	J	74	ILE
12	J	78	ASN
12	J	86	MET
12	J	92	THR
12	J	96	ILE
12	J	100	THR
13	K	14	VAL
13	K	24	SER
13	K	29	ILE
13	K	32	ILE
13	K	81	ASP
13	K	87	THR
13	K	92	GLU
13	K	104	GLN
13	K	105	VAL
13	K	117	ASN
13	K	123	LYS
13	K	124	LYS
14	L	6	ILE
14	L	19	LYS
14	L	26	LEU
14	L	37	THR
14	L	40	ARG
14	L	42	VAL
14	L	51	LEU
14	L	52	ARG
14	L	78	GLU
14	L	84	ILE
14	L	90	LYS

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Mol	Chain	Res	Type
14	L	91	ASP
15	M	32	GLU
15	M	48	LEU
15	M	64	TRP
15	M	93	ARG
15	M	103	THR
15	M	105	THR
15	M	106	ASN
15	M	108	ARG
15	M	115	LYS
16	N	6	LEU
16	N	8	GLU
16	N	16	PHE
16	N	18	VAL
16	N	44	LEU
17	O	4	THR
17	O	5	LYS
17	O	17	ARG
17	O	26	GLU
17	O	27	VAL
17	O	41	GLU
17	O	44	LYS
17	O	65	ARG
17	O	82	ILE
18	P	55	ARG
18	P	62	VAL
18	P	67	THR
18	P	69	THR
18	P	82	GLN
18	P	83	GLU
19	Q	9	VAL
19	Q	10	VAL
19	Q	11	VAL
19	Q	14	LYS
19	Q	38	ARG
19	Q	52	LYS
19	Q	74	LEU
19	Q	100	LYS
20	R	19	LYS
20	R	38	GLU
20	R	45	SER
20	R	47	THR

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Mol	Chain	Res	Type
20	R	53	ARG
20	R	76	LEU
20	R	84	LYS
20	R	87	ARG
20	R	88	LYS
21	S	5	LEU
21	S	6	LYS
21	S	7	LYS
21	S	29	ARG
21	S	30	LEU
21	S	34	TRP
21	S	37	ARG
21	S	44	MET
21	S	49	ILE
21	S	53	ASN
21	S	71	LEU
22	T	22	ARG
22	T	26	ASN
22	T	54	LYS
22	T	62	LEU
22	T	72	LEU
22	T	75	ASN
22	T	82	SER
22	T	84	LEU
23	U	5	ASP
24	X	20	ARG
24	X	24	LYS
24	X	29	ILE
24	X	34	GLN
24	X	36	GLU
24	X	38	ARG
24	X	39	LEU
24	X	42	LEU
24	X	52	TRP
24	X	53	ASN
24	X	59	ARG
24	X	63	GLN
24	X	73	ASP
24	X	75	PHE
24	X	79	GLU
24	X	88	LEU
24	X	90	GLU

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Mol	Chain	Res	Type
24	X	97	ARG
24	X	100	LEU
24	X	105	GLU
24	X	128	ASN
24	X	140	THR
24	X	141	GLU
24	X	143	CYS
24	X	169	LEU
24	X	170	THR
24	X	182	ILE
24	X	192	LEU
24	X	227	VAL
24	X	231	VAL
24	X	238	GLU
24	X	265	VAL
24	X	272	THR
24	X	299	LEU
24	X	300	GLU
24	X	304	ARG
24	X	311	LEU
24	X	316	ARG
24	X	327	TYR
24	X	329	LEU
24	X	344	HIS
24	X	348	ASN
24	X	350	LEU
24	X	353	ASP
24	X	359	TRP

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

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1503/1525 (98%)	282 (18%)	106 (7%)
2	Y	76/77 (98%)	14 (18%)	6 (7%)
2	Z	76/77 (98%)	15 (19%)	5 (6%)
3	V	10/27 (37%)	3 (30%)	3 (30%)
All	All	1665/1706 (97%)	314 (18%)	120 (7%)

All (314) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	22	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	49	U
1	A	51	A
1	A	54	C
1	A	58	C
1	A	60	A
1	A	61	G
1	A	80	G
1	A	88	C
1	A	101	A
1	A	109	A
1	A	115	G
1	A	116	A
1	A	120	A
1	A	121	C
1	A	127	G
1	A	131	C
1	A	169	C
1	A	173	U
1	A	174	C
1	A	181	G
1	A	182	U
1	A	188	U
1	A	195	A
1	A	197	A
1	A	209	U
1	A	210	U
1	A	216	G
1	A	231	G
1	A	244	U
1	A	245	C
1	A	246	A
1	A	247	G
1	A	250	A
1	A	251	G
1	A	266	G

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Mol	Chain	Res	Type
1	A	267	C
1	A	274	A
1	A	289	G
1	A	301	G
1	A	306	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	345	C
1	A	346	G
1	A	347	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	372	C
1	A	382	A
1	A	384	G
1	A	390	C
1	A	397	A
1	A	398	C
1	A	406	G
1	A	411	A
1	A	412	A
1	A	413	G
1	A	414	A
1	A	422	C
1	A	429	U
1	A	430	A
1	A	439	A
1	A	440	A
1	A	452	A
1	A	453	A
1	A	465	A
1	A	467	G
1	A	484	G
1	A	485	G
1	A	496	A
1	A	497	U
1	A	500	G
1	A	505	G

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Mol	Chain	Res	Type
1	A	508	C
1	A	509	A
1	A	510	A
1	A	511	C
1	A	512	U
1	A	518	C
1	A	527	G
1	A	531	U
1	A	533	A
1	A	534	U
1	A	545	C
1	A	547	A
1	A	548	G
1	A	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	563	A
1	A	568	G
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	596	C
1	A	632	A
1	A	642	A
1	A	653	A
1	A	665	A
1	A	687	A
1	A	688	G
1	A	721	G
1	A	722	A
1	A	734	G
1	A	748	C
1	A	749	C
1	A	752	G
1	A	755	G
1	A	766	A
1	A	777	A
1	A	792	A
1	A	793	U

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Mol	Chain	Res	Type
1	A	794	A
1	A	811	C
1	A	816	A
1	A	817	C
1	A	818	G
1	A	819	A
1	A	828	A
1	A	841	U
1	A	842	C
1	A	843	U
1	A	848	C
1	A	851	G
1	A	859	A
1	A	867	G
1	A	884	U
1	A	885	G
1	A	889	A
1	A	890	G
1	A	902	G
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	942	G
1	A	945	G
1	A	960	U
1	A	961	U
1	A	966	G
1	A	968	A
1	A	969	A
1	A	971	G
1	A	972	C
1	A	974	A
1	A	976	G
1	A	977	A
1	A	978	A
1	A	980	C
1	A	981	U
1	A	982	U
1	A	983	A
1	A	984	C
1	A	992	U

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Mol	Chain	Res	Type
1	A	993	G
1	A	994	A
1	A	1004	A
1	A	1024	G
1	A	1045	C
1	A	1050	G
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1056	U
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1081	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1102	A
1	A	1104	G
1	A	1108	G
1	A	1117	G
1	A	1118	C
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1146	A
1	A	1151	A
1	A	1152	A
1	A	1154	G
1	A	1158	C
1	A	1159	U
1	A	1160	G
1	A	1171	G
1	A	1181	G
1	A	1182	G

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Mol	Chain	Res	Type
1	A	1183	A
1	A	1184	G
1	A	1190	G
1	A	1193	G
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1213	A
1	A	1227	A
1	A	1228	C
1	A	1238	A
1	A	1239	A
1	A	1253	G
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1278	U
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1305	G
1	A	1312	G
1	A	1317	C
1	A	1319	A
1	A	1320	C
1	A	1322	C
1	A	1323	G
1	A	1331	G
1	A	1335	C
1	A	1336	C
1	A	1346	A
1	A	1347	G
1	A	1353	G

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Mol	Chain	Res	Type
1	A	136(B)	C
1	A	1364	U
1	A	1365	G
1	A	1370	G
1	A	1378	C
1	A	1402	C
1	A	1419	G
1	A	1430	C
1	A	1443	G
1	A	1446	A
1	A	1447	G
1	A	1452	C
1	A	1453	G
1	A	1487	G
1	A	1492	A
1	A	1493	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1507	A
1	A	1508	G
1	A	1517	G
1	A	1519	A
1	A	1520	G
1	A	1525	G
1	A	1528	U
1	A	1529	G
1	A	1530	G
1	A	1531	A
2	Z	6	G
2	Z	9	G
2	Z	10	G
2	Z	16	C
2	Z	17	C
2	Z	17(A)	U
2	Z	18	G
2	Z	19	G
2	Z	20	U
2	Z	46	G
2	Z	47	U
2	Z	48	C

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Mol	Chain	Res	Type
2	Z	49	G
2	Z	58	A
2	Z	59	A
3	V	22	A
3	V	23	A
3	V	24	A
2	Y	7	G
2	Y	8	U
2	Y	9	G
2	Y	14	A
2	Y	16	C
2	Y	17	C
2	Y	17(A)	U
2	Y	18	G
2	Y	19	G
2	Y	20	U
2	Y	22	G
2	Y	47	U
2	Y	48	C
2	Y	60	U

All (120) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	30	U
1	A	48	C
1	A	49	U
1	A	50	A
1	A	60	A
1	A	108	G
1	A	109	A
1	A	115	G
1	A	119	A
1	A	173	U
1	A	181	G
1	A	208	U
1	A	210	U
1	A	243	A
1	A	244	U
1	A	246	A
1	A	250	A
1	A	266	G

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Mol	Chain	Res	Type
1	A	274	A
1	A	306	G
1	A	328	C
1	A	329	A
1	A	345	C
1	A	351	G
1	A	353	A
1	A	366	C
1	A	412	A
1	A	413	G
1	A	421	U
1	A	428	G
1	A	429	U
1	A	438	G
1	A	465	A
1	A	466	G
1	A	481	G
1	A	484	G
1	A	496	A
1	A	498	A
1	A	509	A
1	A	511	C
1	A	533	A
1	A	547	A
1	A	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	587	G
1	A	595	G
1	A	641	U
1	A	687	A
1	A	721	G
1	A	733	A
1	A	748	C
1	A	793	U
1	A	817	C
1	A	870	U
1	A	884	U
1	A	889	A
1	A	913	A
1	A	971	G

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Mol	Chain	Res	Type
1	A	975	A
1	A	978	A
1	A	982	U
1	A	983	A
1	A	992	U
1	A	1049	U
1	A	1053	G
1	A	1064	G
1	A	1066	C
1	A	1067	A
1	A	1094	G
1	A	1101	A
1	A	1126	U
1	A	1129	C
1	A	1137	C
1	A	1139	G
1	A	1145	C
1	A	1151	A
1	A	1157	A
1	A	1159	U
1	A	1181	G
1	A	1196	U
1	A	1200	C
1	A	1201	A
1	A	1280	A
1	A	1281	U
1	A	1285	A
1	A	1287	A
1	A	1300	G
1	A	1305	G
1	A	1319	A
1	A	1335	C
1	A	1347	G
1	A	1397	C
1	A	1443	G
1	A	1446	A
1	A	1452	C
1	A	1491	G
1	A	1492	A
1	A	1502	A
1	A	1503	A
1	A	1504	G

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Mol	Chain	Res	Type
1	A	1506	U
1	A	1528	U
1	A	1529	G
1	A	1530	G
2	Z	7	G
2	Z	16	C
2	Z	17(A)	U
2	Z	18	G
2	Z	48	C
3	V	15	A
3	V	21	A
3	V	23	A
2	Y	9	G
2	Y	16	C
2	Y	17	C
2	Y	17(A)	U
2	Y	19	G
2	Y	60	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 272 ligands modelled in this entry, 272 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1504/1525 (98%)	0.15	47 (3%) 47 9	34, 99, 199, 271	0
2	Y	77/77 (100%)	-0.17	1 (1%) 74 19	59, 91, 127, 196	0
2	Z	77/77 (100%)	1.01	14 (18%) 2 1	175, 231, 266, 276	0
3	V	10/27 (37%)	1.78	3 (30%) 1 0	63, 104, 143, 196	0
4	B	234/256 (91%)	-0.04	4 (1%) 67 15	91, 127, 174, 204	0
5	C	206/239 (86%)	0.16	11 (5%) 25 5	87, 126, 164, 178	0
6	D	208/209 (99%)	0.40	17 (8%) 12 3	81, 115, 151, 184	0
7	E	151/162 (93%)	0.04	4 (2%) 53 10	71, 100, 145, 173	0
8	F	101/101 (100%)	-0.15	3 (2%) 48 9	64, 94, 131, 149	0
9	G	155/156 (99%)	0.10	5 (3%) 45 9	87, 125, 158, 181	0
10	H	138/138 (100%)	0.22	6 (4%) 34 7	80, 107, 145, 171	0
11	I	127/128 (99%)	0.95	24 (18%) 2 1	105, 140, 173, 227	0
12	J	98/105 (93%)	0.55	9 (9%) 9 2	106, 144, 175, 186	0
13	K	114/129 (88%)	0.31	7 (6%) 21 5	64, 91, 135, 175	0
14	L	122/134 (91%)	0.41	12 (9%) 8 2	57, 89, 131, 185	0
15	M	117/126 (92%)	0.18	5 (4%) 34 7	98, 143, 172, 188	0
16	N	60/61 (98%)	0.91	11 (18%) 2 1	80, 113, 158, 175	0
17	O	88/89 (98%)	-0.05	2 (2%) 57 12	60, 91, 130, 145	0
18	P	83/88 (94%)	0.45	5 (6%) 21 5	90, 123, 155, 202	0
19	Q	99/105 (94%)	0.52	10 (10%) 7 2	76, 105, 140, 159	0
20	R	70/88 (79%)	0.08	2 (2%) 49 9	64, 87, 139, 147	0
21	S	78/93 (83%)	0.79	8 (10%) 7 2	114, 150, 184, 205	0
22	T	99/106 (93%)	0.63	11 (11%) 6 2	87, 117, 160, 184	0
23	U	24/27 (88%)	2.36	12 (50%) 0 0	100, 137, 178, 187	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
24	X	362/378 (95%)	0.17	22 (6%) 21 5	94, 150, 244, 273	0
All	All	4402/4624 (95%)	0.25	255 (5%) 23 5	34, 114, 209, 276	0

All (255) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Z	34	C	10.3
12	J	100	THR	9.7
12	J	3	LYS	9.7
21	S	81	ARG	8.5
24	X	345	ASP	8.3
24	X	344	HIS	8.3
3	V	24	A	8.1
11	I	8	GLY	7.9
5	C	17	ASP	7.3
1	A	841	U	7.1
12	J	73	ASP	7.0
21	S	71	LEU	6.8
2	Z	4	G	6.8
2	Z	33	U	6.7
13	K	118	GLY	6.6
5	C	16	ARG	6.4
23	U	9	ARG	6.3
10	H	98	LYS	6.2
9	G	5	ARG	6.2
11	I	5	TYR	6.1
12	J	5	ARG	6.0
22	T	8	ARG	5.8
9	G	8	GLU	5.4
16	N	14	PRO	5.2
3	V	15	A	5.1
11	I	16	ARG	5.1
23	U	15	ARG	5.1
24	X	353	ASP	5.1
11	I	66	ARG	4.9
23	U	11	GLY	4.8
1	A	1125	U	4.8
1	A	1325	C	4.8
11	I	124	GLN	4.7
2	Z	5	G	4.7
6	D	20	TYR	4.7
16	N	2	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
11	I	17	VAL	4.7
22	T	80	ARG	4.6
2	Z	35	A	4.6
5	C	184	TYR	4.6
16	N	12	ARG	4.6
10	H	54	ASP	4.6
8	F	101	ALA	4.5
1	A	1148	U	4.5
23	U	10	ARG	4.5
11	I	9	ARG	4.5
1	A	1126	U	4.4
13	K	121	PRO	4.4
23	U	8	THR	4.4
2	Z	38	A	4.4
13	K	124	LYS	4.4
6	D	3	ARG	4.4
11	I	29	ASN	4.3
12	J	99	LYS	4.3
2	Z	36	U	4.2
10	H	84	ARG	4.2
6	D	115	ARG	4.2
24	X	173	PRO	4.1
21	S	73	GLU	4.1
23	U	14	TRP	4.1
11	I	18	PHE	4.0
12	J	4	ILE	4.0
1	A	307	C	4.0
6	D	23	GLY	4.0
2	Z	17(A)	U	4.0
1	A	136(B)	C	4.0
6	D	70	ILE	4.0
11	I	62	TYR	4.0
7	E	10	MET	4.0
11	I	7	THR	3.9
5	C	207	VAL	3.9
24	X	322	SER	3.9
23	U	16	GLY	3.9
24	X	321	GLY	3.9
23	U	6	ARG	3.9
24	X	159	ARG	3.9
1	A	308	C	3.9
1	A	1147	C	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	1149	C	3.8
1	A	1394	A	3.8
19	Q	27	PHE	3.8
16	N	11	LYS	3.8
14	L	19	LYS	3.7
1	A	1127	G	3.7
20	R	88	LYS	3.7
24	X	123	PRO	3.7
21	S	8	GLY	3.7
22	T	9	ASN	3.7
12	J	61	GLU	3.7
19	Q	70	ARG	3.6
4	B	232	PRO	3.6
6	D	6	GLY	3.6
11	I	64	THR	3.6
11	I	15	ALA	3.6
7	E	24	ARG	3.5
6	D	24	GLU	3.5
11	I	97	LYS	3.5
5	C	15	THR	3.5
24	X	347	GLU	3.5
1	A	64	G	3.5
6	D	5	ILE	3.5
15	M	99	ARG	3.4
9	G	11	GLN	3.4
1	A	1039	C	3.4
23	U	3	LYS	3.4
3	V	23	A	3.4
11	I	98	PRO	3.3
22	T	34	LYS	3.3
1	A	1364	U	3.3
6	D	4	TYR	3.3
24	X	23	TRP	3.3
1	A	824	C	3.3
13	K	123	LYS	3.3
1	A	1119	C	3.3
6	D	69	GLY	3.3
23	U	5	ASP	3.3
13	K	117	ASN	3.2
1	A	208	U	3.2
24	X	94	ALA	3.2
19	Q	26	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
22	T	83	ARG	3.2
2	Y	17(A)	U	3.2
22	T	79	ARG	3.1
19	Q	42	TYR	3.1
13	K	122	LYS	3.1
1	A	1287	A	3.1
14	L	72	GLU	3.1
17	O	20	GLY	3.1
2	Z	32	C	3.1
21	S	56	GLN	3.0
14	L	63	TYR	3.0
6	D	119	GLN	3.0
15	M	114	ARG	3.0
2	Z	37	A	3.0
5	C	186	PHE	3.0
11	I	28	VAL	2.9
22	T	106	ALA	2.9
11	I	102	LEU	2.9
24	X	290	LYS	2.9
6	D	27	TYR	2.9
11	I	31	GLN	2.9
7	E	9	LYS	2.9
7	E	11	ILE	2.9
19	Q	25	ARG	2.9
22	T	84	LEU	2.9
6	D	65	ARG	2.8
5	C	179	ARG	2.8
11	I	30	GLY	2.8
1	A	41	G	2.8
14	L	52	ARG	2.8
16	N	13	THR	2.8
14	L	27	LYS	2.8
14	L	62	GLY	2.8
21	S	57	HIS	2.7
2	Z	39	C	2.7
1	A	662	G	2.7
16	N	30	ALA	2.7
11	I	65	VAL	2.7
23	U	17	THR	2.7
1	A	790	A	2.7
1	A	743	U	2.7
9	G	32	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
6	D	2	GLY	2.7
13	K	119	CYS	2.7
1	A	1324	A	2.7
1	A	1018	C	2.6
11	I	126	SER	2.6
24	X	210	ALA	2.6
19	Q	24	GLU	2.6
9	G	72	ARG	2.6
4	B	144	ARG	2.6
11	I	117	HIS	2.6
1	A	1395	C	2.6
2	Z	70	G	2.5
6	D	66	ARG	2.5
1	A	1342	C	2.5
19	Q	6	LEU	2.5
5	C	206	GLU	2.5
1	A	843	U	2.4
6	D	22	LYS	2.4
15	M	36	LYS	2.4
1	A	135	C	2.4
21	S	70	LYS	2.4
14	L	28	GLY	2.4
14	L	20	LYS	2.4
14	L	53	LYS	2.4
1	A	366	C	2.4
2	Z	3	C	2.4
18	P	42	ARG	2.4
24	X	122	PHE	2.4
11	I	27	THR	2.4
24	X	124	HIS	2.4
22	T	33	ILE	2.4
1	A	134	A	2.4
24	X	352	GLY	2.4
24	X	356	ASP	2.4
1	A	1113	C	2.3
15	M	35	GLU	2.3
1	A	921	U	2.3
19	Q	38	ARG	2.3
1	A	422	C	2.3
1	A	399	G	2.3
5	C	11	ARG	2.3
1	A	407	G	2.3

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Mol	Chain	Res	Type	RSRZ
15	M	112	GLY	2.3
8	F	94	GLN	2.3
12	J	33	GLN	2.3
20	R	87	ARG	2.3
5	C	45	LYS	2.3
18	P	28	ARG	2.3
19	Q	40	LYS	2.3
1	A	744	C	2.3
14	L	88	ARG	2.3
24	X	343	ARG	2.3
8	F	95	GLU	2.3
4	B	175	ARG	2.2
1	A	42	G	2.2
16	N	58	LYS	2.2
16	N	35	ARG	2.2
24	X	346	PRO	2.2
1	A	325	A	2.2
16	N	26	ARG	2.2
22	T	104	LEU	2.2
24	X	20	ARG	2.2
21	S	9	VAL	2.2
22	T	30	LYS	2.2
1	A	400	C	2.1
17	O	17	ARG	2.1
24	X	49	PRO	2.1
19	Q	28	PRO	2.1
5	C	161	GLU	2.1
11	I	6	GLY	2.1
1	A	46	G	2.1
14	L	42	VAL	2.1
18	P	26	ARG	2.1
6	D	86	LYS	2.1
10	H	101	PRO	2.1
1	A	136	C	2.1
1	A	984	C	2.1
4	B	231	GLU	2.1
2	Z	69	C	2.1
18	P	1	MET	2.1
24	X	18	ALA	2.1
1	A	236	G	2.1
1	A	1069	C	2.1
1	A	575	G	2.0

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Mol	Chain	Res	Type	RSRZ
12	J	43	ARG	2.0
10	H	128	GLY	2.0
10	H	135	CYS	2.0
16	N	21	TYR	2.0
1	A	1260	C	2.0
16	N	22	THR	2.0
23	U	4	GLY	2.0
18	P	44	THR	2.0
14	L	13	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
26	MG	A	5197	1/1	0.29	-	91,91,91,91	0
26	MG	Z	5249	1/1	0.20	-	82,82,82,82	0
26	MG	A	5076	1/1	0.46	-	38,38,38,38	0
26	MG	A	5239	1/1	0.15	-	22,22,22,22	0
26	MG	A	5220	1/1	0.38	-	3,3,3,3	0
26	MG	A	5044	1/1	0.15	-	4,4,4,4	0
26	MG	F	5009	1/1	0.21	-	3,3,3,3	0
26	MG	A	5130	1/1	0.40	-	36,36,36,36	0
26	MG	A	5147	1/1	0.11	-	54,54,54,54	0
26	MG	A	5223	1/1	0.25	-	3,3,3,3	0
26	MG	A	5213	1/1	0.28	-	54,54,54,54	0
26	MG	B	5004	1/1	0.28	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
26	MG	A	5074	1/1	0.15	-	62,62,62,62	0
26	MG	K	5015	1/1	0.37	-	91,91,91,91	0
26	MG	Y	5267	1/1	0.36	-	3,3,3,3	0
26	MG	A	5073	1/1	0.44	-	44,44,44,44	0
26	MG	A	5063	1/1	0.48	-	3,3,3,3	0
26	MG	Y	5271	1/1	0.28	-	27,27,27,27	0
26	MG	A	5107	1/1	0.72	-	68,68,68,68	0
26	MG	A	5179	1/1	0.40	-	66,66,66,66	0
26	MG	G	5011	1/1	1.31	-	82,82,82,82	0
26	MG	K	5014	1/1	0.19	-	70,70,70,70	0
26	MG	F	5092	1/1	0.19	-	57,57,57,57	0
26	MG	Z	5247	1/1	0.20	-	3,3,3,3	0
26	MG	A	5049	1/1	0.16	-	4,4,4,4	0
26	MG	A	5168	1/1	0.38	-	57,57,57,57	0
26	MG	A	5226	1/1	0.26	-	4,4,4,4	0
26	MG	T	5021	1/1	0.30	-	3,3,3,3	0
26	MG	A	5155	1/1	0.37	-	3,3,3,3	0
26	MG	A	5217	1/1	0.60	-	54,54,54,54	0
26	MG	A	5152	1/1	0.37	-	4,4,4,4	0
26	MG	Y	5264	1/1	0.29	-	66,66,66,66	0
26	MG	A	5075	1/1	0.35	-	28,28,28,28	0
26	MG	A	5102	1/1	0.52	-	34,34,34,34	0
26	MG	A	5081	1/1	0.23	-	5,5,5,5	0
26	MG	A	5183	1/1	0.53	-	30,30,30,30	0
26	MG	A	5134	1/1	0.18	-	39,39,39,39	0
26	MG	F	5006	1/1	0.31	-	40,40,40,40	0
26	MG	A	5110	1/1	0.80	-	54,54,54,54	0
26	MG	A	5150	1/1	0.09	-	57,57,57,57	0
26	MG	G	5010	1/1	0.18	-	70,70,70,70	0
26	MG	A	5195	1/1	0.13	-	66,66,66,66	0
26	MG	A	5024	1/1	0.36	-	4,4,4,4	0
26	MG	A	5104	1/1	0.27	-	52,52,52,52	0
26	MG	A	5189	1/1	0.10	-	64,64,64,64	0
26	MG	A	5059	1/1	0.22	-	3,3,3,3	0
26	MG	Y	5263	1/1	0.39	-	52,52,52,52	0
26	MG	A	5208	1/1	0.47	-	67,67,67,67	0
26	MG	A	5051	1/1	0.35	-	3,3,3,3	0
26	MG	A	5023	1/1	0.19	-	5,5,5,5	0
26	MG	A	5233	1/1	0.52	-	79,79,79,79	0
26	MG	A	5064	1/1	0.45	-	3,3,3,3	0
26	MG	A	5182	1/1	0.21	-	18,18,18,18	0
26	MG	A	5187	1/1	0.22	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
26	MG	H	5013	1/1	1.00	-	59,59,59,59	0
26	MG	A	5177	1/1	0.20	-	4,4,4,4	0
26	MG	A	5222	1/1	0.23	-	3,3,3,3	0
26	MG	Z	5257	1/1	0.23	-	36,36,36,36	0
26	MG	A	5088	1/1	0.11	-	58,58,58,58	0
26	MG	A	5095	1/1	0.23	-	49,49,49,49	0
26	MG	A	5135	1/1	0.19	-	80,80,80,80	0
26	MG	A	5039	1/1	0.22	-	4,4,4,4	0
26	MG	A	5069	1/1	0.64	-	33,33,33,33	0
26	MG	A	5180	1/1	0.14	-	78,78,78,78	0
26	MG	C	5005	1/1	0.18	-	3,3,3,3	0
26	MG	Z	5258	1/1	0.34	-	55,55,55,55	0
26	MG	A	5054	1/1	0.36	-	3,3,3,3	0
26	MG	A	5027	1/1	0.15	-	3,3,3,3	0
26	MG	Z	5245	1/1	0.20	-	51,51,51,51	0
26	MG	A	5029	1/1	0.25	-	3,3,3,3	0
26	MG	A	5165	1/1	0.09	-	52,52,52,52	0
26	MG	A	5053	1/1	0.31	-	3,3,3,3	0
26	MG	A	5154	1/1	1.11	-	63,63,63,63	0
26	MG	A	5185	1/1	0.34	-	77,77,77,77	0
26	MG	A	5191	1/1	0.43	-	77,77,77,77	0
26	MG	A	5228	1/1	0.24	-	3,3,3,3	0
26	MG	A	5093	1/1	0.17	-	63,63,63,63	0
26	MG	A	5216	1/1	0.20	-	35,35,35,35	0
26	MG	A	5129	1/1	0.37	-	36,36,36,36	0
26	MG	A	5162	1/1	0.15	-	41,41,41,41	0
26	MG	A	5097	1/1	0.12	-	65,65,65,65	0
26	MG	A	5272	1/1	0.10	-	3,3,3,3	0
26	MG	A	5149	1/1	0.15	-	53,53,53,53	0
26	MG	A	5042	1/1	0.26	-	3,3,3,3	0
26	MG	A	5153	1/1	0.29	-	3,3,3,3	0
26	MG	A	5114	1/1	0.99	-	34,34,34,34	0
26	MG	A	5096	1/1	0.38	-	57,57,57,57	0
26	MG	A	5098	1/1	0.20	-	42,42,42,42	0
26	MG	A	5198	1/1	0.37	-	3,3,3,3	0
26	MG	A	5136	1/1	1.14	-	62,62,62,62	0
26	MG	F	5008	1/1	0.08	-	51,51,51,51	0
26	MG	A	5091	1/1	0.75	-	43,43,43,43	0
26	MG	Z	5248	1/1	0.09	-	74,74,74,74	0
26	MG	A	5146	1/1	0.09	-	36,36,36,36	0
26	MG	A	5100	1/1	0.84	-	49,49,49,49	0
26	MG	Y	5268	1/1	2.09	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
26	MG	A	5142	1/1	0.52	-	27,27,27,27	0
26	MG	Z	5250	1/1	0.17	-	57,57,57,57	0
26	MG	A	5035	1/1	0.15	-	3,3,3,3	0
26	MG	A	5047	1/1	0.24	-	3,3,3,3	0
26	MG	A	5188	1/1	0.13	-	64,64,64,64	0
26	MG	A	5138	1/1	0.38	-	58,58,58,58	0
26	MG	A	5120	1/1	0.16	-	37,37,37,37	0
26	MG	A	5157	1/1	0.40	-	31,31,31,31	0
26	MG	A	5057	1/1	0.27	-	3,3,3,3	0
26	MG	A	5159	1/1	0.11	-	35,35,35,35	0
26	MG	A	5176	1/1	0.29	-	3,3,3,3	0
26	MG	A	5123	1/1	0.43	-	13,13,13,13	0
26	MG	A	5037	1/1	0.13	-	5,5,5,5	0
26	MG	A	5116	1/1	0.38	-	60,60,60,60	0
26	MG	A	5087	1/1	0.30	-	3,3,3,3	0
26	MG	A	5041	1/1	0.20	-	4,4,4,4	0
26	MG	A	5201	1/1	0.39	-	76,76,76,76	0
26	MG	Z	5254	1/1	0.24	-	3,3,3,3	0
26	MG	A	5084	1/1	0.19	-	3,3,3,3	0
26	MG	A	5125	1/1	0.24	-	29,29,29,29	0
26	MG	A	5038	1/1	0.20	-	4,4,4,4	0
26	MG	A	5109	1/1	0.39	-	46,46,46,46	0
26	MG	A	5077	1/1	0.17	-	5,5,5,5	0
26	MG	A	5205	1/1	0.99	-	65,65,65,65	0
26	MG	A	5085	1/1	0.19	-	3,3,3,3	0
26	MG	A	5238	1/1	0.47	-	61,61,61,61	0
26	MG	A	5181	1/1	0.59	-	48,48,48,48	0
26	MG	A	5151	1/1	0.48	-	36,36,36,36	0
26	MG	A	5235	1/1	0.19	-	64,64,64,64	0
26	MG	A	5056	1/1	0.18	-	4,4,4,4	0
26	MG	A	5112	1/1	0.82	-	54,54,54,54	0
26	MG	A	5241	1/1	0.24	-	36,36,36,36	0
26	MG	A	5145	1/1	0.27	-	67,67,67,67	0
26	MG	Z	5253	1/1	0.62	-	68,68,68,68	0
26	MG	A	5026	1/1	0.26	-	3,3,3,3	0
25	ZN	N	5002	1/1	0.07	-	100,100,100,100	0
26	MG	A	5072	1/1	0.47	-	28,28,28,28	0
26	MG	A	5133	1/1	0.26	-	57,57,57,57	0
26	MG	A	5127	1/1	0.29	-	60,60,60,60	0
26	MG	A	5160	1/1	0.10	-	64,64,64,64	0
26	MG	A	5060	1/1	0.21	-	3,3,3,3	0
25	ZN	D	5001	1/1	0.05	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
26	MG	A	5186	1/1	0.15	-	3,3,3,3	0
26	MG	Y	5266	1/1	0.43	-	60,60,60,60	0
26	MG	A	5206	1/1	0.13	-	3,3,3,3	0
26	MG	A	5163	1/1	0.17	-	50,50,50,50	0
26	MG	A	5207	1/1	0.27	-	83,83,83,83	0
26	MG	A	5033	1/1	0.17	-	3,3,3,3	0
26	MG	K	5016	1/1	0.12	-	85,85,85,85	0
26	MG	A	5131	1/1	0.10	-	55,55,55,55	0
26	MG	B	5003	1/1	0.20	-	39,39,39,39	0
26	MG	Z	5251	1/1	0.09	-	69,69,69,69	0
26	MG	A	5067	1/1	0.25	-	3,3,3,3	0
26	MG	A	5237	1/1	0.74	-	63,63,63,63	0
26	MG	Y	5265	1/1	0.30	-	60,60,60,60	0
26	MG	Q	5019	1/1	0.20	-	3,3,3,3	0
26	MG	A	5242	1/1	0.22	-	43,43,43,43	0
26	MG	A	5215	1/1	0.16	-	3,3,3,3	0
26	MG	Y	5261	1/1	0.20	-	31,31,31,31	0
26	MG	A	5034	1/1	0.18	-	3,3,3,3	0
26	MG	A	5243	1/1	0.10	-	29,29,29,29	0
26	MG	A	5172	1/1	0.22	-	4,4,4,4	0
26	MG	A	5236	1/1	0.24	-	66,66,66,66	0
26	MG	A	5196	1/1	0.52	-	82,82,82,82	0
26	MG	A	5126	1/1	0.22	-	63,63,63,63	0
26	MG	A	5078	1/1	0.12	-	3,3,3,3	0
26	MG	A	5164	1/1	0.48	-	54,54,54,54	0
26	MG	A	5231	1/1	0.48	-	3,3,3,3	0
26	MG	A	5234	1/1	0.26	-	36,36,36,36	0
26	MG	A	5045	1/1	0.31	-	3,3,3,3	0
26	MG	A	5167	1/1	0.36	-	36,36,36,36	0
26	MG	A	5032	1/1	0.27	-	3,3,3,3	0
26	MG	A	5156	1/1	0.38	-	29,29,29,29	0
26	MG	A	5058	1/1	0.17	-	4,4,4,4	0
26	MG	A	5219	1/1	0.77	-	28,28,28,28	0
26	MG	Z	5246	1/1	0.21	-	42,42,42,42	0
26	MG	A	5211	1/1	0.25	-	43,43,43,43	0
26	MG	A	5106	1/1	0.47	-	74,74,74,74	0
26	MG	A	5030	1/1	0.23	-	3,3,3,3	0
26	MG	A	5071	1/1	0.48	-	73,73,73,73	0
26	MG	L	5017	1/1	0.52	-	67,67,67,67	0
26	MG	A	5105	1/1	1.40	-	61,61,61,61	0
26	MG	A	5199	1/1	0.23	-	4,4,4,4	0
26	MG	A	5170	1/1	0.34	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
26	MG	A	5090	1/1	0.40	-	79,79,79,79	0
26	MG	A	5068	1/1	0.35	-	3,3,3,3	0
26	MG	A	5227	1/1	0.23	-	3,3,3,3	0
26	MG	A	5221	1/1	0.13	-	5,5,5,5	0
26	MG	A	5117	1/1	0.14	-	59,59,59,59	0
26	MG	A	5224	1/1	0.21	-	3,3,3,3	0
26	MG	A	5103	1/1	0.26	-	3,3,3,3	0
26	MG	A	5113	1/1	1.00	-	45,45,45,45	0
26	MG	A	5202	1/1	0.17	-	51,51,51,51	0
26	MG	A	5209	1/1	0.34	-	57,57,57,57	0
26	MG	A	5144	1/1	0.49	-	49,49,49,49	0
26	MG	Y	5259	1/1	0.30	-	3,3,3,3	0
26	MG	A	5212	1/1	1.08	-	57,57,57,57	0
26	MG	A	5028	1/1	0.23	-	3,3,3,3	0
26	MG	A	5225	1/1	0.31	-	3,3,3,3	0
26	MG	Y	5262	1/1	0.14	-	78,78,78,78	0
26	MG	A	5108	1/1	0.54	-	48,48,48,48	0
26	MG	A	5139	1/1	0.30	-	21,21,21,21	0
26	MG	A	5036	1/1	0.17	-	3,3,3,3	0
26	MG	A	5190	1/1	0.46	-	46,46,46,46	0
26	MG	A	5070	1/1	0.22	-	35,35,35,35	0
26	MG	A	5174	1/1	0.29	-	3,3,3,3	0
26	MG	A	5025	1/1	0.19	-	3,3,3,3	0
26	MG	A	5200	1/1	0.15	-	3,3,3,3	0
26	MG	A	5128	1/1	0.83	-	62,62,62,62	0
26	MG	A	5184	1/1	0.16	-	69,69,69,69	0
26	MG	A	5218	1/1	1.21	-	77,77,77,77	0
26	MG	A	5232	1/1	0.86	-	59,59,59,59	0
26	MG	A	5048	1/1	0.26	-	3,3,3,3	0
26	MG	A	5050	1/1	0.35	-	4,4,4,4	0
26	MG	A	5099	1/1	0.33	-	103,103,103,103	0
26	MG	A	5140	1/1	0.15	-	41,41,41,41	0
26	MG	A	5101	1/1	0.42	-	90,90,90,90	0
26	MG	A	5065	1/1	0.37	-	3,3,3,3	0
26	MG	Y	5270	1/1	0.33	-	3,3,3,3	0
26	MG	A	5169	1/1	0.18	-	3,3,3,3	0
26	MG	A	5066	1/1	0.27	-	6,6,6,6	0
26	MG	A	5083	1/1	0.13	-	4,4,4,4	0
26	MG	A	5118	1/1	0.83	-	60,60,60,60	0
26	MG	A	5094	1/1	0.43	-	3,3,3,3	0
26	MG	Y	5269	1/1	0.42	-	60,60,60,60	0
26	MG	A	5052	1/1	0.19	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
26	MG	S	5020	1/1	0.24	-	3,3,3,3	0
26	MG	A	5204	1/1	0.17	-	3,3,3,3	0
26	MG	Y	5260	1/1	0.39	-	3,3,3,3	0
26	MG	A	5192	1/1	0.43	-	54,54,54,54	0
26	MG	A	5055	1/1	0.30	-	6,6,6,6	0
26	MG	O	5018	1/1	0.27	-	33,33,33,33	0
26	MG	A	5079	1/1	0.24	-	3,3,3,3	0
26	MG	A	5121	1/1	0.26	-	8,8,8,8	0
26	MG	A	5158	1/1	0.25	-	3,3,3,3	0
26	MG	A	5193	1/1	0.23	-	80,80,80,80	0
26	MG	A	5061	1/1	0.26	-	4,4,4,4	0
26	MG	A	5194	1/1	0.46	-	3,3,3,3	0
26	MG	A	5166	1/1	0.13	-	36,36,36,36	0
26	MG	A	5086	1/1	0.36	-	3,3,3,3	0
26	MG	Z	5244	1/1	0.11	-	72,72,72,72	0
26	MG	A	5062	1/1	0.24	-	3,3,3,3	0
26	MG	A	5119	1/1	0.33	-	52,52,52,52	0
26	MG	Z	5252	1/1	0.07	-	95,95,95,95	0
26	MG	A	5178	1/1	0.18	-	3,3,3,3	0
26	MG	A	5229	1/1	0.17	-	3,3,3,3	0
26	MG	A	5031	1/1	0.28	-	4,4,4,4	0
26	MG	Z	5255	1/1	0.39	-	63,63,63,63	0
26	MG	A	5124	1/1	0.29	-	24,24,24,24	0
26	MG	A	5148	1/1	0.27	-	37,37,37,37	0
26	MG	Z	5256	1/1	0.23	-	3,3,3,3	0
26	MG	A	5043	1/1	0.48	-	3,3,3,3	0
26	MG	F	5007	1/1	0.24	-	51,51,51,51	0
26	MG	A	5115	1/1	0.68	-	58,58,58,58	0
26	MG	A	5040	1/1	0.23	-	4,4,4,4	0
26	MG	A	5230	1/1	0.17	-	3,3,3,3	0
26	MG	A	5173	1/1	0.22	-	3,3,3,3	0
26	MG	A	5122	1/1	0.25	-	12,12,12,12	0
26	MG	A	5080	1/1	0.22	-	3,3,3,3	0
26	MG	A	5171	1/1	0.18	-	3,3,3,3	0
26	MG	A	5046	1/1	0.23	-	3,3,3,3	0
26	MG	A	5175	1/1	0.15	-	3,3,3,3	0
26	MG	H	5012	1/1	0.47	-	58,58,58,58	0
26	MG	A	5132	1/1	0.16	-	46,46,46,46	0
26	MG	A	5143	1/1	1.17	-	49,49,49,49	0
26	MG	A	5161	1/1	0.10	-	3,3,3,3	0
26	MG	A	5203	1/1	0.39	-	59,59,59,59	0
26	MG	A	5111	1/1	0.20	-	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
26	MG	A	5082	1/1	0.30	-	3,3,3,3	0
26	MG	A	5210	1/1	0.13	-	94,94,94,94	0
26	MG	A	5240	1/1	0.43	-	59,59,59,59	0
26	MG	A	5022	1/1	0.22	-	3,3,3,3	0
26	MG	A	5214	1/1	0.26	-	3,3,3,3	0
26	MG	A	5089	1/1	0.29	-	3,3,3,3	0
26	MG	A	5141	1/1	0.63	-	60,60,60,60	0
26	MG	A	5137	1/1	0.66	-	40,40,40,40	0

6.5 Other polymers ⓘ

There are no such residues in this entry.