



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:29 AM UTC

PDB ID : 7SYS / pdb_00007sys
EMDB ID : EMD-25539
Title : Structure of the delta dII IRES eIF2-containing 48S initiation complex, closed conformation. Structure 12(delta dII).
Authors : Brown, Z.P.; Abaeva, I.S.; De, S.; Hellen, C.U.T.; Pestova, T.V.; Frank, J.
Deposited on : 2021-11-25
Resolution : 3.50 Å(reported)
Based on initial models : 5FLX, 6D9J, 5K0Y, 6O85, 4KZZ

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

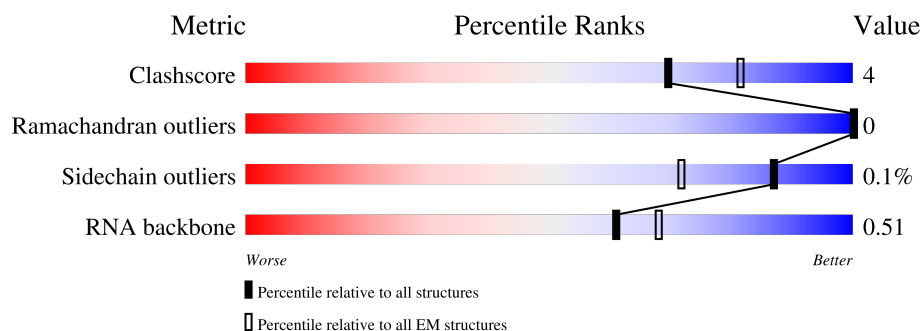
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



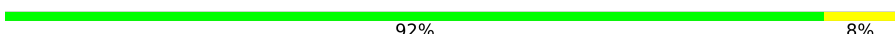
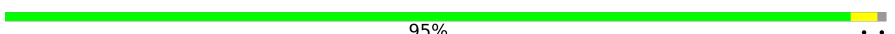
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RNA backbone	8273	3508

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	2	1870	
2	A	144	
3	B	295	
4	C	264	
5	D	221	
6	E	281	
7	F	263	

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Mol	Chain	Length	Quality of chain
8	G	204	
9	H	249	
10	I	432	
11	J	208	
12	K	194	
13	L	149	
14	M	158	
15	N	132	
16	O	151	
17	P	168	
18	Q	145	
19	R	172	
20	S	135	
21	T	152	
22	U	145	
23	V	119	
24	W	83	
25	X	130	
26	Y	143	
27	Z	131	
28	a	124	
29	b	101	
30	c	84	
31	d	69	
32	e	56	

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Mol	Chain	Length	Quality of chain
33	f	133	
34	g	188	
35	h	317	
36	j	315	
37	n	25	
38	z	400	
39	i	75	

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 82981 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1697	Total	C	N	O	P	0	0
			36227	16170	6504	11857	1696		

- Molecule 2 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	99	Total	C	N	O	S	0	0
			798	503	143	148	4		

- Molecule 3 is a protein called uS2 (SA).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	217	Total	C	N	O	S	0	0
			1710	1086	300	316	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	114	THR	ALA	conflict	UNP G1TLT8

- Molecule 4 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 5 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	221	Total	C	N	O	S	0	0
			1716	1111	295	301	9		

- Molecule 6 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	228	Total	C	N	O	S	0	0
			1768	1126	318	316	8		

- Molecule 7 is a protein called eS4 (S4 X isoform).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	25	GLY	SER	conflict	UNP G1TK17
F	51	ARG	LYS	conflict	UNP G1TK17
F	78	THR	ALA	conflict	UNP G1TK17
F	156	VAL	MET	conflict	UNP G1TK17

- Molecule 8 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	191	Total	C	N	O	S	0	0
			1509	943	286	273	7		

- Molecule 9 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 10 is a protein called eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	185	Total	C	N	O	S	0	0
			1488	952	271	264	1		

- Molecule 11 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	206	Total	C	N	O	S	1	0
			1691	1061	333	292	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 12 is a protein called uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 13 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 14 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	151	Total	C	N	O	S	0	0
			1233	785	231	211	6		

- Molecule 15 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	117	Total	C	N	O	S	0	0
			908	570	161	169	8		

- Molecule 16 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 17 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 18 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	120	Total	C	N	O	S	0	0
			997	635	187	168	7		

- Molecule 19 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 20 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 21 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 22 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	141	Total	C	N	O	S	0	0
			1097	688	211	195	3		

- Molecule 23 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 24 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	3	ASN	SER	conflict	UNP G1TM82
W	4	ASP	ASN	conflict	UNP G1TM82
W	33	GLN	PRO	conflict	UNP G1TM82
W	50	PHE	SER	conflict	UNP G1TM82
W	75	ALA	SER	conflict	UNP G1TM82
W	76	ASP	HIS	conflict	UNP G1TM82
W	81	LYS	GLN	conflict	UNP G1TM82

- Molecule 25 is a protein called uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 26 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 27 is a protein called eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

- Molecule 28 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	77	Total	C	N	O	S	0	0
			614	393	114	106	1		

- Molecule 29 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	28	ARG	CYS	conflict	UNP G1TFE8

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Chain	Residue	Modelled	Actual	Comment	Reference
b	56	ALA	VAL	conflict	UNP G1TFE8

- Molecule 30 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 31 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	67	Total	C	N	O	S	0	0
			530	321	108	99	2		

- Molecule 32 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 33 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	57	Total	C	N	O	S	0	0
			457	282	101	73	1		

- Molecule 34 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 35 is a protein called Receptor for Activated C Kinase 1 (RACK1).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 36 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	182	Total	C	N	O	S	0	0
			1221	781	225	212	3		

- Molecule 37 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 38 is a RNA chain called HCV IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	z	188	Total	C	N	O	P	0	0
			4017	1789	721	1319	188		

- Molecule 39 is a RNA chain called Met-tRNA-i-Met.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	75	Total	C	N	O	P	0	0
			1604	717	298	515	74		

- Molecule 40 is ZINC ION (CCD ID: ZN) (formula: Zn).

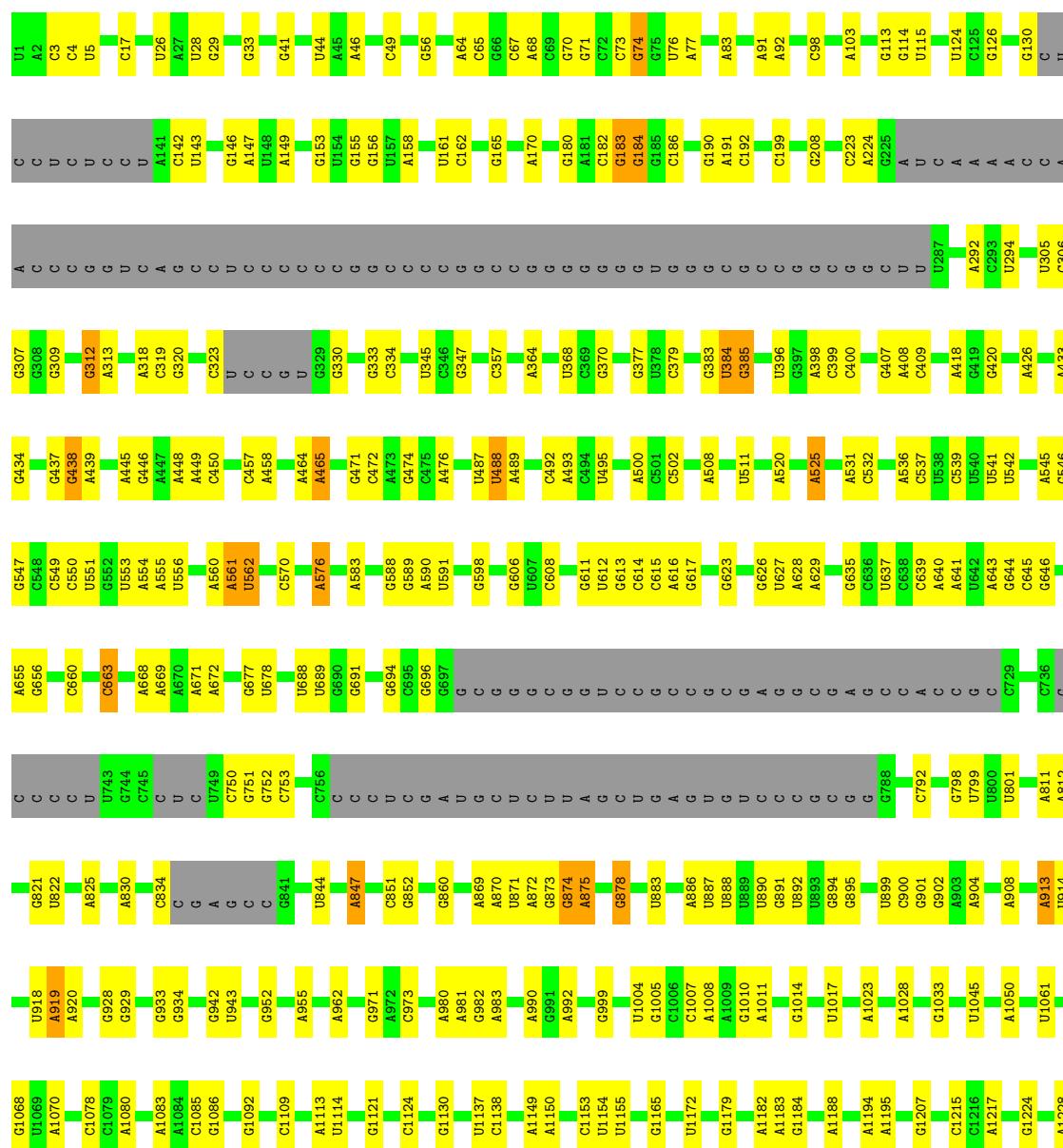
Mol	Chain	Residues	Atoms		AltConf
40	b	1	Total	Zn	0
			1	1	

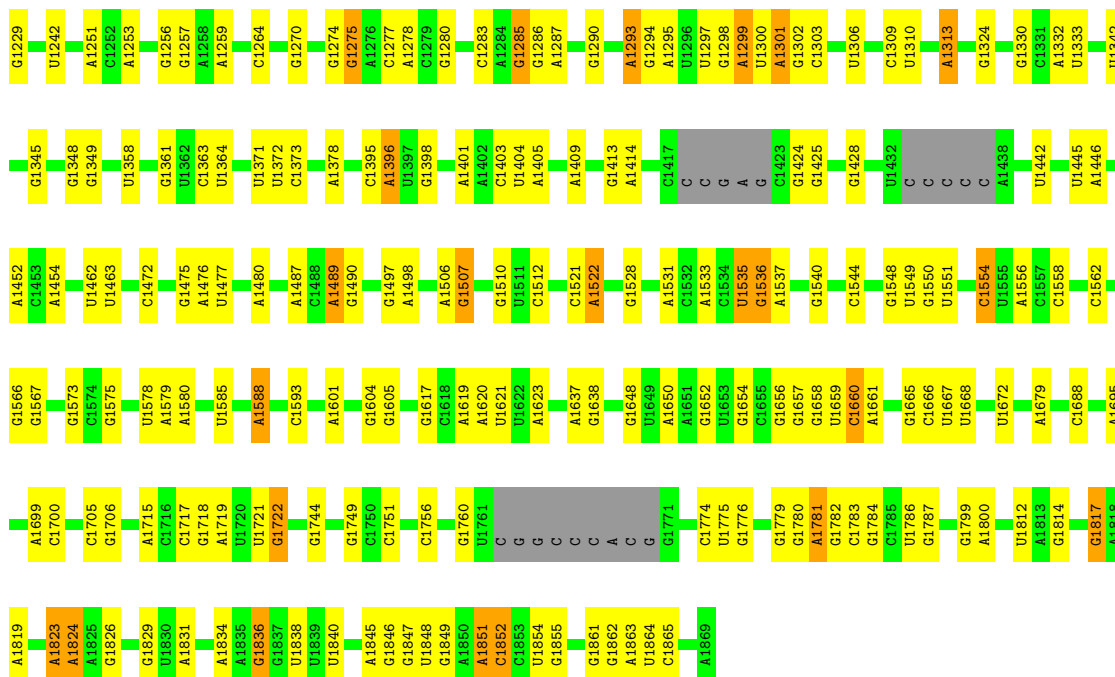
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: 18S rRNA

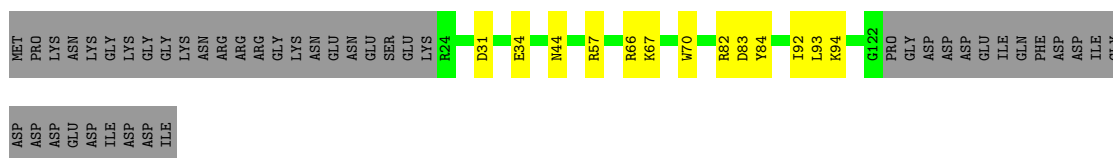
Chain 2: 





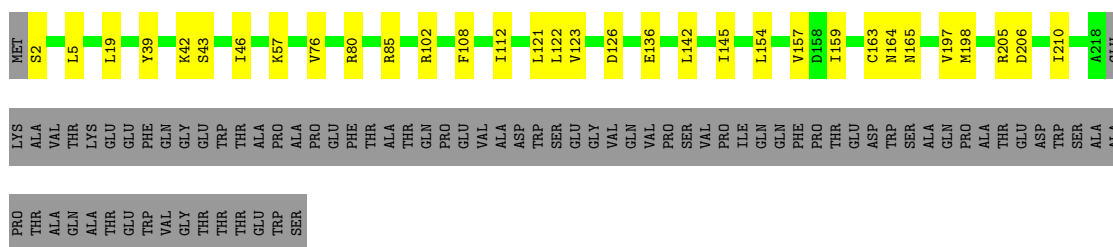
• Molecule 2: Eukaryotic translation initiation factor 1A, X-chromosomal

Chain A: 60% 9% 31%



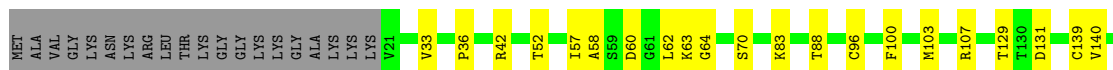
• Molecule 3: uS2 (SA)

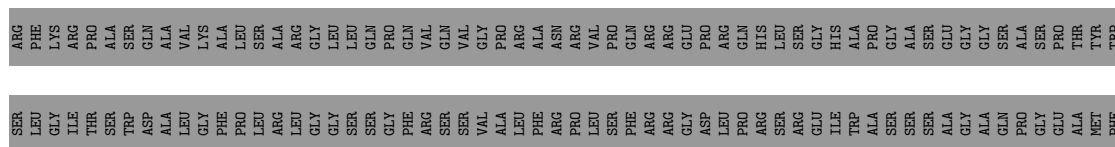
Chain B: 63% 11% 26%



• Molecule 4: eS1

Chain C: 70% 11% 19%





- Molecule 11: eS8

Chain J: 88% 11% .



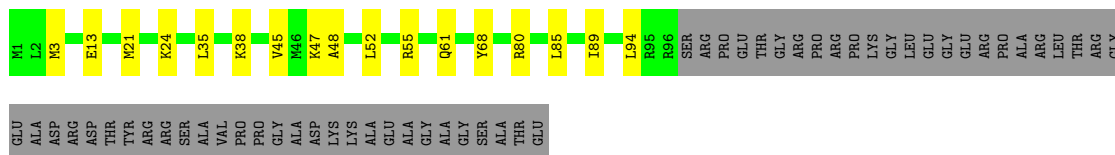
- Molecule 12: uS4

Chain K: 85% 10% 5%



- Molecule 13: eS10

Chain L: 53% 11% 36%



- Molecule 14: uS17

Chain M: 84% 12% .



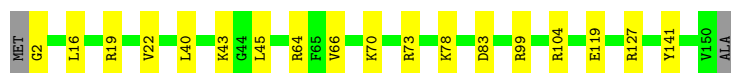
- Molecule 15: eS12

Chain N: 77% 12% 11%



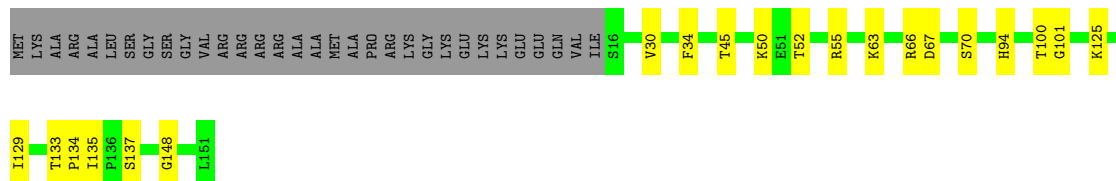
- Molecule 16: uS15

Chain O: 87% 12% .



• Molecule 17: uS11

Chain P: 69% 12% 19%



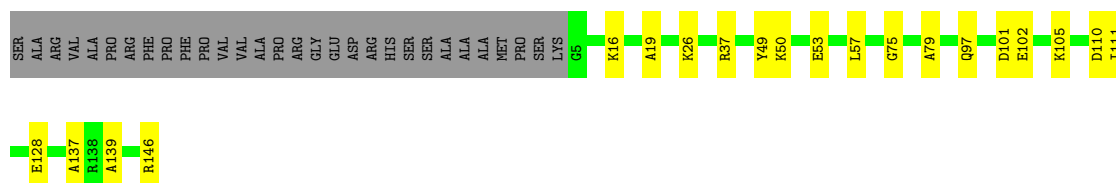
• Molecule 18: uS19

Chain Q: 74% 8% 17%



• Molecule 19: uS9

Chain R: 71% 12% 17%



• Molecule 20: eS17

Chain S: 86% 12% .



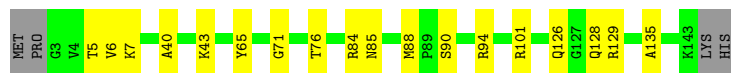
• Molecule 21: uS13

Chain T: 85% 10% 5%



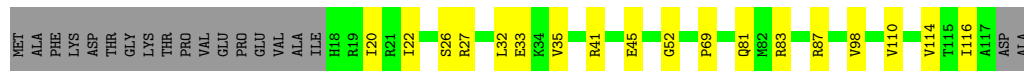
• Molecule 22: eS19

Chain U: 85% 12% .

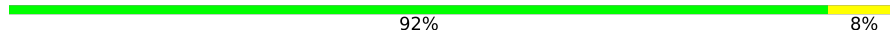


- Molecule 23: uS10

Chain V:  69% 15% 16%



- Molecule 24: eS21

Chain W:  92% 8%

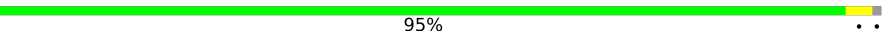


- Molecule 25: uS8

Chain X:  91% 8%



- Molecule 26: uS12

Chain Y:  95%



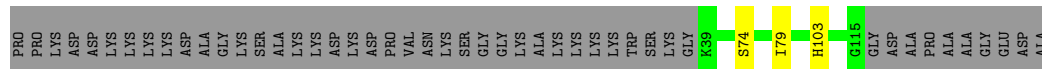
- Molecule 27: eS24

Chain Z:  89% 6% 5%



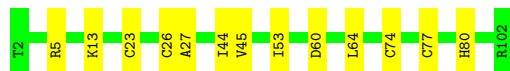
- Molecule 28: eS25

Chain a:  60% 38%



- Molecule 29: eS26

Chain b:  87% 13%



- Molecule 30: eS27

Diagram illustrating the structure of a protein segment, showing residues MET, P2, H19, K22, R23, S27, Q51, R80, and H84. The residues are represented by colored blocks (grey, green, yellow) connected by a horizontal line.

Amino Acid	Information Content (bits)
MET	~0.01
ASP	~0.01
T3	~0.35
K16	~0.35
T21	~0.35
G22	~0.35
R31	~0.35
R44	~0.35
N45	~0.35
D54	~0.35
E60	~0.35
R66	~0.35
R69	~0.35

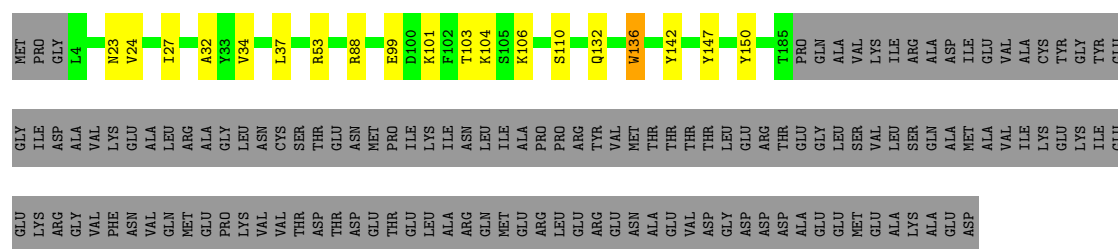
Sequence logo for the 12-mer motif. The y-axis represents information content in bits, ranging from 0 to 1.5. The x-axis shows positions 1 through 12. The sequence METG2W8R22Y34N37Q41C42F43A47D56 is displayed above the bars. MET, W8, N37, Q41, F43, A47, and D56 are highlighted in grey, while G2, R22, Y34, and C42 are highlighted in red.

ALA	LEU	SER	THR	GLY	VAL	VAL	GLN	HIS	THR	LEU	GLY	LYS	VAL	GLY	ARG	GLN	THR	GLY	ARG
R76	L79	A80	R81	K94	K97	R104	Y111	R114	N129	S132	P135	G136	D137	E138	F139	C140	V141	I142	M143

[illegible]

L179	K183	L184	T199	L206	K212	Q215	L218	N222	D231	I235	L239	C240	N244	R245	Y246	V247	L248	I258	Q272	T287	D294	C295	R308	G314	GLY	THR	ARG	PET	T2	E3	T10	V18	T19	Q20	S35	R36	I40	L59	V66	V69	S72	S73	D74	L79	S82	A83	D84	R88	T97	T98	R99	T105	K106	D107	S114	R125	H126	K127	W132	L135	E149	N162	P163	D171
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------

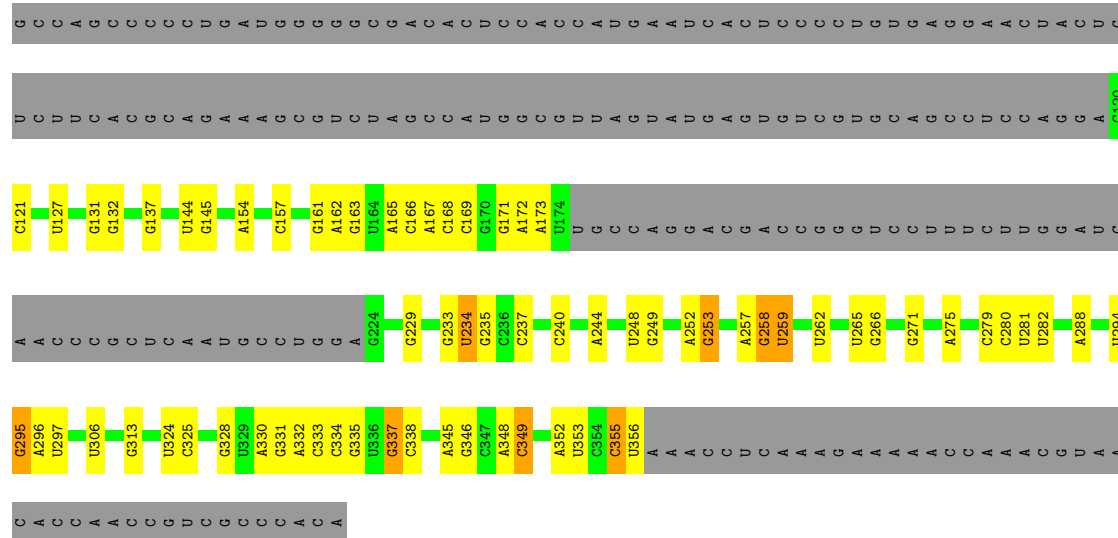
Chain j: 52% 6% 42%



Chain n: 84% 16%



Chain z: 30% 15% . 53%



Chain i: 75% 21% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	103813	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	70.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	56000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	2	0.14	0/40506	0.31	0/63123
2	A	0.16	0/809	0.47	0/1083
3	B	0.21	0/1747	0.53	2/2374 (0.1%)
4	C	0.17	0/1756	0.45	0/2350
5	D	0.18	0/1753	0.42	0/2369
6	E	0.20	0/1796	0.50	0/2417
7	F	0.15	0/2118	0.40	0/2849
8	G	0.17	0/1531	0.49	2/2059 (0.1%)
9	H	0.16	0/1946	0.38	0/2590
10	I	0.18	0/1510	0.47	0/2022
11	J	0.18	0/1723	0.46	0/2298
12	K	0.19	0/1550	0.47	0/2069
13	L	0.23	0/834	0.60	2/1125 (0.2%)
14	M	0.19	0/1254	0.49	0/1677
15	N	0.25	0/918	0.61	0/1233
16	O	0.17	0/1226	0.41	0/1649
17	P	0.15	0/1029	0.38	0/1380
18	Q	0.21	0/1017	0.51	0/1358
19	R	0.22	0/1146	0.52	0/1534
20	S	0.21	0/1082	0.61	2/1452 (0.1%)
21	T	0.20	0/1208	0.50	0/1618
22	U	0.17	0/1115	0.45	0/1493
23	V	0.16	0/805	0.43	0/1081
24	W	0.15	0/643	0.41	0/860
25	X	0.18	0/1051	0.46	0/1406
26	Y	0.19	0/1116	0.49	0/1490
27	Z	0.20	0/1028	0.44	0/1366
28	a	0.19	0/620	0.52	0/831
29	b	0.16	0/828	0.41	0/1109
30	c	0.17	0/665	0.41	0/891
31	d	0.17	0/532	0.44	0/712
32	e	0.15	0/470	0.39	0/623

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	f	0.15	0/462	0.45	0/607
34	g	0.22	0/567	0.47	0/753
35	h	0.16	0/2493	0.46	0/3394
36	j	0.26	0/1239	0.60	3/1680 (0.2%)
37	n	0.19	0/240	0.38	0/305
38	z	0.13	0/4488	0.28	0/6995
39	i	0.12	0/1795	0.26	0/2798
All	All	0.16	0/88616	0.39	11/129023 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	j	136	TRP	CD2-CE3-CZ3	8.48	129.63	118.60
36	j	99	GLU	CA-CB-CG	6.14	126.39	114.10
8	G	141	VAL	CA-C-N	6.01	129.81	120.68
8	G	141	VAL	C-N-CA	6.01	129.81	120.68
36	j	136	TRP	CE2-CD2-CE3	5.92	124.72	118.80
13	L	13	GLU	CA-CB-CG	5.71	125.52	114.10
13	L	13	GLU	N-CA-CB	5.36	119.13	110.40
3	B	43	SER	CA-C-N	5.31	131.68	121.54
3	B	43	SER	C-N-CA	5.31	131.68	121.54
20	S	75	GLU	CA-C-N	5.01	131.11	121.54
20	S	75	GLU	C-N-CA	5.01	131.11	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	36227	0	18299	177	0
2	A	798	0	807	9	0
3	B	1710	0	1708	22	0
4	C	1729	0	1803	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1716	0	1806	13	0
6	E	1768	0	1866	18	0
7	F	2076	0	2177	18	0
8	G	1509	0	1563	12	0
9	H	1923	0	2089	17	0
10	I	1488	0	1582	13	0
11	J	1691	0	1778	14	0
12	K	1525	0	1640	15	0
13	L	810	0	836	11	0
14	M	1233	0	1310	13	0
15	N	908	0	939	11	0
16	O	1202	0	1289	15	0
17	P	1016	0	1039	16	0
18	Q	997	0	1045	9	0
19	R	1128	0	1195	17	0
20	S	1068	0	1121	12	0
21	T	1190	0	1249	10	0
22	U	1097	0	1130	13	0
23	V	795	0	862	12	0
24	W	636	0	637	6	0
25	X	1034	0	1080	7	0
26	Y	1098	0	1167	3	0
27	Z	1011	0	1083	5	0
28	a	614	0	678	2	0
29	b	814	0	863	12	0
30	c	651	0	672	4	0
31	d	530	0	561	7	0
32	e	459	0	452	6	0
33	f	457	0	502	8	0
34	g	555	0	565	5	0
35	h	2436	0	2393	33	0
36	j	1221	0	969	9	0
37	n	239	0	289	5	0
38	z	4017	0	2033	16	0
39	i	1604	0	816	5	0
40	b	1	0	0	0	0
All	All	82981	0	63893	494	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (494) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:318:A:C2	1:2:333:G:N1	2.35	0.95
1:2:1722:G:H1	1:2:1812:U:H3	1.27	0.81
1:2:1656:G:H1	1:2:1668:U:H3	1.32	0.76
1:2:318:A:N1	1:2:333:G:C6	2.52	0.76
1:2:1657:G:H1	1:2:1667:U:H3	1.37	0.71
38:z:145:G:H1	38:z:248:U:H3	1.37	0.71
29:b:23:CYS:SG	29:b:26:CYS:HB3	2.32	0.69
1:2:318:A:C2	1:2:333:G:C6	2.80	0.69
1:2:1554:C:N3	13:L:24:LYS:NZ	2.44	0.66
6:E:116:ARG:NH1	6:E:150:MET:SD	2.71	0.64
1:2:318:A:C2	1:2:333:G:C2	2.86	0.64
35:h:163:PRO:HB2	35:h:179:LEU:HD12	1.83	0.61
1:2:1033:G:H1	1:2:1080:A:HO2'	1.48	0.61
1:2:377:G:H5'	11:J:98:LYS:HB3	1.82	0.61
23:V:26:SER:HB3	23:V:32:LEU:HD12	1.83	0.61
18:Q:80:LEU:HB3	18:Q:83:MET:HE3	1.83	0.60
1:2:1566:G:N7	22:U:101:ARG:NH2	2.49	0.60
17:P:67:ASP:HB2	17:P:70:SER:HB3	1.85	0.59
34:g:141:CYS:SG	34:g:144:CYS:N	2.73	0.59
1:2:334:C:H5	9:H:190:ARG:HH12	1.49	0.59
1:2:1652:G:H1	1:2:1672:U:H3	1.50	0.59
3:B:163:CYS:SG	3:B:164:ASN:N	2.75	0.59
4:C:52:THR:HG22	4:C:58:ALA:H	1.66	0.59
19:R:37:ARG:HB3	22:U:7:LYS:HG2	1.84	0.59
1:2:1700:C:H5	1:2:1836:G:H1	1.52	0.58
1:2:1014:G:N2	30:c:51:GLN:OE1	2.36	0.58
2:A:82:ARG:NH2	2:A:84:TYR:OH	2.36	0.58
7:F:44:LEU:HD21	7:F:72:ILE:HD11	1.85	0.58
7:F:11:ARG:NH2	7:F:21:ASP:OD1	2.36	0.58
1:2:1522:A:H62	18:Q:131:PRO:HG3	1.68	0.58
26:Y:94:ILE:HG12	26:Y:125:VAL:HG21	1.85	0.58
7:F:60:GLU:OE2	27:Z:20:ARG:NH2	2.37	0.58
1:2:1605:G:OP1	22:U:84:ARG:NH2	2.35	0.57
1:2:1658:G:OP2	1:2:1660:C:N4	2.37	0.57
9:H:7:PHE:HB2	9:H:124:LEU:HD23	1.86	0.57
21:T:68:ILE:O	21:T:72:GLN:NE2	2.37	0.57
3:B:19:LEU:HD13	20:S:117:LEU:HD21	1.86	0.57
9:H:5:ILE:HG12	9:H:111:LEU:HD12	1.87	0.57
1:2:1293:A:N6	1:2:1306:U:C2	2.73	0.57
1:2:1824:A:O2'	2:A:67:LYS:NZ	2.37	0.57
7:F:79:ASP:HB3	7:F:82:TYR:HB2	1.86	0.56
29:b:45:VAL:HG11	29:b:53:ILE:HG13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:34:GLU:OE2	2:A:57:ARG:NH1	2.39	0.56
3:B:205:ARG:NH2	20:S:81:ARG:O	2.37	0.56
15:N:51:VAL:HG12	15:N:77:ILE:HB	1.86	0.56
1:2:952:G:H21	17:P:52:THR:HG21	1.70	0.56
1:2:1373:C:O2'	20:S:10:LYS:NZ	2.39	0.56
26:Y:105:PHE:HD1	26:Y:121:LYS:HB3	1.71	0.56
1:2:124:U:OP1	9:H:201:LYS:NZ	2.39	0.55
13:L:80:ARG:NH1	13:L:89:ILE:O	2.40	0.55
1:2:1349:G:H21	3:B:112:ILE:HD11	1.71	0.55
1:2:562:U:OP1	12:K:134:HIS:NE2	2.34	0.55
31:d:44:ARG:HH22	31:d:60:GLU:HG2	1.71	0.55
2:A:83:ASP:OD2	33:f:81:ARG:NH1	2.39	0.55
19:R:16:LYS:HD3	19:R:79:ALA:HA	1.88	0.55
1:2:919:A:OP2	16:O:64:ARG:NH2	2.39	0.55
1:2:851:C:H5''	1:2:852:G:H5'	1.89	0.55
1:2:1396:A:O2'	1:2:1398:G:N7	2.40	0.55
3:B:210:ILE:HD13	20:S:81:ARG:HD2	1.89	0.54
5:D:200:ARG:O	12:K:54:ARG:NH1	2.37	0.54
11:J:165:GLN:HE22	11:J:195:LEU:HD11	1.72	0.54
35:h:105:THR:HG23	35:h:106:LYS:HG2	1.89	0.54
10:I:10:LYS:HD3	10:I:11:PRO:HD2	1.90	0.54
39:i:24:U:H2'	39:i:25:G:H8	1.73	0.54
1:2:153:G:N3	9:H:13:GLN:NE2	2.54	0.54
9:H:137:ARG:HB3	9:H:140:ARG:HG3	1.88	0.54
1:2:1472:C:H42	1:2:1476:A:H62	1.54	0.54
1:2:1718:G:H5'	37:n:21:ARG:HH12	1.72	0.54
38:z:252:A:H4'	38:z:253:G:H5'	1.89	0.54
13:L:35:LEU:HD23	13:L:38:LYS:HD2	1.89	0.54
19:R:102:GLU:HB2	19:R:105:LYS:HE3	1.89	0.54
1:2:637:U:OP2	33:f:97:LYS:NZ	2.41	0.54
35:h:20:GLN:HG2	35:h:69:VAL:H	1.73	0.54
35:h:183:LYS:NZ	35:h:184:LEU:O	2.40	0.54
1:2:913:A:N6	10:I:119:SER:O	2.41	0.54
1:2:1409:A:OP1	19:R:26:LYS:NZ	2.39	0.54
27:Z:17:LEU:HD12	27:Z:18:LEU:HG	1.90	0.54
3:B:126:ASP:OD1	3:B:165:ASN:ND2	2.41	0.53
6:E:105:LEU:HD12	6:E:122:VAL:HG11	1.90	0.53
8:G:49:LEU:HD12	19:R:50:LYS:HG2	1.90	0.53
18:Q:123:TYR:OH	21:T:124:ARG:NH1	2.42	0.53
1:2:511:U:O2'	1:2:576:A:N6	2.41	0.53
1:2:561:A:H5'	12:K:171:GLY:HA3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:138:GLU:HG3	16:O:19:ARG:HE	1.73	0.53
19:R:146:ARG:NH2	39:i:32:C:OP2	2.42	0.53
38:z:127:U:OP1	38:z:313:G:O2'	2.26	0.53
14:M:120:VAL:HG12	14:M:145:VAL:HG11	1.90	0.53
1:2:91:A:H5'	1:2:92:A:H5''	1.91	0.53
1:2:1172:U:O2	1:2:1188:A:N7	2.42	0.53
10:I:65:PRO:HG2	10:I:68:GLN:HB2	1.90	0.53
29:b:26:CYS:SG	29:b:27:ALA:N	2.82	0.53
7:F:187:ALA:O	7:F:245:ARG:NH2	2.42	0.53
1:2:1277:C:H2'	1:2:1278:A:H8	1.74	0.52
1:2:1719:A:N6	1:2:1814:G:O2'	2.42	0.52
1:2:1007:C:O2'	16:O:104:ARG:NH2	2.42	0.52
4:C:149:GLN:NE2	4:C:151:ARG:O	2.42	0.52
6:E:16:ILE:HG21	32:e:22:ARG:HH11	1.74	0.52
3:B:154:LEU:HD22	3:B:157:VAL:HG21	1.91	0.52
7:F:80:ILE:HG23	7:F:81:THR:HG23	1.92	0.52
32:e:43:PHE:O	32:e:47:ALA:HB2	2.08	0.52
1:2:334:C:OP2	9:H:190:ARG:NH2	2.43	0.52
22:U:40:ALA:HB3	22:U:43:LYS:HG2	1.91	0.52
35:h:120:ILE:HB	35:h:132:TRP:HB2	1.92	0.52
10:I:138:GLU:OE2	16:O:19:ARG:NH2	2.43	0.52
1:2:318:A:N1	1:2:333:G:O6	2.43	0.52
22:U:76:THR:HG22	22:U:94:ARG:HB3	1.92	0.52
35:h:215:GLN:NE2	35:h:231:ASP:OD1	2.42	0.52
31:d:44:ARG:NH2	31:d:60:GLU:O	2.43	0.51
38:z:248:U:H2'	38:z:249:G:H8	1.75	0.51
1:2:1179:G:N2	1:2:1182:A:OP2	2.43	0.51
3:B:108:PHE:HB2	3:B:136:GLU:HG2	1.91	0.51
1:2:1310:U:OP1	15:N:36:ARG:NH2	2.43	0.51
1:2:1824:A:N3	2:A:66:ARG:NH1	2.58	0.51
18:Q:41:GLN:HG3	18:Q:84:ILE:HD12	1.92	0.51
7:F:45:ILE:HG13	7:F:61:VAL:HG11	1.92	0.51
2:A:92:ILE:HG22	2:A:93:LEU:HG	1.92	0.51
16:O:70:LYS:HE3	16:O:73:ARG:HE	1.74	0.51
1:2:1124:C:H5''	4:C:150:ILE:HG12	1.92	0.51
1:2:1593:C:OP1	28:a:103:HIS:NE2	2.43	0.51
3:B:2:SER:N	24:W:78:ILE:O	2.44	0.51
23:V:81:GLN:OE1	23:V:83:ARG:NH1	2.41	0.51
1:2:539:C:H42	1:2:545:A:H61	1.59	0.51
1:2:65:C:N4	9:H:134:GLY:O	2.44	0.51
1:2:1847:G:N7	37:n:12:ARG:NH2	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:211:LYS:HG2	5:D:215:MET:HE2	1.93	0.51
1:2:1507:G:N2	34:g:87:THR:OG1	2.39	0.50
13:L:85:LEU:HD21	13:L:89:ILE:HB	1.92	0.50
22:U:5:THR:HG23	22:U:7:LYS:H	1.76	0.50
1:2:396:U:OP2	14:M:79:LYS:NZ	2.44	0.50
1:2:1654:G:OP1	22:U:90:SER:OG	2.28	0.50
12:K:113:GLN:O	12:K:117:LEU:HB2	2.11	0.50
1:2:1130:G:N2	1:2:1130:G:OP2	2.43	0.50
2:A:70:TRP:O	2:A:94:LYS:NZ	2.43	0.50
19:R:97:GLN:HB2	19:R:105:LYS:HG3	1.94	0.50
17:P:30:VAL:HG12	17:P:94:HIS:HB2	1.93	0.50
35:h:72:SER:OG	35:h:74:ASP:OD2	2.29	0.50
35:h:245:ARG:NH1	35:h:295:GLY:O	2.45	0.50
1:2:476:A:N3	1:2:488:U:O2'	2.45	0.50
3:B:80:ARG:NH2	3:B:165:ASN:O	2.45	0.50
38:z:258:G:N2	38:z:259:U:O4	2.45	0.50
1:2:1717:C:O2'	37:n:21:ARG:NH1	2.44	0.50
5:D:187:ARG:HD3	5:D:192:LEU:HD12	1.94	0.50
16:O:40:LEU:HD23	16:O:43:LYS:HD3	1.93	0.50
35:h:247:TRP:HB3	35:h:258:ILE:HD11	1.94	0.50
3:B:85:ARG:NH2	20:S:82:ASP:O	2.44	0.49
16:O:22:VAL:HG22	16:O:66:VAL:HG12	1.93	0.49
36:j:110:SER:OG	39:i:18:G:N7	2.40	0.49
4:C:64:GLY:O	17:P:50:LYS:NZ	2.43	0.49
35:h:99:ARG:NH1	35:h:135:LEU:O	2.45	0.49
35:h:244:ASN:ND2	35:h:294:ASP:O	2.45	0.49
1:2:312:G:O2'	9:H:191:ARG:NH1	2.45	0.49
1:2:1050:A:H62	1:2:1068:G:H21	1.59	0.49
14:M:88:ILE:HD11	14:M:109:MET:HE2	1.94	0.49
1:2:1299:A:O2'	1:2:1301:A:OP1	2.30	0.49
36:j:132:GLN:HA	36:j:136:TRP:HB2	1.93	0.49
24:W:21:ASN:HB3	25:X:67:GLY:HA3	1.93	0.49
1:2:1851:A:H5'	37:n:1:MET:HE2	1.95	0.49
1:2:457:C:H2'	1:2:458:A:H8	1.77	0.49
4:C:139:CYS:SG	4:C:140:VAL:N	2.86	0.49
35:h:212:LYS:HA	35:h:235:ILE:HG13	1.94	0.49
1:2:345:U:OP1	7:F:37:LYS:NZ	2.44	0.49
1:2:464:A:H3'	1:2:465:A:H8	1.77	0.49
1:2:1679:A:H2'	8:G:60:ARG:HG3	1.94	0.49
23:V:35:VAL:HG11	23:V:110:VAL:HG11	1.94	0.49
1:2:860:G:H21	25:X:107:SER:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:495:U:O2'	7:F:27:PHE:O	2.30	0.48
4:C:36:PRO:O	4:C:42:ARG:NH1	2.46	0.48
11:J:48:VAL:HG11	11:J:54:LYS:HD3	1.96	0.48
14:M:93:LEU:HD23	14:M:104:LYS:HB3	1.95	0.48
1:2:64:A:H2	1:2:83:A:H62	1.60	0.48
1:2:161:U:O2'	9:H:87:ARG:NH2	2.46	0.48
35:h:114:SER:HB3	35:h:119:GLN:HB2	1.95	0.48
4:C:107:ARG:NH1	17:P:133:THR:O	2.43	0.48
15:N:82:ASN:HB3	15:N:105:GLY:HA3	1.94	0.48
38:z:294:U:H2'	38:z:295:G:H2'	1.95	0.48
1:2:1401:A:H4'	23:V:52:GLY:HA3	1.94	0.48
22:U:65:TYR:HE1	22:U:128:GLN:HE21	1.61	0.48
38:z:257:A:N6	38:z:275:A:OP2	2.44	0.48
1:2:869:A:OP2	14:M:152:LYS:NZ	2.46	0.48
1:2:1512:C:H5''	32:e:8:TRP:HZ3	1.79	0.48
8:G:21:GLY:HA2	19:R:49:TYR:HE2	1.78	0.48
13:L:85:LEU:HD11	13:L:89:ILE:HD12	1.96	0.48
17:P:101:GLY:HA3	17:P:134:PRO:HG2	1.95	0.48
1:2:155:G:H2'	1:2:156:G:H8	1.78	0.48
1:2:1775:U:N3	1:2:1776:G:O6	2.46	0.48
6:E:142:LEU:HD13	6:E:150:MET:HE2	1.95	0.48
35:h:107:ASP:HB2	35:h:125:ARG:HG3	1.95	0.48
1:2:678:U:OP1	16:O:127:ARG:NH2	2.45	0.48
1:2:1403:C:OP2	1:2:1405:A:N6	2.43	0.48
1:2:1717:C:N3	1:2:1817:G:N2	2.62	0.48
3:B:145:ILE:HG12	3:B:159:ILE:HB	1.96	0.48
7:F:137:PRO:HB2	7:F:150:PRO:HD2	1.95	0.48
14:M:22:ARG:HB2	14:M:25:LEU:HD22	1.96	0.48
15:N:80:ASP:OD1	15:N:80:ASP:N	2.45	0.48
1:2:439:A:H4'	1:2:1799:G:H4'	1.96	0.47
1:2:1113:A:OP1	38:z:295:G:N1	2.45	0.47
1:2:1270:G:O2'	1:2:1301:A:N7	2.47	0.47
24:W:15:ARG:NH1	24:W:33:GLN:OE1	2.43	0.47
35:h:199:THR:HG21	35:h:240:CYS:HA	1.95	0.47
1:2:17:C:O2'	1:2:1194:A:N1	2.46	0.47
1:2:71:G:O6	9:H:170:ARG:NH1	2.47	0.47
35:h:127:LYS:HE3	35:h:149:GLU:HA	1.96	0.47
36:j:23:ASN:HB2	36:j:37:LEU:HD21	1.95	0.47
1:2:520:A:O2'	1:2:825:A:N3	2.42	0.47
13:L:21:MET:HE2	13:L:45:VAL:HG11	1.96	0.47
1:2:1851:A:OP1	37:n:9:ARG:NH1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:61:GLN:HB3	13:L:68:TYR:HB2	1.95	0.47
1:2:615:C:O2'	33:f:79:LEU:O	2.32	0.47
1:2:942:G:N2	17:P:137:SER:O	2.48	0.47
1:2:1549:U:OP1	32:e:34:TYR:OH	2.30	0.47
11:J:114:GLU:OE2	11:J:123:ARG:NH1	2.48	0.47
11:J:173:ALA:HA	11:J:189:VAL:HA	1.97	0.47
15:N:54:SER:OG	15:N:55:ASN:N	2.47	0.47
29:b:74:CYS:SG	29:b:77:CYS:CB	2.92	0.47
1:2:1424:G:H2'	1:2:1425:G:H8	1.80	0.47
20:S:29:HIS:HA	20:S:32:LYS:HE2	1.95	0.47
1:2:3:C:O2	12:K:18:ARG:NH2	2.48	0.47
1:2:1398:G:H4'	35:h:88:ARG:HH22	1.79	0.47
35:h:18:VAL:O	35:h:287:THR:OG1	2.33	0.47
1:2:1540:G:OP2	22:U:43:LYS:NZ	2.47	0.47
4:C:57:ILE:HG23	4:C:60:ASP:H	1.80	0.47
35:h:162:ASN:ND2	35:h:222:ASN:OD1	2.48	0.47
1:2:1092:G:OP1	16:O:2:GLY:N	2.48	0.46
27:Z:58:PHE:HE1	27:Z:74:MET:HE1	1.79	0.46
35:h:35:SER:OG	35:h:36:ARG:N	2.48	0.46
35:h:88:ARG:HD2	35:h:97:THR:HG21	1.97	0.46
1:2:1550:G:H3'	1:2:1579:A:H61	1.80	0.46
5:D:138:GLY:HA3	5:D:162:ILE:HG22	1.97	0.46
11:J:87:ASN:HB3	11:J:90:LEU:HD13	1.97	0.46
13:L:47:LYS:HA	13:L:47:LYS:HD3	1.72	0.46
13:L:52:LEU:HA	13:L:55:ARG:HG2	1.97	0.46
1:2:183:G:O2'	1:2:184:G:O4'	2.32	0.46
1:2:1562:C:H5''	22:U:71:GLY:HA3	1.97	0.46
19:R:97:GLN:HG3	19:R:105:LYS:HE2	1.98	0.46
1:2:570:C:O2'	27:Z:34:THR:O	2.33	0.46
1:2:847:A:OP1	7:F:108:ARG:NH2	2.49	0.46
6:E:127:MET:HE2	6:E:133:GLY:HA2	1.97	0.46
36:j:53:ARG:HG3	36:j:88:ARG:HD2	1.97	0.46
1:2:812:A:H5''	7:F:16:LYS:HD3	1.98	0.46
1:2:1332:A:O2'	6:E:145:GLN:O	2.33	0.46
3:B:5:LEU:HD21	24:W:41:LYS:HA	1.96	0.46
7:F:48:LEU:HD23	7:F:61:VAL:HG23	1.97	0.46
16:O:99:ARG:NH1	16:O:119:GLU:OE2	2.47	0.46
35:h:149:GLU:HG2	35:h:171:ASP:HB3	1.98	0.46
1:2:934:G:H22	1:2:1008:A:H2	1.64	0.46
1:2:1544:C:O2'	19:R:75:GLY:O	2.34	0.46
34:g:104:LYS:HE2	34:g:104:LYS:HB2	1.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1275:G:N2	1:2:1506:A:OP2	2.41	0.45
1:2:1619:A:O2'	18:Q:82:ASP:OD2	2.33	0.45
23:V:26:SER:HB2	23:V:110:VAL:HA	1.98	0.45
1:2:28:U:H2'	1:2:29:G:H8	1.81	0.45
1:2:1854:U:H2'	1:2:1855:G:H8	1.82	0.45
3:B:39:TYR:OH	20:S:104:GLU:OE2	2.31	0.45
5:D:109:ILE:HD11	5:D:151:ILE:HD11	1.98	0.45
11:J:66:SER:HA	11:J:73:THR:HG22	1.98	0.45
10:I:105:THR:HG23	10:I:108:SER:H	1.81	0.45
12:K:60:LEU:HD11	12:K:70:ARG:HA	1.99	0.45
18:Q:34:MET:HB3	18:Q:42:ARG:HG3	1.98	0.45
39:i:19:A:N7	39:i:59:A:N6	2.61	0.45
1:2:616:A:OP1	26:Y:68:LYS:NZ	2.49	0.45
1:2:973:C:O2	17:P:55:ARG:NH1	2.50	0.45
1:2:1705:C:O2	1:2:1851:A:O2'	2.29	0.45
1:2:1722:G:O6	1:2:1812:U:O4	2.34	0.45
4:C:103:MET:HB3	4:C:215:VAL:HB	1.97	0.45
6:E:64:ARG:HE	13:L:94:LEU:HG	1.81	0.45
25:X:31:SER:HB3	25:X:34:ILE:HG13	1.98	0.45
1:2:1283:C:O2'	1:2:1313:A:N1	2.43	0.45
1:2:1445:U:O4	1:2:1446:A:N6	2.49	0.45
3:B:121:LEU:HD21	3:B:145:ILE:HD12	1.98	0.45
15:N:113:ASP:HB3	15:N:116:LYS:HG3	1.99	0.45
29:b:60:ASP:OD1	29:b:60:ASP:N	2.47	0.45
32:e:22:ARG:HH21	32:e:37:ASN:HB2	1.82	0.45
1:2:70:G:OP2	9:H:167:LYS:NZ	2.45	0.45
14:M:125:ILE:HB	14:M:146:THR:HB	1.99	0.45
21:T:34:LYS:HE2	21:T:103:LEU:HD23	1.98	0.45
30:c:80:ARG:HH21	38:z:233:G:H2'	1.81	0.45
39:i:57:A:O2'	39:i:59:A:OP2	2.34	0.45
1:2:1004:U:H2'	1:2:1005:G:H8	1.82	0.45
1:2:1617:G:N2	1:2:1620:A:OP2	2.44	0.45
9:H:230:LYS:HD3	9:H:234:LEU:HD23	1.99	0.45
11:J:101:ILE:HD12	11:J:190:LEU:HD11	1.97	0.45
25:X:53:ILE:HB	25:X:60:LYS:HB2	1.98	0.45
35:h:40:ILE:HB	35:h:59:LEU:HB2	1.99	0.45
1:2:918:U:O2'	1:2:919:A:O4'	2.34	0.45
3:B:102:ARG:HD2	3:B:102:ARG:HA	1.73	0.45
29:b:13:LYS:HA	29:b:13:LYS:HD2	1.86	0.45
23:V:33:GLU:OE2	23:V:87:ARG:NH1	2.49	0.45
36:j:24:VAL:HA	36:j:34:VAL:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1864:U:H3'	29:b:5:ARG:HH21	1.82	0.44
6:E:14:ASP:OD1	6:E:18:LYS:NZ	2.50	0.44
7:F:61:VAL:HA	7:F:64:ILE:HD12	2.00	0.44
1:2:165:G:OP2	1:2:165:G:N2	2.41	0.44
1:2:982:G:H2'	1:2:983:A:H8	1.82	0.44
14:M:111:VAL:HG11	14:M:128:VAL:HG11	1.99	0.44
17:P:45:THR:HG22	17:P:52:THR:HG22	1.99	0.44
18:Q:83:MET:HB2	18:Q:116:LEU:HG	1.99	0.44
22:U:6:VAL:HG12	22:U:135:ALA:HB2	1.99	0.44
1:2:962:A:O2'	36:j:53:ARG:O	2.35	0.44
21:T:25:LYS:O	21:T:29:ALA:N	2.49	0.44
1:2:1324:G:O2'	1:2:1510:G:O2'	2.32	0.44
7:F:87:MET:O	7:F:122:LYS:NZ	2.42	0.44
12:K:65:GLU:OE2	12:K:70:ARG:NH2	2.50	0.44
16:O:16:LEU:O	25:X:57:ARG:NH2	2.50	0.44
23:V:41:ARG:NH1	23:V:45:GLU:OE1	2.51	0.44
24:W:67:ASP:N	24:W:67:ASP:OD1	2.51	0.44
19:R:128:GLU:HG2	19:R:137:ALA:HB1	1.99	0.44
21:T:50:ILE:HD11	21:T:63:GLU:HB2	1.99	0.44
21:T:99:LEU:O	21:T:103:LEU:N	2.46	0.44
34:g:133:ALA:O	34:g:139:HIS:ND1	2.51	0.44
4:C:70:SER:HA	4:C:83:LYS:HG2	2.00	0.44
9:H:70:HIS:HA	9:H:98:ARG:HH12	1.82	0.44
1:2:645:C:H2'	1:2:646:G:H8	1.83	0.44
4:C:62:LEU:O	4:C:88:THR:OG1	2.32	0.44
10:I:70:LYS:HA	10:I:73:GLN:HG3	2.00	0.44
14:M:78:THR:HG22	14:M:79:LYS:HG3	1.99	0.44
1:2:345:U:H1'	7:F:33:THR:HG23	2.00	0.44
1:2:384:U:OP1	14:M:132:ARG:NH1	2.51	0.44
2:A:31:ASP:OD1	2:A:31:ASP:N	2.46	0.44
14:M:26:GLY:H	14:M:30:LYS:HE3	1.83	0.44
1:2:637:U:O2	33:f:129:ASN:ND2	2.42	0.44
5:D:198:ALA:HB3	5:D:221:ASP:HB3	2.00	0.44
1:2:1183:A:H2'	1:2:1184:G:H8	1.83	0.43
1:2:1528:G:O2'	1:2:1666:C:OP1	2.34	0.43
4:C:129:THR:OG1	4:C:131:ASP:OD1	2.36	0.43
15:N:60:MET:SD	15:N:60:MET:N	2.91	0.43
35:h:272:GLN:OE1	35:h:308:ARG:NH1	2.45	0.43
6:E:212:GLU:OE1	20:S:19:LYS:NZ	2.41	0.43
8:G:71:ARG:NH2	8:G:148:ASN:OD1	2.43	0.43
11:J:190:LEU:HB2	11:J:195:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:22:LYS:HD2	12:K:22:LYS:HA	1.84	0.43
19:R:19:ALA:HB2	19:R:75:GLY:HA3	2.00	0.43
38:z:262:U:O2	38:z:271:G:O6	2.36	0.43
1:2:874:G:H2'	1:2:875:A:H8	1.83	0.43
11:J:142:SER:OG	11:J:143:LYS:N	2.51	0.43
13:L:3:MET:HE1	13:L:48:ALA:HB2	1.98	0.43
15:N:33:ARG:H	15:N:33:ARG:HG2	1.59	0.43
38:z:171:G:H3'	38:z:172:A:H8	1.84	0.43
1:2:677:G:H21	1:2:1028:A:H62	1.66	0.43
4:C:33:VAL:HG12	4:C:96:CYS:HB2	2.01	0.43
6:E:151:LYS:HG2	6:E:153:VAL:HG23	2.01	0.43
8:G:169:ILE:HA	8:G:172:CYS:HB2	2.00	0.43
16:O:99:ARG:NH2	16:O:141:TYR:OH	2.52	0.43
38:z:234:U:OP2	38:z:235:G:N2	2.50	0.43
1:2:1544:C:N4	1:2:1588:A:OP2	2.51	0.43
8:G:143:PRO:HG2	31:d:54:ASP:HB2	2.00	0.43
1:2:223:C:H2'	1:2:224:A:C8	2.53	0.43
1:2:928:G:H2'	1:2:929:G:C8	2.53	0.43
1:2:1280:G:OP2	15:N:101:ARG:NH1	2.50	0.43
5:D:94:ILE:HD13	5:D:162:ILE:HG12	2.00	0.43
5:D:205:VAL:O	5:D:224:THR:OG1	2.37	0.43
23:V:26:SER:OG	23:V:27:ARG:N	2.50	0.43
6:E:117:ARG:NH2	38:z:355:C:O2	2.52	0.43
16:O:83:ASP:OD1	16:O:83:ASP:N	2.49	0.43
21:T:68:ILE:HG23	21:T:72:GLN:HE22	1.83	0.43
31:d:21:THR:OG1	31:d:22:GLY:N	2.51	0.43
1:2:1290:G:N7	34:g:95:ARG:NH1	2.67	0.43
4:C:183:GLU:HA	4:C:186:ASN:HB2	2.00	0.43
10:I:95:ILE:HD12	10:I:129:ILE:HG23	2.00	0.43
23:V:22:ILE:HG12	23:V:114:VAL:HG22	2.01	0.43
1:2:1277:C:H2'	1:2:1278:A:C8	2.53	0.43
20:S:21:TYR:HE2	20:S:73:LEU:HD22	1.83	0.43
25:X:11:LEU:HD23	25:X:72:CYS:HB3	2.00	0.43
1:2:613:G:N2	1:2:626:G:OP1	2.47	0.43
20:S:22:THR:O	35:h:212:LYS:NZ	2.42	0.43
6:E:192:TRP:NE1	6:E:201:LYS:O	2.48	0.42
21:T:130:ARG:HA	21:T:130:ARG:HD3	1.89	0.42
35:h:79:LEU:HD22	35:h:120:ILE:HD12	2.01	0.42
12:K:33:GLY:HA3	33:f:111:TYR:CG	2.54	0.42
18:Q:57:LEU:HD11	18:Q:83:MET:HE1	2.01	0.42
29:b:74:CYS:SG	29:b:77:CYS:HB2	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:438:G:H8	1:2:1800:A:H4'	1.84	0.42
1:2:878:G:H22	1:2:908:A:H2	1.66	0.42
1:2:1786:U:H2'	1:2:1787:G:H8	1.84	0.42
12:K:108:ARG:HH21	12:K:149:VAL:HG23	1.84	0.42
17:P:125:LYS:HA	17:P:125:LYS:HD3	1.88	0.42
1:2:1536:G:H2'	1:2:1537:A:H8	1.84	0.42
1:2:1650:A:H5''	19:R:139:ALA:HB2	2.02	0.42
1:2:1823:A:H2'	2:A:44:ASN:HB3	2.01	0.42
1:2:1848:U:H3	1:2:1852:C:N4	2.17	0.42
12:K:79:ARG:HA	12:K:82:VAL:HG12	1.99	0.42
35:h:239:LEU:HD22	35:h:248:LEU:HD11	2.01	0.42
1:2:1285:G:H22	15:N:58:GLU:HG2	1.85	0.42
3:B:42:LYS:HE3	3:B:46:ILE:HB	2.02	0.42
12:K:179:LYS:HE2	12:K:179:LYS:HB2	1.89	0.42
16:O:40:LEU:HD22	16:O:45:LEU:HD12	2.01	0.42
38:z:131:G:H2'	38:z:132:G:H8	1.84	0.42
1:2:639:C:OP1	33:f:114:ARG:NH2	2.53	0.42
1:2:1228:A:H2'	1:2:1229:G:C8	2.55	0.42
5:D:70:VAL:HG11	5:D:93:ILE:HG23	2.02	0.42
6:E:137:VAL:HB	6:E:185:LYS:HB2	2.01	0.42
19:R:49:TYR:O	19:R:53:GLU:HB2	2.19	0.42
30:c:23:ARG:NH1	30:c:27:SER:O	2.52	0.42
1:2:560:A:H5'	12:K:174:LYS:HB2	2.00	0.42
27:Z:44:LEU:HA	27:Z:47:MET:HG2	2.02	0.42
31:d:45:ASN:ND2	31:d:66:ARG:O	2.51	0.42
17:P:148:GLY:HA2	29:b:27:ALA:HB3	2.01	0.42
23:V:20:ILE:HD13	23:V:116:ILE:HB	2.02	0.42
31:d:16:LYS:HG2	31:d:31:ARG:HB3	2.02	0.42
35:h:84:ASP:OD1	35:h:84:ASP:N	2.53	0.42
1:2:943:U:O2'	17:P:135:ILE:O	2.38	0.42
1:2:1535:U:O2'	8:G:82:ASN:OD1	2.31	0.42
1:2:1536:G:H2'	1:2:1537:A:C8	2.54	0.42
3:B:206:ASP:OD1	3:B:206:ASP:N	2.49	0.42
6:E:21:LEU:HD21	6:E:48:ILE:HD13	2.02	0.42
8:G:32:ASP:OD2	8:G:146:ARG:NH2	2.49	0.42
16:O:78:LYS:HD3	16:O:78:LYS:HA	1.84	0.42
19:R:101:ASP:N	19:R:101:ASP:OD2	2.51	0.42
21:T:2:SER:OG	21:T:3:LEU:N	2.52	0.42
21:T:25:LYS:HB3	21:T:28:PHE:HD2	1.85	0.42
22:U:126:GLN:HG3	22:U:129:ARG:HH21	1.85	0.42
36:j:27:ILE:HD12	36:j:32:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:98:C:OP2	1:2:426:A:O2'	2.26	0.41
1:2:751:G:H1	1:2:792:C:H42	1.68	0.41
7:F:125:LYS:HB2	7:F:226:PHE:CD1	2.55	0.41
9:H:120:ASP:OD1	9:H:125:THR:OG1	2.33	0.41
5:D:79:GLU:HG3	24:W:12:TYR:HB3	2.02	0.41
6:E:227:LYS:HE3	35:h:184:LEU:HD23	2.01	0.41
1:2:385:G:O2'	11:J:10:LYS:NZ	2.52	0.41
1:2:433:A:H2'	1:2:434:G:C8	2.55	0.41
1:2:635:G:H5''	33:f:94:LYS:HD2	2.02	0.41
1:2:962:A:H5''	17:P:66:ARG:HG3	2.02	0.41
3:B:197:VAL:HG23	3:B:198:MET:H	1.85	0.41
1:2:379:C:O2	11:J:5:ARG:NE	2.52	0.41
10:I:40:LEU:HD23	10:I:40:LEU:HA	1.95	0.41
22:U:85:ASN:HB2	22:U:88:MET:HB2	2.02	0.41
1:2:611:G:H2'	1:2:612:U:H6	1.86	0.41
1:2:656:G:H21	1:2:663:C:H5''	1.85	0.41
1:2:1705:C:H2'	1:2:1706:G:H8	1.85	0.41
5:D:74:LYS:HA	5:D:74:LYS:HD3	1.86	0.41
8:G:26:ASP:OD1	8:G:26:ASP:N	2.54	0.41
9:H:119:LYS:HA	9:H:119:LYS:HD3	1.89	0.41
10:I:88:SER:OG	10:I:89:GLY:N	2.53	0.41
17:P:34:PHE:HE1	17:P:100:THR:HA	1.84	0.41
18:Q:52:LYS:HE2	18:Q:52:LYS:HB2	1.95	0.41
1:2:980:A:H2'	1:2:981:A:C8	2.56	0.41
10:I:95:ILE:HD11	10:I:133:LEU:HD13	2.02	0.41
19:R:110:ASP:OD1	19:R:111:ILE:N	2.54	0.41
23:V:20:ILE:HG21	23:V:98:VAL:HG21	2.03	0.41
1:2:294:U:C4	14:M:65:ASN:HB3	2.56	0.41
1:2:1845:A:H2'	1:2:1846:G:C8	2.56	0.41
23:V:69:PRO:HB3	32:e:41:GLN:HG2	2.02	0.41
1:2:981:A:H2'	1:2:982:G:C8	2.56	0.41
3:B:57:LYS:HD2	3:B:57:LYS:HA	1.84	0.41
4:C:63:LYS:HD3	4:C:63:LYS:HA	1.86	0.41
4:C:100:PHE:HB3	4:C:181:LEU:HD21	2.02	0.41
7:F:18:TRP:O	7:F:51:ARG:NH2	2.54	0.41
11:J:19:LYS:HD2	11:J:19:LYS:HA	1.90	0.41
17:P:63:LYS:HA	17:P:63:LYS:HD2	1.77	0.41
35:h:206:LEU:HD12	35:h:218:LEU:HD23	2.02	0.41
36:j:101:LYS:HA	36:j:104:LYS:HE2	2.03	0.41
36:j:103:THR:HA	36:j:106:LYS:HG2	2.03	0.41
1:2:640:A:H2'	1:2:641:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:59:LYS:HB2	8:G:62:ARG:HB2	2.03	0.41
25:X:89:TRP:O	25:X:93:LEU:HB3	2.21	0.41
35:h:66:VAL:HA	35:h:82:SER:HA	2.03	0.41
1:2:1550:G:O2'	1:2:1558:C:O2	2.30	0.40
8:G:15:PRO:HG3	19:R:57:LEU:HA	2.03	0.40
10:I:28:LEU:O	10:I:32:MET:HG3	2.21	0.40
17:P:129:ILE:HG21	29:b:44:ILE:HG21	2.03	0.40
20:S:71:ILE:HD11	20:S:74:GLN:HG2	2.02	0.40
35:h:2:THR:OG1	35:h:3:GLU:N	2.53	0.40
1:2:1007:C:H2'	1:2:1008:A:C8	2.56	0.40
1:2:1413:G:H2'	1:2:1414:A:H8	1.86	0.40
6:E:173:ARG:HA	6:E:173:ARG:HD3	1.84	0.40
9:H:157:VAL:HG21	9:H:176:ILE:HD11	2.03	0.40
10:I:15:LYS:HD3	10:I:16:PRO:HD2	2.03	0.40
20:S:41:ILE:HG23	20:S:46:LEU:HD23	2.02	0.40
1:2:1155:U:OP1	5:D:185:THR:OG1	2.37	0.40
1:2:1345:G:OP1	1:2:1688:C:O2'	2.39	0.40
1:2:1705:C:H2'	1:2:1706:G:C8	2.56	0.40
1:2:1705:C:H42	1:2:1829:G:H1	1.67	0.40
1:2:1780:G:H3'	1:2:1781:A:H4'	2.03	0.40
6:E:21:LEU:HD21	6:E:48:ILE:HG21	2.03	0.40
12:K:180:LYS:HD2	12:K:180:LYS:HA	1.85	0.40
29:b:53:ILE:HG21	29:b:64:LEU:HD11	2.04	0.40
29:b:80:HIS:CD2	38:z:337:G:H5'	2.56	0.40
35:h:10:THR:HG22	35:h:308:ARG:HG3	2.03	0.40
1:2:1010:G:H2'	1:2:1011:A:H8	1.86	0.40
1:2:1489:A:N6	38:z:349:C:OP1	2.54	0.40
1:2:1531:A:H4'	1:2:1605:G:H4'	2.03	0.40
3:B:122:LEU:HB2	3:B:142:LEU:HD21	2.03	0.40
6:E:141:LYS:HA	6:E:147:ALA:HA	2.02	0.40
11:J:22:HIS:ND1	11:J:23:LYS:O	2.54	0.40
14:M:30:LYS:HE2	14:M:30:LYS:HB2	1.97	0.40
15:N:120:ALA:HA	15:N:123:VAL:HG12	2.02	0.40
31:d:66:ARG:HA	31:d:66:ARG:HD2	1.90	0.40
1:2:74:G:N2	1:2:77:A:OP1	2.54	0.40
1:2:525:A:O3'	33:f:104:ARG:NH2	2.55	0.40
3:B:76:VAL:HA	3:B:123:VAL:O	2.21	0.40
5:D:196:ILE:HB	5:D:223:TYR:HB2	2.02	0.40
8:G:77:MET:HB3	8:G:89:THR:HG21	2.02	0.40
12:K:136:ARG:HA	12:K:141:VAL:HA	2.04	0.40
28:a:74:SER:HA	28:a:79:ILE:HG12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:c:19:HIS:HB3	30:c:22:LYS:HG3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	97/144 (67%)	92 (95%)	5 (5%)	0	100	100
3	B	215/295 (73%)	202 (94%)	13 (6%)	0	100	100
4	C	211/264 (80%)	198 (94%)	13 (6%)	0	100	100
5	D	219/221 (99%)	216 (99%)	3 (1%)	0	100	100
6	E	226/281 (80%)	219 (97%)	7 (3%)	0	100	100
7	F	260/263 (99%)	250 (96%)	10 (4%)	0	100	100
8	G	189/204 (93%)	181 (96%)	8 (4%)	0	100	100
9	H	235/249 (94%)	231 (98%)	4 (2%)	0	100	100
10	I	181/432 (42%)	173 (96%)	8 (4%)	0	100	100
11	J	205/208 (99%)	191 (93%)	14 (7%)	0	100	100
12	K	183/194 (94%)	181 (99%)	2 (1%)	0	100	100
13	L	94/149 (63%)	86 (92%)	8 (8%)	0	100	100
14	M	149/158 (94%)	136 (91%)	13 (9%)	0	100	100
15	N	115/132 (87%)	106 (92%)	9 (8%)	0	100	100
16	O	147/151 (97%)	145 (99%)	2 (1%)	0	100	100
17	P	134/168 (80%)	122 (91%)	12 (9%)	0	100	100
18	Q	118/145 (81%)	111 (94%)	7 (6%)	0	100	100
19	R	140/172 (81%)	134 (96%)	6 (4%)	0	100	100
20	S	130/135 (96%)	117 (90%)	13 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	T	142/152 (93%)	137 (96%)	5 (4%)	0	100	100
22	U	139/145 (96%)	134 (96%)	5 (4%)	0	100	100
23	V	98/119 (82%)	94 (96%)	4 (4%)	0	100	100
24	W	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
25	X	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
26	Y	139/143 (97%)	137 (99%)	2 (1%)	0	100	100
27	Z	122/131 (93%)	119 (98%)	3 (2%)	0	100	100
28	a	75/124 (60%)	73 (97%)	2 (3%)	0	100	100
29	b	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
30	c	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
31	d	65/69 (94%)	60 (92%)	5 (8%)	0	100	100
32	e	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
33	f	55/133 (41%)	54 (98%)	1 (2%)	0	100	100
34	g	66/188 (35%)	60 (91%)	6 (9%)	0	100	100
35	h	311/317 (98%)	298 (96%)	13 (4%)	0	100	100
36	j	180/315 (57%)	173 (96%)	7 (4%)	0	100	100
37	n	23/25 (92%)	23 (100%)	0	0	100	100
All	All	5104/6280 (81%)	4879 (96%)	225 (4%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	84/123 (68%)	84 (100%)	0	100	100
3	B	180/245 (74%)	180 (100%)	0	100	100
4	C	194/231 (84%)	194 (100%)	0	100	100
5	D	187/187 (100%)	187 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	E	190/232 (82%)	190 (100%)	0	100	100
7	F	224/225 (100%)	224 (100%)	0	100	100
8	G	161/170 (95%)	161 (100%)	0	100	100
9	H	207/218 (95%)	207 (100%)	0	100	100
10	I	165/360 (46%)	165 (100%)	0	100	100
11	J	179/180 (99%)	179 (100%)	0	100	100
12	K	161/168 (96%)	161 (100%)	0	100	100
13	L	87/125 (70%)	87 (100%)	0	100	100
14	M	136/142 (96%)	136 (100%)	0	100	100
15	N	99/108 (92%)	99 (100%)	0	100	100
16	O	130/131 (99%)	130 (100%)	0	100	100
17	P	106/130 (82%)	106 (100%)	0	100	100
18	Q	109/130 (84%)	109 (100%)	0	100	100
19	R	117/140 (84%)	117 (100%)	0	100	100
20	S	119/121 (98%)	119 (100%)	0	100	100
21	T	125/132 (95%)	124 (99%)	1 (1%)	73	77
22	U	111/116 (96%)	111 (100%)	0	100	100
23	V	92/107 (86%)	92 (100%)	0	100	100
24	W	67/67 (100%)	67 (100%)	0	100	100
25	X	112/113 (99%)	112 (100%)	0	100	100
26	Y	113/115 (98%)	113 (100%)	0	100	100
27	Z	107/113 (95%)	107 (100%)	0	100	100
28	a	68/102 (67%)	68 (100%)	0	100	100
29	b	88/88 (100%)	88 (100%)	0	100	100
30	c	75/76 (99%)	75 (100%)	0	100	100
31	d	60/62 (97%)	60 (100%)	0	100	100
32	e	48/49 (98%)	48 (100%)	0	100	100
33	f	47/106 (44%)	47 (100%)	0	100	100
34	g	61/154 (40%)	61 (100%)	0	100	100
35	h	272/275 (99%)	272 (100%)	0	100	100
36	j	84/280 (30%)	81 (96%)	3 (4%)	31	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	n	24/24 (100%)	24 (100%)	0	100	100
All	All	4389/5345 (82%)	4385 (100%)	4 (0%)	87	87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	T	73	ASN
36	j	142	TYR
36	j	147	TYR
36	j	150	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	9	GLN
3	B	50	ASN
3	B	132	GLN
4	C	101	HIS
4	C	179	ASN
4	C	202	GLN
7	F	36	HIS
7	F	67	GLN
7	F	161	GLN
7	F	188	ASN
7	F	209	HIS
8	G	79	HIS
9	H	65	GLN
9	H	110	ASN
9	H	177	GLN
10	I	44	ASN
10	I	68	GLN
11	J	64	ASN
11	J	146	GLN
13	L	7	ASN
13	L	44	HIS
14	M	11	GLN
14	M	19	ASN
14	M	106	HIS
15	N	72	HIS
16	O	105	ASN
18	Q	35	GLN

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Mol	Chain	Res	Type
20	S	93	GLN
20	S	116	ASN
21	T	72	GLN
21	T	76	GLN
22	U	85	ASN
22	U	105	GLN
22	U	128	GLN
23	V	18	HIS
23	V	47	ASN
24	W	49	GLN
25	X	64	ASN
25	X	120	HIS
27	Z	15	ASN
27	Z	89	HIS
28	a	89	GLN
28	a	112	ASN
35	h	159	ASN
35	h	181	ASN
35	h	196	ASN
35	h	215	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1685/1870 (90%)	307 (18%)	10 (0%)
38	z	186/400 (46%)	52 (27%)	0
39	i	74/75 (98%)	15 (20%)	0
All	All	1945/2345 (82%)	374 (19%)	10 (0%)

All (374) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	4	C
1	2	5	U
1	2	26	U
1	2	33	G
1	2	41	G
1	2	44	U
1	2	46	A
1	2	49	C
1	2	56	G

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Mol	Chain	Res	Type
1	2	67	C
1	2	68	A
1	2	73	C
1	2	74	G
1	2	76	U
1	2	103	A
1	2	113	G
1	2	114	G
1	2	115	U
1	2	126	G
1	2	130	G
1	2	142	C
1	2	143	U
1	2	146	G
1	2	147	A
1	2	149	A
1	2	158	A
1	2	162	C
1	2	170	A
1	2	180	G
1	2	182	C
1	2	183	G
1	2	184	G
1	2	186	C
1	2	190	G
1	2	191	A
1	2	192	C
1	2	199	C
1	2	208	G
1	2	292	A
1	2	305	U
1	2	306	C
1	2	307	G
1	2	309	G
1	2	312	G
1	2	313	A
1	2	319	C
1	2	320	G
1	2	323	C
1	2	330	G
1	2	347	G
1	2	357	C

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Mol	Chain	Res	Type
1	2	364	A
1	2	368	U
1	2	370	G
1	2	383	G
1	2	384	U
1	2	385	G
1	2	398	A
1	2	399	C
1	2	400	C
1	2	407	G
1	2	408	A
1	2	409	C
1	2	418	A
1	2	420	G
1	2	437	G
1	2	438	G
1	2	446	G
1	2	448	A
1	2	449	A
1	2	450	C
1	2	465	A
1	2	471	G
1	2	472	C
1	2	474	G
1	2	487	U
1	2	488	U
1	2	489	A
1	2	492	C
1	2	493	A
1	2	500	A
1	2	502	C
1	2	508	A
1	2	525	A
1	2	531	A
1	2	532	C
1	2	536	A
1	2	537	C
1	2	541	U
1	2	542	U
1	2	546	G
1	2	547	G
1	2	549	C

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Mol	Chain	Res	Type
1	2	550	C
1	2	551	U
1	2	554	A
1	2	555	A
1	2	556	U
1	2	561	A
1	2	562	U
1	2	576	A
1	2	583	A
1	2	588	G
1	2	589	G
1	2	590	A
1	2	591	U
1	2	598	G
1	2	606	G
1	2	608	C
1	2	614	C
1	2	617	G
1	2	623	G
1	2	627	U
1	2	628	A
1	2	629	A
1	2	643	A
1	2	644	G
1	2	655	A
1	2	660	C
1	2	663	C
1	2	668	A
1	2	669	A
1	2	671	A
1	2	672	A
1	2	689	U
1	2	691	G
1	2	694	G
1	2	696	G
1	2	750	C
1	2	752	G
1	2	753	C
1	2	798	G
1	2	799	U
1	2	801	U
1	2	811	A

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Mol	Chain	Res	Type
1	2	821	G
1	2	822	U
1	2	830	A
1	2	834	C
1	2	844	U
1	2	847	A
1	2	870	A
1	2	871	U
1	2	872	A
1	2	873	G
1	2	874	G
1	2	875	A
1	2	878	G
1	2	883	U
1	2	886	A
1	2	887	U
1	2	888	U
1	2	890	U
1	2	891	G
1	2	892	U
1	2	894	G
1	2	895	G
1	2	899	U
1	2	900	C
1	2	901	G
1	2	902	G
1	2	904	A
1	2	913	A
1	2	914	U
1	2	919	A
1	2	920	A
1	2	933	G
1	2	955	A
1	2	971	G
1	2	990	A
1	2	992	A
1	2	999	G
1	2	1017	U
1	2	1023	A
1	2	1045	U
1	2	1061	U
1	2	1070	A

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Mol	Chain	Res	Type
1	2	1078	C
1	2	1083	A
1	2	1085	C
1	2	1086	G
1	2	1109	C
1	2	1114	U
1	2	1121	G
1	2	1138	C
1	2	1149	A
1	2	1150	A
1	2	1153	C
1	2	1154	U
1	2	1165	G
1	2	1195	A
1	2	1207	G
1	2	1215	C
1	2	1217	A
1	2	1224	G
1	2	1242	U
1	2	1251	A
1	2	1253	A
1	2	1256	G
1	2	1257	G
1	2	1259	A
1	2	1264	C
1	2	1274	G
1	2	1275	G
1	2	1285	G
1	2	1286	G
1	2	1287	A
1	2	1293	A
1	2	1294	G
1	2	1295	A
1	2	1297	U
1	2	1298	G
1	2	1299	A
1	2	1300	U
1	2	1301	A
1	2	1302	G
1	2	1303	C
1	2	1309	C
1	2	1313	A

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Mol	Chain	Res	Type
1	2	1330	G
1	2	1333	U
1	2	1342	U
1	2	1348	G
1	2	1358	U
1	2	1361	G
1	2	1363	C
1	2	1364	U
1	2	1371	U
1	2	1372	U
1	2	1378	A
1	2	1396	A
1	2	1404	U
1	2	1428	G
1	2	1442	U
1	2	1452	A
1	2	1454	A
1	2	1462	U
1	2	1463	U
1	2	1475	G
1	2	1477	U
1	2	1480	A
1	2	1487	A
1	2	1489	A
1	2	1490	G
1	2	1497	G
1	2	1498	A
1	2	1507	G
1	2	1521	C
1	2	1522	A
1	2	1533	A
1	2	1535	U
1	2	1536	G
1	2	1548	G
1	2	1551	U
1	2	1554	C
1	2	1556	A
1	2	1567	G
1	2	1573	G
1	2	1575	G
1	2	1578	U
1	2	1580	A

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Mol	Chain	Res	Type
1	2	1585	U
1	2	1588	A
1	2	1601	A
1	2	1604	G
1	2	1621	U
1	2	1623	A
1	2	1637	A
1	2	1638	G
1	2	1648	G
1	2	1659	U
1	2	1660	C
1	2	1661	A
1	2	1665	G
1	2	1695	A
1	2	1699	A
1	2	1715	A
1	2	1721	U
1	2	1722	G
1	2	1744	G
1	2	1749	G
1	2	1751	C
1	2	1756	C
1	2	1760	G
1	2	1774	C
1	2	1779	G
1	2	1781	A
1	2	1782	G
1	2	1783	C
1	2	1784	G
1	2	1817	G
1	2	1819	A
1	2	1823	A
1	2	1824	A
1	2	1826	G
1	2	1831	A
1	2	1834	A
1	2	1836	G
1	2	1838	U
1	2	1840	U
1	2	1849	G
1	2	1851	A
1	2	1852	C

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Mol	Chain	Res	Type
1	2	1861	G
1	2	1862	G
1	2	1863	A
1	2	1865	C
38	z	121	C
38	z	137	G
38	z	144	U
38	z	154	A
38	z	157	C
38	z	161	G
38	z	162	A
38	z	163	G
38	z	165	A
38	z	166	C
38	z	167	A
38	z	168	C
38	z	169	C
38	z	173	A
38	z	229	G
38	z	234	U
38	z	237	C
38	z	240	C
38	z	244	A
38	z	253	G
38	z	258	G
38	z	259	U
38	z	265	U
38	z	266	G
38	z	279	C
38	z	280	C
38	z	281	U
38	z	282	U
38	z	288	A
38	z	295	G
38	z	296	A
38	z	297	U
38	z	306	U
38	z	324	U
38	z	325	C
38	z	328	G
38	z	330	A
38	z	331	G

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Mol	Chain	Res	Type
38	z	332	A
38	z	333	C
38	z	334	C
38	z	335	G
38	z	337	G
38	z	338	C
38	z	345	A
38	z	346	G
38	z	348	A
38	z	349	C
38	z	352	A
38	z	353	U
38	z	355	C
38	z	356	U
39	i	4	A
39	i	16	C
39	i	17	G
39	i	18	G
39	i	19	A
39	i	20	A
39	i	47	C
39	i	48	G
39	i	58	A
39	i	59	A
39	i	60	C
39	i	70	C
39	i	73	C
39	i	74	C
39	i	75	A

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	383	G
1	2	445	A
1	2	553	U
1	2	561	A
1	2	688	U
1	2	874	G
1	2	886	A
1	2	1137	U
1	2	1395	C

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Mol	Chain	Res	Type
1	2	1637	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-25539. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit ⓘ

This section was not generated.