Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 04:52 am GMT

PDB ID	:	6ZYM
EMDB ID	:	EMD-11569
Title	:	Human C Complex Spliceosome - High-resolution CORE
Authors	:	Bertram, K.; Kastner, B.
Deposited on	:	2020-08-02
Resolution	:	3.40 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:

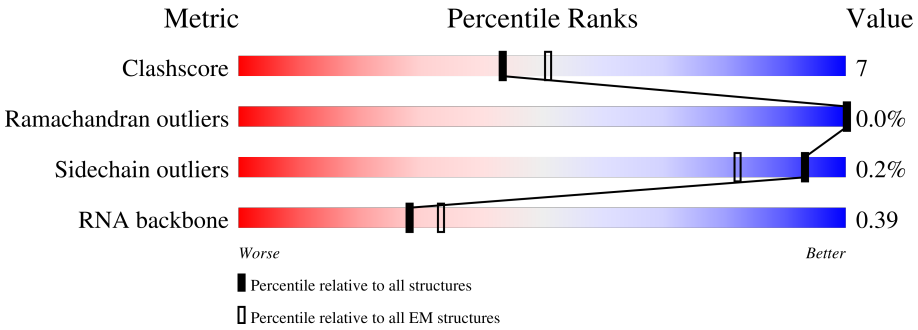
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	2	188	5% 6% · 86%
2	5	116	50% 11% · 36%
3	6	79	· 56% 42% ·
4	9	450	•• 97%
5	A	1755	· 81% 16% ••
6	B	952	75% 18% · 6%
7	C	536	· 36% 5% 58%

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Mol	Chain	Length	Quality of chain
8	D	514	46% 14% 39%
9	E	579	11% 87%
10	F	357	62% 21% 16%
11	L	802	23% 75%
12	O	848	25% 5% 70%
13	P	218	72% 16% 11%
14	Q	144	85% 10%
15	R	229	32% 6% 62%
16	S	2752	99%
17	T	908	19% 78%
18	V	166	81% 17%
19	Y	324	7% 87%
19	Z	324	96%
20	p	654	48% 50%
21	r	1227	97%
22	s	285	7% 93%
23	t	425	13% 87%
24	u	178	83% 5% 12%
25	x	258	12% 88%

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 48271 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	27	575	257	99	192	27	0	0

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	5	74	1548	693	256	525	74	0	0

- Molecule 3 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	6	79	1690	756	312	543	79	0	0

- Molecule 4 is a protein called Corepressor interacting with RBPJ 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	9	14	112	68	21	22	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A	1722	14270	9190	2521	2494	65	0	0

- Molecule 6 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	B	895	6953	4447	1163	1309	34	0	0

- Molecule 7 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	224	Total	C	N	O	S	0	0
			1703	1074	308	312	9		

- Molecule 8 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	315	Total	C	N	O	S	0	0
			2481	1565	451	458	7		

- Molecule 9 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	78	Total	C	N	O	S	0	0
			629	400	107	118	4		

- Molecule 10 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	299	Total	C	N	O	S	0	0
			2230	1407	381	430	12		

- Molecule 11 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	202	Total	C	N	O	S	0	0
			1611	1012	297	296	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	252	Total	C	N	O	S	0	0
			2108	1345	381	377	5		

- Molecule 13 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	195	Total	C	N	O	S	0	0
			1577	991	279	290	17		

- Molecule 14 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	142	Total	C	N	O	S	0	0
			1162	733	216	202	11		

- Molecule 15 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	87	Total	C	N	O	S	0	0
			681	421	134	125	1		

- Molecule 16 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	30	Total	C	N	O	S	0	0
			230	140	49	40	1		

- Molecule 17 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	203	Total	C	N	O	S	0	0
			1669	1071	278	307	13		

- Molecule 18 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	163	Total	C	N	O	S	0	0
			1081	677	200	199	5		

- Molecule 19 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Y	41	Total	C	N	O	P	0	0
			873	391	155	286	41		
19	Z	13	Total	C	N	O	P	0	0
			276	123	50	90	13		

- Molecule 20 is a protein called WD repeat-containing protein 70.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	p	325	Total	C	N	O	S	0	0
			2372	1493	421	442	16		

- Molecule 21 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase

PRP16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	r	35	Total	C	N	O	S	0	0
			259	157	50	51	1		

- Molecule 22 is a protein called Pre-mRNA-splicing factor ISY1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	s	20	Total	C	N	O	S	0	0
			158	96	33	28	1		

- Molecule 23 is a protein called Pre-mRNA-splicing factor CWC25 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	t	56	Total	C	N	O	0	0
			418	259	80	79		

- Molecule 24 is a protein called Splicing factor YJU2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	u	157	Total	C	N	O	S	0	0
			1286	819	226	231	10		

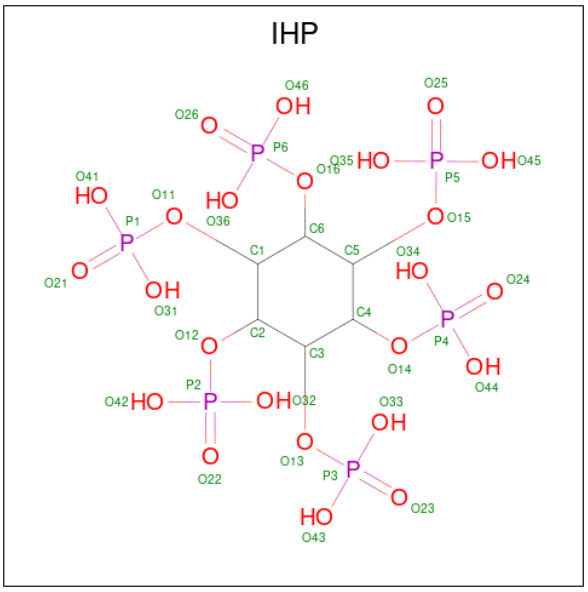
- Molecule 25 is a protein called Protein FRG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	x	30	Total	C	N	O	S	0	0
			239	149	49	40	1		

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

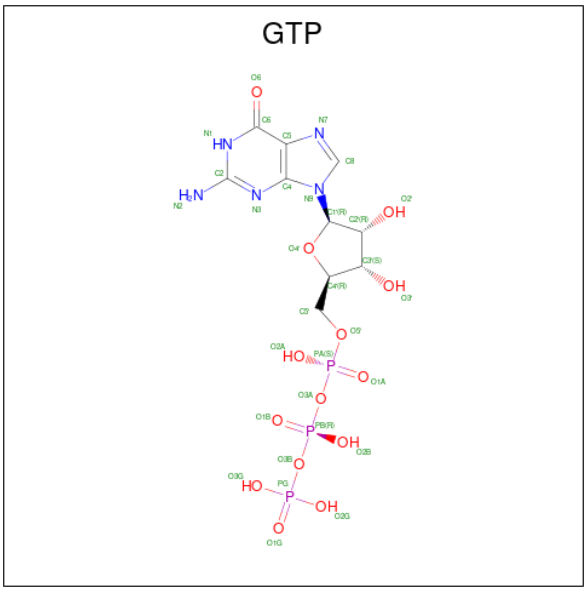
Mol	Chain	Residues	Atoms		AltConf
26	6	5	Total	Mg	0
			5	5	

- Molecule 27 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 28 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 29 is ZINC ION (three-letter code: ZN) (formula: Zn).

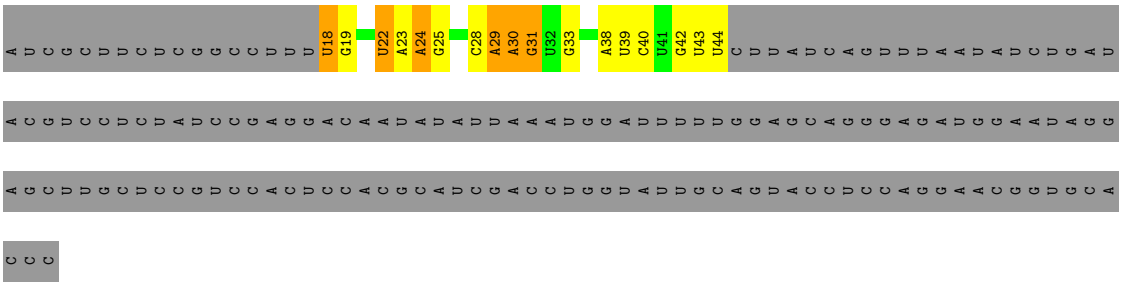
Mol	Chain	Residues	Atoms	AltConf
29	P	3	Total Zn 3 3	0
29	Q	3	Total Zn 3 3	0
29	u	1	Total Zn 1 1	0

3 Residue-property plots (i)

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

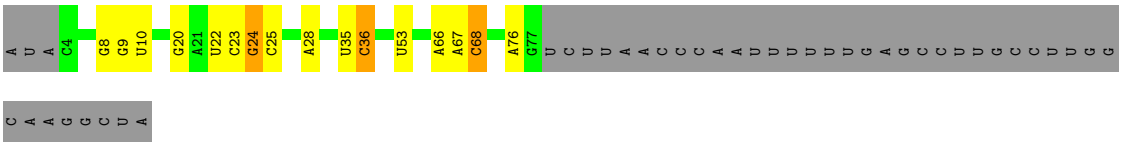
• Molecule 1: U2 snRNA

Chain 2:



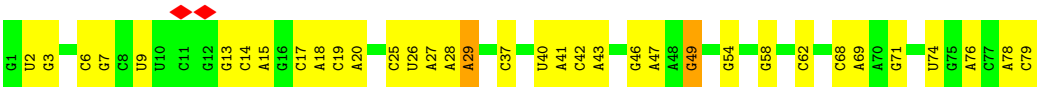
• Molecule 2: U5 snRNA

Chain 5:



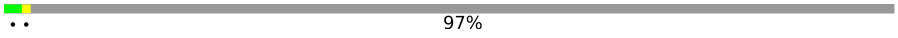
• Molecule 3: U6 snRNA

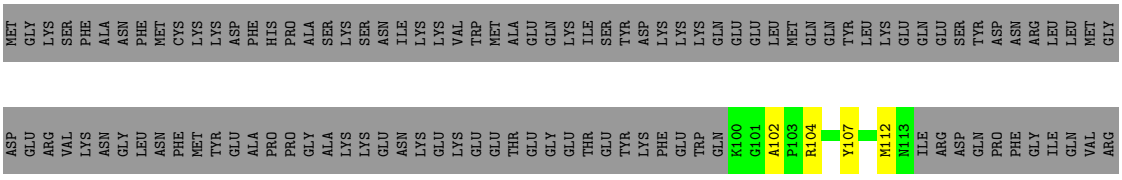
Chain 6:

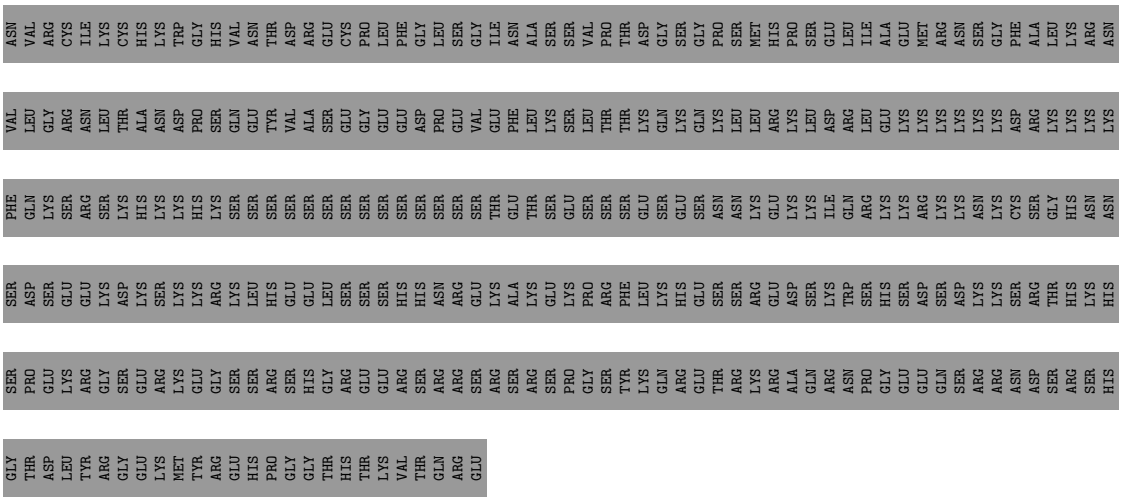


• Molecule 4: Corepressor interacting with RBPJ 1

Chain 9:

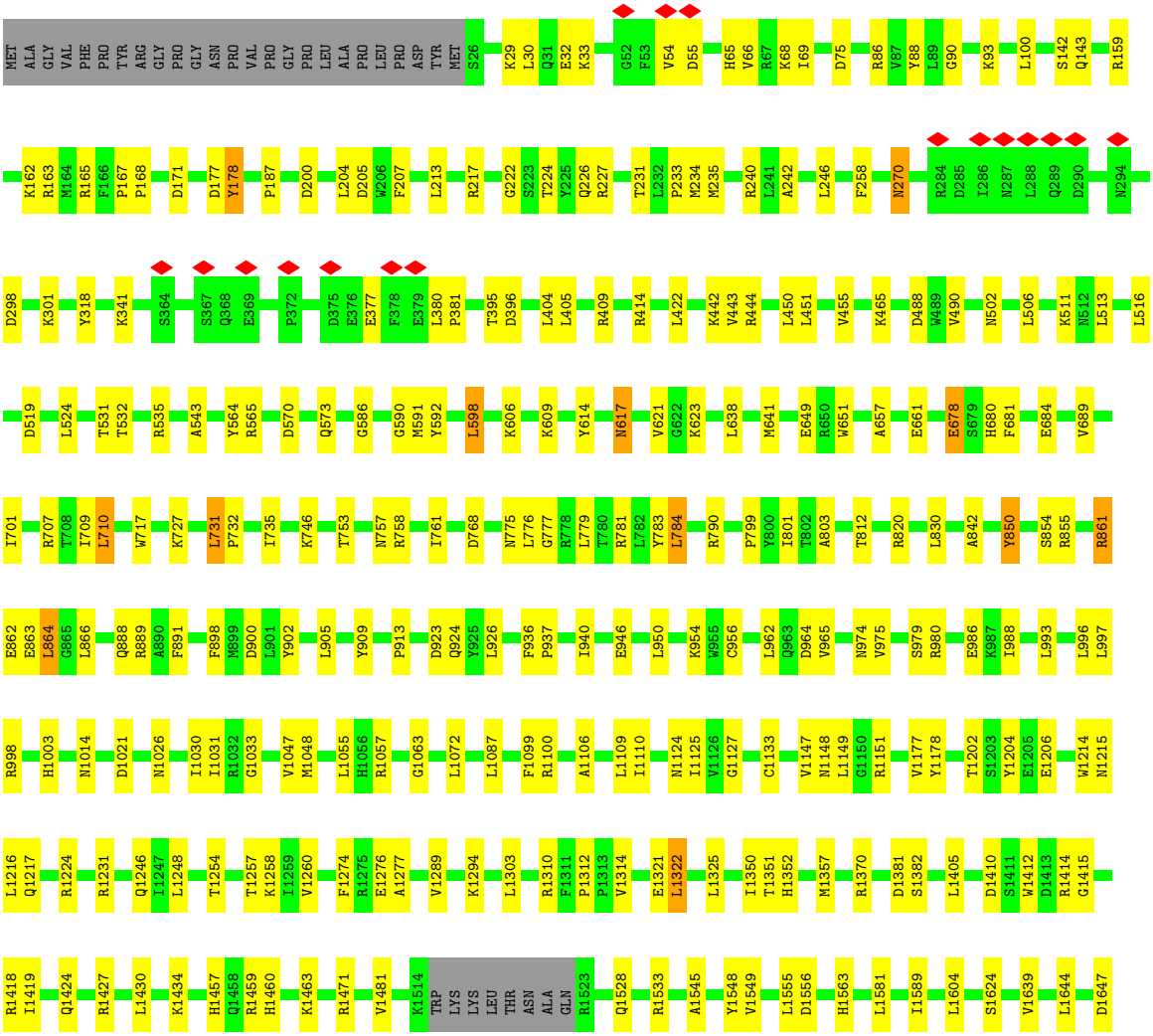






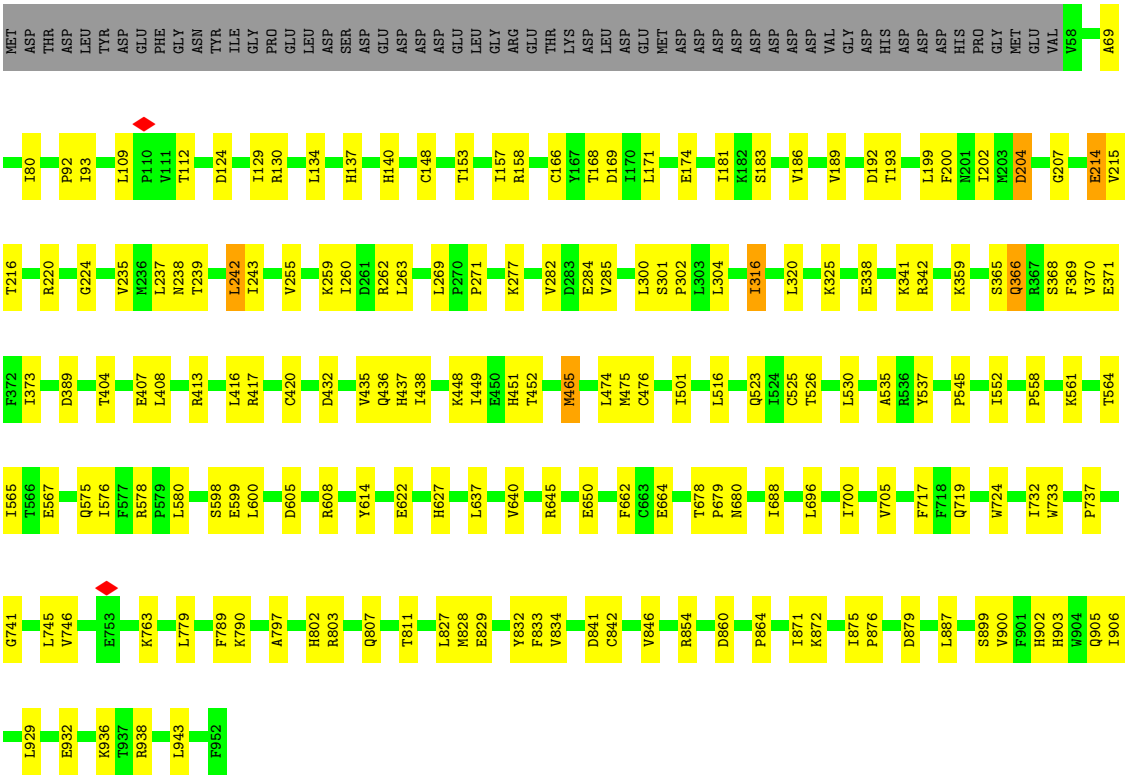
• Molecule 5: Pre-mRNA-processing-splicing factor 8

Chain A:



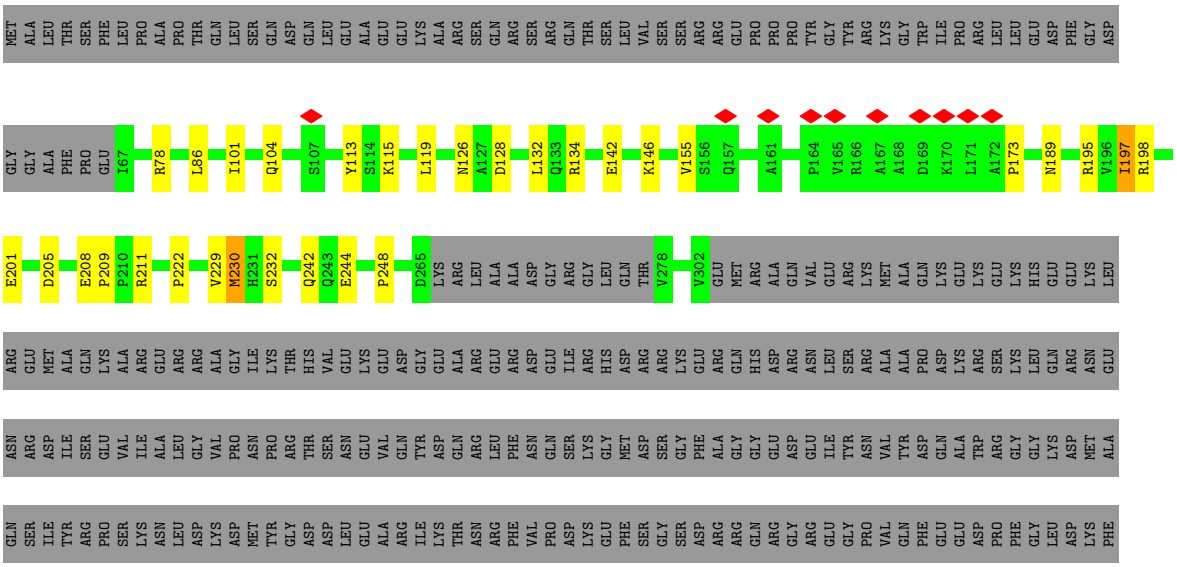
• Molecule 6: 116 kDa U5 small nuclear ribonucleoprotein component

Chain B:

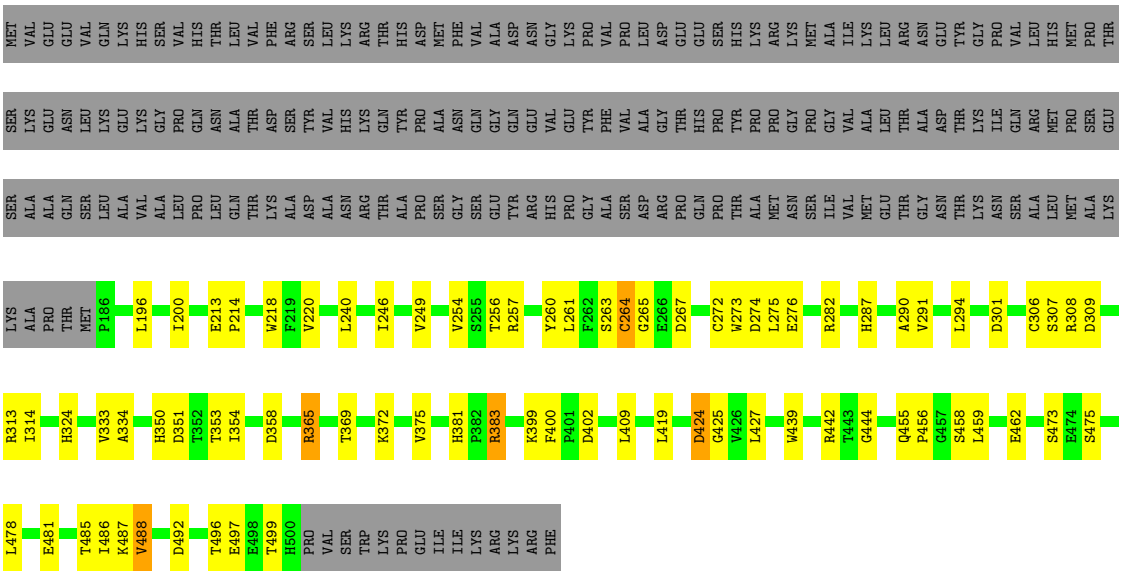


• Molecule 7: SNW domain-containing protein 1

Chain C:



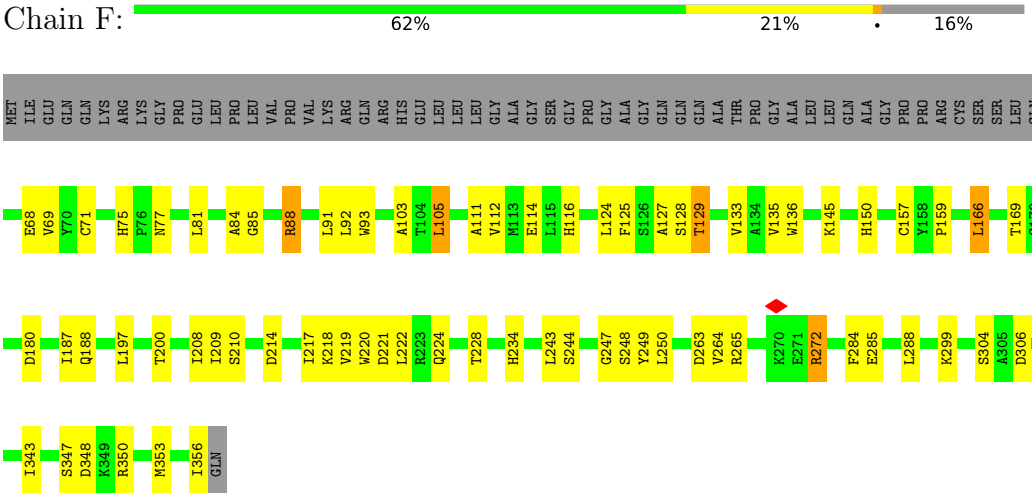
• Molecule 8: Pleiotropic regulator 1



• Molecule 9: Pre-mRNA-processing factor 17

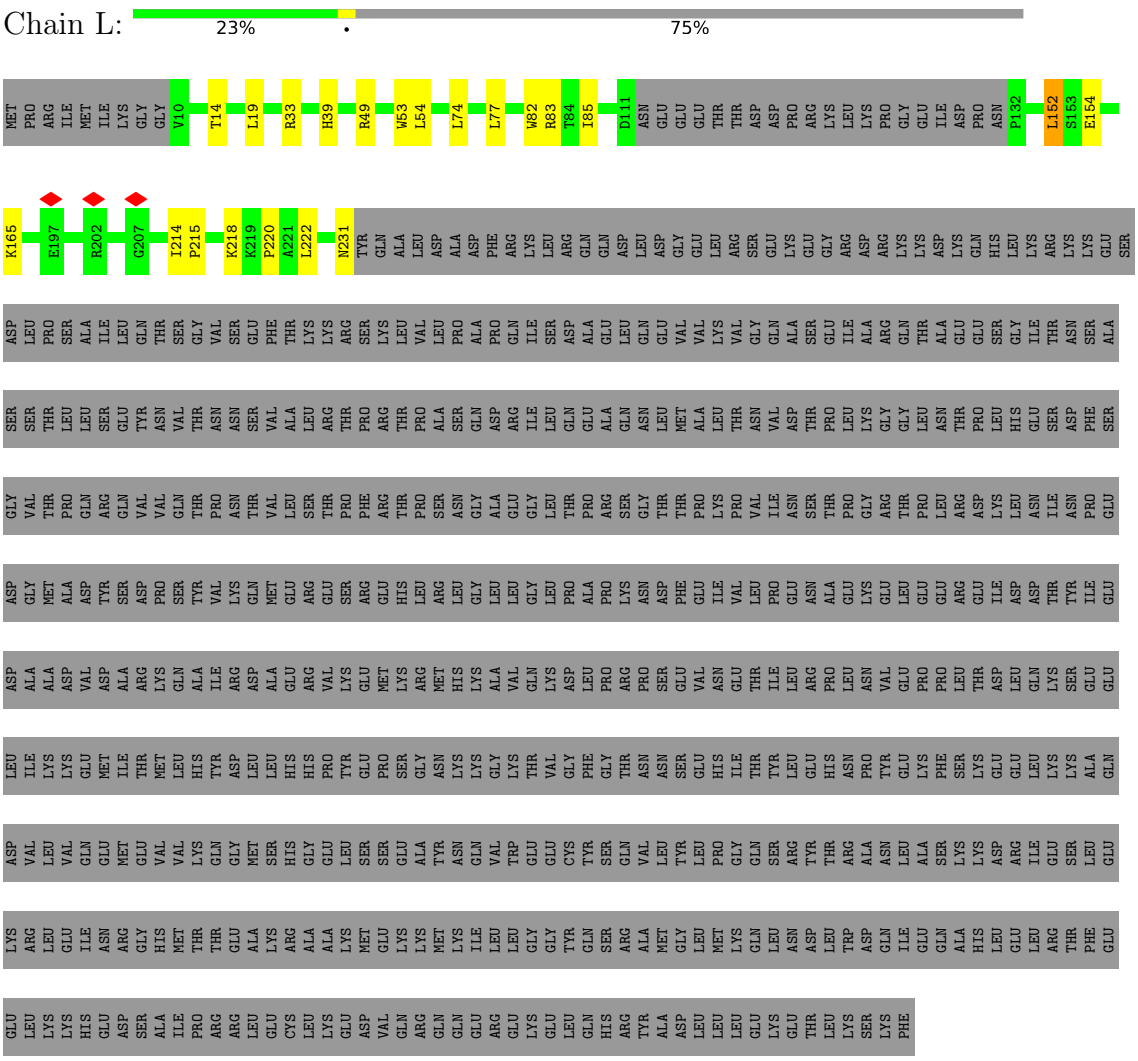
• Molecule 10: U5 small nuclear ribonucleoprotein 40 kDa protein

Chain F:



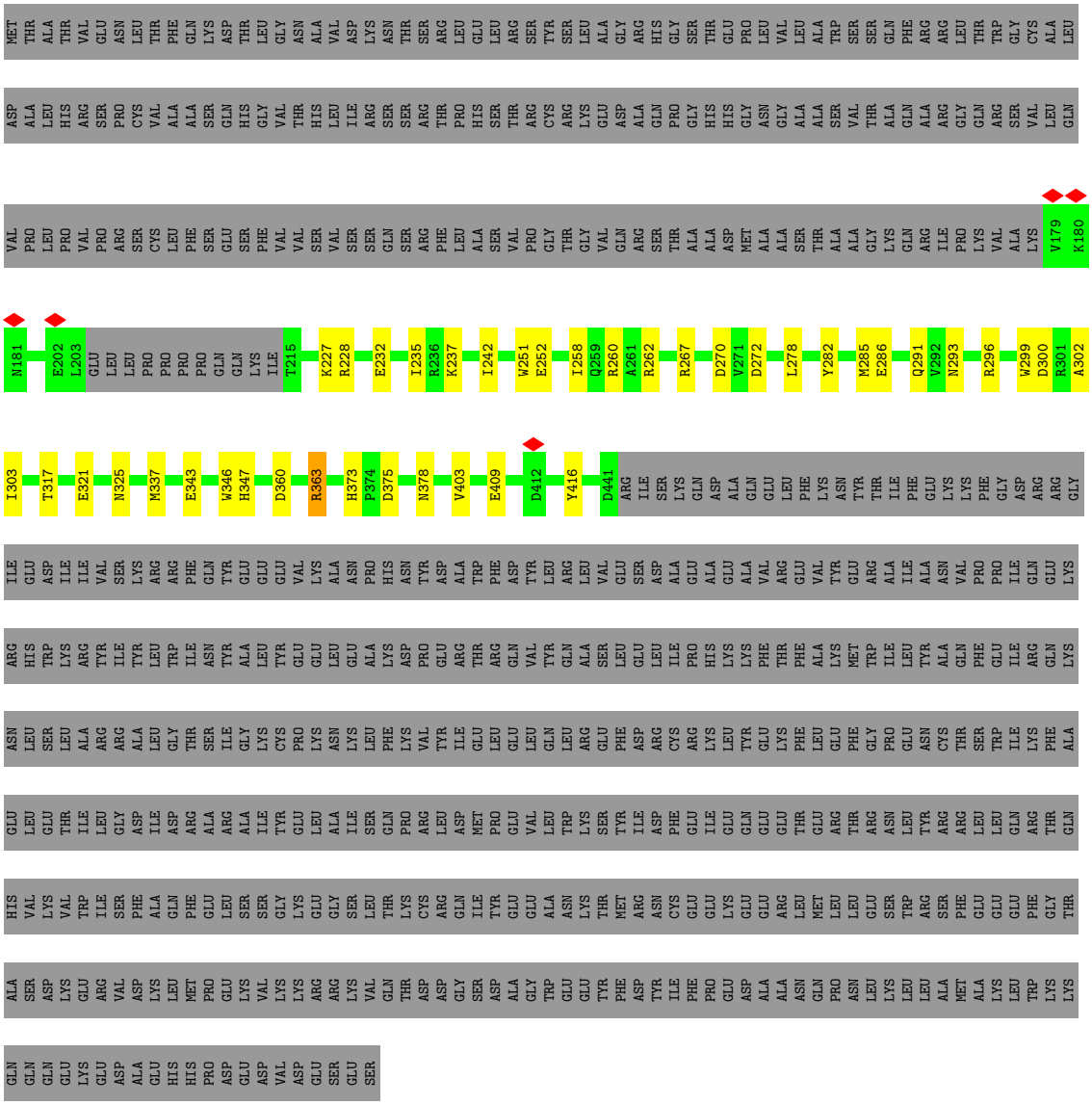
• Molecule 11: Cell division cycle 5-like protein

Chain L:



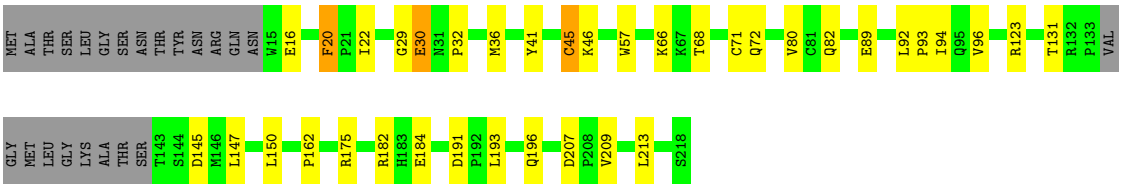
• Molecule 12: Crooked neck-like protein 1

Chain O:



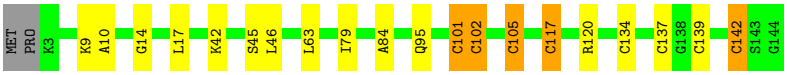
• Molecule 13: Pre-mRNA-splicing factor RBM22

Chain P:



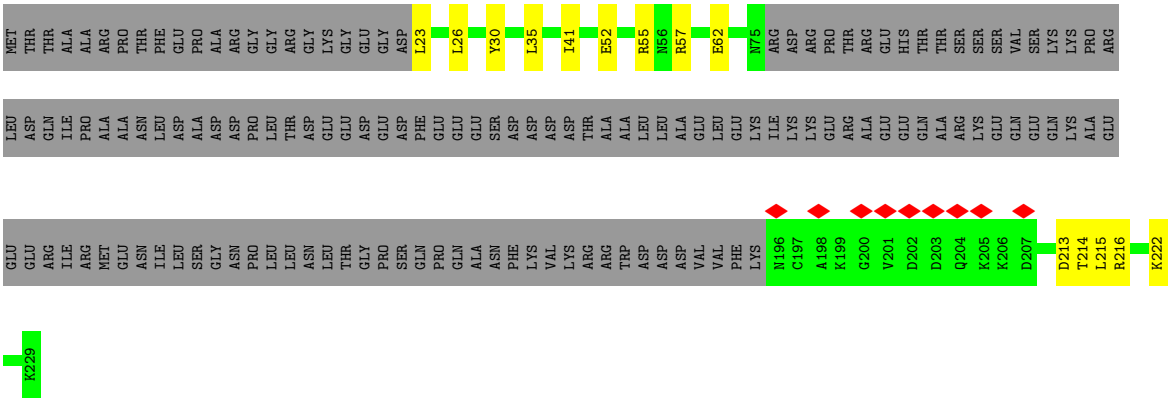
• Molecule 14: Protein BUD31 homolog

Chain Q:



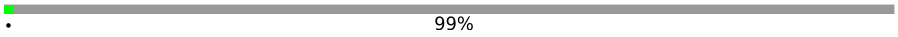
• Molecule 15: Spliceosome-associated protein CWC15 homolog

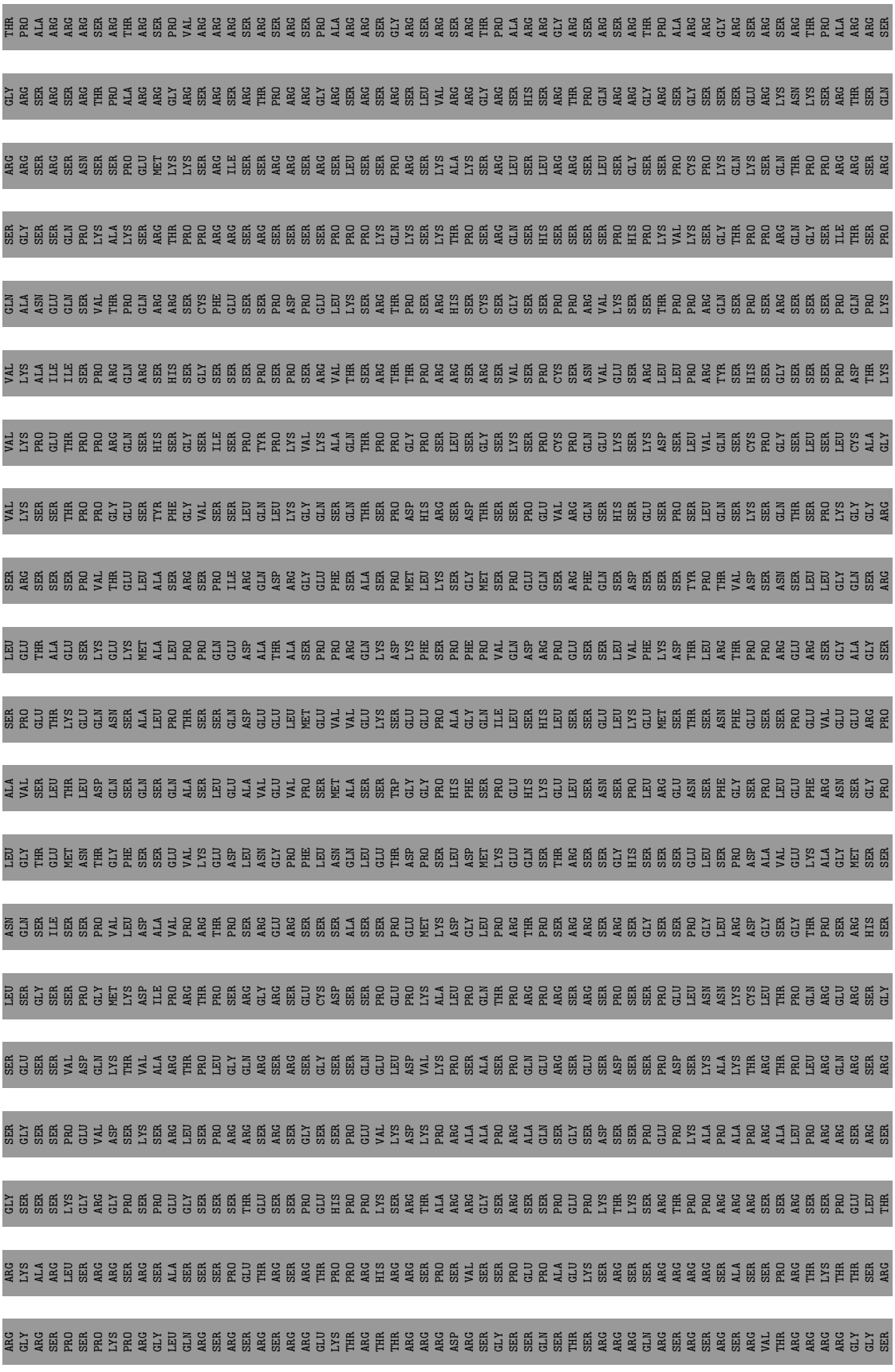
Chain R:

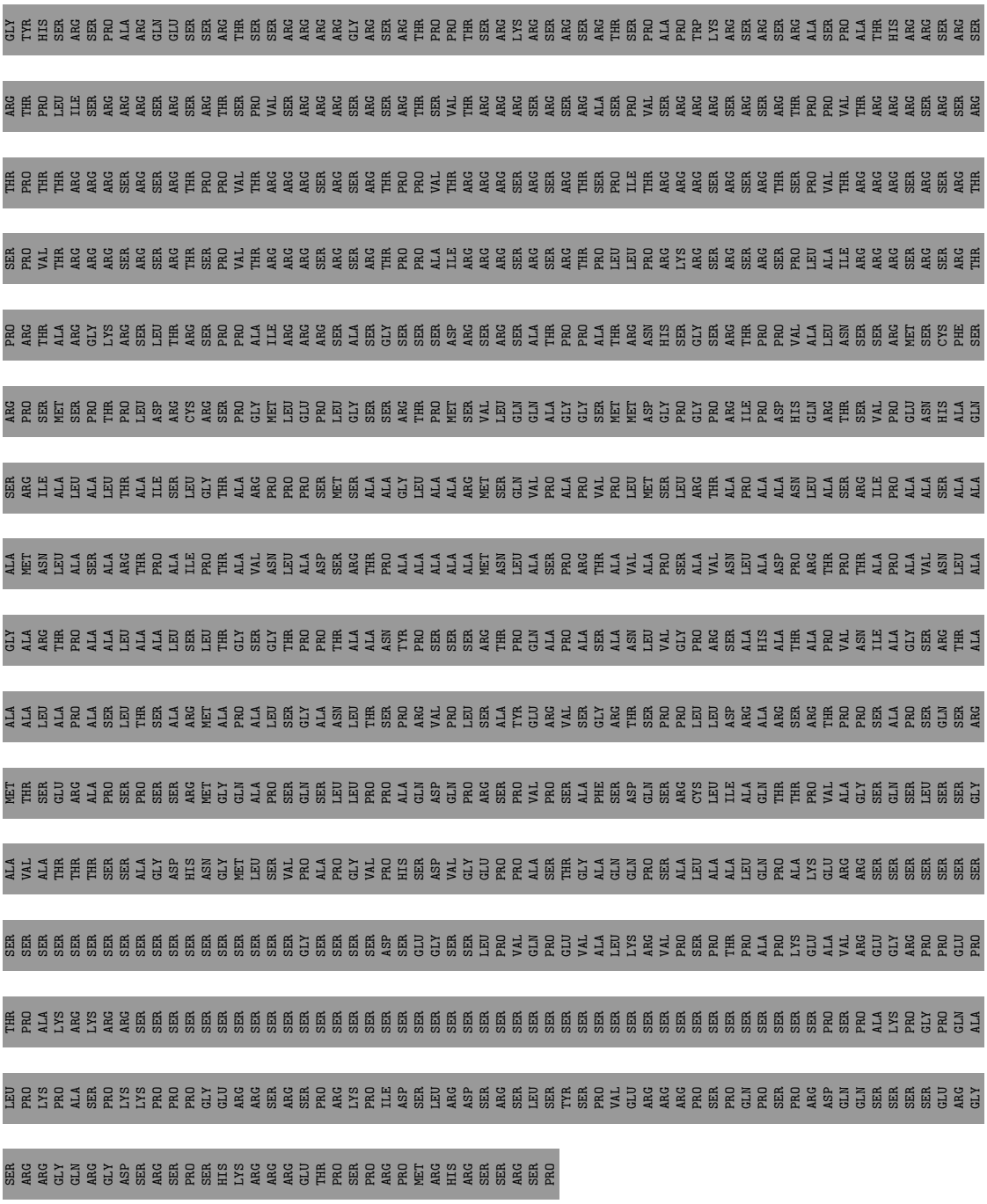


• Molecule 16: Serine/arginine repetitive matrix protein 2

Chain S:

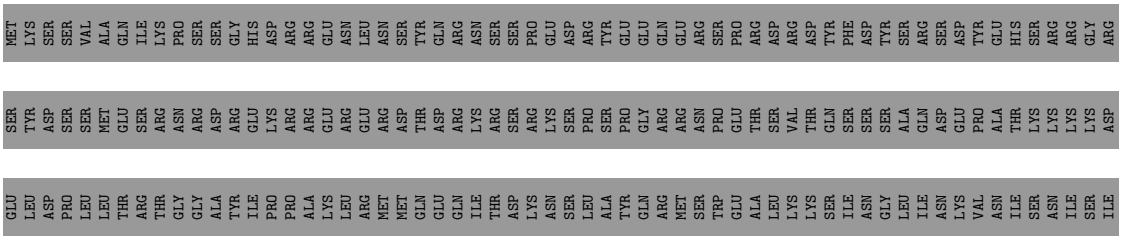


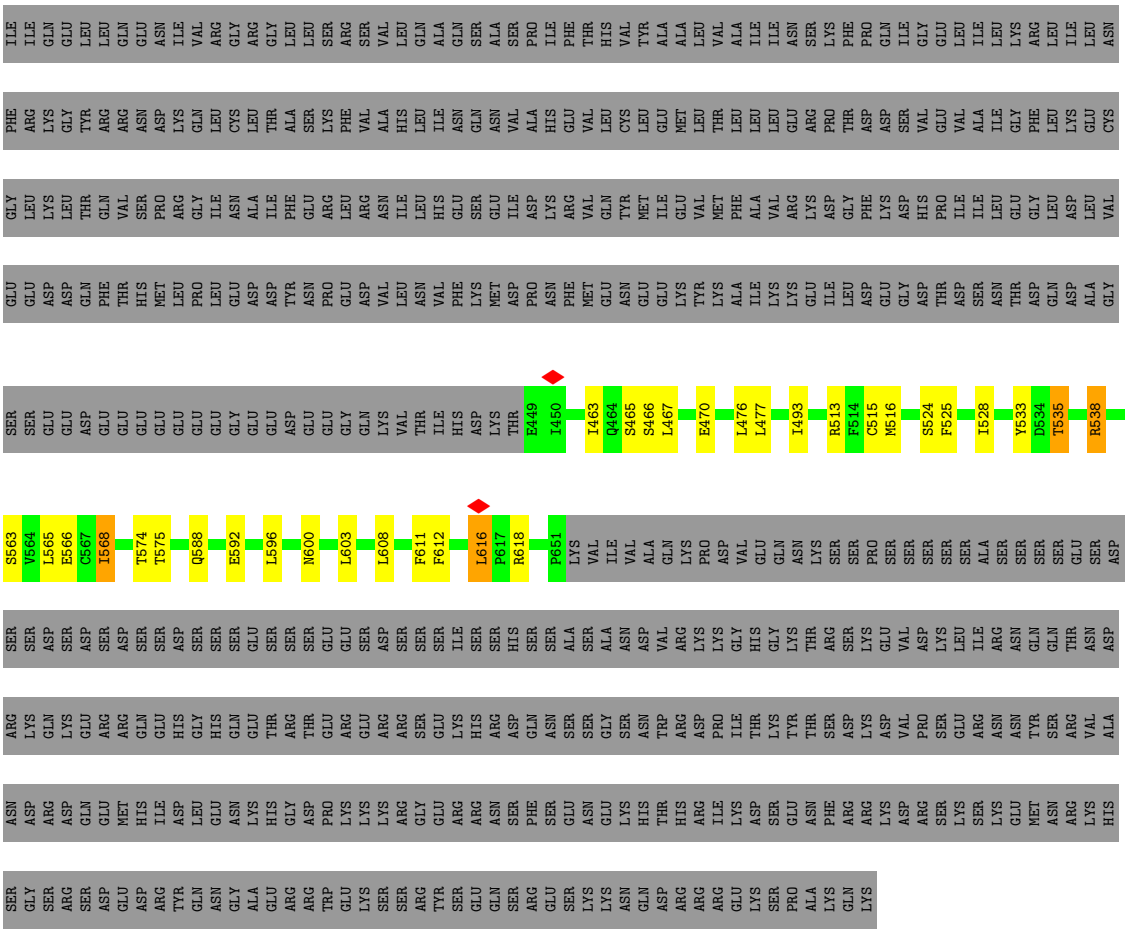




• Molecule 17: Pre-mRNA-splicing factor CWC22 homolog

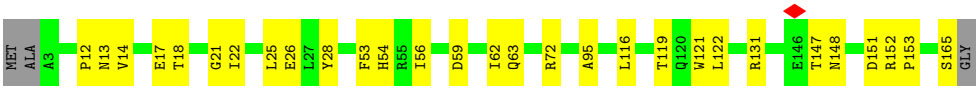
Chain T: 19% 78%





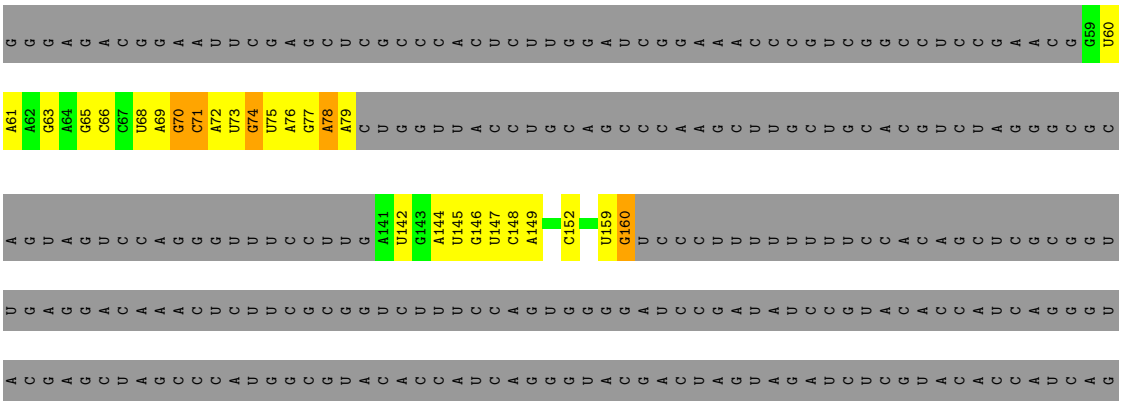
• Molecule 18: Peptidyl-prolyl cis-trans isomerase-like 1

Chain V:

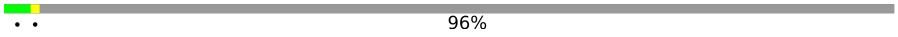


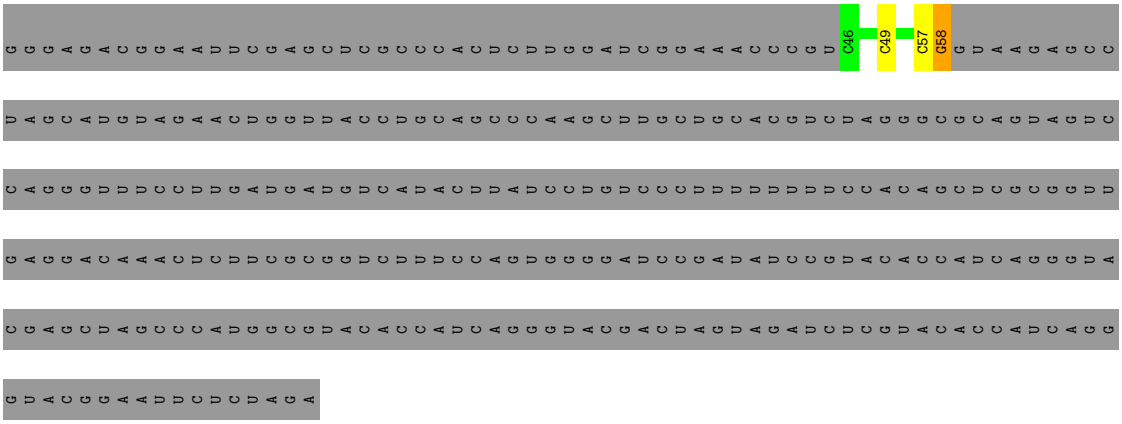
• Molecule 19: pre-mRNA

Chain Y:



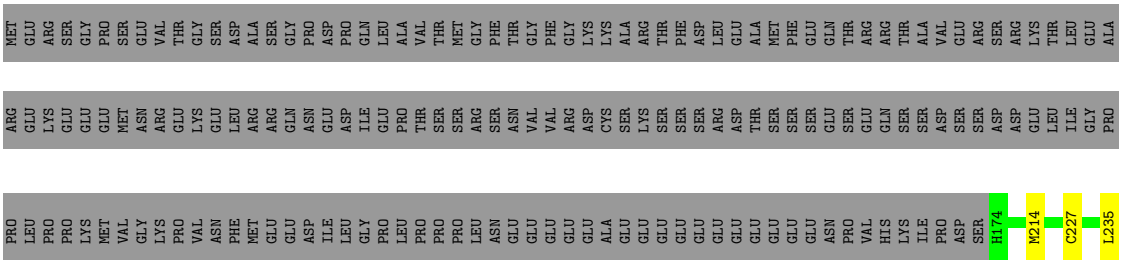
• Molecule 19: pre-mRNA

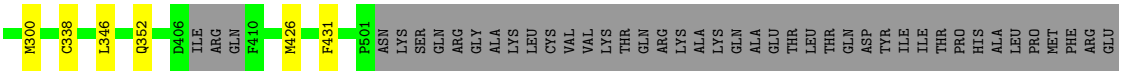
Chain Z: 

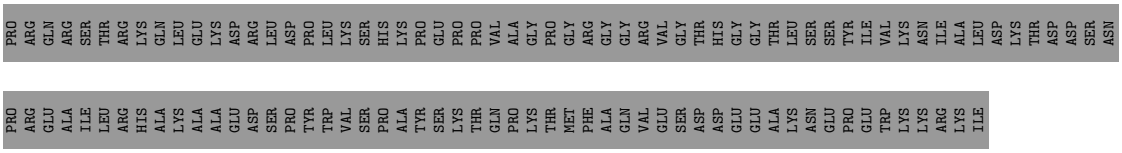


• Molecule 20: WD repeat-containing protein 70

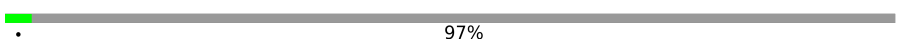
Chain p: 

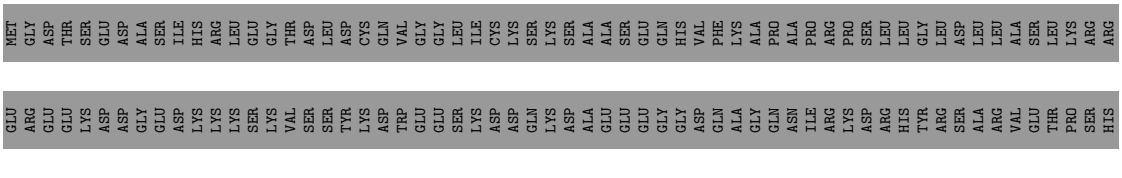


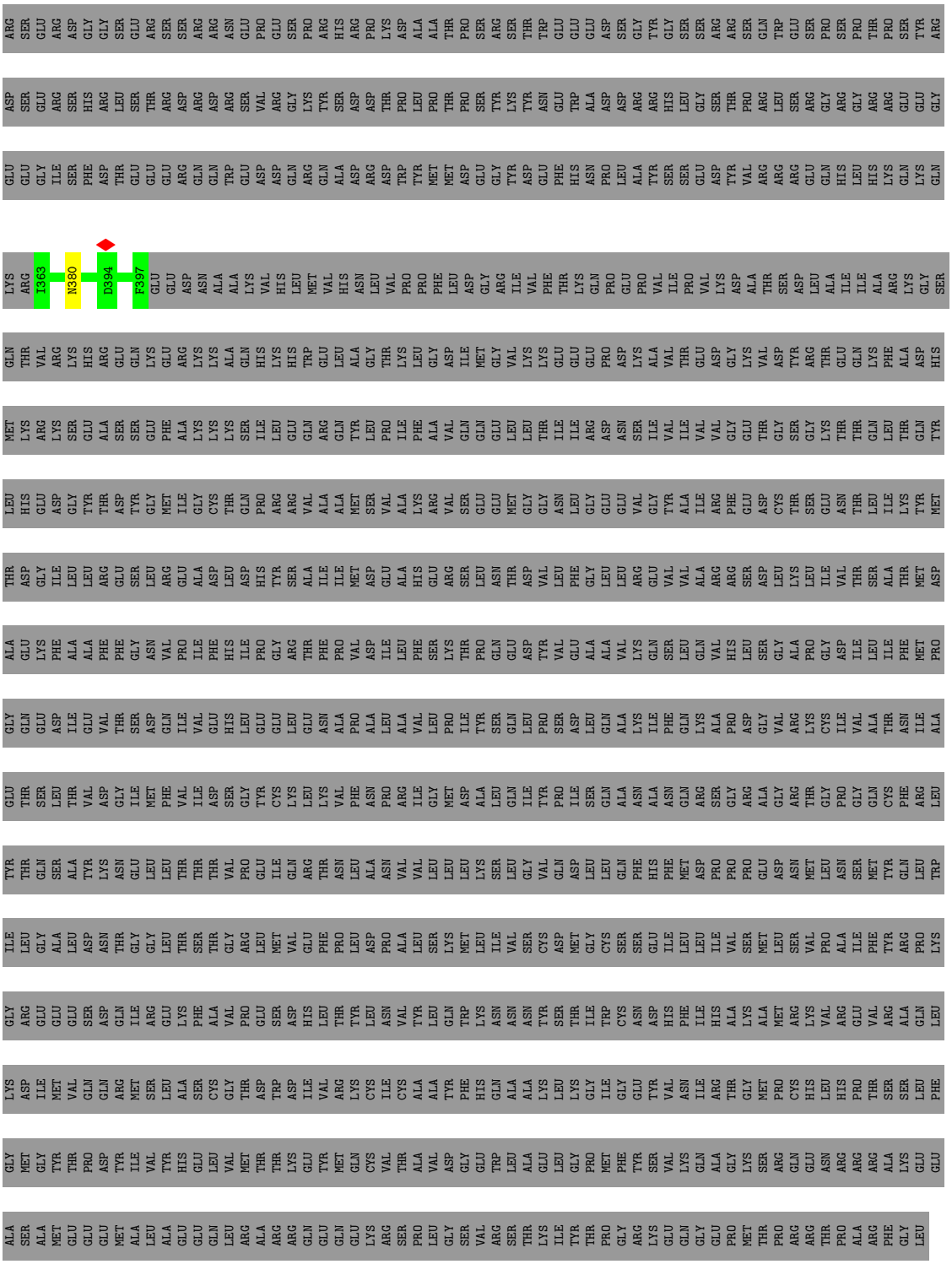




• Molecule 21: Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP16

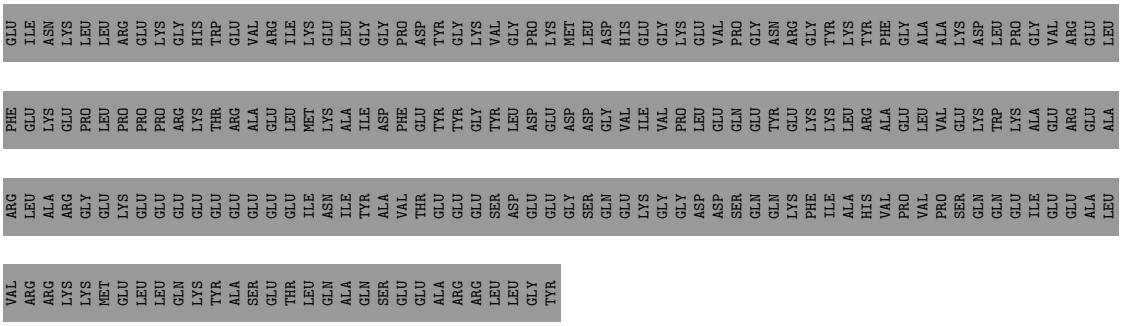
Chain r: 





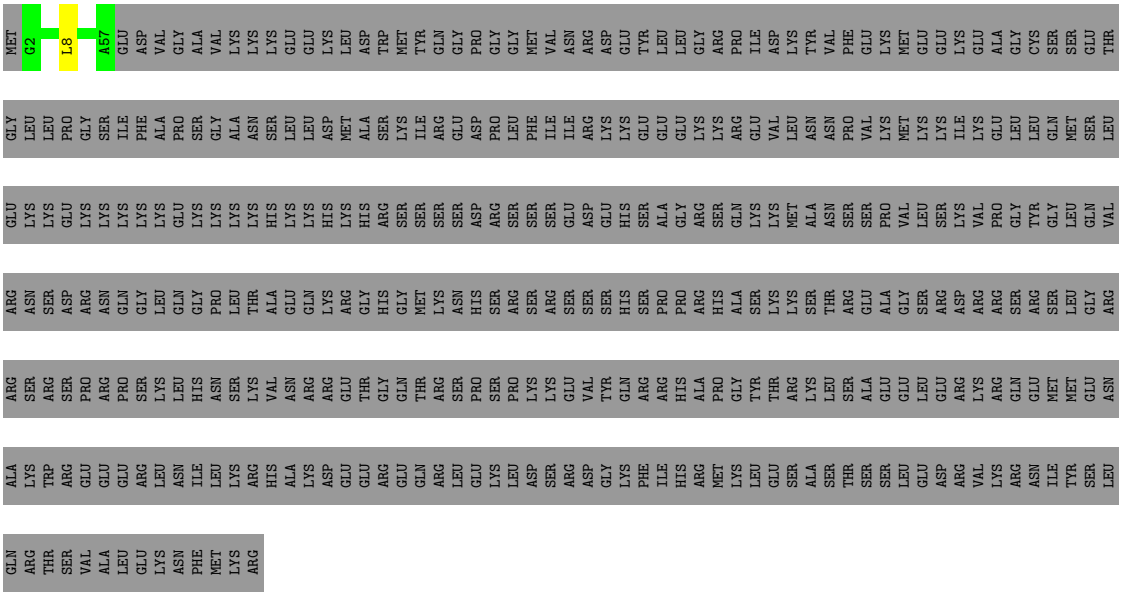
• Molecule 22: Pre-mRNA-splicing factor ISY1 homolog

Chain s: 7% 93%



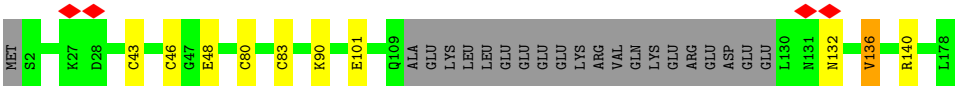
• Molecule 23: Pre-mRNA-splicing factor CWC25 homolog

Chain t:



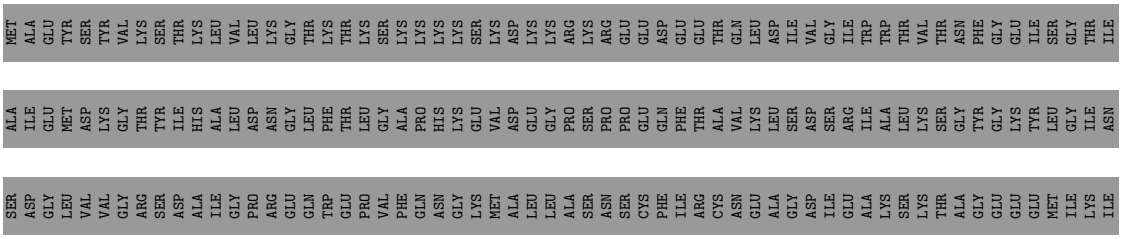
• Molecule 24: Splicing factor YJU2

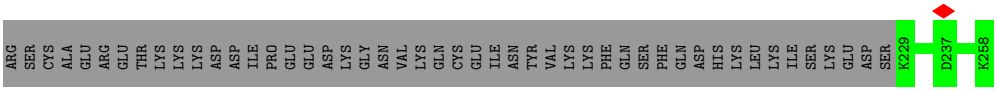
Chain u:



• Molecule 25: Protein FRG1

Chain x:




ARG
SER
CYS
ALA
GLU
ARG
GLU
THR
LYS
LYS
LYS
ASP
ASP
ILE
PRO
GLU
GLU
ASP
LYS
GLY
ASN
VAL
LYS
GLN
CYS
GLU
ILE
ASN
TYR
VAL
LYS
LYS
PHE
GLN
SER
PHE
GLN
ASP
HIS
LYS
LEU
LYS
ILE
SER
LYS
GLU
ASP
SER
K229
D237
K258

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	411539	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	120	Depositor
Minimum defocus (nm)	-1	Depositor
Maximum defocus (nm)	-3	Depositor
Magnification	132000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.336	Depositor
Minimum map value	-0.185	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	466.39996, 466.39996, 466.39996	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	2	0.84	1/642 (0.2%)	1.08	3/998 (0.3%)
2	5	0.77	0/1725	1.04	5/2681 (0.2%)
3	6	0.86	0/1892	0.96	2/2947 (0.1%)
4	9	0.26	0/113	0.45	0/148
5	A	0.55	4/14669 (0.0%)	0.70	23/19894 (0.1%)
6	B	0.47	2/7112 (0.0%)	0.67	9/9681 (0.1%)
7	C	0.48	1/1738 (0.1%)	0.69	4/2353 (0.2%)
8	D	0.68	2/2547 (0.1%)	0.76	4/3471 (0.1%)
9	E	0.39	0/650	0.64	1/886 (0.1%)
10	F	0.47	1/2282 (0.0%)	0.76	9/3109 (0.3%)
11	L	0.46	0/1641	0.65	1/2208 (0.0%)
12	O	0.45	0/2160	0.65	4/2920 (0.1%)
13	P	0.60	2/1613 (0.1%)	0.71	1/2174 (0.0%)
14	Q	0.81	7/1187 (0.6%)	0.96	10/1591 (0.6%)
15	R	0.55	0/690	0.71	0/922
16	S	0.56	0/233	0.70	0/312
17	T	0.50	1/1704 (0.1%)	1.08	10/2291 (0.4%)
18	V	0.33	0/1105	0.58	0/1511
19	Y	0.67	0/975	1.14	9/1514 (0.6%)
19	Z	0.89	0/307	0.87	0/476
20	p	0.48	1/2424 (0.0%)	0.77	5/3295 (0.2%)
21	r	0.36	0/262	0.55	0/356
22	s	0.38	0/158	0.50	0/209
23	t	0.59	0/424	0.74	1/570 (0.2%)
24	u	0.91	9/1312 (0.7%)	1.10	9/1764 (0.5%)
25	x	0.36	0/240	0.58	0/317
All	All	0.58	31/49805 (0.1%)	0.78	110/68598 (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	2
6	B	0	1
20	p	0	3
24	u	0	1
All	All	0	7

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	u	136	VAL	CB-CG1	-15.50	1.20	1.52
14	Q	137	CYS	CB-SG	-12.19	1.61	1.82
24	u	136	VAL	CB-CG2	-9.93	1.31	1.52
24	u	46	CYS	CB-SG	9.92	1.99	1.82
14	Q	134	CYS	CB-SG	-9.87	1.65	1.82
13	P	30	GLU	CD-OE1	-9.68	1.15	1.25
17	T	535	THR	CB-OG1	-8.92	1.25	1.43
14	Q	105	CYS	CB-SG	8.65	1.97	1.82
24	u	48	GLU	CD-OE2	-7.59	1.17	1.25
24	u	101	GLU	CD-OE1	-7.33	1.17	1.25
14	Q	142	CYS	CB-SG	-7.30	1.69	1.82
24	u	80	CYS	CB-SG	6.86	1.94	1.82
20	p	338	CYS	CB-SG	-6.64	1.71	1.82
14	Q	139	CYS	CB-SG	-6.52	1.71	1.82
24	u	140	ARG	CZ-NH2	-6.38	1.24	1.33
8	D	264	CYS	CB-SG	-5.97	1.72	1.81
8	D	488	VAL	CB-CG1	-5.94	1.40	1.52
5	A	88	TYR	CD2-CE2	-5.60	1.30	1.39
6	B	214	GLU	CD-OE1	-5.54	1.19	1.25
5	A	678	GLU	CD-OE2	-5.45	1.19	1.25
10	F	129	THR	CB-CG2	-5.44	1.34	1.52
13	P	20	PHE	CD1-CE1	-5.40	1.28	1.39
24	u	43	CYS	CB-SG	-5.39	1.73	1.81
14	Q	101	CYS	CB-SG	-5.33	1.73	1.81
14	Q	102	CYS	CB-SG	-5.21	1.73	1.81
24	u	83	CYS	CB-SG	5.17	1.91	1.82
7	C	155	VAL	CB-CG2	-5.12	1.42	1.52
5	A	258	PHE	CD2-CE2	-5.08	1.29	1.39
1	2	38	A	C1'-N9	-5.05	1.39	1.46
6	B	622	GLU	CB-CG	-5.04	1.42	1.52
5	A	850	TYR	CD1-CE1	-5.04	1.31	1.39

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	538	ARG	NE-CZ-NH2	-32.07	104.27	120.30
5	A	506	LEU	CB-CG-CD1	-24.98	68.54	111.00
17	T	538	ARG	NE-CZ-NH1	20.37	130.49	120.30
24	u	140	ARG	NE-CZ-NH2	-18.29	111.16	120.30
24	u	136	VAL	CG1-CB-CG2	-17.26	83.29	110.90
14	Q	142	CYS	CA-CB-SG	-14.88	87.22	114.00
24	u	140	ARG	NE-CZ-NH1	12.76	126.68	120.30
2	5	68	C	N1-C2-O2	11.21	125.62	118.90
24	u	80	CYS	CA-CB-SG	10.81	133.46	114.00
14	Q	139	CYS	CA-CB-SG	-10.39	95.31	114.00
6	B	465	MET	CG-SD-CE	-10.36	83.63	100.20
5	A	506	LEU	CB-CG-CD2	9.82	127.69	111.00
10	F	272	ARG	NE-CZ-NH2	-9.78	115.41	120.30
7	C	128	ASP	CB-CG-OD1	9.49	126.84	118.30
20	p	426	MET	CG-SD-CE	9.14	114.83	100.20
24	u	46	CYS	CA-CB-SG	9.10	130.38	114.00
17	T	535	THR	CA-CB-OG1	-9.02	90.07	109.00
14	Q	101	CYS	CA-CB-SG	-8.74	98.27	114.00
24	u	48	GLU	OE1-CD-OE2	-8.53	113.06	123.30
14	Q	117	CYS	CA-CB-SG	-8.41	98.86	114.00
5	A	926	LEU	CB-CG-CD1	-8.21	97.04	111.00
5	A	213	LEU	CA-CB-CG	8.15	134.04	115.30
8	D	424	ASP	CB-CG-OD1	8.09	125.58	118.30
20	p	214	MET	CG-SD-CE	7.94	112.91	100.20
12	O	272	ASP	CB-CG-OD1	7.87	125.38	118.30
14	Q	101	CYS	C-N-CA	-7.61	102.68	121.70
14	Q	137	CYS	CA-CB-SG	-7.44	100.61	114.00
6	B	242	LEU	CB-CG-CD1	-7.35	98.50	111.00
5	A	830	LEU	CB-CG-CD1	-7.31	98.57	111.00
5	A	1322	LEU	CA-CB-CG	7.08	131.59	115.30
2	5	68	C	N3-C2-O2	-7.05	116.97	121.90
5	A	784	LEU	CA-CB-CG	7.03	131.47	115.30
24	u	83	CYS	N-CA-C	-6.89	92.40	111.00
12	O	375	ASP	CB-CG-OD1	6.78	124.41	118.30
14	Q	105	CYS	CA-CB-SG	6.75	126.14	114.00
7	C	86	LEU	CA-CB-CG	6.71	130.73	115.30
10	F	272	ARG	NE-CZ-NH1	6.70	123.65	120.30
10	F	91	LEU	CA-CB-CG	6.70	130.71	115.30
17	T	608	LEU	CA-CB-CG	6.63	130.54	115.30
5	A	598	LEU	CB-CG-CD2	-6.62	99.75	111.00
5	A	731	LEU	CA-CB-CG	6.54	130.33	115.30
5	A	205	ASP	CB-CG-OD1	6.45	124.10	118.30
12	O	363	ARG	CA-CB-CG	6.38	127.43	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	Y	70	G	C8-N9-C4	-6.19	103.92	106.40
17	T	616	LEU	CA-CB-CG	6.17	129.48	115.30
17	T	565	LEU	CA-CB-CG	6.16	129.47	115.30
19	Y	160	G	C4-N9-C1'	6.13	134.47	126.50
5	A	864	LEU	CB-CG-CD2	-6.09	100.64	111.00
14	Q	63	LEU	CA-CB-CG	6.09	129.31	115.30
14	Q	102	CYS	N-CA-C	-6.06	94.64	111.00
5	A	861	ARG	NE-CZ-NH1	6.05	123.33	120.30
23	t	8	LEU	CB-CG-CD1	-6.01	100.78	111.00
6	B	316	ILE	CG1-CB-CG2	-5.99	98.22	111.40
13	P	45	CYS	CA-CB-SG	5.97	124.74	114.00
6	B	650	GLU	OE1-CD-OE2	-5.86	116.26	123.30
1	2	31	G	N7-C8-N9	5.83	116.02	113.10
19	Y	70	G	N7-C8-N9	5.73	115.96	113.10
9	E	139	LEU	CA-CB-CG	5.72	128.45	115.30
19	Y	71	C	N1-C2-O2	5.67	122.30	118.90
20	p	300	MET	CG-SD-CE	-5.67	91.13	100.20
12	O	363	ARG	NE-CZ-NH1	5.62	123.11	120.30
6	B	929	LEU	CA-CB-CG	5.60	128.18	115.30
8	D	383	ARG	NE-CZ-NH1	5.60	123.10	120.30
5	A	178	TYR	CA-CB-CG	5.60	124.04	113.40
5	A	1303	LEU	CA-CB-CG	5.56	128.09	115.30
11	L	152	LEU	CA-CB-CG	5.55	128.08	115.30
5	A	923	ASP	CB-CG-OD1	5.53	123.27	118.30
1	2	18	U	N1-C2-O2	5.51	126.66	122.80
24	u	83	CYS	O-C-N	-5.51	113.88	122.70
19	Y	160	G	N3-C4-C5	-5.50	125.85	128.60
7	C	197	ILE	CG1-CB-CG2	-5.45	99.41	111.40
6	B	269	LEU	CA-CB-CG	5.45	127.83	115.30
14	Q	142	CYS	CB-CA-C	5.42	121.24	110.40
5	A	1048	MET	CG-SD-CE	5.41	108.86	100.20
1	2	31	G	C8-N9-C4	-5.40	104.24	106.40
8	D	365	ARG	NE-CZ-NH2	5.39	123.00	120.30
10	F	105	LEU	CB-CG-CD2	-5.37	101.88	111.00
20	p	235	LEU	CA-CB-CG	5.36	127.63	115.30
5	A	204	LEU	C-N-CA	5.33	135.02	121.70
17	T	535	THR	N-CA-CB	-5.32	100.18	110.30
10	F	88	ARG	CA-CB-CG	5.31	125.09	113.40
2	5	9	G	C4-N9-C1'	5.31	133.40	126.50
24	u	90	LYS	CD-CE-NZ	5.30	123.90	111.70
5	A	864	LEU	CA-CB-CG	5.30	127.49	115.30
6	B	204	ASP	CB-CG-OD1	-5.29	113.54	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	6	42	C	C2-N1-C1'	5.29	124.61	118.80
19	Y	71	C	C2-N1-C1'	5.26	124.59	118.80
5	A	1434	LYS	CD-CE-NZ	-5.26	99.61	111.70
17	T	538	ARG	NH1-CZ-NH2	5.24	125.17	119.40
10	F	166	LEU	CA-CB-CG	5.24	127.35	115.30
3	6	25	C	C2-N1-C1'	5.23	124.55	118.80
5	A	1555	LEU	CB-CG-CD1	-5.22	102.12	111.00
17	T	568	ILE	CG1-CB-CG2	-5.20	99.96	111.40
2	5	36	C	C6-N1-C2	-5.20	118.22	120.30
5	A	710	LEU	CB-CG-CD2	-5.20	102.17	111.00
5	A	784	LEU	CB-CG-CD2	-5.19	102.17	111.00
19	Y	71	C	N3-C2-O2	-5.19	118.27	121.90
6	B	622	GLU	CG-CD-OE1	-5.14	108.01	118.30
17	T	477	LEU	CA-CB-CG	5.14	127.13	115.30
2	5	24	G	O5'-P-OP1	-5.12	101.09	105.70
10	F	129	THR	CA-CB-CG2	-5.10	105.26	112.40
19	Y	160	G	N3-C4-N9	5.10	129.06	126.00
19	Y	160	G	C8-N9-C1'	-5.08	120.39	127.00
5	A	204	LEU	CA-CB-CG	5.07	126.96	115.30
10	F	88	ARG	NE-CZ-NH1	5.07	122.83	120.30
20	p	346	LEU	CA-CB-CG	5.05	126.91	115.30
6	B	416	LEU	CB-CG-CD2	-5.04	102.43	111.00
8	D	459	LEU	CA-CB-CG	5.04	126.89	115.30
7	C	230	MET	CG-SD-CE	-5.03	92.15	100.20
10	F	306	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	A	1649	LYS	Peptide
5	A	380	LEU	Peptide
6	B	366	GLN	Peptide
20	p	227	CYS	Peptide
20	p	352	GLN	Peptide
20	p	431	PHE	Peptide
24	u	132	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	2	575	0	288	7	0
2	5	1548	0	785	3	0
3	6	1690	0	855	12	0
4	9	112	0	109	3	0
5	A	14270	0	14118	188	0
6	B	6953	0	6837	109	0
7	C	1703	0	1692	28	0
8	D	2481	0	2431	52	0
9	E	629	0	572	13	0
10	F	2230	0	2087	52	0
11	L	1611	0	1588	16	0
12	O	2108	0	1963	26	0
13	P	1577	0	1543	30	0
14	Q	1162	0	1163	12	0
15	R	681	0	635	9	0
16	S	230	0	238	3	0
17	T	1669	0	1662	20	0
18	V	1081	0	929	20	0
19	Y	873	0	440	9	0
19	Z	276	0	143	2	0
20	p	2372	0	2209	0	0
21	r	259	0	213	0	0
22	s	158	0	162	0	0
23	t	418	0	379	0	0
24	u	1286	0	1274	0	0
25	x	239	0	252	0	0
26	6	5	0	0	0	0
27	A	36	0	6	4	0
28	B	32	0	12	0	0
29	P	3	0	0	0	0
29	Q	3	0	0	0	0
29	u	1	0	0	0	0
All	All	48271	0	44585	541	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 7.

All (541) 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)
5:A:75:ASP:HA	5:A:502:ASN:HD22	1.45	0.80
13:P:96:VAL:HG21	13:P:213:LEU:HD23	1.65	0.79
5:A:591:MET:HG3	5:A:598:LEU:HD21	1.64	0.78
5:A:993:LEU:O	5:A:997:LEU:HB2	1.83	0.77
18:V:53:PHE:HB3	18:V:56:ILE:HD11	1.67	0.75
10:F:264:VAL:HA	10:F:272:ARG:HH22	1.51	0.74
5:A:902:TYR:HE2	5:A:1246:GLN:HB3	1.53	0.73
7:C:197:ILE:HD11	13:P:20:PHE:CE1	2.24	0.72
10:F:265:ARG:O	10:F:272:ARG:NH1	2.22	0.72
10:F:81:LEU:HD12	10:F:93:TRP:HB2	1.73	0.71
5:A:623:LYS:NZ	5:A:623:LYS:HB3	2.05	0.71
12:O:360:ASP:HA	12:O:363:ARG:HH12	1.54	0.70
5:A:761:ILE:HD12	5:A:775:ASN:HD22	1.57	0.70
11:L:53:TRP:HB3	11:L:54:LEU:HD12	1.73	0.69
7:C:113:TYR:OH	8:D:402:ASP:O	2.11	0.69
6:B:129:ILE:HG22	6:B:199:LEU:HB3	1.75	0.69
5:A:974:ASN:HB2	5:A:1178:TYR:HB3	1.76	0.68
6:B:860:ASP:HA	6:B:871:ILE:HG22	1.74	0.67
8:D:260:TYR:HB3	8:D:274:ASP:HA	1.76	0.67
7:C:197:ILE:HD11	13:P:20:PHE:HE1	1.60	0.67
6:B:137:HIS:HA	6:B:238:ASN:HB3	1.77	0.67
5:A:1214:TRP:NE1	5:A:1276:GLU:OE2	2.28	0.67
5:A:142:SER:HA	5:A:242:ALA:HB2	1.77	0.66
6:B:130:ARG:HH21	6:B:435:VAL:HG13	1.61	0.66
10:F:135:VAL:HB	10:F:145:LYS:HB2	1.77	0.66
6:B:171:LEU:HB2	6:B:174:GLU:HG3	1.78	0.66
13:P:36:MET:HG2	13:P:57:TRP:HB3	1.78	0.66
5:A:30:LEU:HD11	10:F:214:ASP:HA	1.78	0.66
8:D:257:ARG:NH2	8:D:301:ASP:OD2	2.29	0.65
6:B:732:ILE:HG12	6:B:746:VAL:HG12	1.79	0.65
5:A:996:LEU:HD21	5:A:1047:VAL:HG21	1.78	0.65
2:5:20:G:H1'	5:A:465:LYS:HD3	1.80	0.64
6:B:148:CYS:SG	6:B:417:ARG:NH2	2.69	0.64
9:E:111:LEU:HD23	13:P:22:ILE:HD13	1.79	0.64
13:P:162:PRO:O	13:P:182:ARG:NH2	2.30	0.64
8:D:249:VAL:HA	8:D:265:GLY:HA2	1.80	0.64
5:A:1110:ILE:HD11	5:A:1149:LEU:HD13	1.80	0.64
6:B:282:VAL:HA	6:B:285:VAL:HG12	1.80	0.64
6:B:112:THR:OG1	6:B:153:THR:O	2.16	0.63
5:A:1321:GLU:OE2	5:A:1471:ARG:NH1	2.32	0.63
5:A:1660:TYR:OH	5:A:1717:ASN:O	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:208:ILE:HB	10:F:220:TRP:HB2	1.81	0.62
18:V:119:THR:HG22	18:V:122:LEU:HD13	1.80	0.62
5:A:709:ILE:HD11	5:A:735:ILE:HD12	1.81	0.62
6:B:220:ARG:HE	6:B:580:LEU:HD23	1.64	0.62
10:F:208:ILE:HG12	10:F:222:LEU:HD11	1.81	0.62
6:B:69:ALA:HA	8:D:456:PRO:HG3	1.81	0.62
5:A:1424:GLN:HB2	5:A:1427:ARG:HB3	1.82	0.61
8:D:196:LEU:HD11	8:D:487:LYS:HD3	1.82	0.61
5:A:1248:LEU:HD11	5:A:1294:LYS:HB3	1.82	0.61
13:P:66:LYS:NZ	19:Y:76:A:OP1	2.34	0.60
5:A:783:TYR:HD2	5:A:784:LEU:HD12	1.67	0.60
7:C:195:ARG:NH1	13:P:29:GLY:O	2.35	0.60
9:E:124:MET:HG2	10:F:285:GLU:HA	1.84	0.60
19:Z:57:C:H3'	19:Z:58:G:H5"	1.83	0.60
5:A:1312:PRO:HB2	5:A:1314:VAL:HG12	1.82	0.59
10:F:264:VAL:HA	10:F:272:ARG:NH2	2.17	0.59
14:Q:14:GLY:HA2	14:Q:17:LEU:HD13	1.83	0.59
7:C:101:ILE:O	7:C:104:GLN:NE2	2.36	0.59
5:A:623:LYS:HB3	5:A:623:LYS:HZ3	1.68	0.59
5:A:1014:ASN:ND2	5:A:1026:ASN:O	2.30	0.59
5:A:790:ARG:NH1	5:A:986:GLU:O	2.35	0.59
5:A:1125:ILE:HA	5:A:1147:VAL:HG11	1.84	0.59
8:D:306:CYS:HB2	8:D:333:VAL:HG13	1.85	0.59
5:A:217:ARG:HE	5:A:222:GLY:HA2	1.68	0.59
5:A:753:THR:O	5:A:757:ASN:ND2	2.35	0.58
11:L:19:LEU:HD22	11:L:54:LEU:HD22	1.83	0.58
11:L:218:LYS:NZ	12:O:270:ASP:OD2	2.37	0.58
12:O:296:ARG:HH22	12:O:325:ASN:HD22	1.52	0.58
6:B:404:THR:OG1	6:B:407:GLU:OE1	2.17	0.58
10:F:197:LEU:HD22	10:F:288:LEU:HD11	1.85	0.58
15:R:30:TYR:CZ	15:R:35:LEU:HD23	2.39	0.58
9:E:101:THR:OG1	13:P:89:GLU:OE2	2.15	0.58
10:F:340:PRO:HB2	10:F:356:ILE:HB	1.84	0.58
4:9:102:ALA:H	4:9:107:TYR:HD2	1.52	0.58
5:A:235:MET:HB3	5:A:404:LEU:HD21	1.86	0.58
6:B:207:GLY:O	6:B:238:ASN:ND2	2.35	0.58
10:F:69:VAL:HA	10:F:85:GLY:HA3	1.86	0.57
14:Q:79:ILE:HG22	14:Q:84:ALA:HB3	1.85	0.57
6:B:224:GLY:HA3	6:B:438:ILE:HD12	1.86	0.57
6:B:846:VAL:HG13	6:B:887:LEU:HD11	1.87	0.57
7:C:126:ASN:HA	8:D:442:ARG:HD2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:124:LEU:HB2	10:F:136:TRP:HB2	1.87	0.57
12:O:300:ASP:HA	12:O:303:ILE:HG12	1.84	0.57
5:A:231:THR:H	5:A:234:MET:HE3	1.68	0.57
5:A:850:TYR:HE2	5:A:864:LEU:HD21	1.70	0.57
7:C:78:ARG:HD3	18:V:95:ALA:HB3	1.87	0.57
6:B:449:ILE:HG13	6:B:465:MET:HB3	1.86	0.57
13:P:68:THR:HG23	13:P:82:GLN:HB3	1.87	0.57
5:A:909:TYR:HB2	5:A:1033:GLY:HA3	1.87	0.56
6:B:476:CYS:HB2	6:B:565:ILE:HB	1.86	0.56
1:2:24:A:H5"	5:A:781:ARG:HH21	1.70	0.56
5:A:964:ASP:O	5:A:1100:ARG:NH2	2.38	0.56
5:A:200:ASP:OD1	5:A:240:ARG:NH1	2.35	0.56
5:A:1124:ASN:ND2	5:A:1148:ASN:OD1	2.39	0.56
5:A:1204:TYR:HE2	5:A:1206:GLU:HB3	1.70	0.56
7:C:222:PRO:O	13:P:123:ARG:NH1	2.38	0.56
5:A:240:ARG:NH2	5:A:240:ARG:HB3	2.20	0.56
5:A:891:PHE:O	11:L:83:ARG:NH2	2.34	0.56
8:D:478:LEU:HD23	8:D:488:VAL:HG12	1.88	0.56
10:F:127:ALA:HB2	10:F:157:CYS:HB3	1.87	0.56
17:T:533:TYR:CZ	17:T:568:ILE:HG22	2.40	0.56
5:A:414:ARG:NH2	6:B:408:LEU:O	2.39	0.56
15:R:214:THR:HG23	15:R:215:LEU:HG	1.88	0.56
6:B:216:THR:HG22	6:B:580:LEU:HD22	1.88	0.55
6:B:255:VAL:HG12	6:B:300:LEU:HD12	1.86	0.55
18:V:59:ASP:HA	18:V:116:LEU:HD22	1.88	0.55
6:B:525:CYS:SG	6:B:526:THR:N	2.80	0.55
13:P:145:ASP:HB3	13:P:147:LEU:HD23	1.89	0.55
10:F:133:VAL:HG21	10:F:169:THR:HG21	1.88	0.55
3:6:27:A:OP1	13:P:175:ARG:NH2	2.40	0.55
3:6:49:G:N7	11:L:33:ARG:NH2	2.55	0.55
10:F:69:VAL:O	10:F:331:ASN:ND2	2.40	0.55
10:F:166:LEU:HA	10:F:180:ASP:HA	1.88	0.55
5:A:988:ILE:HG21	5:A:1030:ILE:HG23	1.88	0.55
12:O:232:GLU:OE1	12:O:267:ARG:NH1	2.39	0.55
5:A:586:GLY:HA3	5:A:1549:VAL:HG23	1.89	0.54
7:C:205:ASP:OD1	7:C:208:GLU:HB2	2.07	0.54
18:V:17:GLU:HA	18:V:22:ILE:HA	1.89	0.54
6:B:834:VAL:HG21	6:B:875:ILE:HD12	1.88	0.54
5:A:758:ARG:NH2	5:A:900:ASP:OD1	2.33	0.54
5:A:1418:ARG:NH1	5:A:1463:LYS:O	2.40	0.54
5:A:442:LYS:NZ	27:A:3001:IHP:O43	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Q:101:CYS:SG	14:Q:102:CYS:N	2.81	0.54
17:T:566:GLU:HB3	17:T:611:PHE:HB2	1.89	0.54
5:A:1217:GLN:HA	5:A:1224:ARG:HA	1.89	0.54
11:L:214:ILE:HG12	12:O:260:ARG:HG2	1.90	0.54
5:A:270:ASN:O	5:A:270:ASN:ND2	2.41	0.54
5:A:1624:SER:HB2	5:A:1693:SER:HB3	1.89	0.54
12:O:228:ARG:NH2	12:O:252:GLU:OE1	2.36	0.54
13:P:196:GLN:NE2	19:Y:76:A:N3	2.56	0.54
8:D:264:CYS:HB2	8:D:294:LEU:HD13	1.89	0.53
5:A:54:VAL:HG23	5:A:55:ASP:H	1.73	0.53
6:B:366:GLN:HB3	6:B:371:GLU:HB3	1.90	0.53
9:E:97:ASN:ND2	18:V:151:ASP:OD2	2.41	0.53
3:6:14:C:H2'	3:6:15:A:H8	1.74	0.53
5:A:395:THR:OG1	5:A:396:ASP:N	2.39	0.53
12:O:343:GLU:OE2	12:O:347:HIS:NE2	2.41	0.53
5:A:171:ASP:HB2	5:A:519:ASP:HB3	1.90	0.53
10:F:348:ASP:OD2	10:F:350:ARG:NH1	2.41	0.53
11:L:220:PRO:HG3	12:O:262:ARG:HD2	1.90	0.53
6:B:523:GLN:HB3	6:B:558:PRO:HG3	1.90	0.53
18:V:148:ASN:ND2	18:V:152:ARG:O	2.42	0.53
6:B:215:VAL:HG11	6:B:242:LEU:HD22	1.90	0.53
5:A:177:ASP:OD1	5:A:177:ASP:N	2.42	0.52
5:A:227:ARG:NH1	5:A:227:ARG:HB2	2.24	0.52
6:B:832:TYR:HD2	6:B:899:SER:HB3	1.73	0.52
15:R:57:ARG:NH2	15:R:62:GLU:OE1	2.42	0.52
5:A:86:ARG:HH22	7:C:211:ARG:HA	1.73	0.52
5:A:100:LEU:HD13	5:A:641:MET:HB2	1.92	0.52
5:A:1127:GLY:O	5:A:1151:ARG:NH2	2.39	0.52
5:A:1639:VAL:HG12	5:A:1719:PHE:HB3	1.90	0.52
13:P:46:LYS:HD2	19:Y:74:G:H21	1.74	0.52
17:T:524:SER:O	17:T:528:ILE:HG12	2.10	0.52
13:P:22:ILE:HG13	13:P:72:GLN:HE22	1.73	0.52
5:A:975:VAL:HB	5:A:1099:PHE:HB2	1.90	0.52
7:C:134:ARG:NH2	8:D:381:HIS:O	2.40	0.52
1:2:18:U:H3'	5:A:707:ARG:HH22	1.73	0.52
6:B:854:ARG:NH1	6:B:879:ASP:OD2	2.43	0.52
6:B:876:PRO:HG2	6:B:879:ASP:HB2	1.91	0.52
13:P:92:LEU:HA	19:Y:78:A:H61	1.75	0.52
5:A:443:VAL:HG21	5:A:614:TYR:CD1	2.45	0.52
15:R:213:ASP:OD2	15:R:216:ARG:HD3	2.10	0.52
16:S:5:ILE:HD12	16:S:19:VAL:HG11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:24:A:OP1	5:A:781:ARG:NE	2.41	0.52
5:A:298:ASP:OD2	5:A:301:LYS:HE2	2.09	0.52
6:B:260:ILE:HD12	6:B:263:LEU:HD21	1.90	0.52
5:A:143:GLN:NE2	5:A:207:PHE:O	2.39	0.52
5:A:617:ASN:HA	5:A:621:VAL:HG23	1.92	0.52
1:2:29:A:H2'	1:2:30:A:C8	2.44	0.51
4:9:104:ARG:O	4:9:104:ARG:NH1	2.44	0.51
6:B:134:LEU:HB2	6:B:204:ASP:HA	1.92	0.51
6:B:316:ILE:HG22	6:B:420:CYS:HB3	1.92	0.51
10:F:265:ARG:H	10:F:272:ARG:HH12	1.59	0.51
8:D:272:CYS:HB3	8:D:282:ARG:HB2	1.91	0.51
9:E:92:GLU:HG2	18:V:72:ARG:HG2	1.92	0.51
10:F:63:SER:HB2	10:F:350:ARG:HB3	1.90	0.51
10:F:248:SER:O	10:F:264:VAL:N	2.44	0.51
5:A:1382:SER:HA	5:A:1415:GLY:HA2	1.93	0.51
6:B:779:LEU:O	6:B:938:ARG:NH1	2.42	0.51
7:C:142:GLU:HB3	7:C:146:LYS:HZ3	1.75	0.51
9:E:108:ARG:NH2	13:P:131:THR:O	2.44	0.51
6:B:365:SER:OG	6:B:366:GLN:N	2.42	0.51
6:B:501:ILE:HG23	6:B:530:LEU:HD21	1.92	0.51
8:D:358:ASP:HB3	8:D:365:ARG:NH1	2.25	0.51
1:2:22:U:H4'	5:A:678:GLU:OE2	2.11	0.51
5:A:178:TYR:OH	5:A:488:ASP:OD2	2.22	0.50
6:B:183:SER:H	6:B:214:GLU:HG2	1.76	0.50
11:L:39:HIS:NE2	11:L:154:GLU:OE2	2.43	0.50
3:6:20:A:O2'	14:Q:120:ARG:NH1	2.44	0.50
5:A:898:PHE:HD2	5:A:905:LEU:HB3	1.76	0.50
17:T:463:ILE:HD11	17:T:493:ILE:HG22	1.93	0.50
6:B:564:THR:HG21	6:B:576:ILE:HA	1.93	0.50
5:A:162:LYS:NZ	5:A:1690:ASP:OD2	2.43	0.50
5:A:405:LEU:O	6:B:413:ARG:NH2	2.45	0.50
8:D:314:ILE:HD12	8:D:324:HIS:HB2	1.92	0.50
13:P:182:ARG:HG2	13:P:184:GLU:HG3	1.94	0.50
6:B:338:GLU:OE1	6:B:342:ARG:NH1	2.45	0.50
14:Q:105:CYS:HB3	14:Q:117:CYS:HB2	1.94	0.50
8:D:497:GLU:OE1	8:D:497:GLU:N	2.44	0.50
5:A:318:TYR:O	6:B:645:ARG:NH1	2.44	0.49
12:O:409:GLU:O	12:O:416:TYR:OH	2.27	0.49
5:A:511:LYS:HB2	5:A:513:LEU:HD23	1.94	0.49
5:A:956:CYS:HB3	5:A:1216:LEU:HD13	1.94	0.49
6:B:200:PHE:HB3	6:B:202:ILE:HG13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1257:THR:HA	5:A:1260:VAL:HG12	1.94	0.49
15:R:213:ASP:OD1	15:R:214:THR:N	2.45	0.49
5:A:657:ALA:O	5:A:661:GLU:HB2	2.12	0.49
6:B:389:ASP:OD1	6:B:389:ASP:N	2.41	0.49
6:B:664:GLU:HG2	6:B:779:LEU:HB2	1.94	0.49
10:F:187:ILE:HG22	10:F:188:GLN:HG2	1.94	0.49
5:A:758:ARG:HD3	5:A:779:LEU:HD11	1.94	0.49
6:B:664:GLU:HB3	6:B:779:LEU:HD12	1.95	0.49
6:B:932:GLU:OE1	6:B:936:LYS:HD2	2.12	0.49
8:D:291:VAL:HA	8:D:307:SER:HA	1.93	0.49
8:D:473:SER:OG	8:D:475:SER:OG	2.26	0.49
10:F:75:HIS:CE1	10:F:77:ASN:HB2	2.48	0.49
5:A:681:PHE:HE2	5:A:746:LYS:HG3	1.78	0.49
17:T:603:LEU:HD12	17:T:612:PHE:HE2	1.77	0.49
5:A:65:HIS:HD2	14:Q:46:LEU:HD22	1.77	0.49
5:A:623:LYS:NZ	5:A:623:LYS:CB	2.73	0.49
6:B:277:LYS:NZ	6:B:864:PRO:O	2.42	0.49
10:F:105:LEU:HB3	10:F:136:TRP:CZ3	2.48	0.49
6:B:828:MET:HB3	6:B:906:ILE:HD13	1.95	0.48
11:L:215:PRO:O	12:O:267:ARG:NH2	2.46	0.48
12:O:227:LYS:HD2	12:O:251:TRP:CE2	2.47	0.48
5:A:680:HIS:NE2	5:A:684:GLU:OE2	2.45	0.48
5:A:717:TRP:CD2	5:A:746:LYS:HD3	2.48	0.48
9:E:90:ALA:O	18:V:72:ARG:NH1	2.46	0.48
10:F:71:CYS:HB2	10:F:84:ALA:HB3	1.95	0.48
10:F:114:GLU:OE2	10:F:116:HIS:NE2	2.46	0.48
7:C:173:PRO:HG2	7:C:201:GLU:HG3	1.95	0.48
5:A:1289:VAL:HG13	5:A:1357:MET:HG3	1.94	0.48
12:O:337:MET:HE2	12:O:346:TRP:CD2	2.49	0.48
5:A:1667:ARG:NH2	5:A:1673:SER:O	2.40	0.48
3:6:17:C:H2'	3:6:18:A:C8	2.49	0.48
6:B:797:ALA:O	6:B:803:ARG:NH2	2.47	0.48
3:6:78:A:H4'	12:O:237:LYS:HE2	1.95	0.48
5:A:1254:THR:HG21	5:A:1258:LYS:HE2	1.95	0.48
13:P:207:ASP:OD1	13:P:209:VAL:N	2.47	0.48
17:T:596:LEU:O	17:T:600:ASN:HB2	2.12	0.48
5:A:979:SER:OG	5:A:980:ARG:N	2.46	0.48
11:L:231:ASN:HD22	12:O:258:ILE:HB	1.79	0.48
3:6:29:A:N6	19:Y:73:U:O3'	2.47	0.47
5:A:946:GLU:HB2	5:A:950:LEU:HD22	1.96	0.47
10:F:68:GLU:HB2	10:F:347:SER:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:90:GLY:HA3	7:C:209:PRO:HD3	1.95	0.47
9:E:128:GLN:HE22	9:E:139:LEU:HD23	1.79	0.47
10:F:210:SER:O	10:F:218:LYS:N	2.44	0.47
6:B:271:PRO:HB2	6:B:370:VAL:HG13	1.97	0.47
12:O:262:ARG:NH2	12:O:286:GLU:OE1	2.47	0.47
2:5:36:C:O2	16:S:11:ARG:NH1	2.43	0.47
5:A:1260:VAL:HG11	5:A:1325:LEU:HB3	1.96	0.47
11:L:49:ARG:HG3	11:L:54:LEU:HD13	1.97	0.47
5:A:86:ARG:NH2	7:C:211:ARG:HA	2.29	0.47
5:A:377:GLU:HA	5:A:381:PRO:HD3	1.97	0.47
5:A:1204:TYR:CE2	5:A:1206:GLU:HB3	2.49	0.47
6:B:220:ARG:HH11	6:B:452:THR:HG22	1.79	0.47
6:B:235:VAL:HG21	6:B:284:GLU:HG2	1.97	0.47
8:D:351:ASP:HB3	8:D:353:THR:HG22	1.96	0.47
8:D:427:LEU:HB3	8:D:439:TRP:HB2	1.96	0.47
12:O:373:HIS:HB2	12:O:378:ASN:HD21	1.78	0.47
5:A:167:PRO:HA	5:A:168:PRO:HD3	1.81	0.47
5:A:1405:LEU:HD11	5:A:1412:TRP:HD1	1.80	0.47
10:F:343:ILE:HG22	10:F:353:MET:HA	1.97	0.47
5:A:758:ARG:HD2	5:A:758:ARG:HA	1.76	0.47
5:A:1581:LEU:HD22	5:A:1746:ARG:HH11	1.80	0.47
6:B:174:GLU:HG2	6:B:181:ILE:HD12	1.97	0.47
12:O:242:ILE:HD11	12:O:278:LEU:HD22	1.97	0.47
2:5:66:A:H2'	2:5:67:A:H8	1.80	0.46
5:A:962:LEU:HB2	5:A:965:VAL:HB	1.97	0.46
5:A:1350:ILE:HD11	17:T:470:GLU:HB2	1.96	0.46
6:B:302:PRO:HB2	6:B:320:LEU:HD11	1.97	0.46
5:A:710:LEU:HA	5:A:710:LEU:HD23	1.63	0.46
5:A:776:LEU:HD11	5:A:900:ASP:HB2	1.97	0.46
5:A:1701:VAL:HA	5:A:1716:GLY:HA3	1.98	0.46
6:B:696:LEU:O	6:B:700:ILE:HD12	2.14	0.46
10:F:221:ASP:OD2	10:F:228:THR:OG1	2.33	0.46
9:E:128:GLN:HE22	9:E:139:LEU:CD2	2.28	0.46
5:A:1381:ASP:OD2	5:A:1414:ARG:NH1	2.42	0.46
17:T:588:GLN:O	17:T:592:GLU:HG2	2.15	0.46
5:A:516:LEU:HG	5:A:524:LEU:HD11	1.98	0.46
5:A:532:THR:HG21	19:Y:60:U:H3'	1.97	0.46
5:A:863:GLU:HB2	5:A:913:PRO:HB3	1.97	0.46
6:B:166:CYS:HB3	6:B:169:ASP:HB2	1.97	0.46
8:D:246:ILE:HB	8:D:267:ASP:OD2	2.15	0.46
10:F:243:LEU:HD12	10:F:247:GLY:HA2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:213:GLU:HA	8:D:254:VAL:HG11	1.98	0.46
5:A:570:ASP:HB3	5:A:573:GLN:HG3	1.98	0.46
12:O:299:TRP:O	12:O:302:ALA:N	2.48	0.46
4:9:112:MET:SD	4:9:112:MET:N	2.88	0.46
5:A:950:LEU:HD23	5:A:954:LYS:HG3	1.98	0.46
8:D:455:GLN:OE1	8:D:485:THR:OG1	2.34	0.46
6:B:137:HIS:HB3	6:B:140:HIS:CD2	2.51	0.46
15:R:52:GLU:HA	15:R:55:ARG:NH1	2.31	0.46
18:V:28:TYR:OH	18:V:131:ARG:NE	2.33	0.46
5:A:731:LEU:HB3	7:C:248:PRO:HD2	1.97	0.45
6:B:841:ASP:OD1	6:B:842:CYS:N	2.49	0.45
9:E:145:ASN:OD1	9:E:146:HIS:N	2.46	0.45
13:P:191:ASP:OD1	13:P:191:ASP:N	2.46	0.45
17:T:538:ARG:HH21	17:T:538:ARG:HD2	1.28	0.45
5:A:224:THR:HG23	5:A:226:GLN:HG2	1.98	0.45
5:A:946:GLU:HB2	5:A:950:LEU:HB3	1.98	0.45
5:A:1351:THR:HG23	5:A:1352:HIS:ND1	2.31	0.45
6:B:301:SER:HB3	6:B:304:LEU:HD13	1.98	0.45
7:C:142:GLU:HB3	7:C:146:LYS:NZ	2.31	0.45
8:D:309:ASP:OD1	8:D:309:ASP:N	2.48	0.45
6:B:259:LYS:HB3	6:B:262:ARG:HB2	1.98	0.45
6:B:833:PHE:HB2	6:B:902:HIS:CD2	2.51	0.45
9:E:120:ILE:HD13	10:F:284:PHE:HZ	1.81	0.45
18:V:56:ILE:HG23	18:V:62:ILE:HG22	1.98	0.45
6:B:605:ASP:OD1	6:B:608:ARG:NH1	2.50	0.45
17:T:493:ILE:HD11	17:T:525:PHE:HZ	1.82	0.45
17:T:515:CYS:SG	17:T:516:MET:N	2.89	0.45
5:A:1370:ARG:NH1	17:T:467:LEU:O	2.50	0.45
6:B:157:ILE:O	6:B:158:ARG:HD2	2.15	0.45
6:B:436:GLN:HG3	6:B:437:HIS:ND1	2.31	0.45
8:D:307:SER:OG	8:D:309:ASP:OD1	2.21	0.45
10:F:264:VAL:CA	10:F:272:ARG:HH22	2.23	0.45
10:F:304:SER:H	10:F:330:ILE:HB	1.82	0.45
6:B:733:TRP:CZ3	6:B:763:LYS:HA	2.52	0.45
17:T:476:LEU:HD23	17:T:476:LEU:HA	1.84	0.45
5:A:1533:ARG:NH1	5:A:1752:GLN:OE1	2.44	0.45
8:D:481:GLU:OE1	8:D:487:LYS:NZ	2.33	0.45
10:F:243:LEU:HA	10:F:250:LEU:HA	1.99	0.45
11:L:82:TRP:CZ3	11:L:85:ILE:HD11	2.52	0.45
5:A:701:ILE:O	7:C:242:GLN:NE2	2.50	0.45
5:A:812:THR:HG23	5:A:1055:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:474:LEU:HB3	6:B:567:GLU:HG2	1.98	0.45
7:C:189:ASN:HD21	7:C:195:ARG:HG3	1.82	0.45
8:D:354:ILE:HG13	8:D:375:VAL:HG11	1.98	0.45
5:A:29:LYS:O	5:A:33:LYS:HG3	2.17	0.45
5:A:1410:ASP:OD1	5:A:1410:ASP:N	2.50	0.45
6:B:705:VAL:HG22	6:B:717:PHE:HE2	1.81	0.45
8:D:287:HIS:CD2	8:D:313:ARG:HD2	2.52	0.45
8:D:462:GLU:OE2	8:D:462:GLU:N	2.47	0.45
10:F:111:ALA:N	10:F:129:THR:OG1	2.50	0.45
10:F:210:SER:N	10:F:218:LYS:O	2.48	0.45
13:P:16:GLU:H	13:P:41:TYR:HE1	1.64	0.45
5:A:444:ARG:NH1	19:Z:49:C:OP1	2.51	0.44
5:A:1274:PHE:HB3	5:A:1277:ALA:HB3	2.00	0.44
5:A:1644:LEU:HG	5:A:1715:TYR:HD1	1.82	0.44
5:A:799:PRO:HB2	5:A:801:ILE:HG22	1.98	0.44
5:A:1653:ASP:OD1	5:A:1653:ASP:N	2.50	0.44
6:B:600:LEU:HD11	6:B:627:HIS:HE2	1.82	0.44
8:D:399:LYS:HG2	8:D:400:PHE:H	1.82	0.44
9:E:98:PRO:HG2	18:V:121:TRP:HE1	1.83	0.44
6:B:186:VAL:HG12	6:B:535:ALA:HB2	1.98	0.44
6:B:239:THR:O	6:B:243:ILE:HG12	2.17	0.44
8:D:200:ILE:HG13	8:D:486:ILE:HB	2.00	0.44
10:F:171:SER:OG	10:F:172:ASP:N	2.51	0.44
10:F:244:SER:N	10:F:249:TYR:O	2.50	0.44
18:V:147:THR:HA	18:V:153:PRO:HA	1.99	0.44
5:A:1457:HIS:HB3	5:A:1460:HIS:HB2	1.99	0.44
5:A:1718:TRP:HZ3	5:A:1726:ILE:HD12	1.83	0.44
6:B:193:THR:HB	6:B:325:LYS:HD2	1.99	0.44
6:B:109:LEU:HD23	6:B:537:TYR:CD1	2.52	0.44
17:T:535:THR:OG1	17:T:538:ARG:NH2	2.51	0.44
5:A:732:PRO:HB3	7:C:244:GLU:OE2	2.18	0.44
6:B:829:GLU:OE2	6:B:854:ARG:NH2	2.44	0.44
7:C:119:LEU:HD12	7:C:230:MET:CG	2.47	0.44
8:D:496:THR:HG22	8:D:499:THR:HG22	1.99	0.44
3:6:58:G:O6	3:6:76:A:N6	2.51	0.44
11:L:14:THR:HG21	11:L:152:LEU:HD21	1.98	0.44
5:A:29:LYS:O	5:A:32:GLU:HG3	2.18	0.44
5:A:450:LEU:HD23	5:A:450:LEU:HA	1.75	0.44
5:A:854:SER:OG	5:A:855:ARG:N	2.49	0.44
5:A:1133:CYS:SG	5:A:1231:ARG:NE	2.91	0.44
6:B:189:VAL:HG12	6:B:199:LEU:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:531:THR:O	5:A:535:ARG:N	2.51	0.44
5:A:998:ARG:HE	5:A:1003:HIS:HB2	1.82	0.44
5:A:1589:ILE:HD13	5:A:1705:ILE:HD13	2.00	0.44
18:V:28:TYR:HH	18:V:131:ARG:HE	1.60	0.44
3:6:29:A:H62	19:Y:73:U:H1'	1.82	0.43
5:A:66:VAL:HA	5:A:69:ILE:HG22	1.99	0.43
6:B:561:LYS:NZ	6:B:614:TYR:O	2.51	0.43
7:C:115:LYS:O	7:C:230:MET:HE1	2.18	0.43
5:A:490:VAL:HG21	5:A:565:ARG:HG3	2.00	0.43
5:A:609:LYS:CE	27:A:3001:IHP:O44	2.66	0.43
5:A:975:VAL:HG22	5:A:1177:VAL:HG22	2.00	0.43
5:A:1215:ASN:O	5:A:1224:ARG:NE	2.45	0.43
5:A:1604:LEU:HD23	5:A:1719:PHE:HE2	1.83	0.43
5:A:1647:ASP:OD1	5:A:1647:ASP:N	2.52	0.43
6:B:903:HIS:HE1	6:B:905:GLN:HG3	1.83	0.43
8:D:290:ALA:O	8:D:308:ARG:N	2.48	0.43
8:D:424:ASP:OD1	8:D:425:GLY:N	2.50	0.43
6:B:745:LEU:HD23	6:B:789:PHE:HB2	2.00	0.43
12:O:291:GLN:OE1	12:O:291:GLN:N	2.51	0.43
5:A:768:ASP:N	5:A:768:ASP:OD1	2.50	0.43
6:B:530:LEU:HG	6:B:552:ILE:HG22	2.00	0.43
5:A:1057:ARG:HD2	5:A:1057:ARG:HA	1.73	0.43
5:A:1729:ALA:O	5:A:1733:ILE:HG12	2.18	0.43
18:V:12:PRO:HG2	18:V:165:SER:HB3	2.01	0.43
18:V:18:THR:N	18:V:21:GLY:O	2.51	0.43
5:A:1106:ALA:O	5:A:1110:ILE:HD12	2.18	0.43
5:A:1528:GLN:HG2	5:A:1533:ARG:HH22	1.84	0.43
6:B:192:ASP:OD1	6:B:192:ASP:N	2.51	0.43
6:B:193:THR:OG1	6:B:432:ASP:OD2	2.26	0.43
6:B:833:PHE:HZ	6:B:872:LYS:HD3	1.83	0.43
8:D:214:PRO:HG2	8:D:256:THR:HA	2.01	0.43
8:D:218:TRP:HZ3	8:D:220:VAL:HB	1.83	0.43
13:P:80:VAL:HG21	13:P:94:ILE:HD11	2.01	0.43
3:6:2:U:O2	14:Q:95:GLN:NE2	2.33	0.43
5:A:422:LEU:HD12	5:A:422:LEU:H	1.82	0.43
5:A:1430:LEU:HD11	5:A:1459:ARG:HB3	2.01	0.43
6:B:237:LEU:HD21	6:B:900:VAL:HG21	2.00	0.43
6:B:705:VAL:HG22	6:B:717:PHE:CE2	2.54	0.43
5:A:684:GLU:OE1	8:D:308:ARG:NE	2.52	0.43
5:A:689:VAL:HG11	5:A:710:LEU:HD21	2.00	0.43
5:A:842:ALA:HB2	5:A:924:GLN:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1072:LEU:HD22	5:A:1087:LEU:HD22	2.01	0.43
6:B:598:SER:OG	6:B:599:GLU:OE1	2.37	0.43
6:B:737:PRO:HD2	6:B:741:GLY:HA3	2.00	0.43
14:Q:9:LYS:NZ	14:Q:10:ALA:O	2.40	0.43
5:A:163:ARG:HE	5:A:163:ARG:HB3	1.65	0.43
6:B:80:ILE:HB	8:D:200:ILE:HG22	2.01	0.43
6:B:366:GLN:O	6:B:368:SER:N	2.51	0.43
8:D:383:ARG:HG3	8:D:383:ARG:HH11	1.83	0.43
13:P:92:LEU:HD22	13:P:213:LEU:HD21	2.01	0.43
5:A:850:TYR:CE2	5:A:864:LEU:HD21	2.52	0.42
6:B:168:THR:HG21	6:B:204:ASP:OD1	2.19	0.42
17:T:616:LEU:HA	17:T:618:ARG:HG3	2.00	0.42
6:B:637:LEU:HA	6:B:640:VAL:HG22	2.01	0.42
10:F:217:ILE:HD11	10:F:234:HIS:HD2	1.84	0.42
5:A:1749:LYS:HE2	5:A:1749:LYS:HB2	1.86	0.42
6:B:130:ARG:NH2	6:B:435:VAL:O	2.52	0.42
6:B:448:LYS:HA	6:B:448:LYS:HD3	1.92	0.42
8:D:261:LEU:HD23	8:D:275:LEU:HD11	2.00	0.42
10:F:71:CYS:SG	10:F:114:GLU:HA	2.59	0.42
5:A:159:ARG:HD2	5:A:159:ARG:HA	1.86	0.42
5:A:820:ARG:NH1	5:A:1063:GLY:O	2.52	0.42
7:C:232:SER:HB2	8:D:372:LYS:NZ	2.35	0.42
13:P:30:GLU:OE2	13:P:30:GLU:N	2.53	0.42
13:P:93:PRO:HD3	19:Y:78:A:N6	2.34	0.42
13:P:150:LEU:HD21	13:P:213:LEU:HG	2.02	0.42
16:S:24:SER:O	17:T:513:ARG:NH1	2.52	0.42
5:A:68:LYS:NZ	14:Q:45:SER:O	2.48	0.42
5:A:1021:ASP:OD1	5:A:1021:ASP:N	2.53	0.42
10:F:224:GLN:HE21	10:F:228:THR:HG21	1.84	0.42
11:L:165:LYS:HD3	11:L:165:LYS:HA	1.85	0.42
13:P:45:CYS:HB2	13:P:71:CYS:HB3	2.02	0.42
1:2:30:A:H1'	5:A:861:ARG:NH2	2.35	0.42
6:B:93:ILE:HB	8:D:275:LEU:HB3	2.01	0.42
6:B:938:ARG:HG3	6:B:943:LEU:HB2	2.00	0.42
10:F:209:ILE:HG22	10:F:219:VAL:HG22	2.01	0.42
5:A:187:PRO:HB2	5:A:564:TYR:CZ	2.54	0.42
5:A:240:ARG:HB3	5:A:240:ARG:HH21	1.85	0.42
5:A:1310:ARG:NH2	5:A:1563:HIS:O	2.46	0.42
5:A:1545:ALA:N	5:A:1670:ASP:OD2	2.53	0.42
6:B:465:MET:CE	6:B:475:MET:HG3	2.49	0.42
8:D:419:LEU:HD22	8:D:427:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:611:PHE:CE2	17:T:612:PHE:HE1	2.38	0.42
5:A:609:LYS:NZ	27:A:3001:IHP:O44	2.50	0.42
12:O:232:GLU:HA	12:O:235:ILE:HG12	2.02	0.42
5:A:590:GLY:HA2	5:A:592:TYR:CE2	2.55	0.42
7:C:119:LEU:HD12	7:C:230:MET:HG3	2.02	0.42
8:D:354:ILE:HD11	8:D:375:VAL:HG21	2.01	0.42
7:C:229:VAL:O	8:D:369:THR:HG23	2.20	0.42
10:F:125:PHE:HE2	10:F:159:PRO:HB3	1.84	0.42
11:L:74:LEU:HD23	11:L:77:LEU:HD23	2.02	0.42
5:A:727:LYS:HD2	5:A:727:LYS:HA	1.94	0.41
5:A:1026:ASN:HD22	5:A:1031:ILE:HG23	1.85	0.41
5:A:1556:ASP:N	5:A:1556:ASP:OD1	2.53	0.41
6:B:451:HIS:O	6:B:578:ARG:NH2	2.53	0.41
10:F:200:THR:HB	10:F:209:ILE:HD11	2.02	0.41
10:F:249:TYR:CE1	10:F:263:ASP:HB3	2.55	0.41
12:O:363:ARG:HB2	12:O:363:ARG:HH11	1.85	0.41
13:P:193:LEU:O	19:Y:77:G:N2	2.53	0.41
18:V:13:ASN:HA	18:V:26:GLU:HA	2.01	0.41
18:V:54:HIS:NE2	18:V:63:GLN:OE1	2.53	0.41
7:C:198:ARG:HE	7:C:198:ARG:HB2	1.70	0.41
10:F:150:HIS:CE1	10:F:177:LYS:HG3	2.56	0.41
10:F:353:MET:HB2	10:F:353:MET:HE2	1.79	0.41
14:Q:42:LYS:HE3	14:Q:42:LYS:HB2	1.89	0.41
27:A:3001:IHP:P6	27:A:3001:IHP:O45	2.79	0.41
8:D:260:TYR:OH	15:R:41:ILE:HG23	2.20	0.41
10:F:112:VAL:HG12	10:F:128:SER:OG	2.20	0.41
5:A:543:ALA:HB2	5:A:651:TRP:HB3	2.03	0.41
5:A:1322:LEU:HD11	5:A:1481:VAL:HG13	2.02	0.41
6:B:516:LEU:HD13	6:B:575:GLN:HB3	2.01	0.41
6:B:678:THR:O	6:B:680:ASN:N	2.52	0.41
6:B:680:ASN:ND2	6:B:802:HIS:O	2.54	0.41
8:D:334:ALA:HB2	8:D:350:HIS:CE1	2.55	0.41
9:E:98:PRO:HG2	18:V:121:TRP:NE1	2.36	0.41
5:A:231:THR:OG1	6:B:389:ASP:OD2	2.31	0.41
5:A:341:LYS:HE3	5:A:341:LYS:HB3	1.90	0.41
5:A:1624:SER:O	5:A:1624:SER:OG	2.35	0.41
5:A:946:GLU:CB	5:A:950:LEU:HD22	2.50	0.41
6:B:93:ILE:HD11	8:D:240:LEU:CD2	2.50	0.41
15:R:222:LYS:HE3	15:R:222:LYS:HB2	1.86	0.41
3:6:19:C:O2	14:Q:95:GLN:NE2	2.42	0.41
5:A:689:VAL:CG1	5:A:710:LEU:HD21	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:458:SER:HB2	8:D:462:GLU:OE1	2.21	0.41
12:O:293:ASN:HA	12:O:296:ARG:HD2	2.03	0.41
3:6:14:C:H2'	3:6:15:A:C8	2.56	0.41
5:A:93:LYS:O	5:A:649:GLU:HG2	2.20	0.41
5:A:231:THR:HG23	5:A:233:PRO:HD2	2.03	0.41
5:A:246:LEU:HD23	5:A:246:LEU:HA	1.90	0.41
5:A:936:PHE:HB3	5:A:940:ILE:HD11	2.03	0.41
5:A:1650:ASP:OD2	5:A:1723:LYS:NZ	2.37	0.41
6:B:92:PRO:HB3	8:D:276:GLU:HA	2.03	0.41
6:B:359:LYS:HE3	6:B:359:LYS:HB3	1.95	0.41
6:B:679:PRO:HD3	6:B:811:THR:HG21	2.02	0.41
8:D:263:SER:HB3	8:D:273:TRP:HE1	1.85	0.41
8:D:492:ASP:OD1	8:D:492:ASP:N	2.49	0.41
10:F:88:ARG:HB3	10:F:88:ARG:HH11	1.85	0.41
10:F:299:LYS:HE3	10:F:299:LYS:HB3	1.82	0.41
14:Q:120:ARG:HH21	14:Q:142:CYS:HB3	1.86	0.41
18:V:14:VAL:N	18:V:25:LEU:O	2.40	0.41
5:A:888:GLN:O	5:A:889:ARG:NH1	2.49	0.41
5:A:936:PHE:HA	5:A:937:PRO:HD3	1.86	0.41
5:A:1683:LYS:HD3	5:A:1683:LYS:HA	1.93	0.41
6:B:341:LYS:HB3	6:B:341:LYS:HE2	1.77	0.41
6:B:369:PHE:O	6:B:373:ILE:HB	2.21	0.41
6:B:662:PHE:HB3	6:B:827:LEU:HD22	2.03	0.41
12:O:403:VAL:HG13	12:O:416:TYR:HE1	1.86	0.41
5:A:1106:ALA:O	5:A:1109:LEU:N	2.54	0.40
6:B:366:GLN:HA	6:B:370:VAL:HB	2.02	0.40
8:D:409:LEU:HD22	8:D:444:GLY:HA2	2.03	0.40
15:R:23:LEU:HD23	15:R:26:LEU:HD21	2.03	0.40
5:A:638:LEU:HA	5:A:638:LEU:HD23	1.89	0.40
5:A:862:GLU:O	5:A:866:LEU:HD23	2.21	0.40
5:A:1419:ILE:HD13	5:A:1419:ILE:HG21	1.88	0.40
5:A:1604:LEU:HD23	5:A:1719:PHE:CE2	2.56	0.40
6:B:688:ILE:HG22	6:B:790:LYS:HB2	2.03	0.40
7:C:132:LEU:HD23	7:C:132:LEU:HA	1.82	0.40
10:F:92:LEU:HG	10:F:103:ALA:HB3	2.03	0.40
11:L:222:LEU:HD13	11:L:222:LEU:HA	1.95	0.40
12:O:317:THR:O	12:O:321:GLU:HG2	2.22	0.40
17:T:465:SER:OG	17:T:466:SER:N	2.54	0.40
5:A:606:LYS:HD2	5:A:1548:TYR:CZ	2.57	0.40
6:B:124:ASP:HA	6:B:545:PRO:HG2	2.02	0.40
12:O:282:TYR:O	12:O:285:MET:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:563:SER:HA	17:T:611:PHE:CE2	2.56	0.40
5:A:1202:THR:OG1	5:A:1204:TYR:O	2.31	0.40
6:B:719:GLN:HA	6:B:724:TRP:H	1.87	0.40
17:T:574:THR:HG23	17:T:575:THR:H	1.85	0.40
1:2:23:A:H4'	5:A:777:GLY:HA3	2.04	0.40
5:A:451:LEU:O	5:A:455:VAL:HG12	2.22	0.40
6:B:679:PRO:HD2	6:B:807:GLN:HB3	2.03	0.40
7:C:195:ARG:HG2	13:P:32:PRO:HA	2.04	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	
4	9	12/450 (3%)	10 (83%)	2 (17%)	0	100	100
5	A	1718/1755 (98%)	1567 (91%)	150 (9%)	1 (0%)	51	82
6	B	893/952 (94%)	809 (91%)	84 (9%)	0	100	100
7	C	220/536 (41%)	187 (85%)	33 (15%)	0	100	100
8	D	313/514 (61%)	277 (88%)	36 (12%)	0	100	100
9	E	76/579 (13%)	66 (87%)	10 (13%)	0	100	100
10	F	297/357 (83%)	262 (88%)	35 (12%)	0	100	100
11	L	198/802 (25%)	176 (89%)	22 (11%)	0	100	100
12	O	248/848 (29%)	229 (92%)	19 (8%)	0	100	100
13	P	191/218 (88%)	175 (92%)	16 (8%)	0	100	100
14	Q	140/144 (97%)	126 (90%)	14 (10%)	0	100	100
15	R	83/229 (36%)	77 (93%)	6 (7%)	0	100	100
16	S	28/2752 (1%)	23 (82%)	5 (18%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	T	201/908 (22%)	184 (92%)	17 (8%)	0	100	100
18	V	161/166 (97%)	149 (92%)	12 (8%)	0	100	100
20	p	321/654 (49%)	273 (85%)	48 (15%)	0	100	100
21	r	33/1227 (3%)	30 (91%)	3 (9%)	0	100	100
22	s	18/285 (6%)	16 (89%)	2 (11%)	0	100	100
23	t	54/425 (13%)	54 (100%)	0	0	100	100
24	u	153/178 (86%)	131 (86%)	22 (14%)	0	100	100
25	x	28/258 (11%)	26 (93%)	2 (7%)	0	100	100
All	All	5386/14237 (38%)	4847 (90%)	538 (10%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A	803	ALA

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	
4	9	11/411 (3%)	11 (100%)	0	100	100
5	A	1528/1584 (96%)	1524 (100%)	4 (0%)	92	97
6	B	756/847 (89%)	756 (100%)	0	100	100
7	C	173/459 (38%)	173 (100%)	0	100	100
8	D	271/441 (62%)	271 (100%)	0	100	100
9	E	65/502 (13%)	65 (100%)	0	100	100
10	F	231/300 (77%)	231 (100%)	0	100	100
11	L	158/709 (22%)	158 (100%)	0	100	100
12	O	201/751 (27%)	201 (100%)	0	100	100
13	P	175/197 (89%)	175 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	Q	125/130 (96%)	125 (100%)	0	100 100
15	R	64/203 (32%)	64 (100%)	0	100 100
16	S	24/2432 (1%)	24 (100%)	0	100 100
17	T	186/838 (22%)	186 (100%)	0	100 100
18	V	87/134 (65%)	87 (100%)	0	100 100
20	p	234/572 (41%)	234 (100%)	0	100 100
21	r	23/1074 (2%)	22 (96%)	1 (4%)	29 59
22	s	14/240 (6%)	13 (93%)	1 (7%)	14 44
23	t	36/381 (9%)	36 (100%)	0	100 100
24	u	139/167 (83%)	138 (99%)	1 (1%)	84 92
25	x	23/223 (10%)	23 (100%)	0	100 100
All	All	4524/12595 (36%)	4517 (100%)	7 (0%)	93 98

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	165	ARG
5	A	270	ASN
5	A	409	ARG
5	A	617	ASN
21	r	380	ASN
22	s	4	ASN
24	u	136	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	587	GLN
5	A	757	ASN
5	A	775	ASN
6	B	903	HIS
8	D	287	HIS
9	E	128	GLN
12	O	325	ASN
20	p	480	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	26/188 (13%)	13 (50%)	2 (7%)
19	Y	39/324 (12%)	23 (58%)	0
19	Z	12/324 (3%)	1 (8%)	0
2	5	73/116 (62%)	11 (15%)	1 (1%)
3	6	78/79 (98%)	22 (28%)	0
All	All	228/1031 (22%)	70 (30%)	3 (1%)

All (70) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	19	G
1	2	22	U
1	2	24	A
1	2	25	G
1	2	29	A
1	2	30	A
1	2	31	G
1	2	33	G
1	2	39	U
1	2	40	C
1	2	42	G
1	2	43	U
1	2	44	U
2	5	8	G
2	5	10	U
2	5	22	U
2	5	23	C
2	5	24	G
2	5	25	C
2	5	28	A
2	5	35	U
2	5	53	U
2	5	68	C
2	5	76	A
3	6	3	G
3	6	6	C
3	6	7	G
3	6	9	U
3	6	13	G
3	6	26	U
3	6	28	A

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Mol	Chain	Res	Type
3	6	29	A
3	6	37	C
3	6	40	U
3	6	41	A
3	6	43	A
3	6	46	G
3	6	47	A
3	6	49	G
3	6	54	G
3	6	62	C
3	6	68	C
3	6	69	A
3	6	71	G
3	6	74	U
3	6	79	C
19	Y	61	A
19	Y	63	G
19	Y	65	G
19	Y	66	C
19	Y	68	U
19	Y	69	A
19	Y	70	G
19	Y	71	C
19	Y	72	A
19	Y	74	G
19	Y	75	U
19	Y	78	A
19	Y	79	A
19	Y	142	U
19	Y	144	A
19	Y	145	U
19	Y	146	G
19	Y	147	U
19	Y	148	C
19	Y	149	A
19	Y	152	C
19	Y	159	U
19	Y	160	G
19	Z	58	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	28	C
1	2	39	U
2	5	23	C

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 12 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
28	GTP	B	1001	6	26,34,34	1.35	2 (7%)	32,54,54	1.86	8 (25%)
27	IHP	A	3001	-	36,36,36	0.85	0	54,60,60	1.38	6 (11%)

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
28	GTP	B	1001	6	-	8/18/38/38	0/3/3/3
27	IHP	A	3001	-	-	7/30/54/54	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	1001	GTP	C5-C6	-4.92	1.37	1.47
28	B	1001	GTP	C5-C4	-2.08	1.37	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	1001	GTP	C3'-C2'-C1'	4.66	108.00	100.98
27	A	3001	IHP	C6-C1-C2	3.80	118.72	110.41
28	B	1001	GTP	C5-C6-N1	3.54	120.20	113.95
28	B	1001	GTP	C2-N1-C6	-3.45	118.75	125.10
27	A	3001	IHP	C5-C6-C1	3.20	117.42	110.41
28	B	1001	GTP	N2-C2-N1	3.04	123.19	116.71
28	B	1001	GTP	PB-O3B-PG	-3.02	122.47	132.83
28	B	1001	GTP	C8-N7-C5	2.66	108.05	102.99
28	B	1001	GTP	O6-C6-C5	-2.63	119.24	124.37
27	A	3001	IHP	C3-C2-C1	2.54	115.97	110.41
27	A	3001	IHP	O12-C2-C1	2.22	113.92	108.69
28	B	1001	GTP	PA-O3A-PB	-2.20	125.29	132.83
27	A	3001	IHP	O16-C6-C1	2.17	113.80	108.69
27	A	3001	IHP	O15-C5-C6	2.02	113.45	108.69

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	A	3001	IHP	C1-O11-P1-O21
27	A	3001	IHP	C2-O12-P2-O22
27	A	3001	IHP	C4-O14-P4-O24
27	A	3001	IHP	C5-O15-P5-O25
28	B	1001	GTP	C5'-O5'-PA-O3A
28	B	1001	GTP	C5'-O5'-PA-O1A
28	B	1001	GTP	C5'-O5'-PA-O2A
28	B	1001	GTP	PB-O3B-PG-O1G
28	B	1001	GTP	PB-O3B-PG-O3G
27	A	3001	IHP	C2-O12-P2-O42
28	B	1001	GTP	PB-O3A-PA-O2A
27	A	3001	IHP	C5-O15-P5-O45
27	A	3001	IHP	C6-O16-P6-O46
28	B	1001	GTP	O4'-C4'-C5'-O5'
28	B	1001	GTP	C4'-C5'-O5'-PA

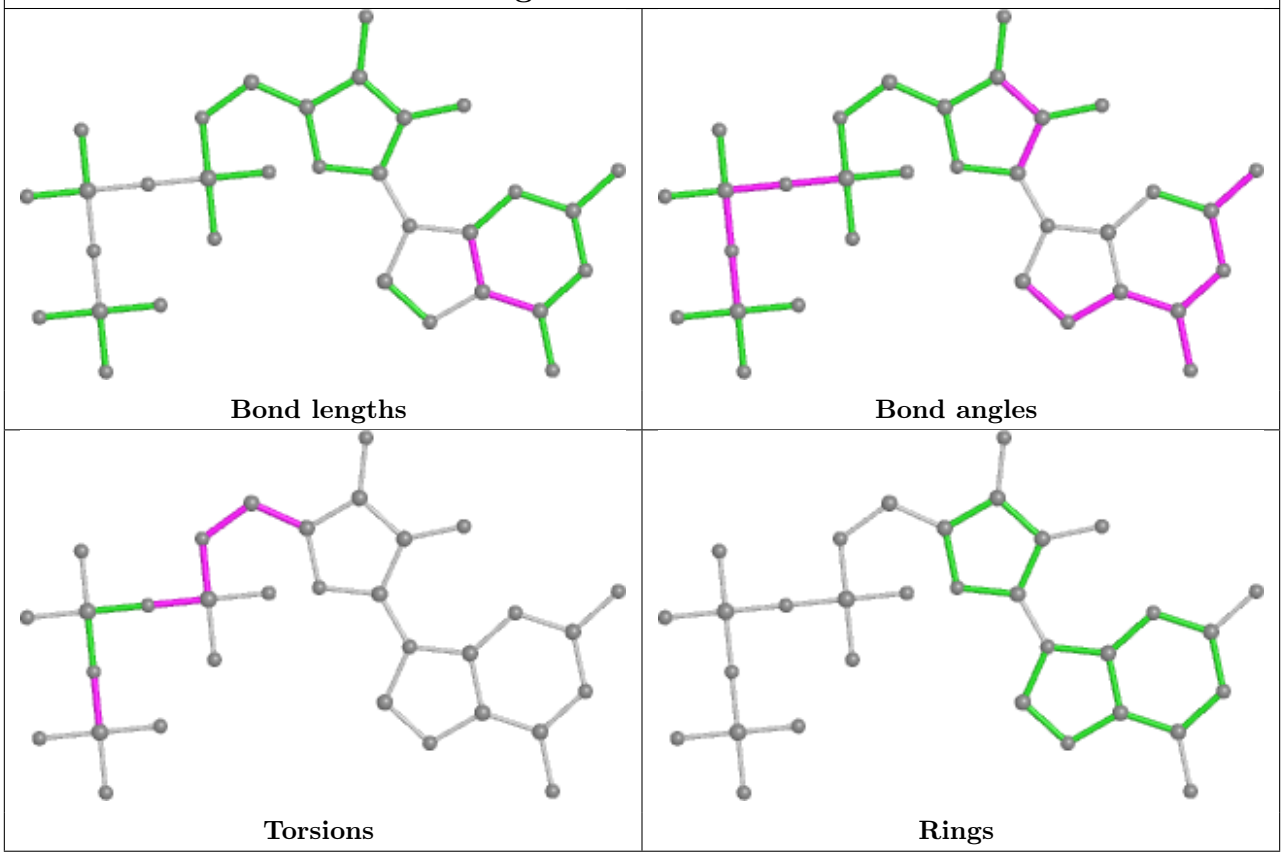
There are no ring outliers.

1 monomer is involved in 4 short contacts:

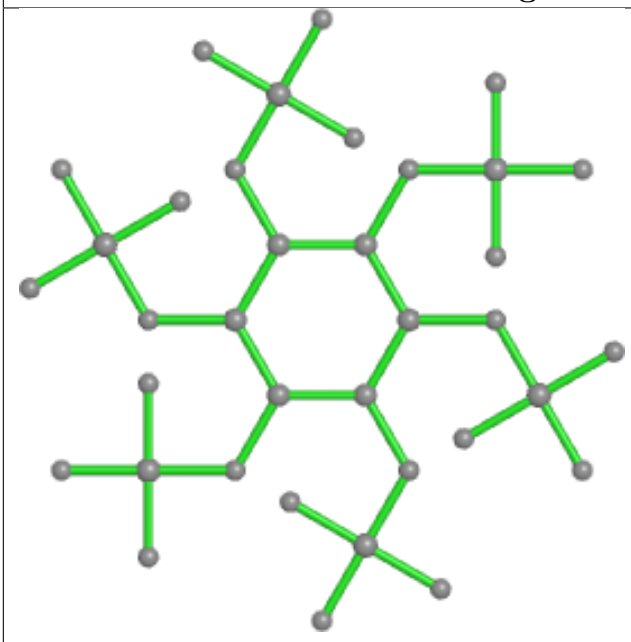
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	A	3001	IHP	4	0

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 then 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.

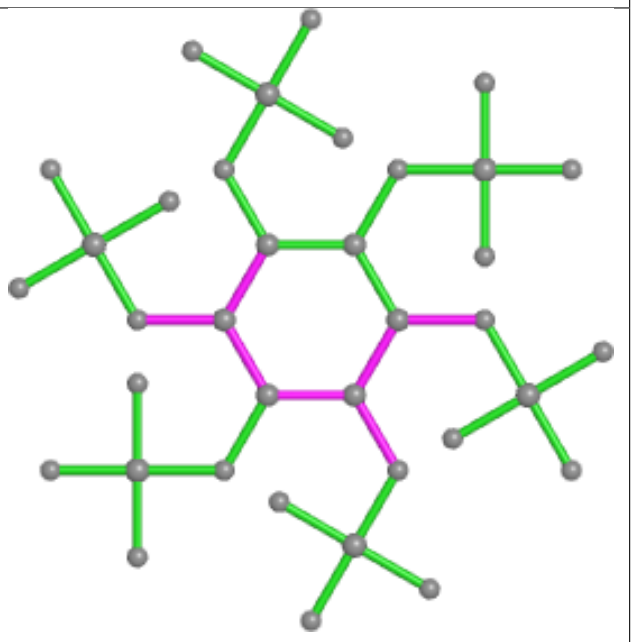
Ligand GTP B 1001



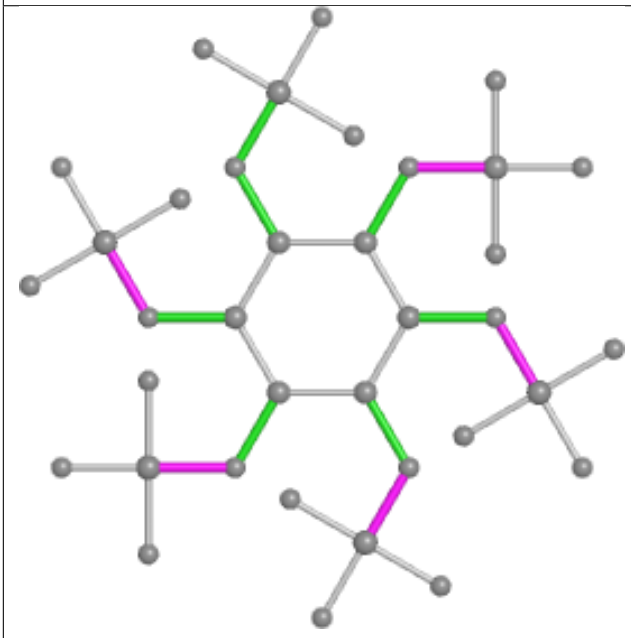
Ligand IHP A 3001



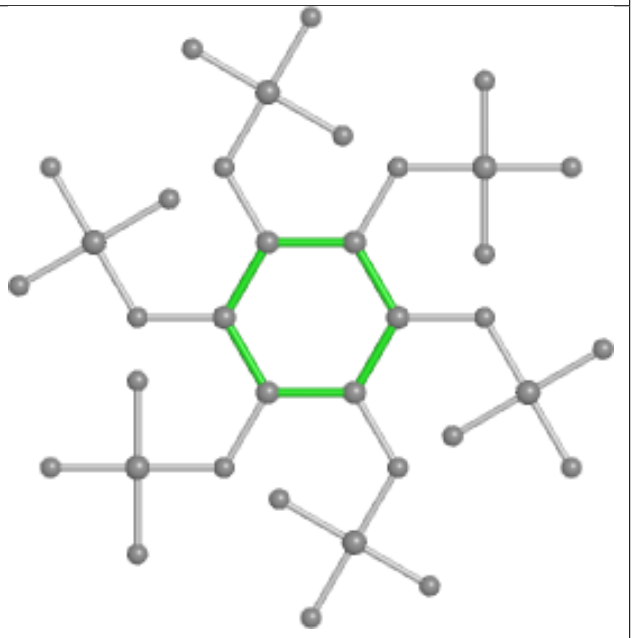
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

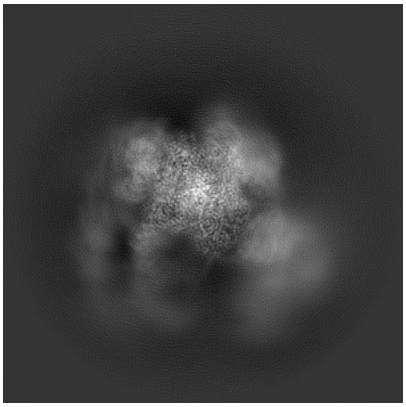
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11569. These allow visual inspection of the internal detail of the map and identification of artifacts.

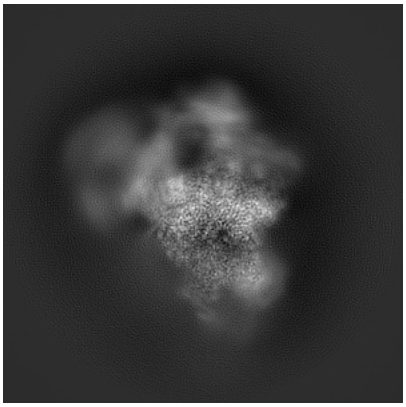
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

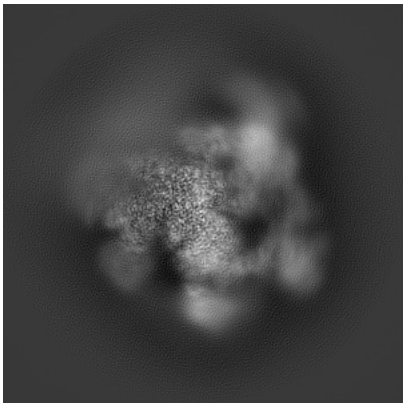
6.1.1 Primary map



X



Y

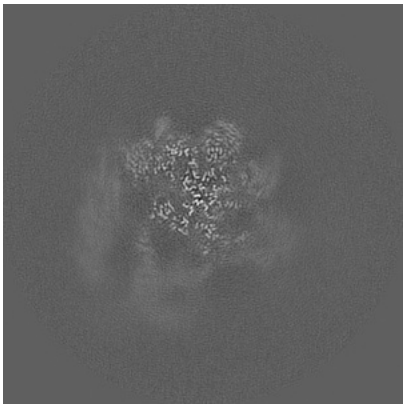


Z

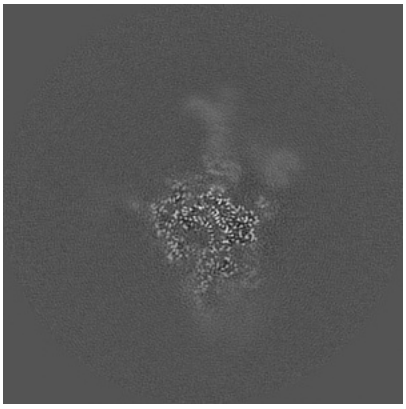
The images above show the map projected in three orthogonal directions.

6.2 Central slices

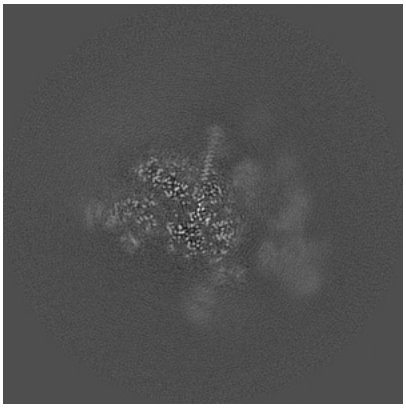
6.2.1 Primary map



X Index: 220



Y Index: 220

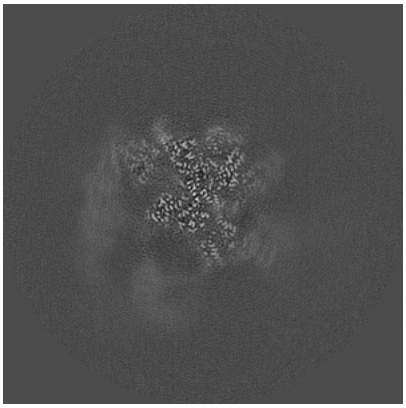


Z Index: 220

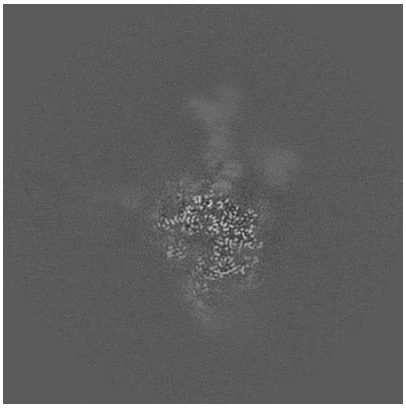
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

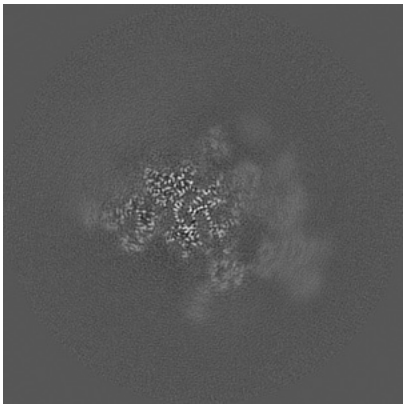
6.3.1 Primary map



X Index: 213



Y Index: 216

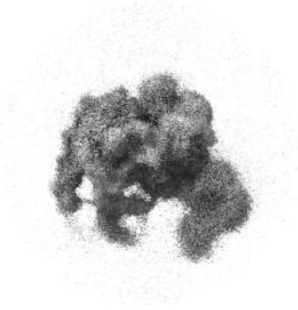


Z Index: 227

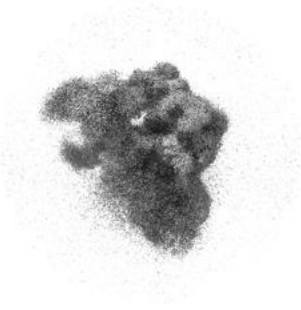
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

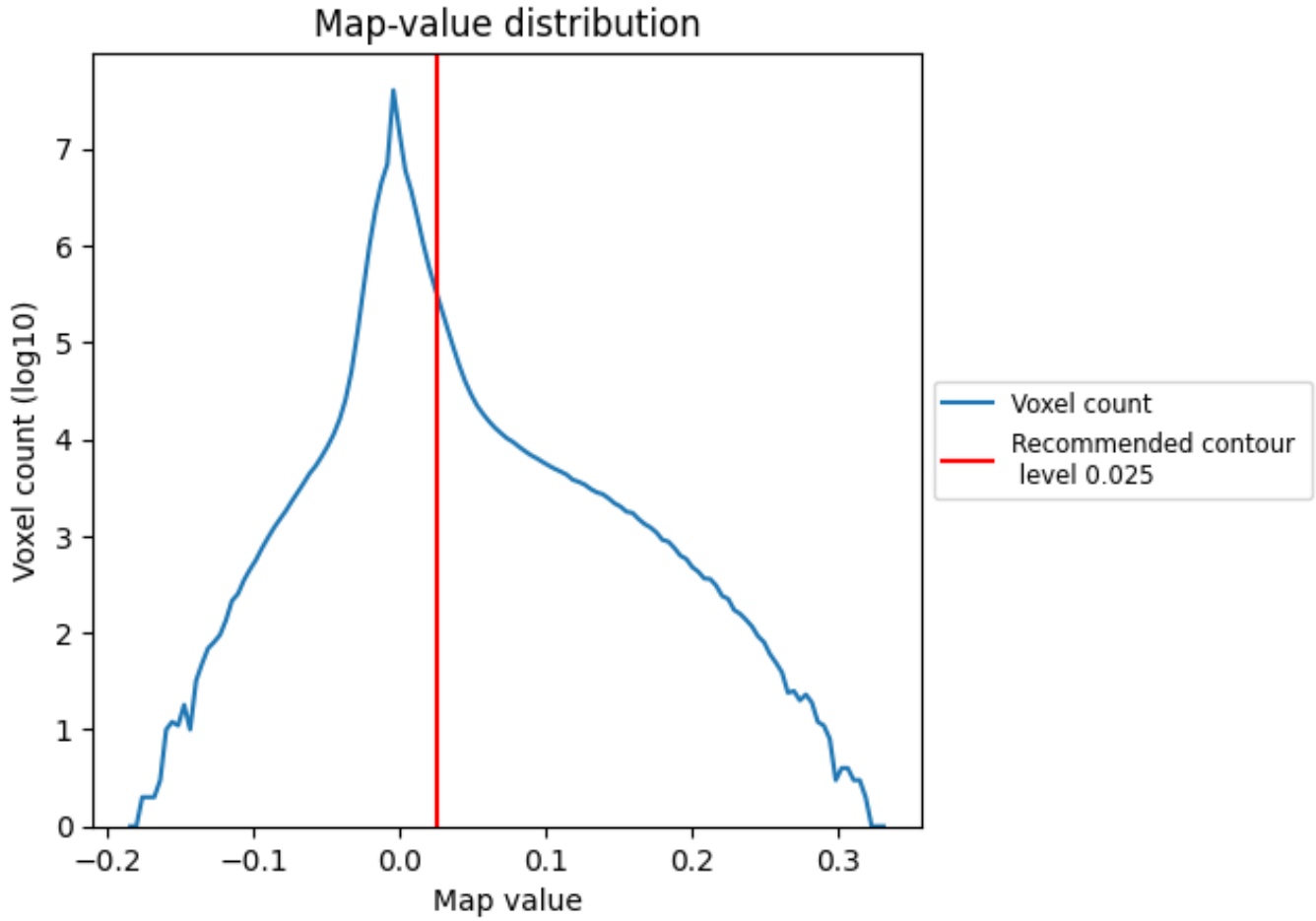
6.5 Mask visualisation (i)

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

7 Map analysis

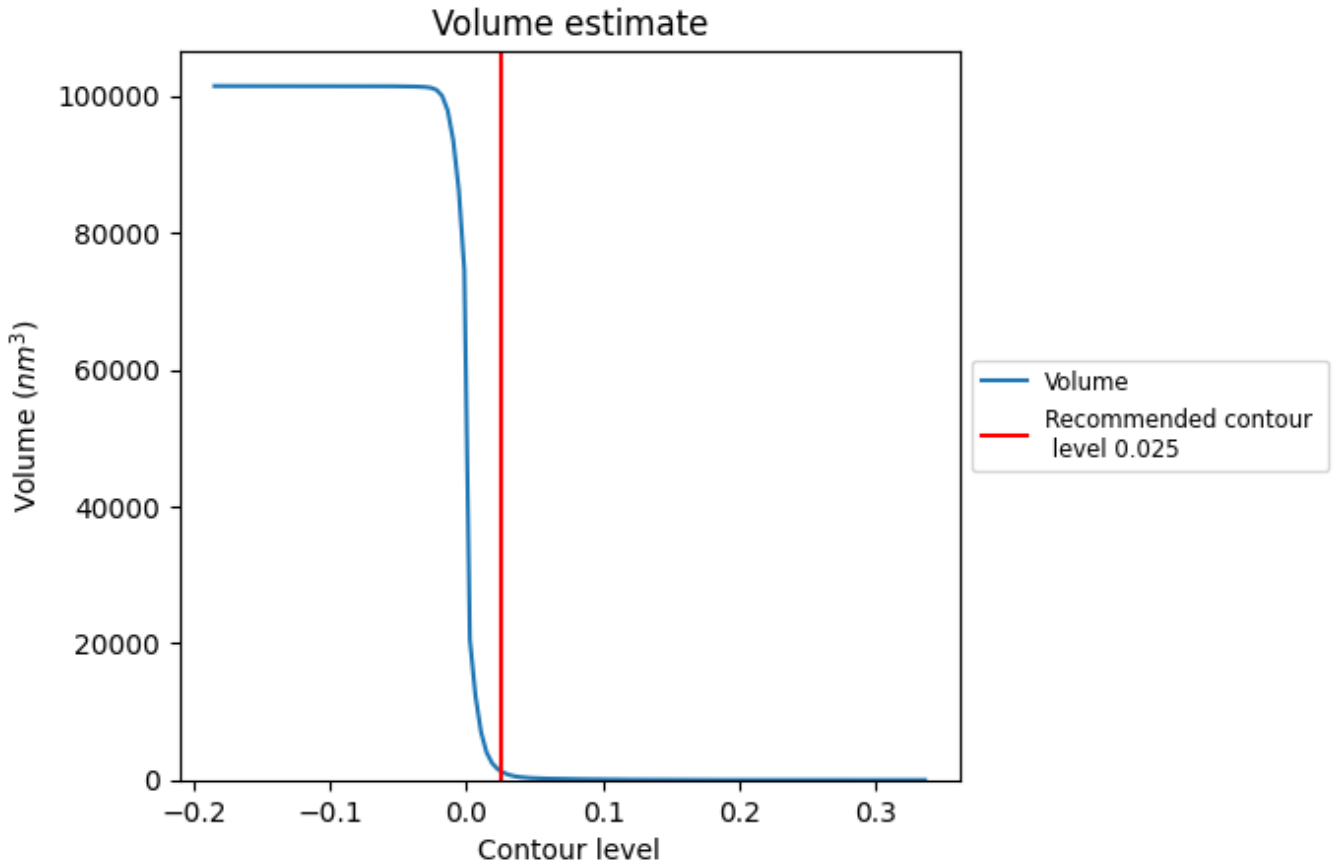
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

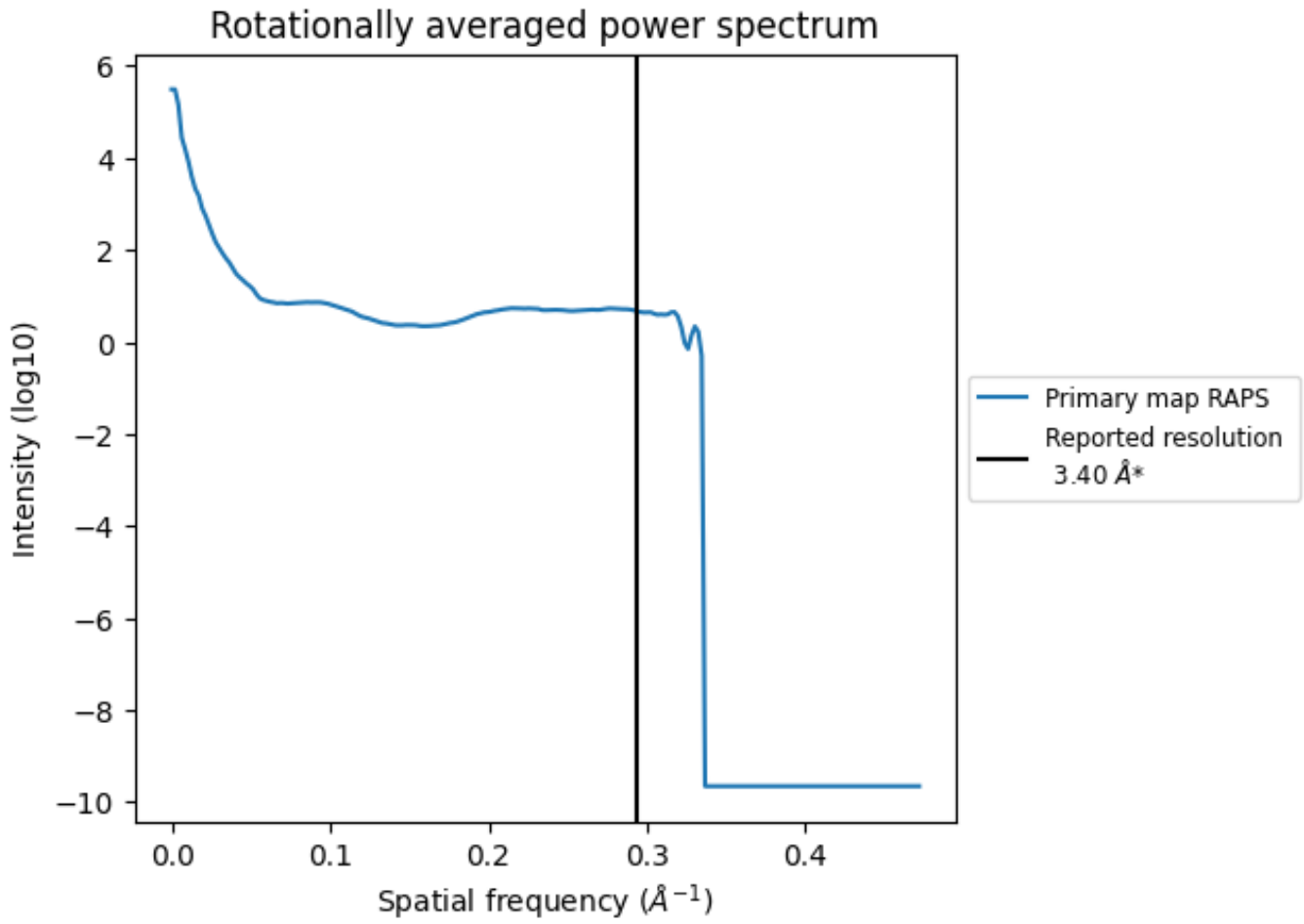
7.2 Volume estimate



The volume at the recommended contour level is 1311 nm^3; this corresponds to an approximate mass of 1184 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 (i)



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

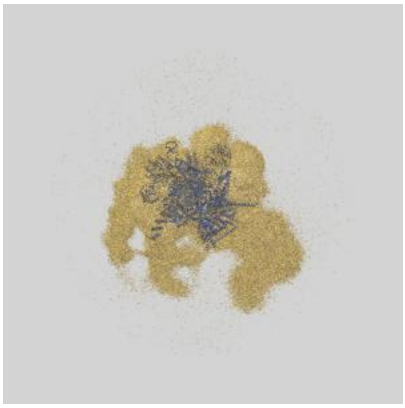
8 Fourier-Shell correlation (i)

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

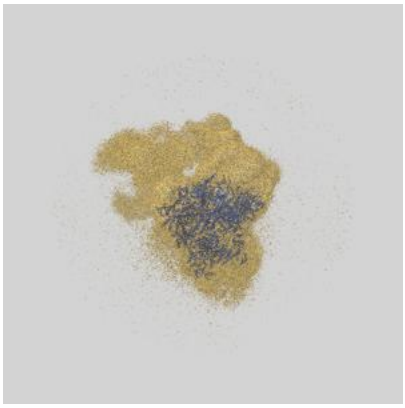
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11569 and PDB model 6ZYM. Per-residue inclusion information can be found in section 3 on page 10.

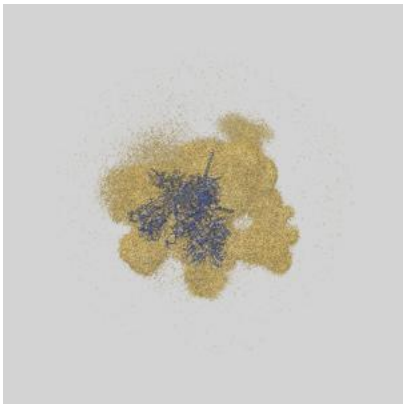
9.1 Map-model overlay



X



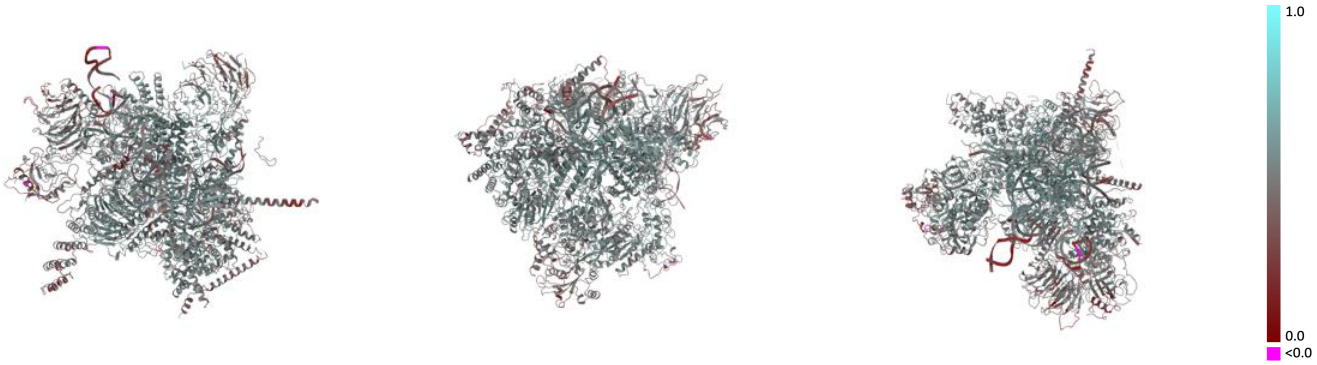
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 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.

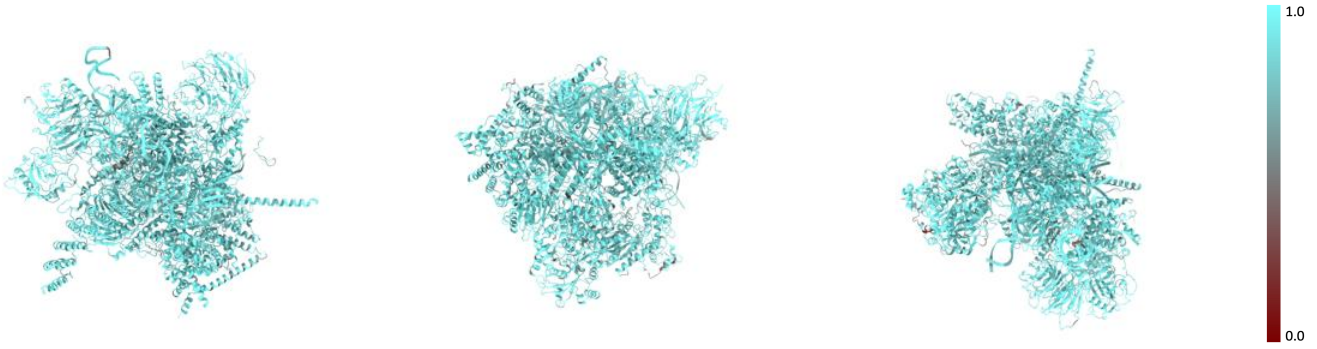
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

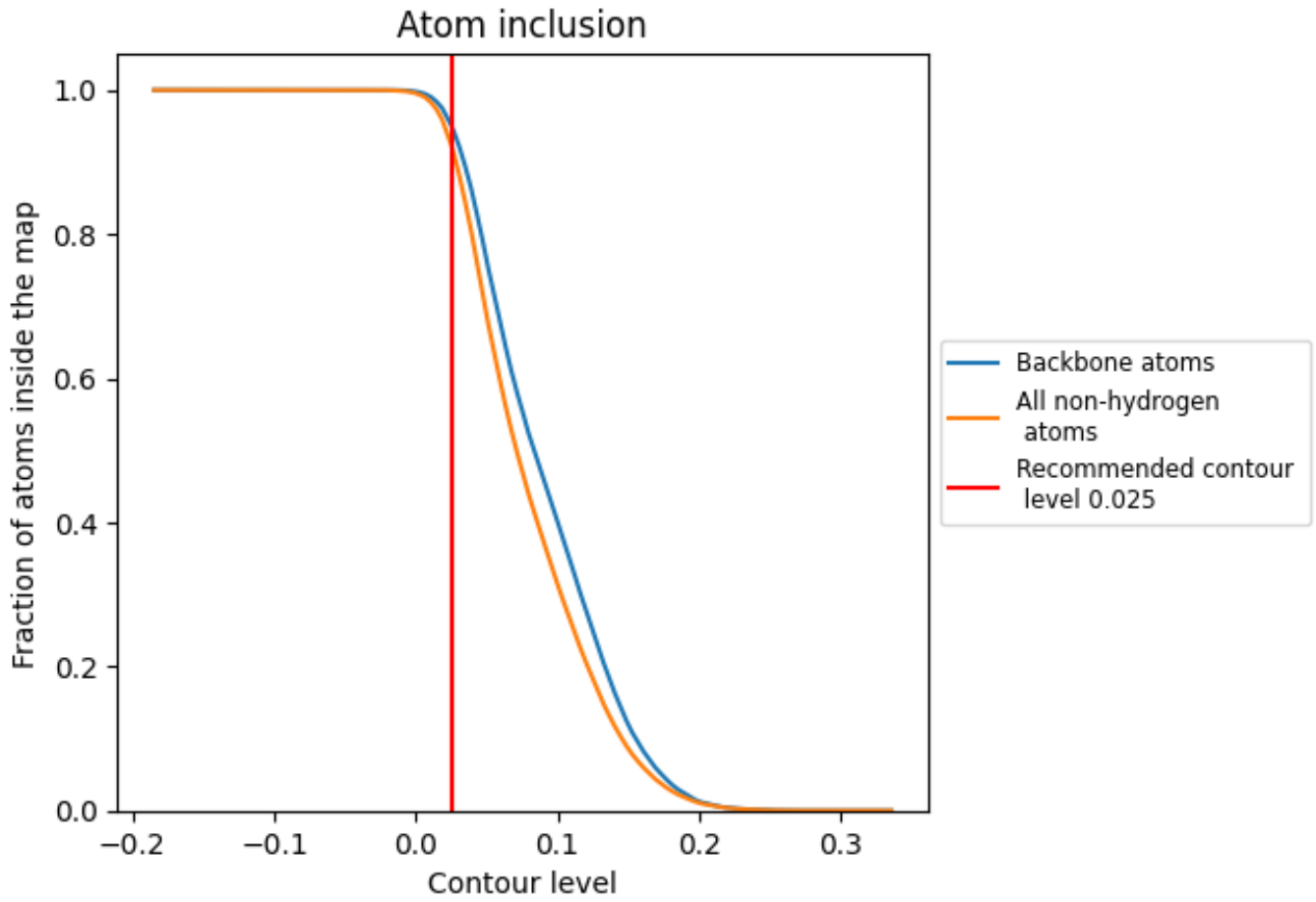
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 92% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9241	0.4980
2	0.9043	0.4570
5	0.9348	0.4550
6	0.9499	0.4720
9	0.6789	0.4240
A	0.9350	0.5390
B	0.9223	0.4880
C	0.8898	0.4710
D	0.9567	0.5520
E	0.9058	0.4900
F	0.9257	0.4340
L	0.8908	0.4840
O	0.9078	0.4660
P	0.9154	0.5070
Q	0.9487	0.5260
R	0.8845	0.4980
S	0.9083	0.5290
T	0.9035	0.4820
V	0.9287	0.4170
Y	0.9267	0.4580
Z	0.9457	0.5490
p	0.9352	0.4540
r	0.8333	0.4610
s	0.9342	0.5570
t	0.8908	0.4500
u	0.8926	0.4830
x	0.8957	0.5330