



wwPDB EM Map/Model Validation Report ⓘ

Oct 3, 2016 – 02:17 PM EDT

PDB ID : 5LJ5
EMDB ID: : EMD-4057
Title : Overall structure 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 : 2016-07-17
Resolution : 3.80 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

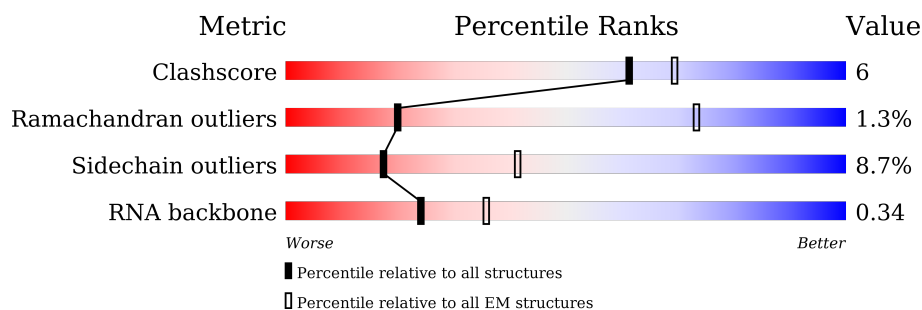
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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.











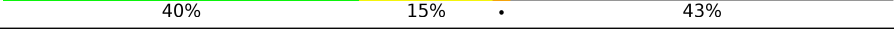

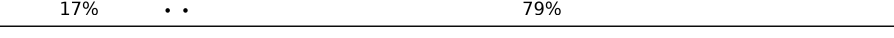
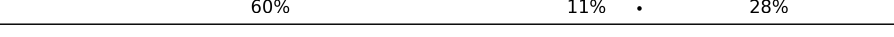

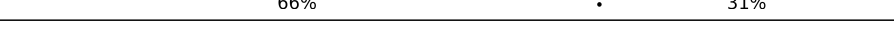


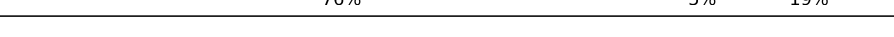

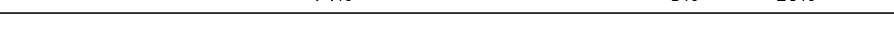






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	33% 36% 9% • 21%
2	E	16	25% 63% 13%
3	I	76	22% 20% • 57%
4	Z	1175	9% 5% 85%
5	V	112	42% 31% 12% • 13%
6	A	2413	73% 15% • 10%
7	B	2163	77% • 21%
8	D	278	34% 7% 59%






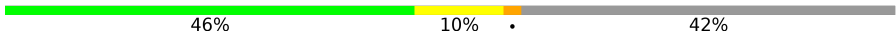






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Mol	Chain	Length	Quality of chain
9	F	179	
10	C	1008	
11	G	235	
12	H	591	
13	J	451	
14	K	379	
15	L	157	
16	M	339	
17	N	364	
18	O	590	
19	P	175	
20	R	135	
21	S	687	
22	T	859	
23	b	196	
23	k	196	
24	d	101	
24	n	101	
25	e	94	
25	p	94	
26	f	86	
26	q	86	
27	g	77	
27	r	77	
28	h	146	

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Mol	Chain	Length	Quality of chain
28	l	146	
29	j	110	
29	m	110	
30	W	238	
31	Y	111	
32	Q	1071	
33	t	503	
33	u	503	
33	v	503	
33	w	503	
34	s	175	
35	x	188	

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
37	ZN	N	401	-	-	X	-
37	ZN	N	402	-	-	X	-

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 85476 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	2168	Total	C	N	O	S	0	0
			16919	10835	2966	3060	58		

- Molecule 7 is a protein called Pre-mRNA-splicing helicase BRR2.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	B	1707	Total	C	N	O	1	0
			8462	5048	1707	1707		

- Molecule 8 is a protein called Protein CWC16.

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

- Molecule 9 is a protein called Pre-mRNA-splicing factor CWC25.

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

- Molecule 10 is a protein called Pre-mRNA-splicing factor SNU114.

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

- Molecule 11 is a protein called Pre-mRNA-splicing factor ISY1.

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

- Molecule 12 is a protein called CWC22.

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

- Molecule 13 is a protein called Pre-mRNA-splicing factor PRP46.

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

- Molecule 14 is a protein called Pre-mRNA-processing protein 45.

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

- Molecule 15 is a protein called Pre-mRNA-splicing factor BUD31.

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

- Molecule 16 is a protein called Pre-mRNA-splicing factor CWC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	252	Total	C	N	O	S	0	0
			2012	1277	354	370	11		

- Molecule 17 is a protein called Pre-mRNA-splicing factor SLT11.

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

- Molecule 18 is a protein called Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	283	Total	C	N	O	S	0	0
			2068	1285	385	392	6		

- Molecule 19 is a protein called CWC15.

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

- Molecule 20 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	R	97	Total	C	N	O	0	0
			544	325	106	113		

- Molecule 21 is a protein called Pre-mRNA-splicing factor CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	464	Total	C	N	O	S	0	0
			3121	1949	581	584	7		

- Molecule 22 is a protein called Pre-mRNA-splicing factor SYF1.

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

- Molecule 23 is a protein called Small nuclear ribonucleoprotein-associated protein B.

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

- Molecule 24 is a protein called Small nuclear ribonucleoprotein Sm D3.

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

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

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

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

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

- Molecule 27 is a protein called Small nuclear ribonucleoprotein G.

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

- Molecule 28 is a protein called Small nuclear ribonucleoprotein Sm D1.

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

- Molecule 29 is a protein called Small nuclear ribonucleoprotein Sm D2.

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

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

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

- Molecule 31 is a protein called U2 small nuclear ribonucleoprotein B''.

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

- Molecule 32 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP16.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Q	619	Total	C	N	O	0	0
			3066	1828	619	619		

- Molecule 33 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	t	438	Total	C	N	O	0	0
			2171	1295	438	438		
33	u	437	Total	C	N	O	0	0
			2166	1292	437	437		
33	v	426	Total	C	N	O	0	0
			2111	1259	426	426		
33	w	435	Total	C	N	O	0	0
			2156	1286	435	435		

- Molecule 34 is a protein called Pre-mRNA-splicing factor SNT309.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	s	110	Total	C	N	O	0	0
			548	328	110	110		

- Molecule 35 is a protein called unknown.

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

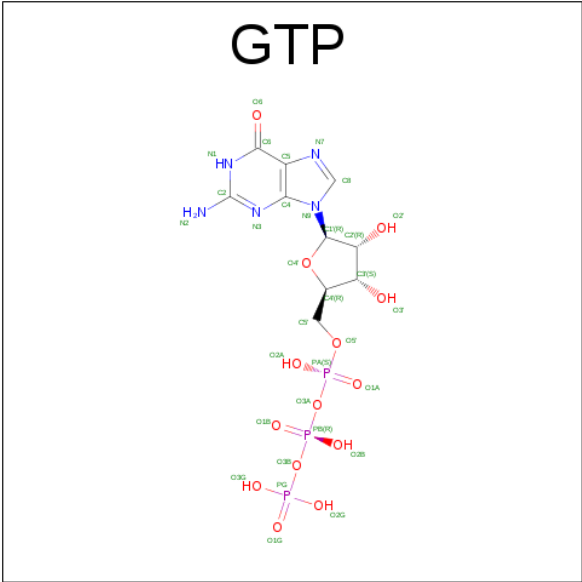
- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 38 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

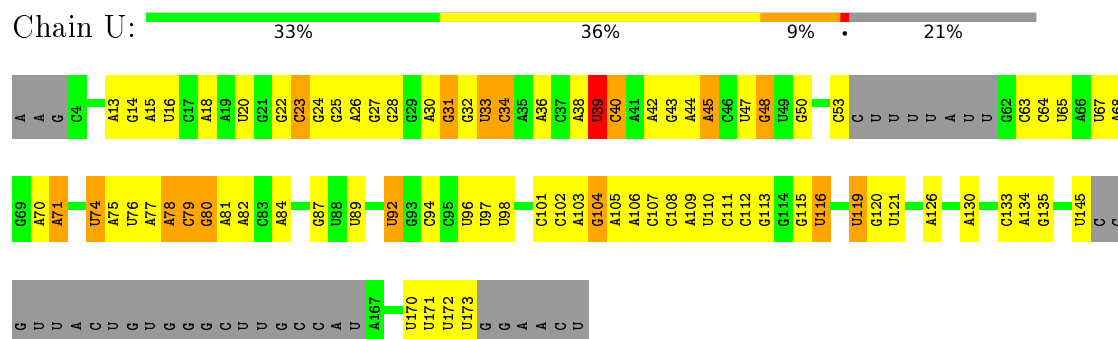


Mol	Chain	Residues	Atoms					AltConf
38	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

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 errors 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.

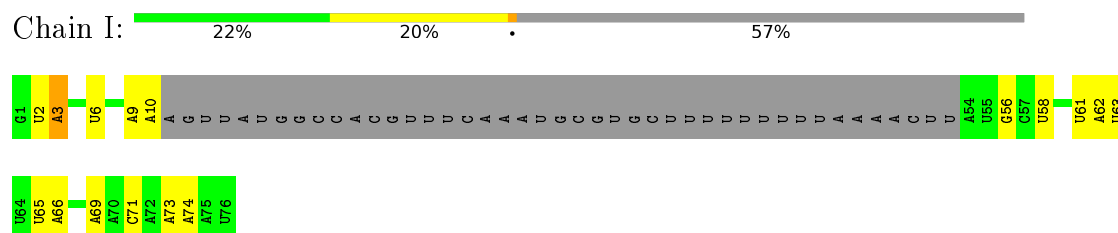
- Molecule 1: U5 snRNA (small nuclear RNA)



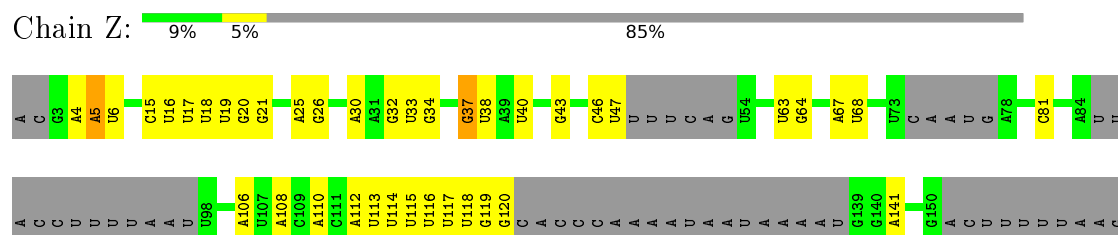
- Molecule 2: Exon 1 (5' exon) of UBC4 pre-mRNA



- Molecule 3: Intron of UBC4 pre-mRNA



- Molecule 4: U2 snRNA (small nuclear RNA)





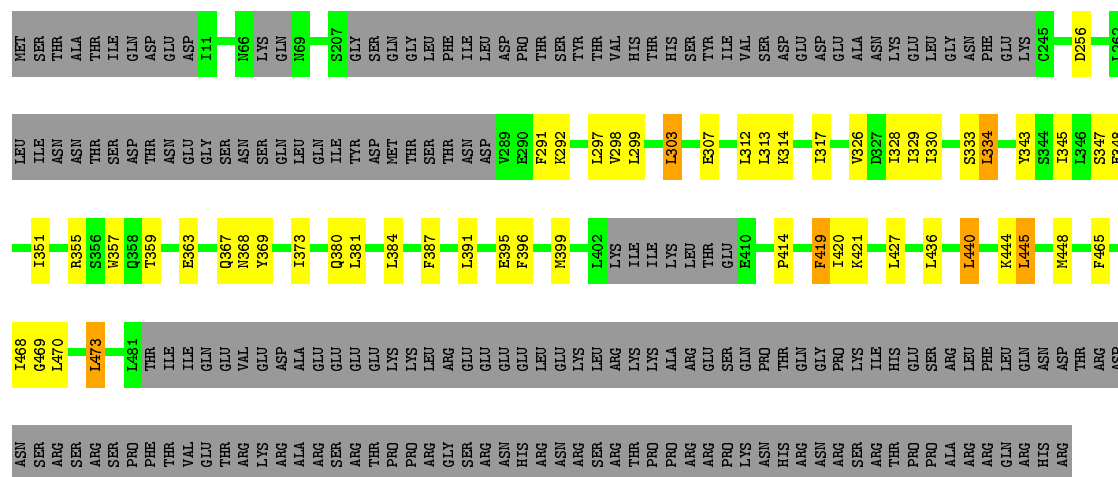

Chain A:  73% 15% 10%

MET	ILE	LYS	K221	I370	Y480	Q648	A753	I882	A1047	V1248	I1367	Y1542	Q1737	V1977	VAL
SER	ASN	ALA	R225	R376	Y493	L649	I753	K889	V1048	V1368	Q1368	R1543	L1738	V1978	ALA
GLY	ALA	ARG	R228	L390	L507	I656	I754	K893	L1049	Y1251	M1369	V1546	D1742	W2048	SER
LEU	GLY	SER	F239	P395	Q508	I659	I756	L912	L1054	N1255	K1371	L1557	S1749	L2060	ASP
PRO	ILE	ASN	P244	V398	Y514	I660	I758	L919	T1064	N1258	L1373	T1560	V1752	E2078	THR
PRO	VAL	LEU	P244	V398	Y514	I660	I758	L919	L1065	L1258	G1374	T1561	F1756	G2085	GLN
PRO	ASP	Y128	P244	V398	Y514	I660	I758	L919	L1066	E1277	L1375	L1562	F1756	G2085	ASN
GLY	THR	P136	P244	V398	Y514	I660	I758	L919	L1067	D1282	K1378	T1565	T1760	G2085	ILE
PHE	LEU	H138	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	SER
GLU	PRO	H139	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	LEU
ASP	PRO	R140	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	LYS
SER	PRO	I141	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	ALA
ASP	PRO	I142	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	PRO
LEU	PRO	I141	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	SER
ALA	GLY	T145	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	VAL
LEU	LEU	M149	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	ARG
PRO	LEU	M153	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	LYS
PRO	GLY	F161	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	ALA
PRO	THR	L165	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	GLU
PRO	ALA	L168	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	LEU
GLY	GLY	P169	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	GLY
TYR	LYS	L172	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	ALA
GLY	VAL	L173	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	ARG
LEU	GLY	L175	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	SER
ASN	HIS	L182	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	GLY
PRO	ARG	V189	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	ASP
MET	LYS	L192	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	LEU
VAL	LEU	Y193	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	LYS
PRO	ILE	A198	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	ALA
SER	GLY	V202	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	LEU
SER	THR	R203	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	ASN
VAL	PHE	T205	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	THR
LEU	ARG	E210	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	VAL
PRO	LYS	P211	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	ILE
PRO	ARG	V212	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	ASN
PRO	LYS	T213	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	ALA
PRO	ARG	T214	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	GLN
PRO	ALA	Q216	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	GLY
PRO	LYS	R217	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	GLY
SER	LYS	S218	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	ILE
ASN	THR	A219	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	VAL
PHE	LYS	L220	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	VAL
GLU	LYS	L220	P244	V398	Y514	I660	I758	L919	N1067	D1282	M1379	T1565	T1760	G2085	VAL



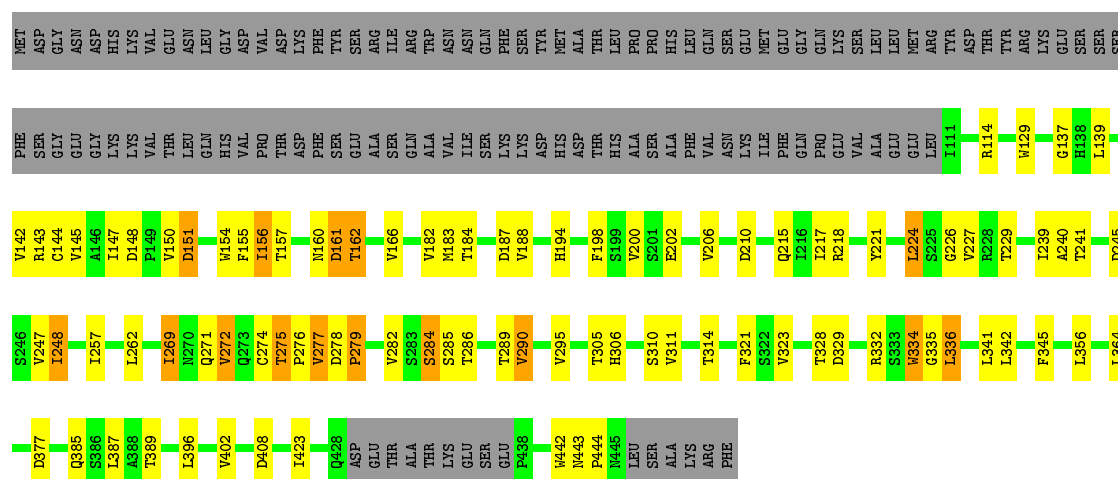
- Molecule 12: CWC22

Chain H: 58% 8% 32%



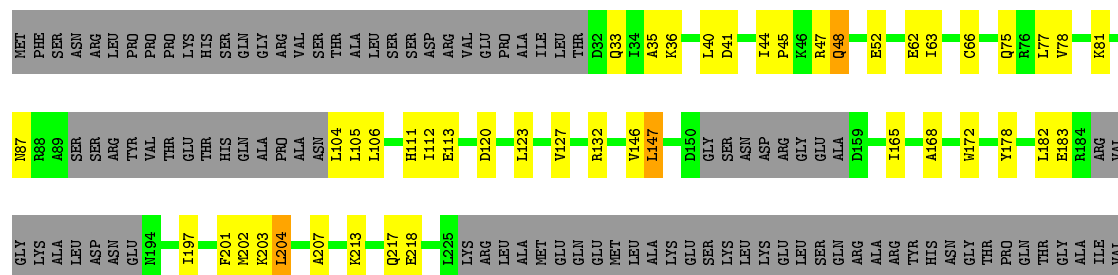
- Molecule 13: Pre-mRNA-splicing factor PRP46

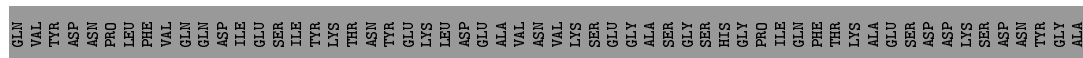
Chain J:  52% 17% 1% 28%



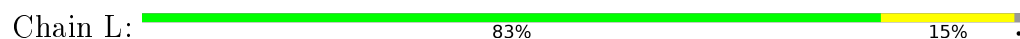
- Molecule 14: Pre-mRNA-processing protein 45

Chain K: 31% 11% . 57%

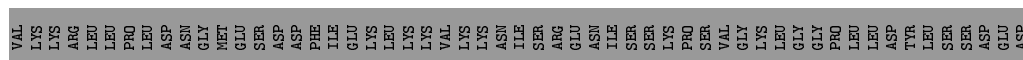
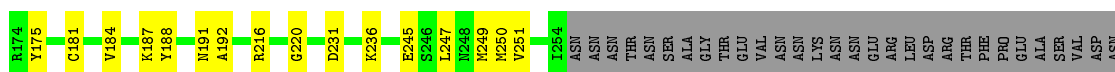




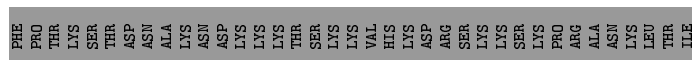
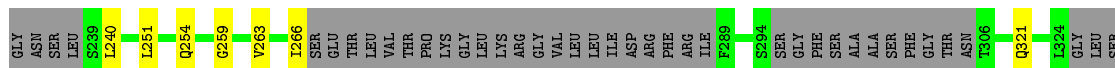
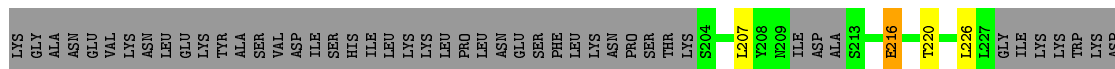
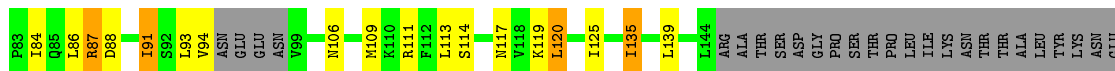
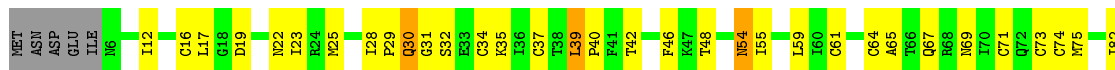
- Molecule 15: Pre-mRNA-splicing factor BUD31



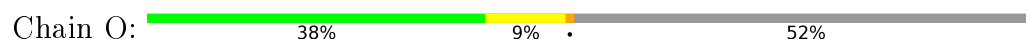
- Molecule 16: Pre-mRNA-splicing factor CWC2

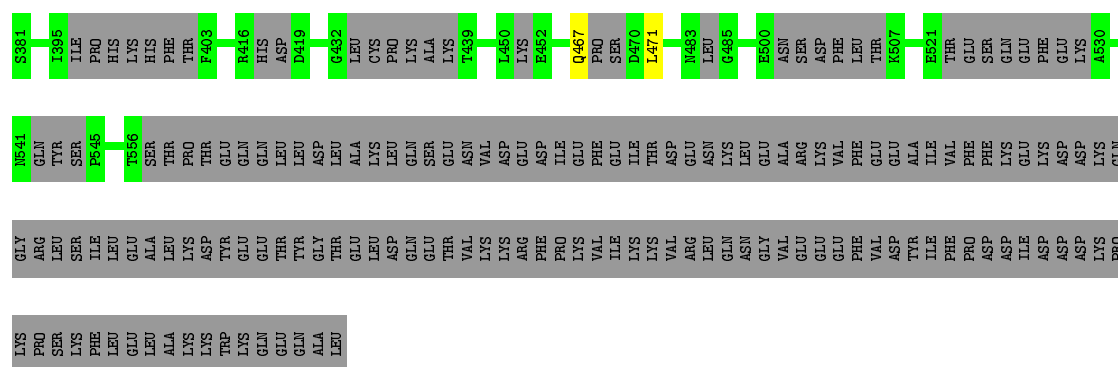


- Molecule 17: Pre-mRNA-splicing factor SLT11



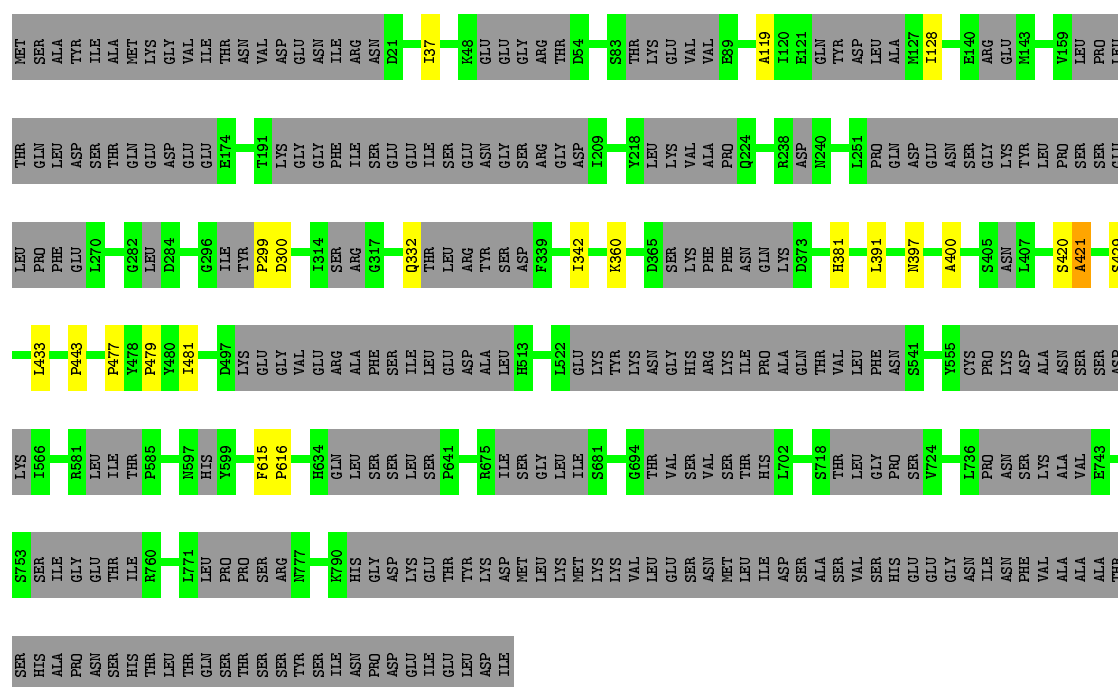
- Molecule 18: Pre-mRNA-splicing factor CEF1





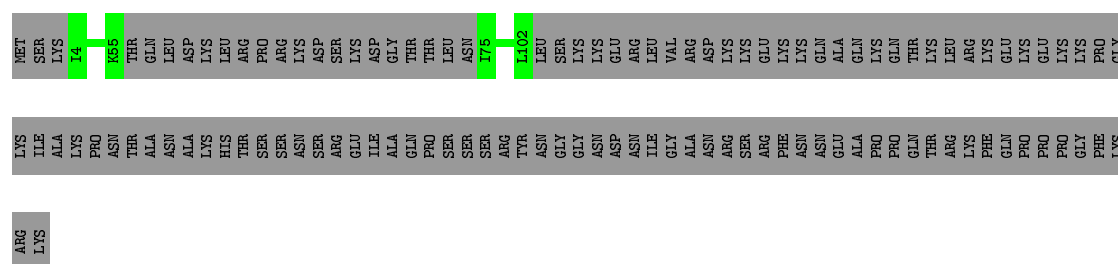
• Molecule 22: Pre-mRNA-splicing factor SYF1

Chain T: 66% 31%



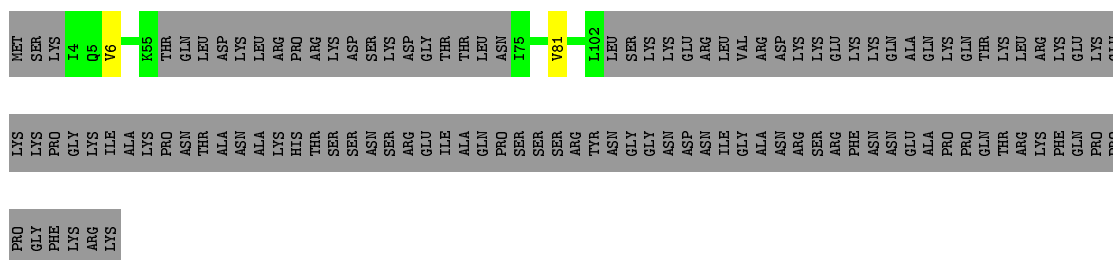
• Molecule 23: Small nuclear ribonucleoprotein-associated protein B

Chain b: 41% 59%



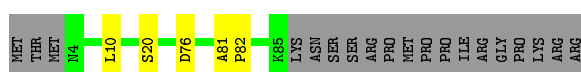
• Molecule 23: Small nuclear ribonucleoprotein-associated protein B

Chain k:  40% 59%




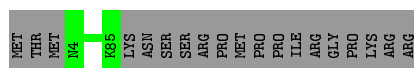
- Molecule 24: Small nuclear ribonucleoprotein Sm D3

Chain d:  76% 5% 19%



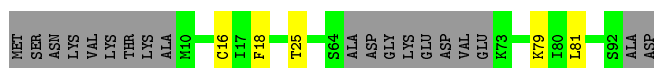
- Molecule 24: Small nuclear ribonucleoprotein Sm D3

Chain n:  81% 19%




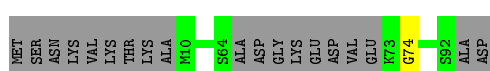
- Molecule 25: Small nuclear ribonucleoprotein E

Chain e:  74% 5% 20%




- Molecule 25: Small nuclear ribonucleoprotein E

Chain p:  79% 20%




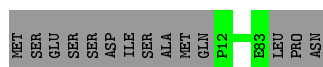
- Molecule 26: Small nuclear ribonucleoprotein F

Chain f:  80% 16%



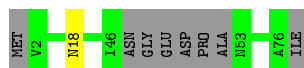
- Molecule 26: Small nuclear ribonucleoprotein F

Chain q:  84% 16%



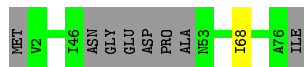
- Molecule 27: Small nuclear ribonucleoprotein G

Chain g: 88% 10%



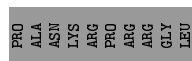
- Molecule 27: Small nuclear ribonucleoprotein G

Chain r: 88% 10%



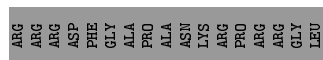
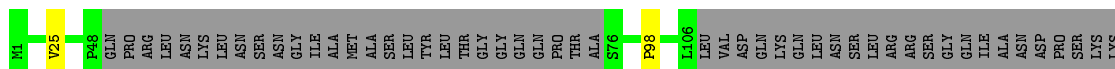
- Molecule 28: Small nuclear ribonucleoprotein Sm D1

Chain h: 56% 44%



- Molecule 28: Small nuclear ribonucleoprotein Sm D1

Chain l: 53% 46%



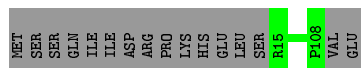
- Molecule 29: Small nuclear ribonucleoprotein Sm D2

Chain j: 83% 15%



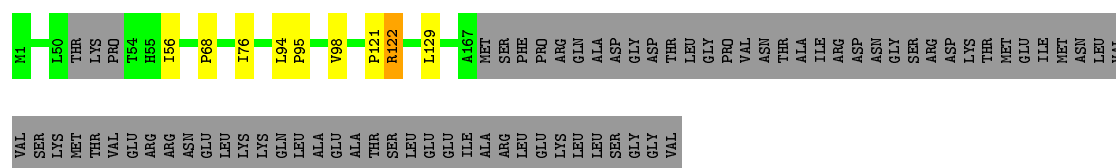
- Molecule 29: Small nuclear ribonucleoprotein Sm D2

Chain m: 85% 15%




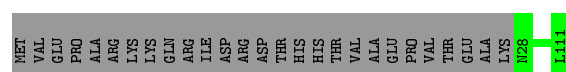
- Molecule 30: U2 small nuclear ribonucleoprotein A'

Chain W:  65% 1% 31%



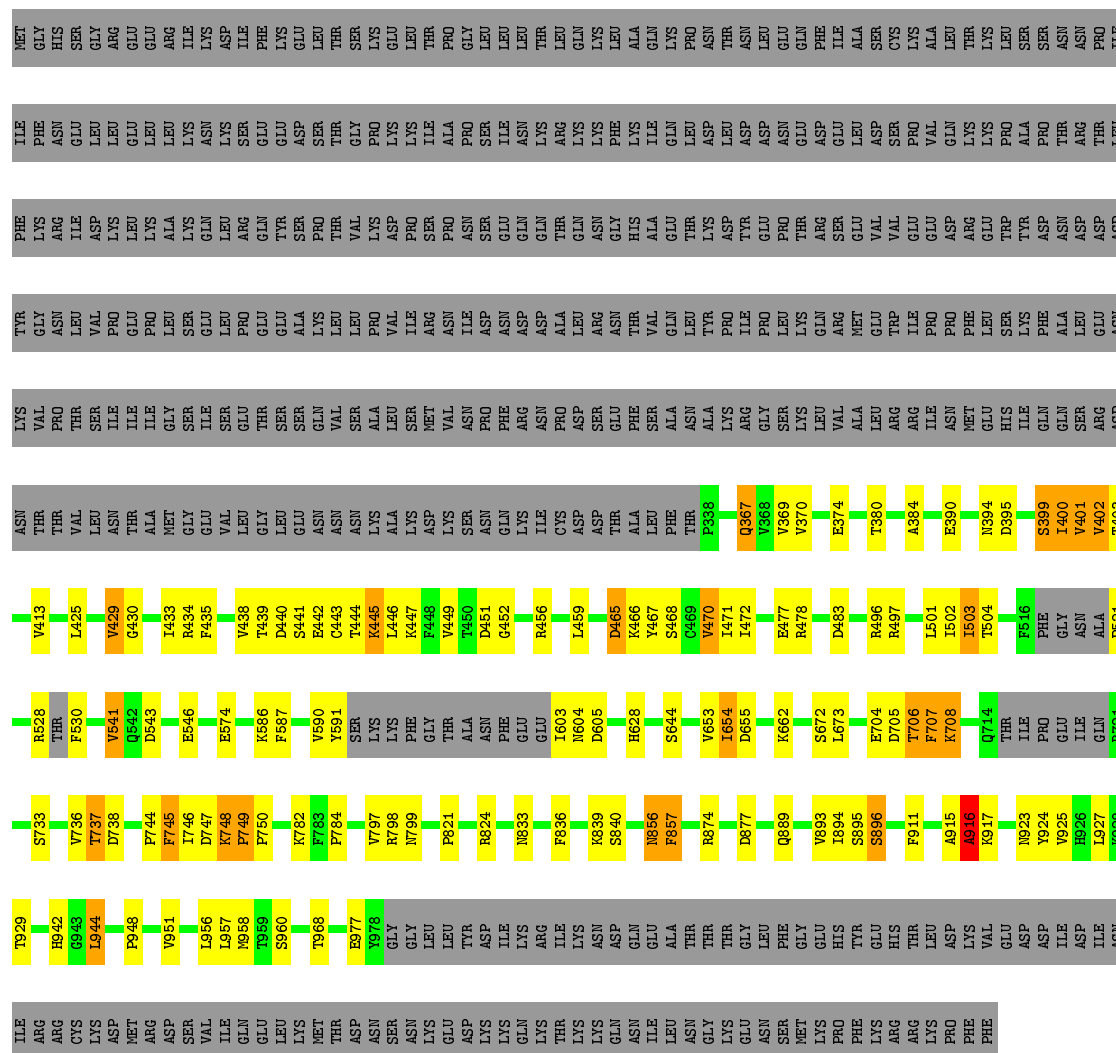
- Molecule 31: U2 small nuclear ribonucleoprotein B''

Chain Y:  76% 24%



- Molecule 32: Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP16

Chain Q: 46% 10% . 42%



- Molecule 33: Pre-mRNA-processing factor 19

Lys	A471	D395	GLU	VAL	ASN	T299	D306	I446	PRO	GLU	PHE	LYS	THR	G492	L467	GLN	SER	ASP	THR	A472	P503																										
HI	C3	V51	GLU	ILE	VAL	PRO	SER	ALA	GLN	GLN	SER	LEU	THR	GLU	SER	THR	ASN	ALA	THR	SER	ILE	P78	G143	ALA	VAL	ILE	THR	ARG	GLU	PHE	LEU	GLN	GLY	LEU	LEU	GLN	SER	SER	ARG	ASP	PHE	VAL	ALA	ARG	GLY	LYS	LEU

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|------|------|-----|-----|-----|------|------|------|-----|-----|-----|-----|-----|------|------|-----|-----|-----|------|------|-----|-----|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| A171 | N295 | G1U | VAL | ASN | T239 | D306 | I416 | PRO | GLU | PHE | LYS | THR | C422 | L467 | GLN | ASP | THR | A472 | P503 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| HI | E52 | ILE | VAL | PRO | SER | ALA | GLN | GLN | ALA | SER | LEU | THR | ASN | SER | ALA | THR | LYS | ALA | ASN | TTR | S76 | K139 | SER | SER | GLN | GLN | ALA | VAL | ALA | ILE | THR | ARG | GLU | GLU | PHE | LEU | GLN | GLY | LEU | LEU | GLN | SER | SER | ARG | ASP | PHE | VAL | ALA | ARG | GLY | LYS | LYS | LEU | LYS |

- [illegible]

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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|-----|-----|-----|------|------|------|-----|-----|-----|-----|------|------|-----|-----|-----|-----|------|------|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| ARG | ASP | PHE | VAL | ALA | ARG | GLY | LYS | LEU | LYS | A471 | T295 | GLU | VAL | ASN | T299 | D306 | I416 | PRO | GLU | PHE | LYS | G422 | I467 | GLN | ASP | ASP | THR | A472 | P503 | HI | P17 | R20 | P99 | V51 | GLU | ILE | VAL | PRO | SER | ALA | GLN | GLN | ALA | SER | LEU | THR | GLU | SER | THR | ASN | SER | ALA | ALA | THR | LEU | LYS | ALA | ASN | ASN | TTR | SER | I77 | S134 | K139 | SER | SER | GLN | GLN | ALA | VAL | ALA | ALA | ILE | THR | ARG | GLU | GLU | PHE | LEU | GLN | GLY | LEU | LEU | GLN | SER |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|-----|-----|-----|------|------|------|-----|-----|-----|-----|------|------|-----|-----|-----|-----|------|------|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| ASP | PHE | ASN | ASP | ASP | ASP | T85 | K94 | P105 | V111 | S119 | L132 | P133 | V136 | R174 | LEU | MET | GLY | ASP | LEU | SER | PHE | VAL | ASP | LYS | GLY | LYS | I112 | I131 | LYS | ARG | GLU | PRO | VAL | HIS | PRO | GLU | ILE | ARG | GLY | ILE | LEU | ALA | LYS | ARG | LYS | ALA | ASP | ASN | SER | VAL | SER | THR | THR | ASN | ALA | LEU | TYR | GLU | THR | LYS | GLN | ARG | ASN | LYS | ARG | THR | PRO |
|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	15872	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	81000	Depositor
Image detector	Not provided	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	C	0.41	0/6902	0.73	0/9386
11	G	0.42	0/839	0.74	0/1126
12	H	0.43	0/2667	0.80	1/3630 (0.0%)
13	J	0.45	0/2613	0.74	0/3551
14	K	0.40	0/1308	0.72	0/1765
15	L	0.40	0/1294	0.75	0/1732
16	M	0.42	0/2058	0.70	0/2769
17	N	0.41	0/1680	0.76	0/2258
18	O	0.49	0/2091	0.86	2/2824 (0.1%)
19	P	0.43	0/282	0.69	0/380
2	E	0.36	0/388	0.69	0/603
20	R	0.40	0/545	0.77	0/748
21	S	0.44	0/3155	0.83	0/4298
22	T	0.38	0/2918	0.74	0/4032
23	b	0.34	0/636	0.59	0/856
23	k	0.28	0/394	0.50	0/546
24	d	0.36	0/634	0.62	1/859 (0.1%)
24	n	0.29	0/403	0.53	0/559
25	e	0.40	0/585	0.56	0/795
25	p	0.30	0/367	0.55	0/507
26	f	0.39	0/585	0.59	0/791
26	q	0.30	0/353	0.53	0/489
27	g	0.36	0/532	0.55	0/715
27	r	0.28	0/338	0.45	0/467
28	h	0.35	0/649	0.54	0/880
28	l	0.30	0/390	0.53	0/541
29	j	0.38	0/753	0.61	0/1013
29	m	0.31	0/466	0.54	0/649
3	I	0.28	0/772	0.71	0/1195
30	W	0.31	0/814	0.53	0/1134
31	Y	0.32	0/415	0.55	0/577

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
32	Q	0.51	0/3061	1.22	18/4260 (0.4%)
33	t	0.46	0/2165	0.67	1/3010 (0.0%)
33	u	0.50	0/2160	0.69	1/3003 (0.0%)
33	v	0.51	0/2104	0.74	4/2923 (0.1%)
33	w	0.47	0/2150	0.68	2/2989 (0.1%)
34	s	0.57	0/546	0.80	0/760
4	Z	0.26	0/4018	0.72	0/6233
5	V	0.32	0/2310	0.77	3/3594 (0.1%)
6	A	0.44	0/17321	0.75	0/23534
7	B	0.52	0/8463	0.72	0/11800
8	D	0.37	0/929	0.67	0/1243
9	F	0.42	0/325	0.74	0/442
All	All	0.43	0/86729	0.75	34/120679 (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
11	G	0	1
16	M	0	1
18	O	0	2
21	S	0	1
32	Q	0	45
33	t	0	1
33	v	0	1
33	w	0	1
34	s	0	2
6	A	0	2
All	All	0	57

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Q	384	ALA	CB-CA-C	8.22	122.43	110.10
1	U	39	U	C2'-C3'-O3'	8.13	127.38	109.50
32	Q	745	PHE	C-N-CA	7.85	141.32	121.70
32	Q	413	VAL	CB-CA-C	7.51	125.67	111.40
32	Q	745	PHE	O-C-N	-6.99	111.52	122.70
5	V	35	A	C5'-C4'-O4'	6.92	117.40	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Q	654	ILE	CB-CA-C	6.74	125.07	111.60
32	Q	916	ALA	N-CA-CB	-6.59	100.87	110.10
32	Q	403	THR	N-CA-C	6.55	128.68	111.00
12	H	440	LEU	CA-CB-CG	6.54	130.33	115.30
24	d	81	ALA	C-N-CD	-6.46	106.39	120.60
32	Q	574	GLU	N-CA-CB	-6.45	98.98	110.60
32	Q	745	PHE	CA-C-N	6.17	130.78	117.20
32	Q	384	ALA	N-CA-CB	6.16	118.72	110.10
18	O	564	TYR	CB-CA-C	6.15	122.71	110.40
33	w	39	PRO	N-CA-CB	6.01	110.51	103.30
33	v	134	SER	CA-C-O	-5.67	108.20	120.10
32	Q	402	VAL	N-CA-C	5.55	125.99	111.00
5	V	35	A	O4'-C4'-C3'	5.43	110.44	106.10
32	Q	394	ASN	CB-CA-C	5.41	121.22	110.40
32	Q	483	ASP	CB-CA-C	5.37	121.14	110.40
32	Q	447	LYS	N-CA-C	5.31	125.33	111.00
32	Q	477	GLU	C-N-CA	5.29	134.93	121.70
33	v	76	SER	N-CA-CB	5.29	118.43	110.50
32	Q	400	ILE	C-N-CA	5.18	134.64	121.70
33	v	134	SER	O-C-N	5.17	130.98	122.70
5	V	92	C	C2'-C3'-O3'	5.13	121.91	113.70
33	u	306	ASP	CB-CA-C	-5.13	100.15	110.40
33	t	306	ASP	CB-CA-C	-5.12	100.17	110.40
33	v	306	ASP	CB-CA-C	-5.11	100.18	110.40
32	Q	445	LYS	CB-CA-C	-5.10	100.20	110.40
33	w	306	ASP	CB-CA-C	-5.10	100.20	110.40
32	Q	470	VAL	C-N-CA	5.09	134.43	121.70
18	O	564	TYR	O-C-N	-5.06	114.61	122.70

There are no chirality outliers.

All (57) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	1325	SER	Peptide
6	A	403	TYR	Peptide
11	G	3	ARG	Peptide
16	M	231	ASP	Peptide
18	O	567	ARG	Mainchain
18	O	83	GLN	Peptide
32	Q	367	GLN	Peptide
32	Q	390	GLU	Peptide
32	Q	399	SER	Peptide

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Mol	Chain	Res	Type	Group
32	Q	429	VAL	Peptide
32	Q	439	THR	Peptide
32	Q	441	SER	Peptide
32	Q	442	GLU	Peptide
32	Q	444	THR	Peptide
32	Q	445	LYS	Peptide
32	Q	446	LEU	Peptide
32	Q	465	ASP	Peptide
32	Q	468	SER	Peptide
32	Q	501	LEU	Peptide
32	Q	541	VAL	Peptide
32	Q	543	ASP	Peptide
32	Q	628	HIS	Peptide
32	Q	662	LYS	Peptide
32	Q	705	ASP	Peptide
32	Q	706	THR	Peptide
32	Q	707	PHE	Peptide
32	Q	733	SER	Peptide
32	Q	736	VAL	Peptide
32	Q	737	THR	Peptide
32	Q	744	PRO	Peptide
32	Q	745	PHE	Peptide
32	Q	747	ASP	Peptide
32	Q	748	LYS	Peptide
32	Q	749	PRO	Peptide
32	Q	797	VAL	Peptide
32	Q	798	ARG	Peptide
32	Q	833	ASN	Peptide
32	Q	856	ASN	Peptide
32	Q	857	PHE	Peptide
32	Q	889	GLN	Peptide
32	Q	893	VAL	Peptide
32	Q	895	SER	Peptide
32	Q	896	SER	Peptide
32	Q	911	PHE	Peptide
32	Q	915	ALA	Peptide
32	Q	916	ALA	Peptide
32	Q	923	ASN	Peptide
32	Q	924	TYR	Peptide
32	Q	944	LEU	Peptide
32	Q	960	SER	Peptide
32	Q	977	GLU	Peptide

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Mol	Chain	Res	Type	Group
21	S	237	ILE	Peptide
34	s	111	VAL	Peptide
34	s	132	LEU	Peptide
33	t	3	CYS	Mainchain
33	v	109	LEU	Mainchain
33	w	134	SER	Mainchain

5.2 Too-close contacts [i](#)

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	1042	23	0
6	A	16919	0	16184	233	0
7	B	8462	0	3706	27	0
8	D	912	0	936	11	0
9	F	321	0	282	3	0
10	C	6756	0	6801	117	0
11	G	823	0	808	10	0
12	H	2639	0	2073	25	0
13	J	2556	0	2551	54	0
14	K	1289	0	1309	17	0
15	L	1270	0	1294	12	0
16	M	2012	0	1968	32	0
17	N	1658	0	1712	59	0
18	O	2068	0	1853	39	0
19	P	275	0	283	4	0
20	R	544	0	345	17	0
21	S	3121	0	2399	55	0
22	T	2946	0	1252	11	0
23	b	631	0	670	0	0
23	k	396	0	169	0	0
24	d	625	0	647	0	0
24	n	404	0	180	0	0
25	e	575	0	597	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	p	369	0	152	0	0
26	f	573	0	572	0	0
26	q	354	0	153	0	0
27	g	529	0	557	0	0
27	r	340	0	152	0	0
28	h	644	0	686	0	0
28	l	392	0	165	0	0
29	j	741	0	778	0	0
29	m	467	0	199	0	0
30	W	816	0	341	1	0
31	Y	416	0	182	0	0
32	Q	3066	0	1345	52	0
33	t	2171	0	945	0	0
33	u	2166	0	942	0	0
33	v	2111	0	917	0	0
33	w	2156	0	938	0	0
34	s	548	0	219	0	0
35	x	660	0	142	0	0
36	E	1	0	0	0	0
36	V	1	0	0	0	0
37	D	1	0	0	1	0
37	L	3	0	0	0	0
37	M	1	0	0	0	0
37	N	2	0	0	5	0
38	C	32	0	12	0	0
All	All	85476	0	62328	741	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 (741) 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)
32:Q:434:ARG:O	32:Q:874:ARG:HA	1.26	1.35
17:N:34:CYS:SG	17:N:37:CYS:SG	1.35	1.34
20:R:36:GLN:O	20:R:40:GLN:N	1.60	1.32
1:U:45:A:N1	1:U:74:U:O4	1.65	1.30
21:S:467:GLN:CA	21:S:471:LEU:HA	1.65	1.24
32:Q:472:ILE:CB	32:Q:503:ILE:H	1.55	1.19
17:N:16:CYS:SG	17:N:73:CYS:HB2	1.85	1.16
32:Q:435:PHE:HA	32:Q:877:ASP:N	1.61	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Q:434:ARG:C	32:Q:874:ARG:HA	1.69	1.13
32:Q:472:ILE:CB	32:Q:503:ILE:N	2.11	1.11
32:Q:472:ILE:CB	32:Q:503:ILE:CA	2.28	1.11
16:M:108:VAL:HG11	17:N:59:LEU:HD13	1.26	1.10
20:R:37:GLN:O	20:R:41:GLN:CB	2.00	1.10
16:M:108:VAL:HG21	17:N:73:CYS:O	1.52	1.09
32:Q:435:PHE:CA	32:Q:877:ASP:H	1.65	1.07
32:Q:672:SER:HA	32:Q:956:LEU:O	1.55	1.05
6:A:2364:THR:H	32:Q:521:PRO:N	1.56	1.03
22:T:360:LYS:CB	22:T:381:HIS:CB	2.36	1.03
21:S:467:GLN:CB	21:S:471:LEU:O	2.07	1.02
21:S:467:GLN:HA	21:S:471:LEU:HA	1.03	1.01
17:N:61:CYS:HG	37:N:401:ZN:ZN	0.67	1.00
21:S:467:GLN:HA	21:S:471:LEU:CA	1.90	0.99
6:A:2364:THR:N	32:Q:521:PRO:N	2.13	0.96
32:Q:435:PHE:HA	32:Q:877:ASP:H	1.14	0.95
17:N:61:CYS:SG	37:N:401:ZN:ZN	1.54	0.94
32:Q:472:ILE:CB	32:Q:503:ILE:HA	1.98	0.92
22:T:429:SER:O	22:T:433:LEU:N	2.03	0.92
21:S:467:GLN:CA	21:S:471:LEU:CA	2.37	0.92
16:M:108:VAL:HG22	17:N:75:MET:HG2	1.53	0.91
21:S:332:GLU:CB	21:S:338:ILE:CB	2.51	0.89
21:S:467:GLN:CB	21:S:471:LEU:HA	2.03	0.89
32:Q:472:ILE:CB	32:Q:503:ILE:O	2.22	0.88
20:R:36:GLN:O	20:R:40:GLN:CB	2.21	0.88
21:S:332:GLU:CB	21:S:334:PHE:O	2.22	0.88
16:M:108:VAL:HG11	17:N:59:LEU:CD1	2.03	0.88
21:S:467:GLN:CB	21:S:471:LEU:CA	2.52	0.87
22:T:420:SER:O	22:T:421:ALA:O	1.93	0.87
32:Q:472:ILE:CB	32:Q:503:ILE:C	2.43	0.86
32:Q:528:ARG:CB	32:Q:530:PHE:N	2.39	0.86
32:Q:673:LEU:H	32:Q:957:LEU:HA	1.38	0.85
8:D:88:CYS:SG	37:D:1001:ZN:ZN	1.65	0.85
7:B:479:GLU:HA	7:B:498:SER:CB	2.07	0.85
6:A:2364:THR:CB	32:Q:521:PRO:N	2.40	0.84
32:Q:587:PHE:O	32:Q:591:TYR:CB	2.26	0.84
17:N:16:CYS:SG	17:N:73:CYS:CB	2.65	0.84
32:Q:434:ARG:O	32:Q:874:ARG:CA	2.21	0.84
16:M:250:MET:HB2	17:N:139:LEU:HD11	1.58	0.83
20:R:28:ASN:O	20:R:32:PRO:CD	2.27	0.83
13:J:210:ASP:HB2	13:J:217:ILE:HD11	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:1182:ALA:O	32:Q:496:ARG:HA	1.80	0.82
16:M:108:VAL:HG22	17:N:75:MET:CG	2.10	0.82
18:O:564:TYR:HA	18:O:566:TYR:H	1.44	0.82
17:N:220:THR:HG22	17:N:240:LEU:HD12	1.62	0.81
6:A:759:ARG:HD2	6:A:783:LEU:HD13	1.61	0.81
18:O:564:TYR:CA	18:O:566:TYR:H	1.93	0.81
21:S:329:LEU:HA	21:S:338:ILE:CB	2.10	0.81
10:C:389:LEU:HD21	10:C:421:LEU:HD12	1.64	0.80
20:R:36:GLN:O	20:R:40:GLN:CA	2.29	0.79
32:Q:459:LEU:CB	32:Q:782:LYS:CB	2.60	0.79
18:O:564:TYR:HA	18:O:566:TYR:N	2.00	0.77
5:V:67:C:H2'	5:V:68:C:O4'	1.85	0.76
32:Q:586:LYS:O	32:Q:590:VAL:N	2.19	0.76
20:R:37:GLN:O	20:R:41:GLN:N	2.19	0.76
16:M:108:VAL:CG1	17:N:59:LEU:HD13	2.14	0.76
13:J:323:VAL:HG12	13:J:336:LEU:HD12	1.67	0.75
1:U:45:A:N1	1:U:74:U:C4	2.54	0.75
17:N:113:LEU:HD11	17:N:120:LEU:HD11	1.69	0.75
16:M:22:ILE:HG23	16:M:23:PRO:HD3	1.67	0.74
17:N:37:CYS:SG	37:N:401:ZN:ZN	1.77	0.74
21:S:332:GLU:CB	21:S:335:PRO:HA	2.18	0.73
32:Q:459:LEU:HA	32:Q:782:LYS:CB	2.17	0.73
18:O:230:THR:HG23	21:S:116:ASN:HD21	1.53	0.73
5:V:76:A:OP2	6:A:749:ARG:NH1	2.21	0.73
16:M:108:VAL:CG1	17:N:59:LEU:HD22	2.20	0.72
17:N:71:CYS:SG	37:N:402:ZN:ZN	1.77	0.72
21:S:467:GLN:CB	21:S:471:LEU:C	2.56	0.72
6:A:1361:VAL:HG21	6:A:1407:ILE:HD11	1.72	0.72
8:D:51:CYS:SG	8:D:88:CYS:HB3	2.30	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
7:B:1163:SER:CA	32:Q:497:ARG:O	2.32	0.71
6:A:1335:TRP:CZ2	6:A:1339:LEU:HD13	2.25	0.71
6:A:745:THR:HA	13:J:182:VAL:HG21	1.73	0.70
6:A:631:LEU:HD21	6:A:663:LEU:HD12	1.73	0.70
10:C:406:VAL:HG11	10:C:427:LEU:HB3	1.71	0.70
16:M:250:MET:CB	17:N:139:LEU:HD11	2.21	0.70
10:C:493:LEU:HD21	10:C:539:VAL:HG21	1.74	0.70
21:S:209:GLU:HB3	21:S:218:THR:HG22	1.75	0.69
32:Q:672:SER:CA	32:Q:956:LEU:O	2.37	0.69
4:Z:34:G:N2	6:A:1325:SER:OG	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
13:J:206:VAL:HG11	13:J:241:THR:HG21	1.76	0.67
16:M:108:VAL:HG13	17:N:59:LEU:HD22	1.76	0.67
32:Q:459:LEU:CA	32:Q:782:LYS:CB	2.72	0.67
20:R:28:ASN:O	20:R:32:PRO:HD3	1.93	0.67
32:Q:435:PHE:CA	32:Q:877:ASP:N	2.34	0.67
7:B:1163:SER:O	7:B:1164:THR:CB	2.43	0.67
10:C:621:ALA:HB2	10:C:664:ALA:HB2	1.76	0.67
10:C:241:VAL:HG11	10:C:273:LEU:HD23	1.76	0.66
18:O:21:LEU:HD12	18:O:40:LEU:HD11	1.76	0.66
10:C:200:CYS:HB3	10:C:436:VAL:HG21	1.78	0.66
13:J:290:VAL:HG12	13: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	13:J:224:LEU:HD22	1.78	0.65
16:M:108:VAL:CG2	17:N:75:MET:HG2	2.24	0.65
6:A:1286:TRP:CE2	6:A:1302:LEU:HD11	2.31	0.65
18:O:60:LEU:HD21	18:O:94:PRO:HB3	1.79	0.65
32:Q:434:ARG:C	32:Q:874:ARG:CA	2.57	0.65
12:H:299:LEU:HD11	12:H:329:ILE:HG12	1.79	0.65
6:A:716:ARG:O	6:A:720:PRO:HD2	1.97	0.64
10:C:193:LEU:HD11	10:C:228:ALA:HB2	1.78	0.64
17:N:125:ILE:HG21	17:N:135:ILE:HD12	1.80	0.64
13:J:282:VAL:HG11	13:J:323:VAL:HG21	1.80	0.64
6:A:1344:THR:O	6:A:1347:ARG:NH1	2.30	0.64
13:J:142:VAL:HG11	13:J:423:ILE:CG2	2.28	0.64
10:C:323:THR:HG21	10:C:438:ALA:HB2	1.81	0.63
6:A:630:LYS:O	6:A:634:ASP:N	2.26	0.63
10:C:501:ILE:HD13	10:C:567:ILE:HG23	1.79	0.63
10:C:872:LEU:HD13	10:C:922:THR:HG22	1.79	0.63
5:V:90:U:O2'	5:V:92:C:C6	2.52	0.63
22:T:429:SER:O	22:T:433:LEU:CB	2.47	0.62
12:H:445:LEU:HD11	12:H:448:MET:HG3	1.80	0.62
21:S:225:ALA:O	21:S:229:VAL:HG23	1.98	0.62
8:D:63:LYS:HE3	9:F:6:LEU:HD22	1.80	0.62
17:N:71:CYS:HG	37: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
5:V:90:U:O2'	5:V:92:C:C5	2.53	0.62
10:C:251:GLN:HG2	10:C:933:TRP:CD2	2.35	0.61
13:J:277:VAL:HG11	13:J:321:PHE:CZ	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:108:VAL:CG2	17:N:73:CYS:O	2.40	0.61
6:A:857:ILE:HD11	6:A:969:ILE:HD11	1.82	0.61
17:N:91:ILE:HD12	17:N:125:ILE:HD12	1.82	0.61
6:A:268:LEU:HD13	6:A:277:LYS:HB2	1.82	0.61
10:C:602:VAL:HG11	10:C:860:PRO:HG3	1.81	0.61
6:A:673:VAL:HG22	6:A:714:PHE:CZ	2.36	0.61
7:B:1162:ALA:O	32:Q:367:GLN:N	2.34	0.61
21:S:149:VAL:O	21:S:152:VAL:HG12	2.01	0.61
32:Q:435:PHE:CB	32:Q:877:ASP:H	2.12	0.61
6:A:1557:LEU:HD13	6:A:1562:PHE:CE2	2.36	0.61
10:C:133:ILE:HD13	10:C:560:GLN:HB3	1.83	0.61
7:B:487:CYS:O	7:B:490:ALA:N	2.33	0.60
1:U:98:U:HO2'	5:V:75:A:H8	1.48	0.60
10:C:270:LEU:HD11	10:C:313:PHE:HB3	1.82	0.60
17:N:39:LEU:HD13	17: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	11:G:1:MET:N	2.34	0.60
7:B:1973:ALA:O	7:B:1976:ALA:HB3	2.01	0.60
13:J:323:VAL:CG1	13:J:336:LEU:HD12	2.32	0.60
15:L:66:LEU:HD13	15:L:73:ILE:HG13	1.83	0.59
8:D:51:CYS:SG	8:D:88:CYS:SG	3.00	0.59
10:C:656:LEU:HD22	10:C:670:ILE:HD11	1.85	0.59
10:C:866:ILE:HB	10:C:902:VAL:HG13	1.83	0.59
6:A:1032:ILE:HG12	6:A:1171:LEU:HD22	1.83	0.59
32:Q:402:VAL:CB	32:Q:449:VAL:H	2.15	0.59
20:R:37:GLN:O	20:R:41:GLN:CA	2.51	0.59
10:C:499:VAL:HG11	10:C:577:LEU:HD13	1.83	0.59
32:Q:452:GLY:O	32:Q:784:PRO:CB	2.50	0.59
21:S:173:VAL:HG23	21:S:188:ILE:HD11	1.85	0.59
6:A:390:LEU:HD21	10:C:605:ILE:HD11	1.85	0.58
13:J:240:ALA:HB1	13:J:248:ILE:HD11	1.82	0.58
13:J:160:ASN:HA	13:J:184:THR:HB	1.85	0.58
17:N:39:LEU:HD23	17:N:111:ARG:HG2	1.85	0.58
12:H:298:VAL:HG11	12:H:312:LEU:HD23	1.84	0.58
6:A:842:LYS:O	6:A:845:VAL:HG12	2.02	0.58
17:N:207:LEU:HD11	17:N:251:LEU:HD11	1.86	0.58
17:N:16:CYS:SG	17:N:71:CYS:SG	3.02	0.58
13:J:248:ILE:HG23	13:J:262:LEU:HB2	1.84	0.58
32:Q:425:LEU:HA	32:Q:429:VAL:CB	2.33	0.58
6:A:1668:ILE:HD13	6:A:1801:SER:HB3	1.86	0.58
18:O:185:LEU:O	18:O:188:ARG:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:16:CYS:HG	17:N:73:CYS:HB2	1.65	0.57
13:J:147:ILE:HD13	13:J:408:ASP:HA	1.84	0.57
20:R:37:GLN:C	20:R:41:GLN:H	2.07	0.57
17:N:16:CYS:SG	17:N:73:CYS:SG	3.02	0.57
6:A:1632:ILE:HG21	6:A:1645:LEU:HD13	1.85	0.57
18:O:185:LEU:O	18: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
15:L:66:LEU:HD13	15: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
10:C:328:VAL:HG21	10:C:345:THR:HG22	1.87	0.56
21:S:229:VAL:HG22	21: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
32:Q:456:ARG:CB	32:Q:784:PRO:CB	2.83	0.56
12:H:465:PHE:HB2	12:H:473:LEU:HD23	1.88	0.56
6:A:948:HIS:CE1	6:A:952:ASN:HD21	2.23	0.56
8:D:51:CYS:SG	8:D:88:CYS:CB	2.94	0.56
5:V:59:A:H2'	5:V:60:G:O4'	2.05	0.56
18:O:33:TRP:CE3	18:O:36:VAL:HG11	2.41	0.56
21:S:184:GLY:O	21:S:188:ILE:HG23	2.05	0.56
21:S:332:GLU:CB	21:S:334:PHE:C	2.74	0.56
13:J:289:THR:HG22	13:J:305:THR:HG22	1.88	0.56
32:Q:673:LEU:N	32:Q:957:LEU:HA	2.17	0.56
17:N:226:LEU:HD13	17:N:266:ILE:HD11	1.87	0.56
32:Q:434:ARG:CB	32:Q:874:ARG:O	2.54	0.56
6:A:878:GLU:O	6:A:882:ILE:HG23	2.06	0.56
8:D:11:TYR:CD1	11:G:12:LEU:HD21	2.41	0.56
18:O:230:THR:HG21	21:S:117:HIS:ND1	2.21	0.56
20:R:31:ARG:N	20:R:32:PRO:CD	2.68	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
13:J:277:VAL:HG13	13:J:278:ASP:N	2.20	0.55
17:N:106:ASN:HD21	18:O:208:GLY:HA2	1.71	0.55
6:A:137:GLU:CD	15:L:30:LEU:HG	2.26	0.55
15:L:94:LYS:HD2	15:L:109:ILE:HD11	1.87	0.55
6:A:1000:TRP:CZ2	6:A:1510:ILE:HG21	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:1795:SER:O	7:B:1798:GLY:N	2.39	0.55
18:O:37:ALA:HB2	18:O:45:ALA:HA	1.88	0.55
6:A:724:ARG:O	6:A:728:ASN:HB2	2.07	0.55
10:C:472:VAL:HB	10:C:575:ALA:HB3	1.88	0.55
16:M:163:VAL:HG23	16: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
32:Q:587:PHE:O	32:Q:591:TYR:N	2.39	0.55
20:R:28:ASN:O	20:R:32:PRO:HD2	2.04	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	10:C:893:LYS:HB3	2.42	0.54
17:N:106:ASN:HB2	18: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
17:N:17:LEU:CD2	17:N:23:ILE:HD12	2.37	0.54
6:A:2364:THR:CA	32:Q:521:PRO:N	2.70	0.54
20:R:31:ARG:N	20:R:32:PRO:HD2	2.23	0.54
6:A:1562:PHE:O	6:A:1565:THR:OG1	2.24	0.54
17:N:29:PRO:HA	17:N:42:THR:HG22	1.90	0.54
18:O:211:ILE:HD13	21:S:44:ARG:HG3	1.89	0.54
21:S:99:ILE:N	21:S:100:PRO:CD	2.70	0.54
30:W:121:PRO:O	30:W:122:ARG:CB	2.56	0.54
18:O:16:VAL:HG22	18:O:152:LEU:HD21	1.88	0.54
6:A:141:LYS:HG3	15: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	14:K:207:ALA:HB1	2.08	0.54
10:C:861:ILE:HD11	10:C:938:ARG:HB2	1.89	0.54
1:U:92:U:O2	20:R:12:LYS:NZ	2.39	0.54
1:U:103:A:O2'	1:U:104:G:O4'	2.24	0.54
10:C:138:VAL:HG23	10:C:236:LEU:HB2	1.90	0.53
10:C:265:PHE:HB2	10:C:311:ILE:HD13	1.89	0.53
10:C:191:ILE:HG23	10:C:221:PHE:CE2	2.44	0.53
1:U:102:C:OP1	6:A:675:HIS:NE2	2.42	0.53
10:C:241:VAL:HG22	10:C:267:ILE:CG2	2.38	0.53
5:V:35:A:C8	15:L:41:LEU:HD13	2.43	0.53
17:N:64:CYS:SG	17:N:114:SER:HB2	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
13:J:277:VAL:HG11	13:J:321:PHE:HZ	1.71	0.53
1:U:45:A:N6	1:U:74:U:N3	2.55	0.53
10:C:864:VAL:HG22	10:C:930:LEU:HD23	1.90	0.53
6:A:882:ILE:HD11	6:A:1065:LEU:HD21	1.90	0.53
13:J:306:HIS:CE1	14: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
8:D:101:PRO:HB2	9:F:23:VAL:HG21	1.90	0.53
13:J:142:VAL:HG11	13: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
10:C:201:THR:HG22	10:C:207:SER:HB3	1.90	0.53
7:B:1502:LEU:O	7:B:1503:GLU:C	2.47	0.53
10:C:126:MET:SD	10:C:132:ARG:NH2	2.82	0.53
6:A:937:LEU:HD22	6:A:1590:LEU:CD2	2.39	0.52
7:B:1928:LEU:O	7:B:1931:GLN:N	2.40	0.52
11:G:55:SER:O	11:G:58:ILE:HG22	2.10	0.52
10:C:836:SER:O	10:C:840:PRO:HD2	2.09	0.52
13:J:341:LEU:HD23	13:J:342:LEU:N	2.24	0.52
22:T:119:ALA:HB1	22: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
6:A:1375:LEU:HD12	6:A:1383:PHE:CE1	2.44	0.52
1:U:45:A:H2'	1:U:45:A:N3	2.24	0.52
14:K:201:PHE:CD2	18:O:80:LEU:HD21	2.45	0.52
6:A:1339:LEU:HD11	6:A:1360:LEU:HD22	1.92	0.52
13:J:335:GLY:H	13:J:342:LEU:HD13	1.74	0.52
7:B:1163:SER:N	32:Q:497:ARG:O	2.42	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
10:C:539:VAL:HG13	10:C:564:ILE:HG23	1.92	0.52
6:A:785:HIS:NE2	14:K:168:ALA:HB2	2.24	0.52
6:A:1654:TRP:CZ3	6:A:1779:LEU:HD12	2.45	0.51
32:Q:673:LEU:O	32:Q:958:MET:CB	2.58	0.51
21:S:199:MET:SD	21:S:246:LEU:HD22	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
10:C:626:SER:HB3	10:C:634:ILE:HD12	1.91	0.51
6:A:808:ILE:HG21	14:K:165:ILE:HD12	1.91	0.51
12:H:333:SER:HA	12:H:343:TYR:CE2	2.46	0.51
10:C:664:ALA:HB1	10:C:666:ILE:CD1	2.39	0.51
10:C:664:ALA:HB1	10:C:666:ILE:HD12	1.92	0.51
12:H:347:SER:O	12:H:351:ILE:HG12	2.09	0.51
18:O:16:VAL:CG2	18: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:HD12	6:A:249:LEU:O	2.11	0.51
7:B:2036:SER:O	7:B:2039:ALA:HB3	2.11	0.51
6:A:660:ILE:HG21	6:A:711:TRP:CH2	2.45	0.51
22:T:420:SER:O	22:T:421:ALA:C	2.49	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
7:B:1399:ASN:O	7:B:1448:THR:HA	2.10	0.51
10:C:255:GLN:HG2	10:C:598:ILE:HD12	1.92	0.51
13:J:206:VAL:CG1	13:J:241:THR:HG21	2.40	0.51
10:C:963:SER:O	10:C:967:VAL:HG23	2.10	0.51
3:I:2:U:H3'	6:A:607:THR:OG1	2.11	0.51
32:Q:425:LEU:O	32:Q:429:VAL:CB	2.59	0.51
22:T:299:PRO:O	22:T:300:ASP:C	2.49	0.51
6:A:1329:THR:HG21	6:A:1601:ILE:HB	1.93	0.51
6:A:458:PHE:CZ	10:C:336:ILE:HD11	2.45	0.51
10:C:872:LEU:HD13	10:C:922:THR:CG2	2.41	0.51
12:H:326:VAL:O	12:H:330:ILE:HG12	2.10	0.51
13:J:275:THR:OG1	13:J:279:PRO:O	2.29	0.51
6:A:350:PRO:HD3	6:A:526:LEU:HD13	1.92	0.50
6:A:741:ILE:CD1	13:J:224:LEU:HD22	2.41	0.50
21:S:172:PHE:CD2	21:S:188:ILE:HD13	2.46	0.50
21:S:332:GLU:CB	21:S:335:PRO:CA	2.87	0.50
5:V:27:U:O2'	15: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
10:C:139:ILE:HG12	10:C:225:THR:HG23	1.93	0.50
3:I:3:A:OP2	11:G:3:ARG:HA	2.11	0.50
32:Q:840:SER:HA	32:Q:968:THR:HA	1.94	0.50
1:U:71:A:N3	1:U:116:U:O2'	2.33	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
10:C:493:LEU:HD22	10:C:542:ILE:HD11	1.93	0.50
6:A:912:LEU:HD22	6:A:951:LEU:HG	1.94	0.50
10:C:615:LEU:N	10:C:616:PRO:HD2	2.26	0.50
10:C:617:LYS:HB3	10: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:N	6:A:410:ILE:HD12	2.27	0.50
6:A:175:LEU:HD23	6:A:564:TRP:CZ2	2.46	0.50
6:A:674:MET:CE	6:A:674:MET:HA	2.42	0.50
10:C:133:ILE:HG23	10:C:209:MET:SD	2.52	0.50
10:C:864:VAL:HG22	10:C:930:LEU:CD2	2.42	0.50
18:O:230:THR:HG21	21:S:117:HIS:CE1	2.47	0.50
32:Q:433:ILE:O	32:Q:877:ASP:CB	2.60	0.50
6:A:1344:THR:HG21	6:A:1537:TRP:CD2	2.46	0.50
16:M:108:VAL:CG1	17:N:59:LEU:CD2	2.90	0.50
13:J:156:ILE:HG22	13:J:166:VAL:HG22	1.93	0.50
13:J:200:VAL:CG2	13:J:227:VAL:HB	2.41	0.50
10:C:231:ALA:HB2	10: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	16:M:75:PHE:CZ	3.00	0.49
16:M:108:VAL:HG22	17:N:75:MET:HG3	1.91	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
18:O:230:THR:HG22	21:S:114:CYS:SG	2.53	0.49
11:G:28:ASP:OD1	11:G:28:ASP:N	2.44	0.49
12:H:291:PHE:CE1	12:H:317:ILE:HG21	2.47	0.49
6:A:937:LEU:HD13	6:A:1590:LEU:HD11	1.93	0.49
10:C:116:THR:HG21	10:C:118:TYR:CZ	2.47	0.49
10:C:544:LEU:HD23	10:C:562:VAL:HG12	1.94	0.49
9:F:27:GLU:O	9:F:31:ILE:HG12	2.13	0.49
13:J:145:VAL:HG22	13:J:157:THR:HG22	1.94	0.49
6:A:137:GLU:CD	15:L:52:ILE:HG23	2.33	0.49
6:A:1400:ILE:HG22	6:A:1400:ILE:O	2.12	0.49
10:C:137:GLY:O	10:C:139:ILE:HD12	2.13	0.49
18:O:20:ILE:HD11	18:O:152:LEU:HD22	1.95	0.49
21:S:99:ILE:HD11	21:S:132:VAL:HG11	1.95	0.49
6:A:1795:LYS:N	6:A:1796:PRO:CD	2.75	0.49
13:J:150:VAL:HG13	13:J:151:ASP:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:332:GLN:CB	22:T:342:ILE:CB	2.91	0.49
5:V:52:G:H2'	5:V:53:A:C8	2.47	0.49
10:C:607:LEU:HD11	10:C:644:ILE:HD11	1.96	0.48
18:O:24:ALA:O	18:O:28:TYR:N	2.37	0.48
6:A:1557:LEU:HD13	6:A:1562:PHE:CD2	2.48	0.48
7:B:479:GLU:CA	7:B:498:SER:CB	2.86	0.48
10:C:213:LEU:HD11	10:C:561:ILE:HD13	1.95	0.48
12:H:427:LEU:HD23	12:H:436:LEU:HD11	1.95	0.48
6:A:724:ARG:CD	19:P:31:LEU:HD11	2.43	0.48
12:H:368:ASN:ND2	12:H:384:LEU:HD11	2.29	0.48
32:Q:430:GLY:HA3	32:Q:438:VAL:O	2.14	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
13:J:277:VAL:HG22	13: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
13:J:147:ILE:HG22	13:J:155:PHE:HB3	1.94	0.48
17:N:65:ALA:O	17:N:69:ASN:N	2.47	0.48
13:J:272:VAL:HG13	13:J:272:VAL:O	2.14	0.48
10:C:241:VAL:HG23	10:C:268:ASN:O	2.14	0.48
17:N:17:LEU:HD21	17: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
15:L:22:THR:HG21	15:L:62:TYR:CE1	2.49	0.48
16:M:137:LEU:HD21	16:M:192:ALA:HB1	1.96	0.48
18:O:218:VAL:HB	21:S:89:GLU:HB3	1.96	0.48
5:V:32:U:C4	17:N:28:ILE:HG21	2.49	0.48
6:A:857:ILE:CD1	6:A:969:ILE:HD11	2.44	0.47
10:C:273:LEU:HD12	10:C:274:ILE:N	2.29	0.47
10:C:625:ILE:HG22	10:C:634:ILE:HD11	1.95	0.47
21:S:140:LEU:HD22	21:S:156:TYR:CE2	2.49	0.47
6:A:1222:LEU:O	6:A:1226:VAL:HG23	2.15	0.47
10:C:229:LEU:HB3	10:C:259:ASN:HD21	1.79	0.47
14:K:41:ASP:HA	14:K:44:ILE:HD12	1.96	0.47
10:C:211:ASN:N	10:C:211:ASN:HD22	2.12	0.47
10:C:873:LEU:HD21	10:C:891:THR:HG21	1.94	0.47
12:H:355:ARG:O	12:H:359:THR:HG23	2.14	0.47
18:O:33:TRP:HA	18:O:36:VAL:HG12	1.96	0.47
21:S:112:VAL:HG13	21:S:114:CYS:HB2	1.96	0.47
22:T:119:ALA:HB1	22:T:128:ILE:HA	1.94	0.47
6:A:1066:LEU:HD11	6:A:1113:ILE:HG23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:522:TYR:CE2	6:A:686:ILE:HD12	2.50	0.47
10:C:136:VAL:O	10:C:234:LEU:O	2.33	0.47
13:J:341:LEU:HD22	14:K:45:PRO:HB3	1.96	0.47
18:O:564:TYR:C	18:O:566:TYR:H	2.18	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
10:C:193:LEU:HD12	10:C:213:LEU:HB3	1.97	0.47
10:C:504:THR:HG23	10:C:574:SER:O	2.15	0.47
32:Q:465:ASP:C	32:Q:467:TYR:H	2.18	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
21:S:229:VAL:HG11	21:S:243:VAL:CG2	2.45	0.47
7:B:990:ASP:O	7:B:994:ASP:N	2.45	0.47
6:A:687:ILE:HD11	6:A:706:PRO:HG3	1.97	0.47
8:D:23:LEU:HG	11:G:18:GLN:HE22	1.80	0.47
13:J:144:CYS:SG	13:J:187:ASP:HA	2.55	0.47
21:S:225:ALA:O	21:S:228:THR:HG22	2.15	0.47
6:A:1345:TYR:O	6:A:1345:TYR:HD1	1.98	0.46
6:A:468:LEU:HD22	6:A:469:ILE:HG23	1.97	0.46
7:B:496:THR:O	7:B:497:THR:CB	2.63	0.46
14:K:104:LEU:HD12	14:K:113:GLU:HA	1.97	0.46
18:O:541:CYS:O	18:O:544:LEU:O	2.33	0.46
32:Q:401:VAL:O	32:Q:402:VAL:CB	2.62	0.46
21:S:193:VAL:HG11	21:S:202:TRP:CZ2	2.50	0.46
6:A:1417:GLN:CG	6:A:1418:THR:HG23	2.45	0.46
7:B:1105:ALA:O	7:B:1106:GLY:C	2.54	0.46
13:J:269:ILE:HA	13:J:285:SER:HA	1.97	0.46
6:A:876:PRO:HA	14:K:204:LEU:HD22	1.97	0.46
6:A:319:ARG:O	6:A:321:GLU:N	2.48	0.46
8:D:31:LEU:HD11	11:G:31:ARG:NH2	2.30	0.46
20:R:36:GLN:C	20:R:40:GLN:CB	2.82	0.46
10:C:312:ILE:HD13	10:C:435:LEU:HG	1.98	0.46
18:O:214:ASN:HB2	18:O:217:ILE:HD11	1.97	0.46
18:O:25:VAL:HG11	18:O:52:TRP:CH2	2.50	0.46
6:A:1881:THR:HG21	6:A:1920:LEU:CD2	2.46	0.46
13:J:144:CYS:SG	13:J:145:VAL:N	2.89	0.46
32:Q:706:THR:C	32:Q:708:LYS:N	2.69	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
7:B:781:LEU:O	7:B:785:ALA:N	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:369:TYR:CE1	12:H:420:ILE:HD11	2.51	0.46
12:H:465:PHE:CB	12:H:473:LEU:HD23	2.46	0.46
16:M:17:GLU:HB2	16: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
10:C:493:LEU:CD2	10:C:539:VAL:HG21	2.45	0.46
15:L:94:LYS:CD	15:L:109:ILE:HD11	2.45	0.46
5:V:32:U:O4	17:N:28:ILE:HG21	2.16	0.46
10:C:873:LEU:N	10:C:874:PRO:CD	2.79	0.46
10:C:928:CYS:SG	10:C:929:GLN:N	2.89	0.46
13:J:248:ILE:HG13	13:J:262:LEU:HD12	1.98	0.46
18:O:230:THR:HG21	21:S:117:HIS:CG	2.51	0.46
12:H:334:LEU:HD21	12:H:384:LEU:HD12	1.98	0.46
16:M:99:ILE:HD13	16:M:188:TYR:CD2	2.51	0.46
18:O:530:VAL:O	18:O:533:LEU:N	2.48	0.46
6:A:1020:ILE:HB	6:A:1022:PRO:HD2	1.98	0.45
6:A:1357:LEU:HD11	12:H:303:LEU:HD22	1.98	0.45
10:C:501:ILE:CD1	10: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
10:C:837:GLN:HA	10:C:837:GLN:HE21	1.81	0.45
12:H:351:ILE:HG21	12:H:395:GLU:HG3	1.98	0.45
13:J:144:CYS:SG	13:J:188:VAL:N	2.88	0.45
13:J:284:SER:OG	13: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:O	6:A:783:LEU:HD12	2.16	0.45
10:C:492:LEU:O	10:C:492:LEU:HD12	2.16	0.45
12:H:330:ILE:HG22	12:H:334:LEU:CD2	2.46	0.45
32:Q:435:PHE:CB	32:Q:874:ARG:C	2.85	0.45
21:S:169:TRP:CE3	21:S:192:TYR:HB2	2.51	0.45
6:A:1282:ASP:C	12: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
10:C:274:ILE:HG21	10:C:385:PHE:CD2	2.51	0.45
10:C:470:ALA:HB1	10:C:486:VAL:HG12	1.98	0.45
10:C:936:ILE:HG23	10:C:936:ILE:O	2.16	0.45
17:N:216:GLU:O	17:N:220:THR:HG23	2.17	0.45
6:A:1461:TYR:CE1	6:A:1494:LEU:HD13	2.51	0.45
7:B:1343:PHE:O	7:B:1345:PHE:N	2.49	0.45
12:H:312:LEU:CD1	12:H:329:ILE:HD11	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
13:J:229:THR:HG21	13:J:271:GLN:HA	1.98	0.45
4:Z:5:A:H2'	4:Z:6:U:O4'	2.16	0.45
13:J:161:ASP:O	13:J:162:THR:HB	2.17	0.45
21:S:202:TRP:CZ2	21:S:228:THR:HG21	2.52	0.45
6:A:1214:ARG:N	6:A:1255:ASN:OD1	2.50	0.45
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
10:C:862:TYR:CE2	10:C:908:VAL:HG13	2.51	0.45
16:M:81:CYS:SG	16: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
21:S:140:LEU:HD23	21: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
7:B:479:GLU:HA	7:B:498:SER:CA	2.46	0.44
17:N:16:CYS:HB2	17:N:71:CYS:SG	2.57	0.44
7:B:1382:LEU:O	7:B:1385:LEU:N	2.50	0.44
10:C:241:VAL:CG1	10:C:273:LEU:HD23	2.46	0.44
10:C:808:LEU:HD22	10:C:944:VAL:HG21	1.99	0.44
17:N:12:ILE:HG23	17: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
10:C:223:ASP:OD1	10:C:224:GLU:N	2.50	0.44
11:G:18:GLN:HG3	11:G:19:GLN:N	2.32	0.44
12:H:292:LYS:CD	12: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	10:C:336:ILE:HD11	2.52	0.44
6:A:719:ILE:HB	6:A:720:PRO:CD	2.47	0.44
10:C:444:GLN:N	10:C:445:PRO:CD	2.81	0.44
6:A:724:ARG:HD3	19:P:31:LEU:HD11	1.99	0.44
6:A:687:ILE:HD11	6:A:706:PRO:CG	2.48	0.44
10:C:905:GLN:NE2	10:C:936:ILE:HD13	2.32	0.44
13:J:248:ILE:HD13	13: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
10:C:708:ILE:N	10:C:708:ILE:HD12	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
16:M:114:ARG:NE	16:M:127:ILE:HG21	2.32	0.44
16:M:173:ILE:HG12	16:M:184:VAL:HG13	1.99	0.44
21:S:140:LEU:CD2	21:S:155:LEU:HD22	2.48	0.44
21:S:160:CYS:HB3	21: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
10:C:658:ASP:HB3	10:C:663:TYR:CE2	2.52	0.43
16:M:74:LEU:HA	16:M:112:PHE:CE1	2.53	0.43
17:N:125:ILE:HG21	17:N:135:ILE:CD1	2.45	0.43
6:A:2278:SER:O	6:A:2282:ALA:HB2	2.18	0.43
6:A:268:LEU:HD13	6:A:277:LYS:CB	2.47	0.43
13:J:156:ILE:HD11	13:J:188:VAL:HG21	2.00	0.43
13:J:277:VAL:HG13	13:J:279:PRO:HD2	2.00	0.43
13:J:129:TRP:HB2	13:J:385:GLN:HE22	1.83	0.43
21:S:229:VAL:HG22	21: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
10:C:862:TYR:CG	10:C:908:VAL:HG22	2.53	0.43
8:D:43:LEU:HD21	8:D:86:ILE:CD1	2.47	0.43
13:J:142:VAL:HG12	13:J:142:VAL:O	2.18	0.43
17:N:91:ILE:CD1	17:N:125:ILE:HD12	2.48	0.43
21:S:193:VAL:HG11	21:S:202:TRP:CH2	2.54	0.43
21:S:467:GLN:CB	21:S:471:LEU:CB	2.93	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
10:C:225:THR:HG21	10:C:252:LEU:CD2	2.48	0.43
17:N:67:GLN:HB3	17:N:120:LEU:HD23	2.00	0.43
14:K:35:ALA:CB	21:S:158:LYS:HE3	2.48	0.43
4:Z:34:G:H21	6:A:1325:SER:HG	1.59	0.43
10:C:335:SER:HB2	10:C:336:ILE:HD12	1.99	0.43
17:N:71:CYS:HB3	17:N:74:CYS:HB2	2.00	0.43
6:A:1085:LYS:O	6:A:1088:VAL:HG13	2.18	0.43
12:H:381:LEU:HD21	12: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
10:C:888:ILE:HG23	10:C:902:VAL:HG23	2.00	0.43
8:D:11:TYR:CE1	11:G:12:LEU:HD21	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:73:ILE:HG23	15:L:77:LEU:HD23	2.00	0.43
16:M:250:MET:SD	17:N:139:LEU:HD21	2.59	0.43
6:A:954:ILE:HG23	6:A:991:THR:HG23	2.00	0.43
16:M:247:LEU:HA	16:M:250:MET:HG2	1.99	0.43
18:O:211:ILE:O	21:S:83:ARG:NH2	2.52	0.43
6:A:136:PRO:HB3	6:A:562:ILE:HD13	2.01	0.43
10:C:905:GLN:HE22	10:C:936:ILE:HD13	1.84	0.43
10:C:94:VAL:HG12	13:J:154:TRP:CZ2	2.54	0.43
7:B:1163:SER:O	32:Q:367:GLN:CB	2.67	0.43
21:S:72:ALA:HB1	21: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
10:C:242:VAL:HG22	10:C:277:LEU:HD11	2.01	0.43
10:C:381:LEU:HA	10:C:384:ILE:HD12	1.99	0.43
10:C:78:MET:N	10:C:78:MET:SD	2.92	0.43
14:K:127:VAL:HG13	17:N:31:GLY:O	2.18	0.43
6:A:1737:GLN:HE21	6:A:1737:GLN:HA	1.84	0.42
6:A:305:LEU:HD22	10:C:390:SER:HA	2.01	0.42
10:C:861:ILE:HA	10:C:907:PRO:HA	2.01	0.42
6:A:785:HIS:CE1	14:K:168:ALA:HB2	2.54	0.42
18:O:211:ILE:HD12	21: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
7:B:1182:ALA:O	32:Q:496:ARG:CA	2.59	0.42
10:C:599:THR:HG23	10:C:599:THR:O	2.18	0.42
6:A:556:TYR:CG	14: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:2388:ARG:O	6:A:2389:PRO:C	2.57	0.42
6:A:852:LEU:HD23	6:A:978:ILE:HD11	2.01	0.42
10:C:104:THR:HG23	10:C:105:ILE:HG23	2.00	0.42
10:C:791:TYR:O	10:C:791:TYR:CG	2.72	0.42
11:G:51:LYS:O	11:G:54:VAL:HG12	2.19	0.42
13:J:200:VAL:HG22	13:J:227:VAL:HB	2.01	0.42
17:N:88:ASP:O	17:N:91:ILE:HG23	2.20	0.42
20:R:13:GLY:O	20:R:15:SER:N	2.52	0.42
18:O:211:ILE:CD1	21:S:48:ARG:HB2	2.49	0.42
1:U:74:U:O2	1:U:78:A:C2	2.72	0.42
10:C:710:VAL:HG22	10:C:820:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:119:THR:HG22	15:L:120:CYS:N	2.34	0.42
17:N:67:GLN:HA	17:N:119:LYS:HA	2.02	0.42
22:T:119:ALA:HB1	22: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:C	6:A:783:LEU:HD12	2.39	0.42
10:C:605:ILE:HD12	10: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	10:C:909:ILE:HG21	2.01	0.42
6:A:719:ILE:HB	6:A:720:PRO:HD2	2.01	0.42
10:C:470:ALA:HB2	10:C:488:ILE:HA	2.02	0.42
10:C:472:VAL:HG21	10:C:567:ILE:HG21	2.01	0.42
6:A:1357:LEU:HD11	12:H:303:LEU:CD2	2.49	0.42
1:U:23:C:O2	1:U:23:C:O4'	2.37	0.42
5:V:55:G:N7	18:O:35:LYS:HB3	2.35	0.42
6:A:1064:THR:HG22	18: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
13:J:114:ARG:HB3	14: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
17:N:259:GLY:O	17:N:263:VAL:HG23	2.20	0.42
14:K:120:ASP:OD2	14:K:123:LEU:HD13	2.20	0.42
16:M:249:MET:SD	17:N:86:LEU:HD13	2.60	0.42
18:O:564:TYR:CB	18:O:566:TYR:H	2.33	0.42
6:A:929:LEU:HD12	6:A:1589:LYS:CG	2.50	0.42
10:C:400:LEU:HD12	10:C:408:LEU:HD21	2.02	0.42
16:M:114:ARG:CD	16:M:127:ILE:HG21	2.50	0.42
18:O:22:LYS:HB2	18:O:56:LEU:HD12	2.02	0.42
20:R:32:PRO:HB3	20:R:35:SER:CB	2.50	0.42
5:V:36:U:O2	5:V:36:U:C2'	2.68	0.42
10:C:418:GLN:HB3	10:C:419:PRO:HD3	2.02	0.41
13:J:334:TRP:CD1	13:J:334:TRP:N	2.88	0.41
17:N:25:MET:HB3	17:N:46:PHE:HB3	2.01	0.41
17:N:16:CYS:CB	17:N:71:CYS:SG	3.08	0.41
6:A:756:LEU:CD1	19:P:12:ARG:HD3	2.50	0.41
21:S:140:LEU:HD21	21:S:155:LEU:HD22	2.01	0.41
10:C:225:THR:HG21	10:C:252:LEU:HD21	2.02	0.41
10:C:608:GLN:HE21	10:C:641:GLU:HG2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:276:PRO:HB2	14:K:63:ILE:HD12	2.02	0.41
16:M:247:LEU:HA	16:M:250:MET:CG	2.51	0.41
16:M:48:VAL:HG22	16:M:220:GLY:N	2.36	0.41
6:A:756:LEU:HD11	19:P:12:ARG:HD3	2.03	0.41
21:S:332:GLU:HA	21:S:334:PHE:CB	2.50	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	13:J:221:TYR:CD2	3.07	0.41
22:T:397:ASN:O	22:T:400:ALA:HB3	2.20	0.41
7:B:1610:LEU:O	7:B:1660:ALA:O	2.38	0.41
10:C:273:LEU:HA	10:C:277:LEU:HD12	2.02	0.41
10:C:621:ALA:CB	10:C:664:ALA:HB2	2.48	0.41
32:Q:916:ALA:HB3	32:Q:951:VAL:H	1.85	0.41
6:A:565:VAL:CG1	6:A:637:VAL:HG22	2.51	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
12:H:334:LEU:HD12	12:H:380:GLN:HB3	2.02	0.41
6:A:252:GLU:HA	6:A:255:ILE:HD12	2.02	0.41
12:H:330:ILE:HD12	12:H:387:PHE:HE2	1.86	0.41
32:Q:603:ILE:C	32:Q:605:ASP:H	2.24	0.41
6:A:1609:TRP:CE3	6:A:1823:LEU:HD13	2.56	0.41
10:C:314:ALA:CB	10:C:321:THR:HG22	2.50	0.41
12:H:292:LYS:HD3	12:H:328:ILE:HD11	2.01	0.41
16:M:156:ILE:HG21	16: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	10:C:318:LEU:HD21	2.20	0.41
17:N:82:ILE:HG22	17: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
10:C:287:LYS:HE3	10: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
10:C:152:LEU:HD11	10:C:319:GLY:HA2	2.02	0.40
10:C:632:VAL:HG12	10:C:634:ILE:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:390:LEU:N	10:C:653:ASP:OD1	2.54	0.40
10:C:677:PHE:HB3	10:C:857:LEU:HD22	2.03	0.40
21:S:189:TYR:O	21:S:192:TYR:HB3	2.21	0.40
6:A:1620:TYR:CD2	6:A:1621:VAL:HG13	2.56	0.40
10:C:223:ASP:O	10:C:227:VAL:HG23	2.21	0.40
10:C:749:LYS:O	10:C:753:THR:HG23	2.21	0.40
18:O:211:ILE:CD1	21: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
7:B:1795:SER:O	7:B:1796:PRO:C	2.60	0.40
1:U:45:A:OP1	10:C:108:GLN:O	2.40	0.40
10:C:234:LEU:HD13	10:C:439:ILE:HG23	2.03	0.40
10:C:264:CYS:SG	10:C:312:ILE:HD11	2.61	0.40
10:C:561:ILE:O	10:C:562:VAL:HG13	2.22	0.40
14:K:75:GLN:HA	14: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
7:B:833:THR:O	7:B:834:LEU:C	2.58	0.40
7:B:960:ILE:O	7:B:964:GLY:N	2.54	0.40
10:C:241:VAL:HG22	10:C:267:ILE:HG23	2.04	0.40
13:J:345:PHE:CE2	13:J:364:LEU:HD22	2.57	0.40
20:R:31:ARG:O	20:R:33:GLN:N	2.47	0.40
5:V:86:G:C2	21:S:57:TYR:CE2	3.10	0.40
4:Z:1102:C:C2'	4:Z:1102:C:O2	2.69	0.40
6:A:1054:LEU:HD13	6:A:1121:ILE:HG21	2.03	0.40
6:A:1491:ILE:HD13	6:A:1491:ILE:HA	1.97	0.40
13:J:198:PHE:CD1	13:J:239:ILE:HD13	2.57	0.40
13:J:321:PHE:CE1	13:J:336:LEU:CD2	3.05	0.40
16:M:109:LEU:HA	16:M:116:LYS:HG2	2.03	0.40
17:N:84:ILE:O	17:N:87:ARG:HG3	2.21	0.40
18:O:148:GLU:O	18:O:152:LEU:HD23	2.21	0.40
18:O:211:ILE:HD12	21: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	2160/2413 (90%)	1997 (92%)	152 (7%)	11 (0%)	34	77
7	B	1704/2163 (79%)	1585 (93%)	111 (6%)	8 (0%)	34	77
8	D	112/278 (40%)	93 (83%)	17 (15%)	2 (2%)	11	55
9	F	44/179 (25%)	41 (93%)	3 (7%)	0	100	100
10	C	872/1008 (86%)	777 (89%)	82 (9%)	13 (2%)	13	59
11	G	95/235 (40%)	89 (94%)	5 (5%)	1 (1%)	17	65
12	H	389/591 (66%)	362 (93%)	23 (6%)	4 (1%)	19	66
13	J	322/451 (71%)	263 (82%)	47 (15%)	12 (4%)	4	40
14	K	155/379 (41%)	146 (94%)	8 (5%)	1 (1%)	30	74
15	L	153/157 (98%)	136 (89%)	15 (10%)	2 (1%)	15	61
16	M	250/339 (74%)	228 (91%)	19 (8%)	3 (1%)	16	63
17	N	195/364 (54%)	178 (91%)	14 (7%)	3 (2%)	13	59
18	O	277/590 (47%)	248 (90%)	24 (9%)	5 (2%)	11	55
19	P	34/175 (19%)	28 (82%)	5 (15%)	1 (3%)	6	46
20	R	93/135 (69%)	81 (87%)	11 (12%)	1 (1%)	17	65
21	S	432/687 (63%)	416 (96%)	14 (3%)	2 (0%)	34	77
22	T	536/859 (62%)	506 (94%)	21 (4%)	9 (2%)	11	56
23	b	76/196 (39%)	70 (92%)	6 (8%)	0	100	100
23	k	76/196 (39%)	65 (86%)	9 (12%)	2 (3%)	7	48
24	d	80/101 (79%)	72 (90%)	7 (9%)	1 (1%)	15	61
24	n	80/101 (79%)	66 (82%)	14 (18%)	0	100	100
25	e	71/94 (76%)	68 (96%)	3 (4%)	0	100	100
25	p	71/94 (76%)	63 (89%)	7 (10%)	1 (1%)	14	59
26	f	70/86 (81%)	66 (94%)	3 (4%)	1 (1%)	14	59
26	q	70/86 (81%)	61 (87%)	9 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	g	65/77 (84%)	64 (98%)	1 (2%)	0	100	100
27	r	65/77 (84%)	55 (85%)	9 (14%)	1 (2%)	13	59
28	h	78/146 (53%)	74 (95%)	4 (5%)	0	100	100
28	l	75/146 (51%)	63 (84%)	10 (13%)	2 (3%)	6	48
29	j	92/110 (84%)	87 (95%)	5 (5%)	0	100	100
29	m	92/110 (84%)	84 (91%)	8 (9%)	0	100	100
30	W	160/238 (67%)	117 (73%)	35 (22%)	8 (5%)	3	31
31	Y	82/111 (74%)	77 (94%)	5 (6%)	0	100	100
32	Q	609/1071 (57%)	486 (80%)	73 (12%)	50 (8%)	1	18
33	t	426/503 (85%)	417 (98%)	9 (2%)	0	100	100
33	u	425/503 (84%)	413 (97%)	12 (3%)	0	100	100
33	v	412/503 (82%)	403 (98%)	6 (2%)	3 (1%)	26	72
33	w	423/503 (84%)	414 (98%)	7 (2%)	2 (0%)	34	77
34	s	106/175 (61%)	92 (87%)	8 (8%)	6 (6%)	2	28
All	All	11527/16230 (71%)	10551 (92%)	821 (7%)	155 (1%)	20	61

All (155) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	A	320	ASP
6	A	737	ARG
7	B	766	ILE
12	H	414	PRO
16	M	127	ILE
17	N	120	LEU
20	R	14	SER
22	T	421	ALA
22	T	477	PRO
22	T	481	ILE
22	T	616	PRO
30	W	76	ILE
28	l	98	PRO
27	r	68	ILE
32	Q	370	VAL
32	Q	380	THR
32	Q	399	SER
32	Q	400	ILE

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Mol	Chain	Res	Type
32	Q	401	VAL
32	Q	440	ASP
32	Q	443	CYS
32	Q	466	LYS
32	Q	470	VAL
32	Q	471	ILE
32	Q	478	ARG
32	Q	502	ILE
32	Q	503	ILE
32	Q	546	GLU
32	Q	653	VAL
32	Q	654	ILE
32	Q	655	ASP
32	Q	707	PHE
32	Q	737	THR
32	Q	748	LYS
32	Q	749	PRO
32	Q	799	ASN
32	Q	836	PHE
32	Q	917	LYS
32	Q	925	VAL
32	Q	948	PRO
34	s	94	LYS
34	s	111	VAL
34	s	133	PRO
6	A	588	LEU
6	A	1424	HIS
6	A	1639	PRO
6	A	1763	ASN
7	B	1693	HIS
10	C	76	VAL
10	C	172	TRP
10	C	269	LYS
10	C	432	GLN
10	C	535	PRO
10	C	901	GLU
12	H	469	GLY
13	J	162	THR
13	J	245	ASP
13	J	277	VAL
13	J	328	THR
16	M	23	PRO

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Mol	Chain	Res	Type
18	O	81	PRO
19	P	9	LEU
30	W	122	ARG
23	k	81	VAL
32	Q	369	VAL
32	Q	374	GLU
32	Q	395	ASP
32	Q	856	ASN
32	Q	857	PHE
32	Q	894	ILE
32	Q	896	SER
32	Q	942	HIS
33	v	109	LEU
34	s	105	PRO
34	s	136	VAL
6	A	1593	ALA
7	B	492	PRO
7	B	1936	ARG
8	D	76	LEU
10	C	574	SER
12	H	445	LEU
13	J	442	TRP
15	L	38	SER
17	N	30	GLN
17	N	54	ASN
18	O	214	ASN
18	O	546	HIS
21	S	238	TRP
30	W	95	PRO
28	l	25	VAL
32	Q	451	ASP
32	Q	604	ASN
32	Q	644	SER
32	Q	746	ILE
32	Q	824	ARG
32	Q	929	THR
32	Q	944	LEU
33	v	20	ARG
6	A	660	ILE
7	B	1555	GLU
7	B	1968	ASN
18	O	206	LYS

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Mol	Chain	Res	Type
21	S	112	VAL
22	T	479	PRO
22	T	615	PHE
30	W	68	PRO
30	W	94	LEU
30	W	129	LEU
23	k	6	VAL
32	Q	504	THR
32	Q	738	ASP
32	Q	839	LYS
32	Q	927	LEU
33	w	20	ARG
34	s	119	SER
6	A	457	ASP
6	A	1491	ILE
8	D	34	MET
10	C	100	LEU
10	C	459	PRO
11	G	41	VAL
13	J	310	SER
13	J	444	PRO
16	M	4	TRP
18	O	216	ASP
22	T	443	PRO
32	Q	541	VAL
32	Q	704	GLU
32	Q	708	LYS
33	w	17	PRO
7	B	622	LEU
10	C	137	GLY
10	C	807	PRO
12	H	303	LEU
13	J	226	GLY
22	T	391	LEU
32	Q	821	PRO
13	J	137	GLY
32	Q	750	PRO
7	B	791	PRO
10	C	185	ILE
10	C	301	GLY
13	J	279	PRO
14	K	146	VAL

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Mol	Chain	Res	Type
15	L	117	GLY
26	f	15	PRO
25	p	74	GLY
13	J	443	ASN
22	T	37	ILE
30	W	56	ILE
30	W	98	VAL
33	v	36	GLY
6	A	774	ILE
13	J	272	VAL
24	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%)	18	59
8	D	100/256 (39%)	91 (91%)	9 (9%)	12	49
9	F	26/163 (16%)	25 (96%)	1 (4%)	40	76
10	C	722/910 (79%)	659 (91%)	63 (9%)	13	50
11	G	89/216 (41%)	81 (91%)	8 (9%)	12	49
12	H	185/552 (34%)	164 (89%)	21 (11%)	7	37
13	J	283/397 (71%)	250 (88%)	33 (12%)	7	36
14	K	143/328 (44%)	115 (80%)	28 (20%)	1	13
15	L	138/141 (98%)	129 (94%)	9 (6%)	21	62
16	M	213/296 (72%)	189 (89%)	24 (11%)	7	38
17	N	194/332 (58%)	175 (90%)	19 (10%)	10	44
18	O	174/525 (33%)	152 (87%)	22 (13%)	5	32
19	P	26/152 (17%)	21 (81%)	5 (19%)	2	13
20	R	23/121 (19%)	19 (83%)	4 (17%)	2	18
21	S	208/633 (33%)	181 (87%)	27 (13%)	5	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	b	70/176 (40%)	70 (100%)	0	100	100
24	d	69/89 (78%)	66 (96%)	3 (4%)	35	74
25	e	65/83 (78%)	60 (92%)	5 (8%)	16	56
26	f	63/77 (82%)	61 (97%)	2 (3%)	46	79
27	g	58/66 (88%)	57 (98%)	1 (2%)	68	89
28	h	77/129 (60%)	77 (100%)	0	100	100
29	j	79/103 (77%)	76 (96%)	3 (4%)	40	76
All	All	4706/7927 (59%)	4298 (91%)	408 (9%)	17	50

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
8	D	3	GLU
8	D	8	ASN
8	D	25	ARG
8	D	47	PHE
8	D	49	MET
8	D	71	LEU
8	D	79	ILE
8	D	99	THR
8	D	114	ARG
9	F	20	ARG
10	C	92	GLU
10	C	100	LEU
10	C	103	HIS
10	C	109	LEU
10	C	124	LEU
10	C	132	ARG
10	C	139	ILE
10	C	153	LEU
10	C	156	ASP
10	C	206	LYS
10	C	211	ASN
10	C	219	VAL
10	C	233	ASP
10	C	234	LEU
10	C	255	GLN
10	C	272	ARG
10	C	273	LEU
10	C	283	ASP
10	C	315	SER
10	C	347	ARG
10	C	358	ASN
10	C	359	PHE
10	C	362	LYS

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Mol	Chain	Res	Type
10	C	381	LEU
10	C	400	LEU
10	C	401	ARG
10	C	431	GLN
10	C	447	GLU
10	C	453	THR
10	C	458	ILE
10	C	468	LEU
10	C	469	TRP
10	C	471	HIS
10	C	474	LYS
10	C	475	THR
10	C	534	THR
10	C	545	LEU
10	C	562	VAL
10	C	576	THR
10	C	590	LYS
10	C	602	VAL
10	C	610	LEU
10	C	673	PRO
10	C	758	ASP
10	C	768	PHE
10	C	774	LEU
10	C	784	SER
10	C	791	TYR
10	C	794	GLN
10	C	799	PHE
10	C	803	VAL
10	C	830	ASN
10	C	837	GLN
10	C	851	LEU
10	C	861	ILE
10	C	902	VAL
10	C	927	MET
10	C	933	TRP
10	C	965	ASP
10	C	970	THR
10	C	971	ARG
10	C	989	LEU
10	C	992	TYR
11	G	4	ASN
11	G	18	GLN

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Mol	Chain	Res	Type
11	G	28	ASP
11	G	31	ARG
11	G	33	GLN
11	G	74	GLN
11	G	78	LEU
11	G	94	TRP
12	H	256	ASP
12	H	297	LEU
12	H	307	GLU
12	H	313	LEU
12	H	314	LYS
12	H	334	LEU
12	H	348	GLU
12	H	357	TRP
12	H	363	GLU
12	H	367	GLN
12	H	373	ILE
12	H	391	LEU
12	H	396	PHE
12	H	399	MET
12	H	419	PHE
12	H	421	LYS
12	H	440	LEU
12	H	444	LYS
12	H	468	ILE
12	H	470	LEU
12	H	473	LEU
13	J	139	LEU
13	J	143	ARG
13	J	148	ASP
13	J	151	ASP
13	J	156	ILE
13	J	161	ASP
13	J	183	MET
13	J	194	HIS
13	J	202	GLU
13	J	215	GLN
13	J	218	ARG
13	J	224	LEU
13	J	247	VAL
13	J	248	ILE
13	J	257	ILE

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Mol	Chain	Res	Type
13	J	269	ILE
13	J	274	CYS
13	J	275	THR
13	J	284	SER
13	J	286	THR
13	J	290	VAL
13	J	295	VAL
13	J	314	THR
13	J	329	ASP
13	J	332	ARG
13	J	334	TRP
13	J	336	LEU
13	J	356	LEU
13	J	377	ASP
13	J	387	LEU
13	J	389	THR
13	J	396	LEU
13	J	402	VAL
14	K	33	GLN
14	K	36	LYS
14	K	40	LEU
14	K	47	ARG
14	K	48	GLN
14	K	52	GLU
14	K	62	GLU
14	K	66	CYS
14	K	77	LEU
14	K	81	LYS
14	K	87	ASN
14	K	105	LEU
14	K	106	LEU
14	K	111	HIS
14	K	112	ILE
14	K	132	ARG
14	K	147	LEU
14	K	172	TRP
14	K	178	TYR
14	K	182	LEU
14	K	183	GLU
14	K	197	ILE
14	K	202	MET
14	K	203	LYS

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Mol	Chain	Res	Type
14	K	204	LEU
14	K	213	LYS
14	K	217	GLN
14	K	218	GLU
15	L	3	ARG
15	L	37	LYS
15	L	54	GLN
15	L	59	ARG
15	L	61	ARG
15	L	85	LYS
15	L	123	ARG
15	L	139	GLN
15	L	142	PHE
16	M	5	ARG
16	M	10	LYS
16	M	18	LEU
16	M	26	THR
16	M	33	TRP
16	M	38	SER
16	M	44	ASN
16	M	109	LEU
16	M	111	CYS
16	M	114	ARG
16	M	116	LYS
16	M	127	ILE
16	M	132	LYS
16	M	135	LYS
16	M	136	THR
16	M	149	LYS
16	M	172	ARG
16	M	181	CYS
16	M	187	LYS
16	M	191	ASN
16	M	216	ARG
16	M	236	LYS
16	M	245	GLU
16	M	251	VAL
17	N	19	ASP
17	N	22	ASN
17	N	30	GLN
17	N	32	SER
17	N	35	LYS

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Mol	Chain	Res	Type
17	N	39	LEU
17	N	48	THR
17	N	54	ASN
17	N	55	ILE
17	N	87	ARG
17	N	91	ILE
17	N	93	LEU
17	N	94	VAL
17	N	109	MET
17	N	117	ASN
17	N	135	ILE
17	N	216	GLU
17	N	254	GLN
17	N	321	GLN
18	O	27	LYS
18	O	35	LYS
18	O	40	LEU
18	O	44	THR
18	O	46	ARG
18	O	53	ASN
18	O	65	PHE
18	O	73	LEU
18	O	91	MET
18	O	93	ARG
18	O	156	ARG
18	O	158	ARG
18	O	170	LYS
18	O	175	MET
18	O	184	GLU
18	O	188	ARG
18	O	192	LYS
18	O	196	ILE
18	O	204	LYS
18	O	205	LYS
18	O	206	LYS
18	O	247	LYS
19	P	8	GLN
19	P	9	LEU
19	P	16	LYS
19	P	29	ARG
19	P	40	ARG
20	R	6	ILE

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Mol	Chain	Res	Type
20	R	8	LEU
20	R	15	SER
20	R	16	THR
21	S	60	ARG
21	S	67	GLN
21	S	71	TYR
21	S	77	GLU
21	S	78	GLN
21	S	86	SER
21	S	92	LEU
21	S	117	HIS
21	S	139	TYR
21	S	143	GLU
21	S	144	GLU
21	S	152	VAL
21	S	156	TYR
21	S	158	LYS
21	S	173	VAL
21	S	188	ILE
21	S	189	TYR
21	S	192	TYR
21	S	209	GLU
21	S	216	GLU
21	S	224	LEU
21	S	226	ILE
21	S	234	ASN
21	S	257	GLN
21	S	260	TYR
21	S	263	SER
21	S	266	LEU
24	d	10	LEU
24	d	20	SER
24	d	76	ASP
25	e	16	CYS
25	e	18	PHE
25	e	25	THR
25	e	79	LYS
25	e	81	LEU
26	f	36	THR
26	f	79	LEU
27	g	18	ASN
29	j	24	PHE

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Mol	Chain	Res	Type
29	j	49	ARG
29	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
6	A	1603	ASN
6	A	1737	GLN
6	A	2018	ASN
10	C	158	HIS
10	C	260	ASN
10	C	289	ASN
10	C	358	ASN
10	C	418	GLN
10	C	608	GLN
10	C	776	ASN
10	C	837	GLN
11	G	9	ASN
11	G	33	GLN
13	J	273	GLN
14	K	33	GLN
14	K	174	ASN
14	K	210	ASN
16	M	25	GLN
16	M	44	ASN
17	N	22	ASN
18	O	82	ASN
21	S	61	ASN

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Mol	Chain	Res	Type
21	S	78	GLN
21	S	79	HIS
21	S	200	GLN
21	S	214	ASN
21	S	234	ASN
21	S	236	GLN
24	d	41	ASN
25	e	15	ASN
25	e	34	GLN
26	f	24	ASN
27	g	18	ASN
27	g	66	ASN
28	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%)
3	I	31/76 (40%)	15 (48%)	0
4	Z	162/1175 (13%)	58 (35%)	11 (6%)
5	V	96/112 (85%)	35 (36%)	6 (6%)
All	All	442/1558 (28%)	184 (41%)	32 (7%)

All (184) 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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
5	V	93	A
5	V	99	A

All (32) 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
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	V	92	C

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 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$
38	GTP	C	1101	-	26,34,34	1.00	2 (7%)	29,54,54	1.91	5 (17%)

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
38	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)
38	C	1101	GTP	C5-C4	2.50	1.46	1.40
38	C	1101	GTP	C6-C5	3.09	1.47	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	C	1101	GTP	C1'-N9-C4	-4.67	121.59	126.81
38	C	1101	GTP	N3-C2-N1	-3.74	122.47	127.56
38	C	1101	GTP	C6-C5-C4	-3.43	116.94	120.86
38	C	1101	GTP	C5-C6-N1	-3.42	119.06	123.52
38	C	1101	GTP	C6-N1-C2	4.91	121.63	115.88

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

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
35	x	4

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