



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 12:15 AM UTC

PDB ID : 6ICZ / pdb_00006icz
EMDB ID : EMD-9645
Title : Cryo-EM structure of a human post-catalytic spliceosome (P complex) at 3.0 angstrom
Authors : Zhang, X.; Zhan, X.; Yan, C.; Shi, Y.
Deposited on : 2018-09-07
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

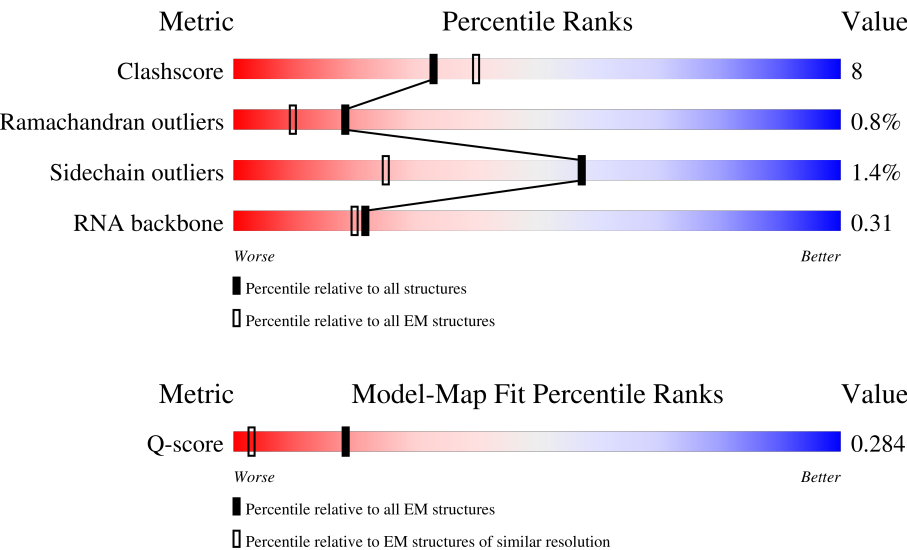
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.00 Å.

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



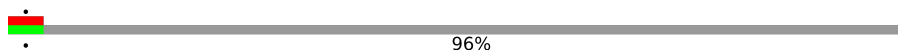
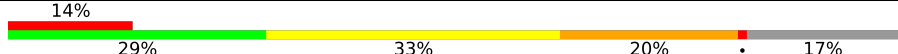
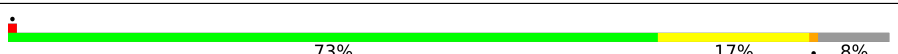
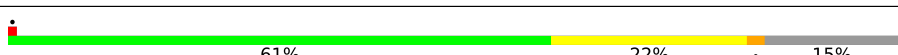
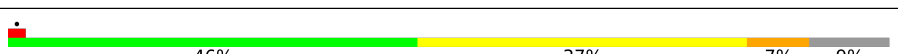
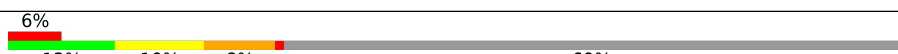
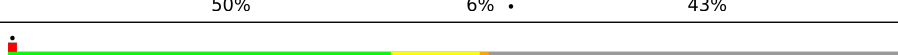
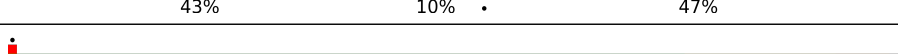
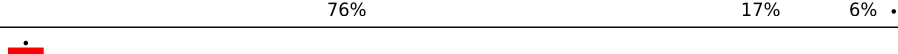
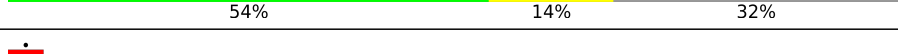
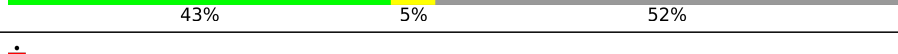
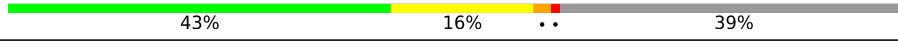
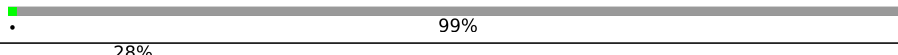
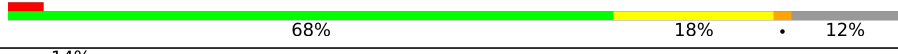
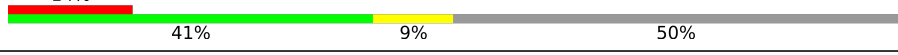
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 (2.50 - 3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	v	148	97% 91%6%
2	w	174	52% 47%5%48%
3	u	411	94% 89%5%6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	x	703	
5	A	2335	
6	B	117	
7	C	972	
8	E	357	
9	F	107	
10	G	273	
11	H	188	
12	J	848	
13	L	802	
14	M	243	
15	N	144	
16	O	420	
17	P	229	
18	R	536	
19	S	166	
20	T	514	
21	U	2752	
22	V	908	
23	W	579	
24	X	184	
25	Z	586	
26	I	855	
27	y	301	
28	Q	1485	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	a	126	
29	h	126	
30	b	231	
30	i	231	
31	c	119	
31	j	119	
32	d	118	
32	k	118	
33	f	86	
33	m	86	
34	e	92	
34	l	92	
35	g	76	
35	n	76	
36	o	255	
37	p	225	
38	Y	1220	
39	K	225	
40	q	504	
40	r	504	
40	s	504	
40	t	504	
41	D	2136	

2 Entry composition

There are 46 unique types of molecules in this entry. The entry contains 97900 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 protein called Protein mago nashi homolog 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	v	144	Total	C	N	O	0	0
			711	423	144	144		

- Molecule 2 is a protein called RNA-binding protein 8A.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	w	91	Total	C	N	O	0	0
			445	263	91	91		

- Molecule 3 is a protein called Eukaryotic initiation factor 4A-III.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	u	386	Total	C	N	O	0	0
			1907	1135	386	386		

- Molecule 4 is a protein called Protein CASC3.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	x	25	Total	C	N	O	0	0
			124	74	25	25		

- Molecule 5 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	2253	Total	C	N	O	S	0	0
			17837	11432	3157	3177	71		

- Molecule 6 is a RNA chain called U5snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	97	Total	C	N	O	P	0	0
			2040	914	339	690	97		

- Molecule 7 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	894	Total	C	N	O	S	0	0
			7066	4520	1178	1334	34		

- Molecule 8 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	303	Total	C	N	O	S	0	0
			2366	1487	415	451	13		

- Molecule 9 is a RNA chain called U6snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	97	Total	C	N	O	P	0	0
			2075	928	381	669	97		

- Molecule 10 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	84	Total	C	N	O	P	0	0
			1549	684	218	563	84		

- Molecule 11 is a RNA chain called U2snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	140	Total	C	N	O	P	0	0
			2966	1326	510	990	140		

- Molecule 12 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	571	Total	C	N	O	S	0	0
			3829	2385	720	718	6		

- Molecule 13 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	454	Total	C	N	O	S	0	0
			3064	1884	596	578	6		

- Molecule 14 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	130	Total	C	N	O	S	0	0
			1098	684	204	208	2		

- Molecule 15 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	143	Total	C	N	O	S	0	0
			1184	746	217	209	12		

- Molecule 16 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	285	Total	C	N	O	S	0	0
			2296	1442	408	426	20		

- Molecule 17 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	110	Total	C	N	O	S	0	0
			929	569	182	176	2		

- Molecule 18 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	261	Total	C	N	O	P S	0	0
			2073	1300	373	386	2 12		

- Molecule 19 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	159	Total	C	N	O	S	0	0
			1236	787	215	227	7		

- Molecule 20 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	313	Total	C	N	O	S	0	0
			2461	1554	447	452	8		

- Molecule 21 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	26	Total	C	N	O	S	0	0
			193	120	36	36	1		

- Molecule 22 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	452	Total	C	N	O	S	0	0
			2765	1723	508	523	11		

- Molecule 23 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	508	Total	C	N	O	S	0	0
			4122	2623	714	761	24		

- Molecule 24 is a protein called PRKR-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	92	Total	C	N	O	S	0	0
			701	432	133	132	4		

- Molecule 25 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	242	Total	C	N	O	S	0	0
			1999	1260	357	374	8		

- Molecule 26 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	I	564	Total	C	N	O	0	0
			2782	1654	564	564		

- Molecule 27 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	y	79	Total	C	N	O	0	0
			390	232	79	79		

- Molecule 28 is a protein called RNA helicase aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	Q	1322	Total	C	N	O	4	0
			6562	3918	1322	1322		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	h	81	Total	C	N	O	0	0
			398	236	81	81		
29	a	81	Total	C	N	O	0	0
			399	237	81	81		

- Molecule 30 is a protein called Small nuclear ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	i	86	Total	C	N	O	0	0
			424	252	86	86		
30	b	86	Total	C	N	O	0	0
			424	252	86	86		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	j	82	Total	C	N	O	0	0
			406	242	82	82		
31	c	82	Total	C	N	O	0	0
			406	242	82	82		

- Molecule 32 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	k	85	Total	C	N	O	0	0
			422	252	85	85		
32	d	97	Total	C	N	O	0	0
			480	286	97	97		

- Molecule 33 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	m	73	Total	C	N	O	0	0
			356	210	73	73		
33	f	74	Total	C	N	O	0	0
			361	213	74	74		

- Molecule 34 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	l	79	Total	C	N	O	0	0
			391	233	79	79		
34	e	79	Total	C	N	O	0	0
			391	233	79	79		

- Molecule 35 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	n	69	Total	C	N	O	0	0
			339	201	69	69		
35	g	74	Total	C	N	O	0	0
			363	215	74	74		

- Molecule 36 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	o	162	Total	C	N	O	0	0
			804	480	162	162		

- Molecule 37 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	p	94	Total	C	N	O	0	0
			464	276	94	94		

- Molecule 38 is a protein called ATP-dependent RNA helicase DHX8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Y	713	Total	C	N	O	S	0	0
			2917	1486	716	714	1		

- Molecule 39 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	K	152	Total	C	N	O	0	0
			757	453	152	152		

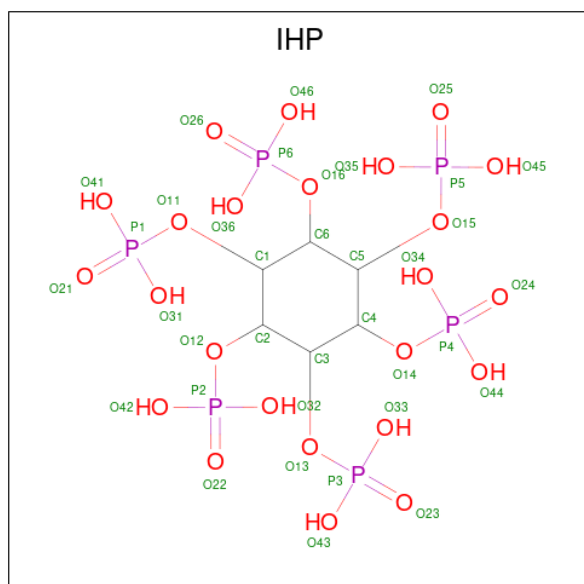
- Molecule 40 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	q	132	Total	C	N	O	0	0
			659	395	132	132		
40	r	131	Total	C	N	O	0	0
			654	392	131	131		
40	s	67	Total	C	N	O	0	0
			335	201	67	67		
40	t	67	Total	C	N	O	0	0
			335	201	67	67		

- Molecule 41 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

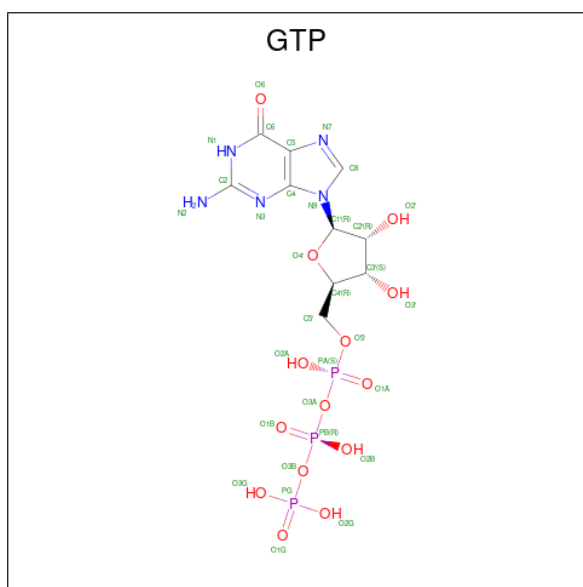
Mol	Chain	Residues	Atoms				AltConf	Trace
41	D	1722	Total	C	N	O	0	0
			8530	5086	1722	1722		

- Molecule 42 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms				AltConf
42	A	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 43 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

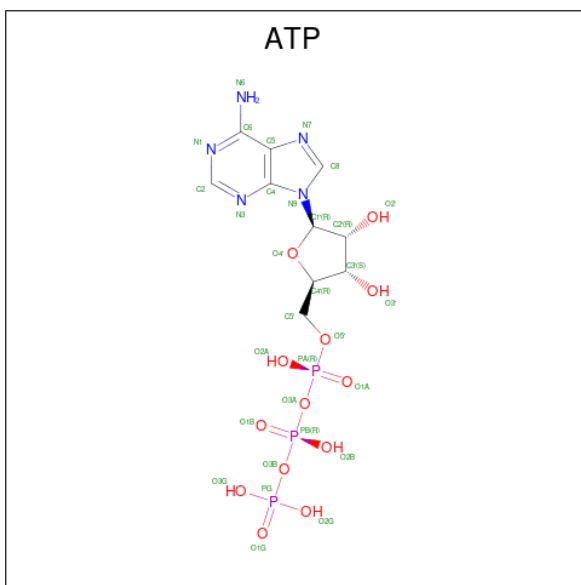
- Molecule 44 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
44	C	1	Total	Mg	0
			1	1	
44	F	6	Total	Mg	0
			6	6	
44	Q	2	Total	Mg	0
			2	2	

- Molecule 45 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
45	N	3	Total	Zn	0
			3	3	
45	O	3	Total	Zn	0
			3	3	
45	Z	1	Total	Zn	0
			1	1	

- Molecule 46 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

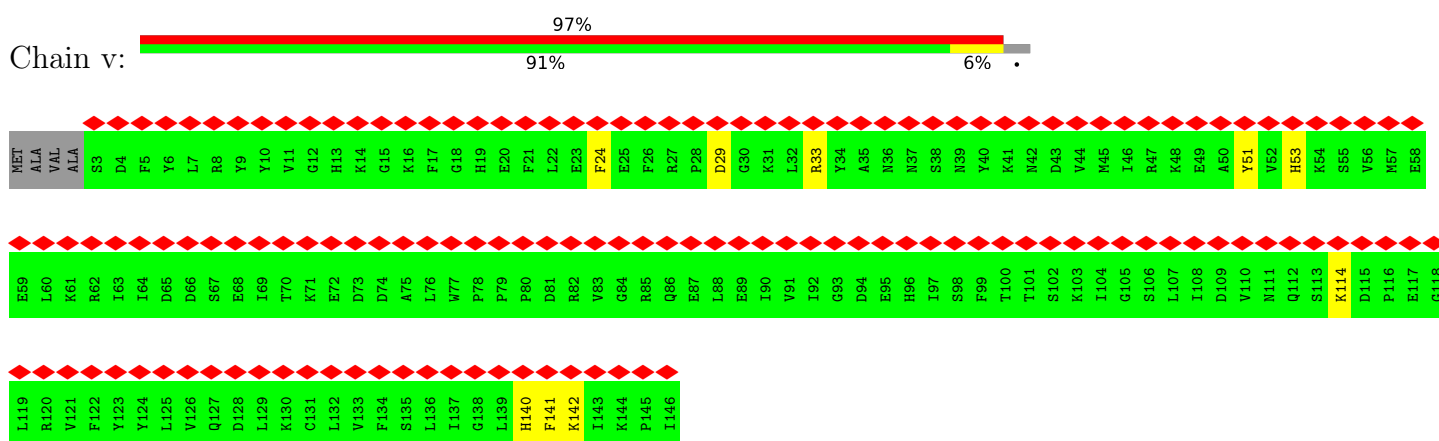


Mol	Chain	Residues	Atoms					AltConf
46	Q	1	Total 31	C 10	N 5	O 13	P 3	0

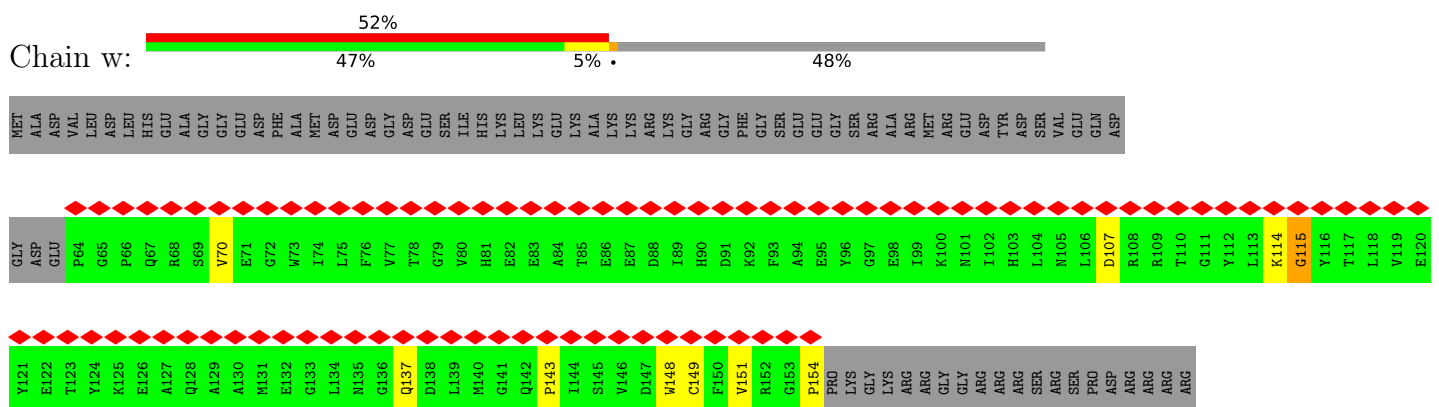
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Protein mago nashi homolog 2



• Molecule 2: RNA-binding protein 8A



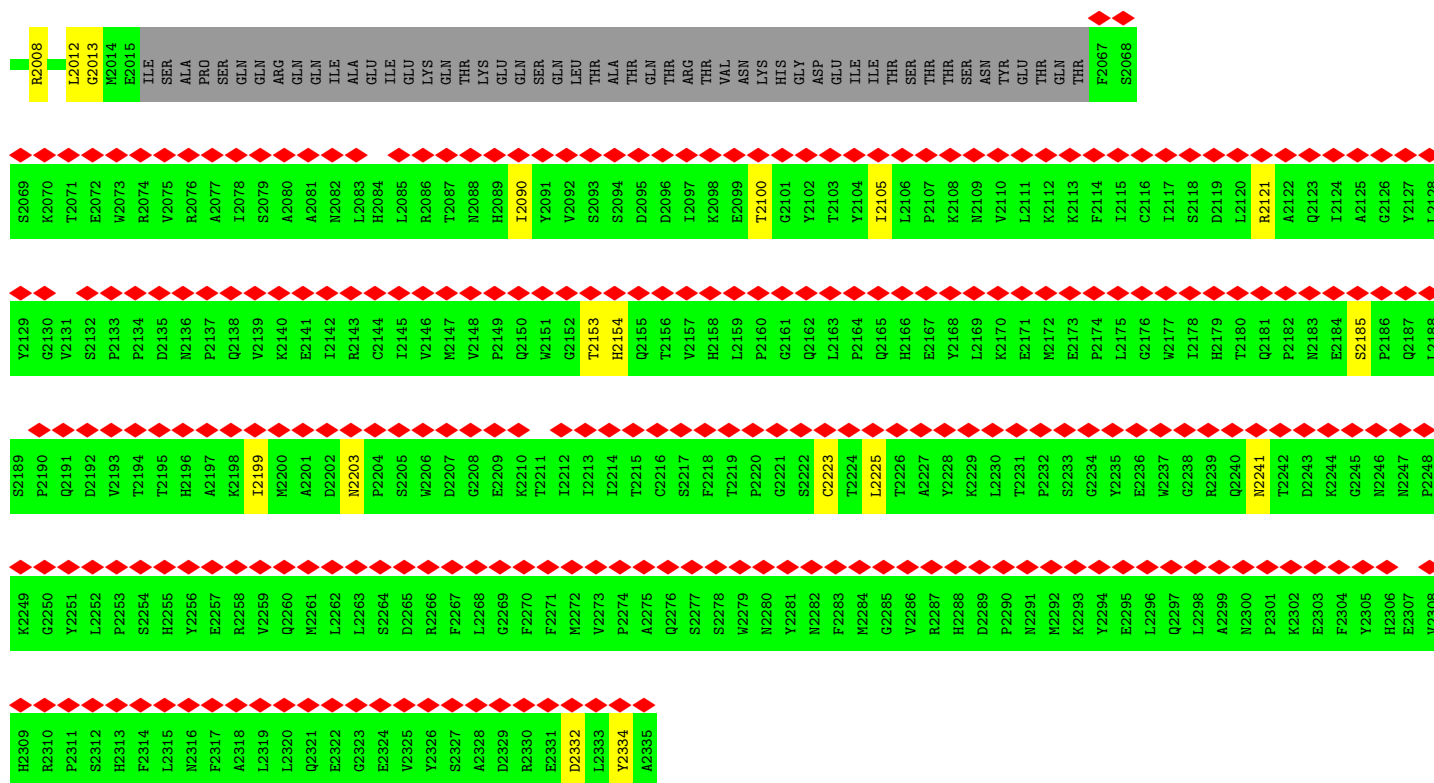


WORLD WIDE
PDB
PROTEIN DATA BANK

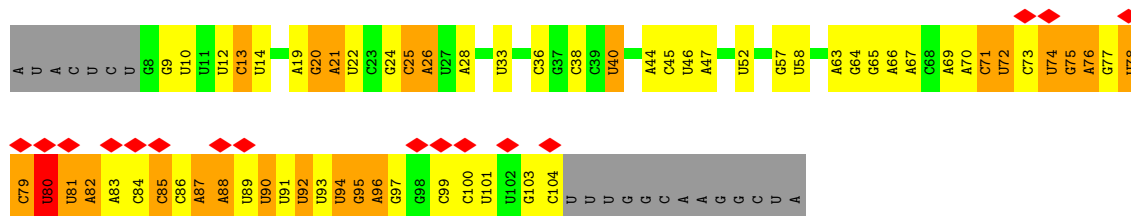
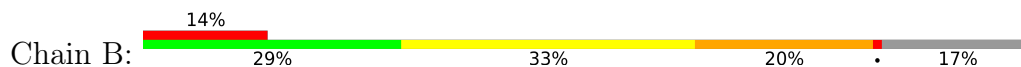
TYR	GLY	GLY	VAL	THR	TYR	ASN	ALA	GLN	GLN	GLN	VAL	GLN	PRO	LYS	PRO	SER	PRO	PRO	ARG	ARG	THR	PRO	GLN	PRO	VAL	THR	ILE	LYS	PRO	PRO	PRO	GLU	VAL	VAL	SER	ARG	GLY	SER	SER
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

Chain A: 12% 81% 15%

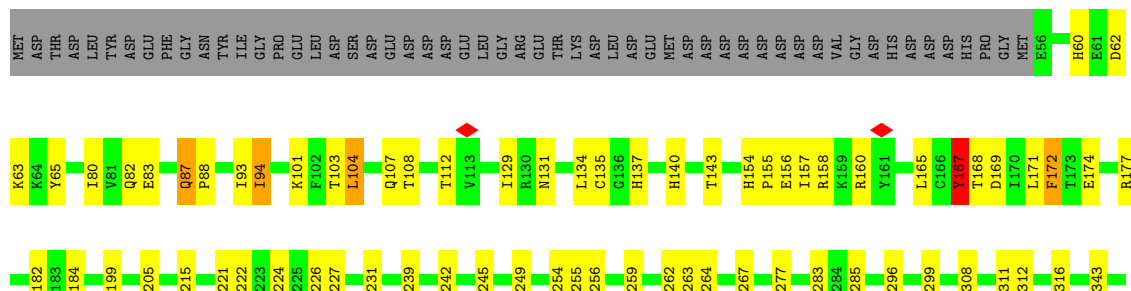




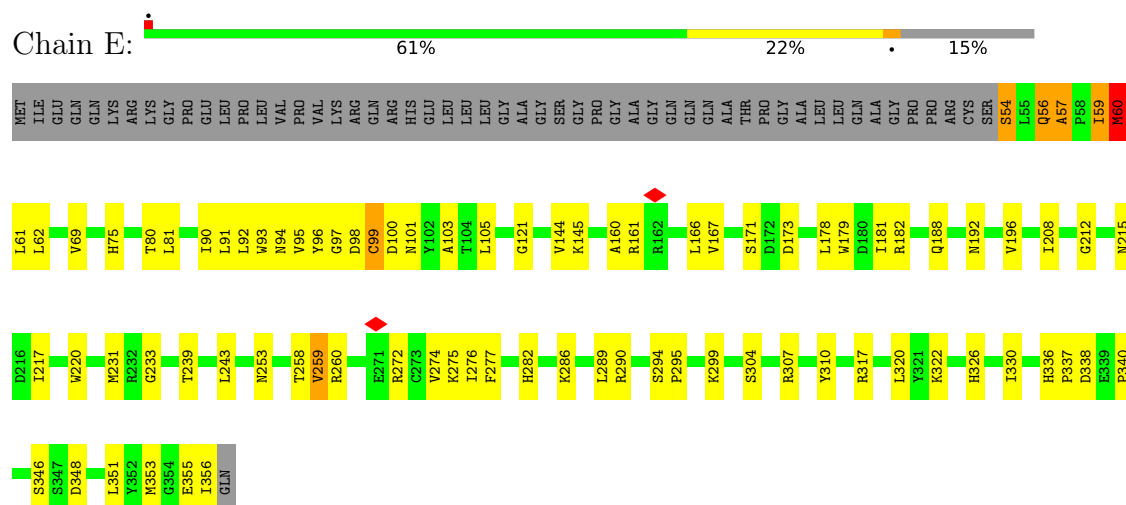
• Molecule 6: U5snRNA



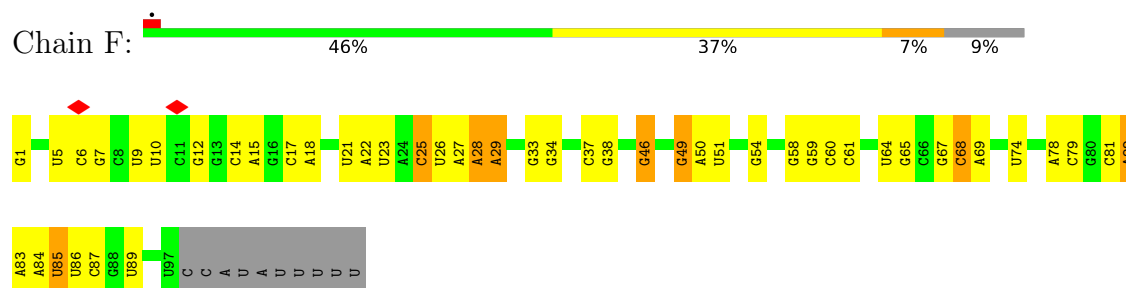
• Molecule 7: 116 kDa U5 small nuclear ribonucleoprotein component



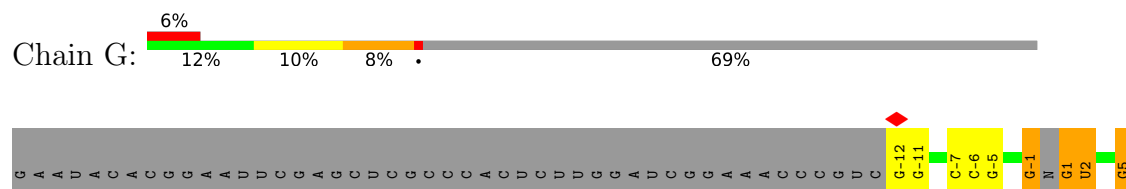
- Molecule 8: U5 small nuclear ribonucleoprotein 40 kDa protein.



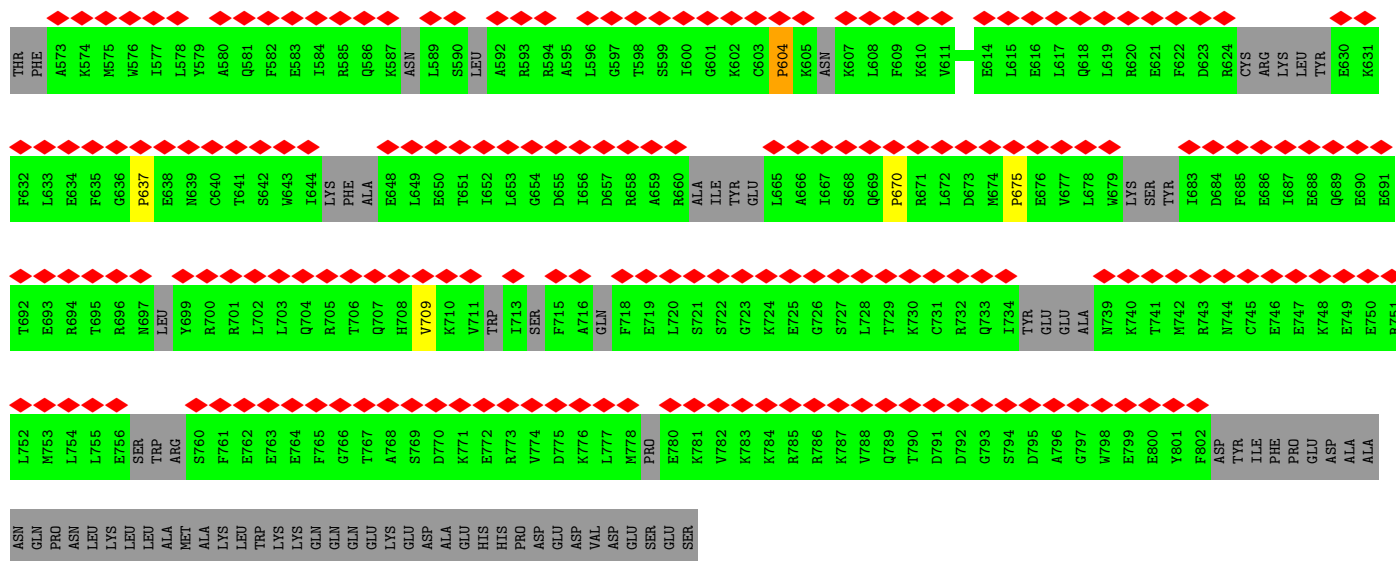
- Molecule 9: U6snRNA



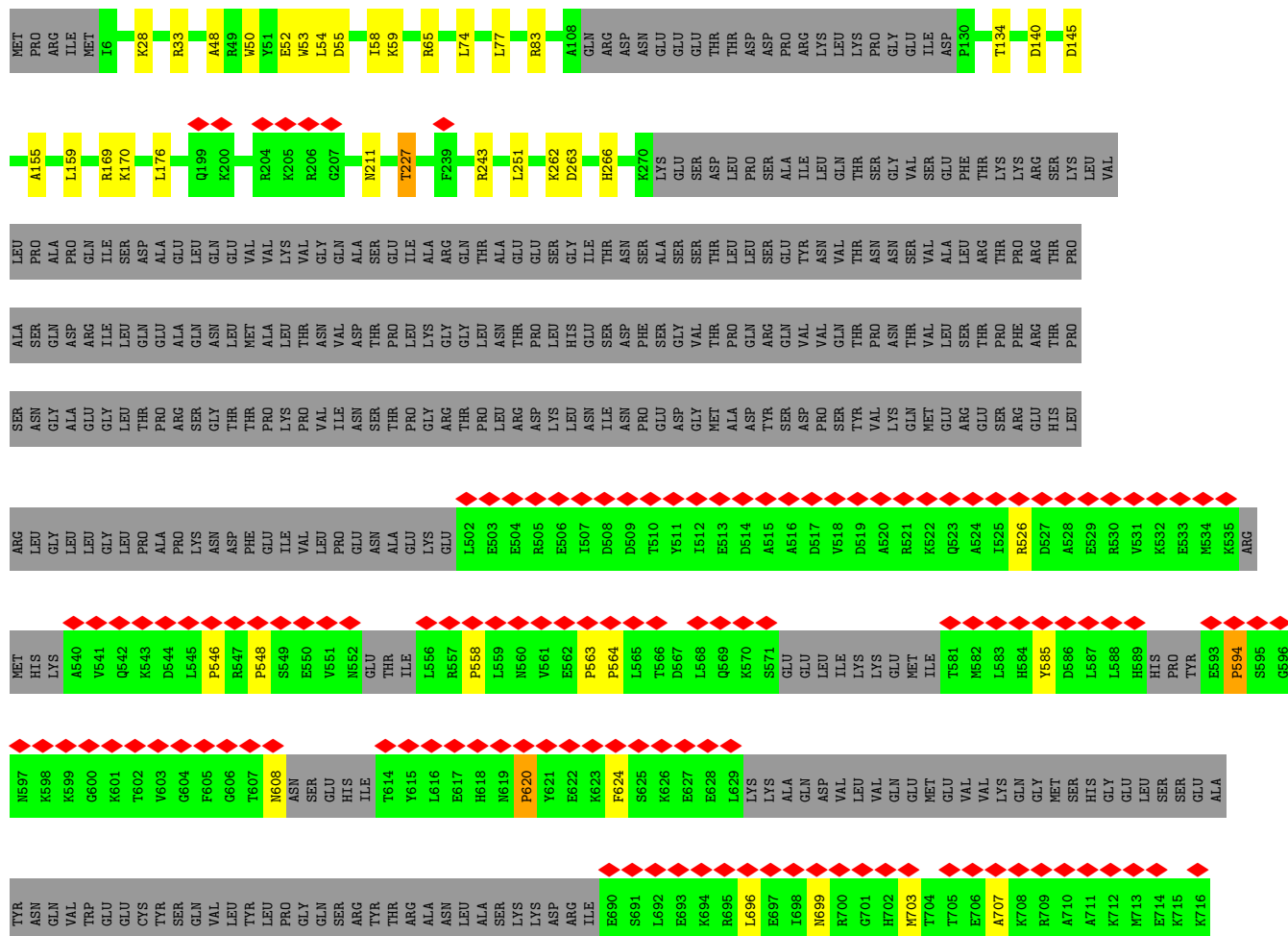
- Molecule 10: pre-mRNA

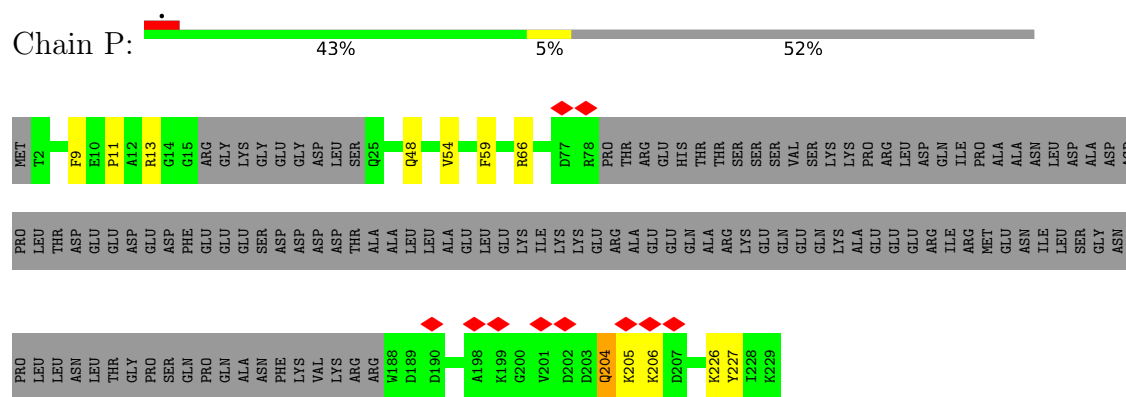




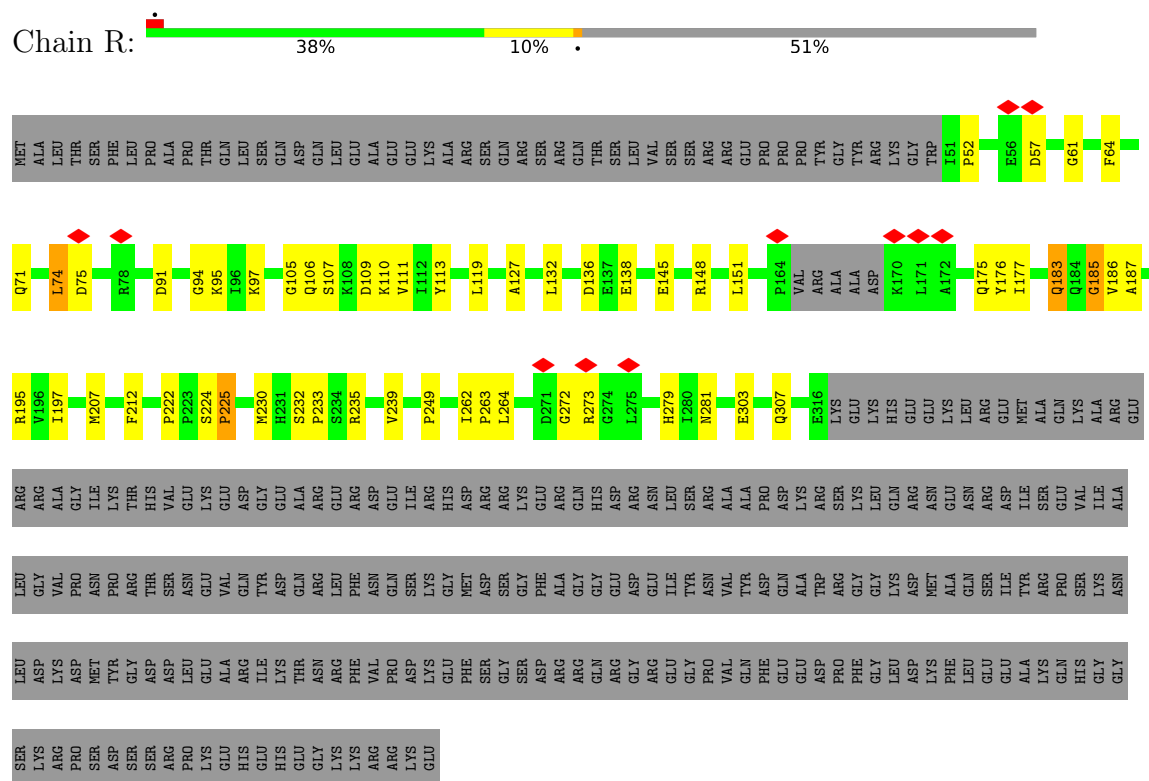


● Molecule 13: Cell division cycle 5-like protein

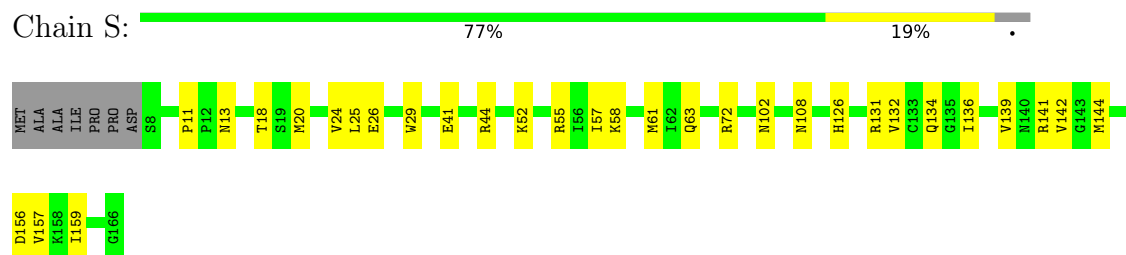




- Molecule 18: SNW domain-containing protein 1



- Molecule 19: Peptidyl-prolyl cis-trans isomerase-like 1



- Molecule 20: Pleiotropic regulator 1







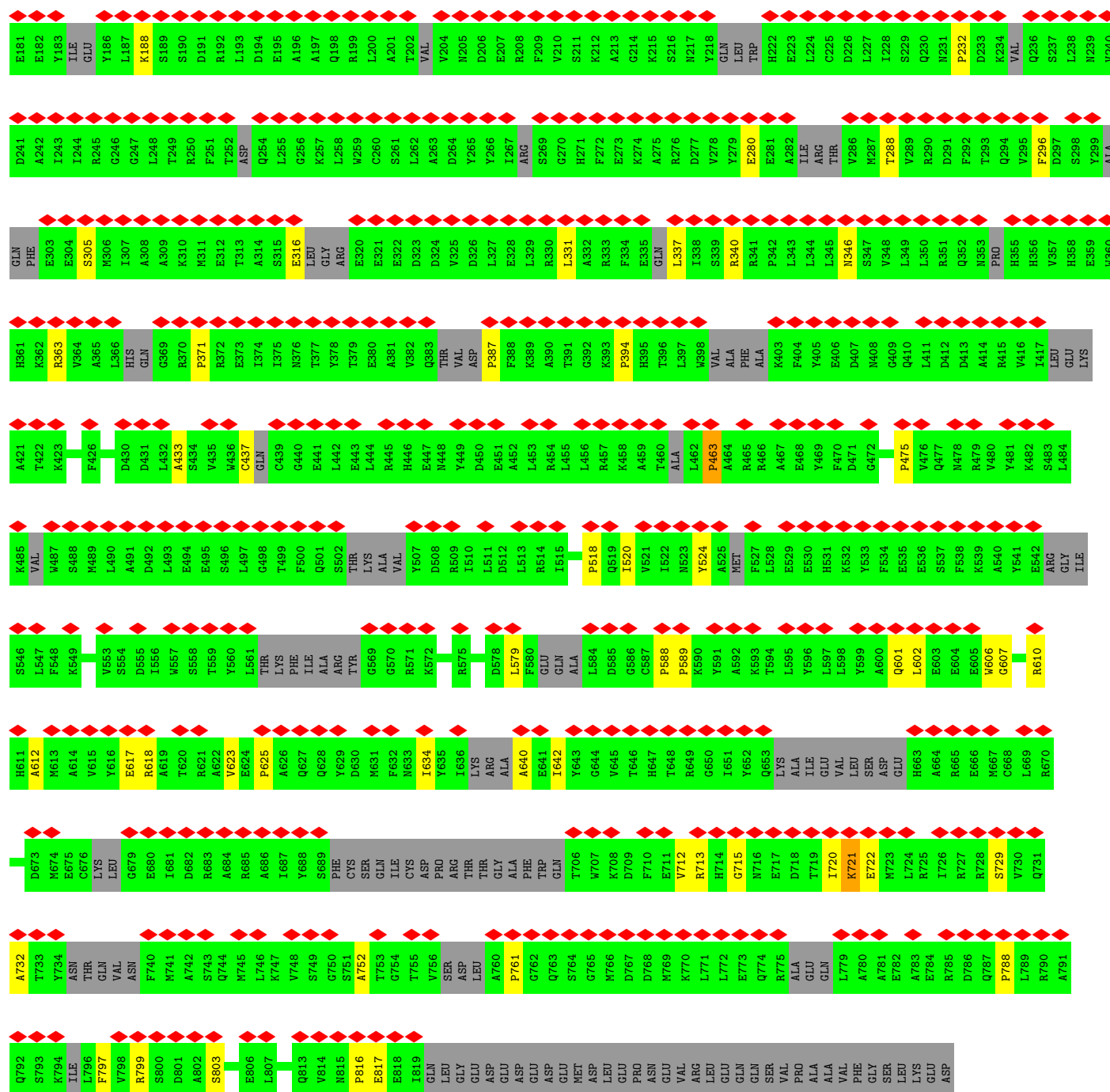
[illegible]

- Molecule 22: Pre-mRNA-splicing factor CWC22 homolog

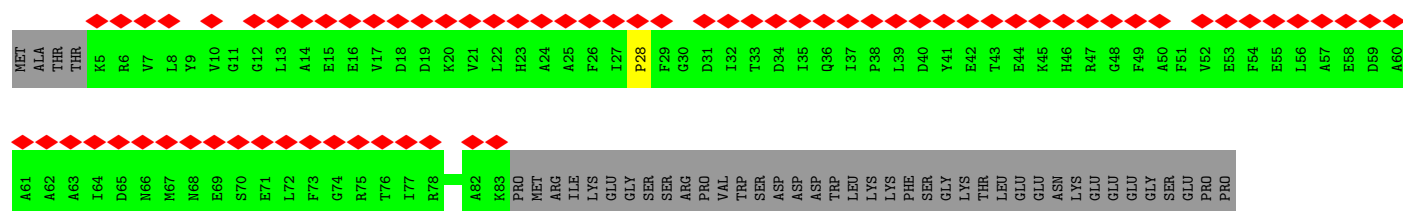


I181	I182	Q183	E184	L185	L186	Q187	E188	N189	I190	R191	G193	R194	G195	L196	L197	S198	R199	S200	V201	L202	Q203	A204	Q205	S206	A207	S208	P209	I210	F211	T212	H213	V214	Y215	A216	A217	L218	V219	A220	I221	I222	N223	S224	K225	F226				
LEU	ASP	PRO	LEU	LEU	THR	ARG	GLY	ALA	TTR	ILE	PRO	ALA	LYS	LEU	MET	GLN	GLU	ILE	ASP	K149	M150	S151	L152	A153	Y154	Q155	R156	M157	S158	W159	E160	A161	L162	K163	K164	S165	I166	M167	G168	L169	I170	M171	K172					
TYR	ASP	SER	SER	MET	GLU	SER	ARG	ASP	ARG	GLY	LYS	ARG	ARG	GLU	ARG	THR	ASP	LYS	SER	LYS	ARG	PRO	SER	PRO	GLY	ARG	ARG	ASN	GLU	THR	SER	VAL	THR	GLN	SER	SER	ALA	GLN	ASP	GLU	PRO	ALA	THR	LYS	LYS	ARG	LYS	ASP



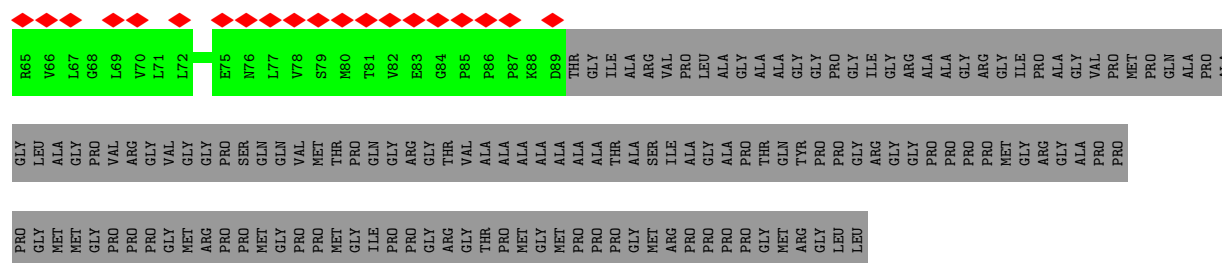


• Molecule 27: Peptidyl-prolyl cis-trans isomerase E

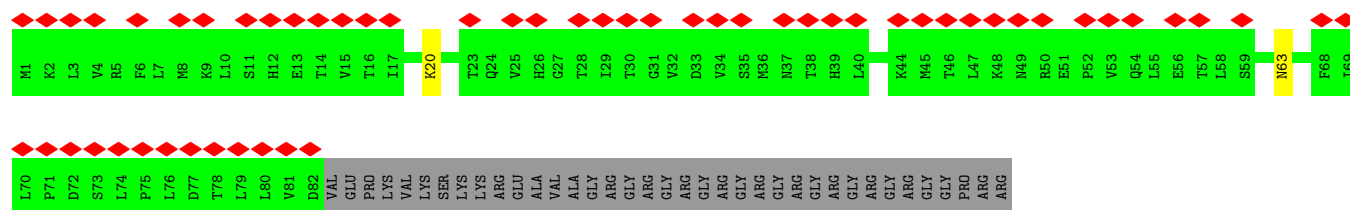




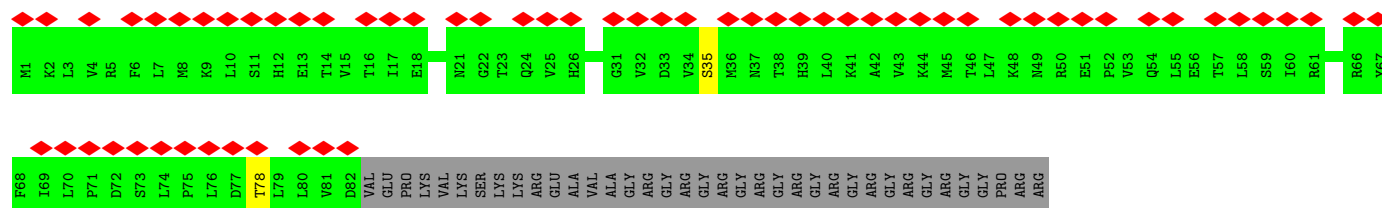
MET	THR	VAL																																																						
G4	K5	K6	K7	K8		Q11	I12	I13	D14	I15	R16	M17	R18	C19	L20	L21	Q22	D23	G24	R25	L26	F27	I28	G29	T30	F31	K32	A33	F34	D35	K36		N39	L40	I41	L42	C43		E47	F48	R49	K50	I51	K52	P53	K54	N55	S56	K57	Q58	A59	E60	R61	E62	E63	K64



• Molecule 31: Small nuclear ribonucleoprotein Sm D1



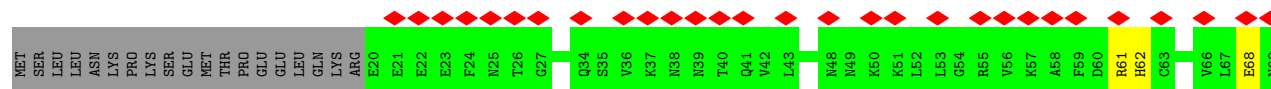
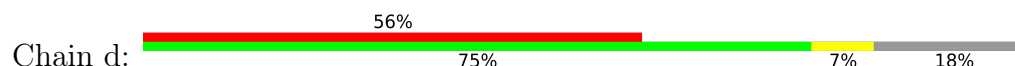
• Molecule 31: Small nuclear ribonucleoprotein Sm D1

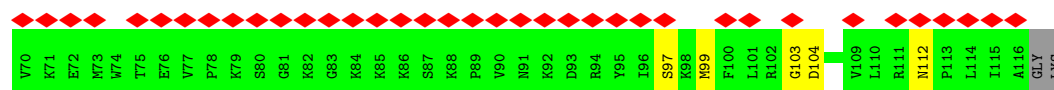


• Molecule 32: Small nuclear ribonucleoprotein Sm D2

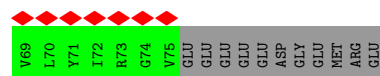
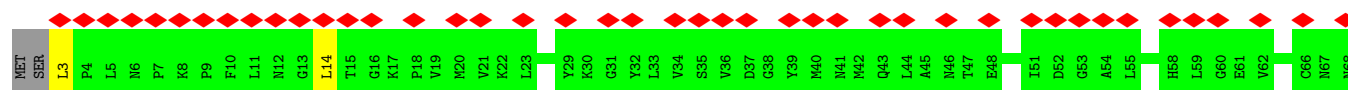
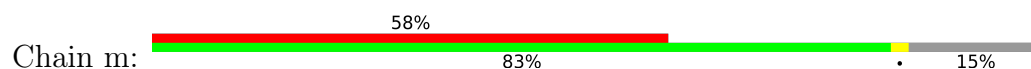


• Molecule 32: Small nuclear ribonucleoprotein Sm D2

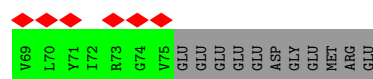
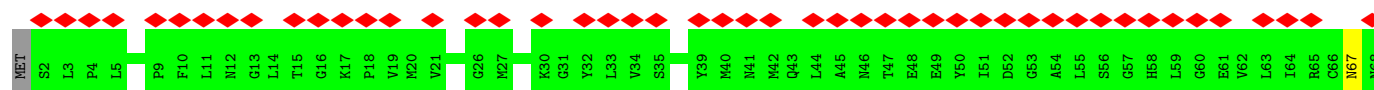
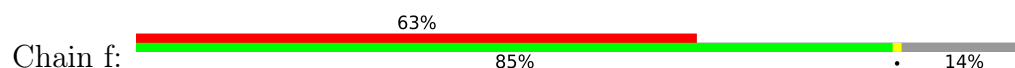




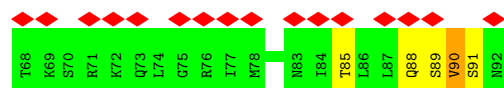
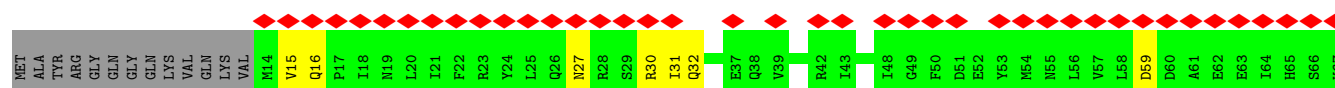
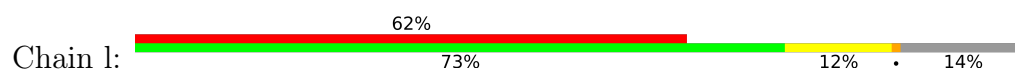
• Molecule 33: Small nuclear ribonucleoprotein F



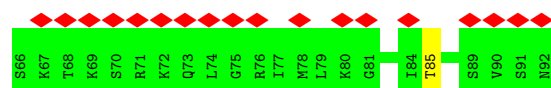
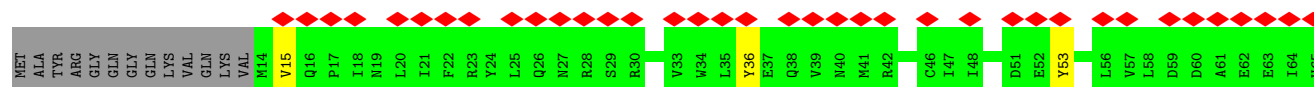
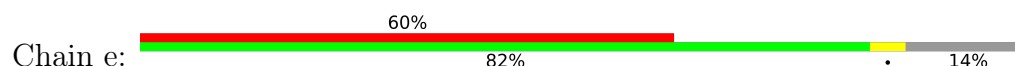
• Molecule 33: Small nuclear ribonucleoprotein F



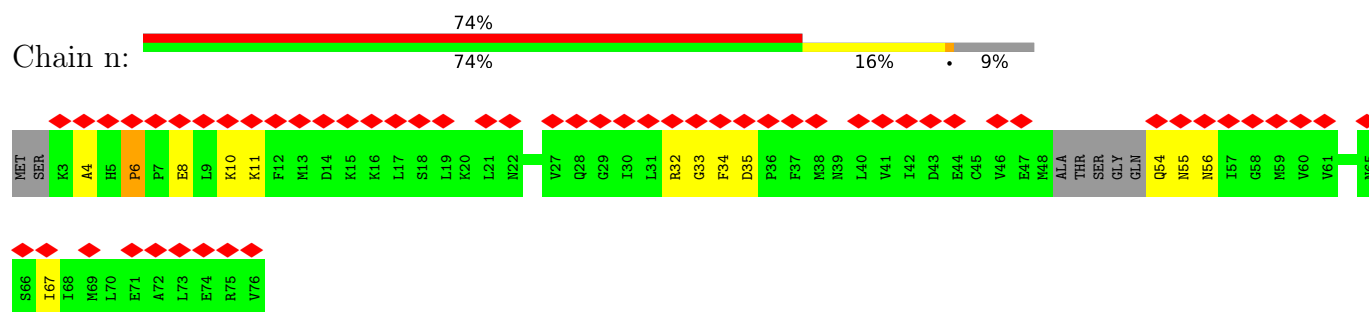
• Molecule 34: Small nuclear ribonucleoprotein E



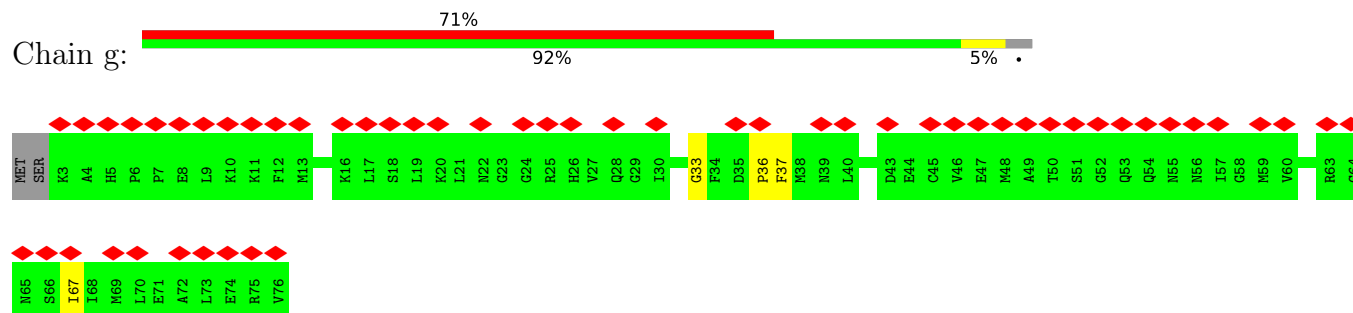
• Molecule 34: Small nuclear ribonucleoprotein E



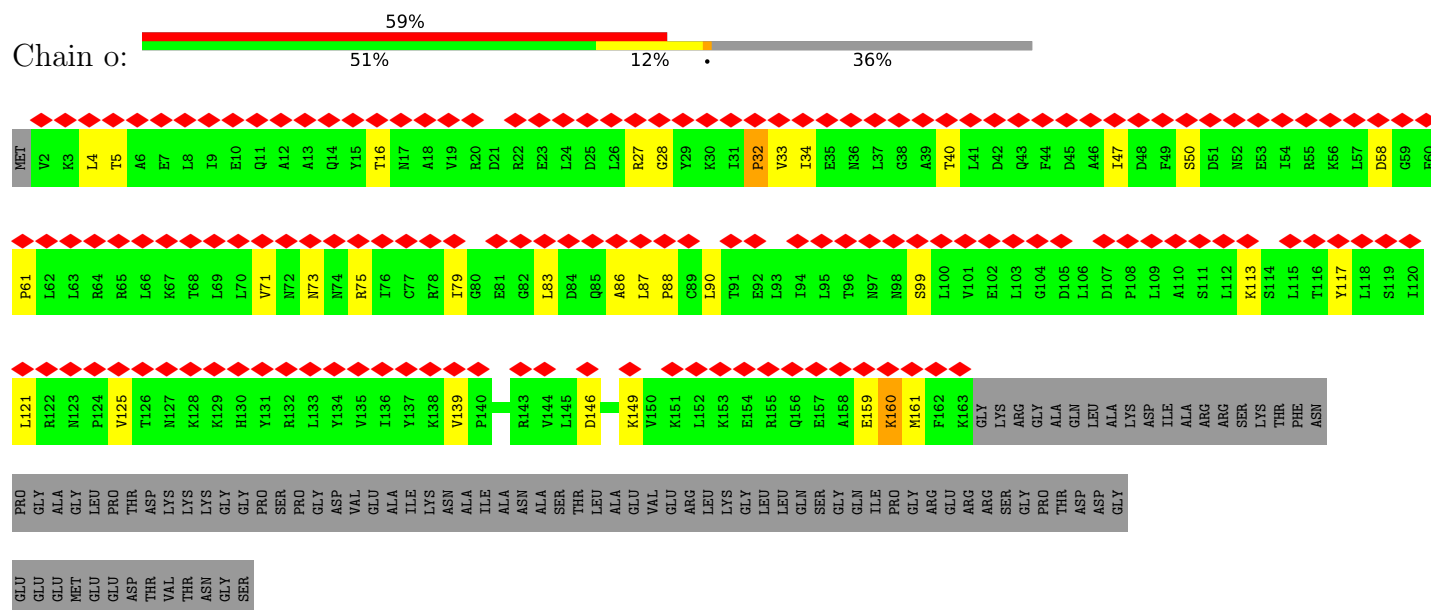
• Molecule 35: Small nuclear ribonucleoprotein G



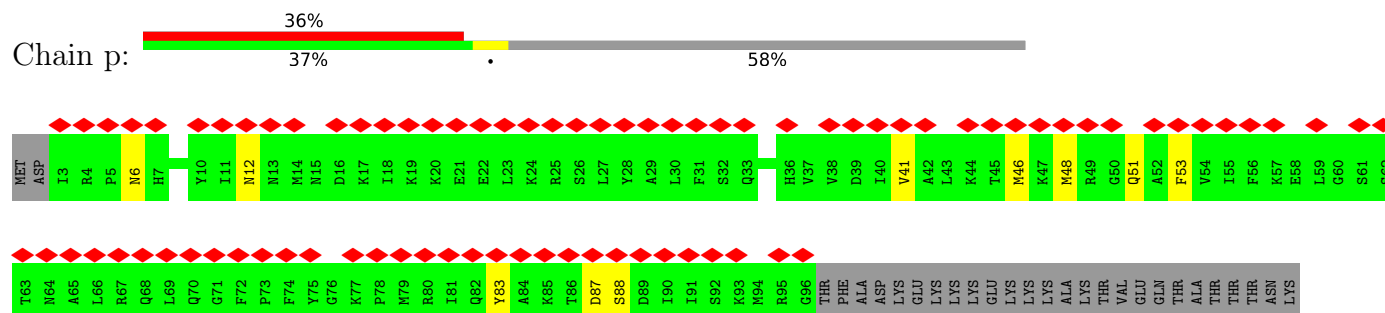
• Molecule 35: Small nuclear ribonucleoprotein G

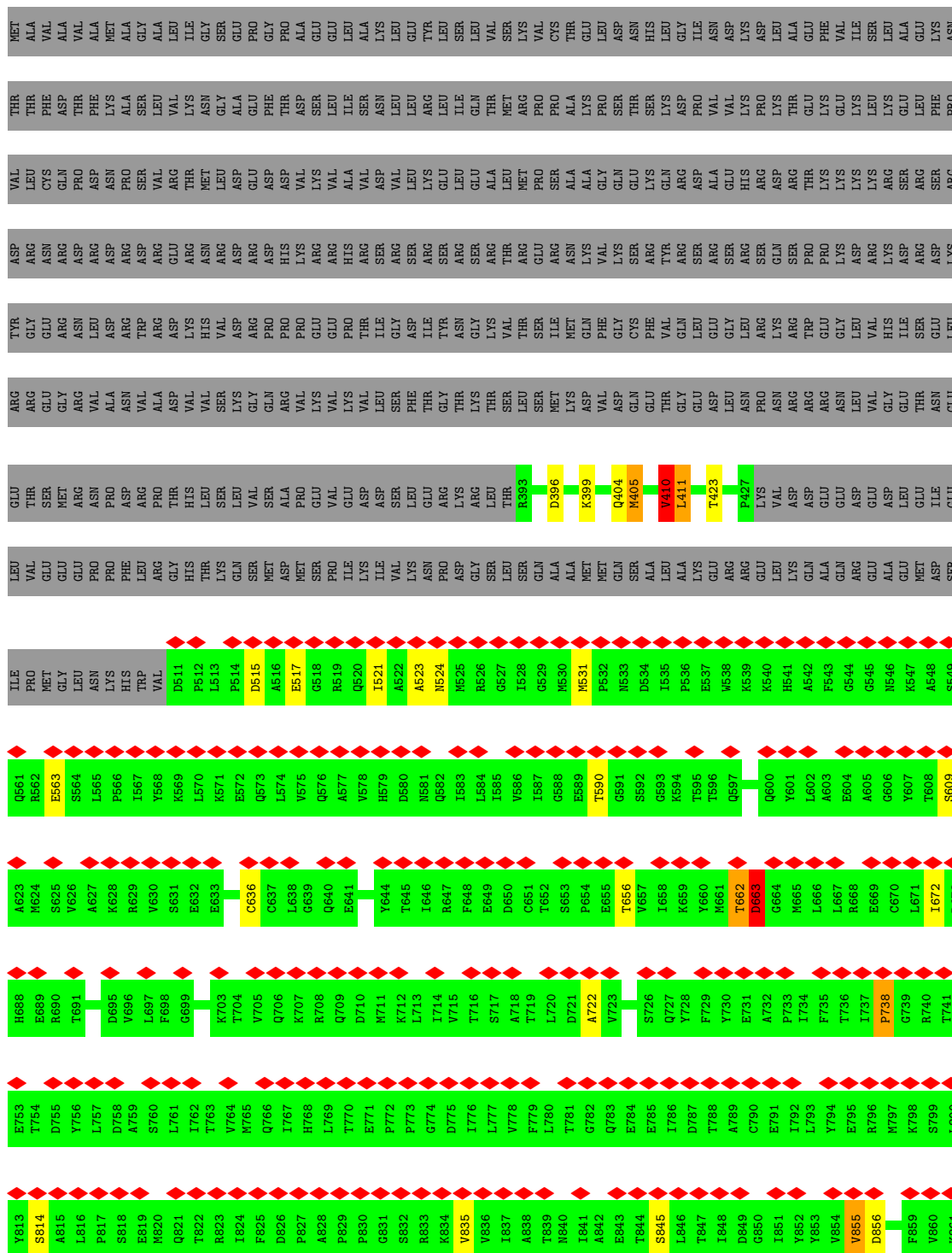


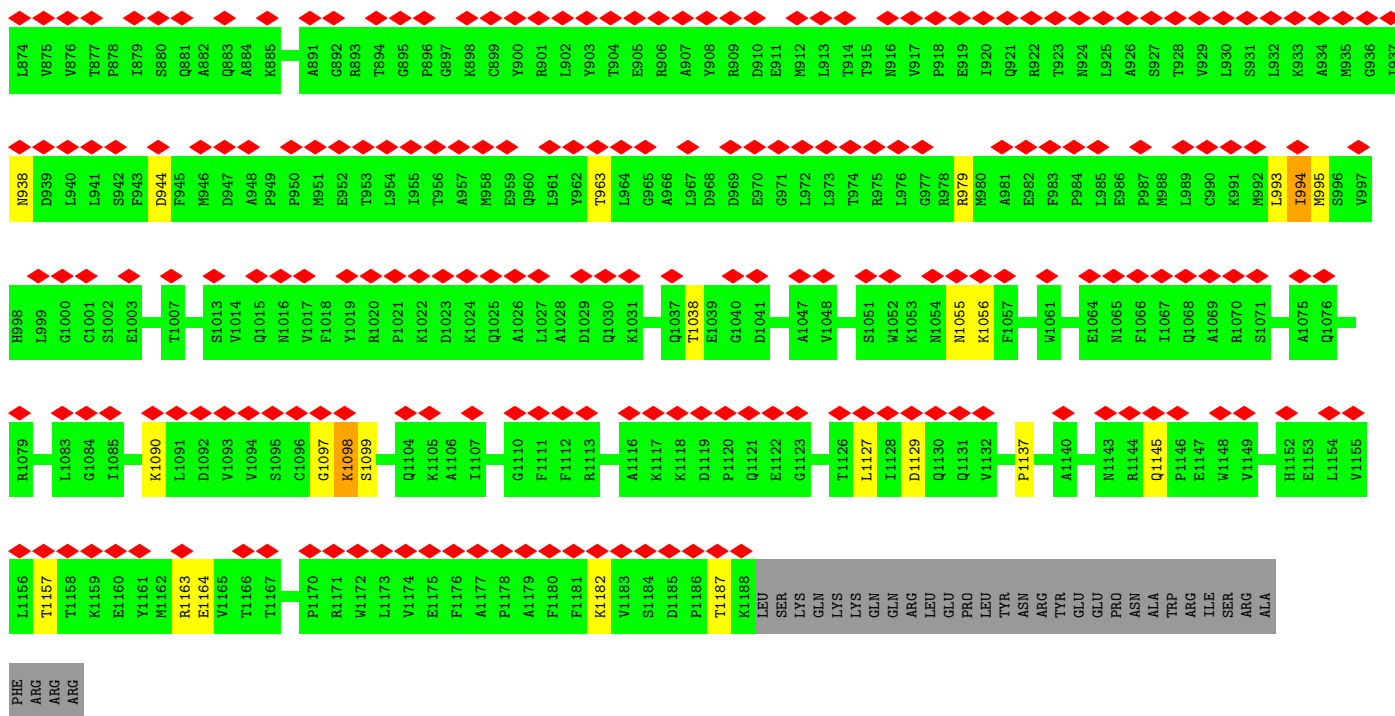
• Molecule 36: U2 small nuclear ribonucleoprotein A'



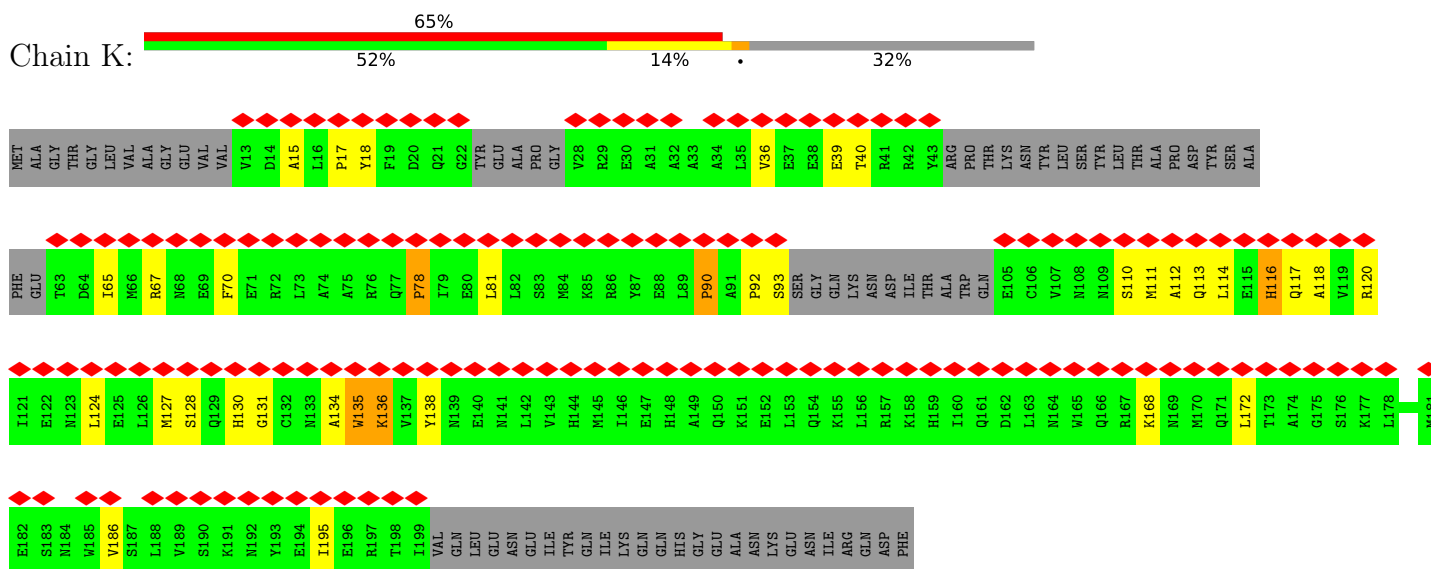
• Molecule 37: U2 small nuclear ribonucleoprotein B''



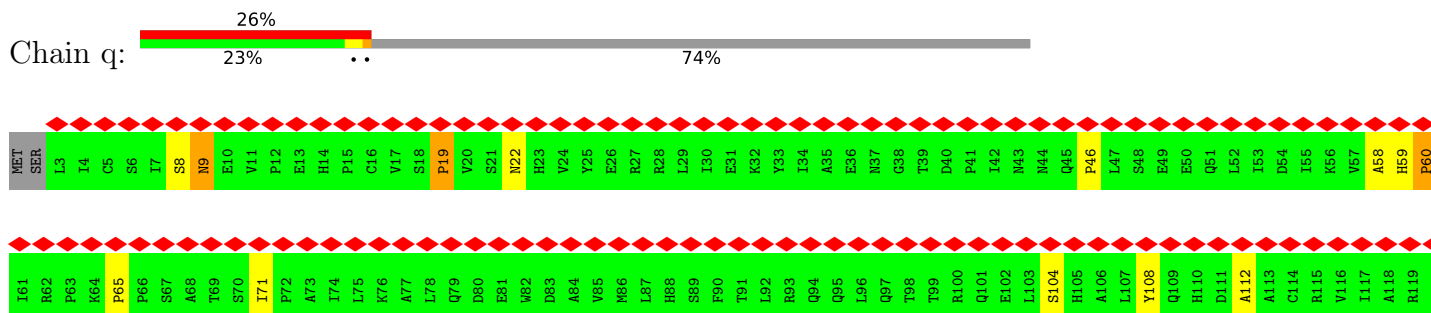




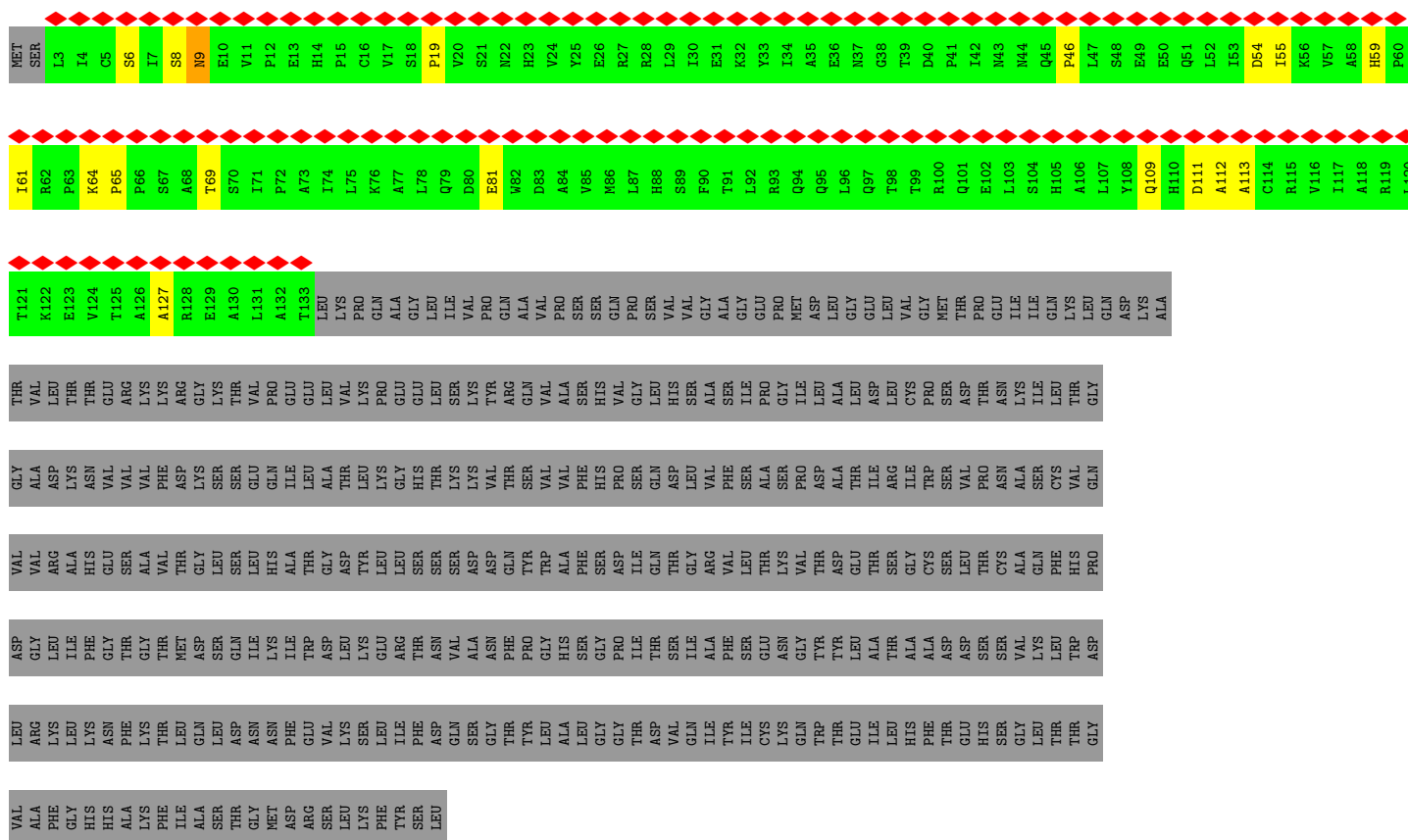
• Molecule 39: Pre-mRNA-splicing factor SPF27



• Molecule 40: Pre-mRNA-processing factor 19



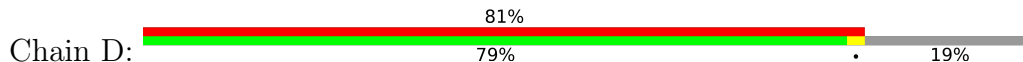
- Molecule 40: Pre-mRNA-processing factor 19



- Molecule 40: Pre-mRNA-processing factor 19

LEU	ARG	LEU	LYS	ASN	PRO	THR	LEU	ASP	ASN	ASP	GLU	VAL	LYS	SER	LEU	ILE	PRO	ASP	GLN	SER	GLY	THR	LEU	ALA	GLY	GLY	THR	ASP	VAL	GLN	ILE	TYR	ILE	CYS	LYS	GLN	TRP	THR	THR	GLU	ILE	LEU	HIS	PRO	THR	THR	GLY	LEU	THR	THR	GLY
VAL	ALA	PRO	GLY	HIS	HIS	ALA	LYS	PRO	ILE	ALA	SER	SER	ARG	ASP	MET	ASN	ASP	ARG	SER	LEU	LYS	PRO	THR	SER	LEU																										

- Molecule 41: U5 small nuclear ribonucleoprotein 200 kDa helicase



NET	ALA	ASP	VAL	THR	ALA	ARG	SER	GLN	LEU	GLU	TYR	LYS	ASN	SER	ASN	LEU	VAL	LEU	GLN	ALA	ASP	ARG	SER	LEU	ILE	ASP	ARG	THR	ARG	ASP	GLU	PRO	THR	GLY	GLY	VAL	LEU	SER	LEU	VAL	GLY	LYS	LEU	GLU	GLY	THR	ARG	MET	GLY	ASP	LYS	ALA	GLN	ARG	THR	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

PRO GLN MET MET GLN GLU GLU ARG ARG ARG ALA LYS ARG ARG LYS ASP ARG ASP ASP ARG HIS ASP ILE ASN MET MET LYS GLY TYR THR LEU LEU LEU SER SER GLU GLY ILE ILE ILE ILE TYR LYS PRO LYS LYS THR THR LYS GLU THR VAL LEU LEU SER LEU PHE ILE

GLN	ALA	ALA	GLY	ASP	GLN	GLN	PRO	ARG	ASP	ASP	ILE	GLY	CYS	GLY	ALA	ALA	ASP	GLU	VAL	LEU	LEU	ALA	ALA	VAL	LEU	LEU	LYS	ASN	GLU	LYS	ARG	ASP	LYS	GLU	GLU	ASP	ILE	GLU	LEU	LEU	GLY	GLN	THR	ASP	ASP	THR	ARG	TYR	HIS	VAL	LEU	LEU	VAL	ASN	LEU	GLY	LYS	LYS	ILE	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ASP TYR GLY GLY ASP LYS GLU ILE GLN ASN MET ASP ASP ASN ILE ASP ASP GLU THR TYR GLY VAL ASN VAL VAL GLN PHE GLU SER ASP ASP GLU GLU GLY GLY ASP GLU VAL ASP ASP TYR GLY GLU VAL ARG GLU GLU ALA SER ASP ASP ASP MET GLU GLY ASP ASP ALA VAL VAL ARG CYS THR THR

SER	ALA	ASN	LEU	VAL	ALA	SER	GLY	LEU	LEU	MET	SER	SER	LYS	LYS	ASP	LEU	HIS	PRO	ARG	ASP	ILE	ASP	ALA	THR	PHE	LEU	GLN	ARG	GLN	LEU	SER	ARG	PHE	TYR	ASP	ASP	ALA	ALA	ILE	VAL	SER	GLN	LYS	LYS	ALA	ALA	ASP	GLU	VAL	LEU	GLU	ILE	LEU	LEU	LYS	THR	SER	ASP	ASP	ARG
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

GLU CYS GLU ASN GLN LEU VAL PHE THR PHE ASP PHE ILE LYS VAL LEU ARG LEU GLN HIS ARG MET MET ILE TYR CYS THR LEU LEU ALA SER ALA GLN SER SER GLU GLU GLY GLU ARG ILE LEU MET MET GLY LYS MET GLU ASP PRO LEU LEU SER LYS PHE LEU

TVR	GLN	LEU	HIS	GLU	THR	GLU	LYS	ASP	LEU	TLE	ARG	GLU	ARG	SER	ARG	ARG	GLU	ARG	VAL	ARG	GLN	SER	ARG	MET	ASP	THR	ASP	LEU	GLU	THR	MET	ASP	LEU	ASP	GLN	GLY	GLY	GLU	ALA	LEU	A404	P405	P406	P407	P408	P409	P410	P411	P412	P413	P414	P415	P416	P417	P418	P419	P420
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

H421	F422	M423	A424	N425	K426	R427	C428	Q429	L430	P431	D432	G433	S434	F435	R436	R437	Q438	R439	K440	G441	Y442	E443	E444	V445	H446	V447	P448	A449	L450	K451	P452	K453	P454	F455	G456	S457	E458	E459	Q460	L461	L462	P463	V464	E465	K466	L467	P468	K469	Y470	A471	Q472	A473	G474	G475	E476	G477	F478	K479	T480
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

L481	N482	R483	I484	Q485	S486	K487	L488	Y489	R490	A491	A492	L493	E494	T495	D496	E497	N498	L499	L500	L501	C502	A503	P504	T505	G506	A507	K509	T510	N511	V512	A513	L514	M515	C516	M517	L518	R519	E520	I521	G522	K523	H524	I525	N526	M527	D528	G529	T530	I531	N532	V533	D534	D535	F536	K537	I538	I539	Y540
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

I541	A542	P543	M544	R545	S546	V547	V548	Q549	E550	M551	V552	G553	S554	F555	G556	K557	R558	L559	A560	T561	Y562	G563	I564	T565	V566	A567	E568	L569	T570	G571	D572	H573	Q574	L575	C576	K577	E578	E579	I580	S581	A582	T583	Q584	I586	I586	V587	C588	T589	P590	E591	K592	W593	D594	I595	I596	T597	R598	K599	G600
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

G601	E602	R603	T604	Y605	T606	Q607	L608	V609	R610	L611	I612	I613	L614	D615	E616	I617	H618	L619	L620	H621	D622	D623	R624	G625	P626	V627	L628	E629	A630	L631	V632	A633	R634	A635	I636	R637	N638	I639	E640	M641	T642	Q643	E644	D645	V646	R647	L648	I649	G650	L651	S652	A653	T654	L655	P656	N657	Y658	E659	D660
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

V661	A662	T663	F664	L665	R666	D667	S668	P669	A670	K671	G672	L673	F674	Y675	F676	D677	N678	S679	F680	R681	P682	V683	P684	L685	E686	K687	T688	Y689	V690	G691	I692	T693	E694	K695	K696	A697	T698	K699	R700	F701	Q702	I703	M704	N705	E706	I707	V708	Y709	E710	K711	I712	M713	E714	H715	A716	G717	K718	N719	O720
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

V721	L722	V723	F724	V725	H726	S727	R728	K729	E730	T731	G732	K733	T734	A735	R736	A737	I738	R739	D740	H741	G742	L743	E744	K745	D746	T747	L748	G749	L750	F751	L752	R753	E754	G755	S756	A757	S758	T759	E760	V761	L762	R763	T764	E765	A766	F767	Q768	G769	K770	N771	L772	E773	L774	D775	K776	L777	L778	F779	V780
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

A1501	H1502	Q1441	P1381	Y1321	P1261	E1201	K1141	M1081	S1021	A961	L901	W841	G781
H1503	R1442	R1443	M1382	Q1322	L1262	L1202	K1142	V1082	S1022	L962	N902	T842	F782
L1504	K1443	K1444	E1383	D1323	T1263	T1203	I1143	Y1083	E1023	M963	E904	E843	A783
G1505	N1444	N1445	A1384	K1324	I1204	I1204	E1144	V1084	F1024	L964	I905	L844	I784
S1507	V1445	Q1446	L1385	F1325	P1265	P1206	K1145	T1085	K1025	D965	V906	G845	H785
A1508	Q1447	T1448	E1387	F1327	F1267	D1207	K1146	Q1086	N1026	K966	L847	A846	H786
T1509	T1448	T1448	Q1388	F1328	I1268	F1208	F1148	A1088	T1028	N967	G908	D848	A787
S1510	N1449	N1449	V1389	N1329	A1269	Q1209	F1149	A1089	V1029	N968	N909	M849	G788
T1511	L1450	F1451	Y1390	P1330	W1210	W1210	F1150	R1090	E1030	V970	V910	L850	T790
F1512	F1452	F1451	M1391	I1331	D1211	D1211	E1151	L1091	E1031	K971	Q911	Q851	R791
M1513	V1453	V1453	D1392	Q1332	E1212	E1212	R1152	M1092	E1032	Y972	N912	M852	V792
F1514	D1454	D1454	W1393	T1333	K1213	K1213	L1153	R1093	E1033	D973	A913	L854	D793
H1515	E1455	E1455	F1394	Q1334	V1214	V1214	Y1154	A1094	K1034	K974	K914	G854	R794
P1516	V1456	V1456	E1395	V1335	H1215	H1215	D1155	I1095	L1035	K975	D915	R855	T795
M1517	H1457	H1457	K1396	F1336	G1216	G1216	L1156	F1096	E1036	T976	A916	A856	L796
V1518	L1458	L1458	F1397	N1337	S1217	S1217	M1157	E1097	L1037	G977	V917	G857	V797
R1519	I1459	I1459	Q1398	T1338	S1218	S1218	H1158	I1098	Q1038	N978	N918	R858	E798
P1520	G1460	G1461	D1399	V1339	E1219	E1219	M1159	V1099	K1039	F979	W919	P859	D799
V1521	G1461	G1461	R1400	Y1340	A1220	A1220	E1160	L1100	L1040	Q980	L920	Q860	L800
F1522	E1462	E1462	L1401	N1341	F1221	F1221	I1161	M1101	L1041	Y981	G921	Y861	F801
L1523	N1463	N1463	M1402	S1342	W1222	W1222	G1162	I1102	E1042	T982	Y922	D862	A802
E1524	K1464	K1464	K1403	D1343	I1223	I1223	E1163	G1103	R1043	E983	A923	T863	D803
L1525	P1465	P1465	K1404	D1344	L1224	L1224	L1164	W1104	Y1044	L984	Y924	K864	K804
H1526	V1466	V1466	V1405	N1345	V1225	V1225	I1165	A1105	P1045	G985	L925	G865	H805
I1527	L1467	L1467	F1406	V1346	E1226	E1226	R1166	Q1106	I1046	R986	Y926	E866	I806
Q1528	E1468	E1468	L1407	F1347	D1227	D1227	M1167	L1107	P1047	T987	I927	G867	Q807
G1529	V1469	V1469	H1408	V1348	V1228	V1228	P1168	T1108	V1048	A988	R928	I868	V808
F1530	I1470	I1470	T1409	G1349	D1229	D1229	K1169	I1109	Y1049	S989	M929	L869	L809
M1531	C1471	C1471	G1410	A1350	S1230	S1230	M1170	K1110	E1050	H990	L930	I870	W810
I1532	S1472	S1472	E1411	P1351	E1231	E1231	G1171	T1111	S1051	Y991	R931	T871	S811
S1533	R1473	R1473	T1412	T1352	V1232	V1232	K1172	M1112	I1052	Y992	S932	S872	T812
H1534	M1474	M1474	S1413	G1353	I1233	I1233	T1173	N1113	E1053	Y993	P933	H873	A813
T1535	R1475	R1475	D1415	G1355	H1235	H1235	H1175	C1115	P1055	T994	T934	G874	T814
Q1536	Y1476	Y1476	L1416	K1356	H1236	H1236	K1176	K1116	S1056	D996	Y936	E875	L815
T1537	I1477	I1477	K1417	T1357	E1237	E1237	Y1177	M1117	A1057	T997	G937	L876	A816
R1538	S1478	S1478	L1418	I1358	V1238	V1238	V1178	I1118	K1058	V998	I938	Y877	W817
L1539	S1479	S1479	L1419	C1359	F1239	F1239	H1179	D1119	I1059	Q999	S939	Y878	G818
L1540	Q1480	Q1480	G1420	A1360	L1240	L1240	L1180	K1120	N1060	T1000	H940	Y879	V819
S1541	I1481	I1481	K1421	E1361	L1241	L1241	F1181	R1121	V1061	Y1001	D941	S881	L821
M1542	E1482	E1482	G1422	F1362	K1242	K1242	P1182	M1122	L1062	M1002	D942	L882	P822
A1543	R1483	R1483	N1423	A1363	A1243	A1243	K1183	W1123	L1063	Q1003	L943	L883	A823
K1544	P1484	P1484	I1424	I1364	K1244	K1244	L1184	Q1124	Q1064	L1004	K944	N884	H824
P1545	L1485	L1485	I1425	L1365	Y1245	Y1245	E1185	S1125	A1065	L1005	G945	Q885	T825
V1546	R1486	R1486	I1426	P1366	A1246	A1246	L1186	M1126	F1066	K1006	D946	Q886	W826
Y1547	I1487	I1487	S1427	M1367	Q1247	Q1247	S1187	C1127	I1067	P1007	P947	L887	I827
H1548	V1488	V1488	T1428	L1368	D1248	D1248	V1188	P1128	S1068	T1008	L948	P888	I828
A1549	L1489	L1489	P1429	L1369	E1249	E1249	H1189	L1129	Q1069	L1009	L949	P889	K829
I1550	L1490	L1490	S1310	Q1370	H1250	H1250	L1190	R1130	L1070	S1010	D950	E890	G830
T1551	S1491	S1491	K1431	S1371	L1251	L1251	Q1191	Q1131	K1071	E1011	Q951	S891	T831
K1552	S1492	S1492	W1432	S1372	I1252	I1252	P1192	F1132	L1072	I1012	R952	Q892	Q832
H1553	S1493	S1493	D1433	E1373	T1253	T1253	L1193	K1133	E1073	R953	M893	V894	R834
S1554	L1494	L1494	I1434	G1374	F1254	F1254	T1194	K1134	G1074	L1014	L954	Y894	Y834
P1555	S1495	S1495	L1435	R1375	F1255	F1255	R1195	L1135	F1075	F1015	D955	S895	S835
K1556	N1496	N1496	S1436	C1376	V1256	V1256	S1196	P1136	A1076	R1016	L956	K896	P836
L1557	A1497	A1497	R1437	V1377	P1257	P1257	T1197	E1137	L1077	V1017	L897	E837	E837
P1558	L1498	L1498	L1438	V1378	E1258	E1258	L1198	E1138	M1078	F1018	P898	K838	K838
V1559	D1499	D1499	W1439	I1379	F1259	F1259	K1199	V1139	A1079	S1019	T959	D899	G839
I1560	V1500	V1500	L1440	T1380	L1320	L1320	V1200	V1140	D1080	L1020	A960	M900	R840

V1561	H1621	I1681	V1741	C1801	R1861	R1921	S1981	L2041	A2101
F1562	E1622	Y1682	T1742	I1802	H1862	L1922	V1982	E2042	H2102
V1563	G1623	D1683	K1743	S1803	H1863	I1923	F1983	R2043	M2103
P1564	L1624	V1684	T1744	I1804	E1864	Q1924	D1984	E2044	Y2104
S1565	L1625	L1685	I1745	D1806	D1865	C1926	I1985	E2045	T2105
R1566	P1626	Q1686	E1746	D1807	N1866	C1926	M1986	E2046	L2106
K1567	M1627	M1687	N1747	E1807	L1867	V1927	E1987	V2047	Y2107
Q1568	E1628	V1688	K1748	M1808	L1868	D1928	M1988	T2048	F2108
T1569	R1629	H1689	Q1749	D1809	R1869	V1929	E1989	G2049	M2109
R1570	R1630	H1690	D1750	V1810	Q1870	L1930	D1990	P2050	S2110
L1571	L1631	A1691	A1751	A1811	L1871	S1931	E1991	V2051	D2111
T1572	V1632	N1692	V1752	P1812	A1872	S1932	E1992	I2052	A2112
A1573	E1633	R1693	D1753	L1813	Q1873	N1933	R1993	A2053	Y2113
I1574	Q1634	P1694	Y1754	M1814	K1874	G1934	N1994	P2054	M2114
D1575	L1635	L1695	L1755	L1815	V1875	W1935	A1995	L2055	G2115
I1576	F1636	Q1696	T1756	Q1816	P1876	L1936	L1996	F2056	C2116
L1577	S1637	D1697	W1757	M1817	H1877	S1937	L1997	P2057	D2117
T1578	S1638	D1698	T1758	I1818	K1878	P1938	Q1998	Q2058	Q2118
T1579	G1639	E1699	F1759	A1819	L1879	A1939	L1999	K2059	E2119
C1580	A1640	G1700	L1760	A1820	N1880	L1940	T2000	R2060	Y2120
A1581	I1641	A1701	Y1761	Y1821	M1881	A1941	D2001	E2061	K2121
A1582	Q1642	C1702	R1762	Y1822	P1882	A1942	S2002	E2062	F2122
D1583	V1643	V1703	R1763	Y1823	K1883	M1943	Q2003	G2063	S2123
I1584	V1644	I1704	M1764	I1824	F1884	E1944	T2004	W2064	V2124
Q1585	V1645	M1705	T1765	N1825	L1885	L1945	A2005	W2065	D2125
R1586	A1646	C1706	Q1766	Y1826	D1886	A1946	D2006	V2066	VAL
Q1587	S1647	Q1707	N1767	T1827	P1887	Q1947	V2007	V2067	LYS
R1588	R1648	G1708	P1768	I1828	H1888	M1948	A2008	I2068	GLU
F1589	S1649	S1709	N1769	I1829	V1889	V1949	R2009	G2069	ALA
L1590	L1650	K1710	Y1770	E1830	K1890	T1950	F2010	D2070	THR
H1591	C1651	K1711	Y1771	L1831	T1891	Q1951	C2011	A2071	ASP
C1592	W1652	D1712	N1772	F1832	N1892	A1952	N2012	K2072	SER
T1593	G1653	F1713	L1773	S1833	L1893	M1953	R2013	S2073	ASP
E1594	M1654	F1714	Q1774	M1834	L1894	W1954	Y2014	N2074	SER
K1595	N1655	K1715	G1775	S1835	L1895	S1955	P2015	S2075	ASP
D1596	V1656	K1716	I1776	L1836	Q1896	K1956	N2016	L2076	ASP
L1597	A1657	F1717	S1777	M1837	A1897	D1957	I2017	I2077	ASP
I1598	A1658	L1718	H1778	A1838	H1898	S1958	E2018	S2078	ASP
P1599	H1659	Y1719	R1779	K1839	L1899	Y1959	L2019	I2079	ASP
Y1600	L1660	E1720	H1780	T1840	S1900	L1960	S2020	K2080	ASP
L1601	V1661	L1721	L1781	K1841	N1901	K1961	Y2021	R2081	ASP
E1602	L1662	P1722	S1782	L1842	M1902	Q1962	E2022	L2082	ASP
K1603	I1663	P1723	D1783	R1843	Q1903	L1963	V2023	T2083	ASP
L1604	M1664	V1724	H1784	G1844	L1904	P1964	V2024	L2084	ASP
S1605	D1665	E1725	L1785	L1845	S1905	H1965	D2025	Q2085	ASP
D1606	T1666	S1726	S1786	I1846	A1906	F1966	K2026	Q2086	ASP
S1607	Q1667	H1727	E1787	E1847	E1907	T1967	D2027	K2087	ASP
T1608	Y1668	L1728	L1788	I1848	L1908	S1968	S2028	A2088	ASP
L1609	Y1669	D1729	V1789	I1849	Q1909	E1969	I2029	K2089	ASP
K1610	N1670	H1730	E1790	S1850	Q1910	H1970	R2030	V2090	ASP
E1611	G1671	C1731	Q1791	N1851	D1911	I1971	S2031	K2091	ASP
T1612	K1672	M1732	T1792	A1852	T1912	K1972	G2032	L2092	ASP
L1613	I1673	H1733	L1793	A1853	E1913	R1973	G2033	D2093	ASP
L1614	H1674	D1734	S1794	E1854	L1914	C1974	P2034	F2094	ASP
N1615	A1675	H1735	D1795	Y1855	I1915	T1975	V2035	V2095	ASP
G1616	Y1676	F1736	L1796	E1856	L1916	D1976	V2036	A2096	ASP
V1617	V1677	Q1737	E1797	N1857	S1917	K1977	V2037	F2097	ASP
G1618	D1678	M1738	Q1798	I1858	L1918	G1978	L2038	A2098	ASP
Y1619	Y1679	E1739	S1799	P1859	A1919	V1979	V2039	T2099	ASP
L1620	P1680	I1740	K1800	I1860	I1920	E1980	Q2040	G2100	ASP

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	143320	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.552	Depositor
Minimum map value	-0.288	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.338, 1.338, 1.338	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: IHP, SEP, GTP, ZN, ATP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	v	0.46	0/710	1.03	3/987 (0.3%)
2	w	0.46	0/444	1.21	4/614 (0.7%)
3	u	0.51	0/1906	1.20	13/2653 (0.5%)
4	x	0.53	0/123	1.12	0/170
5	A	0.52	1/18287 (0.0%)	0.81	25/24842 (0.1%)
6	B	0.48	1/2274 (0.0%)	0.61	2/3535 (0.1%)
7	C	1.55	10/7225 (0.1%)	0.86	18/9818 (0.2%)
8	E	0.30	0/2420	0.77	3/3281 (0.1%)
9	F	0.47	0/2323	0.59	0/3619
10	G	0.41	0/1716	0.78	5/2656 (0.2%)
11	H	0.79	24/3305 (0.7%)	1.29	46/5130 (0.9%)
12	J	0.48	0/3870	0.86	15/5252 (0.3%)
13	L	0.47	1/3091 (0.0%)	0.83	10/4178 (0.2%)
14	M	0.39	0/1119	0.72	0/1497
15	N	1.04	1/1210 (0.1%)	0.99	5/1622 (0.3%)
16	O	0.40	0/2344	0.74	2/3163 (0.1%)
17	P	0.41	0/943	0.70	0/1255
18	R	0.46	0/2091	0.81	2/2809 (0.1%)
19	S	0.29	0/1268	0.62	0/1714
20	T	0.63	0/2526	0.94	7/3443 (0.2%)
21	U	0.29	0/196	0.64	0/265
22	V	0.39	0/2784	0.77	0/3791
23	W	0.36	0/4230	0.82	7/5713 (0.1%)
24	X	0.30	0/714	0.64	0/959
25	Z	0.34	0/2049	0.80	6/2757 (0.2%)
26	I	0.53	0/2749	0.96	20/3773 (0.5%)
27	y	0.43	0/389	1.01	0/540
28	Q	0.38	0/6565	0.86	4/9143 (0.0%)
29	a	0.78	0/397	1.00	0/549
29	h	0.78	0/396	0.99	0/547
30	b	0.85	0/423	1.14	3/587 (0.5%)
30	i	0.84	0/423	1.14	3/587 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	c	0.88	0/405	1.12	1/563 (0.2%)
31	j	0.87	0/405	1.11	0/563
32	d	1.12	0/479	1.25	1/666 (0.2%)
32	k	1.14	0/420	1.24	1/583 (0.2%)
33	f	1.20	0/360	1.25	0/497
33	m	1.21	1/355 (0.3%)	1.24	0/490
34	e	1.04	0/390	1.24	1/542 (0.2%)
34	l	1.00	0/390	1.33	2/542 (0.4%)
35	g	0.86	0/362	1.08	1/501 (0.2%)
35	n	0.80	0/337	1.05	1/465 (0.2%)
36	o	0.98	0/803	2.25	43/1119 (3.8%)
37	p	0.93	0/463	1.85	6/643 (0.9%)
38	Y	0.82	0/2917	1.65	22/3670 (0.6%)
39	K	0.62	1/753 (0.1%)	1.07	3/1046 (0.3%)
40	q	0.63	0/658	0.97	3/919 (0.3%)
40	r	0.57	0/653	1.07	6/912 (0.7%)
40	s	0.50	0/334	0.91	0/466
40	t	0.56	0/334	0.82	0/466
41	D	0.56	0/8529	1.12	27/11891 (0.2%)
All	All	0.68	40/99857 (0.0%)	0.96	321/137993 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	A	0	6
7	C	0	7
8	E	0	1
11	H	0	1
12	J	0	3
14	M	0	1
16	O	0	1
17	P	0	1
18	R	0	2
20	T	0	3
23	W	0	3
25	Z	0	2
32	d	0	1
32	k	0	1
38	Y	0	15

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
41	D	0	1
All	All	0	49

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	104	LEU	CB-CG	55.56	2.64	1.53
7	C	172	PHE	CE1-CZ	53.27	2.98	1.38
7	C	172	PHE	CD1-CE1	52.29	2.95	1.38
7	C	172	PHE	CD2-CE2	51.50	2.93	1.38
7	C	172	PHE	CE2-CZ	50.12	2.89	1.38
7	C	172	PHE	CG-CD1	34.22	2.10	1.38
7	C	172	PHE	CG-CD2	34.14	2.10	1.38
11	H	142	C	C1'-N1	7.72	1.60	1.48
11	H	77	C	C1'-N1	7.53	1.59	1.48
39	K	186	VAL	CA-CB	-7.35	1.44	1.54
11	H	69	U	C1'-N1	7.23	1.59	1.48
11	H	54	U	C1'-N1	7.21	1.59	1.48
11	H	91	U	C1'-N1	7.19	1.59	1.48
6	B	103	G	C1'-N9	-7.17	1.37	1.48
11	H	60	U	C1'-N1	7.11	1.59	1.48
11	H	74	U	C1'-N1	7.08	1.59	1.48
11	H	89	U	C1'-N1	7.07	1.59	1.48
11	H	72	U	C1'-N1	7.06	1.59	1.48
11	H	150	U	C1'-N1	6.99	1.58	1.48
11	H	55	U	C1'-N1	6.99	1.58	1.48
11	H	92	U	C1'-N1	6.96	1.58	1.48
11	H	182	U	C1'-N1	6.95	1.58	1.48
11	H	58	U	C1'-N1	6.93	1.58	1.48
7	C	104	LEU	CG-CD1	6.65	1.74	1.52
11	H	73	C	C1'-N1	6.61	1.58	1.48
11	H	78	C	C1'-N1	6.56	1.58	1.48
11	H	151	C	C1'-N1	6.55	1.58	1.48
11	H	141	C	C1'-N1	6.54	1.58	1.48
7	C	104	LEU	CG-CD2	6.52	1.74	1.52
11	H	184	C	C1'-N1	6.49	1.58	1.48
11	H	67	C	C1'-N1	6.44	1.58	1.48
11	H	84	C	C1'-N1	6.44	1.58	1.48
11	H	148	C	C1'-N1	6.44	1.58	1.48
11	H	71	C	C1'-N1	6.42	1.58	1.48
11	H	70	C	C1'-N1	6.38	1.58	1.48
7	C	926	ALA	C-N	6.37	1.41	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	N	137	CYS	CB-SG	-5.96	1.61	1.81
13	L	793	LEU	CA-CB	-5.35	1.44	1.53
5	A	2105	ILE	CA-CB	-5.15	1.48	1.54
33	m	14	LEU	CA-C	5.07	1.59	1.52

All (321) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	104	LEU	CD1-CG-CD2	-12.80	82.65	110.80
10	G	131	U	C2'-C3'-O3'	-12.13	95.51	113.70
7	C	104	LEU	CA-CB-CG	11.85	157.76	116.30
5	A	624	GLY	CA-C-N	10.96	131.27	119.87
5	A	624	GLY	C-N-CA	10.96	131.27	119.87
34	l	90	VAL	N-CA-C	10.93	120.91	110.42
38	Y	396	ASP	CA-C-N	10.71	130.94	119.05
38	Y	396	ASP	C-N-CA	10.71	130.94	119.05
3	u	37	THR	CA-C-N	10.64	130.41	119.56
3	u	37	THR	C-N-CA	10.64	130.41	119.56
20	T	405	PHE	N-CA-C	10.49	122.72	111.28
2	w	114	LYS	N-CA-C	-10.46	93.67	110.20
6	B	104	C	C2'-C3'-O3'	-10.04	94.44	109.50
7	C	104	LEU	CB-CG-CD1	9.35	138.75	110.70
11	H	39	U	C2'-C3'-O3'	8.80	126.90	113.70
11	H	54	U	O3'-P-O5'	-8.69	90.97	104.00
11	H	82	G	O3'-P-O5'	-8.69	90.97	104.00
40	r	46	PRO	N-CA-CB	8.68	111.08	103.27
11	H	150	U	O3'-P-O5'	-8.67	91.00	104.00
11	H	84	C	O3'-P-O5'	-8.66	91.00	104.00
11	H	88	A	O3'-P-O5'	-8.66	91.00	104.00
11	H	93	A	O3'-P-O5'	-8.65	91.03	104.00
11	H	78	C	O3'-P-O5'	-8.64	91.04	104.00
11	H	73	C	O3'-P-O5'	-8.63	91.05	104.00
11	H	55	U	O3'-P-O5'	-8.62	91.06	104.00
11	H	83	A	O3'-P-O5'	-8.62	91.06	104.00
7	C	104	LEU	CB-CG-CD2	8.62	136.56	110.70
11	H	67	C	O3'-P-O5'	-8.62	91.07	104.00
11	H	181	G	O3'-P-O5'	-8.62	91.07	104.00
11	H	92	U	O3'-P-O5'	-8.61	91.08	104.00
11	H	141	C	O3'-P-O5'	-8.61	91.09	104.00
11	H	74	U	O3'-P-O5'	-8.60	91.10	104.00
11	H	80	A	O3'-P-O5'	-8.60	91.11	104.00
11	H	180	G	O3'-P-O5'	-8.59	91.12	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	H	59	A	O3'-P-O5'	-8.58	91.12	104.00
11	H	56	A	O3'-P-O5'	-8.58	91.13	104.00
11	H	79	G	O3'-P-O5'	-8.58	91.13	104.00
11	H	57	A	O3'-P-O5'	-8.57	91.14	104.00
11	H	69	U	O3'-P-O5'	-8.55	91.17	104.00
11	H	148	C	O3'-P-O5'	-8.55	91.17	104.00
11	H	182	U	O3'-P-O5'	-8.55	91.18	104.00
11	H	149	A	O3'-P-O5'	-8.54	91.19	104.00
11	H	89	U	O3'-P-O5'	-8.53	91.20	104.00
11	H	72	U	O3'-P-O5'	-8.53	91.20	104.00
40	q	46	PRO	N-CA-CB	8.53	111.27	103.34
11	H	91	U	O3'-P-O5'	-8.53	91.21	104.00
11	H	183	G	O3'-P-O5'	-8.53	91.21	104.00
11	H	58	U	O3'-P-O5'	-8.52	91.22	104.00
26	I	601	GLN	N-CA-C	8.52	122.90	108.67
11	H	70	C	O3'-P-O5'	-8.52	91.22	104.00
11	H	71	C	O3'-P-O5'	-8.52	91.23	104.00
11	H	68	G	O3'-P-O5'	-8.51	91.24	104.00
11	H	81	G	O3'-P-O5'	-8.51	91.24	104.00
11	H	90	A	O3'-P-O5'	-8.50	91.24	104.00
11	H	77	C	O3'-P-O5'	-8.48	91.28	104.00
36	o	5	THR	N-CA-CB	-8.48	98.34	111.05
7	C	172	PHE	CD1-CG-CD2	8.43	131.24	118.60
6	B	80	U	C2'-C3'-O3'	8.13	121.70	109.50
10	G	137	C	C3'-C2'-O2'	8.12	122.88	110.70
36	o	16	THR	CA-C-O	-8.03	111.77	120.36
25	Z	163	TYR	N-CA-C	-7.99	102.52	111.14
36	o	99	SER	N-CA-C	7.92	122.71	112.26
36	o	117	TYR	CA-C-O	7.71	128.50	120.40
28	Q	1379	TYR	N-CA-C	7.61	122.65	112.30
13	L	563	PRO	N-CA-CB	7.60	110.45	103.08
39	K	90	PRO	N-CA-CB	7.56	111.19	103.25
40	q	60	PRO	N-CA-CB	7.37	110.98	103.25
5	A	623	LYS	N-CA-C	-7.32	96.58	108.52
39	K	78	PRO	N-CA-CB	7.32	110.94	103.25
41	D	1044	VAL	CA-C-N	7.28	126.78	118.85
41	D	1044	VAL	C-N-CA	7.28	126.78	118.85
26	I	588	PRO	N-CA-CB	7.26	110.12	103.08
10	G	137	C	C2'-C3'-O3'	7.24	124.56	113.70
36	o	71	VAL	CA-C-N	7.24	131.68	120.75
36	o	71	VAL	C-N-CA	7.24	131.68	120.75
23	W	257	ILE	CA-C-N	7.22	128.87	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	257	ILE	C-N-CA	7.22	128.87	119.84
41	D	1666	THR	N-CA-C	7.18	121.48	112.87
12	J	522	PRO	N-CA-CB	7.15	110.01	103.08
36	o	47	ILE	N-CA-CB	7.13	123.13	111.58
3	u	77	ASP	N-CA-C	-7.10	99.77	110.28
12	J	187	VAL	CA-C-N	7.09	135.09	121.54
12	J	187	VAL	C-N-CA	7.09	135.09	121.54
7	C	678	THR	N-CA-C	-7.05	99.78	110.50
41	D	533	VAL	N-CA-C	7.05	118.92	112.29
36	o	121	LEU	CA-C-O	6.93	128.93	121.44
26	I	589	PRO	N-CA-CB	6.91	110.85	103.39
36	o	4	LEU	N-CA-C	-6.89	97.99	108.67
18	R	225	PRO	CA-C-N	6.88	126.84	119.76
18	R	225	PRO	C-N-CA	6.88	126.84	119.76
26	I	475	PRO	N-CA-CB	6.87	110.80	103.52
13	L	594	PRO	N-CA-CB	6.86	110.46	103.25
26	I	160	PRO	N-CA-CB	6.86	110.45	103.25
40	r	19	PRO	N-CA-CB	6.83	110.41	102.76
12	J	604	PRO	N-CA-CB	6.80	110.39	103.25
13	L	558	PRO	N-CA-CB	6.77	110.70	103.52
37	p	53	PHE	CA-C-O	-6.76	112.88	120.32
12	J	637	PRO	N-CA-CB	6.76	110.68	103.52
36	o	58	ASP	N-CA-CB	-6.74	100.58	111.24
40	q	19	PRO	N-CA-CB	6.72	110.31	103.25
12	J	675	PRO	N-CA-CB	6.71	110.30	103.25
26	I	162	PRO	N-CA-CB	6.69	110.62	103.52
26	I	232	PRO	N-CA-CB	6.69	110.61	103.52
26	I	387	PRO	N-CA-CB	6.68	110.35	103.00
26	I	602	LEU	N-CA-C	6.67	118.55	111.28
26	I	722	GLU	N-CA-C	6.67	118.55	111.28
26	I	816	PRO	N-CA-CB	6.63	110.55	103.52
12	J	488	PRO	N-CA-CB	6.62	110.20	103.25
12	J	523	PRO	N-CA-CB	6.58	110.49	103.52
13	L	620	PRO	N-CA-CB	6.57	110.14	103.25
3	u	38	PRO	N-CA-C	6.56	122.37	113.84
12	J	239	ARG	CA-C-N	6.54	134.04	121.54
12	J	239	ARG	C-N-CA	6.54	134.04	121.54
26	I	518	PRO	N-CA-CB	6.46	110.37	103.52
15	N	35	GLU	N-CA-C	-6.44	100.03	109.50
38	Y	1038	THR	N-CA-C	6.41	118.84	111.02
26	I	371	PRO	N-CA-CB	6.40	110.61	103.44
26	I	463	PRO	N-CA-CB	6.39	109.96	103.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	I	394	PRO	N-CA-CB	6.38	110.59	103.44
11	H	40	C	C4'-C3'-O3'	6.38	122.57	113.00
20	T	342	GLU	CA-C-N	6.37	127.80	119.84
20	T	342	GLU	C-N-CA	6.37	127.80	119.84
26	I	788	PRO	N-CA-CB	6.37	110.57	103.44
11	H	104	U	C2'-C3'-O3'	6.37	123.25	113.70
26	I	177	PRO	N-CA-CB	6.37	110.57	103.44
13	L	546	PRO	N-CA-CB	6.34	110.54	103.44
5	A	1019	TYR	N-CA-C	-6.33	99.71	109.14
36	o	87	LEU	CA-C-N	6.33	126.24	119.28
36	o	87	LEU	C-N-CA	6.33	126.24	119.28
12	J	670	PRO	N-CA-CB	6.33	110.53	103.44
36	o	40	THR	CA-C-N	6.31	131.56	122.40
36	o	40	THR	C-N-CA	6.31	131.56	122.40
13	L	564	PRO	N-CA-CB	6.29	110.19	103.52
3	u	68	ALA	N-CA-C	6.28	119.42	111.69
23	W	318	VAL	N-CA-C	6.28	116.96	110.36
7	C	756	LYS	N-CA-C	6.27	118.63	111.11
5	A	1091	TYR	N-CA-C	-6.19	100.21	110.17
1	v	142	LYS	N-CA-C	6.13	118.62	109.25
28	Q	522	VAL	N-CA-C	-6.12	99.61	108.17
13	L	548	PRO	N-CA-CB	6.11	110.29	103.44
36	o	73	ASN	N-CA-C	6.11	119.78	111.17
41	D	1006	LYS	CA-C-N	6.09	126.27	119.32
41	D	1006	LYS	C-N-CA	6.09	126.27	119.32
38	Y	994	ILE	O-C-N	-6.09	114.95	122.57
5	A	1362	ASP	CA-C-N	6.08	130.37	121.31
5	A	1362	ASP	C-N-CA	6.08	130.37	121.31
10	G	1	G	C4'-C3'-O3'	6.07	122.10	113.00
12	J	551	PRO	N-CA-CB	6.06	110.23	103.44
3	u	339	ARG	N-CA-C	6.05	119.58	109.95
36	o	75	ARG	N-CA-CB	-6.03	102.59	111.51
12	J	566	PRO	N-CA-CB	6.03	110.19	103.44
13	L	753	GLU	N-CA-C	-6.03	104.34	111.03
3	u	178	THR	N-CA-C	6.00	120.73	113.17
26	I	761	PRO	N-CA-CB	5.99	109.86	103.39
40	r	59	HIS	CA-C-N	5.98	127.31	119.84
40	r	59	HIS	C-N-CA	5.98	127.31	119.84
36	o	79	ILE	CA-C-N	5.97	125.77	120.10
36	o	79	ILE	C-N-CA	5.97	125.77	120.10
20	T	342	GLU	C-N-CD	-5.96	100.57	125.00
23	W	251	GLY	N-CA-C	-5.93	99.12	113.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2199	ILE	CB-CA-C	-5.90	104.28	112.02
36	o	113	LYS	N-CA-C	5.89	118.45	111.33
37	p	46	MET	N-CA-C	-5.89	104.77	111.07
38	Y	672	ILE	CA-C-N	5.88	127.45	122.28
38	Y	672	ILE	C-N-CA	5.88	127.45	122.28
41	D	1291	LEU	CA-C-N	5.86	126.19	119.92
41	D	1291	LEU	C-N-CA	5.86	126.19	119.92
36	o	27	ARG	CB-CA-C	-5.86	98.76	109.54
35	n	67	ILE	CB-CA-C	-5.85	104.91	111.23
36	o	50	SER	CA-C-O	5.85	127.75	121.55
26	I	625	PRO	N-CA-CB	5.82	109.73	103.33
35	g	67	ILE	CB-CA-C	-5.82	104.94	111.23
38	Y	811	PRO	CA-C-N	5.78	130.79	121.95
38	Y	811	PRO	C-N-CA	5.78	130.79	121.95
3	u	336	VAL	N-CA-C	-5.75	103.99	112.04
41	D	782	PHE	N-CA-C	5.74	118.14	109.41
36	o	149	LYS	CB-CA-C	-5.74	101.89	110.16
12	J	205	LEU	CA-C-N	5.72	135.76	121.80
12	J	205	LEU	C-N-CA	5.72	135.76	121.80
5	A	2153	THR	N-CA-C	-5.69	101.76	109.95
3	u	210	PRO	N-CA-C	5.65	121.38	113.53
15	N	41	ARG	N-CA-C	-5.64	100.80	108.24
36	o	27	ARG	CA-C-N	5.63	128.62	120.11
36	o	27	ARG	C-N-CA	5.63	128.62	120.11
36	o	71	VAL	O-C-N	-5.63	115.53	122.57
41	D	1048	VAL	N-CA-C	-5.63	106.30	113.22
41	D	1135	LEU	CA-C-N	5.62	125.55	119.76
41	D	1135	LEU	C-N-CA	5.62	125.55	119.76
38	Y	663	ASP	O-C-N	-5.61	115.12	122.59
7	C	710	ASN	CA-C-N	5.61	128.06	120.38
7	C	710	ASN	C-N-CA	5.61	128.06	120.38
36	o	159	GLU	N-CA-C	-5.59	104.81	111.69
1	v	114	LYS	N-CA-C	-5.59	100.56	109.96
10	G	1	G	C2'-C3'-O3'	5.59	122.09	113.70
7	C	800	PRO	CA-C-N	5.57	128.53	120.79
7	C	800	PRO	C-N-CA	5.57	128.53	120.79
38	Y	410	VAL	N-CA-C	5.56	116.33	110.72
16	O	105	ASP	CA-C-N	5.55	128.98	120.82
16	O	105	ASP	C-N-CA	5.55	128.98	120.82
5	A	2225	LEU	N-CA-C	5.54	117.81	109.23
11	H	165	A	N9-C1'-C2'	5.53	120.30	112.00
5	A	2241	ASN	N-CA-C	5.52	118.32	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	52	LYS	CA-C-N	-5.52	114.24	119.76
30	b	52	LYS	C-N-CA	-5.52	114.24	119.76
8	E	60	MET	N-CA-C	5.52	119.04	111.54
38	Y	1097	GLY	CA-C-N	5.51	132.07	121.54
38	Y	1097	GLY	C-N-CA	5.51	132.07	121.54
5	A	2203	ASN	N-CA-C	5.51	120.85	109.11
11	H	157	G	P-O5'-C5'	-5.51	112.64	120.90
38	Y	738	PRO	N-CA-C	5.50	123.81	112.47
3	u	384	ASP	N-CA-C	5.50	117.70	111.11
36	o	32	PRO	CA-C-N	5.49	130.62	122.99
36	o	32	PRO	C-N-CA	5.49	130.62	122.99
30	i	52	LYS	CA-C-N	-5.49	114.27	119.76
30	i	52	LYS	C-N-CA	-5.49	114.27	119.76
36	o	16	THR	O-C-N	5.49	129.48	123.22
30	i	5	LYS	N-CA-C	5.47	118.17	111.82
5	A	1189	MET	CA-C-N	5.46	131.97	121.54
5	A	1189	MET	C-N-CA	5.46	131.97	121.54
36	o	34	ILE	CA-C-O	-5.46	114.30	120.74
2	w	115	GLY	N-CA-C	5.45	126.11	113.18
39	K	116	HIS	N-CA-C	-5.45	105.25	111.14
11	H	160	A	P-O5'-C5'	-5.44	112.74	120.90
25	Z	111	ILE	CA-C-N	5.44	128.73	120.13
25	Z	111	ILE	C-N-CA	5.44	128.73	120.13
26	I	601	GLN	CB-CA-C	-5.41	109.87	117.23
41	D	1228	VAL	CB-CA-C	-5.40	104.96	112.04
36	o	40	THR	N-CA-C	-5.38	106.22	112.89
5	A	2100	THR	N-CA-C	-5.37	106.73	113.28
38	Y	869	THR	CA-C-N	5.36	131.92	121.41
38	Y	869	THR	C-N-CA	5.36	131.92	121.41
41	D	1228	VAL	N-CA-C	5.36	116.73	110.62
8	E	57	ALA	CA-C-N	5.35	125.42	119.32
8	E	57	ALA	C-N-CA	5.35	125.42	119.32
7	C	560	VAL	N-CA-C	-5.35	102.07	109.46
41	D	2096	ALA	CA-C-N	5.35	125.56	120.31
41	D	2096	ALA	C-N-CA	5.35	125.56	120.31
41	D	1693	ARG	CA-C-N	5.35	125.16	119.28
41	D	1693	ARG	C-N-CA	5.35	125.16	119.28
5	A	619	GLY	CA-C-N	5.34	124.97	119.05
5	A	619	GLY	C-N-CA	5.34	124.97	119.05
30	b	5	LYS	N-CA-C	5.31	117.98	111.82
7	C	167	TYR	N-CA-C	5.31	117.65	110.06
41	D	488	LEU	N-CA-C	5.30	119.85	113.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	485	ASP	N-CA-C	5.30	116.75	110.97
25	Z	164	ASP	N-CA-C	5.30	117.06	111.28
36	o	88	PRO	CB-CA-C	-5.30	103.95	112.21
36	o	125	VAL	CA-C-N	5.29	127.90	120.28
36	o	125	VAL	C-N-CA	5.29	127.90	120.28
37	p	6	ASN	N-CA-CB	-5.29	101.69	111.53
41	D	749	GLY	N-CA-C	-5.29	108.40	114.69
7	C	83	GLU	CA-C-N	5.28	131.62	121.54
7	C	83	GLU	C-N-CA	5.28	131.62	121.54
23	W	317	GLU	CA-C-N	5.27	127.40	120.60
23	W	317	GLU	C-N-CA	5.27	127.40	120.60
36	o	33	VAL	N-CA-CB	-5.27	103.83	111.52
38	Y	609	SER	CA-C-N	5.26	131.59	121.54
38	Y	609	SER	C-N-CA	5.26	131.59	121.54
36	o	146	ASP	CA-C-N	5.26	130.02	122.40
36	o	146	ASP	C-N-CA	5.26	130.02	122.40
40	r	111	ASP	CA-C-N	5.25	127.32	120.28
40	r	111	ASP	C-N-CA	5.25	127.32	120.28
38	Y	979	ARG	CA-C-N	5.25	127.26	120.44
38	Y	979	ARG	C-N-CA	5.25	127.26	120.44
11	H	39	U	O4'-C1'-C2'	-5.23	102.37	107.60
3	u	163	THR	N-CA-C	-5.21	103.61	110.39
5	A	669	ALA	N-CA-C	5.21	117.01	110.91
5	A	1203	SER	CA-C-N	5.21	128.63	120.82
5	A	1203	SER	C-N-CA	5.21	128.63	120.82
37	p	48	MET	N-CA-C	5.20	119.63	113.28
5	A	848	GLU	CA-C-N	5.20	127.50	120.38
5	A	848	GLU	C-N-CA	5.20	127.50	120.38
41	D	1127	CYS	CA-C-N	5.19	125.49	119.47
41	D	1127	CYS	C-N-CA	5.19	125.49	119.47
23	W	257	ILE	N-CA-C	5.18	120.07	108.88
3	u	367	ARG	N-CA-C	-5.18	106.23	112.54
37	p	51	GLN	N-CA-C	5.17	117.54	109.52
41	D	811	SER	N-CA-C	5.17	114.96	108.45
15	N	35	GLU	CA-C-N	-5.15	113.40	119.84
15	N	35	GLU	C-N-CA	-5.15	113.40	119.84
38	Y	656	THR	CA-C-N	5.15	128.86	121.55
38	Y	656	THR	C-N-CA	5.15	128.86	121.55
20	T	407	GLN	N-CA-C	5.14	118.33	110.36
11	H	160	A	C4'-C3'-C2'	-5.14	97.46	102.60
3	u	342	ASP	N-CA-C	5.13	117.07	107.99
41	D	572	ASP	N-CA-C	-5.13	103.38	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	749	THR	CA-C-N	5.12	127.34	120.58
7	C	749	THR	C-N-CA	5.12	127.34	120.58
41	D	1875	VAL	CA-C-N	5.12	124.57	119.24
41	D	1875	VAL	C-N-CA	5.12	124.57	119.24
2	w	148	TRP	N-CA-C	-5.12	103.28	110.50
36	o	90	LEU	O-C-N	5.12	129.40	122.59
36	o	90	LEU	CA-C-O	-5.12	113.19	120.51
32	k	99	MET	N-CA-C	5.12	116.84	108.76
28	Q	568	ARG	CA-C-N	5.11	125.11	119.90
28	Q	568	ARG	C-N-CA	5.11	125.11	119.90
13	L	145	ASP	CA-C-N	5.11	128.85	120.63
13	L	145	ASP	C-N-CA	5.11	128.85	120.63
38	Y	814	SER	N-CA-C	5.10	118.28	111.75
5	A	2185	SER	CA-C-N	-5.10	116.50	121.65
5	A	2185	SER	C-N-CA	-5.10	116.50	121.65
11	H	156	U	C4'-C3'-C2'	5.10	107.70	102.60
2	w	107	ASP	N-CA-C	-5.09	102.10	109.59
15	N	34	THR	N-CA-C	5.09	119.64	113.38
37	p	83	TYR	CA-C-O	-5.08	115.25	121.05
25	Z	112	ILE	CA-C-N	5.07	129.76	122.35
25	Z	112	ILE	C-N-CA	5.07	129.76	122.35
1	v	141	PHE	N-CA-C	5.06	120.11	113.88
32	d	99	MET	N-CA-C	5.06	116.75	108.76
36	o	139	VAL	CA-C-N	5.04	124.70	119.56
36	o	139	VAL	C-N-CA	5.04	124.70	119.56
11	H	155	C	P-O3'-C3'	5.03	127.75	120.20
36	o	83	LEU	N-CA-C	5.03	117.42	111.33
34	l	85	THR	N-CA-C	-5.03	106.00	112.68
20	T	401	PRO	CA-C-N	5.02	134.96	125.66
20	T	401	PRO	C-N-CA	5.02	134.96	125.66
31	c	78	THR	CB-CA-C	-5.02	103.00	110.88
34	e	85	THR	N-CA-C	-5.02	106.01	112.68
41	D	574	GLN	N-CA-C	5.02	117.86	111.69
5	A	903	SER	N-CA-C	-5.01	108.20	114.56
36	o	28	GLY	N-CA-C	5.00	120.78	113.48

There are no chirality outliers.

All (49) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	A	1070	ASP	Peptide
5	A	1091	TYR	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
5	A	1209	HIS	Peptide
5	A	1502	PHE	Peptide
5	A	851	SER	Peptide
5	A	941	LYS	Peptide
7	C	103	THR	Peptide
7	C	167	TYR	Peptide
7	C	439	PRO	Peptide
7	C	456	GLY	Peptide
7	C	534	VAL	Peptide
7	C	560	VAL	Peptide
7	C	93	ILE	Peptide
41	D	430	LEU	Peptide
8	E	192	ASN	Peptide
11	H	40	C	Sidechain
12	J	205	LEU	Peptide
12	J	240	THR	Peptide
12	J	241	VAL	Peptide
14	M	124	PHE	Peptide
16	O	133	PRO	Peptide
17	P	204	GLN	Peptide
18	R	183	GLN	Peptide
18	R	185	GLY	Peptide
20	T	185	MET	Peptide
20	T	400	PHE	Peptide
20	T	457	GLY	Peptide
23	W	198	LYS	Peptide
23	W	242	HIS	Peptide
23	W	245	GLU	Peptide
38	Y	1098	LYS	Peptide
38	Y	1127	LEU	Peptide
38	Y	1163	ARG	Peptide
38	Y	1187	THR	Peptide
38	Y	515	ASP	Peptide
38	Y	550	TYR	Peptide
38	Y	563	GLU	Peptide
38	Y	636	CYS	Peptide
38	Y	662	THR	Peptide
38	Y	811	PRO	Peptide
38	Y	855	VAL	Peptide
38	Y	868	LYS	Peptide
38	Y	938	ASN	Peptide
38	Y	963	THR	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
38	Y	993	LEU	Peptide
25	Z	135	GLU	Peptide
25	Z	92	GLN	Peptide
32	d	112	ASN	Peptide
32	k	112	ASN	Peptide

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	v	711	0	299	6	0
2	w	445	0	203	6	0
3	u	1907	0	845	2	0
4	x	124	0	51	0	0
5	A	17837	0	17053	242	0
6	B	2040	0	1034	66	0
7	C	7066	0	7084	131	0
8	E	2366	0	2303	67	0
9	F	2075	0	1048	27	0
10	G	1549	0	784	51	0
11	H	2966	0	1505	256	0
12	J	3829	0	2907	40	0
13	L	3064	0	2521	53	0
14	M	1098	0	1082	24	0
15	N	1184	0	1189	41	0
16	O	2296	0	2284	36	0
17	P	929	0	910	7	0
18	R	2073	0	2119	37	0
19	S	1236	0	1210	25	0
20	T	2461	0	2420	70	0
21	U	193	0	196	5	0
22	V	2765	0	1955	17	0
23	W	4122	0	4031	154	0
24	X	701	0	631	56	0
25	Z	1999	0	1951	35	0
26	I	2782	0	1245	54	0
27	y	390	0	190	1	0
28	Q	6562	0	2836	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	a	399	0	173	0	0
29	h	398	0	172	1	0
30	b	424	0	179	1	0
30	i	424	0	179	3	0
31	c	406	0	170	1	0
31	j	406	0	170	3	0
32	d	480	0	200	8	0
32	k	422	0	175	5	0
33	f	361	0	158	1	0
33	m	356	0	156	1	0
34	e	391	0	163	5	0
34	l	391	0	163	28	0
35	g	363	0	160	4	0
35	n	339	0	145	45	0
36	o	804	0	350	2	0
37	p	464	0	205	16	0
38	Y	2917	0	857	15	0
39	K	757	0	338	52	0
40	q	659	0	296	23	0
40	r	654	0	294	33	0
40	s	335	0	168	5	0
40	t	335	0	168	8	0
41	D	8530	0	3747	12	0
42	A	36	0	6	3	0
43	C	32	0	12	2	0
44	C	1	0	0	0	0
44	F	6	0	0	0	0
44	Q	2	0	0	0	0
45	N	3	0	0	0	0
45	O	3	0	0	0	0
45	Z	1	0	0	0	0
46	Q	31	0	12	0	0
All	All	97900	0	70702	1400	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 8.

All (1400) 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)
23:W:266:ARG:HB2	34:I:16:GLN:CB	1.23	1.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:104:LEU:CG	7:C:104:LEU:CD1	1.74	1.61
12:J:466:ARG:CB	26:I:607:GLY:HA2	1.44	1.47
23:W:257:ILE:HG13	35:n:10:LYS:CB	1.47	1.45
23:W:264:ASN:HB3	35:n:35:ASP:CA	1.43	1.44
8:E:56:GLN:NE2	8:E:97:GLY:HA2	1.35	1.40
7:C:172:PHE:CD1	7:C:172:PHE:CG	2.10	1.39
7:C:172:PHE:CG	7:C:172:PHE:CD2	2.10	1.39
23:W:257:ILE:HD12	23:W:258:PRO:CD	1.51	1.36
23:W:257:ILE:CD1	23:W:258:PRO:HD2	1.54	1.34
24:X:109:PHE:CE2	34:l:91:SER:CB	2.10	1.33
11:H:150:U:O3'	24:X:124:THR:HG22	1.31	1.27
26:I:331:LEU:CB	26:I:340:ARG:CB	2.12	1.26
39:K:39:GLU:CB	40:r:112:ALA:HB1	1.67	1.25
11:H:167:U:O4	37:p:41:VAL:HA	1.34	1.24
39:K:81:LEU:CB	40:t:72:PRO:HA	1.67	1.24
39:K:113:GLN:O	39:K:117:GLN:CB	1.87	1.22
23:W:266:ARG:CB	34:l:16:GLN:CB	2.17	1.21
23:W:264:ASN:CB	35:n:35:ASP:HA	1.70	1.19
40:q:22:ASN:CB	40:r:55:ILE:HA	1.72	1.18
23:W:264:ASN:ND2	35:n:35:ASP:CB	2.08	1.17
23:W:258:PRO:CG	23:W:265:LEU:HD22	1.74	1.16
20:T:342:GLU:CB	20:T:343:PRO:HD2	1.63	1.15
23:W:258:PRO:HG3	23:W:265:LEU:CD2	1.74	1.15
24:X:109:PHE:CD2	34:l:91:SER:CB	2.29	1.14
11:H:165:A:H61	37:p:87:ASP:C	1.54	1.14
20:T:399:LYS:HB2	20:T:406:ILE:HD11	1.14	1.13
12:J:427:LYS:NZ	26:I:579:LEU:CB	2.12	1.13
26:I:612:ALA:CB	26:I:623:VAL:CB	2.26	1.12
12:J:484:VAL:CB	26:I:642:ILE:CB	2.28	1.12
13:L:608:ASN:HA	40:q:112:ALA:CB	1.77	1.12
11:H:165:A:H61	37:p:88:SER:N	1.48	1.11
24:X:109:PHE:CZ	34:l:89:SER:O	2.03	1.11
39:K:112:ALA:O	39:K:116:HIS:CB	1.98	1.11
24:X:109:PHE:HE2	34:l:91:SER:CB	1.54	1.10
7:C:104:LEU:CD1	7:C:104:LEU:CD2	2.30	1.10
26:I:296:PHE:HA	26:I:305:SER:CB	1.80	1.10
26:I:346:ASN:CB	28:Q:524:LYS:CB	2.30	1.10
11:H:165:A:N6	37:p:87:ASP:C	2.08	1.10
11:H:150:U:H5''	24:X:124:THR:CB	1.81	1.10
12:J:466:ARG:CB	26:I:607:GLY:CA	2.30	1.09
39:K:39:GLU:C	40:r:112:ALA:CB	2.23	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:427:LYS:CE	26:I:579:LEU:CB	2.30	1.09
24:X:110:GLN:HG3	34:I:91:SER:O	1.53	1.08
10:G:138:A:C2	11:H:39:U:O2	2.07	1.08
26:I:612:ALA:HB2	26:I:623:VAL:CB	1.84	1.07
11:H:150:U:H5''	24:X:124:THR:HB	1.31	1.07
23:W:257:ILE:HD12	23:W:258:PRO:N	1.67	1.07
39:K:39:GLU:CA	40:r:112:ALA:HB1	1.84	1.07
11:H:156:U:H6	11:H:156:U:H5''	1.09	1.07
11:H:150:U:H5''	24:X:124:THR:CG2	1.84	1.06
7:C:104:LEU:CB	7:C:104:LEU:HG	1.86	1.06
23:W:264:ASN:HB3	35:n:35:ASP:CB	1.84	1.05
23:W:264:ASN:HD22	35:n:35:ASP:CB	1.68	1.05
39:K:36:VAL:CB	40:r:113:ALA:HB2	1.86	1.05
39:K:39:GLU:C	40:r:112:ALA:HB2	1.80	1.05
8:E:56:GLN:HE22	8:E:97:GLY:CA	1.67	1.05
11:H:98:G:C6	32:k:61:ARG:CB	2.39	1.04
23:W:262:GLY:HA3	35:n:4:ALA:O	1.55	1.04
11:H:151:C:OP1	24:X:123:GLN:HB2	1.55	1.03
11:H:101:U:O2	29:h:66:SER:CB	2.06	1.03
20:T:342:GLU:HB3	20:T:343:PRO:CD	1.88	1.03
23:W:257:ILE:CG1	35:n:10:LYS:CB	2.35	1.03
8:E:60:MET:HG3	8:E:353:MET:SD	1.99	1.03
39:K:39:GLU:CB	40:r:112:ALA:CB	2.38	1.02
7:C:104:LEU:HD11	7:C:104:LEU:HD21	1.40	1.01
11:H:105:G:O6	31:j:20:LYS:CB	2.10	0.99
8:E:56:GLN:NE2	8:E:97:GLY:CA	2.23	0.99
5:A:1976:TRP:O	5:A:1980:GLU:HG3	1.62	0.99
11:H:106:G:H4'	11:H:107:A:OP1	1.62	0.99
5:A:1945:VAL:HG11	5:A:1990:ASP:CG	1.86	0.99
23:W:257:ILE:HD12	23:W:258:PRO:HD2	1.05	0.98
24:X:120:ALA:O	24:X:124:THR:HG23	1.64	0.97
1:v:29:ASP:CB	2:w:154:PRO:CB	2.42	0.97
11:H:102:U:C2	30:i:37:HIS:CB	2.47	0.97
11:H:151:C:P	24:X:124:THR:HG22	2.05	0.96
8:E:60:MET:HB3	8:E:353:MET:HB2	1.45	0.96
39:K:15:ALA:CB	40:s:112:ALA:O	2.14	0.95
23:W:264:ASN:CB	35:n:35:ASP:CB	2.43	0.95
13:L:608:ASN:HA	40:q:112:ALA:HB1	1.48	0.95
23:W:261:VAL:C	35:n:6:PRO:CB	2.39	0.94
11:H:156:U:H5''	11:H:156:U:C6	2.02	0.94
5:A:1673:SER:CB	25:Z:164:ASP:OD1	2.15	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:150:U:C5'	24:X:124:THR:HB	1.97	0.93
39:K:81:LEU:CB	40:t:72:PRO:CA	2.46	0.93
11:H:150:U:OP1	24:X:124:THR:HB	1.69	0.93
23:W:257:ILE:HD13	23:W:258:PRO:HD2	1.51	0.92
8:E:54:SER:N	8:E:96:TYR:HE1	1.66	0.92
11:H:108:G:H2'	11:H:109:C:H6	1.31	0.92
16:O:72:GLN:HG3	16:O:82:GLN:HE22	1.35	0.92
39:K:39:GLU:C	40:r:112:ALA:HB1	1.91	0.92
23:W:257:ILE:HG12	35:n:10:LYS:HA	1.52	0.92
40:q:22:ASN:CB	40:r:55:ILE:CA	2.49	0.91
26:I:188:LYS:CB	27:y:28:PRO:CB	2.48	0.91
11:H:165:A:N1	37:p:88:SER:HA	1.86	0.91
23:W:264:ASN:CG	35:n:35:ASP:CB	2.44	0.91
6:B:93:U:O2	32:d:104:ASP:CB	2.18	0.91
26:I:280:GLU:C	26:I:288:THR:CB	2.43	0.91
11:H:106:G:H5'	11:H:106:G:H8	1.36	0.90
20:T:342:GLU:CB	20:T:343:PRO:CD	2.47	0.90
13:L:65:ARG:NH2	26:I:799:ARG:O	2.04	0.90
8:E:56:GLN:HE22	8:E:97:GLY:HA2	1.07	0.90
24:X:116:ASN:HB3	35:n:55:ASN:CB	2.02	0.89
10:G:138:A:N1	11:H:39:U:O2	2.05	0.89
11:H:100:U:H5'	11:H:100:U:C6	2.07	0.89
10:G:129:G:O3'	23:W:541:LYS:HE3	1.72	0.88
39:K:120:ARG:CB	40:r:69:THR:CB	2.51	0.88
11:H:104:U:O2	31:j:63:ASN:CB	2.21	0.88
20:T:399:LYS:CB	20:T:406:ILE:HD11	2.02	0.88
5:A:1673:SER:HB2	25:Z:164:ASP:OD1	1.74	0.88
20:T:342:GLU:HB3	20:T:343:PRO:HD2	0.91	0.88
39:K:39:GLU:CB	40:r:112:ALA:CA	2.51	0.88
23:W:262:GLY:HA2	35:n:6:PRO:CB	2.04	0.87
26:I:612:ALA:HB1	26:I:623:VAL:CB	2.04	0.87
11:H:154:C:O2	11:H:176:G:N2	2.07	0.87
11:H:98:G:C5	32:k:61:ARG:CB	2.58	0.87
13:L:732:MET:CB	40:q:65:PRO:CB	2.52	0.87
11:H:156:U:H6	11:H:156:U:C5'	1.89	0.86
11:H:166:G:N2	11:H:166:G:OP2	2.08	0.86
11:H:165:A:N1	37:p:88:SER:CB	2.37	0.86
8:E:56:GLN:HE21	8:E:97:GLY:HA2	1.36	0.86
7:C:104:LEU:HB3	7:C:172:PHE:CE1	2.11	0.85
39:K:131:GLY:O	39:K:135:TRP:CB	2.24	0.85
24:X:102:LYS:HE3	34:l:27:ASN:O	1.75	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:K:40:THR:N	40:r:112:ALA:HB2	1.91	0.85
23:W:266:ARG:HB2	34:l:16:GLN:CA	2.07	0.85
38:Y:405:MET:CE	38:Y:411:LEU:HD23	2.06	0.85
11:H:165:A:C6	37:p:88:SER:HA	2.09	0.85
38:Y:405:MET:CE	38:Y:411:LEU:CD2	2.54	0.85
8:E:54:SER:N	8:E:96:TYR:CE1	2.44	0.85
11:H:163:G:O6	37:p:12:ASN:CB	2.25	0.85
7:C:104:LEU:CD1	7:C:104:LEU:HD21	2.03	0.84
39:K:40:THR:N	40:r:112:ALA:CB	2.41	0.84
26:I:280:GLU:O	26:I:288:THR:CB	2.25	0.84
11:H:41:U:H5''	11:H:41:U:H6	1.43	0.83
11:H:98:G:H4'	11:H:98:G:OP2	1.78	0.83
11:H:152:G:N2	11:H:153:A:N7	2.26	0.83
11:H:165:A:N1	37:p:88:SER:CA	2.41	0.83
12:J:427:LYS:HE2	26:I:579:LEU:CB	2.09	0.83
23:W:257:ILE:CG1	35:n:10:LYS:HA	2.08	0.83
6:B:80:U:H2'	6:B:80:U:OP1	1.79	0.83
6:B:90:U:N3	35:g:37:PHE:HA	1.94	0.82
6:B:90:U:H3	35:g:37:PHE:HA	1.45	0.81
11:H:150:U:C3'	24:X:124:THR:HG22	2.10	0.81
23:W:257:ILE:HG13	35:n:10:LYS:CA	2.10	0.81
11:H:152:G:H5''	11:H:153:A:OP2	1.80	0.81
39:K:114:LEU:O	39:K:118:ALA:N	2.13	0.81
11:H:106:G:H5'	11:H:106:G:C8	2.16	0.81
5:A:1831:LYS:HG2	10:G:2:U:OP2	1.80	0.80
11:H:151:C:OP2	24:X:124:THR:HA	1.80	0.80
24:X:109:PHE:HD2	34:l:91:SER:CB	1.94	0.80
23:W:265:LEU:HD23	23:W:300:SER:CB	2.12	0.80
10:G:126:C:H4'	10:G:127:U:OP1	1.82	0.79
11:H:108:G:H2'	11:H:109:C:C6	2.17	0.79
10:G:130:A:O2'	10:G:131:U:OP2	1.99	0.79
5:A:1945:VAL:CG1	5:A:1990:ASP:CG	2.55	0.79
23:W:252:ARG:HH11	23:W:252:ARG:HG2	1.46	0.79
6:B:88:A:N3	34:e:53:TYR:CB	2.46	0.78
11:H:153:A:H2'	11:H:154:C:H5'	1.65	0.78
23:W:264:ASN:CB	35:n:35:ASP:CA	2.39	0.78
10:G:138:A:H2	11:H:39:U:O2	1.65	0.78
6:B:87:A:N7	32:d:61:ARG:CB	2.46	0.78
5:A:1980:GLU:OE1	25:Z:347:PRO:HD2	1.84	0.78
8:E:61:LEU:HG	8:E:62:LEU:N	1.97	0.78
11:H:150:U:OP1	24:X:124:THR:CB	2.32	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:142:U:O2'	10:G:143:U:OP1	2.01	0.77
28:Q:523:ALA:HB3	28:Q:534:ARG:H	1.48	0.77
5:A:1979:VAL:HA	5:A:1982:GLN:OE1	1.83	0.77
20:T:342:GLU:OE2	20:T:342:GLU:HA	1.82	0.77
23:W:264:ASN:HB3	35:n:35:ASP:HA	0.78	0.77
11:H:107:A:N3	11:H:107:A:H3'	2.00	0.77
11:H:177:A:H5''	11:H:178:A:OP1	1.84	0.77
12:J:427:LYS:HZ1	26:I:579:LEU:CB	1.95	0.77
11:H:102:U:O2	30:i:37:HIS:CB	2.33	0.76
20:T:399:LYS:HB2	20:T:406:ILE:CD1	2.07	0.76
11:H:150:U:H5''	24:X:124:THR:HG21	1.66	0.76
8:E:56:GLN:HE22	8:E:97:GLY:C	1.93	0.76
6:B:75:G:N7	6:B:76:A:C8	2.54	0.76
23:W:257:ILE:CG1	35:n:10:LYS:CA	2.62	0.76
11:H:143:A:H3'	11:H:143:A:N3	2.00	0.76
11:H:165:A:N6	37:p:88:SER:N	2.26	0.76
12:J:427:LYS:HZ3	26:I:579:LEU:CB	1.95	0.76
16:O:72:GLN:HG3	16:O:82:GLN:NE2	2.01	0.76
40:q:8:SER:O	40:q:9:ASN:CB	2.34	0.76
7:C:474:LEU:HA	7:C:498:SER:O	1.86	0.75
6:B:72:U:H1'	6:B:74:U:H1'	1.68	0.75
6:B:81:U:O2'	6:B:82:A:OP2	2.02	0.75
38:Y:405:MET:HE3	38:Y:411:LEU:HD23	1.67	0.75
10:G:129:G:H4'	23:W:541:LYS:CD	2.16	0.75
20:T:346:ILE:HD12	20:T:356:LEU:HD12	1.66	0.75
7:C:104:LEU:CG	7:C:104:LEU:CB	2.64	0.75
23:W:252:ARG:NH2	35:n:10:LYS:O	2.20	0.75
6:B:94:U:OP2	33:f:67:ASN:CB	2.35	0.74
24:X:116:ASN:CB	35:n:55:ASN:CB	2.65	0.74
26:I:720:ILE:O	26:I:721:LYS:CB	2.34	0.74
23:W:266:ARG:O	34:l:16:GLN:CB	2.35	0.74
12:J:493:ALA:HB1	12:J:499:ARG:CB	2.18	0.74
11:H:153:A:C2'	11:H:154:C:H5'	2.17	0.74
23:W:258:PRO:HB2	23:W:265:LEU:HD13	1.69	0.74
11:H:150:U:P	24:X:124:THR:HB	2.28	0.74
15:N:38:GLU:OE2	15:N:38:GLU:HA	1.87	0.74
39:K:36:VAL:O	40:r:112:ALA:HB3	1.87	0.74
6:B:87:A:C5	32:d:61:ARG:CB	2.71	0.74
11:H:165:A:N6	37:p:87:ASP:O	2.19	0.73
39:K:111:MET:O	40:t:90:PHE:CB	2.35	0.73
11:H:151:C:OP1	24:X:123:GLN:CB	2.36	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:41:U:H2'	11:H:42:G:C8	2.23	0.73
12:J:463:GLY:O	26:I:610:ARG:CB	2.37	0.73
39:K:15:ALA:HB3	40:s:112:ALA:O	1.88	0.73
5:A:1945:VAL:CG1	5:A:1990:ASP:OD2	2.37	0.73
23:W:257:ILE:CG2	35:n:10:LYS:CB	2.67	0.73
23:W:541:LYS:HB2	23:W:541:LYS:HZ2	1.54	0.73
11:H:179:C:H2'	11:H:180:G:H8	1.53	0.72
24:X:109:PHE:HZ	34:l:89:SER:O	1.67	0.72
7:C:104:LEU:HB2	7:C:172:PHE:CD1	2.25	0.72
11:H:153:A:H2'	11:H:154:C:C5'	2.19	0.72
5:A:1673:SER:HB3	25:Z:164:ASP:OD1	1.88	0.72
11:H:150:U:O3'	24:X:124:THR:CG2	2.24	0.72
24:X:102:LYS:CE	34:l:27:ASN:O	2.38	0.72
6:B:74:U:O4	6:B:75:G:O6	2.07	0.71
7:C:104:LEU:HB2	7:C:172:PHE:CG	2.25	0.71
11:H:39:U:C5'	11:H:39:U:H6	2.03	0.71
39:K:130:HIS:O	39:K:134:ALA:HB3	1.90	0.71
11:H:151:C:P	24:X:124:THR:CG2	2.78	0.71
5:A:1946:ASN:HD22	5:A:1986:LEU:HD11	1.54	0.71
11:H:105:G:N3	11:H:105:G:H2'	2.05	0.71
10:G:138:A:N1	11:H:39:U:C2	2.58	0.71
11:H:151:C:OP1	24:X:120:ALA:O	2.09	0.71
6:B:96:A:C6	6:B:97:G:C5	2.78	0.71
39:K:135:TRP:O	39:K:136:LYS:CB	2.38	0.71
34:l:15:VAL:O	35:n:33:GLY:HA3	1.90	0.71
7:C:104:LEU:HG	7:C:172:PHE:CE2	2.26	0.70
11:H:152:G:OP2	24:X:123:GLN:NE2	2.19	0.70
11:H:168:A:N6	35:n:54:GLN:CB	2.55	0.70
6:B:78:U:H6	6:B:78:U:H3'	1.57	0.70
39:K:70:PHE:CB	40:t:71:ILE:CB	2.70	0.70
23:W:252:ARG:HG3	23:W:253:SER:N	2.05	0.70
28:Q:523:ALA:HB3	28:Q:534:ARG:N	2.07	0.70
11:H:154:C:H2'	11:H:155:C:C6	2.26	0.70
23:W:258:PRO:HD2	23:W:266:ARG:HH12	1.56	0.69
5:A:1935:ARG:HH21	25:Z:348:THR:HG21	1.56	0.69
13:L:65:ARG:CZ	26:I:799:ARG:O	2.40	0.69
24:X:110:GLN:CG	34:l:91:SER:O	2.36	0.69
11:H:153:A:N6	11:H:177:A:C2	2.60	0.69
13:L:620:PRO:CB	40:q:108:TYR:CB	2.71	0.69
40:q:71:ILE:HA	40:r:81:GLU:CB	2.23	0.69
6:B:93:U:HI'	32:d:104:ASP:CB	2.22	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:671:THR:O	5:A:676:ARG:NH1	2.26	0.69
23:W:261:VAL:O	35:n:6:PRO:CB	2.41	0.69
11:H:97:G:H4'	11:H:99:A:OP1	1.91	0.69
11:H:150:U:H3	11:H:181:G:H1	1.41	0.68
23:W:257:ILE:CD1	23:W:258:PRO:CD	2.33	0.68
11:H:168:A:C6	35:n:54:GLN:CB	2.76	0.68
20:T:356:LEU:HD22	20:T:366:VAL:HB	1.74	0.68
11:H:150:U:C5'	24:X:124:THR:CG2	2.69	0.68
39:K:39:GLU:CB	40:r:112:ALA:O	2.41	0.68
10:G:137:C:C5'	10:G:137:C:H6	2.06	0.68
12:J:512:GLU:CB	26:I:640:ALA:N	2.57	0.68
13:L:65:ARG:NH2	26:I:799:ARG:HA	2.09	0.68
38:Y:405:MET:HE3	38:Y:411:LEU:CD2	2.21	0.68
11:H:152:G:O3'	11:H:153:A:O4'	2.11	0.67
5:A:1986:LEU:HD23	5:A:1986:LEU:C	2.19	0.67
11:H:143:A:H2'	11:H:144:C:H6	1.59	0.67
13:L:28:LYS:HE2	13:L:50:TRP:HE1	1.60	0.67
23:W:265:LEU:HD23	23:W:300:SER:HB2	1.76	0.67
20:T:329:HIS:ND1	20:T:349:SER:OG	2.27	0.67
26:I:337:LEU:CB	26:I:363:ARG:O	2.43	0.67
23:W:266:ARG:HD3	23:W:266:ARG:N	2.10	0.67
11:H:108:G:O2'	11:H:109:C:H5'	1.95	0.67
11:H:151:C:O2	11:H:152:G:C8	2.48	0.67
39:K:113:GLN:O	39:K:117:GLN:N	2.27	0.67
5:A:663:ARG:NH1	9:F:64:U:OP2	2.28	0.66
7:C:623:GLU:H	7:C:941:LYS:HZ2	1.41	0.66
23:W:262:GLY:CA	35:n:6:PRO:CB	2.73	0.66
6:B:96:A:O2'	6:B:97:G:H5'	1.95	0.66
20:T:270:VAL:HB	20:T:284:TYR:HB2	1.77	0.66
11:H:67:C:H42	11:H:85:A:H61	1.44	0.66
6:B:92:U:O4	30:b:36:LYS:O	2.14	0.66
13:L:65:ARG:NE	26:I:799:ARG:O	2.29	0.66
24:X:116:ASN:HD21	35:n:56:ASN:H	1.41	0.66
11:H:151:C:H2'	11:H:152:G:H8	1.59	0.66
23:W:541:LYS:HB2	23:W:541:LYS:NZ	2.10	0.66
11:H:151:C:C2	11:H:152:G:C8	2.84	0.66
34:l:30:ARG:O	34:l:90:VAL:N	2.28	0.66
6:B:96:A:C6	6:B:97:G:C6	2.84	0.66
5:A:761:ILE:HD12	5:A:775:ASN:HD22	1.61	0.66
20:T:314:ILE:HD11	20:T:326:LEU:HD21	1.78	0.65
11:H:153:A:C3'	11:H:154:C:H5'	2.25	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:266:ARG:HG3	34:I:15:VAL:O	1.97	0.65
26:I:296:PHE:CA	26:I:305:SER:CB	2.66	0.65
38:Y:405:MET:HE1	38:Y:411:LEU:HD23	1.78	0.65
11:H:75:A:H61	11:H:77:C:H42	1.43	0.65
23:W:445:TRP:HE1	23:W:452:ASP:HB3	1.62	0.65
5:A:1594:CYS:SG	25:Z:268:ARG:NH2	2.68	0.65
23:W:252:ARG:HH11	23:W:252:ARG:CG	2.10	0.65
5:A:188:LEU:HD22	5:A:567:GLY:HA2	1.79	0.65
8:E:56:GLN:HG2	8:E:57:ALA:N	2.11	0.65
5:A:1699:THR:HA	5:A:1717:ASN:HD22	1.62	0.65
23:W:257:ILE:HG23	35:n:10:LYS:CB	2.27	0.65
5:A:44:ARG:HH22	8:E:286:LYS:HB2	1.60	0.65
16:O:78:LYS:O	16:O:97:ARG:NH2	2.29	0.65
5:A:1945:VAL:HG13	5:A:1990:ASP:OD2	1.97	0.65
5:A:1437:ARG:NH1	5:A:1455:TRP:O	2.30	0.64
7:C:817:TYR:O	7:C:821:LEU:HB2	1.97	0.64
11:H:98:G:N3	11:H:98:G:H3'	2.13	0.64
23:W:258:PRO:HB2	23:W:265:LEU:CD1	2.26	0.64
11:H:153:A:H3'	11:H:154:C:H5'	1.79	0.64
39:K:39:GLU:CB	40:r:112:ALA:C	2.69	0.64
20:T:282:ARG:HB2	20:T:320:LYS:HD3	1.79	0.64
39:K:39:GLU:CB	40:r:112:ALA:HA	2.27	0.64
10:G:129:G:C4'	23:W:541:LYS:HE3	2.28	0.64
20:T:314:ILE:HD12	20:T:324:HIS:HB2	1.78	0.64
7:C:829:GLU:HB2	7:C:907:VAL:HG22	1.80	0.64
14:M:239:ARG:HD3	26:I:817:GLU:CB	2.28	0.64
23:W:313:ILE:HB	23:W:328:PHE:HB2	1.80	0.63
11:H:147:G:H2'	11:H:148:C:H6	1.62	0.63
20:T:458:SER:OG	20:T:459:LEU:N	2.32	0.63
23:W:258:PRO:HG3	23:W:265:LEU:HD22	0.82	0.63
5:A:270:ASN:HD21	21:U:8:PRO:HB3	1.63	0.63
7:C:224:GLY:HA3	7:C:438:ILE:HD12	1.81	0.63
10:G:137:C:H2'	10:G:138:A:C8	2.34	0.63
16:O:50:ARG:NH1	16:O:122:GLU:OE1	2.32	0.63
41:D:1992:GLU:HA	41:D:1995:ALA:HB3	1.80	0.63
5:A:200:ASP:OD1	5:A:240:ARG:NH2	2.32	0.63
11:H:154:C:H2'	11:H:155:C:H6	1.62	0.63
24:X:116:ASN:CG	35:n:55:ASN:CB	2.72	0.62
5:A:1615:HIS:HB3	5:A:1618:LYS:HB3	1.82	0.62
5:A:1667:ARG:HH12	5:A:1674:HIS:HA	1.64	0.62
12:J:512:GLU:CB	26:I:640:ALA:HA	2.30	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:485:ILE:HB	23:W:502:PHE:HB2	1.80	0.62
13:L:608:ASN:CA	40:q:112:ALA:CB	2.68	0.62
14:M:178:GLU:OE2	14:M:181:ARG:NH2	2.32	0.62
40:r:8:SER:O	40:r:9:ASN:CB	2.47	0.62
5:A:1476:GLN:OE1	22:V:457:ARG:NH1	2.32	0.62
11:H:112:G:H2'	11:H:113:G:H8	1.64	0.62
11:H:157:G:H8	11:H:157:G:H5''	1.65	0.62
39:K:15:ALA:HB1	40:s:112:ALA:O	1.99	0.62
5:A:907:PRO:HG2	5:A:1032:ARG:HH21	1.65	0.62
39:K:134:ALA:O	39:K:136:LYS:N	2.33	0.62
8:E:61:LEU:HG	8:E:62:LEU:H	1.64	0.62
11:H:151:C:OP2	24:X:124:THR:CA	2.48	0.62
11:H:152:G:C2	11:H:153:A:C5	2.87	0.62
5:A:443:VAL:HG12	5:A:610:HIS:HB3	1.81	0.62
6:B:74:U:N3	6:B:75:G:C6	2.68	0.62
11:H:143:A:H2'	11:H:144:C:C6	2.35	0.62
19:S:61:MET:HE2	19:S:63:GLN:HB2	1.81	0.62
8:E:217:ILE:HB	8:E:231:MET:HB2	1.81	0.62
11:H:156:U:C6	11:H:156:U:C5'	2.72	0.62
5:A:974:ASN:HB2	5:A:1178:TYR:HB3	1.81	0.62
42:A:3000:IHP:O24	25:Z:167:ARG:NH2	2.29	0.62
6:B:90:U:N3	35:g:36:PRO:O	2.33	0.62
19:S:72:ARG:HD3	23:W:90:ALA:HB3	1.81	0.62
23:W:266:ARG:C	34:l:16:GLN:CB	2.73	0.62
5:A:1809:ILE:HB	5:A:1818:PHE:HB2	1.81	0.61
23:W:265:LEU:CD2	23:W:300:SER:HB2	2.29	0.61
9:F:46:G:OP1	13:L:169:ARG:NH1	2.32	0.61
13:L:65:ARG:HG2	26:I:803:SER:CB	2.30	0.61
13:L:764:PRO:O	13:L:765:ARG:CB	2.48	0.61
11:H:142:C:C2'	11:H:143:A:H5'	2.30	0.61
11:H:166:G:H2'	11:H:166:G:N3	2.15	0.61
23:W:341:ASN:OD1	23:W:388:GLN:NE2	2.32	0.61
5:A:274:PRO:HG3	21:U:1:MET:HB3	1.83	0.61
7:C:737:PRO:HB3	7:C:775:ARG:HB3	1.82	0.61
19:S:131:ARG:NH1	19:S:132:VAL:O	2.34	0.61
12:J:466:ARG:CB	26:I:606:TRP:O	2.47	0.61
16:O:234:LEU:HB2	16:O:272:ILE:HB	1.81	0.61
5:A:419:ARG:NH2	5:A:423:ASP:O	2.33	0.61
15:N:101:CYS:SG	15:N:102:CYS:N	2.73	0.61
15:N:120:ARG:HH11	15:N:142:CYS:CB	2.13	0.61
23:W:258:PRO:CD	23:W:266:ARG:HH12	2.12	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:153:A:N6	11:H:177:A:H2	1.98	0.61
39:K:124:LEU:O	39:K:128:SER:N	2.27	0.61
7:C:172:PHE:CE2	7:C:172:PHE:CZ	2.89	0.61
8:E:90:ILE:HB	8:E:105:LEU:HB2	1.81	0.61
8:E:60:MET:HE3	8:E:97:GLY:O	2.01	0.61
9:F:29:A:N6	10:G:17:U:OP2	2.34	0.60
11:H:151:C:P	24:X:124:THR:N	2.74	0.60
20:T:210:ILE:HG12	20:T:221:THR:HG22	1.83	0.60
20:T:349:SER:OG	20:T:351:ASP:OD1	2.17	0.60
5:A:1248:LEU:O	5:A:1298:ARG:NH1	2.34	0.60
11:H:108:G:O5'	11:H:108:G:H8	1.84	0.60
23:W:391:PHE:O	23:W:402:GLN:HA	2.01	0.60
10:G:130:A:O2'	10:G:131:U:P	2.60	0.60
11:H:18:U:OP2	14:M:221:LYS:NZ	2.32	0.60
23:W:565:LYS:HD2	23:W:577:LEU:HD21	1.83	0.60
25:Z:124:GLY:HA3	25:Z:149:ILE:HG23	1.83	0.60
22:V:628:ILE:HG12	22:V:640:THR:HB	1.84	0.60
5:A:43:LYS:O	5:A:49:ARG:NH1	2.33	0.60
13:L:155:ALA:O	13:L:159:LEU:HB2	2.00	0.60
6:B:88:A:C2	34:e:53:TYR:CB	2.85	0.60
7:C:684:LYS:HB3	7:C:795:VAL:HB	1.82	0.60
5:A:506:LEU:O	5:A:510:ARG:HB2	2.02	0.60
7:C:449:ILE:HG13	7:C:465:MET:HB3	1.84	0.60
8:E:144:VAL:HG12	8:E:145:LYS:HG3	1.84	0.60
13:L:732:MET:HA	40:q:65:PRO:CB	2.31	0.60
10:G:138:A:O5'	10:G:138:A:H8	1.83	0.59
14:M:239:ARG:HG2	26:I:817:GLU:CB	2.32	0.59
24:X:51:LYS:HE2	34:l:59:ASP:CB	2.32	0.59
20:T:347:THR:HG22	20:T:357:TRP:HE1	1.66	0.59
39:K:112:ALA:O	39:K:116:HIS:N	2.35	0.59
11:H:167:U:C4	37:p:41:VAL:HA	2.32	0.59
11:H:165:A:C6	37:p:88:SER:CA	2.83	0.59
23:W:436:THR:HG21	23:W:464:MET:HB2	1.85	0.59
5:A:975:VAL:HB	5:A:1099:PHE:HB2	1.83	0.59
5:A:1946:ASN:ND2	5:A:1986:LEU:HD21	2.17	0.59
8:E:274:VAL:HG12	8:E:275:LYS:HG3	1.83	0.59
23:W:262:GLY:N	35:n:6:PRO:CB	2.65	0.59
15:N:40:LYS:CG	15:N:41:ARG:H	2.15	0.59
7:C:277:LYS:NZ	7:C:864:PRO:O	2.36	0.59
13:L:608:ASN:CA	40:q:112:ALA:HB1	2.28	0.59
10:G:134:U:C5'	10:G:135:G:OP2	2.51	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:104:U:H6	11:H:104:U:H3'	1.66	0.59
5:A:1860:GLN:HG2	5:A:1883:VAL:HB	1.85	0.59
10:G:134:U:C5	10:G:135:G:N2	2.71	0.59
24:X:116:ASN:ND2	35:n:56:ASN:H	1.99	0.59
5:A:1136:ARG:HA	5:A:1139:ARG:HE	1.67	0.58
6:B:96:A:N6	6:B:97:G:C6	2.71	0.58
40:q:22:ASN:CB	40:r:55:ILE:CB	2.81	0.58
10:G:137:C:C5'	10:G:137:C:C6	2.85	0.58
23:W:265:LEU:HD21	23:W:302:HIS:HB2	1.84	0.58
16:O:197:ASN:HB3	16:O:200:ASP:HB2	1.84	0.58
19:S:72:ARG:NH2	23:W:73:ASP:O	2.35	0.58
20:T:345:ILE:HD11	20:T:359:LEU:HD13	1.85	0.58
23:W:304:LEU:HB3	23:W:316:TRP:HB2	1.85	0.58
15:N:118:ILE:HD13	15:N:132:ILE:CG2	2.32	0.58
7:C:245:HIS:O	7:C:249:GLU:HB2	2.03	0.58
9:F:49:G:OP1	13:L:33:ARG:NH1	2.37	0.58
23:W:257:ILE:HD12	23:W:257:ILE:C	2.25	0.58
5:A:650:ARG:HH21	5:A:651:TRP:HE1	1.51	0.58
5:A:1784:ASN:HD22	5:A:1897:LEU:HD12	1.69	0.58
7:C:343:LEU:HD13	7:C:373:ILE:HD11	1.85	0.58
15:N:118:ILE:HD13	15:N:132:ILE:HG23	1.86	0.58
20:T:261:LEU:HB2	20:T:273:TRP:HB2	1.85	0.58
6:B:13:C:C2	6:B:65:G:C2	2.92	0.57
7:C:221:ILE:HG23	7:C:495:ARG:HB2	1.84	0.57
10:G:129:G:H4'	23:W:541:LYS:HD2	1.86	0.57
11:H:105:G:N1	11:H:107:A:H5'	2.19	0.57
6:B:96:A:C5	6:B:97:G:N7	2.73	0.57
7:C:104:LEU:CB	7:C:172:PHE:CE1	2.86	0.57
19:S:13:ASN:HA	19:S:25:LEU:O	2.03	0.57
20:T:250:ARG:NH1	20:T:266:GLU:OE2	2.36	0.57
11:H:165:A:N6	37:p:88:SER:CA	2.67	0.57
13:L:65:ARG:NH2	26:I:799:ARG:CA	2.67	0.57
19:S:26:GLU:OE1	19:S:131:ARG:NH2	2.37	0.57
20:T:356:LEU:CD2	20:T:366:VAL:HB	2.34	0.57
5:A:1781:ASP:HB3	5:A:1808:PHE:HB3	1.86	0.57
6:B:40:U:H3	10:G:-1:G:H22	1.52	0.57
6:B:87:A:H2'	6:B:87:A:N3	2.19	0.57
13:L:263:ASP:OD2	14:M:199:ARG:NH2	2.33	0.57
5:A:617:ASN:HB2	5:A:622:GLY:O	2.04	0.57
10:G:127:U:P	23:W:547:LYS:NZ	2.78	0.57
5:A:474:ARG:HD2	6:B:14:U:H5'	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1072:LEU:HD22	5:A:1087:LEU:HD22	1.86	0.57
7:C:846:VAL:HG22	7:C:887:LEU:HD11	1.86	0.57
11:H:152:G:N2	11:H:153:A:C5	2.73	0.57
11:H:154:C:O2'	11:H:155:C:H5'	2.04	0.57
16:O:72:GLN:CG	16:O:82:GLN:NE2	2.67	0.57
23:W:347:PHE:HD2	23:W:359:TRP:HB2	1.68	0.57
39:K:113:GLN:O	39:K:117:GLN:CA	2.53	0.57
6:B:96:A:C2'	6:B:97:G:H5'	2.34	0.57
11:H:169:C:O5'	11:H:169:C:H6	1.88	0.57
19:S:102:ASN:ND2	19:S:108:ASN:OD1	2.29	0.57
20:T:318:ARG:HD3	20:T:319:THR:HG23	1.87	0.57
25:Z:121:GLU:HB2	25:Z:130:LYS:HD3	1.87	0.57
5:A:798:GLY:HA3	18:R:281:ASN:HD22	1.70	0.57
20:T:272:CYS:HB3	20:T:282:ARG:HG2	1.86	0.57
6:B:78:U:H3'	6:B:78:U:C6	2.40	0.56
11:H:77:C:H2'	11:H:78:C:H6	1.70	0.56
11:H:98:G:O6	32:k:61:ARG:CB	2.53	0.56
11:H:179:C:H2'	11:H:180:G:C8	2.38	0.56
23:W:258:PRO:CB	23:W:265:LEU:HD13	2.35	0.56
5:A:1193:GLU:HB3	5:A:1231:ARG:HB3	1.86	0.56
5:A:1386:TRP:HB3	38:Y:410:VAL:HG21	1.88	0.56
7:C:172:PHE:CD2	7:C:172:PHE:CE2	2.93	0.56
8:E:239:THR:O	8:E:290:ARG:NH1	2.37	0.56
10:G:136:U:OP2	10:G:136:U:H6	1.88	0.56
11:H:71:C:C2	11:H:72:U:C5	2.94	0.56
11:H:77:C:C2	11:H:78:C:C5	2.93	0.56
11:H:141:C:C2	11:H:142:C:C5	2.94	0.56
11:H:149:A:H2'	11:H:150:U:H6	1.71	0.56
20:T:311:THR:HG22	20:T:327:SER:HB3	1.88	0.56
34:l:32:GLN:N	34:l:88:GLN:O	2.35	0.56
11:H:181:G:H2'	11:H:182:U:H6	1.70	0.56
16:O:27:CYS:SG	16:O:83:THR:OG1	2.63	0.56
23:W:262:GLY:HA2	35:n:6:PRO:CA	2.36	0.56
6:B:96:A:C4	6:B:97:G:C8	2.93	0.56
11:H:73:C:C2	11:H:74:U:C5	2.94	0.56
11:H:183:G:H2'	11:H:184:C:H6	1.71	0.56
20:T:312:ALA:HB3	20:T:326:LEU:HD12	1.87	0.56
24:X:54:GLU:OE2	33:m:3:LEU:HA	2.05	0.56
8:E:94:ASN:HB2	8:E:99:CYS:HA	1.88	0.56
11:H:72:U:C2	11:H:73:C:C5	2.94	0.56
11:H:83:A:H2'	11:H:84:C:H6	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:466:ARG:CA	26:I:607:GLY:HA2	2.29	0.56
5:A:409:ARG:HH11	6:B:25:C:H2'	1.71	0.56
7:C:104:LEU:CB	7:C:172:PHE:CZ	2.89	0.56
11:H:70:C:C2	11:H:71:C:C5	2.93	0.56
11:H:70:C:H2'	11:H:71:C:H6	1.70	0.56
12:J:344:GLN:HG2	14:M:132:LEU:HD21	1.87	0.56
39:K:67:ARG:CB	40:s:81:GLU:CB	2.84	0.56
40:q:58:ALA:HB1	40:r:6:SER:HA	1.87	0.56
40:q:71:ILE:CB	40:r:81:GLU:CB	2.84	0.56
5:A:788:GLN:HG2	5:A:1024:HIS:HB3	1.88	0.56
11:H:57:A:H2'	11:H:58:U:H6	1.70	0.56
11:H:69:U:C2	11:H:70:C:C5	2.94	0.56
11:H:73:C:H2'	11:H:74:U:H6	1.70	0.56
15:N:120:ARG:NH1	15:N:142:CYS:HB3	2.20	0.56
23:W:330:GLY:O	23:W:357:LYS:NZ	2.37	0.56
11:H:152:G:N2	11:H:153:A:C8	2.73	0.56
5:A:112:GLN:HE21	5:A:189:GLU:HA	1.71	0.56
8:E:60:MET:HB3	8:E:353:MET:CB	2.27	0.56
11:H:91:U:C2	11:H:92:U:C5	2.94	0.56
13:L:65:ARG:NH2	26:I:799:ARG:C	2.64	0.56
23:W:531:LYS:HG2	23:W:547:LYS:HA	1.88	0.56
25:Z:285:TYR:HD1	25:Z:292:MET:HG2	1.71	0.56
11:H:54:U:C2	11:H:55:U:C5	2.94	0.55
11:H:68:G:H2'	11:H:69:U:H6	1.71	0.55
11:H:150:U:H2'	11:H:151:C:H6	1.71	0.55
16:O:223:LEU:HD22	16:O:285:GLU:HG2	1.86	0.55
18:R:94:GLY:O	19:S:141:ARG:NH1	2.38	0.55
18:R:106:GLN:HG2	18:R:110:LYS:HD3	1.88	0.55
5:A:1986:LEU:HD23	5:A:1986:LEU:O	2.07	0.55
11:H:141:C:H2'	11:H:142:C:H6	1.71	0.55
13:L:59:LYS:HA	14:M:243:VAL:H	1.71	0.55
7:C:813:ARG:NH2	7:C:817:TYR:OH	2.40	0.55
11:H:91:U:H2'	11:H:92:U:H6	1.71	0.55
11:H:150:U:C2	11:H:151:C:C5	2.94	0.55
11:H:165:A:N6	37:p:88:SER:HA	2.21	0.55
11:H:183:G:C4	11:H:184:C:C5	2.94	0.55
15:N:40:LYS:CG	15:N:41:ARG:N	2.70	0.55
18:R:91:ASP:OD1	18:R:91:ASP:N	2.39	0.55
5:A:1980:GLU:OE1	25:Z:347:PRO:HG2	2.06	0.55
6:B:20:G:H1'	6:B:21:A:H5''	1.89	0.55
6:B:74:U:H5'	6:B:75:G:O5'	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:488:VAL:HG13	7:C:609:LYS:HE2	1.87	0.55
23:W:266:ARG:HG3	34:I:15:VAL:C	2.31	0.55
5:A:1431:ALA:O	5:A:1434:LYS:NZ	2.40	0.55
11:H:40:C:H2'	11:H:41:U:C6	2.40	0.55
11:H:90:A:H2'	11:H:91:U:H6	1.71	0.55
11:H:147:G:C4	11:H:148:C:C5	2.94	0.55
11:H:69:U:H2'	11:H:70:C:H6	1.71	0.55
11:H:88:A:H2'	11:H:89:U:H6	1.70	0.55
5:A:608:LEU:HD13	5:A:632:ALA:HB1	1.87	0.55
5:A:1773:SER:O	5:A:1813:ARG:NH1	2.37	0.55
11:H:54:U:H2'	11:H:55:U:H6	1.71	0.55
11:H:71:C:H2'	11:H:72:U:H6	1.70	0.55
11:H:90:A:C4	11:H:91:U:C5	2.95	0.55
18:R:145:GLU:OE1	18:R:148:ARG:NH2	2.40	0.55
38:Y:405:MET:HE1	38:Y:411:LEU:CD2	2.36	0.55
5:A:1593:LEU:HD12	5:A:1664:ILE:HD11	1.89	0.55
7:C:172:PHE:CD1	7:C:172:PHE:CE1	2.95	0.55
8:E:196:VAL:HA	8:E:212:GLY:HA2	1.88	0.55
11:H:149:A:C4	11:H:150:U:C5	2.95	0.55
5:A:293:TRP:HB2	5:A:1136:ARG:HH22	1.71	0.55
5:A:1491:LYS:O	5:A:1710:ASN:ND2	2.40	0.55
5:A:1816:GLN:HE21	5:A:1916:LEU:HD21	1.71	0.55
7:C:312:SER:OG	43:C:1500:GTP:N7	2.40	0.55
11:H:59:A:H2'	11:H:60:U:H6	1.70	0.55
11:H:171:U:H6	11:H:171:U:H5'	1.72	0.55
5:A:909:TYR:HB2	5:A:1033:GLY:HA3	1.89	0.54
5:A:1476:GLN:NE2	25:Z:85:GLN:OE1	2.37	0.54
6:B:85:C:H3'	6:B:85:C:OP1	2.07	0.54
7:C:169:ASP:HB2	7:C:174:GLU:HB3	1.89	0.54
10:G:137:C:H6	10:G:137:C:O5'	1.90	0.54
11:H:68:G:C4	11:H:69:U:C5	2.95	0.54
11:H:181:G:C4	11:H:182:U:C5	2.95	0.54
14:M:226:TYR:O	14:M:230:THR:N	2.39	0.54
26:I:280:GLU:CB	26:I:288:THR:CB	2.85	0.54
9:F:78:A:OP2	13:L:170:LYS:NZ	2.38	0.54
7:C:561:LYS:NZ	7:C:614:TYR:O	2.36	0.54
11:H:72:U:H2'	11:H:73:C:H6	1.71	0.54
12:J:466:ARG:CB	26:I:606:TRP:C	2.80	0.54
16:O:239:LEU:O	16:O:296:ARG:NH1	2.34	0.54
23:W:268:THR:HG22	23:W:270:PRO:HD2	1.88	0.54
24:X:116:ASN:ND2	35:n:56:ASN:N	2.56	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:680:HIS:NE2	5:A:684:GLU:OE2	2.40	0.54
6:B:100:C:H2'	6:B:101:U:C6	2.42	0.54
7:C:172:PHE:CD1	7:C:172:PHE:HA	2.43	0.54
15:N:97:TYR:HA	15:N:120:ARG:HH22	1.72	0.54
23:W:505:HIS:HB2	23:W:527:ASP:HB3	1.88	0.54
40:q:71:ILE:CA	40:r:81:GLU:CB	2.84	0.54
10:G:129:G:C3'	23:W:541:LYS:HE3	2.37	0.54
11:H:57:A:C4	11:H:58:U:C5	2.95	0.54
11:H:153:A:C3'	11:H:154:C:C5'	2.86	0.54
13:L:624:PHE:CB	40:q:104:SER:HA	2.38	0.54
16:O:173:CYS:HB3	23:W:206:ALA:HB3	1.89	0.54
38:Y:405:MET:HE3	38:Y:411:LEU:CG	2.37	0.54
5:A:942:PRO:HD3	5:A:1091:TYR:HA	1.88	0.54
11:H:83:A:C4	11:H:84:C:C5	2.95	0.54
11:H:88:A:C4	11:H:89:U:C5	2.95	0.54
41:D:1048:VAL:O	41:D:1050:GLU:N	2.40	0.54
5:A:1980:GLU:OE1	25:Z:347:PRO:CD	2.54	0.54
7:C:143:THR:HG23	7:C:168:THR:HB	1.89	0.54
12:J:214:ILE:HG23	12:J:219:GLU:HB2	1.89	0.54
13:L:732:MET:CA	40:q:65:PRO:CB	2.86	0.54
5:A:361:HIS:NE2	7:C:283:ASP:OD2	2.40	0.54
5:A:1848:LEU:HD13	5:A:1914:MET:HE3	1.90	0.54
7:C:104:LEU:CB	7:C:172:PHE:CD1	2.91	0.54
8:E:208:ILE:HG23	8:E:220:TRP:HB2	1.89	0.54
11:H:59:A:C4	11:H:60:U:C5	2.95	0.54
20:T:185:MET:SD	20:T:442:ARG:NH1	2.80	0.54
5:A:1433:ASP:OD1	5:A:1439:ARG:NH2	2.40	0.54
8:E:304:SER:H	8:E:330:ILE:HB	1.72	0.54
22:V:483:GLU:O	22:V:486:THR:OG1	2.24	0.54
5:A:58:LYS:NZ	5:A:479:THR:O	2.34	0.54
5:A:1210:LYS:HG3	22:V:509:LEU:HD13	1.90	0.54
5:A:1945:VAL:HG11	5:A:1990:ASP:OD2	2.02	0.54
20:T:346:ILE:CD1	20:T:356:LEU:HD12	2.36	0.54
40:q:22:ASN:CB	40:r:54:ASP:O	2.56	0.54
5:A:1904:ASP:OD1	24:X:86:ARG:NH2	2.40	0.53
6:B:79:C:H2'	6:B:79:C:O2	2.07	0.53
23:W:442:LEU:HB2	23:W:456:ILE:HB	1.89	0.53
5:A:266:SER:OG	5:A:271:MET:O	2.23	0.53
5:A:579:GLN:HG3	5:A:629:PHE:H	1.74	0.53
5:A:781:ARG:HH21	11:H:24:A:H5''	1.73	0.53
7:C:718:PHE:HB3	7:C:724:TRP:HB3	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:171:SER:OG	8:E:173:ASP:OD1	2.27	0.53
24:X:109:PHE:HE2	34:l:91:SER:CA	2.16	0.53
25:Z:179:MET:O	25:Z:182:VAL:HB	2.08	0.53
25:Z:342:HIS:HB3	25:Z:345:ALA:HB3	1.91	0.53
5:A:1132:LYS:HA	5:A:1139:ARG:HH12	1.73	0.53
5:A:1889:LEU:HB2	5:A:2013:GLY:HA3	1.90	0.53
6:B:87:A:C6	32:d:61:ARG:CB	2.91	0.53
5:A:48:LYS:HG3	5:A:49:ARG:HD2	1.90	0.53
5:A:1807:ILE:HB	5:A:1820:LYS:HB3	1.90	0.53
5:A:1942:ALA:CB	5:A:1983:LEU:HD22	2.37	0.53
6:B:78:U:O2'	6:B:79:C:OP1	2.21	0.53
7:C:704:VAL:HG23	7:C:705:VAL:HG22	1.91	0.53
13:L:608:ASN:HA	40:q:112:ALA:HB3	1.84	0.53
16:O:88:LEU:O	18:R:183:GLN:NE2	2.42	0.53
25:Z:273:LYS:HB3	25:Z:292:MET:HG3	1.90	0.53
5:A:725:PRO:HB2	18:R:272:GLY:HA3	1.90	0.53
12:J:343:GLU:HG3	12:J:369:PHE:HZ	1.73	0.53
7:C:501:ILE:O	7:C:543:ARG:HA	2.09	0.53
20:T:346:ILE:HD12	20:T:356:LEU:CD1	2.38	0.53
22:V:603:LEU:HD12	22:V:639:LEU:HD13	1.91	0.53
6:B:13:C:C2	6:B:65:G:N2	2.77	0.53
19:S:11:PRO:O	19:S:29:TRP:NE1	2.31	0.53
5:A:79:ARG:O	5:A:82:ARG:HB2	2.09	0.53
5:A:829:PRO:O	5:A:882:LYS:NZ	2.38	0.53
7:C:104:LEU:CB	7:C:172:PHE:CE2	2.92	0.53
9:F:28:A:H1'	15:N:40:LYS:O	2.09	0.53
39:K:81:LEU:CB	40:t:72:PRO:CB	2.87	0.53
5:A:65:HIS:HD2	15:N:46:LEU:HD22	1.73	0.53
20:T:210:ILE:HG13	20:T:480:ALA:HB2	1.91	0.53
7:C:259:LYS:HG2	43:C:1500:GTP:C6	2.43	0.52
11:H:147:G:H2'	11:H:148:C:C6	2.43	0.52
23:W:259:GLN:OE1	35:n:34:PHE:N	2.42	0.52
34:l:31:ILE:HA	34:l:89:SER:HA	1.90	0.52
8:E:160:ALA:HB2	8:E:166:LEU:H	1.72	0.52
11:H:153:A:H3'	11:H:154:C:C5'	2.38	0.52
6:B:96:A:N6	6:B:97:G:O6	2.42	0.52
23:W:265:LEU:HD23	23:W:300:SER:OG	2.08	0.52
25:Z:127:THR:OG1	25:Z:153:GLU:OE1	2.26	0.52
12:J:294:HIS:HE2	13:L:227:THR:HG1	1.51	0.52
6:B:71:C:H5''	6:B:72:U:C6	2.45	0.52
23:W:392:VAL:HG22	23:W:402:GLN:HG2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:41:GLU:OE2	19:S:44:ARG:NH2	2.41	0.52
23:W:260:ASP:O	35:n:6:PRO:CB	2.58	0.52
23:W:427:VAL:HG23	23:W:490:ALA:HB1	1.91	0.52
39:K:120:ARG:HA	40:r:69:THR:HA	1.92	0.52
11:H:39:U:H6	11:H:39:U:H5''	1.72	0.52
20:T:353:THR:HG22	20:T:369:THR:HG22	1.91	0.52
18:R:61:GLY:HA2	19:S:136:ILE:HB	1.90	0.52
25:Z:87:PRO:HB2	25:Z:91:LYS:HD3	1.91	0.52
5:A:57:GLN:NE2	5:A:59:GLU:OE2	2.37	0.52
9:F:14:C:H2'	9:F:15:A:H8	1.73	0.52
10:G:136:U:OP2	10:G:136:U:C6	2.62	0.52
10:G:137:C:C6	10:G:137:C:H5''	2.45	0.52
11:H:108:G:C4	11:H:109:C:C5	2.98	0.52
12:J:355:ARG:HH21	14:M:139:THR:HG23	1.75	0.52
18:R:107:SER:OG	18:R:109:ASP:OD1	2.28	0.52
5:A:855:ARG:HD2	5:A:1523:ARG:HH12	1.75	0.52
5:A:2090:ILE:HA	5:A:2223:CYS:O	2.10	0.52
6:B:75:G:C8	6:B:76:A:C8	2.97	0.52
7:C:172:PHE:CE1	7:C:172:PHE:CZ	2.98	0.52
7:C:508:LYS:HE3	7:C:510:LEU:HD21	1.91	0.52
22:V:456:ARG:HG3	22:V:492:MET:HG3	1.92	0.52
23:W:265:LEU:HG	23:W:300:SER:HB2	1.90	0.52
39:K:39:GLU:O	40:r:112:ALA:HB2	2.08	0.52
39:K:111:MET:C	40:t:90:PHE:CB	2.83	0.52
39:K:138:TYR:CB	40:r:61:ILE:CB	2.88	0.52
9:F:22:A:H5''	15:N:115:THR:OG1	2.10	0.51
13:L:526:ARG:CB	13:L:594:PRO:CB	2.88	0.51
23:W:354:ARG:NH1	23:W:373:ARG:O	2.44	0.51
38:Y:405:MET:HE3	38:Y:411:LEU:HG	1.92	0.51
39:K:114:LEU:O	39:K:118:ALA:HB2	2.10	0.51
6:B:99:C:H2'	6:B:100:C:C6	2.45	0.51
11:H:143:A:N3	11:H:143:A:C3'	2.73	0.51
11:H:150:U:O5'	24:X:124:THR:HB	2.10	0.51
5:A:1921:ASP:HB3	5:A:1966:HIS:CD2	2.44	0.51
6:B:46:U:O2	21:U:11:ARG:NH2	2.43	0.51
8:E:80:THR:HA	8:E:93:TRP:O	2.11	0.51
20:T:307:SER:OG	20:T:308:ARG:N	2.44	0.51
23:W:265:LEU:CG	23:W:300:SER:HB2	2.40	0.51
1:v:53:HIS:CB	2:w:149:CYS:O	2.58	0.51
8:E:259:VAL:HB	8:E:277:PHE:HB2	1.92	0.51
8:E:326:HIS:HD1	8:E:346:SER:HG	1.57	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:696:LEU:HA	39:K:110:SER:CB	2.40	0.51
23:W:500:LYS:HA	23:W:540:THR:HG21	1.93	0.51
5:A:71:ARG:NH1	15:N:34:THR:HG22	2.26	0.51
5:A:658:ARG:NH1	9:F:67:G:OP1	2.35	0.51
8:E:91:LEU:HD22	8:E:101:ASN:HD21	1.74	0.51
11:H:105:G:N3	11:H:105:G:C2'	2.72	0.51
12:J:466:ARG:CB	26:I:610:ARG:CB	2.89	0.51
5:A:1776:ILE:HB	5:A:1858:PRO:HA	1.92	0.51
10:G:127:U:P	23:W:547:LYS:HZ3	2.33	0.51
11:H:108:G:C4	11:H:109:C:C6	2.98	0.51
23:W:252:ARG:HH22	35:n:11:LYS:C	2.19	0.51
23:W:266:ARG:N	23:W:266:ARG:CD	2.73	0.51
26:I:729:SER:O	26:I:732:ALA:HB3	2.09	0.51
10:G:130:A:HO2'	10:G:131:U:P	2.34	0.51
5:A:584:HIS:HE1	42:A:3000:IHP:O22	1.93	0.51
7:C:734:ALA:HB2	7:C:767:VAL:HG22	1.93	0.51
7:C:926:ALA:HA	7:C:929:LEU:HG	1.92	0.51
20:T:477:LEU:HB3	20:T:489:TYR:HB2	1.92	0.51
5:A:552:ARG:NH1	5:A:589:THR:O	2.44	0.51
5:A:711:GLN:HE22	11:H:18:U:H3'	1.76	0.51
12:J:512:GLU:CB	26:I:640:ALA:CA	2.88	0.51
18:R:52:PRO:HB3	18:R:57:ASP:HB3	1.93	0.51
5:A:109:PRO:HG3	5:A:630:TRP:HE1	1.76	0.50
6:B:78:U:C6	6:B:78:U:C3'	2.94	0.50
7:C:445:ALA:HA	7:C:448:LYS:HB3	1.93	0.50
23:W:267:SER:O	23:W:268:THR:O	2.28	0.50
40:q:127:ALA:HB1	40:t:127:ALA:HB1	1.93	0.50
5:A:984:MET:HG3	5:A:1048:MET:HE1	1.94	0.50
7:C:448:LYS:O	7:C:452:THR:HB	2.11	0.50
7:C:622:GLU:OE1	7:C:941:LYS:NZ	2.38	0.50
15:N:18:ILE:HG21	15:N:70:ILE:HD11	1.93	0.50
15:N:120:ARG:NH1	15:N:142:CYS:CB	2.75	0.50
23:W:552:VAL:HG13	23:W:571:TRP:CD1	2.46	0.50
25:Z:122:ASN:O	25:Z:138:ARG:NH2	2.44	0.50
5:A:329:LEU:HD12	7:C:177:ARG:HD2	1.92	0.50
5:A:425:PRO:HG3	6:B:26:A:H5'	1.93	0.50
7:C:104:LEU:CB	7:C:172:PHE:CD2	2.94	0.50
20:T:427:LEU:HB3	20:T:439:TRP:HB2	1.93	0.50
23:W:252:ARG:HD2	23:W:257:ILE:HG22	1.94	0.50
5:A:108:MET:O	5:A:110:TRP:N	2.44	0.50
5:A:663:ARG:NH2	9:F:65:G:N7	2.58	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:74:U:N3	6:B:75:G:C5	2.80	0.50
13:L:48:ALA:O	13:L:52:GLU:CB	2.60	0.50
20:T:289:SER:OG	20:T:308:ARG:NE	2.36	0.50
23:W:387:LYS:HD3	23:W:390:LEU:HD12	1.93	0.50
23:W:534:ILE:HB	23:W:544:SER:HB3	1.94	0.50
23:W:541:LYS:NZ	23:W:541:LYS:CB	2.73	0.50
11:H:100:U:H4'	11:H:101:U:H5'	1.93	0.50
12:J:294:HIS:CD2	13:L:227:THR:HG1	2.29	0.50
16:O:176:GLY:HA2	23:W:206:ALA:HB2	1.94	0.50
16:O:283:ALA:O	16:O:287:SER:HB3	2.11	0.50
21:U:1:MET:SD	21:U:1:MET:N	2.80	0.50
5:A:658:ARG:NH2	9:F:65:G:OP2	2.43	0.50
7:C:725:ASP:O	7:C:729:ALA:N	2.43	0.50
10:G:129:G:H4'	23:W:541:LYS:CE	2.41	0.50
20:T:213:GLU:HG3	20:T:218:TRP:CE2	2.47	0.50
7:C:481:MET:HE2	7:C:490:PHE:HB2	1.94	0.50
8:E:69:VAL:HG11	8:E:351:LEU:HD21	1.94	0.50
10:G:129:G:C4'	23:W:541:LYS:CE	2.90	0.50
11:H:168:A:H3'	11:H:169:C:C5	2.47	0.50
5:A:1318:THR:HB	5:A:1324:GLY:HA3	1.94	0.50
5:A:1676:ILE:HD13	5:A:1706:ASP:HB2	1.93	0.50
7:C:129:ILE:HG22	7:C:199:LEU:HB3	1.93	0.50
8:E:258:THR:HG22	8:E:260:ARG:HG3	1.94	0.50
34:e:15:VAL:O	35:g:33:GLY:HA3	2.12	0.50
5:A:160:HIS:HE1	25:Z:170:TRP:HA	1.77	0.50
5:A:161:PHE:CE2	5:A:626:GLY:HA2	2.47	0.50
5:A:1137:ASP:O	5:A:1141:ARG:NH1	2.43	0.50
22:V:530:LYS:NZ	22:V:564:VAL:O	2.45	0.50
39:K:127:MET:CB	40:r:64:LYS:O	2.60	0.50
5:A:380:LEU:HD12	5:A:384:VAL:HG21	1.92	0.49
5:A:1949:ARG:NH2	24:X:62:GLU:OE1	2.45	0.49
7:C:168:THR:HG23	7:C:184:THR:HB	1.93	0.49
12:J:427:LYS:HE3	26:I:579:LEU:CB	2.36	0.49
5:A:224:THR:N	6:B:12:U:OP1	2.39	0.49
5:A:409:ARG:HE	5:A:413:LEU:HD21	1.77	0.49
7:C:485:ASP:OD1	7:C:485:ASP:N	2.44	0.49
9:F:85:U:H5'	14:M:193:ARG:HD2	1.94	0.49
11:H:110:A:H2'	11:H:111:G:C2	2.46	0.49
23:W:252:ARG:CG	23:W:252:ARG:NH1	2.73	0.49
39:K:114:LEU:O	39:K:118:ALA:CB	2.60	0.49
7:C:137:HIS:HB3	7:C:140:HIS:CD2	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:834:VAL:HG21	7:C:883:PHE:HE2	1.78	0.49
18:R:151:LEU:HD22	20:T:323:VAL:HG11	1.92	0.49
20:T:335:THR:O	20:T:347:THR:OG1	2.29	0.49
5:A:1275:ARG:HD2	5:A:1375:TRP:CE2	2.47	0.49
7:C:171:LEU:HD11	7:C:182:LYS:HD2	1.94	0.49
7:C:774:THR:HA	7:C:784:ILE:HD12	1.94	0.49
12:J:466:ARG:HA	26:I:606:TRP:C	2.37	0.49
23:W:267:SER:O	23:W:268:THR:C	2.56	0.49
24:X:109:PHE:HE2	34:I:91:SER:N	2.10	0.49
5:A:1275:ARG:NH1	5:A:1373:GLN:O	2.39	0.49
5:A:1984:LYS:HG2	5:A:1988:LEU:HD12	1.94	0.49
6:B:79:C:C6	6:B:79:C:C5'	2.95	0.49
9:F:21:U:H1'	15:N:121:VAL:CG2	2.42	0.49
9:F:21:U:O4'	15:N:121:VAL:HG23	2.12	0.49
16:O:26:THR:HG22	16:O:155:PRO:HB3	1.93	0.49
5:A:1972:THR:OG1	5:A:1975:GLU:OE1	2.24	0.49
7:C:476:CYS:HB2	7:C:565:ILE:HB	1.95	0.49
7:C:747:ASP:HB3	7:C:791:ILE:HB	1.94	0.49
23:W:257:ILE:HG12	35:n:10:LYS:CA	2.28	0.49
10:G:126:C:O3'	23:W:547:LYS:NZ	2.46	0.49
15:N:119:CYS:SG	15:N:139:CYS:HB3	2.53	0.49
23:W:531:LYS:HD3	23:W:547:LYS:HG2	1.93	0.49
16:O:56:ARG:HG2	16:O:67:LYS:HB3	1.95	0.49
28:Q:523:ALA:O	28:Q:532:PRO:HA	2.13	0.49
5:A:118:VAL:HG21	5:A:487:LEU:HD12	1.94	0.49
5:A:1219:GLU:O	5:A:1222:LYS:NZ	2.42	0.49
5:A:1576:ILE:O	5:A:1746:ARG:NH1	2.38	0.49
5:A:1894:GLN:NE2	24:X:69:GLY:O	2.46	0.49
14:M:239:ARG:CG	26:I:817:GLU:CB	2.91	0.49
16:O:34:ILE:HB	18:R:197:ILE:HG12	1.94	0.49
5:A:379:GLU:HG2	7:C:355:LYS:HB3	1.92	0.49
5:A:1215:ASN:HB3	5:A:1224:ARG:HD2	1.95	0.49
6:B:44:A:O2'	10:G:-5:G:N2	2.43	0.49
14:M:210:TYR:HB3	14:M:219:ASN:HD22	1.78	0.49
17:P:13:ARG:NH1	20:T:329:HIS:O	2.45	0.49
18:R:132:LEU:HA	20:T:399:LYS:HE3	1.95	0.49
20:T:342:GLU:CG	20:T:343:PRO:CD	2.91	0.49
39:K:36:VAL:O	40:r:112:ALA:CB	2.58	0.49
12:J:221:ASN:ND2	13:L:211:ASN:OD1	2.46	0.48
13:L:65:ARG:HE	26:I:803:SER:CB	2.26	0.48
20:T:339:GLN:NE2	20:T:342:GLU:O	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1066:GLN:CG	38:Y:423:THR:O	2.61	0.48
5:A:1615:HIS:HD2	5:A:1616:PRO:HD2	1.78	0.48
7:C:135:CYS:HB2	7:C:242:LEU:HD13	1.95	0.48
7:C:137:HIS:HB2	7:C:239:THR:HG23	1.94	0.48
11:H:107:A:N3	11:H:107:A:C3'	2.74	0.48
20:T:422:ASN:HB3	20:T:424:ASP:H	1.78	0.48
5:A:699:GLU:OE1	18:R:235:ARG:NH2	2.46	0.48
13:L:784:LEU:CB	39:K:195:ILE:CB	2.90	0.48
18:R:74:LEU:HD23	18:R:75:ASP:H	1.76	0.48
40:r:127:ALA:O	40:s:127:ALA:HB1	2.13	0.48
5:A:1610:GLN:NE2	5:A:1612:GLU:OE2	2.46	0.48
13:L:608:ASN:HA	40:q:112:ALA:HB2	1.83	0.48
23:W:258:PRO:CB	23:W:265:LEU:CD1	2.91	0.48
6:B:96:A:C2	6:B:97:G:C4	3.02	0.48
5:A:768:ASP:OD1	6:B:40:U:O2'	2.27	0.48
5:A:854:SER:OG	5:A:855:ARG:N	2.47	0.48
8:E:233:GLY:O	8:E:260:ARG:NH1	2.46	0.48
34:l:30:ARG:C	34:l:90:VAL:H	2.20	0.48
8:E:92:LEU:HD12	8:E:103:ALA:HB3	1.93	0.48
10:G:136:U:H2'	10:G:137:C:C5	2.49	0.48
20:T:394:ASN:OD1	20:T:396:LYS:NZ	2.47	0.48
24:X:116:ASN:CG	35:n:55:ASN:HA	2.39	0.48
6:B:88:A:C4	34:e:53:TYR:CB	2.97	0.48
5:A:1865:ARG:NH1	10:G:147:C:OP1	2.47	0.48
6:B:92:U:C2	31:c:35:SER:CB	2.97	0.48
11:H:101:U:H4'	11:H:102:U:OP1	2.14	0.48
13:L:59:LYS:HG2	14:M:243:VAL:HA	1.96	0.48
16:O:276:THR:HG23	16:O:279:ALA:H	1.78	0.48
23:W:252:ARG:CZ	35:n:10:LYS:O	2.62	0.48
8:E:260:ARG:HG2	8:E:276:ILE:HG12	1.96	0.48
11:H:151:C:OP2	24:X:124:THR:N	2.46	0.48
13:L:74:LEU:HD23	13:L:77:LEU:HD12	1.94	0.48
16:O:27:CYS:SG	16:O:66:LYS:NZ	2.81	0.48
5:A:325:HIS:HD2	5:A:326:HIS:HD2	1.60	0.47
5:A:522:PHE:O	5:A:548:ARG:NH2	2.38	0.47
5:A:1768:TYR:CZ	5:A:2012:LEU:HD11	2.49	0.47
7:C:226:VAL:HA	7:C:254:THR:O	2.14	0.47
5:A:211:GLN:OE1	5:A:214:ARG:NH1	2.47	0.47
5:A:1214:TRP:CE2	5:A:1230:LEU:HD11	2.49	0.47
5:A:1560:ILE:HG21	5:A:1573:LEU:HD13	1.95	0.47
20:T:248:THR:HB	20:T:266:GLU:HG3	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Q:523:ALA:CB	28:Q:534:ARG:O	2.63	0.47
1:v:24:PHE:HA	1:v:33:ARG:O	2.14	0.47
1:v:140:HIS:O	2:w:70:VAL:CB	2.62	0.47
5:A:356:ILE:HD13	7:C:867:PRO:HD3	1.96	0.47
5:A:1831:LYS:HG2	10:G:2:U:P	2.53	0.47
5:A:1962:THR:HG22	5:A:1969:PRO:HA	1.96	0.47
7:C:440:SER:O	7:C:443:VAL:N	2.47	0.47
11:H:44:U:H2'	11:H:45:C:C6	2.48	0.47
12:J:323:LEU:HD22	14:M:179:ILE:HG22	1.96	0.47
14:M:237:LEU:HD11	18:R:264:LEU:HD22	1.95	0.47
19:S:18:THR:HG22	19:S:159:ILE:HG12	1.96	0.47
7:C:506:PRO:HA	7:C:526:THR:HA	1.96	0.47
7:C:938:ARG:HE	7:C:945:GLU:HA	1.80	0.47
8:E:167:VAL:HB	8:E:179:TRP:HB2	1.96	0.47
11:H:42:G:H8	11:H:42:G:O5'	1.98	0.47
11:H:151:C:C2	11:H:152:G:N7	2.82	0.47
18:R:185:GLY:O	18:R:187:ALA:N	2.47	0.47
23:W:258:PRO:HD2	23:W:266:ARG:NH1	2.28	0.47
5:A:1775:GLN:HG2	5:A:1859:LYS:HD2	1.97	0.47
6:B:93:U:H4'	6:B:94:U:H5''	1.97	0.47
10:G:138:A:H2'	10:G:139:U:C6	2.49	0.47
14:M:221:LYS:HE3	18:R:249:PRO:HB3	1.96	0.47
5:A:1251:SER:O	5:A:1298:ARG:NH2	2.33	0.47
8:E:60:MET:SD	8:E:60:MET:C	2.96	0.47
16:O:123:ARG:NH1	18:R:222:PRO:O	2.46	0.47
39:K:40:THR:CB	40:r:109:GLN:HA	2.45	0.47
5:A:62:PRO:HG3	15:N:53:HIS:CD2	2.50	0.47
5:A:425:PRO:HB2	5:A:428:LYS:HB2	1.97	0.47
5:A:555:LYS:NZ	5:A:559:ASP:OD2	2.43	0.47
10:G:129:G:H4'	23:W:541:LYS:HE3	1.95	0.47
11:H:153:A:C8	11:H:154:C:H5'	2.50	0.47
20:T:416:ILE:HA	20:T:431:ALA:HA	1.95	0.47
22:V:565:LEU:HG	22:V:568:ILE:HD12	1.95	0.47
9:F:25:C:N4	16:O:39:GLU:OE1	2.47	0.47
11:H:98:G:N3	11:H:98:G:C3'	2.78	0.47
11:H:141:C:H2'	11:H:142:C:C6	2.50	0.47
11:H:183:G:H2'	11:H:184:C:C6	2.50	0.47
20:T:342:GLU:CG	20:T:343:PRO:HD2	2.37	0.47
8:E:60:MET:CG	8:E:353:MET:SD	2.89	0.47
11:H:91:U:H2'	11:H:92:U:C6	2.50	0.47
11:H:149:A:H2'	11:H:150:U:C6	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:133:CYS:SG	25:Z:134:PHE:N	2.88	0.47
34:l:15:VAL:CB	35:n:32:ARG:O	2.63	0.47
5:A:143:GLN:NE2	5:A:207:PHE:O	2.45	0.47
5:A:668:VAL:HB	9:F:68:C:H5''	1.96	0.47
5:A:1763:LEU:HG	5:A:1862:ILE:HD13	1.96	0.47
7:C:205:THR:HB	7:C:215:VAL:HG22	1.97	0.47
8:E:95:VAL:C	8:E:96:TYR:CD2	2.93	0.47
11:H:41:U:H5''	11:H:41:U:C6	2.35	0.47
16:O:22:ILE:HG23	23:W:112:SER:HB3	1.97	0.47
22:V:470:GLU:OE2	22:V:513:ARG:NH1	2.47	0.47
23:W:372:ASN:HD22	23:W:395:MET:HE2	1.80	0.47
26:I:712:VAL:O	26:I:713:ARG:C	2.57	0.47
5:A:1350:ILE:HD12	22:V:470:GLU:HG3	1.97	0.46
5:A:1806:ALA:HA	5:A:1820:LYS:O	2.14	0.46
9:F:82:A:N6	11:H:19:G:OP1	2.48	0.46
10:G:134:U:H5''	10:G:135:G:OP2	2.15	0.46
11:H:38:A:H2'	11:H:39:U:H5''	1.97	0.46
11:H:72:U:H2'	11:H:73:C:C6	2.50	0.46
19:S:52:LYS:HE3	19:S:156:ASP:HA	1.97	0.46
22:V:536:ILE:H	22:V:536:ILE:HG13	1.49	0.46
23:W:562:GLU:OE1	23:W:565:LYS:NZ	2.43	0.46
7:C:448:LYS:O	7:C:452:THR:CB	2.63	0.46
7:C:692:LEU:HD12	7:C:786:ASN:HA	1.96	0.46
13:L:48:ALA:O	13:L:52:GLU:HB3	2.15	0.46
24:X:116:ASN:HD21	35:n:56:ASN:N	2.11	0.46
25:Z:334:ALA:O	25:Z:338:GLY:N	2.44	0.46
5:A:164:MET:HE2	5:A:569:VAL:HG11	1.97	0.46
8:E:326:HIS:CE1	8:E:346:SER:HG	2.32	0.46
12:J:466:ARG:CB	26:I:607:GLY:N	2.75	0.46
14:M:239:ARG:CD	26:I:817:GLU:CB	2.92	0.46
23:W:524:ILE:HD11	23:W:558:TRP:HE3	1.79	0.46
5:A:762:ARG:HH12	17:P:226:LYS:HZ1	1.63	0.46
5:A:856:LEU:HD23	5:A:860:GLN:HB3	1.97	0.46
7:C:156:GLU:OE2	7:C:167:TYR:OH	2.33	0.46
11:H:57:A:H2'	11:H:58:U:C6	2.50	0.46
11:H:150:U:H2'	11:H:151:C:C6	2.49	0.46
18:R:127:ALA:HB2	20:T:442:ARG:HD3	1.97	0.46
5:A:103:LEU:HD11	5:A:554:THR:HG22	1.97	0.46
5:A:1986:LEU:C	5:A:1986:LEU:CD2	2.85	0.46
11:H:41:U:H6	11:H:41:U:C5'	2.20	0.46
11:H:90:A:H2'	11:H:91:U:C6	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:182:U:H2'	11:H:183:G:H8	1.81	0.46
12:J:193:GLN:O	12:J:196:ARG:HB3	2.16	0.46
12:J:221:ASN:HD22	12:J:221:ASN:HA	1.54	0.46
23:W:400:ILE:HD12	23:W:445:TRP:CZ3	2.51	0.46
23:W:506:MET:H	23:W:527:ASP:HB2	1.81	0.46
5:A:976:MET:HG2	5:A:1187:PHE:HB3	1.97	0.46
5:A:1045:GLY:HA3	5:A:1090:ARG:NH2	2.29	0.46
11:H:105:G:O6	31:j:20:LYS:C	2.59	0.46
24:X:109:PHE:HE2	34:l:90:VAL:C	2.24	0.46
36:o:61:PRO:O	36:o:86:ALA:HB1	2.16	0.46
5:A:542:ASN:O	5:A:546:LEU:HB2	2.15	0.46
5:A:944:ASP:HA	5:A:1437:ARG:HE	1.81	0.46
5:A:1312:PRO:HG2	5:A:1314:VAL:HG12	1.98	0.46
7:C:698:GLU:O	7:C:702:ASN:N	2.49	0.46
8:E:338:ASP:OD1	8:E:338:ASP:N	2.49	0.46
9:F:21:U:OP1	15:N:116:ASN:ND2	2.49	0.46
11:H:70:C:H2'	11:H:71:C:C6	2.49	0.46
11:H:104:U:H4'	11:H:105:G:C4'	2.45	0.46
11:H:108:G:H8	11:H:108:G:P	2.39	0.46
11:H:181:G:H2'	11:H:182:U:C6	2.50	0.46
22:V:539:LEU:HD12	22:V:544:LEU:HD23	1.98	0.46
23:W:400:ILE:HD11	23:W:421:VAL:HG11	1.98	0.46
5:A:320:TYR:OH	7:C:634:GLU:OE2	2.30	0.46
5:A:852:VAL:O	5:A:854:SER:N	2.49	0.46
5:A:1418:ARG:HE	5:A:1464:LEU:HD23	1.80	0.46
8:E:98:ASP:HB3	8:E:100:ASP:OD1	2.16	0.46
11:H:81:G:H2'	11:H:82:G:H8	1.80	0.46
11:H:142:C:H2'	11:H:143:A:H5'	1.98	0.46
14:M:209:ASP:HB2	18:R:263:PRO:HG3	1.98	0.46
39:K:111:MET:CB	40:t:90:PHE:CB	2.94	0.46
41:D:1349:GLY:HA2	41:D:1491:SER:O	2.16	0.46
7:C:935:ILE:O	7:C:939:ARG:N	2.46	0.46
11:H:68:G:H2'	11:H:69:U:C6	2.50	0.46
11:H:69:U:H2'	11:H:70:C:C6	2.49	0.46
11:H:78:C:H2'	11:H:79:G:H8	1.81	0.46
12:J:367:GLU:OE2	12:J:382:TYR:OH	2.33	0.46
13:L:140:ASP:OD1	13:L:140:ASP:N	2.49	0.46
23:W:434:VAL:HG21	23:W:476:LEU:HD11	1.98	0.46
11:H:152:G:O2'	11:H:153:A:H1'	2.16	0.46
16:O:236:VAL:O	16:O:269:CYS:HA	2.16	0.46
6:B:87:A:N6	32:d:61:ARG:CB	2.79	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:56:A:H2'	11:H:57:A:H8	1.81	0.45
11:H:104:U:H3'	11:H:104:U:C6	2.49	0.45
26:I:712:VAL:O	26:I:715:GLY:N	2.49	0.45
5:A:359:ILE:HA	7:C:864:PRO:HB3	1.97	0.45
5:A:603:ARG:O	5:A:606:LYS:HB2	2.16	0.45
5:A:1242:ASN:OD1	5:A:1245:ARG:NH2	2.42	0.45
11:H:54:U:H2'	11:H:55:U:C6	2.50	0.45
11:H:71:C:H2'	11:H:72:U:C6	2.50	0.45
5:A:1382:SER:HA	5:A:1415:GLY:HA2	1.98	0.45
7:C:104:LEU:CB	7:C:172:PHE:CG	2.97	0.45
7:C:227:LEU:HB3	7:C:255:VAL:HG22	1.98	0.45
9:F:1:G:O2'	15:N:99:ASN:ND2	2.50	0.45
10:G:137:C:C5	10:G:137:C:OP2	2.69	0.45
11:H:102:U:OP2	11:H:102:U:H3'	2.16	0.45
11:H:171:U:H2'	11:H:172:C:O4'	2.16	0.45
41:D:441:GLY:O	41:D:693:THR:N	2.36	0.45
1:v:53:HIS:N	2:w:149:CYS:O	2.34	0.45
5:A:2121:ARG:O	5:A:2154:HIS:HA	2.15	0.45
7:C:87:GLN:HE21	20:T:239:LYS:HB3	1.81	0.45
11:H:88:A:H2'	11:H:89:U:C6	2.50	0.45
11:H:92:U:H2'	11:H:93:A:H8	1.82	0.45
18:R:303:GLU:OE2	18:R:307:GLN:NE2	2.49	0.45
8:E:75:HIS:NE2	8:E:121:GLY:O	2.46	0.45
11:H:58:U:H2'	11:H:59:A:H8	1.82	0.45
11:H:74:U:H2'	11:H:75:A:H8	1.81	0.45
11:H:79:G:H2'	11:H:80:A:H8	1.81	0.45
11:H:82:G:H2'	11:H:83:A:H8	1.81	0.45
16:O:280:ALA:HB1	16:O:302:TRP:HH2	1.81	0.45
5:A:338:VAL:HG12	7:C:262:ARG:HH21	1.82	0.45
5:A:1048:MET:HE3	5:A:1048:MET:HB2	1.77	0.45
6:B:96:A:N1	6:B:97:G:C5	2.84	0.45
9:F:22:A:OP2	23:W:130:ARG:NH2	2.50	0.45
10:G:139:U:O4	10:G:140:A:N6	2.50	0.45
11:H:73:C:H2'	11:H:74:U:C6	2.50	0.45
11:H:148:C:H2'	11:H:149:A:H8	1.82	0.45
13:L:28:LYS:NZ	18:R:273:ARG:HH22	2.15	0.45
15:N:118:ILE:CD1	15:N:132:ILE:HG23	2.46	0.45
16:O:68:THR:HA	16:O:83:THR:HG22	1.99	0.45
18:R:94:GLY:HA3	19:S:141:ARG:HD3	1.97	0.45
5:A:1908:LYS:HE3	23:W:448:ASP:HB3	1.98	0.45
7:C:566:THR:OG1	7:C:567:GLU:N	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:604:LEU:HD23	7:C:607:LEU:HD12	1.98	0.45
8:E:95:VAL:HB	8:E:96:TYR:HD2	1.81	0.45
11:H:89:U:H2'	11:H:90:A:H8	1.82	0.45
11:H:100:U:C6	11:H:100:U:C5'	2.93	0.45
5:A:1980:GLU:OE1	25:Z:347:PRO:CG	2.64	0.45
7:C:158:ARG:HB2	7:C:165:LEU:HB3	1.99	0.45
8:E:95:VAL:C	8:E:96:TYR:HD2	2.25	0.45
10:G:120:G:O4'	26:I:316:GLU:O	2.34	0.45
11:H:80:A:H2'	11:H:81:G:H8	1.81	0.45
15:N:118:ILE:H	15:N:118:ILE:HG13	1.62	0.45
16:O:233:THR:HA	16:O:272:ILE:O	2.17	0.45
40:q:71:ILE:CB	40:r:81:GLU:CA	2.94	0.45
6:B:69:A:N6	6:B:70:A:N3	2.64	0.45
7:C:94:ILE:H	7:C:94:ILE:HG13	1.45	0.45
7:C:887:LEU:HD23	7:C:897:SER:HB2	1.98	0.45
11:H:67:C:H2'	11:H:68:G:H8	1.81	0.45
19:S:20:MET:HE3	19:S:141:ARG:HG2	1.99	0.45
19:S:72:ARG:HH22	23:W:74:PRO:HA	1.82	0.45
20:T:373:LYS:HD2	20:T:392:PRO:HB2	1.99	0.45
7:C:221:ILE:O	7:C:495:ARG:NH1	2.50	0.45
13:L:52:GLU:OE2	13:L:134:THR:OG1	2.34	0.45
13:L:717:MET:O	13:L:721:LEU:N	2.48	0.45
20:T:418:THR:HG21	20:T:468:CYS:H	1.81	0.45
23:W:257:ILE:HG23	23:W:257:ILE:O	2.17	0.45
23:W:514:VAL:HA	23:W:524:ILE:O	2.16	0.45
39:K:112:ALA:O	39:K:116:HIS:CA	2.62	0.45
3:u:82:SER:O	3:u:219:ALA:HA	2.17	0.44
5:A:1490:PHE:O	5:A:1493:THR:OG1	2.35	0.44
5:A:1513:MET:HE3	10:G:164:A:H61	1.82	0.44
11:H:106:G:C4'	11:H:107:A:OP1	2.45	0.44
12:J:224:LYS:NZ	12:J:257:GLU:OE2	2.47	0.44
22:V:499:GLN:HG2	25:Z:72:TRP:CG	2.52	0.44
41:D:721:VAL:HA	41:D:825:THR:O	2.17	0.44
8:E:355:GLU:H	23:W:82:ASN:ND2	2.16	0.44
11:H:84:C:H2'	11:H:85:A:H8	1.82	0.44
11:H:93:A:H2'	11:H:94:A:H8	1.82	0.44
17:P:204:GLN:O	17:P:206:LYS:N	2.50	0.44
23:W:420:ALA:O	23:W:438:ASP:N	2.46	0.44
41:D:419:GLY:C	41:D:421:HIS:H	2.24	0.44
5:A:417:ARG:NH1	6:B:58:U:O3'	2.44	0.44
6:B:20:G:H8	6:B:21:A:H2'	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:63:LYS:HE3	7:C:65:TYR:HE1	1.82	0.44
9:F:23:U:OP1	15:N:115:THR:HG21	2.17	0.44
11:H:180:G:H2'	11:H:181:G:H8	1.81	0.44
13:L:699:ASN:CB	39:K:114:LEU:CB	2.95	0.44
7:C:112:THR:HG23	7:C:154:HIS:CD2	2.53	0.44
11:H:55:U:H2'	11:H:56:A:H8	1.82	0.44
11:H:59:A:H2'	11:H:60:U:C6	2.50	0.44
11:H:170:C:C6	11:H:170:C:OP2	2.70	0.44
12:J:251:TRP:CE3	12:J:252:GLU:HG3	2.53	0.44
18:R:64:PHE:H	18:R:71:GLN:HE22	1.65	0.44
20:T:405:PHE:O	20:T:405:PHE:CD1	2.70	0.44
23:W:181:PHE:HD1	23:W:200:VAL:HG12	1.83	0.44
23:W:264:ASN:ND2	23:W:267:SER:HB2	2.32	0.44
38:Y:405:MET:CE	38:Y:411:LEU:HD21	2.43	0.44
5:A:348:PRO:HB3	5:A:394:TYR:CZ	2.52	0.44
5:A:976:MET:HE2	5:A:1098:PHE:HD1	1.82	0.44
5:A:1497:THR:OG1	5:A:1499:GLU:OE1	2.26	0.44
42:A:3000:IHP:H3	42:A:3000:IHP:O32	2.17	0.44
11:H:153:A:C2'	11:H:154:C:C5'	2.86	0.44
13:L:55:ASP:HB3	13:L:58:ILE:HG13	2.00	0.44
14:M:162:PRO:HA	14:M:167:LEU:HD12	1.98	0.44
18:R:105:GLY:HA3	18:R:225:PRO:HG2	1.99	0.44
20:T:294:LEU:HD12	20:T:303:LEU:HD11	2.00	0.44
23:W:462:HIS:CE1	23:W:482:ASP:HB3	2.52	0.44
24:X:109:PHE:CE2	34:I:90:VAL:C	2.95	0.44
5:A:89:LEU:O	5:A:92:LEU:HB3	2.18	0.44
5:A:121:HIS:HD2	18:R:207:MET:HG3	1.82	0.44
5:A:721:LYS:O	5:A:781:ARG:NH1	2.51	0.44
5:A:1214:TRP:NE1	5:A:1276:GLU:OE1	2.50	0.44
11:H:83:A:H2'	11:H:84:C:C6	2.49	0.44
18:R:91:ASP:O	18:R:95:LYS:NZ	2.43	0.44
19:S:58:LYS:HE2	19:S:144:MET:HG2	2.00	0.44
5:A:620:PRO:HG2	25:Z:134:PHE:HE2	1.83	0.44
5:A:1494:TYR:HB3	5:A:1744:ARG:HD3	2.00	0.44
5:A:2008:ARG:O	5:A:2012:LEU:HB2	2.18	0.44
7:C:82:GLN:HE21	20:T:238:LEU:H	1.66	0.44
7:C:311:SER:HB3	7:C:316:ILE:HB	2.00	0.44
11:H:77:C:H2'	11:H:78:C:C6	2.50	0.44
11:H:143:A:OP2	11:H:143:A:C2	2.71	0.44
18:R:136:ASP:HB3	18:R:138:GLU:H	1.82	0.44
8:E:299:LYS:HE3	8:E:320:LEU:HD13	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:346:SER:OG	8:E:348:ASP:OD1	2.36	0.44
11:H:169:C:O5'	11:H:169:C:C6	2.70	0.44
15:N:118:ILE:CD1	15:N:132:ILE:CG2	2.95	0.44
9:F:21:U:C1'	15:N:121:VAL:CG2	2.96	0.44
9:F:28:A:C1'	15:N:40:LYS:O	2.66	0.44
11:H:108:G:C5	11:H:109:C:C5	3.06	0.44
11:H:114:A:C8	11:H:114:A:OP2	2.70	0.44
11:H:153:A:H2'	11:H:154:C:H5''	2.00	0.44
12:J:232:GLU:OE2	12:J:267:ARG:NH2	2.44	0.44
13:L:65:ARG:CZ	26:I:799:ARG:C	2.90	0.44
5:A:787:GLU:OE2	5:A:790:ARG:NH2	2.43	0.43
5:A:1286:ASP:OD1	5:A:1354:ARG:NH2	2.51	0.43
11:H:150:U:C4'	24:X:124:THR:HG22	2.48	0.43
11:H:154:C:O2'	11:H:155:C:C5'	2.66	0.43
20:T:354:ILE:HD11	20:T:389:SER:CB	2.48	0.43
5:A:106:MET:HA	5:A:107:PRO:HD3	1.84	0.43
5:A:1199:LYS:HD3	5:A:1206:GLU:HG3	2.00	0.43
8:E:336:HIS:CD2	8:E:337:PRO:HD2	2.52	0.43
9:F:21:U:C1'	15:N:121:VAL:HG23	2.48	0.43
13:L:703:MET:O	13:L:707:ALA:HB3	2.18	0.43
20:T:289:SER:OG	20:T:290:ALA:N	2.51	0.43
23:W:456:ILE:HG22	23:W:461:MET:HE1	1.99	0.43
26:I:433:ALA:O	26:I:437:CYS:N	2.50	0.43
7:C:101:LYS:HG2	7:C:172:PHE:HE2	1.83	0.43
7:C:107:GLN:HG3	7:C:108:THR:H	1.83	0.43
10:G:143:U:H2'	10:G:145:U:C5	2.53	0.43
20:T:297:HIS:HB2	20:T:302:VAL:HG12	2.00	0.43
5:A:1070:ASP:OD1	5:A:1073:SER:OG	2.28	0.43
5:A:1454:TRP:CD1	5:A:1454:TRP:H	2.36	0.43
7:C:747:ASP:OD1	7:C:747:ASP:N	2.50	0.43
11:H:178:A:N3	11:H:178:A:H2'	2.33	0.43
16:O:133:PRO:HB2	16:O:136:MET:HB3	2.00	0.43
20:T:345:ILE:O	20:T:357:TRP:HD1	2.01	0.43
7:C:134:LEU:HD23	7:C:226:VAL:HB	2.00	0.43
7:C:296:GLU:HB2	7:C:299:ILE:HD11	2.01	0.43
10:G:134:U:H3'	10:G:135:G:H21	1.84	0.43
11:H:104:U:C6	11:H:104:U:C3'	3.01	0.43
11:H:157:G:H2'	11:H:158:G:O4'	2.18	0.43
11:H:166:G:OP2	11:H:166:G:C2	2.72	0.43
1:v:51:TYR:CB	2:w:151:VAL:O	2.66	0.43
7:C:264:ILE:HG12	7:C:378:TYR:CE1	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:231:MET:HE2	8:E:272:ARG:HH11	1.82	0.43
9:F:17:C:H2'	9:F:18:A:H8	1.84	0.43
11:H:142:C:O2'	11:H:143:A:H5'	2.18	0.43
11:H:163:G:C6	37:p:12:ASN:CB	3.00	0.43
12:J:228:ARG:NE	12:J:252:GLU:OE2	2.51	0.43
5:A:1945:VAL:HG11	5:A:1990:ASP:CB	2.46	0.43
6:B:74:U:O2	6:B:74:U:H2'	2.18	0.43
12:J:213:LYS:HA	13:L:243:ARG:HA	2.01	0.43
15:N:133:GLU:OE2	15:N:140:ARG:NH2	2.36	0.43
16:O:76:LYS:HG2	23:W:111:LEU:HD22	2.00	0.43
18:R:119:LEU:HD21	18:R:230:MET:HB3	2.01	0.43
19:S:72:ARG:HG3	23:W:72:LEU:HD13	2.00	0.43
5:A:624:GLY:HA2	5:A:625:PRO:HD3	1.69	0.43
5:A:1130:ASN:HB3	5:A:1132:LYS:HE3	2.00	0.43
5:A:1803:ILE:HG13	5:A:1804:ASN:H	1.84	0.43
7:C:242:LEU:HD23	7:C:242:LEU:HA	1.87	0.43
7:C:255:VAL:HG21	7:C:285:VAL:HG11	2.00	0.43
13:L:53:TRP:HD1	13:L:54:LEU:HD12	1.84	0.43
16:O:196:GLN:HE22	16:O:209:VAL:HG23	1.83	0.43
23:W:360:ASP:HB2	23:W:367:ILE:HD11	2.01	0.43
23:W:452:ASP:OD1	23:W:452:ASP:N	2.52	0.43
13:L:227:THR:O	13:L:227:THR:OG1	2.37	0.43
19:S:55:ARG:HH21	19:S:57:ILE:HD11	1.82	0.43
3:u:254:PHE:HA	3:u:401:ASP:O	2.18	0.43
5:A:893:GLU:OE2	5:A:1018:ASN:ND2	2.52	0.43
7:C:669:THR:HG22	7:C:690:GLU:HG3	2.01	0.43
8:E:59:ILE:HD12	8:E:59:ILE:HA	1.87	0.43
8:E:178:LEU:HB2	8:E:188:GLN:HB3	2.01	0.43
8:E:310:TYR:HE1	8:E:322:LYS:HG3	1.84	0.43
13:L:65:ARG:CG	26:I:803:SER:CB	2.97	0.43
14:M:125:SER:HB3	18:R:239:VAL:HG22	2.00	0.43
16:O:235:TYR:HD2	16:O:301:LYS:HB2	1.84	0.43
23:W:348:LEU:HD11	23:W:356:LEU:HD21	2.00	0.43
5:A:549:GLU:HB3	5:A:591:MET:HG2	2.00	0.42
8:E:277:PHE:HE1	8:E:317:ARG:HG2	1.83	0.42
11:H:43:U:H2'	11:H:44:U:C6	2.53	0.42
15:N:118:ILE:HD13	15:N:132:ILE:HG21	2.01	0.42
15:N:120:ARG:HA	15:N:120:ARG:HD2	1.43	0.42
7:C:80:ILE:HG22	7:C:82:GLN:HG2	2.01	0.42
7:C:924:GLN:HG3	7:C:932:GLU:HG3	2.01	0.42
8:E:307:ARG:NE	8:E:326:HIS:O	2.42	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:119:G:H4'	10:G:120:G:OP1	2.19	0.42
15:N:40:LYS:HE2	15:N:40:LYS:HB2	1.26	0.42
23:W:258:PRO:CG	23:W:266:ARG:NH1	2.82	0.42
23:W:264:ASN:CG	23:W:267:SER:HB2	2.43	0.42
5:A:25:MET:SD	8:E:215:ASN:ND2	2.91	0.42
11:H:106:G:C8	11:H:106:G:C5'	2.96	0.42
22:V:455:PHE:O	22:V:459:ILE:HG12	2.19	0.42
5:A:167:PRO:HA	5:A:168:PRO:HD3	1.90	0.42
5:A:1891:LEU:HD22	5:A:1937:ILE:HD12	2.01	0.42
7:C:160:ARG:NH1	7:C:410:LEU:HD22	2.34	0.42
7:C:711:ARG:NH2	7:C:730:ARG:O	2.37	0.42
11:H:39:U:H2'	11:H:40:C:C6	2.55	0.42
11:H:151:C:OP2	24:X:123:GLN:C	2.63	0.42
18:R:177:ILE:HG13	18:R:197:ILE:HB	2.01	0.42
23:W:399:LYS:HA	23:W:414:TYR:O	2.19	0.42
23:W:530:GLY:HA2	23:W:552:VAL:HA	2.01	0.42
38:Y:399:LYS:HB2	38:Y:399:LYS:HE3	1.59	0.42
32:d:68:GLU:HA	32:d:97:SER:O	2.19	0.42
5:A:523:ASN:OD1	5:A:552:ARG:NH2	2.53	0.42
5:A:2332:ASP:C	5:A:2334:TYR:H	2.28	0.42
6:B:74:U:C4	6:B:75:G:C6	3.07	0.42
8:E:181:ILE:HG13	8:E:182:ARG:HG3	2.00	0.42
11:H:112:G:H2'	11:H:113:G:C8	2.50	0.42
16:O:31:ASN:O	18:R:195:ARG:NH1	2.52	0.42
17:P:54:VAL:HG13	17:P:59:PHE:HZ	1.83	0.42
22:V:540:GLU:O	22:V:544:LEU:N	2.45	0.42
23:W:465:PRO:HG2	23:W:481:MET:HE3	2.02	0.42
25:Z:265:LEU:HB3	25:Z:266:ARG:H	1.71	0.42
5:A:569:VAL:HG12	5:A:573:GLN:HB2	2.02	0.42
5:A:793:ASN:HD22	7:C:60:HIS:CD2	2.38	0.42
5:A:1017:ILE:HD11	5:A:1031:ILE:HD11	2.02	0.42
7:C:277:LYS:HD2	7:C:865:GLY:HA3	2.00	0.42
7:C:442:LYS:HG2	7:C:468:CYS:HB2	2.02	0.42
11:H:155:C:H2'	11:H:156:U:H5''	2.02	0.42
15:N:22:LEU:HD23	15:N:22:LEU:HA	1.82	0.42
15:N:121:VAL:HA	15:N:122:PRO:HD3	1.88	0.42
23:W:258:PRO:CG	23:W:265:LEU:HD13	2.49	0.42
25:Z:84:HIS:ND1	25:Z:85:GLN:OE1	2.53	0.42
41:D:1583:ASP:C	41:D:1585:GLN:H	2.26	0.42
2:w:137:GLN:O	2:w:143:PRO:HA	2.19	0.42
5:A:155:LYS:HZ3	5:A:624:GLY:H	1.67	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1260:VAL:HG21	5:A:1325:LEU:HB3	2.01	0.42
7:C:264:ILE:HG21	7:C:381:LEU:HD12	2.01	0.42
8:E:96:TYR:CD2	8:E:96:TYR:N	2.88	0.42
13:L:83:ARG:HA	13:L:83:ARG:HD3	1.87	0.42
15:N:37:HIS:CG	15:N:37:HIS:O	2.70	0.42
32:k:68:GLU:HA	32:k:97:SER:O	2.19	0.42
36:o:160:LYS:O	36:o:161:MET:C	2.63	0.42
5:A:67:ARG:HD2	15:N:33:GLU:OE2	2.20	0.42
5:A:451:LEU:HD23	5:A:451:LEU:HA	1.89	0.42
5:A:1275:ARG:NH2	5:A:1464:LEU:O	2.43	0.42
12:J:287:MET:HB3	14:M:186:LEU:HD11	2.00	0.42
12:J:311:GLN:HG3	14:M:131:GLN:HG2	2.02	0.42
15:N:22:LEU:HD11	15:N:60:ILE:HD11	2.02	0.42
18:R:113:TYR:OH	20:T:402:ASP:O	2.33	0.42
5:A:156:ARG:HD3	25:Z:153:GLU:HG2	2.02	0.42
5:A:723:ASN:ND2	5:A:788:GLN:OE1	2.52	0.42
10:G:137:C:OP2	10:G:137:C:H5	2.02	0.42
14:M:176:THR:HA	14:M:179:ILE:HG12	2.02	0.42
38:Y:411:LEU:HD23	38:Y:411:LEU:HA	1.84	0.42
5:A:546:LEU:HD22	5:A:648:LEU:HD11	2.02	0.42
5:A:1507:SER:HB2	5:A:1511:GLU:HG3	2.01	0.42
6:B:63:A:H2'	6:B:64:G:C8	2.55	0.42
9:F:22:A:C8	15:N:121:VAL:HG21	2.54	0.42
10:G:142:U:HO2'	10:G:143:U:P	2.38	0.42
15:N:102:CYS:HB3	15:N:104:ARG:H	1.84	0.42
18:R:175:GLN:NE2	18:R:176:TYR:O	2.52	0.42
19:S:102:ASN:H	19:S:126:HIS:CE1	2.38	0.42
20:T:371:HIS:NE2	20:T:389:SER:OG	2.35	0.42
22:V:459:ILE:HD12	22:V:489:LEU:HD23	2.00	0.42
25:Z:79:ARG:O	25:Z:81:THR:N	2.53	0.42
5:A:533:LYS:NZ	10:G:5:G:OP2	2.34	0.41
5:A:1772:PHE:HB3	25:Z:320:ASP:HB2	2.01	0.41
7:C:62:ASP:OD1	7:C:62:ASP:N	2.33	0.41
7:C:131:ASN:HB3	7:C:222:SER:HA	2.01	0.41
8:E:81:LEU:HB2	8:E:93:TRP:HB2	2.02	0.41
8:E:161:ARG:HH22	8:E:243:LEU:HD12	1.85	0.41
12:J:242:ILE:HD13	12:J:275:ASN:ND2	2.35	0.41
20:T:314:ILE:CD1	20:T:326:LEU:HD21	2.47	0.41
20:T:329:HIS:ND1	20:T:349:SER:CB	2.82	0.41
23:W:475:TRP:CD1	23:W:489:GLY:HA2	2.55	0.41
5:A:1807:ILE:HG12	5:A:1841:THR:HG23	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:623:GLU:H	7:C:941:LYS:NZ	2.14	0.41
8:E:340:PRO:HB2	8:E:356:ILE:HB	2.01	0.41
10:G:21:A:N6	16:O:91:GLY:O	2.43	0.41
13:L:262:LYS:HE3	13:L:266:HIS:CE1	2.55	0.41
19:S:20:MET:HG3	19:S:142:VAL:HG22	2.02	0.41
21:U:23:LEU:HD12	22:V:477:LEU:HD13	2.02	0.41
23:W:264:ASN:CA	35:n:35:ASP:HA	2.43	0.41
23:W:305:LEU:HD21	23:W:313:ILE:HG23	2.02	0.41
23:W:506:MET:HE3	23:W:506:MET:HB2	1.78	0.41
26:I:296:PHE:CB	26:I:305:SER:O	2.68	0.41
5:A:99:VAL:HG13	5:A:554:THR:HG21	2.02	0.41
5:A:531:THR:HG23	5:A:534:GLU:H	1.84	0.41
5:A:620:PRO:HG2	25:Z:134:PHE:CE2	2.55	0.41
5:A:762:ARG:NH2	17:P:227:TYR:OH	2.53	0.41
5:A:1976:TRP:HA	5:A:1979:VAL:HG22	2.03	0.41
13:L:699:ASN:HA	39:K:114:LEU:CB	2.50	0.41
14:M:212:ASN:HB3	14:M:215:ASN:H	1.85	0.41
23:W:126:GLU:HB3	23:W:130:ARG:NH1	2.35	0.41
5:A:866:LEU:HD12	5:A:913:PRO:HB2	2.02	0.41
5:A:1174:PHE:HE2	5:A:1176:SER:HB2	1.85	0.41
11:H:113:G:C2'	11:H:114:A:H5'	2.50	0.41
19:S:24:VAL:HB	19:S:134:GLN:HB3	2.02	0.41
38:Y:405:MET:HE3	38:Y:405:MET:HB3	1.78	0.41
5:A:506:LEU:O	5:A:510:ARG:CB	2.68	0.41
5:A:738:MET:HB3	5:A:738:MET:HE3	1.85	0.41
8:E:294:SER:HB3	8:E:299:LYS:HB2	2.02	0.41
11:H:43:U:OP2	11:H:43:U:C6	2.74	0.41
11:H:151:C:OP1	24:X:124:THR:N	2.54	0.41
5:A:764:GLY:HA2	5:A:1245:ARG:NH1	2.36	0.41
7:C:441:PRO:O	7:C:445:ALA:HB2	2.20	0.41
11:H:157:G:H5''	11:H:157:G:C8	2.50	0.41
39:K:18:TYR:CB	39:K:168:LYS:HA	2.50	0.41
5:A:902:TYR:OH	5:A:1249:MET:SD	2.68	0.41
6:B:70:A:H5''	6:B:70:A:H8	1.85	0.41
23:W:84:THR:O	23:W:87:THR:OG1	2.35	0.41
10:G:163:C:H2'	10:G:164:A:O4'	2.20	0.41
11:H:37:U:H2'	11:H:38:A:H8	1.85	0.41
11:H:102:U:H4'	30:i:75:GLU:CB	2.50	0.41
15:N:120:ARG:HH11	15:N:142:CYS:HB2	1.86	0.41
16:O:240:GLY:H	16:O:268:GLN:HB3	1.86	0.41
5:A:707:ARG:HG2	17:P:9:PHE:CZ	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:835:ASP:OD1	5:A:921:TYR:OH	2.33	0.41
5:A:1088:PHE:HD1	5:A:1097:ILE:HG12	1.85	0.41
5:A:1590:VAL:HG22	5:A:1664:ILE:HD12	2.03	0.41
5:A:2332:ASP:O	5:A:2334:TYR:N	2.54	0.41
7:C:87:GLN:HA	7:C:88:PRO:HD2	1.97	0.41
7:C:743:ASN:HB3	7:C:770:PHE:CZ	2.56	0.41
11:H:152:G:H2'	11:H:153:A:C1'	2.51	0.41
16:O:110:SER:OG	16:O:113:ASN:ND2	2.53	0.41
23:W:97:ASN:OD1	23:W:97:ASN:N	2.54	0.41
23:W:304:LEU:HD11	23:W:567:ILE:HG21	2.02	0.41
23:W:387:LYS:NZ	23:W:430:ASN:OD1	2.49	0.41
23:W:393:ALA:HB3	23:W:403:TRP:HZ3	1.86	0.41
25:Z:178:HIS:O	25:Z:181:ILE:HB	2.21	0.41
28:Q:529:GLU:C	28:Q:531:TRP:H	2.29	0.41
32:k:62:HIS:O	32:k:103:GLY:HA3	2.21	0.41
38:Y:662:THR:C	38:Y:663:ASP:O	2.61	0.41
39:K:92:PRO:O	39:K:93:SER:C	2.64	0.41
40:q:71:ILE:CB	40:r:81:GLU:HA	2.51	0.41
41:D:538:ILE:O	41:D:585:ILE:HA	2.21	0.41
41:D:577:LYS:O	41:D:581:SER:N	2.54	0.41
41:D:1481:ILE:C	41:D:1483:ARG:H	2.28	0.41
5:A:192:GLN:H	5:A:192:GLN:HG2	1.69	0.41
5:A:1790:ILE:HD13	24:X:76:SER:HB2	2.03	0.41
7:C:618:THR:HB	7:C:630:LEU:HB2	2.03	0.41
7:C:637:LEU:HD23	7:C:637:LEU:HA	1.94	0.41
7:C:833:PHE:HB2	7:C:902:HIS:ND1	2.36	0.41
9:F:17:C:H2'	9:F:18:A:C8	2.56	0.41
11:H:102:U:OP2	11:H:102:U:H2'	2.21	0.41
20:T:366:VAL:HG21	20:T:402:ASP:HA	2.03	0.41
23:W:341:ASN:HB3	23:W:344:GLY:H	1.86	0.41
5:A:913:PRO:HA	5:A:916:LYS:HD3	2.04	0.40
5:A:1244:VAL:HG11	5:A:1291:CYS:HB3	2.03	0.40
5:A:1946:ASN:HD22	5:A:1986:LEU:HD21	1.83	0.40
7:C:101:LYS:HG2	7:C:172:PHE:CE2	2.56	0.40
7:C:112:THR:H	7:C:155:PRO:HD2	1.87	0.40
7:C:169:ASP:OD1	7:C:169:ASP:N	2.54	0.40
7:C:843:VAL:HG13	7:C:871:ILE:HD11	2.03	0.40
11:H:152:G:H2'	11:H:152:G:N3	2.36	0.40
11:H:153:A:C8	11:H:154:C:O4'	2.74	0.40
12:J:493:ALA:CB	12:J:499:ARG:CB	2.96	0.40
16:O:230:THR:H	16:O:277:ARG:NH1	2.18	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:136:ILE:HA	19:S:139:VAL:HG12	2.03	0.40
20:T:193:PRO:HD2	20:T:495:ALA:HB1	2.03	0.40
20:T:483:ASP:OD1	20:T:485:THR:OG1	2.34	0.40
24:X:116:ASN:CG	35:n:55:ASN:CA	2.94	0.40
25:Z:106:VAL:HG12	25:Z:153:GLU:HG3	2.03	0.40
25:Z:162:ASP:HB2	25:Z:165:GLY:H	1.85	0.40
41:D:642:THR:C	41:D:644:GLU:H	2.29	0.40
6:B:85:C:H3'	6:B:85:C:P	2.61	0.40
7:C:706:GLN:HG3	7:C:707:ILE:H	1.86	0.40
8:E:253:ASN:HB3	8:E:259:VAL:HG13	2.02	0.40
8:E:295:PRO:HG3	8:E:337:PRO:HA	2.03	0.40
16:O:64:ARG:HD2	16:O:163:HIS:CE1	2.56	0.40
17:P:66:ARG:HH22	20:T:217:GLN:HE22	1.68	0.40
19:S:25:LEU:HA	19:S:132:VAL:HA	2.03	0.40
23:W:162:ASN:HB3	23:W:165:LEU:HG	2.03	0.40
23:W:257:ILE:HG21	35:n:10:LYS:CB	2.50	0.40
5:A:1241:HIS:HB2	5:A:1287:LEU:HD21	2.02	0.40
5:A:1590:VAL:HG11	5:A:1614:ILE:HD11	2.04	0.40
7:C:104:LEU:HG	7:C:172:PHE:CD2	2.56	0.40
7:C:231:ALA:O	7:C:277:LYS:HE3	2.21	0.40
7:C:263:LEU:HD23	7:C:267:LEU:HD12	2.02	0.40
11:H:149:A:C6	11:H:150:U:C4	3.09	0.40
11:H:183:G:C6	11:H:184:C:N4	2.89	0.40
15:N:70:ILE:HG12	15:N:74:LEU:HD23	2.03	0.40
20:T:314:ILE:O	20:T:323:VAL:N	2.54	0.40
32:d:62:HIS:O	32:d:103:GLY:HA3	2.21	0.40
5:A:1803:ILE:O	5:A:1824:THR:HG22	2.22	0.40
7:C:104:LEU:CG	7:C:172:PHE:CE2	3.01	0.40
7:C:506:PRO:HG2	7:C:568:PRO:HG3	2.03	0.40
11:H:57:A:C6	11:H:58:U:C4	3.10	0.40
13:L:176:LEU:HD22	23:W:440:LYS:HE3	2.04	0.40
18:R:91:ASP:HB3	18:R:97:LYS:HE3	2.02	0.40
19:S:142:VAL:HG13	19:S:157:VAL:HG11	2.04	0.40
20:T:438:LEU:HB2	20:T:448:GLN:HB3	2.03	0.40
26:I:729:SER:HA	26:I:732:ALA:HB3	2.04	0.40
41:D:420:SER:CB	41:D:622:ASP:HA	2.52	0.40
5:A:156:ARG:NH1	25:Z:153:GLU:OE2	2.55	0.40
5:A:796:LYS:HD3	18:R:279:HIS:HE1	1.87	0.40
5:A:1330:MET:HG3	5:A:1367:ASN:OD1	2.21	0.40
5:A:1403:LEU:HD23	5:A:1403:LEU:HA	1.92	0.40
6:B:95:G:C5	34:e:36:TYR:O	2.74	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:104:LEU:HB3	7:C:172:PHE:CZ	2.56	0.40
8:E:95:VAL:HG23	8:E:96:TYR:H	1.85	0.40
8:E:282:HIS:NE2	8:E:289:LEU:HD12	2.36	0.40
20:T:320:LYS:HB2	20:T:320:LYS:HE3	1.85	0.40
26:I:520:ILE:O	26:I:524:TYR:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	v	142/148 (96%)	138 (97%)	4 (3%)	0	100	100
2	w	89/174 (51%)	87 (98%)	1 (1%)	1 (1%)	11	43
3	u	384/411 (93%)	372 (97%)	9 (2%)	3 (1%)	16	50
4	x	23/703 (3%)	22 (96%)	1 (4%)	0	100	100
5	A	2247/2335 (96%)	2091 (93%)	147 (6%)	9 (0%)	30	65
7	C	892/972 (92%)	798 (90%)	90 (10%)	4 (0%)	30	65
8	E	301/357 (84%)	273 (91%)	28 (9%)	0	100	100
12	J	530/848 (62%)	491 (93%)	32 (6%)	7 (1%)	9	38
13	L	436/802 (54%)	405 (93%)	27 (6%)	4 (1%)	14	48
14	M	128/243 (53%)	124 (97%)	3 (2%)	1 (1%)	16	50
15	N	141/144 (98%)	126 (89%)	13 (9%)	2 (1%)	9	36
16	O	283/420 (67%)	260 (92%)	22 (8%)	1 (0%)	30	65
17	P	104/229 (45%)	86 (83%)	15 (14%)	3 (3%)	3	20
18	R	255/536 (48%)	229 (90%)	24 (9%)	2 (1%)	16	50
19	S	157/166 (95%)	148 (94%)	9 (6%)	0	100	100
20	T	311/514 (60%)	281 (90%)	23 (7%)	7 (2%)	5	25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	U	24/2752 (1%)	23 (96%)	1 (4%)	0	100	100
22	V	444/908 (49%)	429 (97%)	14 (3%)	1 (0%)	43	76
23	W	506/579 (87%)	441 (87%)	60 (12%)	5 (1%)	12	45
24	X	90/184 (49%)	84 (93%)	6 (7%)	0	100	100
25	Z	238/586 (41%)	214 (90%)	24 (10%)	0	100	100
26	I	498/855 (58%)	481 (97%)	10 (2%)	7 (1%)	9	36
27	y	77/301 (26%)	75 (97%)	2 (3%)	0	100	100
28	Q	1308/1485 (88%)	1282 (98%)	26 (2%)	0	100	100
29	a	77/126 (61%)	76 (99%)	1 (1%)	0	100	100
29	h	77/126 (61%)	76 (99%)	1 (1%)	0	100	100
30	b	84/231 (36%)	82 (98%)	2 (2%)	0	100	100
30	i	84/231 (36%)	82 (98%)	2 (2%)	0	100	100
31	c	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
31	j	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
32	d	95/118 (80%)	91 (96%)	4 (4%)	0	100	100
32	k	81/118 (69%)	78 (96%)	3 (4%)	0	100	100
33	f	72/86 (84%)	69 (96%)	3 (4%)	0	100	100
33	m	71/86 (83%)	68 (96%)	3 (4%)	0	100	100
34	e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
34	l	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
35	g	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
35	n	65/76 (86%)	59 (91%)	4 (6%)	2 (3%)	3	19
36	o	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	9	38
37	p	92/225 (41%)	90 (98%)	2 (2%)	0	100	100
38	Y	709/1220 (58%)	616 (87%)	61 (9%)	32 (4%)	2	12
39	K	144/225 (64%)	129 (90%)	8 (6%)	7 (5%)	1	10
40	q	130/504 (26%)	119 (92%)	7 (5%)	4 (3%)	3	19
40	r	129/504 (26%)	119 (92%)	8 (6%)	2 (2%)	7	34
40	s	65/504 (13%)	62 (95%)	2 (3%)	1 (2%)	8	35
40	t	65/504 (13%)	64 (98%)	0	1 (2%)	8	35
41	D	1720/2136 (80%)	1633 (95%)	84 (5%)	3 (0%)	43	76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	13914/24425 (57%)	12995 (93%)	808 (6%)	111 (1%)	18	50

All (111) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	u	383	ASN
15	N	36	PRO
18	R	233	PRO
20	T	343	PRO
20	T	458	SER
23	W	268	THR
26	I	463	PRO
26	I	721	LYS
26	I	797	PHE
38	Y	531	MET
38	Y	610	ARG
38	Y	855	VAL
38	Y	944	ASP
38	Y	995	MET
38	Y	1090	LYS
38	Y	1098	LYS
38	Y	1099	SER
38	Y	1129	ASP
38	Y	1145	GLN
38	Y	1164	GLU
39	K	78	PRO
39	K	90	PRO
39	K	135	TRP
40	q	59	HIS
40	q	60	PRO
40	s	71	ILE
40	t	69	THR
41	D	957	VAL
41	D	1584	ILE
2	w	115	GLY
3	u	340	GLY
3	u	385	ASP
7	C	94	ILE
12	J	188	GLN
12	J	241	VAL
12	J	709	VAL
13	L	765	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	N	37	HIS
17	P	205	LYS
18	R	186	VAL
23	W	243	VAL
23	W	258	PRO
26	I	618	ARG
26	I	634	ILE
36	o	160	LYS
38	Y	517	GLU
38	Y	845	SER
38	Y	870	GLY
38	Y	1182	LYS
39	K	136	LYS
39	K	172	LEU
40	q	9	ASN
12	J	205	LEU
17	P	48	GLN
20	T	186	PRO
20	T	328	GLY
26	I	752	ALA
35	n	6	PRO
38	Y	524	ASN
38	Y	550	TYR
38	Y	806	GLU
38	Y	994	ILE
38	Y	1055	ASN
38	Y	1056	LYS
40	q	19	PRO
40	r	9	ASN
5	A	1092	ILE
5	A	1190	CYS
12	J	604	PRO
13	L	585	TYR
20	T	406	ILE
23	W	74	PRO
26	I	617	GLU
35	n	8	GLU
36	o	32	PRO
38	Y	590	THR
38	Y	663	ASP
38	Y	722	ALA
38	Y	835	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	K	65	ILE
5	A	56	ALA
5	A	108	MET
5	A	570	ASP
12	J	341	PRO
14	M	125	SER
22	V	597	PRO
38	Y	811	PRO
5	A	109	PRO
5	A	853	LYS
5	A	1503	TRP
13	L	763	ILE
16	O	20	PHE
17	P	11	PRO
38	Y	523	ALA
38	Y	856	ASP
38	Y	1157	THR
7	C	87	GLN
7	C	441	PRO
13	L	764	PRO
38	Y	738	PRO
38	Y	1137	PRO
39	K	17	PRO
40	r	65	PRO
5	A	852	VAL
12	J	206	LEU
20	T	185	MET
20	T	401	PRO
38	Y	521	ILE
23	W	271	PRO
41	D	585	ILE
7	C	440	SER

5.3.2 Protein sidechains [i](#)

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	
5	A	1795/2108 (85%)	1783 (99%)	12 (1%)	76	86
7	C	793/866 (92%)	788 (99%)	5 (1%)	78	88
8	E	259/300 (86%)	253 (98%)	6 (2%)	44	74
12	J	241/751 (32%)	240 (100%)	1 (0%)	84	90
13	L	208/709 (29%)	206 (99%)	2 (1%)	68	84
14	M	117/209 (56%)	115 (98%)	2 (2%)	53	78
15	N	130/130 (100%)	124 (95%)	6 (5%)	24	58
16	O	255/361 (71%)	251 (98%)	4 (2%)	55	79
17	P	99/203 (49%)	99 (100%)	0	100	100
18	R	219/457 (48%)	215 (98%)	4 (2%)	51	77
19	S	129/134 (96%)	129 (100%)	0	100	100
20	T	269/441 (61%)	260 (97%)	9 (3%)	33	67
21	U	21/2432 (1%)	20 (95%)	1 (5%)	23	57
22	V	140/838 (17%)	134 (96%)	6 (4%)	26	60
23	W	447/502 (89%)	440 (98%)	7 (2%)	55	79
24	X	62/157 (40%)	58 (94%)	4 (6%)	15	47
25	Z	214/520 (41%)	211 (99%)	3 (1%)	59	80
38	Y	8/1085 (1%)	4 (50%)	4 (50%)	0	0
All	All	5406/12203 (44%)	5330 (99%)	76 (1%)	57	80

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	258	PHE
5	A	283	VAL
5	A	413	LEU
5	A	623	LYS
5	A	668	VAL
5	A	735	ILE
5	A	1109	LEU
5	A	1763	LEU
5	A	1790	ILE
5	A	1981	VAL
5	A	1984	LYS
5	A	1985	ASP
7	C	157	ILE
7	C	256	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	C	308	CYS
7	C	559	ILE
7	C	678	THR
8	E	54	SER
8	E	56	GLN
8	E	59	ILE
8	E	60	MET
8	E	99	CYS
8	E	259	VAL
12	J	221	ASN
13	L	227	THR
13	L	251	LEU
14	M	184	ILE
14	M	212	ASN
15	N	38	GLU
15	N	40	LYS
15	N	118	ILE
15	N	119	CYS
15	N	120	ARG
15	N	121	VAL
16	O	72	GLN
16	O	73	THR
16	O	75	SER
16	O	147	LEU
18	R	74	LEU
18	R	111	VAL
18	R	212	PHE
18	R	262	ILE
20	T	327	SER
20	T	339	GLN
20	T	342	GLU
20	T	344	GLN
20	T	356	LEU
20	T	404	SER
20	T	406	ILE
20	T	407	GLN
20	T	412	HIS
21	U	23	LEU
22	V	458	THR
22	V	489	LEU
22	V	536	ILE
22	V	539	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	V	583	VAL
22	V	597	PRO
23	W	252	ARG
23	W	257	ILE
23	W	260	ASP
23	W	266	ARG
23	W	427	VAL
23	W	541	LYS
23	W	552	VAL
24	X	104	LYS
24	X	105	LEU
24	X	111	LYS
24	X	113	LEU
25	Z	74	ILE
25	Z	164	ASP
25	Z	166	LYS
38	Y	404	GLN
38	Y	405	MET
38	Y	410	VAL
38	Y	411	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	97	HIS
5	A	160	HIS
5	A	181	ASN
5	A	270	ASN
5	A	294	ASN
5	A	325	HIS
5	A	326	HIS
5	A	328	HIS
5	A	368	GLN
5	A	483	GLN
5	A	617	ASN
5	A	659	GLN
5	A	704	ASN
5	A	723	ASN
5	A	775	ASN
5	A	957	GLN
5	A	994	ASN
5	A	1023	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	1075	GLN
5	A	1117	HIS
5	A	1124	ASN
5	A	1145	HIS
5	A	1246	GLN
5	A	1359	HIS
5	A	1468	ASN
5	A	1487	HIS
5	A	1615	HIS
5	A	1674	HIS
5	A	1717	ASN
5	A	1766	GLN
5	A	1774	ASN
5	A	1816	GLN
5	A	1835	GLN
5	A	1918	ASN
5	A	1946	ASN
5	A	1966	HIS
7	C	60	HIS
7	C	82	GLN
7	C	87	GLN
7	C	107	GLN
7	C	152	GLN
7	C	154	HIS
7	C	297	ASN
7	C	627	HIS
7	C	642	HIS
7	C	892	GLN
8	E	56	GLN
8	E	101	ASN
8	E	202	ASN
8	E	225	ASN
8	E	287	ASN
12	J	221	ASN
12	J	238	ASN
12	J	275	ASN
12	J	331	GLN
12	J	347	HIS
13	L	186	GLN
13	L	211	ASN
13	L	266	HIS
14	M	172	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	M	212	ASN
15	N	53	HIS
15	N	99	ASN
15	N	136	HIS
16	O	72	GLN
16	O	79	ASN
16	O	82	GLN
16	O	163	HIS
17	P	29	GLN
17	P	75	ASN
17	P	212	ASN
18	R	71	GLN
18	R	175	GLN
18	R	183	GLN
18	R	276	GLN
18	R	279	HIS
19	S	10	GLN
20	T	278	ASN
20	T	339	GLN
20	T	384	HIS
20	T	446	ASN
21	U	3	ASN
22	V	499	GLN
23	W	82	ASN
23	W	147	GLN
23	W	162	ASN
23	W	242	HIS
23	W	250	GLN
23	W	462	HIS
23	W	491	GLN
23	W	492	ASN
23	W	529	ASN
23	W	533	ASN
24	X	103	GLN
24	X	116	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	G	82/273 (30%)	44 (53%)	7 (8%)
11	H	133/188 (70%)	45 (33%)	9 (6%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	B	96/117 (82%)	46 (47%)	8 (8%)
9	F	96/107 (89%)	33 (34%)	6 (6%)
All	All	407/685 (59%)	168 (41%)	30 (7%)

All (168) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	B	9	G
6	B	10	U
6	B	13	C
6	B	19	A
6	B	20	G
6	B	21	A
6	B	22	U
6	B	24	G
6	B	25	C
6	B	26	A
6	B	28	A
6	B	33	U
6	B	36	C
6	B	38	C
6	B	40	U
6	B	45	C
6	B	47	A
6	B	52	U
6	B	57	G
6	B	66	A
6	B	67	A
6	B	71	C
6	B	72	U
6	B	73	C
6	B	74	U
6	B	75	G
6	B	76	A
6	B	77	G
6	B	78	U
6	B	79	C
6	B	80	U
6	B	81	U
6	B	82	A
6	B	83	A
6	B	84	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	B	85	C
6	B	86	C
6	B	87	A
6	B	88	A
6	B	89	U
6	B	90	U
6	B	91	U
6	B	92	U
6	B	94	U
6	B	95	G
6	B	96	A
9	F	6	C
9	F	7	G
9	F	9	U
9	F	10	U
9	F	12	G
9	F	26	U
9	F	27	A
9	F	28	A
9	F	29	A
9	F	33	G
9	F	34	G
9	F	37	C
9	F	38	G
9	F	46	G
9	F	49	G
9	F	51	U
9	F	54	G
9	F	58	G
9	F	59	G
9	F	60	C
9	F	61	C
9	F	68	C
9	F	69	A
9	F	74	U
9	F	79	C
9	F	81	C
9	F	82	A
9	F	83	A
9	F	84	A
9	F	85	U
9	F	86	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	F	87	C
9	F	89	U
10	G	-11	G
10	G	-7	C
10	G	-6	C
10	G	-1	G
10	G	2	U
10	G	5	G
10	G	8	C
10	G	11	A
10	G	13	C
10	G	17	U
10	G	18	A
10	G	21	A
10	G	22	C
10	G	23	U
10	G	25	G
10	G	27	U
10	G	120	G
10	G	123	U
10	G	124	U
10	G	125	C
10	G	126	C
10	G	127	U
10	G	128	U
10	G	129	G
10	G	130	A
10	G	131	U
10	G	134	U
10	G	135	G
10	G	136	U
10	G	137	C
10	G	138	A
10	G	139	U
10	G	140	A
10	G	141	C
10	G	142	U
10	G	143	U
10	G	144	A
10	G	145	U
10	G	146	C
10	G	149	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	G	163	C
10	G	164	A
10	G	166	A
10	G	167	G
11	H	14	C
11	H	15	U
11	H	16	U
11	H	17	U
11	H	19	G
11	H	20	G
11	H	24	A
11	H	25	G
11	H	29	A
11	H	30	A
11	H	31	G
11	H	33	G
11	H	38	A
11	H	39	U
11	H	40	C
11	H	41	U
11	H	42	G
11	H	43	U
11	H	98	G
11	H	99	A
11	H	100	U
11	H	101	U
11	H	102	U
11	H	103	U
11	H	104	U
11	H	105	G
11	H	106	G
11	H	107	A
11	H	111	G
11	H	112	G
11	H	114	A
11	H	115	G
11	H	143	A
11	H	147	G
11	H	152	G
11	H	153	A
11	H	154	C
11	H	156	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	H	157	G
11	H	168	A
11	H	170	C
11	H	171	U
11	H	177	A
11	H	178	A
11	H	179	C

All (30) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	B	20	G
6	B	21	A
6	B	78	U
6	B	79	C
6	B	80	U
6	B	88	A
6	B	92	U
6	B	95	G
9	F	5	U
9	F	25	C
9	F	26	U
9	F	33	G
9	F	50	A
9	F	58	G
10	G	-12	G
10	G	1	G
10	G	16	G
10	G	21	A
10	G	137	C
10	G	138	A
10	G	142	U
11	H	29	A
11	H	39	U
11	H	40	C
11	H	100	U
11	H	104	U
11	H	105	G
11	H	106	G
11	H	156	U
11	H	168	A

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
18	SEP	R	232	18	8,9,10	1.52	1 (12%)	7,12,14	1.81	1 (14%)
18	SEP	R	224	18	8,9,10	0.84	0	7,12,14	1.54	1 (14%)

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
18	SEP	R	232	18	-	2/6/8/10	-
18	SEP	R	224	18	-	1/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	232	SEP	P-O1P	3.33	1.60	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	232	SEP	OG-CB-CA	4.37	112.39	108.14
18	R	224	SEP	OG-CB-CA	-2.59	105.63	108.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	R	232	SEP	N-CA-CB-OG
18	R	232	SEP	C-CA-CB-OG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	R	224	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 16 are monoatomic - leaving 3 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	$\# Z > 2$
42	IHP	A	3000	-	36,36,36	0.84	0	60,60,60	1.08	2 (3%)
46	ATP	Q	1501	44	32,33,33	2.06	7 (21%)	48,52,52	1.89	16 (33%)
43	GTP	C	1500	44	33,34,34	1.00	2 (6%)	50,54,54	1.60	9 (18%)

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
42	IHP	A	3000	-	-	5/30/54/54	0/1/1/1
46	ATP	Q	1501	44	-	4/22/38/38	0/3/3/3
43	GTP	C	1500	44	-	4/22/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	Q	1501	ATP	PB-O3B	7.43	1.67	1.59
46	Q	1501	ATP	C6-N6	4.57	1.45	1.34
46	Q	1501	ATP	C4-N3	3.31	1.40	1.34
46	Q	1501	ATP	C2'-C3'	-2.82	1.45	1.53
46	Q	1501	ATP	C3'-C4'	-2.24	1.47	1.53
43	C	1500	GTP	C5-N7	-2.18	1.34	1.39
46	Q	1501	ATP	O2'-C2'	-2.15	1.37	1.43
43	C	1500	GTP	O4'-C4'	-2.09	1.40	1.45
46	Q	1501	ATP	C8-N7	2.08	1.35	1.31

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	Q	1501	ATP	C5-C4-N3	-4.96	119.89	126.72
43	C	1500	GTP	C5-C4-N3	-4.54	121.16	128.39
43	C	1500	GTP	C2-N3-C4	4.53	120.10	112.30
46	Q	1501	ATP	N3-C2-N1	-4.33	122.02	128.58
46	Q	1501	ATP	N3-C4-N9	3.79	133.62	127.17
46	Q	1501	ATP	N9-C8-N7	-3.40	109.11	113.94
46	Q	1501	ATP	C2-N3-C4	3.32	119.93	111.83
43	C	1500	GTP	N9-C8-N7	-3.25	107.38	113.40
43	C	1500	GTP	C2-N1-C6	-3.13	119.44	125.11
46	Q	1501	ATP	C4-N9-C8	2.95	108.83	105.74
46	Q	1501	ATP	C5-N7-C8	2.94	108.06	103.45
43	C	1500	GTP	N9-C4-N3	2.78	131.52	125.95
43	C	1500	GTP	C5-C6-N1	2.72	120.18	113.25
46	Q	1501	ATP	C4-C5-N7	-2.71	107.49	110.58
43	C	1500	GTP	C8-N7-C5	2.66	109.00	104.26
42	A	3000	IHP	O13-C3-C2	2.58	114.24	108.76
43	C	1500	GTP	O6-C6-C5	-2.58	119.73	126.53
46	Q	1501	ATP	O2A-PA-O1A	-2.55	100.58	112.44
46	Q	1501	ATP	O2G-PG-O1G	-2.44	101.31	110.83
46	Q	1501	ATP	O2G-PG-O3B	2.31	112.39	104.64
46	Q	1501	ATP	O2B-PB-O1B	-2.26	101.93	112.44
46	Q	1501	ATP	O2A-PA-O3A	2.24	113.33	107.27
46	Q	1501	ATP	O5'-C5'-C4'	2.13	116.25	108.99
42	A	3000	IHP	O44-P4-O34	2.10	115.67	107.80
43	C	1500	GTP	C2'-C3'-C4'	2.10	106.66	102.61
46	Q	1501	ATP	O4'-C1'-N9	2.09	112.11	108.09
46	Q	1501	ATP	O3G-PG-O3B	2.06	111.56	104.64

There are no chirality outliers.

All (13) torsion outliers are listed below:

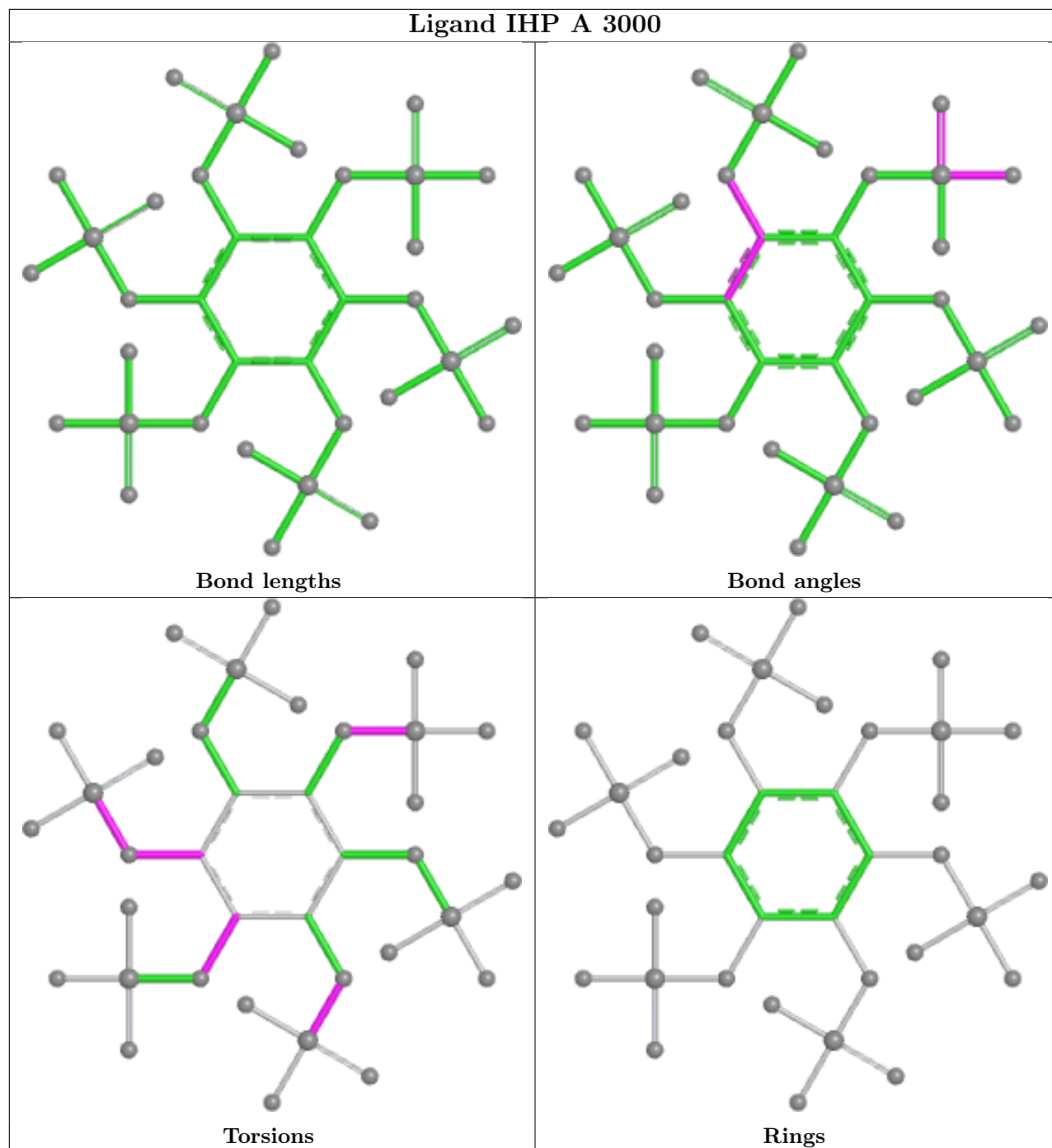
Mol	Chain	Res	Type	Atoms
43	C	1500	GTP	PB-O3B-PG-O3G
46	Q	1501	ATP	C5'-O5'-PA-O1A
46	Q	1501	ATP	C5'-O5'-PA-O2A
46	Q	1501	ATP	C5'-O5'-PA-O3A
43	C	1500	GTP	C3'-C4'-C5'-O5'
43	C	1500	GTP	O4'-C4'-C5'-O5'
42	A	3000	IHP	C2-O12-P2-O22
42	A	3000	IHP	C3-C2-O12-P2
42	A	3000	IHP	C4-O14-P4-O44
46	Q	1501	ATP	PB-O3A-PA-O2A
43	C	1500	GTP	PB-O3A-PA-O2A
42	A	3000	IHP	C2-C1-O11-P1
42	A	3000	IHP	C6-O16-P6-O26

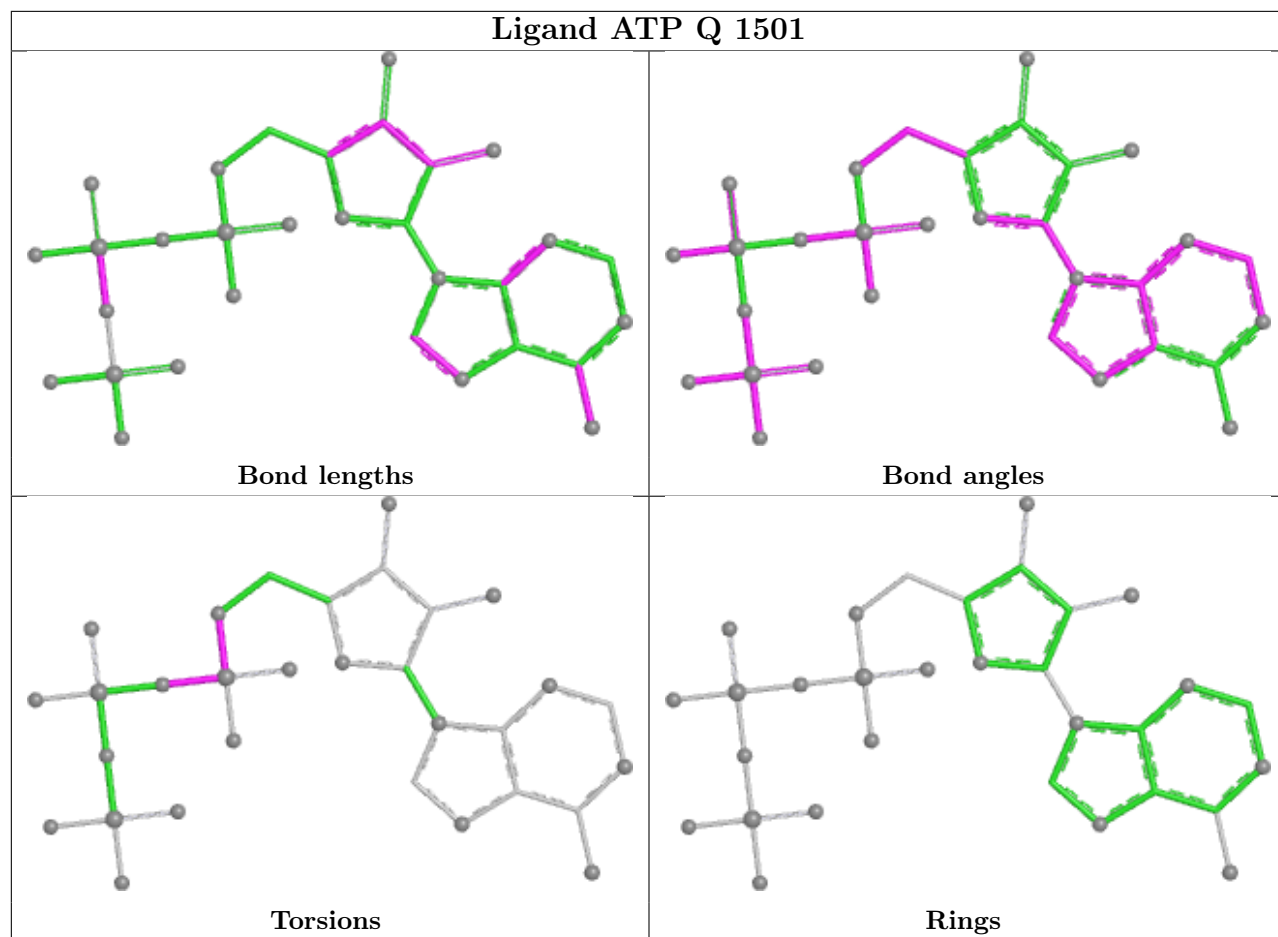
There are no ring outliers.

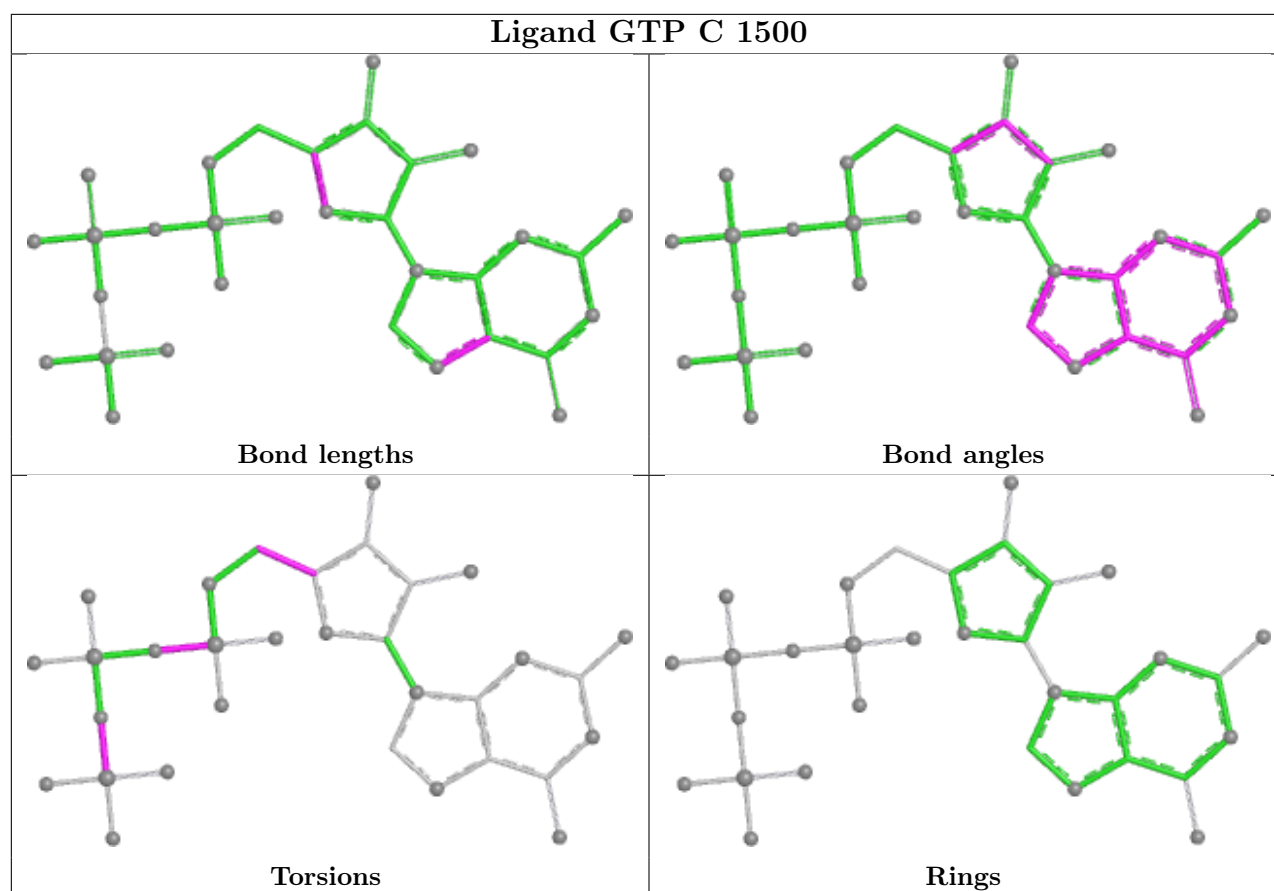
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	A	3000	IHP	3	0
43	C	1500	GTP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

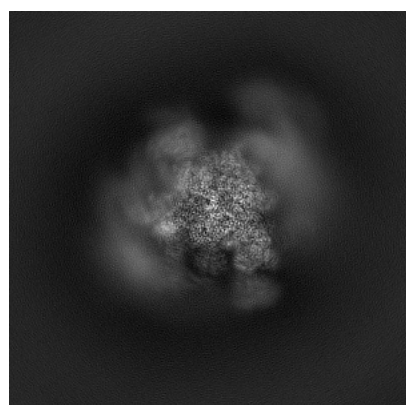
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9645. These allow visual inspection of the internal detail of the map and identification of artifacts.

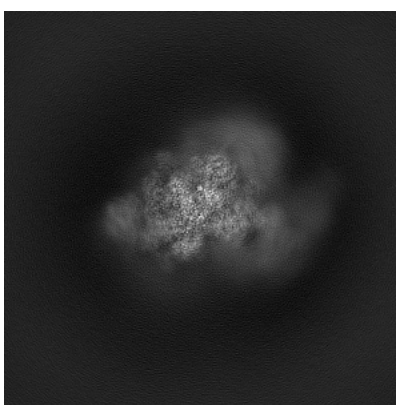
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

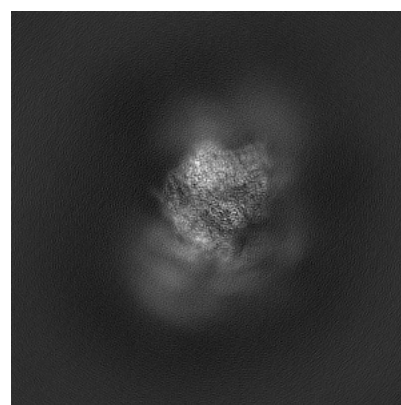
6.1.1 Primary map



X



Y

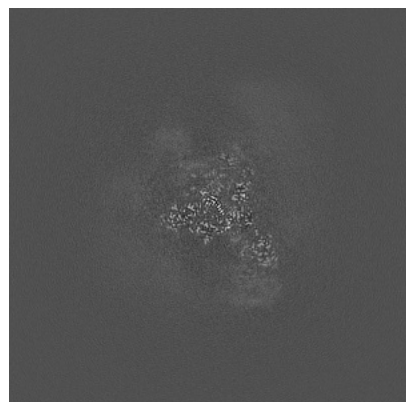


Z

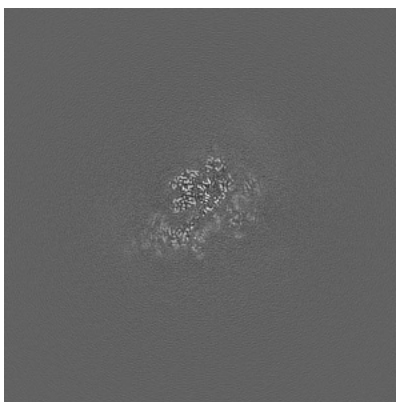
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

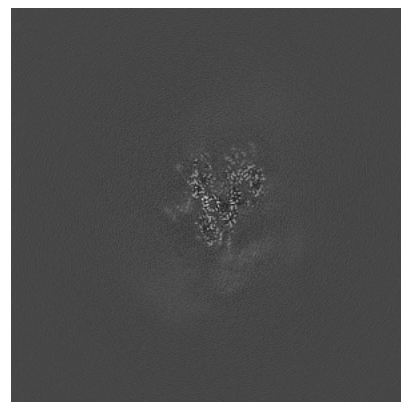
6.2.1 Primary map



X Index: 200



Y Index: 200

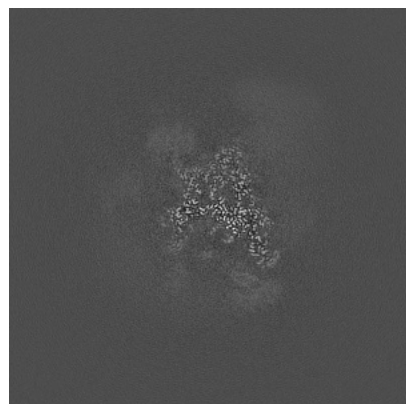


Z Index: 200

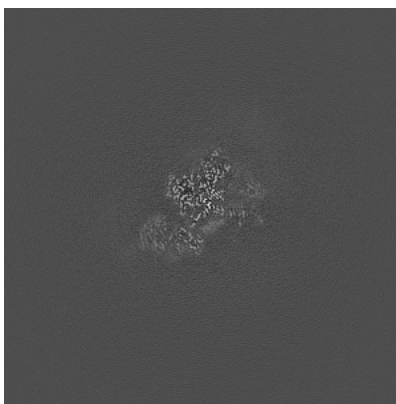
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

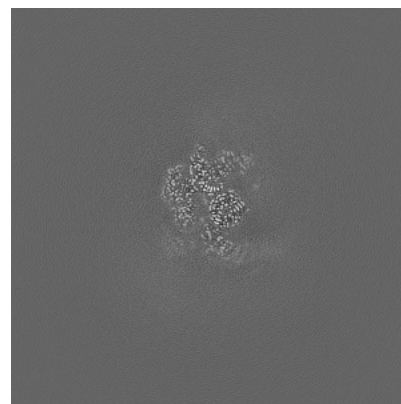
6.3.1 Primary map



X Index: 193



Y Index: 205

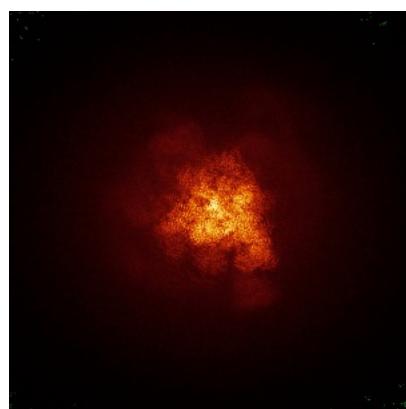


Z Index: 180

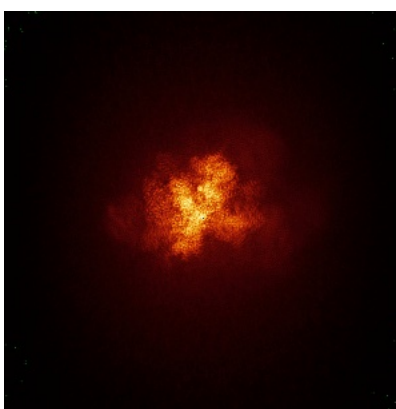
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

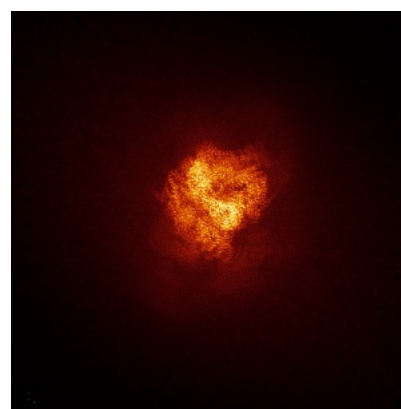
6.4.1 Primary map



X



Y

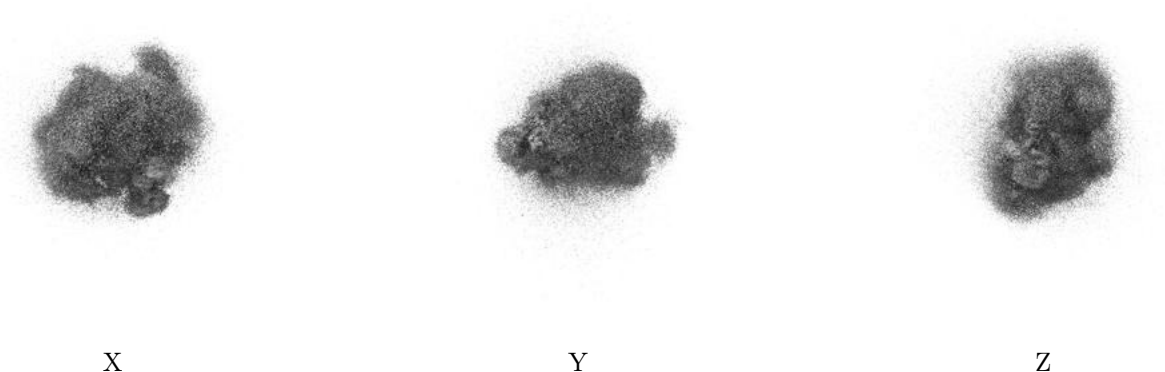


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

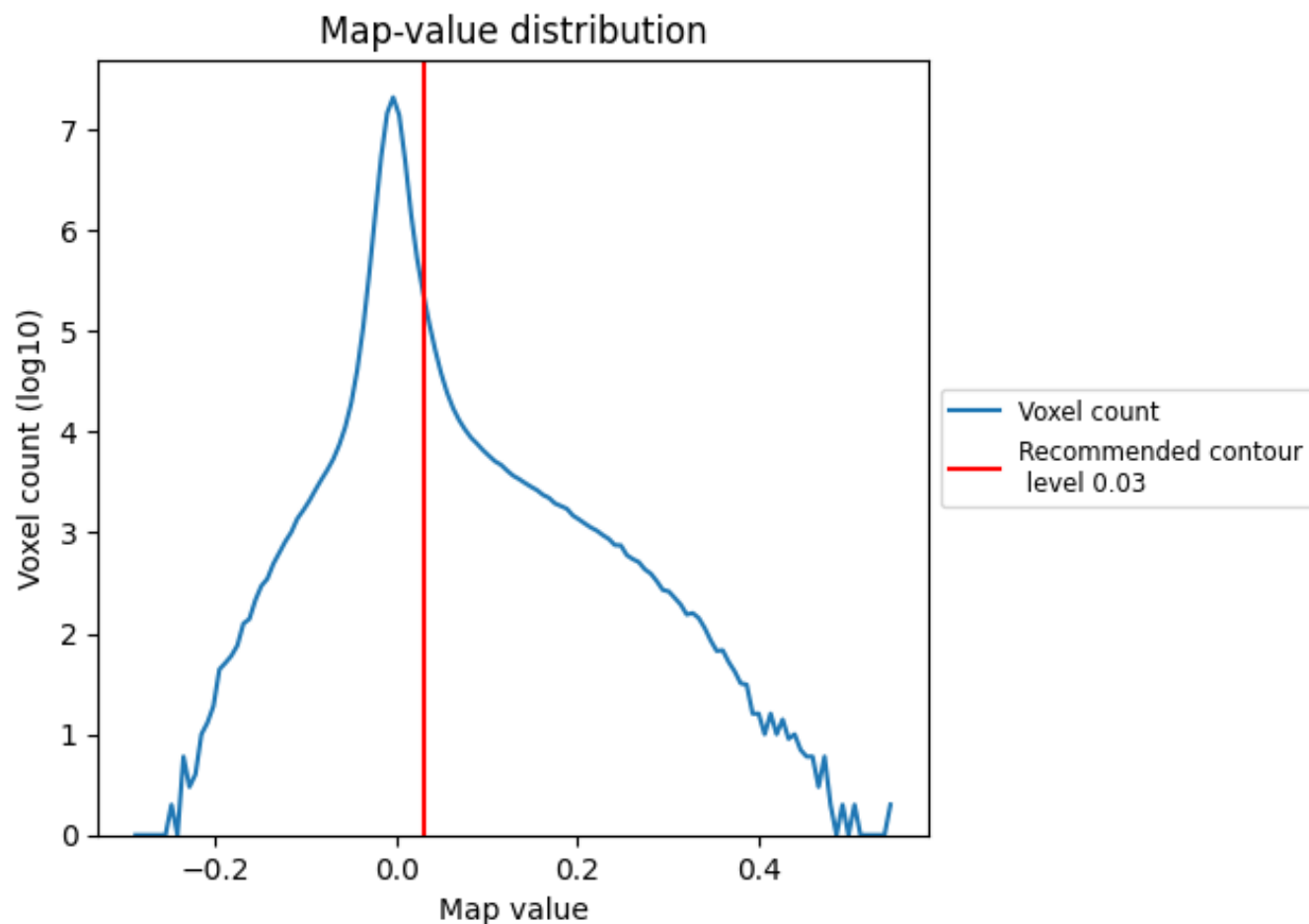
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

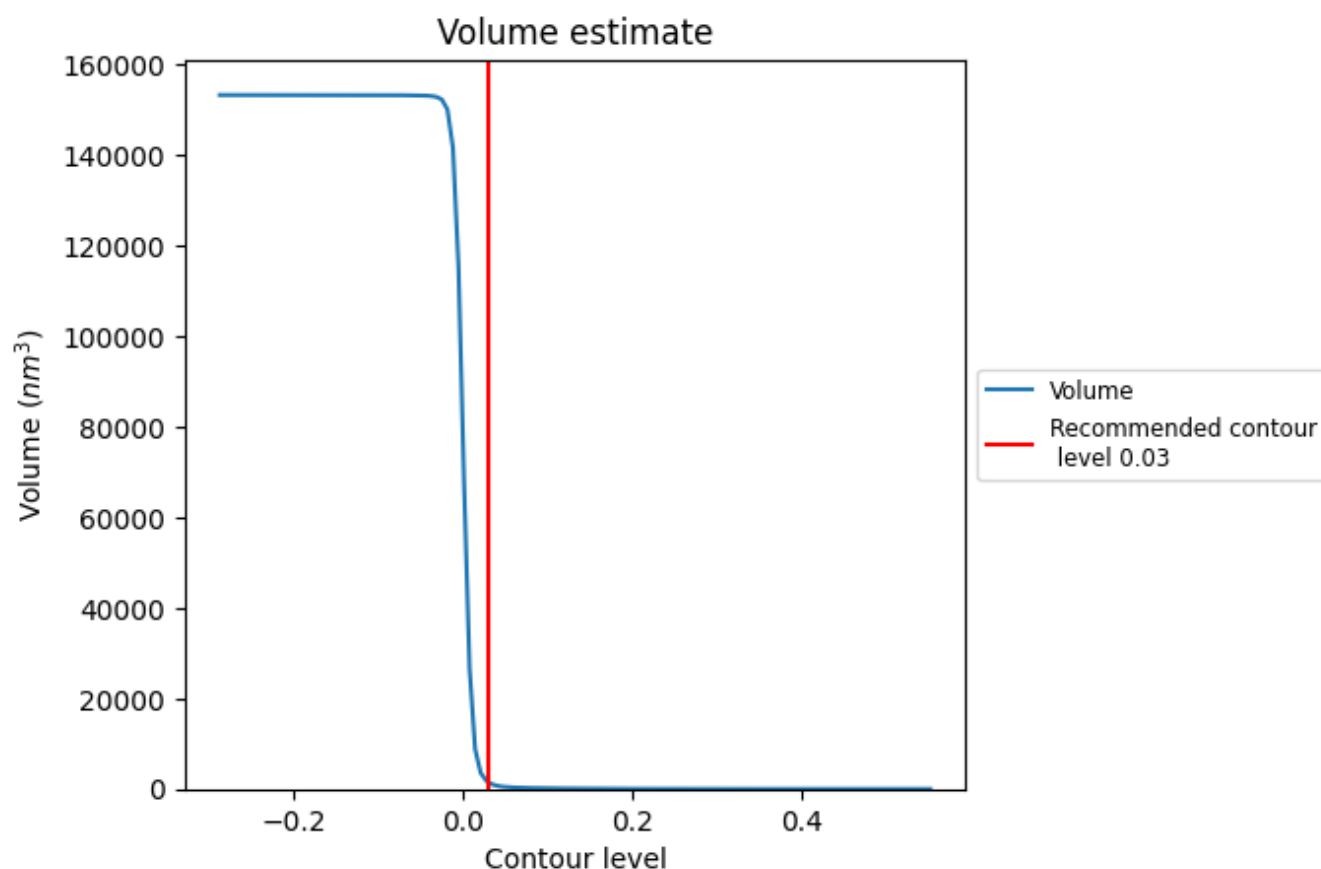
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

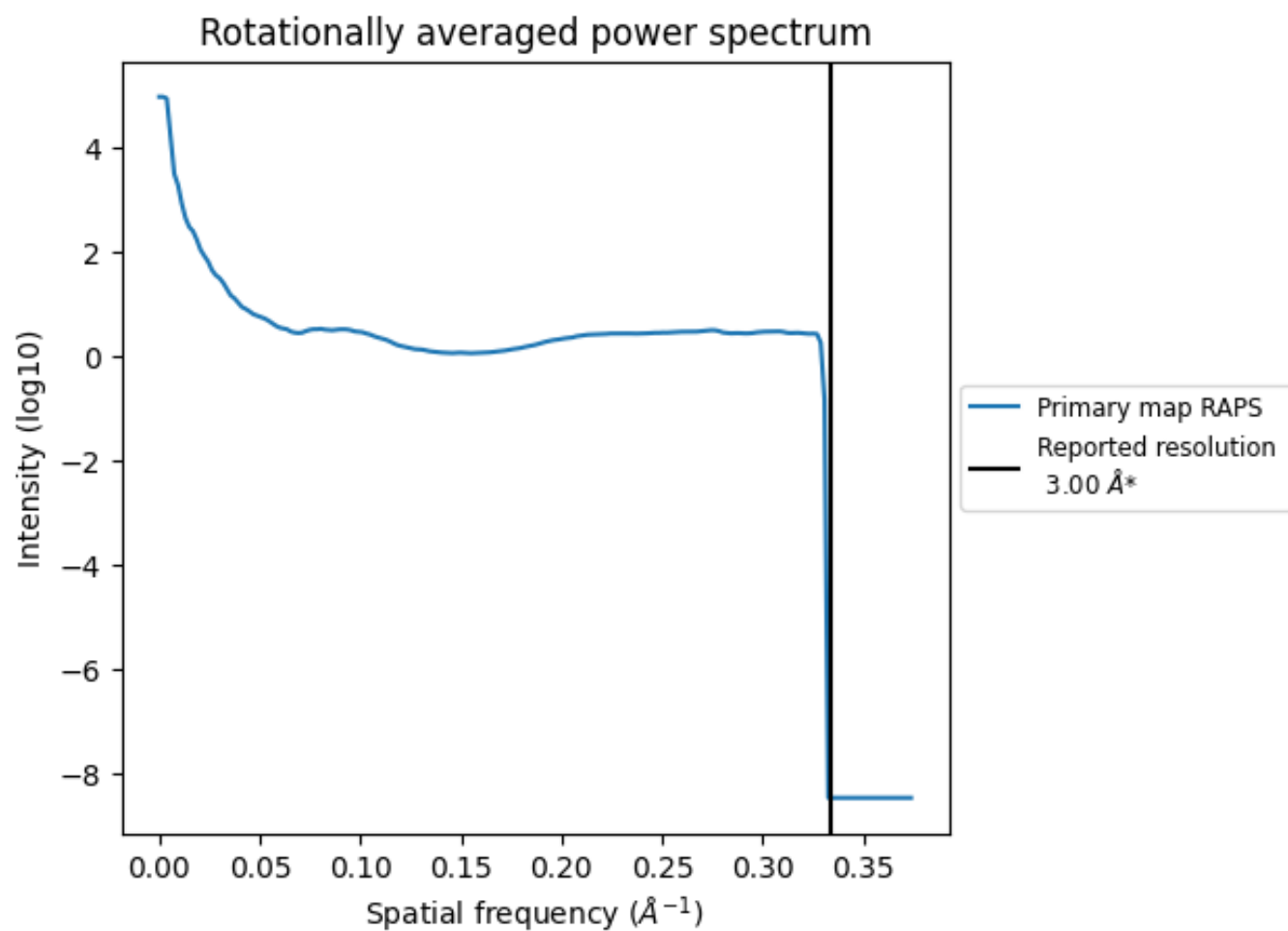
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1504 nm³; this corresponds to an approximate mass of 1358 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

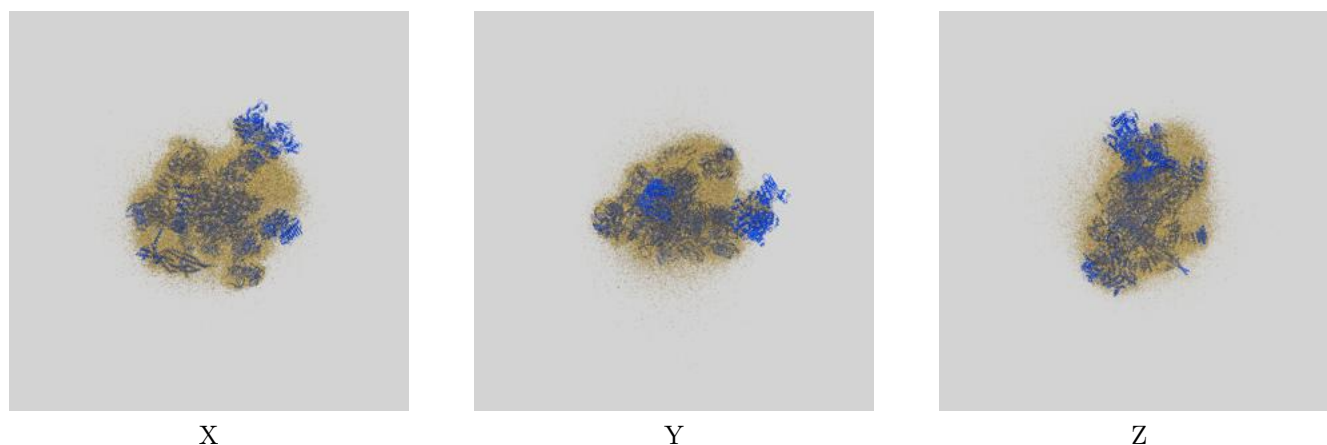
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

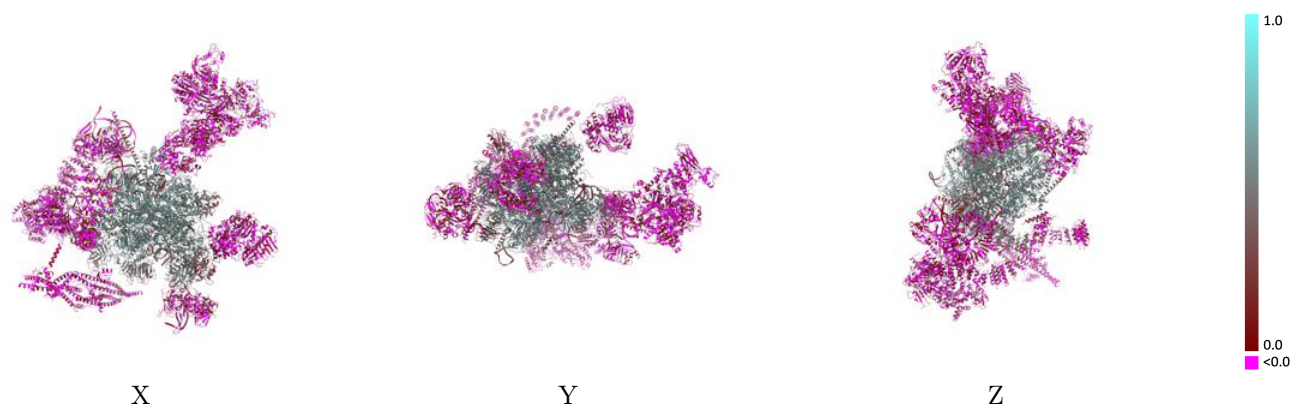
This section contains information regarding the fit between EMDB map EMD-9645 and PDB model 6ICZ. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



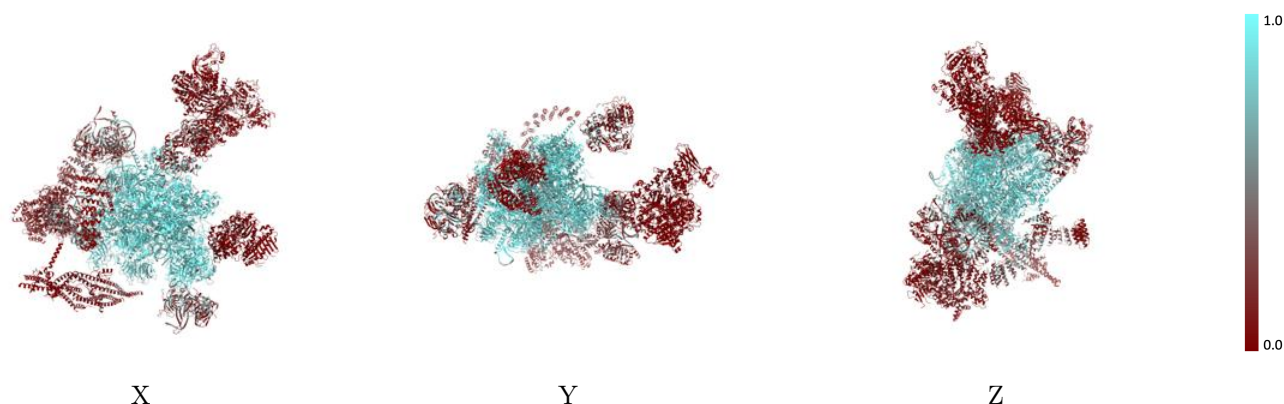
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



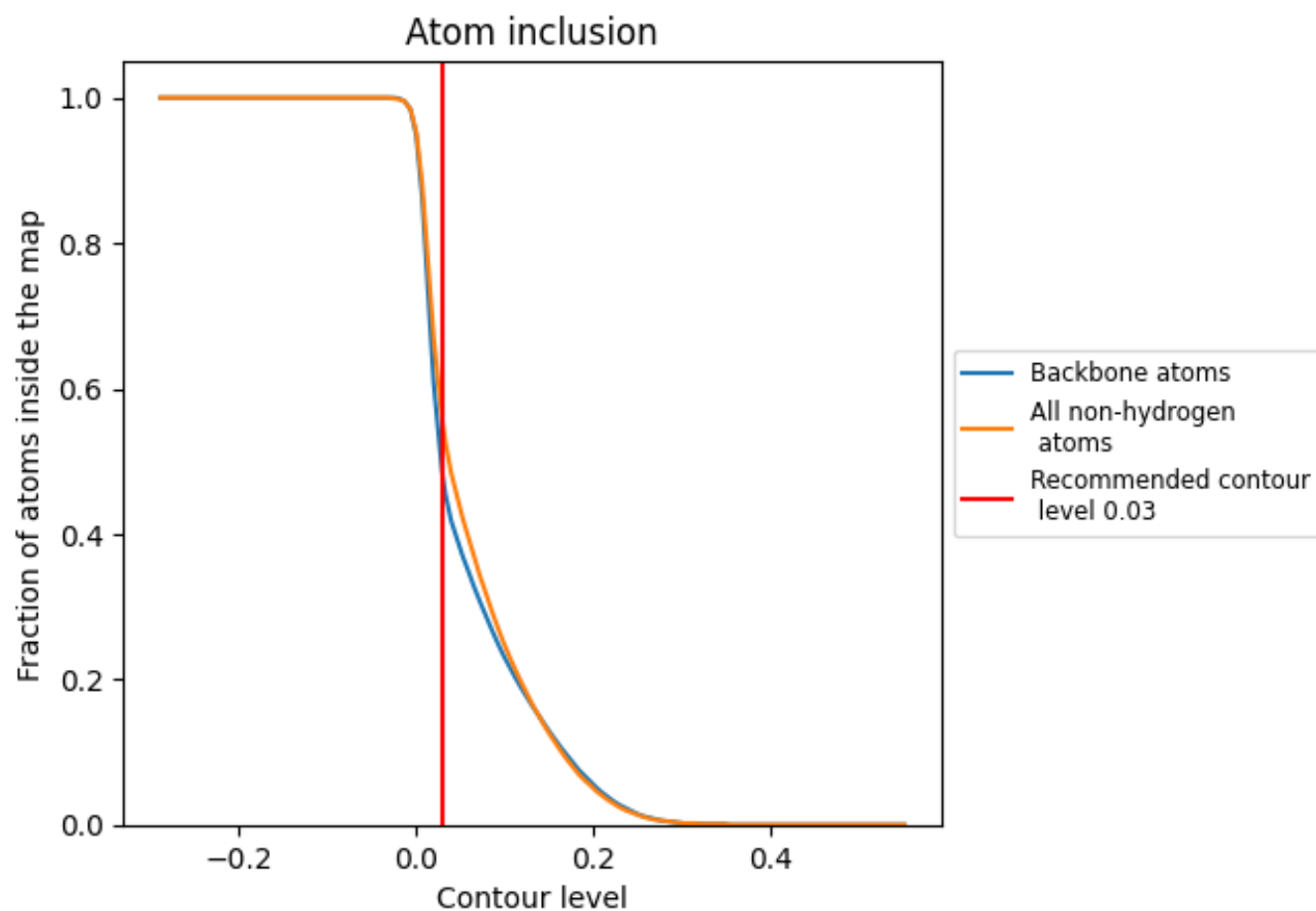
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 49% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5600	 0.2840
A	 0.8720	 0.5070
B	 0.7660	 0.3530
C	 0.8960	 0.4650
D	 0.0170	 0.0020
E	 0.8600	 0.4140
F	 0.9330	 0.4850
G	 0.7650	 0.3440
H	 0.4880	 0.1340
I	 0.2180	 0.0190
J	 0.5970	 0.3190
K	 0.1120	 -0.0060
L	 0.6000	 0.3280
M	 0.8730	 0.4830
N	 0.9350	 0.5390
O	 0.8170	 0.4200
P	 0.8340	 0.4750
Q	 0.0290	 0.0020
R	 0.8770	 0.4780
S	 0.8670	 0.4200
T	 0.9650	 0.5840
U	 0.8240	 0.5200
V	 0.4890	 0.2780
W	 0.8310	 0.4190
X	 0.5930	 0.3250
Y	 0.2630	 0.0450
Z	 0.7970	 0.4390
a	 0.3460	 0.0120
b	 0.3260	 0.0300
c	 0.2930	 0.0150
d	 0.3210	 0.0150
e	 0.3220	 0.0560
f	 0.3020	 0.0360
g	 0.3000	 0.0160
h	 0.1990	 -0.0100



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.2030	 0.0080
j	 0.3640	 0.0370
k	 0.2940	 -0.0060
l	 0.3040	 0.0530
m	 0.3820	 0.0410
n	 0.2270	 -0.0020
o	 0.1490	 0.0120
p	 0.2390	 -0.0180
q	 0.0430	 -0.0060
r	 0.0690	 0.0010
s	 0.1190	 0.0440
t	 0.0570	 -0.0170
u	 0.0290	 -0.0080
v	 0.0010	 0.0100
w	 0.0000	 0.0450
x	 0.0000	 0.0520
y	 0.1870	 -0.0070