



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Aug 21, 2017 – 11:42 PM EDT

PDB ID : 5LJ3
EMDB ID: : EMD-4055
Title : Structure of the core of the yeast spliceosome immediately after branching
Authors : Galej, W.P.; Wilkinson, M.F.; Fica, S.M.; Oubridge, C.; Newman, A.J.; Nagai, K.
Deposited on : unknown
Resolution : 3.80 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

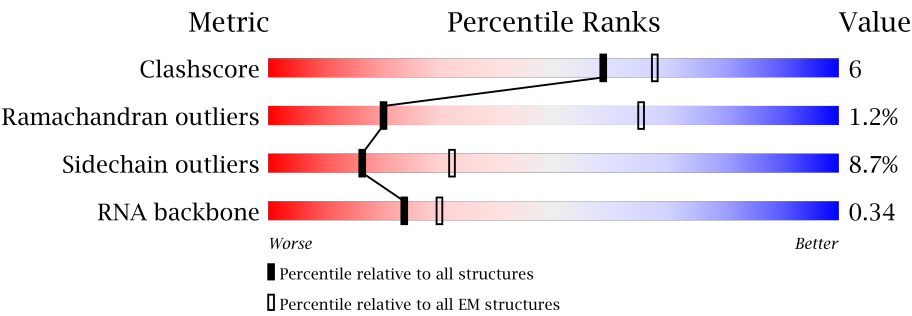
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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.










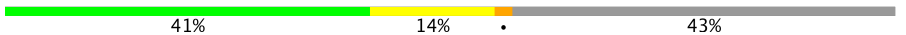

















Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	U	179	<div><div>33%36%9%•21%</div></div>
2	E	16	<div><div>25%63%13%</div></div>
3	I	76	<div><div>22%20%•57%</div></div>
4	Z	1175	<div><div>9%5%85%</div></div>
5	V	112	<div><div>44%30%12%•13%</div></div>
6	A	2413	<div><div>63%15%•20%</div></div>
7	D	278	<div><div>34%7%59%</div></div>
8	F	179	<div><div>23%•74%</div></div>

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Mol	Chain	Length	Quality of chain
9	C	1008	
10	G	235	
11	H	591	
12	J	451	
13	K	379	
14	L	157	
15	M	339	
16	N	364	
17	O	590	
18	P	175	
19	R	135	
20	S	687	
21	T	859	
22	b	196	
22	k	196	
23	d	101	
23	n	101	
24	e	94	
24	p	94	
25	f	86	
25	q	86	
26	g	77	
26	r	77	
27	h	146	
27	l	146	

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Mol	Chain	Length	Quality of chain
28	j	110	 83% 15%
28	m	110	 85% 15%
29	W	238	 65% 31%
30	Y	111	 76% 24%
31	x	132	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	ZN	N	401	-	-	X	-
33	ZN	N	402	-	-	X	-

2 Entry composition [i](#)

There are 34 unique types of molecules in this entry. The entry contains 63161 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 U5 snRNA (small nuclear RNA).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	141	Total	C	N	O	P	0	0
			2999	1342	530	986	141		

- Molecule 2 is a RNA chain called Exon 1 (5' exon) of UBC4 pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	16	Total	C	N	O	P	0	0
			346	155	66	109	16		

- Molecule 3 is a RNA chain called Intron of UBC4 pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	33	Total	C	N	O	P	0	0
			693	312	116	232	33		

- Molecule 4 is a RNA chain called U2 snRNA (small nuclear RNA).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Z	171	Total	C	N	O	P	0	0
			3610	1614	604	1221	171		

- Molecule 5 is a RNA chain called U6 snRNA (small nuclear RNA).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	V	97	Total	C	N	O	P	0	0
			2066	925	368	676	97		

- Molecule 6 is a protein called Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1922	Total	C	N	O	S	0	0
			15704	10112	2720	2814	58		

- Molecule 7 is a protein called Protein CWC16.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	114	Total	C	N	O	S	0	0
			912	577	165	162	8		

- Molecule 8 is a protein called Pre-mRNA-splicing factor CWC25.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	46	Total	C	N	O		0	0
			321	203	61	57			

- Molecule 9 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	882	Total	C	N	O	S	0	0
			6756	4393	1133	1203	27		

- Molecule 10 is a protein called ISY1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	97	Total	C	N	O	S	0	0
			823	513	154	155	1		

- Molecule 11 is a protein called CWC22.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	399	Total	C	N	O	S	0	0
			2639	1657	468	506	8		

- Molecule 12 is a protein called PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	326	Total	C	N	O	S	0	0
			2556	1616	454	476	10		

- Molecule 13 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	163	Total	C	N	O	S	0	0
			1289	808	236	240	5		

- Molecule 14 is a protein called Pre-mRNA-splicing factor BUD31.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	155	Total	C	N	O	S	0	0
			1270	797	238	225	10		

- Molecule 15 is a protein called CWC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	252	Total	C	N	O	S	0	0
			2010	1275	354	370	11		

- Molecule 16 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	209	Total	C	N	O	S	0	0
			1658	1055	287	301	15		

- Molecule 17 is a protein called CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	198	Total	C	N	O	S	0	0
			1645	1032	300	307	6		

- Molecule 18 is a protein called CWC15.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	P	36	Total	C	N	O	0	0
			275	176	53	46		

- Molecule 19 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	R	97	Total	C	N	O	0	0
			550	328	109	113		

- Molecule 20 is a protein called CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	464	Total	C	N	O	S	0	0
			3120	1948	581	584	7		

- Molecule 21 is a protein called SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	T	592	Total	C	N	O	0	0
			2946	1762	592	592		

- Molecule 22 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	b	80	Total	C	N	O	S	0	0
			631	403	114	111	3		
22	k	80	Total	C	N	O		0	0
			396	236	80	80			

- Molecule 23 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	82	Total	C	N	O	S	0	0
			625	399	109	115	2		
23	n	82	Total	C	N	O		0	0
			404	240	82	82			

- Molecule 24 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	e	75	Total	C	N	O	S	0	0
			575	379	92	101	3		
24	p	75	Total	C	N	O		0	0
			369	219	75	75			

- Molecule 25 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	f	72	Total	C	N	O	S	0	0
			573	368	101	103	1		
25	q	72	Total	C	N	O		0	0
			354	210	72	72			

- Molecule 26 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	g	69	Total	C	N	O	S	0	0
			529	337	93	97	2		
26	r	69	Total	C	N	O		0	0
			340	202	69	69			

- Molecule 27 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	h	82	Total	C	N	O	S	0	0
			644	409	110	123	2		
27	l	79	Total	C	N	O		0	0
			392	234	79	79			

- Molecule 28 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	j	94	Total	C	N	O	S	0	0
			741	477	141	119	4		
28	m	94	Total	C	N	O		0	0
			467	279	94	94			

- Molecule 29 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	W	164	Total	C	N	O	0	0
			816	488	164	164		

- Molecule 30 is a protein called U2 small nuclear ribonucleoprotein B''.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	Y	84	Total	C	N	O	0	0
			416	248	84	84		

- Molecule 31 is a protein called unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	x	132	Total	C	N	O	0	0
			660	396	132	132		

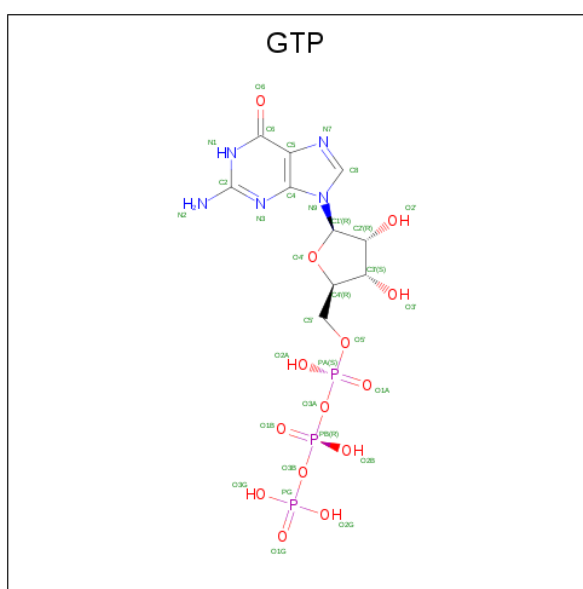
- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
32	V	1	Total	Mg	0
			1	1	
32	E	1	Total	Mg	0
			1	1	

- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
33	L	3	Total	Zn	0
			3	3	
33	D	1	Total	Zn	0
			1	1	
33	N	2	Total	Zn	0
			2	2	
33	M	1	Total	Zn	0
			1	1	

- Molecule 34 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

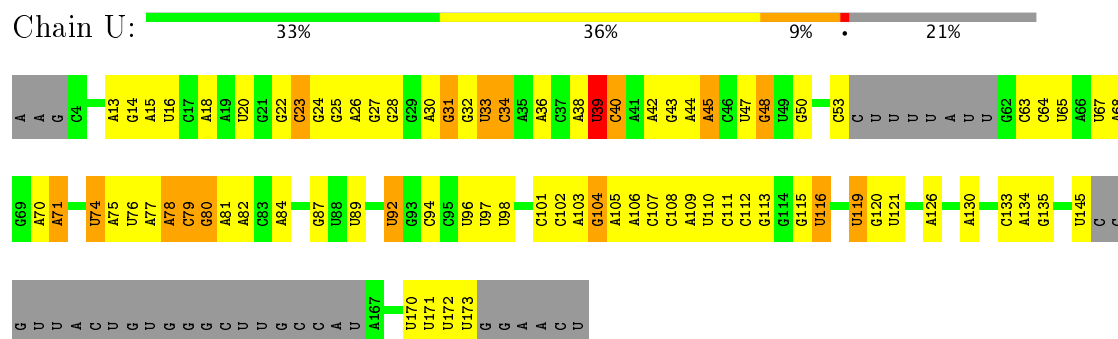


Mol	Chain	Residues	Atoms					AltConf
34	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

3 Residue-property plots [i](#)

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

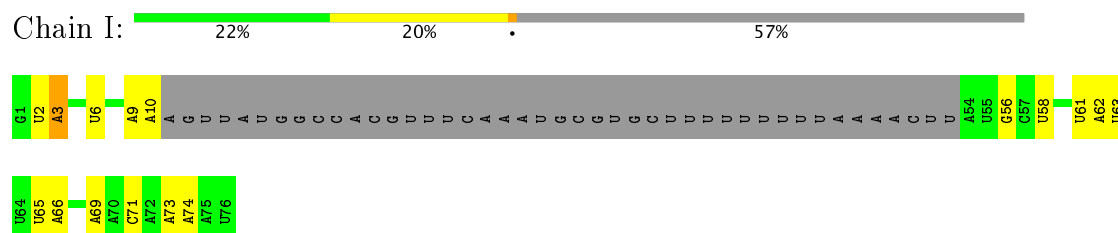
- Molecule 1: U5 snRNA (small nuclear RNA)



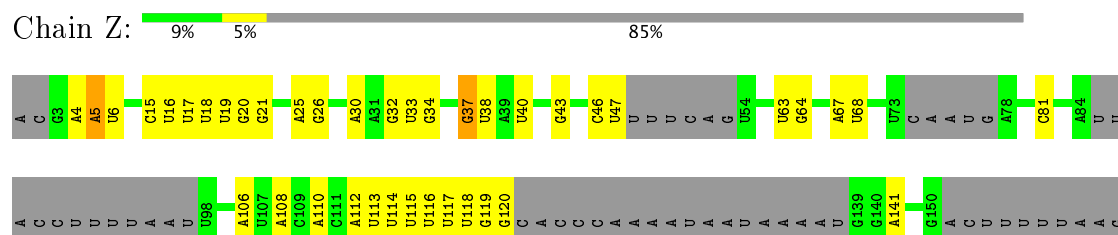
- Molecule 2: Exon 1 (5' exon) of UBC4 pre-mRNA

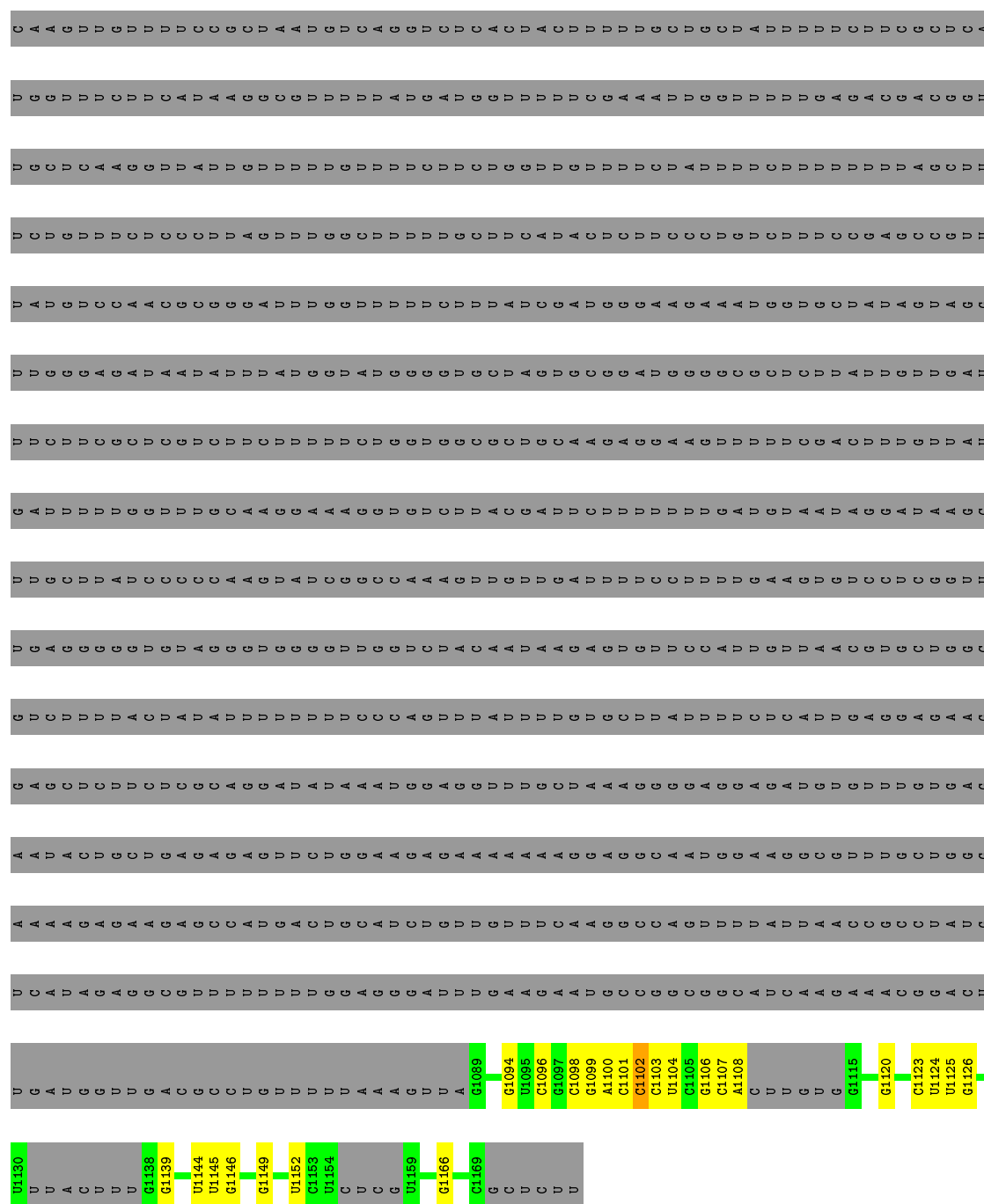


- Molecule 3: Intron of UBC4 pre-mRNA



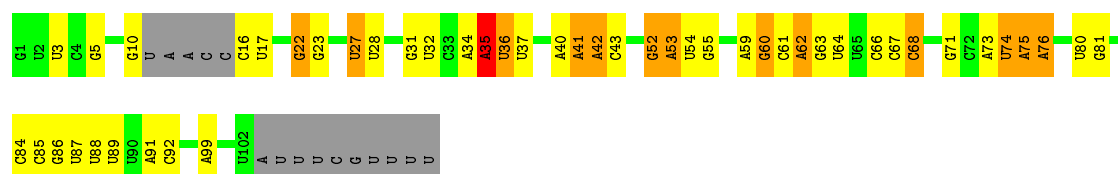
- Molecule 4: U2 snRNA (small nuclear RNA)





- Molecule 5: U6 snRNA (small nuclear RNA)

Chain V: 44% 30% 12% 13%



- Molecule 6: Pre-mRNA-splicing factor 8

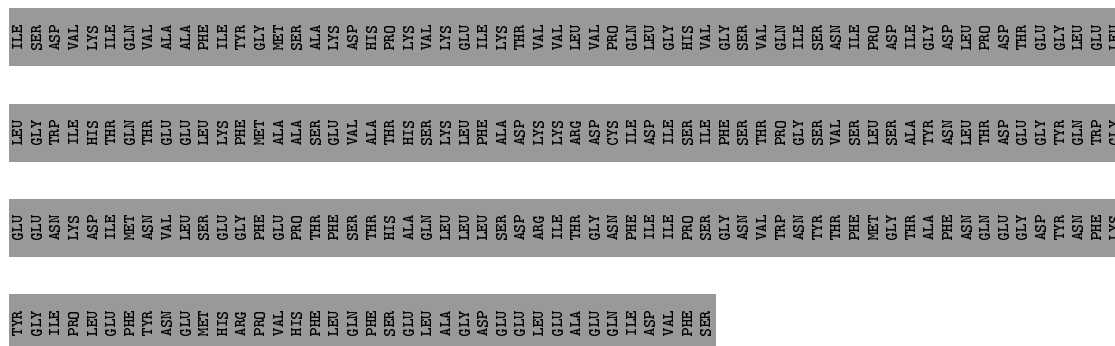
Chain A:

63%

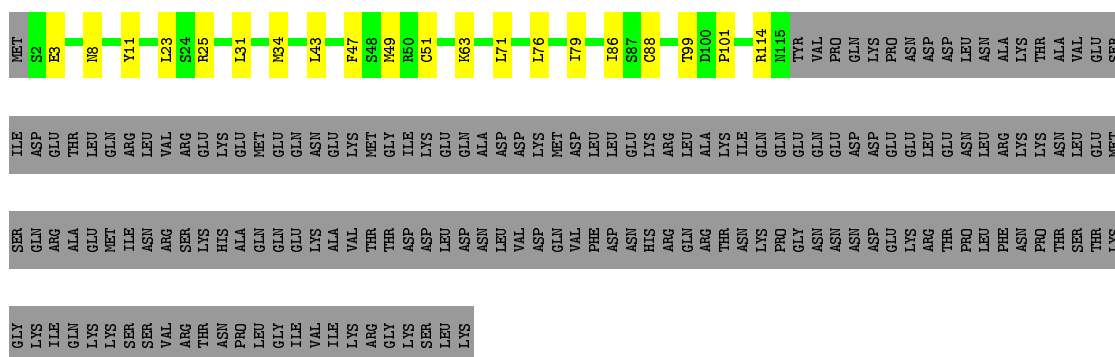
15%

20%

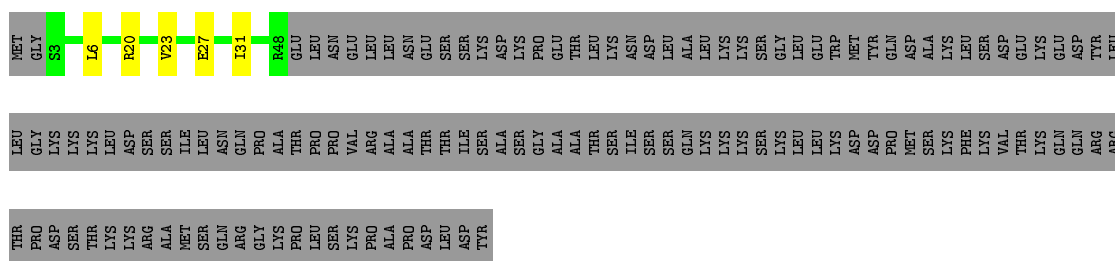
VAL	VAL	V1977	Q1737	Y1542	I1367	V1248	A1047	I882	A753	Q648	Y480	I370	K221	LYS	ILE
ALA	ALA	V1978	L1738	R1543	Q1368	V1249	V1048	K889	I753	L649	K493	R376	R225	ALA	ASN
ALA	ALA	W2048	D1742	V1546	M1369	Y1251	L1049	K893	I754	I656	D755	L507	R228	ARG	GLU
ASP	ASP	L2060	S1749	L1557	K1371	N1255	L1054	L912	L756	H659	L508	L390	F239	SER	GLU
GLU	GLU	E2078	V1752	T1560	L1373	L1258	T1064	L919	L758	I660	Y514	P395	P239	ASN	ILE
SER	SER	G2085	F1756	L1561	G1374	E1277	L1065	V922	K759	I663	S521	P398	P244	LEU	ASP
THR	THR	GLN	T1760	F1562	L1375	E1277	L1066	V922	I766	T664	Y522	V398	P244	THR	PHE
PHE	PHE	ASN	T1760	T1565	K1378	D1282	N1067	V922	I766	I666	Y522	V398	P244	LEU	GLU
SER	SER	ILE	M1763	V1570	M1379	D1282	I1078	V922	M770	I666	Y522	V398	P244	PRO	PRO
LYS	LYS	LYS	N1763	V1570	R1382	V1286	T1083	L929	M770	V673	Y526	N403	E252	PRO	GLU
ASN	ASN	ALA	L1779	F1574	F1383	D1287	A1084	L937	I774	M674	Y529	N405	E256	ASP	LEU
GLU	GLU	TRP	K1795	K1589	V1387	L1288	K1085	Y944	R775	H675	K555	I410	I255	PRO	PRO
ARG	ARG	VAL	P1796	L1590	F1388	L1302	V1088	B948	K778	D682	Y556	Q412	I257	ALA	ALA
LYS	LYS	LYS	S1801	A1593	K1392	I1309	V1089	B948	I782	I686	I562	F424	L261	LEU	LEU
GLN	GLN	ARG	M1802	L1600	E1393	K1310	I1090	I951	L783	I687	D563	D425	I264	PRO	PRO
ILE	ILE	ILE	R1803	L1598	L1394	R1315	V1098	N952	L784	I687	Y564	I410	I264	ASP	GLY
ALA	ALA	ALA	M1806	S1599	L1397	I1316	M1098	N953	I784	K690	Y565	Q412	I264	GLU	GLU
GLU	GLU	GLU	M1806	T1601	L1397	R1317	L1103	I954	K785	I695	Y565	Q412	I264	LEU	LEU
LEU	LEU	LEU	L1815	P1602	T1400	S1323	I1104	I954	K785	I695	Y565	Q412	I264	GLY	GLY
GLU	GLU	GLU	R1820	R1604	I1407	G1324	I1113	I954	L785	I695	Y565	Q412	I264	ASP	LEU
ALA	ALA	ALA	R1820	R1604	I1407	G1324	I1113	I954	L785	I695	Y565	Q412	I264	PRO	PRO
ARG	ARG	ARG	L1823	V1609	A1409	T1326	I1121	N972	K785	I695	Y565	Q412	I264	LEU	LEU
SER	SER	SER	Q1824	V1610	Q1417	T1327	F1144	Q976	I811	I711	I591	ASN	L268	PRO	PRO
LYS	LYS	LYS	Q1824	V1610	T1418	T1329	F1144	Q976	I811	I711	I591	ASN	L268	PRO	PRO
ILE	ILE	ILE	Q1827	I1614	T1418	T1329	F1144	Q976	I811	I711	I591	ASN	L268	PRO	PRO
VAL	VAL	VAL	SER	V1620	H1424	W1335	T1162	I977	A820	L712	K600	ASN	L286	GLY	GLY
SER	SER	SER	VAL	V1621	M1429	T1337	L1165	Y982	B831	F714	L605	LEU	E287	ASN	ASN
ALA	ALA	ALA	GLN	V1621	M1429	T1337	D1166	Y982	B831	L715	L605	LEU	E287	ASN	ASN
ASP	ASP	ASP	GLU	V1632	D1433	S1338	R1167	Y991	B833	R716	T607	VAL	L305	ARG	ARG
PHE	PHE	PHE	GLU	V1639	E1434	L1339	L1168	W1000	B834	Q717	T718	ASN	L305	LYS	LYS
VAL	VAL	VAL	LEU	V1643	L1436	L1342	L1171	W1000	B834	T718	T719	VAL	L305	LYS	LYS
GLU	GLU	GLU	ASN	S1643	L1436	L1342	L1171	W1000	B834	P720	S613	ASN	L305	VAL	VAL
GLU	GLU	GLU	SER	S1644	E1447	T1344	W1207	D1004	V845	R724	L626	ASN	L305	ASP	ASP
GLN	GLN	GLN	THR	L1646	E1448	Y1345	P1208	H1011	B847	N728	L626	GLY	L305	THR	THR
ASN	ASN	ASN	MET	I1646	E1448	F1346	K1209	K1014	B847	L729	K627	ASP	L305	PHE	PHE
VAL	VAL	VAL	THR	Q1647	Y1461	R1347	R1212	P1015	L849	I730	K629	PHE	L305	THR	THR
THR	THR	THR	THR	V1654	Y1461	R1347	R1212	P1015	L849	T731	K630	LEU	L305	LEU	LEU
LYS	LYS	LYS	LYS	W1654	I1491	I1350	M1213	E1019	L852	R737	K631	PRO	L305	LYS	LYS
THR	THR	THR	THR	V1657	L1494	E1354	R1214	I1020	T863	R737	L631	PRO	L305	PRO	PRO
ILE	ILE	ILE	ILE	V1657	L1494	P1355	R1217	P1021	T863	R737	L631	PRO	L305	PRO	PRO
LYS	LYS	LYS	LYS	V1657	L1494	P1355	R1217	P1021	T863	R737	L631	PRO	L305	PRO	PRO
ASN	ASN	ASN	ASN	V1669	I1510	L1356	L1222	P1022	T863	R737	L631	PRO	L305	PRO	PRO
ALA	ALA	ALA	ALA	L1669	I1510	L1357	L1023	L1023	T863	R737	L631	PRO	L305	PRO	PRO
GLN	GLN	GLN	GLN	L1669	I1510	L1357	L1023	L1023	T863	R737	L631	PRO	L305	PRO	PRO
GLY	GLY	GLY	GLY	M1948	K1515	D1358	G1223	L1024	T863	R737	L631	PRO	L305	PRO	PRO
LEU	LEU	LEU	LEU	V1681	K1515	L1359	V1226	V1025	T863	R737	L631	PRO	L305	PRO	PRO
LYS	LYS	LYS	LYS	V1681	K1515	L1360	V1226	V1025	T863	R737	L631	PRO	L305	PRO	PRO
LYS	LYS	LYS	LYS	V1681	K1515	L1360	V1226	V1025	T863	R737	L631	PRO	L305	PRO	PRO
PHE	PHE	PHE	PHE	H1707	E1520	V1361	V1234	W1028	T863	R737	L631	PRO	L305	PRO	PRO
ILE	ILE	ILE	ILE	E1708	W1537	E1364	V1234	W1028	T863	R737	L631	PRO	L305	PRO	PRO
GLU	GLU	GLU	GLU	L1974	W1537	E1364	T1239	I1032	T881	D751	F647	L479	L355	GLU	GLU



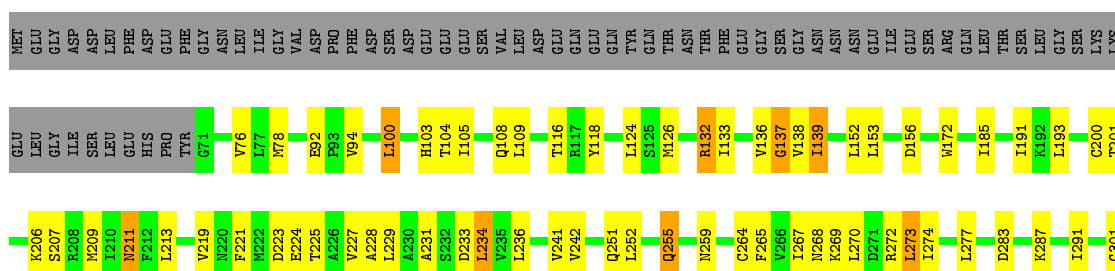
- Molecule 7: Protein CWC16



- Molecule 8: Pre-mRNA-splicing factor CWC25



- Molecule 9: Pre-mRNA-splicing factor SNU114



Response	Percentage
Yes, the government should do more to protect the environment	52%
No, the government should not do more to protect the environment	17%
Don't know	1%
Other	28%



Response	Percentage
Used	31%
Not used	11%
Don't know	57%



83% 15%



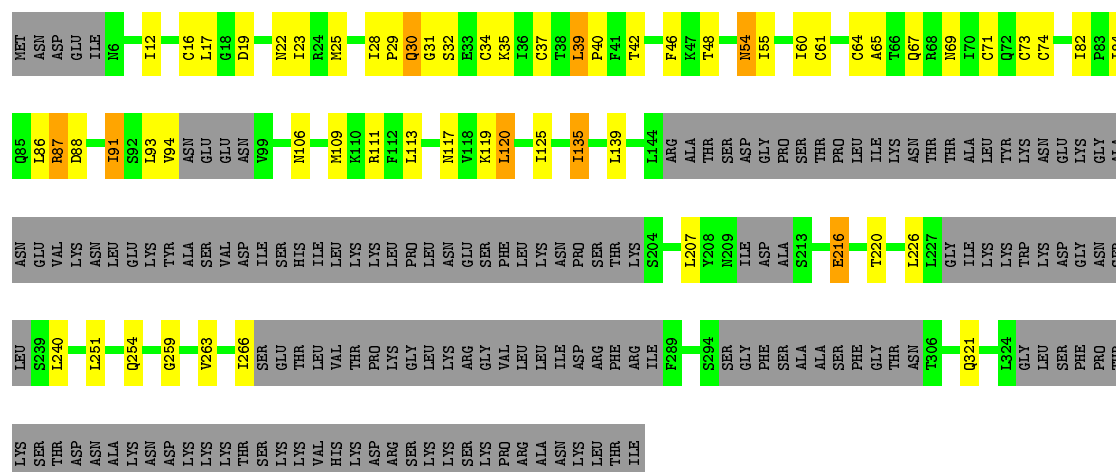
Response	Percentage
Yes	60%
No	13%
Don't know	26%



LYS LYS ARG LEU LEU PRO ASP ASN GLY MET GLU SER ASP ASP PHE LEU GLU LYS LYS LYS LYS ASN ILE SER ARG GLU ASN LYS SER SER LYS PRO SER VAL GLY LYS LEU LEU GLY PRO LEU LEU ASP TYR LYS LEU SER SER ASP GLU

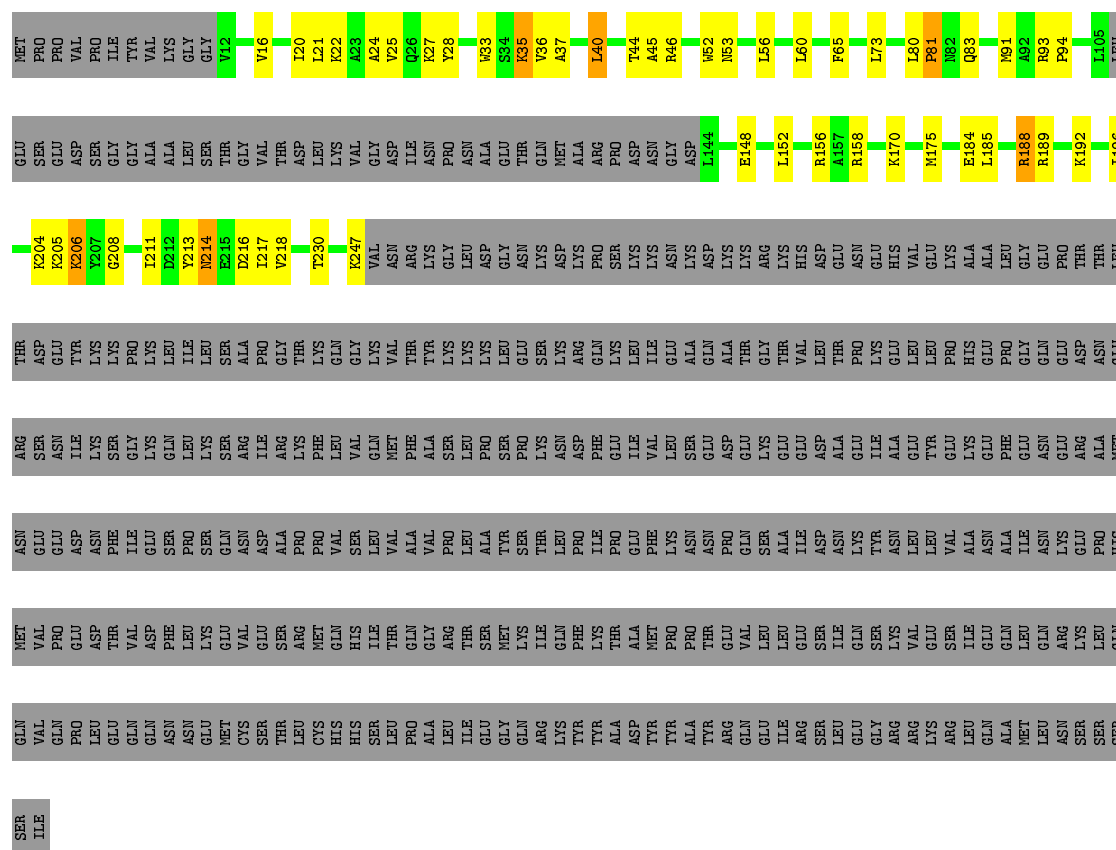
- Molecule 16: Pre-mRNA-splicing factor SLT11

Chain N: 41% 14% . 43%



- Molecule 17: CEF1

Chain 0:  25% 8% 66%



- Molecule 18: CWC15

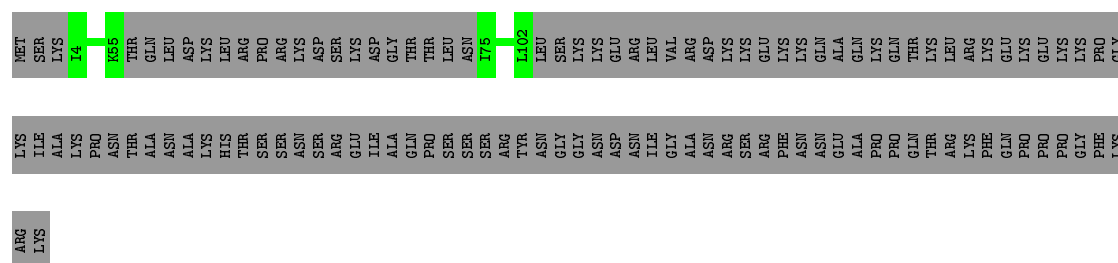
[illegible]

MET
S2
I6
G7
L8
K12
G13
S14
S15
T16
S50
HIS
ASP
LYS
ALA
SER
ARG
PRO
LEU
ALA
VAL
GLN
LYS
GLN
T64
G111
GIU
GLN
GLN
ARG
MET
MET
SER
SER
LEU
TYR
THR
PRO
ARG
LYS
ALA
ARG
LEU
THR
THR
GIU
GLU
GLN
HIS
ARG
HIS
ILV

[illegible][illegible]

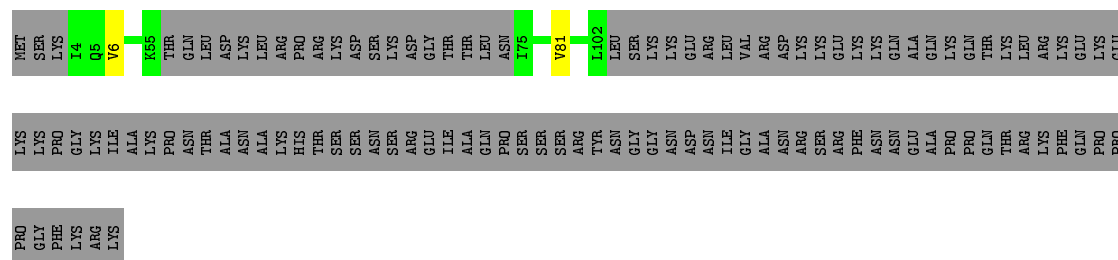
- Molecule 22: Small nuclear ribonucleoprotein-associated protein B

Chain b: 41% 59%

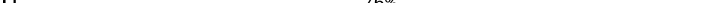


- Molecule 22: Small nuclear ribonucleoprotein-associated protein B

Chain k: 40% 59%



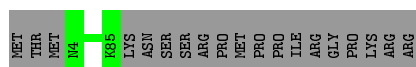
- Molecule 23: Small nuclear ribonucleoprotein Sm D3

Chain d:  76% 5% 19%



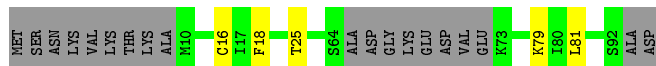
- Molecule 23: Small nuclear ribonucleoprotein Sm D3

Chain n: 81% 19%



- Molecule 24: Small nuclear ribonucleoprotein E

Chain e: 74% 5% 20%



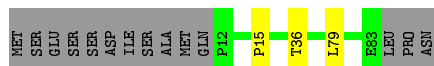
- Molecule 24: Small nuclear ribonucleoprotein E

Chain p: 79% 0% 20%



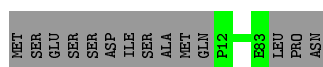
- Molecule 25: Small nuclear ribonucleoprotein F

Chain f: 80% 0% 16%



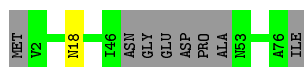
- Molecule 25: Small nuclear ribonucleoprotein F

Chain q: 84% 0% 16%



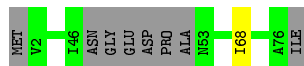
- Molecule 26: Small nuclear ribonucleoprotein G

Chain g: 88% 0% 10%



- Molecule 26: Small nuclear ribonucleoprotein G

Chain r: 88% 0% 10%



- Molecule 27: Small nuclear ribonucleoprotein Sm D1

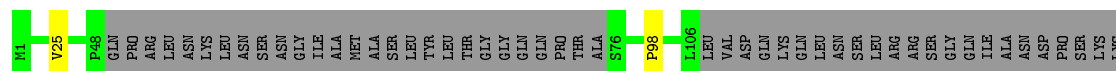
Chain h: 56% 0% 44%



PRO
ALA
ASN
LYS
ARG
PRO
ARG
ARG
GLY
LEU

- Molecule 27: Small nuclear ribonucleoprotein Sm D1

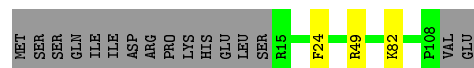
Chain 1:  53% . 46%



ARG
ARG
ARG
ASP
PHE
GLY
ALA
PRO
ALA
ASN
LYS
ARG
PRO
ARG
ARG
GLY
LEU

- Molecule 28: Small nuclear ribonucleoprotein Sm D2

Chain j: 83% • 15%



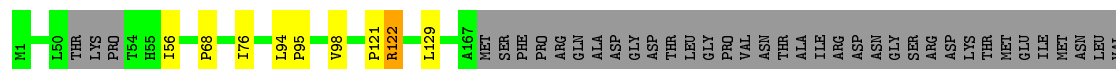
- Molecule 28: Small nuclear ribonucleoprotein Sm D2

Chain m: 85% 15%



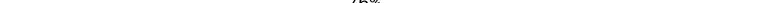
- Molecule 29: U2 small nuclear ribonucleoprotein A'

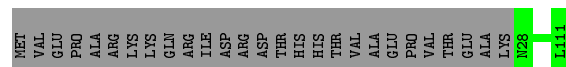
Chain W:  65% . 31%



VAL	SER	LYS	MET	THR	VAL	GLU	ARG	ARG	ASN	GLU	LEU	LYS	LYS	GLN	LEU	ALA	GLU	ALA	THR	SER	LEU	GLU	GLU	ILE	ALA	ARG	LEU	GLU	LYS	LEU	LEU	SER	GLY	GLY	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 30: U2 small nuclear ribonucleoprotein B''

Chain Y:  76% 24%



- Molecule 31: unknown

Chain x: 100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	93106	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	35714	Depositor
Image detector	GATAN K2 QUANTUM (4k 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: GTP, 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 >2	RMSZ	# Z >2
1	U	0.31	0/3351	0.75	1/5213 (0.0%)
10	G	0.42	0/839	0.74	0/1126
11	H	0.43	0/2667	0.80	1/3630 (0.0%)
12	J	0.45	0/2613	0.74	0/3551
13	K	0.40	0/1308	0.72	0/1765
14	L	0.40	0/1294	0.75	0/1732
15	M	0.42	0/2056	0.70	0/2766
16	N	0.41	0/1680	0.76	0/2258
17	O	0.43	0/1669	0.81	0/2236
18	P	0.43	0/282	0.69	0/380
19	R	0.40	0/550	0.76	0/752
2	E	0.36	0/388	0.69	0/603
20	S	0.44	0/3154	0.83	0/4297
21	T	0.38	0/2916	0.74	0/4026
22	b	0.34	0/636	0.59	0/856
22	k	0.28	0/394	0.50	0/546
23	d	0.36	0/634	0.62	1/859 (0.1%)
23	n	0.29	0/403	0.53	0/559
24	e	0.40	0/585	0.56	0/795
24	p	0.30	0/367	0.55	0/507
25	f	0.39	0/585	0.59	0/791
25	q	0.30	0/353	0.53	0/489
26	g	0.36	0/532	0.55	0/715
26	r	0.28	0/338	0.45	0/467
27	h	0.35	0/649	0.54	0/880
27	l	0.30	0/390	0.53	0/541
28	j	0.38	0/753	0.61	0/1013
28	m	0.31	0/466	0.54	0/649
29	W	0.31	0/814	0.53	0/1134
3	I	0.28	0/772	0.71	0/1195
30	Y	0.32	0/415	0.55	0/577
4	Z	0.26	0/4018	0.72	0/6233

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
5	V	0.31	0/2309	0.76	2/3590 (0.1%)
6	A	0.43	0/16107	0.75	0/21845
7	D	0.37	0/929	0.67	0/1243
8	F	0.42	0/325	0.74	0/442
9	C	0.41	0/6902	0.73	0/9386
All	All	0.39	0/64443	0.73	5/89647 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	G	0	1
15	M	0	1
17	O	0	1
20	S	0	1
6	A	0	2
All	All	0	6

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	39	U	C2'-C3'-O3'	8.13	127.38	109.50
5	V	35	A	C5'-C4'-O4'	6.92	117.40	109.10
11	H	440	LEU	CA-CB-CG	6.54	130.33	115.30
23	d	81	ALA	C-N-CD	-6.46	106.39	120.60
5	V	35	A	O4'-C4'-C3'	5.43	110.44	106.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	1325	SER	Peptide
6	A	403	TYR	Peptide
10	G	3	ARG	Peptide
15	M	231	ASP	Peptide
17	O	83	GLN	Peptide
20	S	237	ILE	Peptide

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	U	2999	0	1515	24	0
2	E	346	0	173	5	0
3	I	693	0	351	3	0
4	Z	3610	0	1831	10	0
5	V	2066	0	1043	21	0
6	A	15704	0	15649	227	0
7	D	912	0	936	11	0
8	F	321	0	282	3	0
9	C	6756	0	6801	117	0
10	G	823	0	808	10	0
11	H	2639	0	2073	25	0
12	J	2556	0	2551	54	0
13	K	1289	0	1309	17	0
14	L	1270	0	1294	12	0
15	M	2010	0	1964	20	0
16	N	1658	0	1713	49	0
17	O	1645	0	1672	32	0
18	P	275	0	283	4	0
19	R	550	0	356	2	0
20	S	3120	0	2397	39	0
21	T	2946	0	1250	6	0
22	b	631	0	670	0	0
22	k	396	0	169	0	0
23	d	625	0	647	0	0
23	n	404	0	180	0	0
24	e	575	0	597	0	0
24	p	369	0	152	0	0
25	f	573	0	572	0	0
25	q	354	0	153	0	0
26	g	529	0	557	0	0
26	r	340	0	152	0	0
27	h	644	0	686	0	0
27	l	392	0	165	0	0
28	j	741	0	778	0	0
28	m	467	0	199	0	0
29	W	816	0	341	1	0
30	Y	416	0	182	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	x	660	0	142	0	0
32	E	1	0	0	0	0
32	V	1	0	0	0	0
33	D	1	0	0	1	0
33	L	3	0	0	0	0
33	M	1	0	0	0	0
33	N	2	0	0	4	0
34	C	32	0	12	0	0
All	All	63161	0	52605	611	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 6.

All (611) 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)
16:N:34:CYS:SG	16:N:37:CYS:SG	1.40	1.39
1:U:45:A:N1	1:U:74:U:O4	1.65	1.30
16:N:16:CYS:SG	16:N:73:CYS:HB2	1.85	1.16
21:T:360:LYS:CB	21:T:381:HIS:CB	2.36	1.03
16:N:61:CYS:SG	33:N:401:ZN:ZN	1.54	0.94
7:D:88:CYS:SG	33:D:1001:ZN:ZN	1.65	0.85
16:N:16:CYS:SG	16:N:73:CYS:CB	2.65	0.84
15:M:250:MET:HB2	16:N:139:LEU:HD11	1.58	0.83
12:J:210:ASP:HB2	12:J:217:ILE:HD11	1.61	0.83
16:N:61:CYS:O	16:N:64:CYS:SG	2.37	0.82
16:N:220:THR:HG22	16:N:240:LEU:HD12	1.62	0.81
6:A:759:ARG:HD2	6:A:783:LEU:HD13	1.61	0.81
9:C:389:LEU:HD21	9:C:421:LEU:HD12	1.64	0.80
5:V:67:C:H2'	5:V:68:C:O4'	1.85	0.76
12:J:323:VAL:HG12	12:J:336:LEU:HD12	1.67	0.75
1:U:45:A:N1	1:U:74:U:C4	2.54	0.75
16:N:113:LEU:HD11	16:N:120:LEU:HD11	1.69	0.75
15:M:22:ILE:HG23	15:M:23:PRO:HD3	1.67	0.74
16:N:37:CYS:SG	33:N:401:ZN:ZN	1.77	0.74
17:O:230:THR:HG23	20:S:116:ASN:HD21	1.53	0.73
5:V:76:A:OP2	6:A:749:ARG:NH1	2.21	0.73
16:N:71:CYS:SG	33:N:402:ZN:ZN	1.77	0.72
6:A:1361:VAL:HG21	6:A:1407:ILE:HD11	1.72	0.72
6:A:1335:TRP:CD1	6:A:1367:ILE:HG13	2.24	0.72
6:A:853:THR:HG23	6:A:971:MET:HG3	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1335:TRP:CZ2	6:A:1339:LEU:HD13	2.25	0.71
6:A:745:THR:HA	12:J:182:VAL:HG21	1.73	0.70
6:A:631:LEU:HD21	6:A:663:LEU:HD12	1.73	0.70
9:C:406:VAL:HG11	9:C:427:LEU:HB3	1.71	0.70
15:M:250:MET:CB	16:N:139:LEU:HD11	2.21	0.70
9:C:493:LEU:HD21	9:C:539:VAL:HG21	1.74	0.70
20:S:209:GLU:HB3	20:S:218:THR:HG22	1.75	0.69
4:Z:34:G:N2	6:A:1325:SER:OG	2.22	0.68
6:A:1067:ASN:HB2	6:A:1083:THR:HG21	1.76	0.68
6:A:1342:LEU:CD2	6:A:1360:LEU:HD21	2.24	0.68
12:J:206:VAL:HG11	12:J:241:THR:HG21	1.76	0.67
9:C:621:ALA:HB2	9:C:664:ALA:HB2	1.76	0.67
9:C:241:VAL:HG11	9:C:273:LEU:HD23	1.76	0.66
17:O:21:LEU:HD12	17:O:40:LEU:HD11	1.76	0.66
9:C:200:CYS:HB3	9:C:436:VAL:HG21	1.78	0.66
12:J:290:VAL:HG12	12:J:311:VAL:HG11	1.77	0.66
1:U:110:U:H2'	1:U:111:C:O4'	1.95	0.66
6:A:741:ILE:HD11	12:J:224:LEU:HD22	1.78	0.65
6:A:1286:TRP:CE2	6:A:1302:LEU:HD11	2.31	0.65
17:O:60:LEU:HD21	17:O:94:PRO:HB3	1.79	0.65
11:H:299:LEU:HD11	11:H:329:ILE:HG12	1.79	0.65
6:A:716:ARG:O	6:A:720:PRO:HD2	1.97	0.64
9:C:193:LEU:HD11	9:C:228:ALA:HB2	1.78	0.64
16:N:125:ILE:HG21	16:N:135:ILE:HD12	1.80	0.64
12:J:282:VAL:HG11	12:J:323:VAL:HG21	1.80	0.64
6:A:1344:THR:O	6:A:1347:ARG:NH1	2.30	0.64
12:J:142:VAL:HG11	12:J:423:ILE:CG2	2.28	0.64
9:C:323:THR:HG21	9:C:438:ALA:HB2	1.81	0.63
6:A:630:LYS:O	6:A:634:ASP:N	2.26	0.63
9:C:501:ILE:HD13	9:C:567:ILE:HG23	1.79	0.63
9:C:872:LEU:HD13	9:C:922:THR:HG22	1.79	0.63
16:N:60:ILE:HB	16:N:64:CYS:SG	2.39	0.63
11:H:445:LEU:HD11	11:H:448:MET:HG3	1.80	0.62
20:S:225:ALA:O	20:S:229:VAL:HG23	1.98	0.62
7:D:63:LYS:HE3	8:F:6:LEU:HD22	1.80	0.62
16:N:71:CYS:HG	33:N:402:ZN:ZN	1.13	0.62
6:A:213:TYR:HA	6:A:216:GLN:HE21	1.63	0.62
6:A:673:VAL:HG22	6:A:714:PHE:CE1	2.34	0.62
9:C:251:GLN:HG2	9:C:933:TRP:CD2	2.35	0.61
12:J:277:VAL:HG11	12:J:321:PHE:CZ	2.36	0.61
6:A:857:ILE:HD11	6:A:969:ILE:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:91:ILE:HD12	16:N:125:ILE:HD12	1.82	0.61
6:A:268:LEU:HD13	6:A:277:LYS:HB2	1.82	0.61
9:C:602:VAL:HG11	9:C:860:PRO:HG3	1.81	0.61
6:A:673:VAL:HG22	6:A:714:PHE:CZ	2.36	0.61
20:S:149:VAL:O	20:S:152:VAL:HG12	2.01	0.61
6:A:1557:LEU:HD13	6:A:1562:PHE:CE2	2.36	0.61
9:C:133:ILE:HD13	9:C:560:GLN:HB3	1.83	0.61
1:U:98:U:HO2'	5:V:75:A:H8	1.48	0.60
9:C:270:LEU:HD11	9:C:313:PHE:HB3	1.82	0.60
16:N:39:LEU:HD13	16:N:40:PRO:HD2	1.84	0.60
6:A:1738:LEU:HD13	6:A:1779:LEU:HD11	1.84	0.60
4:Z:38:U:O2	10:G:1:MET:N	2.34	0.60
12:J:323:VAL:CG1	12:J:336:LEU:HD12	2.32	0.60
14:L:66:LEU:HD13	14:L:73:ILE:HG13	1.83	0.59
9:C:656:LEU:HD22	9:C:670:ILE:HD11	1.85	0.59
9:C:866:ILE:HB	9:C:902:VAL:HG13	1.83	0.59
6:A:1032:ILE:HG12	6:A:1171:LEU:HD22	1.83	0.59
9:C:499:VAL:HG11	9:C:577:LEU:HD13	1.83	0.59
20:S:173:VAL:HG23	20:S:188:ILE:HD11	1.85	0.59
6:A:390:LEU:HD21	9:C:605:ILE:HD11	1.85	0.58
12:J:240:ALA:HB1	12:J:248:ILE:HD11	1.82	0.58
12:J:160:ASN:HA	12:J:184:THR:HB	1.85	0.58
16:N:39:LEU:HD23	16:N:111:ARG:HG2	1.85	0.58
11:H:298:VAL:HG11	11:H:312:LEU:HD23	1.84	0.58
6:A:842:LYS:O	6:A:845:VAL:HG12	2.02	0.58
16:N:207:LEU:HD11	16:N:251:LEU:HD11	1.86	0.58
16:N:16:CYS:SG	16:N:71:CYS:SG	3.02	0.58
12:J:248:ILE:HG23	12:J:262:LEU:HB2	1.84	0.58
6:A:1668:ILE:HD13	6:A:1801:SER:HB3	1.86	0.58
17:O:185:LEU:O	17:O:188:ARG:HG3	2.03	0.58
16:N:16:CYS:HG	16:N:73:CYS:HB2	1.65	0.57
12:J:147:ILE:HD13	12:J:408:ASP:HA	1.84	0.57
16:N:16:CYS:SG	16:N:73:CYS:SG	3.02	0.57
6:A:1632:ILE:HG21	6:A:1645:LEU:HD13	1.85	0.57
17:O:185:LEU:O	17:O:189:ARG:HG2	2.03	0.57
6:A:395:PRO:HB2	6:A:398:VAL:HG21	1.87	0.57
6:A:305:LEU:HD21	6:A:476:ALA:HB2	1.85	0.57
14:L:66:LEU:HD13	14:L:73:ILE:CG1	2.34	0.57
6:A:1557:LEU:HD11	6:A:1570:TRP:HB2	1.86	0.56
6:A:322:VAL:HG23	6:A:508:GLN:HE21	1.70	0.56
6:A:342:LEU:HB3	6:A:344:ASN:HD22	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:328:VAL:HG21	9:C:345:THR:HG22	1.87	0.56
20:S:229:VAL:HG22	20:S:238:TRP:HZ2	1.69	0.56
6:A:370:ILE:HB	6:A:1418:THR:HG21	1.87	0.56
6:A:969:ILE:HG22	6:A:982:TYR:HA	1.86	0.56
6:A:1049:LEU:HB2	6:A:1258:LEU:HD11	1.86	0.56
11:H:465:PHE:HB2	11:H:473:LEU:HD23	1.88	0.56
6:A:948:HIS:CE1	6:A:952:ASN:HD21	2.23	0.56
5:V:59:A:H2'	5:V:60:G:O4'	2.05	0.56
17:O:33:TRP:CE3	17:O:36:VAL:HG11	2.41	0.56
20:S:184:GLY:O	20:S:188:ILE:HG23	2.05	0.56
12:J:289:THR:HG22	12:J:305:THR:HG22	1.88	0.56
16:N:226:LEU:HD13	16:N:266:ILE:HD11	1.87	0.56
6:A:878:GLU:O	6:A:882:ILE:HG23	2.06	0.56
7:D:11:TYR:CD1	10:G:12:LEU:HD21	2.41	0.56
17:O:230:THR:HG21	20:S:117:HIS:ND1	2.21	0.56
6:A:1417:GLN:HG2	6:A:1418:THR:HG23	1.88	0.55
6:A:172:ILE:HD13	6:A:625:LEU:HB3	1.88	0.55
6:A:521:SER:HB2	6:A:682:ASP:HA	1.88	0.55
12:J:277:VAL:HG13	12:J:278:ASP:N	2.20	0.55
16:N:106:ASN:HD21	17:O:208:GLY:HA2	1.71	0.55
6:A:137:GLU:CD	14:L:30:LEU:HG	2.26	0.55
14:L:94:LYS:HD2	14:L:109:ILE:HD11	1.87	0.55
6:A:1000:TRP:CZ2	6:A:1510:ILE:HG21	2.41	0.55
17:O:37:ALA:HB2	17:O:45:ALA:HA	1.88	0.55
6:A:724:ARG:O	6:A:728:ASN:HB2	2.07	0.55
9:C:472:VAL:HB	9:C:575:ALA:HB3	1.88	0.55
15:M:163:VAL:HG23	15:M:164:PHE:HD1	1.71	0.55
6:A:168:LEU:N	6:A:169:PRO:CD	2.69	0.55
6:A:588:LEU:HD13	6:A:591:LEU:CD2	2.37	0.55
6:A:1209:LYS:HA	6:A:1212:ARG:HG2	1.89	0.55
6:A:168:LEU:HD21	6:A:626:LEU:HD21	1.89	0.55
6:A:1542:TYR:O	6:A:1546:VAL:HG23	2.07	0.54
6:A:424:PHE:CE1	9:C:893:LYS:HB3	2.42	0.54
16:N:106:ASN:HB2	17:O:213:TYR:CG	2.42	0.54
6:A:628:MET:HE3	6:A:660:ILE:HG23	1.88	0.54
1:U:45:A:C2	1:U:74:U:O4	2.54	0.54
6:A:228:LYS:HD2	6:A:695:LEU:HD11	1.90	0.54
2:E:-5:G:HO2'	2:E:-4:A:H8	1.55	0.54
16:N:17:LEU:CD2	16:N:23:ILE:HD12	2.37	0.54
6:A:1562:PHE:O	6:A:1565:THR:OG1	2.24	0.54
16:N:29:PRO:HA	16:N:42:THR:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:211:ILE:HD13	20:S:44:ARG:HG3	1.89	0.54
20:S:99:ILE:N	20:S:100:PRO:CD	2.70	0.54
29:W:121:PRO:O	29:W:122:ARG:CB	2.56	0.54
17:O:16:VAL:HG22	17:O:152:LEU:HD21	1.88	0.54
6:A:141:LYS:HG3	14:L:52:ILE:HD11	1.90	0.54
6:A:1335:TRP:CH2	6:A:1364:GLU:HG2	2.42	0.54
6:A:1756:PHE:CE1	6:A:1760:THR:HG21	2.43	0.54
6:A:880:THR:OG1	13:K:207:ALA:HB1	2.08	0.54
9:C:861:ILE:HD11	9:C:938:ARG:HB2	1.89	0.54
7:D:51:CYS:SG	7:D:88:CYS:SG	3.06	0.54
1:U:92:U:O2	19:R:12:LYS:NZ	2.39	0.54
1:U:103:A:O2'	1:U:104:G:O4'	2.24	0.54
9:C:138:VAL:HG23	9:C:236:LEU:HB2	1.90	0.53
9:C:265:PHE:HB2	9:C:311:ILE:HD13	1.89	0.53
9:C:191:ILE:HG23	9:C:221:PHE:CE2	2.44	0.53
1:U:102:C:OP1	6:A:675:HIS:NE2	2.42	0.53
9:C:241:VAL:HG22	9:C:267:ILE:CG2	2.38	0.53
5:V:35:A:C8	14:L:41:LEU:HD13	2.43	0.53
6:A:929:LEU:HD11	6:A:1590:LEU:HD23	1.91	0.53
6:A:674:MET:CE	6:A:1621:VAL:HG11	2.38	0.53
6:A:2060:LEU:HD21	6:A:2078:GLU:HG3	1.89	0.53
12:J:277:VAL:HG11	12:J:321:PHE:HZ	1.71	0.53
1:U:45:A:N6	1:U:74:U:N3	2.55	0.53
9:C:864:VAL:HG22	9:C:930:LEU:HD23	1.90	0.53
6:A:882:ILE:HD11	6:A:1065:LEU:HD21	1.90	0.53
12:J:306:HIS:CE1	13:K:147:LEU:HD11	2.44	0.53
6:A:210:GLU:O	6:A:214:THR:HG23	2.09	0.53
6:A:588:LEU:HD13	6:A:591:LEU:HD22	1.91	0.53
7:D:101:PRO:HB2	8:F:23:VAL:HG21	1.90	0.53
12:J:142:VAL:HG11	12:J:423:ILE:HG23	1.91	0.53
6:A:161:PHE:HA	6:A:198:ALA:HB1	1.91	0.53
6:A:308:MET:HG3	6:A:479:LEU:HD11	1.89	0.53
9:C:201:THR:HG22	9:C:207:SER:HB3	1.90	0.53
9:C:126:MET:SD	9:C:132:ARG:NH2	2.82	0.53
6:A:937:LEU:HD22	6:A:1590:LEU:CD2	2.39	0.52
10:G:55:SER:O	10:G:58:ILE:HG22	2.10	0.52
9:C:836:SER:O	9:C:840:PRO:HD2	2.09	0.52
12:J:341:LEU:HD23	12:J:342:LEU:N	2.24	0.52
21:T:119:ALA:HB1	21:T:128:ILE:CA	2.39	0.52
1:U:32:G:H3'	1:U:33:U:C5'	2.38	0.52
6:A:937:LEU:HD22	6:A:1590:LEU:HD22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1375:LEU:HD12	6:A:1383:PHE:CE1	2.44	0.52
1:U:45:A:N3	1:U:45:A:H2'	2.24	0.52
13:K:201:PHE:CD2	17:O:80:LEU:HD21	2.45	0.52
6:A:1339:LEU:HD11	6:A:1360:LEU:HD22	1.92	0.52
12:J:335:GLY:H	12:J:342:LEU:HD13	1.74	0.52
6:A:1207:TRP:O	6:A:1212:ARG:NH1	2.42	0.52
6:A:1090:ILE:HD11	6:A:1104:ILE:CD1	2.40	0.52
6:A:1393:GLU:O	6:A:1394:LEU:HD23	2.10	0.52
6:A:1974:LEU:O	6:A:1977:VAL:HG22	2.10	0.52
6:A:730:ILE:HD12	6:A:731:THR:N	2.25	0.52
9:C:539:VAL:HG13	9:C:564:ILE:HG23	1.92	0.52
6:A:785:HIS:NE2	13:K:168:ALA:HB2	2.24	0.52
6:A:1654:TRP:CZ3	6:A:1779:LEU:HD12	2.45	0.51
7:D:51:CYS:SG	7:D:88:CYS:HB3	2.50	0.51
20:S:199:MET:SD	20:S:246:LEU:HD22	2.50	0.51
6:A:212:VAL:HG22	6:A:311:LEU:HD11	1.92	0.51
6:A:718:THR:O	6:A:719:ILE:C	2.48	0.51
9:C:626:SER:HB3	9:C:634:ILE:HD12	1.91	0.51
6:A:808:ILE:HG21	13:K:165:ILE:HD12	1.91	0.51
11:H:333:SER:HA	11:H:343:TYR:CE2	2.46	0.51
9:C:664:ALA:HB1	9:C:666:ILE:CD1	2.39	0.51
9:C:664:ALA:HB1	9:C:666:ILE:HD12	1.92	0.51
11:H:347:SER:O	11:H:351:ILE:HG12	2.09	0.51
16:N:61:CYS:N	16:N:64:CYS:SG	2.84	0.51
17:O:16:VAL:CG2	17:O:152:LEU:HD21	2.40	0.51
3:I:2:U:O4	4:Z:37:G:H1'	2.10	0.51
6:A:249:LEU:O	6:A:249:LEU:HD12	2.11	0.51
6:A:660:ILE:HG21	6:A:711:TRP:CH2	2.45	0.51
6:A:1047:ALA:HB3	6:A:1251:TYR:HB3	1.92	0.51
6:A:1375:LEU:HD12	6:A:1383:PHE:HE1	1.76	0.51
6:A:172:ILE:HG23	6:A:629:MET:HG2	1.93	0.51
9:C:255:GLN:HG2	9:C:598:ILE:HD12	1.92	0.51
12:J:206:VAL:CG1	12:J:241:THR:HG21	2.40	0.51
9:C:963:SER:O	9:C:967:VAL:HG23	2.10	0.51
3:I:2:U:H3'	6:A:607:THR:OG1	2.11	0.51
6:A:1329:THR:HG21	6:A:1601:ILE:HB	1.93	0.51
6:A:458:PHE:CZ	9:C:336:ILE:HD11	2.45	0.51
9:C:872:LEU:HD13	9:C:922:THR:CG2	2.41	0.51
11:H:326:VAL:O	11:H:330:ILE:HG12	2.10	0.51
12:J:275:THR:OG1	12:J:279:PRO:O	2.29	0.51
6:A:350:PRO:HD3	6:A:526:LEU:HD13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:741:ILE:CD1	12:J:224:LEU:HD22	2.41	0.50
20:S:172:PHE:CD2	20:S:188:ILE:HD13	2.46	0.50
5:V:27:U:O2'	14:L:124:VAL:HA	2.11	0.50
6:A:1893:ILE:HD12	6:A:1978:VAL:HG22	1.92	0.50
6:A:659:HIS:O	6:A:660:ILE:C	2.49	0.50
6:A:713:ASN:O	6:A:716:ARG:HB3	2.11	0.50
9:C:139:ILE:HG12	9:C:225:THR:HG23	1.93	0.50
3:I:3:A:OP2	10:G:3:ARG:HA	2.11	0.50
1:U:71:A:N3	1:U:116:U:O2'	2.33	0.50
4:Z:4:A:H2'	4:Z:5:A:H5'	1.91	0.50
6:A:249:LEU:HD11	6:A:637:VAL:HG11	1.93	0.50
9:C:493:LEU:HD22	9:C:542:ILE:HD11	1.93	0.50
6:A:912:LEU:HD22	6:A:951:LEU:HG	1.94	0.50
9:C:615:LEU:N	9:C:616:PRO:HD2	2.26	0.50
9:C:617:LYS:HB3	9:C:666:ILE:HD11	1.94	0.50
6:A:182:PRO:HG2	6:A:220:THR:HG21	1.94	0.50
6:A:410:ILE:HD12	6:A:410:ILE:N	2.27	0.50
6:A:175:LEU:HD23	6:A:564:TRP:CZ2	2.46	0.50
6:A:674:MET:HA	6:A:674:MET:CE	2.42	0.50
9:C:133:ILE:HG23	9:C:209:MET:SD	2.52	0.50
9:C:864:VAL:HG22	9:C:930:LEU:CD2	2.42	0.50
17:O:230:THR:HG21	20:S:117:HIS:CE1	2.47	0.50
6:A:1344:THR:HG21	6:A:1537:TRP:CD2	2.46	0.50
12:J:156:ILE:HG22	12:J:166:VAL:HG22	1.93	0.50
12:J:200:VAL:CG2	12:J:227:VAL:HB	2.41	0.50
9:C:231:ALA:HB2	9:C:473:LEU:HD13	1.93	0.49
6:A:138:HIS:NE2	6:A:142:ILE:HD11	2.27	0.49
5:V:35:A:C8	15:M:75:PHE:CZ	3.00	0.49
1:U:32:G:C6	1:U:34:C:C4	3.01	0.49
4:Z:4:A:C2'	4:Z:5:A:H5'	2.42	0.49
6:A:1309:ILE:CG2	6:A:1359:ILE:HD12	2.42	0.49
6:A:793:TRP:CZ2	6:A:820:ALA:HB1	2.48	0.49
17:O:230:THR:HG22	20:S:114:CYS:SG	2.53	0.49
10:G:28:ASP:OD1	10:G:28:ASP:N	2.44	0.49
11:H:291:PHE:CE1	11:H:317:ILE:HG21	2.47	0.49
16:N:37:CYS:SG	16:N:61:CYS:SG	3.11	0.49
6:A:937:LEU:HD13	6:A:1590:LEU:HD11	1.93	0.49
9:C:116:THR:HG21	9:C:118:TYR:CZ	2.47	0.49
9:C:544:LEU:HD23	9:C:562:VAL:HG12	1.94	0.49
8:F:27:GLU:O	8:F:31:ILE:HG12	2.13	0.49
12:J:145:VAL:HG22	12:J:157:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:137:GLU:CD	14:L:52:ILE:HG23	2.33	0.49
6:A:1400:ILE:HG22	6:A:1400:ILE:O	2.12	0.49
9:C:137:GLY:O	9:C:139:ILE:HD12	2.13	0.49
17:O:20:ILE:HD11	17:O:152:LEU:HD22	1.95	0.49
20:S:99:ILE:HD11	20:S:132:VAL:HG11	1.95	0.49
6:A:1795:LYS:N	6:A:1796:PRO:CD	2.75	0.49
12:J:150:VAL:HG13	12:J:151:ASP:HB3	1.95	0.49
21:T:332:GLN:CB	21:T:342:ILE:CB	2.91	0.49
5:V:52:G:H2'	5:V:53:A:C8	2.47	0.49
9:C:607:LEU:HD11	9:C:644:ILE:HD11	1.96	0.48
17:O:24:ALA:O	17:O:28:TYR:N	2.37	0.48
6:A:1557:LEU:HD13	6:A:1562:PHE:CD2	2.48	0.48
9:C:213:LEU:HD11	9:C:561:ILE:HD13	1.95	0.48
11:H:427:LEU:HD23	11:H:436:LEU:HD11	1.95	0.48
6:A:724:ARG:CD	18:P:31:LEU:HD11	2.43	0.48
11:H:368:ASN:ND2	11:H:384:LEU:HD11	2.29	0.48
5:V:41:A:H2'	5:V:42:A:O4'	2.14	0.48
6:A:1669:LEU:HB3	6:A:1681:VAL:HG21	1.95	0.48
12:J:277:VAL:HG22	12:J:278:ASP:H	1.79	0.48
6:A:1223:GLY:CA	6:A:1248:VAL:HG11	2.43	0.48
6:A:708:TRP:CE2	6:A:712:LEU:HD11	2.49	0.48
12:J:147:ILE:HG22	12:J:155:PHE:HB3	1.94	0.48
16:N:65:ALA:O	16:N:69:ASN:N	2.47	0.48
12:J:272:VAL:O	12:J:272:VAL:HG13	2.14	0.48
9:C:241:VAL:HG23	9:C:268:ASN:O	2.14	0.48
16:N:17:LEU:HD21	16:N:23:ILE:HD12	1.96	0.48
6:A:1028:TRP:CZ3	6:A:1162:THR:HG22	2.49	0.48
6:A:522:TYR:CZ	6:A:686:ILE:HD12	2.48	0.48
14:L:22:THR:HG21	14:L:62:TYR:CE1	2.49	0.48
15:M:137:LEU:HD21	15:M:192:ALA:HB1	1.96	0.48
17:O:218:VAL:HB	20:S:89:GLU:HB3	1.96	0.48
5:V:32:U:C4	16:N:28:ILE:HG21	2.49	0.48
6:A:857:ILE:CD1	6:A:969:ILE:HD11	2.44	0.47
9:C:273:LEU:HD12	9:C:274:ILE:N	2.29	0.47
9:C:625:ILE:HG22	9:C:634:ILE:HD11	1.95	0.47
20:S:140:LEU:HD22	20:S:156:TYR:CE2	2.49	0.47
6:A:1222:LEU:O	6:A:1226:VAL:HG23	2.15	0.47
9:C:229:LEU:HB3	9:C:259:ASN:HD21	1.79	0.47
13:K:41:ASP:HA	13:K:44:ILE:HD12	1.96	0.47
9:C:211:ASN:HD22	9:C:211:ASN:N	2.12	0.47
9:C:873:LEU:HD21	9:C:891:THR:HG21	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:355:ARG:O	11:H:359:THR:HG23	2.14	0.47
17:O:33:TRP:HA	17:O:36:VAL:HG12	1.96	0.47
20:S:112:VAL:HG13	20:S:114:CYS:HB2	1.96	0.47
21:T:119:ALA:HB1	21:T:128:ILE:HA	1.94	0.47
6:A:1066:LEU:HD11	6:A:1113:ILE:HG23	1.95	0.47
6:A:522:TYR:CE2	6:A:686:ILE:HD12	2.50	0.47
9:C:136:VAL:O	9:C:234:LEU:O	2.33	0.47
12:J:341:LEU:HD22	13:K:45:PRO:HB3	1.96	0.47
6:A:628:MET:CE	6:A:664:THR:HB	2.45	0.47
6:A:1388:PHE:CD1	6:A:1397:LEU:HD12	2.50	0.47
9:C:193:LEU:HD12	9:C:213:LEU:HB3	1.97	0.47
9:C:504:THR:HG23	9:C:574:SER:O	2.15	0.47
6:A:1234:VAL:HG11	6:A:1239:THR:HG22	1.95	0.47
6:A:1347:ARG:HD2	6:A:1447:TRP:CE2	2.49	0.47
2:E:-5:G:O2'	2:E:-4:A:H8	1.98	0.47
20:S:229:VAL:HG11	20:S:243:VAL:CG2	2.45	0.47
6:A:687:ILE:HD11	6:A:706:PRO:HG3	1.97	0.47
7:D:23:LEU:HG	10:G:18:GLN:HE22	1.80	0.47
12:J:144:CYS:SG	12:J:187:ASP:HA	2.55	0.47
20:S:225:ALA:O	20:S:228:THR:HG22	2.15	0.47
6:A:1345:TYR:HD1	6:A:1345:TYR:O	1.98	0.46
6:A:468:LEU:HD22	6:A:469:ILE:HG23	1.97	0.46
13:K:104:LEU:HD12	13:K:113:GLU:HA	1.97	0.46
20:S:193:VAL:HG11	20:S:202:TRP:CZ2	2.50	0.46
6:A:1417:GLN:CG	6:A:1418:THR:HG23	2.45	0.46
12:J:269:ILE:HA	12:J:285:SER:HA	1.97	0.46
6:A:876:PRO:HA	13:K:204:LEU:HD22	1.97	0.46
6:A:319:ARG:O	6:A:321:GLU:N	2.48	0.46
7:D:31:LEU:HD11	10:G:31:ARG:NH2	2.30	0.46
9:C:312:ILE:HD13	9:C:435:LEU:HG	1.98	0.46
17:O:214:ASN:HB2	17:O:217:ILE:HD11	1.97	0.46
17:O:25:VAL:HG11	17:O:52:TRP:CH2	2.50	0.46
6:A:1881:THR:HG21	6:A:1920:LEU:CD2	2.46	0.46
12:J:144:CYS:SG	12:J:145:VAL:N	2.89	0.46
5:V:71:G:H21	5:V:75:A:H2	1.62	0.46
6:A:286:LEU:HD13	6:A:287:GLU:N	2.30	0.46
11:H:369:TYR:CE1	11:H:420:ILE:HD11	2.51	0.46
11:H:465:PHE:CB	11:H:473:LEU:HD23	2.46	0.46
15:M:17:GLU:HB2	15:M:18:LEU:HD13	1.97	0.46
6:A:1350:ILE:HD13	6:A:1356:LEU:CD2	2.46	0.46
6:A:929:LEU:HD11	6:A:1590:LEU:CD2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:493:LEU:CD2	9:C:539:VAL:HG21	2.45	0.46
14:L:94:LYS:CD	14:L:109:ILE:HD11	2.45	0.46
5:V:32:U:O4	16:N:28:ILE:HG21	2.16	0.46
9:C:873:LEU:N	9:C:874:PRO:CD	2.79	0.46
9:C:928:CYS:SG	9:C:929:GLN:N	2.89	0.46
12:J:248:ILE:HG13	12:J:262:LEU:HD12	1.98	0.46
17:O:230:THR:HG21	20:S:117:HIS:CG	2.51	0.46
11:H:334:LEU:HD21	11:H:384:LEU:HD12	1.98	0.46
15:M:99:ILE:HD13	15:M:188:TYR:CD2	2.51	0.46
6:A:1020:ILE:HB	6:A:1022:PRO:HD2	1.98	0.45
6:A:1357:LEU:HD11	11:H:303:LEU:HD22	1.98	0.45
9:C:501:ILE:CD1	9:C:567:ILE:HG23	2.46	0.45
1:U:119:U:C2	1:U:120:G:C8	3.04	0.45
6:A:1354:GLU:N	6:A:1355:PRO:CD	2.78	0.45
9:C:837:GLN:HA	9:C:837:GLN:HE21	1.81	0.45
11:H:351:ILE:HG21	11:H:395:GLU:HG3	1.98	0.45
12:J:144:CYS:SG	12:J:188:VAL:N	2.88	0.45
12:J:284:SER:OG	12:J:311:VAL:O	2.35	0.45
1:U:47:U:H2'	1:U:48:G:C8	2.52	0.45
6:A:783:LEU:HD12	6:A:783:LEU:O	2.16	0.45
9:C:492:LEU:O	9:C:492:LEU:HD12	2.16	0.45
11:H:330:ILE:HG22	11:H:334:LEU:CD2	2.46	0.45
20:S:169:TRP:CE3	20:S:192:TYR:HB2	2.51	0.45
6:A:1282:ASP:C	11:H:345:ILE:HD11	2.36	0.45
6:A:1286:TRP:CD1	6:A:1448:GLU:HB2	2.52	0.45
2:E:-4:A:H2'	2:E:-3:A:C8	2.51	0.45
6:A:210:GLU:N	6:A:211:PRO:HD2	2.32	0.45
9:C:274:ILE:HG21	9:C:385:PHE:CD2	2.51	0.45
9:C:470:ALA:HB1	9:C:486:VAL:HG12	1.98	0.45
9:C:936:ILE:O	9:C:936:ILE:HG23	2.16	0.45
16:N:216:GLU:O	16:N:220:THR:HG23	2.17	0.45
6:A:1461:TYR:CE1	6:A:1494:LEU:HD13	2.51	0.45
11:H:312:LEU:CD1	11:H:329:ILE:HD11	2.47	0.45
6:A:1049:LEU:CB	6:A:1258:LEU:HD11	2.47	0.45
6:A:507:LEU:HD21	6:A:529:TYR:CE2	2.52	0.45
6:A:583:ILE:HG23	6:A:588:LEU:HD12	1.98	0.45
12:J:229:THR:HG21	12:J:271:GLN:HA	1.98	0.45
4:Z:5:A:H2'	4:Z:6:U:O4'	2.16	0.45
12:J:161:ASP:O	12:J:162:THR:HB	2.17	0.45
20:S:202:TRP:CZ2	20:S:228:THR:HG21	2.52	0.45
6:A:1214:ARG:N	6:A:1255:ASN:OD1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1657:ILE:CD1	6:A:1815:LEU:HD22	2.47	0.45
6:A:889:TRP:CH2	6:A:893:ARG:HD3	2.52	0.45
9:C:862:TYR:CE2	9:C:908:VAL:HG13	2.51	0.45
15:M:81:CYS:SG	15:M:91:HIS:CE1	3.10	0.45
5:V:63:G:H2'	5:V:64:U:H6	1.82	0.45
6:A:1560:THR:HG21	6:A:1609:TRP:NE1	2.32	0.44
20:S:140:LEU:HD23	20:S:152:VAL:HG22	1.99	0.44
6:A:173:LEU:HA	6:A:715:LEU:HD13	1.98	0.44
6:A:639:PHE:CG	6:A:649:LEU:HD22	2.52	0.44
16:N:16:CYS:HB2	16:N:71:CYS:SG	2.57	0.44
9:C:241:VAL:CG1	9:C:273:LEU:HD23	2.46	0.44
9:C:808:LEU:HD22	9:C:944:VAL:HG21	1.99	0.44
16:N:12:ILE:HG23	16:N:16:CYS:SG	2.57	0.44
6:A:1090:ILE:HD11	6:A:1104:ILE:HD11	1.99	0.44
6:A:1336:ASN:HB3	6:A:1400:ILE:HD12	1.99	0.44
6:A:1820:ARG:O	6:A:1824:GLN:N	2.50	0.44
6:A:264:ILE:HD11	6:A:647:PHE:N	2.33	0.44
9:C:223:ASP:OD1	9:C:224:GLU:N	2.50	0.44
10:G:18:GLN:HG3	10:G:19:GLN:N	2.32	0.44
11:H:292:LYS:CD	11:H:328:ILE:HD11	2.47	0.44
1:U:39:U:H2'	1:U:40:C:O4'	2.18	0.44
6:A:458:PHE:CE2	9:C:336:ILE:HD11	2.52	0.44
6:A:719:ILE:HB	6:A:720:PRO:CD	2.47	0.44
9:C:444:GLN:N	9:C:445:PRO:CD	2.81	0.44
6:A:724:ARG:HD3	18:P:31:LEU:HD11	1.99	0.44
6:A:687:ILE:HD11	6:A:706:PRO:CG	2.48	0.44
9:C:905:GLN:NE2	9:C:936:ILE:HD13	2.32	0.44
12:J:248:ILE:HD13	12:J:272:VAL:HG21	2.00	0.44
6:A:1371:VAL:HG11	6:A:1397:LEU:HD11	1.98	0.44
6:A:759:ARG:CD	6:A:783:LEU:HD13	2.41	0.44
9:C:708:ILE:N	9:C:708:ILE:HD12	2.33	0.44
2:E:-4:A:H2'	2:E:-3:A:H8	1.83	0.44
6:A:189:VAL:CG2	6:A:202:VAL:HG13	2.48	0.44
6:A:588:LEU:HD22	6:A:613:SER:HA	2.00	0.44
15:M:114:ARG:NE	15:M:127:ILE:HG21	2.32	0.44
15:M:173:ILE:HG12	15:M:184:VAL:HG13	1.99	0.44
20:S:140:LEU:CD2	20:S:155:LEU:HD22	2.48	0.44
20:S:160:CYS:HB3	20:S:169:TRP:CH2	2.53	0.44
6:A:1372:LYS:HD2	6:A:1378:LYS:HA	2.00	0.43
6:A:1944:LEU:HD23	6:A:1956:ILE:HG23	2.00	0.43
9:C:658:ASP:HB3	9:C:663:TYR:CE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:74:LEU:HA	15:M:112:PHE:CE1	2.53	0.43
16:N:125:ILE:HG21	16:N:135:ILE:CD1	2.45	0.43
6:A:268:LEU:HD13	6:A:277:LYS:CB	2.47	0.43
12:J:156:ILE:HD11	12:J:188:VAL:HG21	2.00	0.43
12:J:277:VAL:HG13	12:J:279:PRO:HD2	2.00	0.43
12:J:129:TRP:HB2	12:J:385:GLN:HE22	1.83	0.43
20:S:229:VAL:HG22	20:S:238:TRP:CZ2	2.50	0.43
6:A:1021:PRO:O	6:A:1025:VAL:HG23	2.17	0.43
6:A:1409:ALA:HB3	6:A:1424:HIS:O	2.18	0.43
9:C:862:TYR:CG	9:C:908:VAL:HG22	2.53	0.43
7:D:43:LEU:HD21	7:D:86:ILE:CD1	2.47	0.43
12:J:142:VAL:O	12:J:142:VAL:HG12	2.18	0.43
16:N:91:ILE:CD1	16:N:125:ILE:HD12	2.48	0.43
20:S:193:VAL:HG11	20:S:202:TRP:CH2	2.54	0.43
6:A:1375:LEU:CD1	6:A:1614:ILE:HD13	2.49	0.43
6:A:239:PHE:CE1	6:A:656:ILE:HD11	2.53	0.43
6:A:796:ASN:HD22	6:A:858:LYS:HG3	1.82	0.43
9:C:225:THR:HG21	9:C:252:LEU:CD2	2.48	0.43
16:N:67:GLN:HB3	16:N:120:LEU:HD23	2.00	0.43
13:K:35:ALA:CB	20:S:158:LYS:HE3	2.48	0.43
4:Z:34:G:H21	6:A:1325:SER:HG	1.59	0.43
9:C:335:SER:HB2	9:C:336:ILE:HD12	1.99	0.43
16:N:71:CYS:HB3	16:N:74:CYS:HB2	2.00	0.43
6:A:1085:LYS:O	6:A:1088:VAL:HG13	2.18	0.43
11:H:381:LEU:HD21	11:H:419:PHE:CA	2.49	0.43
1:U:79:C:H3'	1:U:80:G:C5'	2.49	0.43
6:A:834:ILE:CD1	6:A:845:VAL:HG23	2.49	0.43
9:C:888:ILE:HG23	9:C:902:VAL:HG23	2.00	0.43
7:D:11:TYR:CE1	10:G:12:LEU:HD21	2.54	0.43
14:L:73:ILE:HG23	14:L:77:LEU:HD23	2.00	0.43
15:M:250:MET:SD	16:N:139:LEU:HD21	2.59	0.43
6:A:954:ILE:HG23	6:A:991:THR:HG23	2.00	0.43
15:M:247:LEU:HA	15:M:250:MET:HG2	1.99	0.43
17:O:211:ILE:O	20:S:83:ARG:NH2	2.52	0.43
6:A:136:PRO:HB3	6:A:562:ILE:HD13	2.01	0.43
9:C:905:GLN:HE22	9:C:936:ILE:HD13	1.84	0.43
9:C:94:VAL:HG12	12:J:154:TRP:CZ2	2.54	0.43
20:S:72:ALA:HB1	20:S:88:PHE:CZ	2.54	0.43
6:A:1347:ARG:HD2	6:A:1447:TRP:CD2	2.54	0.43
6:A:1387:VAL:HG12	6:A:1610:TRP:CD2	2.53	0.43
6:A:849:LEU:C	6:A:849:LEU:HD13	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:242:VAL:HG22	9:C:277:LEU:HD11	2.01	0.43
9:C:381:LEU:HA	9:C:384:ILE:HD12	1.99	0.43
9:C:78:MET:N	9:C:78:MET:SD	2.92	0.43
13:K:127:VAL:HG13	16:N:31:GLY:O	2.18	0.43
6:A:1737:GLN:HA	6:A:1737:GLN:HE21	1.84	0.42
6:A:305:LEU:HD22	9:C:390:SER:HA	2.01	0.42
9:C:861:ILE:HA	9:C:907:PRO:HA	2.01	0.42
6:A:785:HIS:CE1	13:K:168:ALA:HB2	2.54	0.42
17:O:211:ILE:HD12	20:S:48:ARG:CZ	2.49	0.42
1:U:105:A:H2'	1:U:106:A:C8	2.54	0.42
4:Z:26:G:C2	5:V:59:A:C5	3.07	0.42
6:A:1089:VAL:HG22	6:A:1098:VAL:HG22	2.01	0.42
9:C:599:THR:O	9:C:599:THR:HG23	2.18	0.42
6:A:556:TYR:CG	13:K:120:ASP:HB3	2.54	0.42
6:A:139:LEU:HD13	6:A:193:TYR:CD2	2.55	0.42
6:A:1921:VAL:HG21	6:A:1948:MET:HE1	2.00	0.42
6:A:852:LEU:HD23	6:A:978:ILE:HD11	2.01	0.42
9:C:104:THR:HG23	9:C:105:ILE:HG23	2.00	0.42
9:C:791:TYR:O	9:C:791:TYR:CG	2.72	0.42
10:G:51:LYS:O	10:G:54:VAL:HG12	2.19	0.42
12:J:200:VAL:HG22	12:J:227:VAL:HB	2.01	0.42
16:N:88:ASP:O	16:N:91:ILE:HG23	2.20	0.42
19:R:13:GLY:O	19:R:15:SER:N	2.52	0.42
17:O:211:ILE:CD1	20:S:48:ARG:HB2	2.49	0.42
1:U:74:U:O2	1:U:78:A:C2	2.72	0.42
9:C:710:VAL:HG22	9:C:820:LEU:HD23	2.01	0.42
14:L:119:THR:HG22	14:L:120:CYS:N	2.34	0.42
16:N:67:GLN:HA	16:N:119:LYS:HA	2.02	0.42
21:T:119:ALA:HB1	21:T:128:ILE:CB	2.50	0.42
6:A:172:ILE:HG23	6:A:629:MET:CG	2.49	0.42
6:A:783:LEU:HD12	6:A:783:LEU:C	2.39	0.42
9:C:605:ILE:HD12	9:C:652:MET:HG3	2.01	0.42
1:U:30:A:H2'	1:U:31:G:O4'	2.20	0.42
5:V:86:G:C2	5:V:87:U:H1'	2.54	0.42
6:A:1342:LEU:HD23	6:A:1360:LEU:HD21	2.02	0.42
6:A:376:ARG:HG3	9:C:909:ILE:HG21	2.01	0.42
6:A:719:ILE:HB	6:A:720:PRO:HD2	2.01	0.42
9:C:470:ALA:HB2	9:C:488:ILE:HA	2.02	0.42
9:C:472:VAL:HG21	9:C:567:ILE:HG21	2.01	0.42
6:A:1357:LEU:HD11	11:H:303:LEU:CD2	2.49	0.42
1:U:23:C:O2	1:U:23:C:O4'	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:55:G:N7	17:O:35:LYS:HB3	2.35	0.42
6:A:1064:THR:HG22	17:O:81:PRO:HD2	2.02	0.42
6:A:1369:ASN:O	6:A:1373:LEU:N	2.46	0.42
4:Z:38:U:OP2	6:A:1643:ILE:HD11	2.20	0.42
2:E:-3:A:H2'	2:E:-2:A:O4'	2.19	0.42
12:J:114:ARG:HB3	13:K:48:GLN:HE22	1.85	0.42
6:A:218:SER:O	6:A:221:TRP:HB3	2.20	0.42
6:A:644:VAL:HG22	6:A:648:GLN:HB2	2.02	0.42
16:N:259:GLY:O	16:N:263:VAL:HG23	2.20	0.42
13:K:120:ASP:OD2	13:K:123:LEU:HD13	2.20	0.42
15:M:249:MET:SD	16:N:86:LEU:HD13	2.60	0.42
6:A:929:LEU:HD12	6:A:1589:LYS:CG	2.50	0.42
9:C:400:LEU:HD12	9:C:408:LEU:HD21	2.02	0.42
15:M:114:ARG:CD	15:M:127:ILE:HG21	2.50	0.42
17:O:22:LYS:HB2	17:O:56:LEU:HD12	2.02	0.42
5:V:36:U:C2'	5:V:36:U:O2	2.68	0.42
9:C:418:GLN:HB3	9:C:419:PRO:HD3	2.02	0.41
12:J:334:TRP:CD1	12:J:334:TRP:N	2.88	0.41
16:N:25:MET:HB3	16:N:46:PHE:HB3	2.01	0.41
16:N:16:CYS:CB	16:N:71:CYS:SG	3.08	0.41
6:A:756:LEU:CD1	18:P:12:ARG:HD3	2.50	0.41
20:S:140:LEU:HD21	20:S:155:LEU:HD22	2.01	0.41
9:C:225:THR:HG21	9:C:252:LEU:HD21	2.02	0.41
9:C:608:GLN:HE21	9:C:641:GLU:HG2	1.85	0.41
12:J:276:PRO:HB2	13:K:63:ILE:HD12	2.02	0.41
15:M:247:LEU:HA	15:M:250:MET:CG	2.51	0.41
15:M:48:VAL:HG22	15:M:220:GLY:N	2.36	0.41
6:A:756:LEU:HD11	18:P:12:ARG:HD3	2.03	0.41
1:U:38:A:H2'	1:U:39:U:O4'	2.20	0.41
5:V:61:C:H2'	5:V:62:A:O4'	2.19	0.41
6:A:168:LEU:N	6:A:169:PRO:HD2	2.35	0.41
5:V:74:U:C5	12:J:221:TYR:CD2	3.07	0.41
21:T:397:ASN:O	21:T:400:ALA:HB3	2.20	0.41
9:C:273:LEU:HA	9:C:277:LEU:HD12	2.02	0.41
9:C:621:ALA:CB	9:C:664:ALA:HB2	2.48	0.41
6:A:565:VAL:CG1	6:A:637:VAL:HG22	2.51	0.41
7:D:51:CYS:SG	7:D:88:CYS:CB	3.08	0.41
6:A:1316:ILE:HD13	6:A:1316:ILE:HA	1.94	0.41
6:A:1749:SER:O	6:A:1752:VAL:HG22	2.20	0.41
11:H:334:LEU:HD12	11:H:380:GLN:HB3	2.02	0.41
6:A:252:GLU:HA	6:A:255:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:330:ILE:HD12	11:H:387:PHE:HE2	1.86	0.41
6:A:1609:TRP:CE3	6:A:1823:LEU:HD13	2.56	0.41
9:C:314:ALA:CB	9:C:321:THR:HG22	2.50	0.41
11:H:292:LYS:HD3	11:H:328:ILE:HD11	2.01	0.41
15:M:156:ILE:HG21	15:M:175:TYR:CE1	2.55	0.41
6:A:758:LEU:HD23	6:A:759:ARG:N	2.36	0.41
6:A:831:ARG:CD	6:A:848:ASN:HD21	2.34	0.41
6:A:976:GLN:HG3	6:A:1310:LYS:HB3	2.02	0.41
6:A:480:TYR:OH	9:C:318:LEU:HD21	2.20	0.41
16:N:82:ILE:HG22	16:N:86:LEU:HB2	2.02	0.41
6:A:1014:LYS:N	6:A:1015:PRO:CD	2.84	0.41
6:A:937:LEU:HD13	6:A:1590:LEU:HD21	2.01	0.41
6:A:562:ILE:HG22	6:A:563:ASP:O	2.21	0.41
6:A:666:ILE:HG22	6:A:673:VAL:HG21	2.03	0.41
9:C:287:LYS:HE3	9:C:291:ILE:HD11	2.03	0.41
5:V:22:G:H2'	5:V:23:G:O4'	2.21	0.41
6:A:1011:ASN:HD22	6:A:1144:PHE:HA	1.86	0.40
6:A:370:ILE:HD12	6:A:1418:THR:OG1	2.21	0.40
6:A:831:ARG:HD3	6:A:848:ASN:HD21	1.86	0.40
9:C:152:LEU:HD11	9:C:319:GLY:HA2	2.02	0.40
9:C:632:VAL:HG12	9:C:634:ILE:HG13	2.03	0.40
6:A:390:LEU:N	9:C:653:ASP:OD1	2.54	0.40
9:C:677:PHE:HB3	9:C:857:LEU:HD22	2.03	0.40
20:S:189:TYR:O	20:S:192:TYR:HB3	2.21	0.40
6:A:1620:TYR:CD2	6:A:1621:VAL:HG13	2.56	0.40
9:C:223:ASP:O	9:C:227:VAL:HG23	2.21	0.40
9:C:749:LYS:O	9:C:753:THR:HG23	2.21	0.40
17:O:211:ILE:CD1	20:S:44:ARG:HG3	2.50	0.40
1:U:45:A:N6	1:U:74:U:H3	2.19	0.40
6:A:1756:PHE:CZ	6:A:1760:THR:HG21	2.56	0.40
1:U:45:A:OP1	9:C:108:GLN:O	2.40	0.40
9:C:234:LEU:HD13	9:C:439:ILE:HG23	2.03	0.40
9:C:264:CYS:SG	9:C:312:ILE:HD11	2.61	0.40
9:C:561:ILE:O	9:C:562:VAL:HG13	2.22	0.40
13:K:75:GLN:HA	13:K:78:VAL:HG12	2.03	0.40
6:A:1223:GLY:HA2	6:A:1248:VAL:HG11	2.02	0.40
6:A:1392:LYS:HB3	6:A:1601:ILE:HD11	2.03	0.40
6:A:1603:ASN:HD22	6:A:1604:ARG:N	2.19	0.40
6:A:175:LEU:HD22	6:A:629:MET:CE	2.52	0.40
6:A:1881:THR:HG21	6:A:1920:LEU:HD23	2.02	0.40
6:A:766:ILE:HG21	6:A:782:ILE:HD13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:241:VAL:HG22	9:C:267:ILE:HG23	2.04	0.40
12:J:345:PHE:CE2	12:J:364:LEU:HD22	2.57	0.40
5:V:86:G:C2	20:S:57:TYR:CE2	3.10	0.40
4:Z:1102:C:O2	4:Z:1102:C:C2'	2.69	0.40
6:A:1054:LEU:HD13	6:A:1121:ILE:HG21	2.03	0.40
6:A:1491:ILE:HA	6:A:1491:ILE:HD13	1.97	0.40
12:J:198:PHE:CD1	12:J:239:ILE:HD13	2.57	0.40
12:J:321:PHE:CE1	12:J:336:LEU:CD2	3.05	0.40
15:M:109:LEU:HA	15:M:116:LYS:HG2	2.03	0.40
16:N:84:ILE:O	16:N:87:ARG:HG3	2.21	0.40
17:O:148:GLU:O	17:O:152:LEU:HD23	2.21	0.40
17:O:211:ILE:HD12	20:S:48:ARG:NE	2.36	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 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	
6	A	1916/2413 (79%)	1762 (92%)	143 (8%)	11 (1%)	28	70
7	D	112/278 (40%)	93 (83%)	17 (15%)	2 (2%)	10	50
8	F	44/179 (25%)	41 (93%)	3 (7%)	0	100	100
9	C	872/1008 (86%)	777 (89%)	82 (9%)	13 (2%)	12	53
10	G	95/235 (40%)	89 (94%)	5 (5%)	1 (1%)	17	60
11	H	389/591 (66%)	362 (93%)	23 (6%)	4 (1%)	18	61
12	J	322/451 (71%)	263 (82%)	47 (15%)	12 (4%)	4	36
13	K	155/379 (41%)	146 (94%)	8 (5%)	1 (1%)	28	70
14	L	153/157 (98%)	136 (89%)	15 (10%)	2 (1%)	14	56
15	M	250/339 (74%)	228 (91%)	19 (8%)	3 (1%)	15	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	N	195/364 (54%)	178 (91%)	14 (7%)	3 (2%)	12	53
17	O	194/590 (33%)	173 (89%)	17 (9%)	4 (2%)	8	47
18	P	34/175 (19%)	28 (82%)	5 (15%)	1 (3%)	5	41
19	R	91/135 (67%)	80 (88%)	10 (11%)	1 (1%)	17	60
20	S	432/687 (63%)	416 (96%)	14 (3%)	2 (0%)	32	73
21	T	532/859 (62%)	504 (95%)	20 (4%)	8 (2%)	12	53
22	b	76/196 (39%)	70 (92%)	6 (8%)	0	100	100
22	k	76/196 (39%)	65 (86%)	9 (12%)	2 (3%)	6	43
23	d	80/101 (79%)	72 (90%)	7 (9%)	1 (1%)	14	56
23	n	80/101 (79%)	66 (82%)	14 (18%)	0	100	100
24	e	71/94 (76%)	68 (96%)	3 (4%)	0	100	100
24	p	71/94 (76%)	63 (89%)	7 (10%)	1 (1%)	13	54
25	f	70/86 (81%)	66 (94%)	3 (4%)	1 (1%)	13	54
25	q	70/86 (81%)	61 (87%)	9 (13%)	0	100	100
26	g	65/77 (84%)	64 (98%)	1 (2%)	0	100	100
26	r	65/77 (84%)	55 (85%)	9 (14%)	1 (2%)	12	53
27	h	78/146 (53%)	74 (95%)	4 (5%)	0	100	100
27	l	75/146 (51%)	63 (84%)	10 (13%)	2 (3%)	6	43
28	j	92/110 (84%)	87 (95%)	5 (5%)	0	100	100
28	m	92/110 (84%)	84 (91%)	8 (9%)	0	100	100
29	W	160/238 (67%)	117 (73%)	35 (22%)	8 (5%)	2	30
30	Y	82/111 (74%)	77 (94%)	5 (6%)	0	100	100
All	All	7089/10809 (66%)	6428 (91%)	577 (8%)	84 (1%)	20	58

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	A	320	ASP
6	A	737	ARG
11	H	414	PRO
15	M	127	ILE
16	N	120	LEU
19	R	14	SER
21	T	477	PRO

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Mol	Chain	Res	Type
21	T	481	ILE
21	T	616	PRO
29	W	76	ILE
27	l	98	PRO
26	r	68	ILE
6	A	588	LEU
6	A	1424	HIS
6	A	1639	PRO
6	A	1763	ASN
9	C	76	VAL
9	C	172	TRP
9	C	269	LYS
9	C	432	GLN
9	C	535	PRO
9	C	901	GLU
11	H	469	GLY
12	J	162	THR
12	J	245	ASP
12	J	277	VAL
12	J	328	THR
15	M	23	PRO
17	O	81	PRO
18	P	9	LEU
29	W	122	ARG
22	k	81	VAL
6	A	1593	ALA
7	D	76	LEU
9	C	574	SER
11	H	445	LEU
12	J	442	TRP
14	L	38	SER
16	N	30	GLN
16	N	54	ASN
17	O	214	ASN
20	S	238	TRP
29	W	95	PRO
27	l	25	VAL
6	A	660	ILE
17	O	206	LYS
20	S	112	VAL
21	T	479	PRO
21	T	615	PHE

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Mol	Chain	Res	Type
29	W	68	PRO
29	W	94	LEU
29	W	129	LEU
22	k	6	VAL
6	A	457	ASP
6	A	1491	ILE
7	D	34	MET
9	C	100	LEU
9	C	459	PRO
10	G	41	VAL
12	J	310	SER
12	J	444	PRO
15	M	4	TRP
17	O	216	ASP
21	T	443	PRO
9	C	137	GLY
9	C	807	PRO
11	H	303	LEU
12	J	226	GLY
21	T	391	LEU
12	J	137	GLY
9	C	185	ILE
9	C	301	GLY
12	J	279	PRO
13	K	146	VAL
14	L	117	GLY
25	f	15	PRO
24	p	74	GLY
12	J	443	ASN
21	T	37	ILE
29	W	56	ILE
29	W	98	VAL
6	A	774	ILE
12	J	272	VAL
23	d	82	PRO

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	
6	A	1701/2182 (78%)	1580 (93%)	121 (7%)	17	55
7	D	100/256 (39%)	91 (91%)	9 (9%)	11	45
8	F	26/163 (16%)	25 (96%)	1 (4%)	38	70
9	C	722/910 (79%)	659 (91%)	63 (9%)	12	46
10	G	89/216 (41%)	81 (91%)	8 (9%)	11	45
11	H	185/552 (34%)	164 (89%)	21 (11%)	7	34
12	J	283/398 (71%)	250 (88%)	33 (12%)	6	33
13	K	143/328 (44%)	115 (80%)	28 (20%)	1	12
14	L	138/141 (98%)	129 (94%)	9 (6%)	20	57
15	M	212/295 (72%)	188 (89%)	24 (11%)	7	34
16	N	194/332 (58%)	175 (90%)	19 (10%)	9	40
17	O	174/526 (33%)	152 (87%)	22 (13%)	5	29
18	P	26/152 (17%)	21 (81%)	5 (19%)	1	12
19	R	24/121 (20%)	20 (83%)	4 (17%)	2	19
20	S	208/633 (33%)	181 (87%)	27 (13%)	5	28
22	b	70/176 (40%)	70 (100%)	0	100	100
23	d	69/89 (78%)	66 (96%)	3 (4%)	33	68
24	e	65/83 (78%)	60 (92%)	5 (8%)	15	52
25	f	63/77 (82%)	61 (97%)	2 (3%)	44	74
26	g	58/66 (88%)	57 (98%)	1 (2%)	66	85
27	h	77/129 (60%)	77 (100%)	0	100	100
28	j	79/103 (77%)	76 (96%)	3 (4%)	38	70
All	All	4706/7928 (59%)	4298 (91%)	408 (9%)	16	46

All (408) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	A	128	TYR
6	A	145	THR
6	A	149	MET
6	A	153	MET
6	A	165	LEU
6	A	173	LEU

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Mol	Chain	Res	Type
6	A	175	LEU
6	A	192	LEU
6	A	204	GLU
6	A	205	THR
6	A	225	ARG
6	A	228	LYS
6	A	244	ASP
6	A	257	ASN
6	A	261	LEU
6	A	265	ASN
6	A	282	ASP
6	A	284	ARG
6	A	286	LEU
6	A	296	THR
6	A	297	SER
6	A	310	ASN
6	A	319	ARG
6	A	326	ASN
6	A	353	GLU
6	A	355	LEU
6	A	405	ASN
6	A	412	GLN
6	A	425	ASP
6	A	479	LEU
6	A	493	MET
6	A	514	TYR
6	A	555	LYS
6	A	571	LEU
6	A	572	CYS
6	A	591	LEU
6	A	600	LYS
6	A	605	LEU
6	A	615	LEU
6	A	630	LYS
6	A	631	LEU
6	A	663	LEU
6	A	674	MET
6	A	690	LYS
6	A	705	GLN
6	A	728	ASN
6	A	737	ARG
6	A	743	LYS

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Mol	Chain	Res	Type
6	A	749	ARG
6	A	751	ASP
6	A	753	TYR
6	A	755	ASP
6	A	758	LEU
6	A	760	ASN
6	A	770	MET
6	A	775	ARG
6	A	778	LYS
6	A	783	LEU
6	A	785	HIS
6	A	811	ILE
6	A	821	ASP
6	A	832	GLU
6	A	846	LYS
6	A	852	LEU
6	A	919	LEU
6	A	922	VAL
6	A	944	TYR
6	A	968	ASP
6	A	971	MET
6	A	972	MET
6	A	1004	ASP
6	A	1019	GLU
6	A	1020	ILE
6	A	1024	LEU
6	A	1078	ILE
6	A	1099	ASN
6	A	1103	LEU
6	A	1165	LEU
6	A	1167	ARG
6	A	1168	ILE
6	A	1212	ARG
6	A	1217	ARG
6	A	1277	GLU
6	A	1282	ASP
6	A	1288	LEU
6	A	1315	ARG
6	A	1317	ARG
6	A	1323	SER
6	A	1326	THR
6	A	1327	THR

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Mol	Chain	Res	Type
6	A	1338	SER
6	A	1345	TYR
6	A	1346	PHE
6	A	1347	ARG
6	A	1354	GLU
6	A	1373	LEU
6	A	1378	LYS
6	A	1379	MET
6	A	1382	ARG
6	A	1429	MET
6	A	1433	ASP
6	A	1434	GLU
6	A	1436	LEU
6	A	1515	LYS
6	A	1520	GLU
6	A	1543	ARG
6	A	1574	PHE
6	A	1589	LYS
6	A	1598	LEU
6	A	1600	GLN
6	A	1603	ASN
6	A	1644	SER
6	A	1647	GLN
6	A	1668	ILE
6	A	1707	HIS
6	A	1708	GLU
6	A	1737	GLN
6	A	1742	ASP
6	A	1803	ARG
6	A	1806	MET
6	A	2048	TRP
7	D	3	GLU
7	D	8	ASN
7	D	25	ARG
7	D	47	PHE
7	D	49	MET
7	D	71	LEU
7	D	79	ILE
7	D	99	THR
7	D	114	ARG
8	F	20	ARG
9	C	92	GLU

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Mol	Chain	Res	Type
9	C	100	LEU
9	C	103	HIS
9	C	109	LEU
9	C	124	LEU
9	C	132	ARG
9	C	139	ILE
9	C	153	LEU
9	C	156	ASP
9	C	206	LYS
9	C	211	ASN
9	C	219	VAL
9	C	233	ASP
9	C	234	LEU
9	C	255	GLN
9	C	272	ARG
9	C	273	LEU
9	C	283	ASP
9	C	315	SER
9	C	347	ARG
9	C	358	ASN
9	C	359	PHE
9	C	362	LYS
9	C	381	LEU
9	C	400	LEU
9	C	401	ARG
9	C	431	GLN
9	C	447	GLU
9	C	453	THR
9	C	458	ILE
9	C	468	LEU
9	C	469	TRP
9	C	471	HIS
9	C	474	LYS
9	C	475	THR
9	C	534	THR
9	C	545	LEU
9	C	562	VAL
9	C	576	THR
9	C	590	LYS
9	C	602	VAL
9	C	610	LEU
9	C	673	PRO

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Mol	Chain	Res	Type
9	C	758	ASP
9	C	768	PHE
9	C	774	LEU
9	C	784	SER
9	C	791	TYR
9	C	794	GLN
9	C	799	PHE
9	C	803	VAL
9	C	830	ASN
9	C	837	GLN
9	C	851	LEU
9	C	861	ILE
9	C	902	VAL
9	C	927	MET
9	C	933	TRP
9	C	965	ASP
9	C	970	THR
9	C	971	ARG
9	C	989	LEU
9	C	992	TYR
10	G	4	ASN
10	G	18	GLN
10	G	28	ASP
10	G	31	ARG
10	G	33	GLN
10	G	74	GLN
10	G	78	LEU
10	G	94	TRP
11	H	256	ASP
11	H	297	LEU
11	H	307	GLU
11	H	313	LEU
11	H	314	LYS
11	H	334	LEU
11	H	348	GLU
11	H	357	TRP
11	H	363	GLU
11	H	367	GLN
11	H	373	ILE
11	H	391	LEU
11	H	396	PHE
11	H	399	MET

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Mol	Chain	Res	Type
11	H	419	PHE
11	H	421	LYS
11	H	440	LEU
11	H	444	LYS
11	H	468	ILE
11	H	470	LEU
11	H	473	LEU
12	J	139	LEU
12	J	143	ARG
12	J	148	ASP
12	J	151	ASP
12	J	156	ILE
12	J	161	ASP
12	J	183	MET
12	J	194	HIS
12	J	202	GLU
12	J	215	GLN
12	J	218	ARG
12	J	224	LEU
12	J	247	VAL
12	J	248	ILE
12	J	257	ILE
12	J	269	ILE
12	J	274	CYS
12	J	275	THR
12	J	284	SER
12	J	286	THR
12	J	290	VAL
12	J	295	VAL
12	J	314	THR
12	J	329	ASP
12	J	332	ARG
12	J	334	TRP
12	J	336	LEU
12	J	356	LEU
12	J	377	ASP
12	J	387	LEU
12	J	389	THR
12	J	396	LEU
12	J	402	VAL
13	K	33	GLN
13	K	36	LYS

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Mol	Chain	Res	Type
13	K	40	LEU
13	K	47	ARG
13	K	48	GLN
13	K	52	GLU
13	K	62	GLU
13	K	66	CYS
13	K	77	LEU
13	K	81	LYS
13	K	87	ASN
13	K	105	LEU
13	K	106	LEU
13	K	111	HIS
13	K	112	ILE
13	K	132	ARG
13	K	147	LEU
13	K	172	TRP
13	K	178	TYR
13	K	182	LEU
13	K	183	GLU
13	K	197	ILE
13	K	202	MET
13	K	203	LYS
13	K	204	LEU
13	K	213	LYS
13	K	217	GLN
13	K	218	GLU
14	L	3	ARG
14	L	37	LYS
14	L	54	GLN
14	L	59	ARG
14	L	61	ARG
14	L	85	LYS
14	L	123	ARG
14	L	139	GLN
14	L	142	PHE
15	M	5	ARG
15	M	10	LYS
15	M	18	LEU
15	M	26	THR
15	M	33	TRP
15	M	38	SER
15	M	44	ASN

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Mol	Chain	Res	Type
15	M	109	LEU
15	M	111	CYS
15	M	114	ARG
15	M	116	LYS
15	M	127	ILE
15	M	132	LYS
15	M	135	LYS
15	M	136	THR
15	M	149	LYS
15	M	172	ARG
15	M	181	CYS
15	M	187	LYS
15	M	191	ASN
15	M	216	ARG
15	M	236	LYS
15	M	245	GLU
15	M	251	VAL
16	N	19	ASP
16	N	22	ASN
16	N	30	GLN
16	N	32	SER
16	N	35	LYS
16	N	39	LEU
16	N	48	THR
16	N	54	ASN
16	N	55	ILE
16	N	87	ARG
16	N	91	ILE
16	N	93	LEU
16	N	94	VAL
16	N	109	MET
16	N	117	ASN
16	N	135	ILE
16	N	216	GLU
16	N	254	GLN
16	N	321	GLN
17	O	27	LYS
17	O	35	LYS
17	O	40	LEU
17	O	44	THR
17	O	46	ARG
17	O	53	ASN

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Mol	Chain	Res	Type
17	O	65	PHE
17	O	73	LEU
17	O	91	MET
17	O	93	ARG
17	O	156	ARG
17	O	158	ARG
17	O	170	LYS
17	O	175	MET
17	O	184	GLU
17	O	188	ARG
17	O	192	LYS
17	O	196	ILE
17	O	204	LYS
17	O	205	LYS
17	O	206	LYS
17	O	247	LYS
18	P	8	GLN
18	P	9	LEU
18	P	16	LYS
18	P	29	ARG
18	P	40	ARG
19	R	6	ILE
19	R	8	LEU
19	R	15	SER
19	R	16	THR
20	S	60	ARG
20	S	67	GLN
20	S	71	TYR
20	S	77	GLU
20	S	78	GLN
20	S	86	SER
20	S	92	LEU
20	S	117	HIS
20	S	139	TYR
20	S	143	GLU
20	S	144	GLU
20	S	152	VAL
20	S	156	TYR
20	S	158	LYS
20	S	173	VAL
20	S	188	ILE
20	S	189	TYR

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Mol	Chain	Res	Type
20	S	192	TYR
20	S	209	GLU
20	S	216	GLU
20	S	224	LEU
20	S	226	ILE
20	S	234	ASN
20	S	257	GLN
20	S	260	TYR
20	S	263	SER
20	S	266	LEU
23	d	10	LEU
23	d	20	SER
23	d	76	ASP
24	e	16	CYS
24	e	18	PHE
24	e	25	THR
24	e	79	LYS
24	e	81	LEU
25	f	36	THR
25	f	79	LEU
26	g	18	ASN
28	j	24	PHE
28	j	49	ARG
28	j	82	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
6	A	194	HIS
6	A	216	GLN
6	A	310	ASN
6	A	326	ASN
6	A	344	ASN
6	A	412	GLN
6	A	508	GLN
6	A	733	GLN
6	A	760	ASN
6	A	848	ASN
6	A	948	HIS
6	A	1368	GLN
6	A	1449	ASN
6	A	1568	ASN

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Mol	Chain	Res	Type
6	A	1603	ASN
6	A	1737	GLN
6	A	2018	ASN
9	C	158	HIS
9	C	260	ASN
9	C	289	ASN
9	C	358	ASN
9	C	418	GLN
9	C	608	GLN
9	C	776	ASN
9	C	837	GLN
10	G	9	ASN
10	G	33	GLN
12	J	273	GLN
13	K	33	GLN
13	K	174	ASN
13	K	210	ASN
15	M	25	GLN
15	M	44	ASN
16	N	22	ASN
17	O	82	ASN
20	S	61	ASN
20	S	78	GLN
20	S	79	HIS
20	S	200	GLN
20	S	214	ASN
20	S	234	ASN
20	S	236	GLN
23	d	41	ASN
24	e	15	ASN
24	e	34	GLN
25	f	24	ASN
26	g	18	ASN
26	g	66	ASN
27	h	86	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	U	138/179 (77%)	66 (47%)	13 (9%)
2	E	15/16 (93%)	10 (66%)	2 (13%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	I	31/76 (40%)	15 (48%)	0
4	Z	162/1175 (13%)	58 (35%)	11 (6%)
5	V	95/112 (84%)	34 (35%)	5 (5%)
All	All	441/1558 (28%)	183 (41%)	31 (7%)

All (183) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	U	13	A
1	U	14	G
1	U	15	A
1	U	16	U
1	U	18	A
1	U	20	U
1	U	22	G
1	U	23	C
1	U	24	G
1	U	25	G
1	U	26	A
1	U	27	G
1	U	28	G
1	U	31	G
1	U	33	U
1	U	34	C
1	U	36	A
1	U	40	C
1	U	42	A
1	U	43	G
1	U	44	A
1	U	48	G
1	U	50	G
1	U	53	C
1	U	63	C
1	U	65	U
1	U	67	U
1	U	68	A
1	U	70	A
1	U	71	A
1	U	74	U
1	U	75	A
1	U	76	U
1	U	77	A

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Mol	Chain	Res	Type
1	U	78	A
1	U	79	C
1	U	80	G
1	U	81	A
1	U	82	A
1	U	84	A
1	U	87	G
1	U	89	U
1	U	92	U
1	U	94	C
1	U	96	U
1	U	97	U
1	U	101	C
1	U	104	G
1	U	107	C
1	U	108	C
1	U	109	A
1	U	112	C
1	U	113	G
1	U	115	G
1	U	116	U
1	U	119	U
1	U	121	U
1	U	126	A
1	U	130	A
1	U	133	C
1	U	134	A
1	U	135	G
1	U	145	U
1	U	170	U
1	U	171	U
1	U	173	U
2	E	-14	A
2	E	-11	G
2	E	-10	A
2	E	-9	U
2	E	-8	C
2	E	-7	U
2	E	-6	A
2	E	-5	G
2	E	-4	A
2	E	-1	G

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Mol	Chain	Res	Type
3	I	3	A
3	I	6	U
3	I	9	A
3	I	10	A
3	I	56	G
3	I	58	U
3	I	61	U
3	I	62	A
3	I	63	U
3	I	65	U
3	I	66	A
3	I	69	A
3	I	71	C
3	I	73	A
3	I	74	A
4	Z	5	A
4	Z	15	C
4	Z	16	U
4	Z	17	U
4	Z	18	U
4	Z	19	U
4	Z	20	G
4	Z	21	G
4	Z	25	A
4	Z	30	A
4	Z	32	G
4	Z	33	U
4	Z	37	G
4	Z	40	U
4	Z	43	G
4	Z	46	C
4	Z	47	U
4	Z	63	U
4	Z	64	G
4	Z	67	A
4	Z	68	U
4	Z	81	C
4	Z	106	A
4	Z	108	A
4	Z	110	A
4	Z	112	A
4	Z	113	U

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Mol	Chain	Res	Type
4	Z	114	U
4	Z	115	U
4	Z	116	U
4	Z	117	U
4	Z	119	G
4	Z	120	G
4	Z	141	A
4	Z	1094	G
4	Z	1096	C
4	Z	1098	C
4	Z	1099	G
4	Z	1100	A
4	Z	1101	C
4	Z	1102	C
4	Z	1103	C
4	Z	1104	U
4	Z	1106	G
4	Z	1107	C
4	Z	1108	A
4	Z	1120	G
4	Z	1123	C
4	Z	1124	U
4	Z	1125	U
4	Z	1126	G
4	Z	1139	G
4	Z	1144	U
4	Z	1145	U
4	Z	1146	G
4	Z	1149	G
4	Z	1152	U
4	Z	1166	G
5	V	3	U
5	V	5	G
5	V	10	G
5	V	17	U
5	V	22	G
5	V	27	U
5	V	28	U
5	V	31	G
5	V	34	A
5	V	35	A
5	V	36	U

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Mol	Chain	Res	Type
5	V	37	U
5	V	40	A
5	V	41	A
5	V	42	A
5	V	43	C
5	V	52	G
5	V	54	U
5	V	62	A
5	V	66	C
5	V	68	C
5	V	73	A
5	V	74	U
5	V	75	A
5	V	76	A
5	V	80	U
5	V	81	G
5	V	84	C
5	V	85	C
5	V	88	U
5	V	89	U
5	V	91	A
5	V	92	C
5	V	99	A

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	U	23	C
1	U	24	G
1	U	26	A
1	U	27	G
1	U	33	U
1	U	39	U
1	U	43	G
1	U	45	A
1	U	64	C
1	U	76	U
1	U	78	A
1	U	96	U
1	U	172	U
2	E	-10	A
2	E	-9	U

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Mol	Chain	Res	Type
4	Z	16	U
4	Z	19	U
4	Z	20	G
4	Z	32	G
4	Z	112	A
4	Z	114	U
4	Z	115	U
4	Z	118	U
4	Z	1123	C
4	Z	1124	U
4	Z	1145	U
5	V	16	C
5	V	53	A
5	V	60	G
5	V	74	U
5	V	84	C

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
34	GTP	C	1101	-	27,34,34	0.99	2 (7%)	27,54,54	2.03	7 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	GTP	C	1101	-	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	C	1101	GTP	C5-C4	2.50	1.46	1.40
34	C	1101	GTP	C6-C5	3.25	1.47	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	C	1101	GTP	C6-C5-C4	-3.92	116.94	120.84
34	C	1101	GTP	N3-C2-N1	-3.42	122.47	127.46
34	C	1101	GTP	C5-C6-N1	-3.11	119.06	123.48
34	C	1101	GTP	C1'-N9-C4	-2.92	121.59	126.64
34	C	1101	GTP	C4-C5-N7	-2.52	106.97	109.41
34	C	1101	GTP	C6-N1-C2	3.87	121.63	116.06
34	C	1101	GTP	C2-N3-C4	5.00	121.00	115.16

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
31	x	4
21	T	2

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Mol	Chain	Number of breaks
19	R	1
5	V	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	x	54:UNK	C	55:UNK	N	111.76
1	x	110:UNK	C	111:UNK	N	53.94
1	x	36:UNK	C	37:UNK	N	49.39
1	x	87:UNK	C	88:UNK	N	31.03
1	T	419:LYS	C	420:SER	N	5.13
1	R	35:SER	C	36:GLN	N	4.69
1	V	92:C	O3'	93:A	P	3.22
1	T	431:ALA	C	432:ILE	N	3.17