wwPDB EM Map/Model Validation Report (i)

Jun 14, 2016 – 01:45 PM EDT

PDB ID	:	5IY9
EMDB ID:	:	EMD-8134
Title	:	Human holo-PIC in the initial transcribing state (no IIS)
Authors	:	He, Y.; Yan, C.; Fang, J.; Inouye, C.; Tjian, R.; Ivanov, I.; Nogales, E.
Deposited on	:	2016-03-24
Resolution	:	6.30 Å(reported)
Based on PDB ID	:	?

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

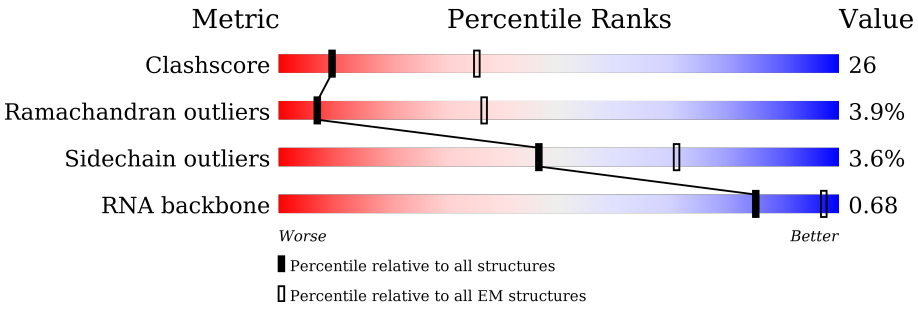
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

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 6.30 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1970	50% 21% • • 26%
2	B	1174	61% 34% • ••
3	C	275	66% 31% •
4	D	142	75% 15% • 9%
5	E	210	72% 26% ••
6	F	127	57% 11% 32%
7	G	172	69% 29% ••
8	H	150	56% 39% 5% •

Continued on next page...

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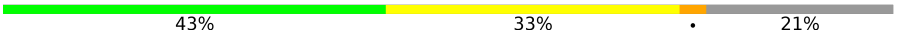
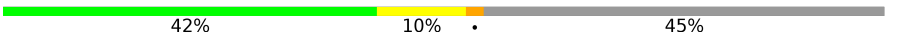
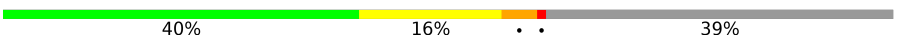
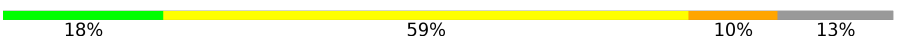
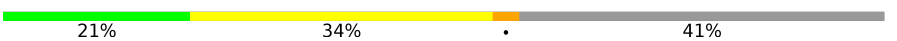
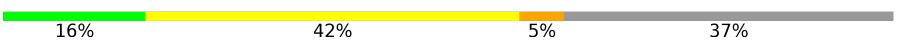
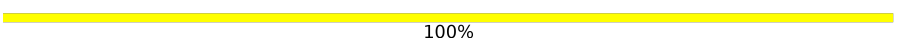
Mol	Chain	Length	Quality of chain
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	316	
14	N	376	
15	O	109	
16	P	339	
17	Q	439	
18	R	291	
19	S	517	
20	T	249	
21	V	782	
22	W	760	
23	0	395	
24	1	71	
25	2	462	
26	3	308	
27	X	83	
28	Y	83	
29	Z	6	

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 61725 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 DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1454	11515	7234	2058	2150	73	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1165	9317	5878	1637	1738	64	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	275	2213	1386	380	440	7	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	129	1062	665	179	214	4	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	210	1723	1088	301	325	9	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	86	689	437	120	127	5	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	150	Total	C	N	O	S	0	0
			1205	764	196	239	6		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	125	Total	C	N	O	S	0	0
			1013	626	177	198	12		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			937	604	154	177	2		

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 13 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	310	Total	C	N	O	S	0	0
			2391	1490	426	457	18		

- Molecule 14 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	113	Total	C	N	O	S	0	0
			930	585	152	189	4		

- Molecule 15 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	99	Total	C	N	O	S	0	0
			806	510	142	151	3		

- Molecule 16 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	185	Total	C	N	O	S	0	0
			1462	946	257	252	7		

- Molecule 17 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	180	Total	C	N	O	S	0	0
			1484	938	262	273	11		

- Molecule 18 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	165	Total	C	N	O	S	0	0
			1357	865	235	253	4		

- Molecule 19 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	138	Total	C	N	O	S	0	0
			1138	719	208	208	3		

- Molecule 20 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	222	Total	C	N	O	S	0	0
			1788	1127	320	338	3		

- Molecule 21 is a protein called TFIIH basal transcription factor complex helicase XPB subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	475	Total	C	N	O	S	0	0
			3855	2454	663	712	26		

- Molecule 22 is a protein called TFIIH basal transcription factor complex helicase XPD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	665	Total	C	N	O	S	0	0
			5348	3415	932	975	26		

- Molecule 23 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	0	188	Total	C	N	O	S	0	0
			1479	935	258	276	10		

- Molecule 24 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1	62	Total	C	N	O	S	0	0
			491	317	77	93	4		

- Molecule 25 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	2	274	Total	C	N	O	S	0	0
			2196	1417	377	392	10		

- Molecule 26 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	3	193	Total	C	N	O	S	0	0
			1526	978	252	284	12		

- Molecule 27 is a DNA chain called SCP-X.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	83	Total	C	N	O	P	0	0
			1710	815	307	506	82		

- Molecule 28 is a DNA chain called SCP-Y.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y	83	Total	C	N	O	P	0	0
			1681	798	300	501	82		

- Molecule 29 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	6	Total	C	N	O	P	0	0
			125	57	23	40	5		

- Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
30	A	2	Total	Mg	0
			2	2	

- Molecule 31 is ZINC ION (three-letter code: ZN) (formula: Zn).

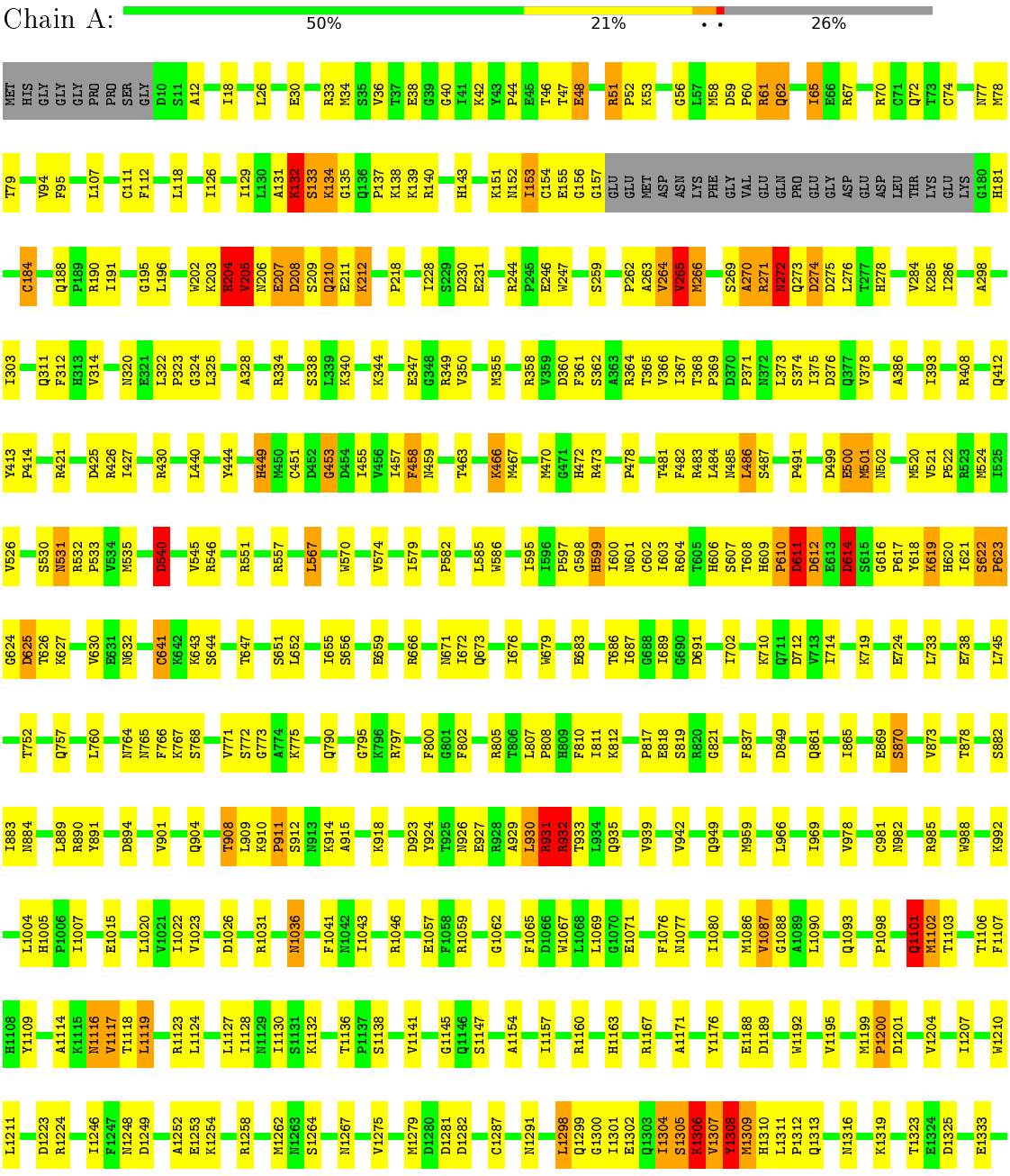
Mol	Chain	Residues	Atoms		AltConf
31	J	1	Total	Zn	0
			1	1	
31	Q	1	Total	Zn	0
			1	1	
31	B	1	Total	Zn	0
			1	1	
31	I	2	Total	Zn	0
			2	2	
31	C	1	Total	Zn	0
			1	1	
31	A	2	Total	Zn	0
			2	2	
31	L	1	Total	Zn	0
			1	1	
31	M	1	Total	Zn	0
			1	1	

3 Residue-property plots (i)

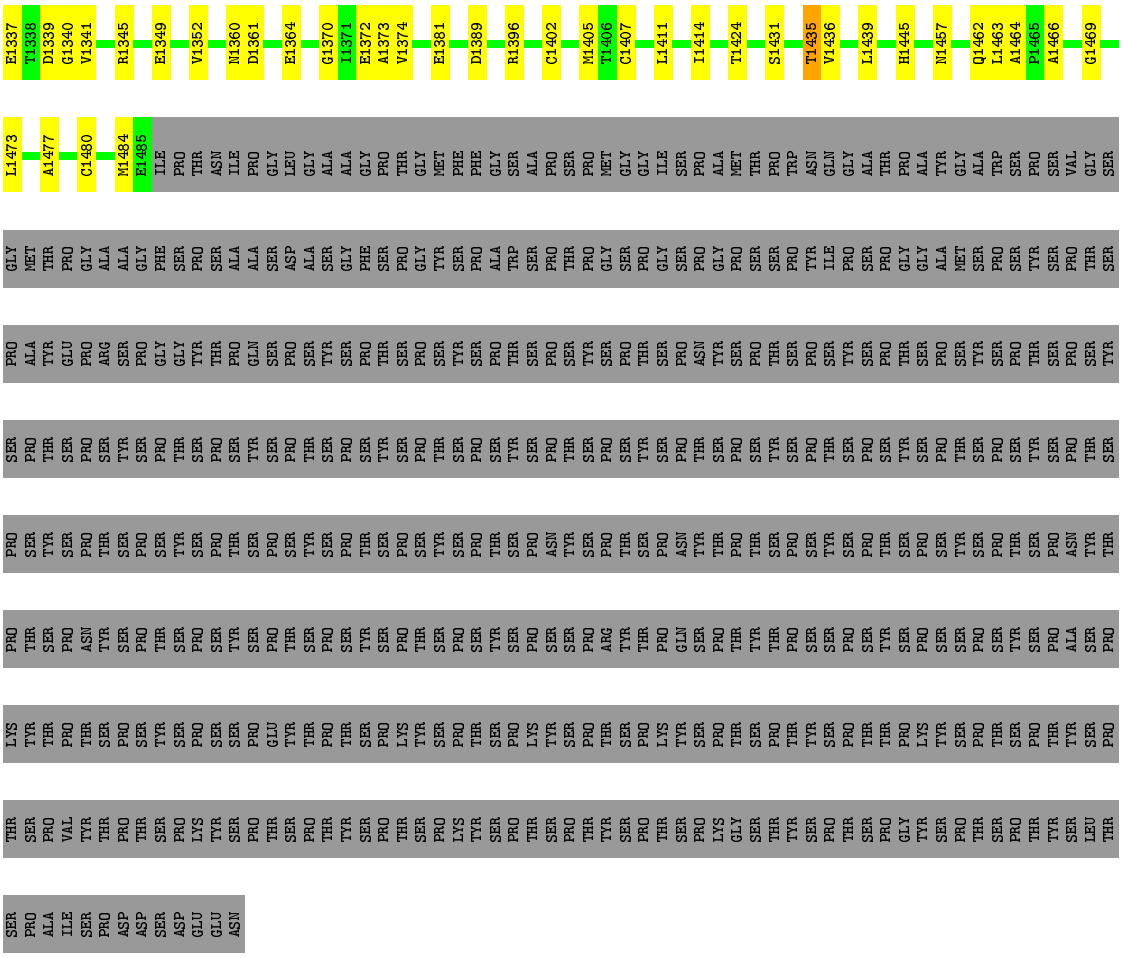
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

Chain A:

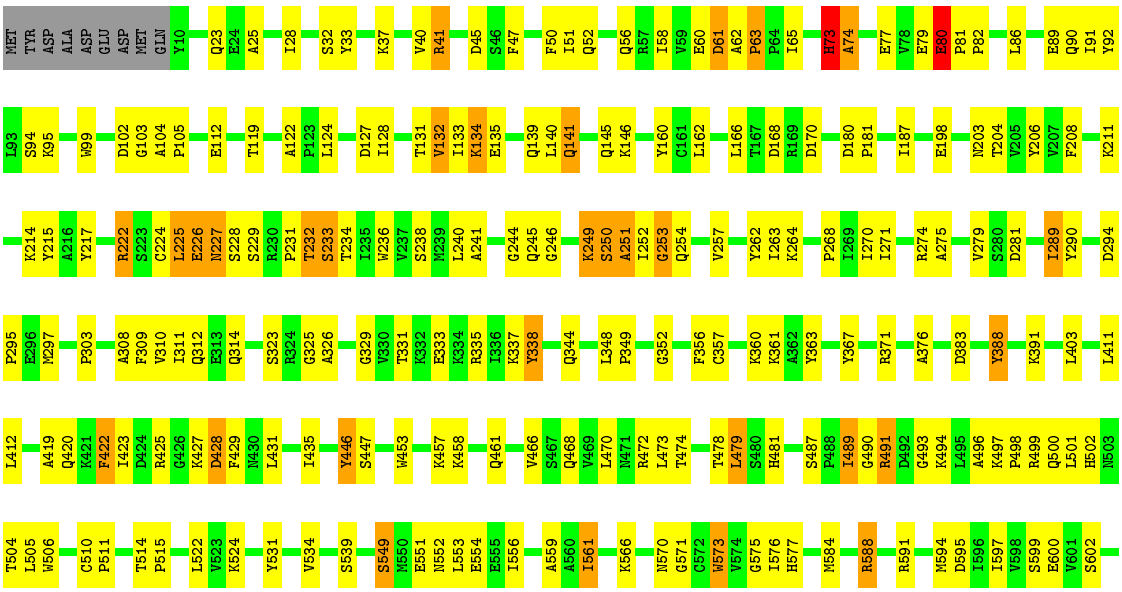


WORLDWIDE PDB PROTEIN DATA BANK
EMDataBank Unified Data Resource for 3DEM

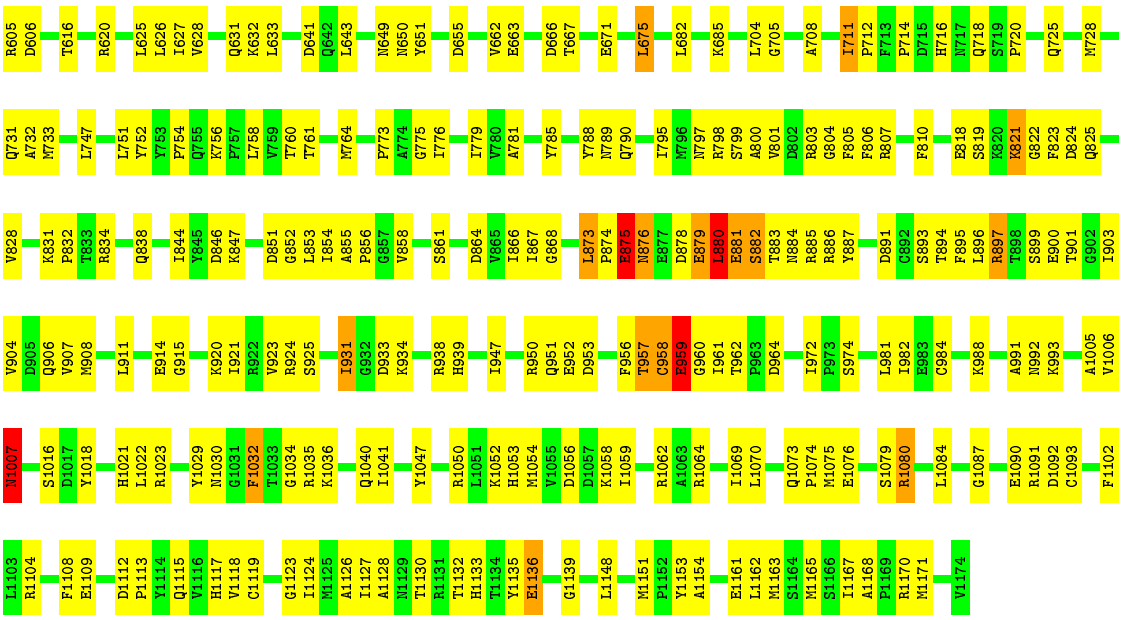


• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

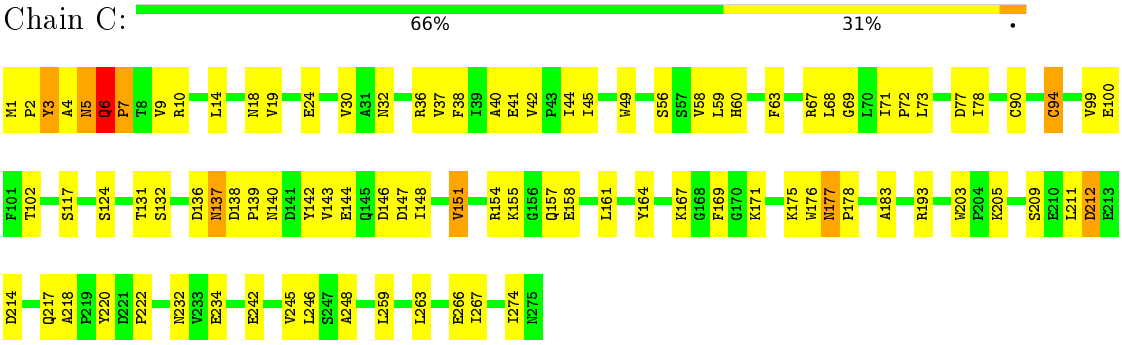
Chain B:



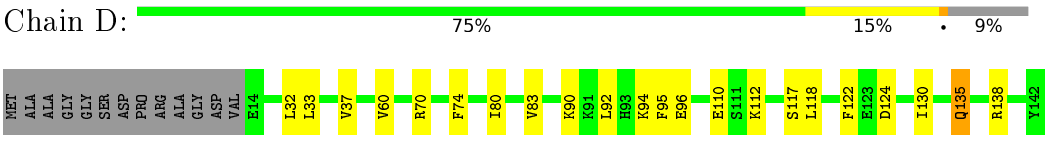
WORLDWIDE PDB PROTEIN DATA BANK
EMDataBank Unified Data Resource for 3DEM



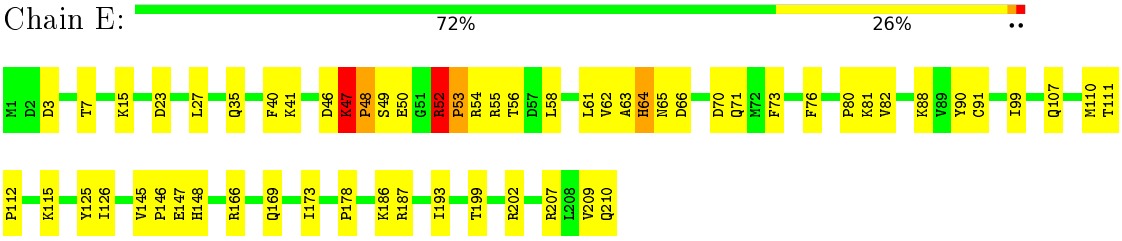
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

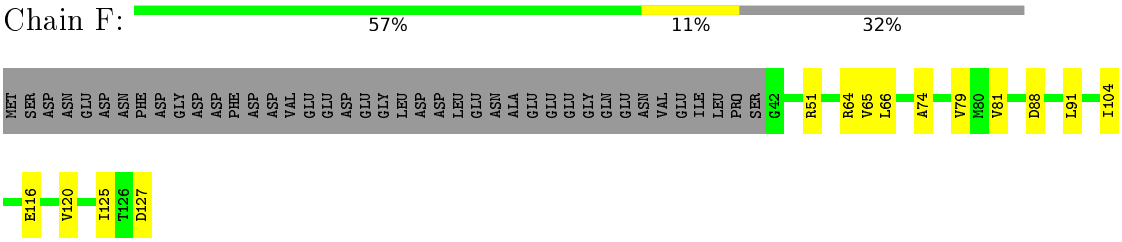


• Molecule 5: DNA-directed RNA polymerase II subunit RPB5



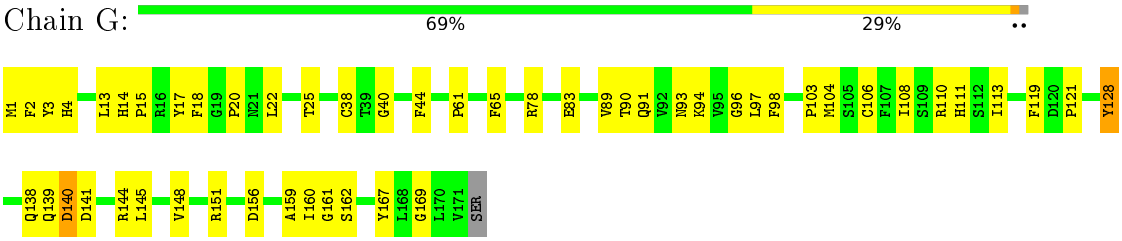
• Molecule 6: DNA-directed RNA polymerase II subunit RPB6

Chain F:



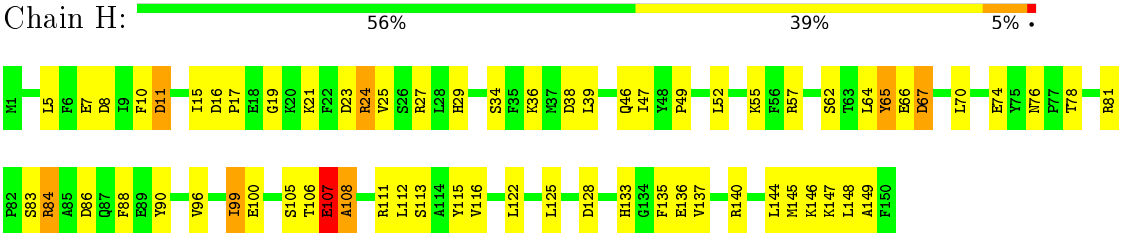
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:



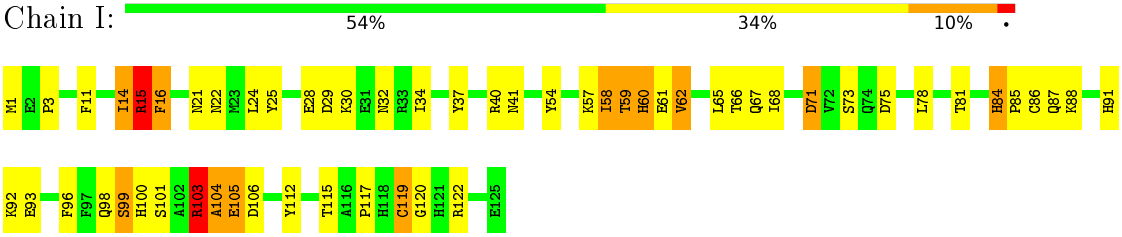
- Molecule 8: DNA-directed RNA polymerase II subunit RPB8

Chain H:



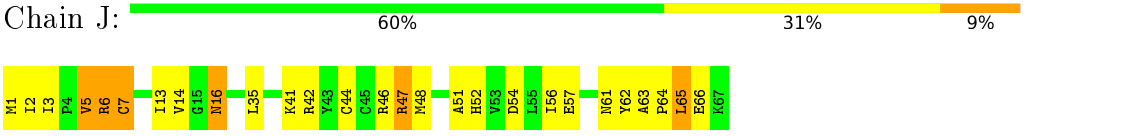
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:



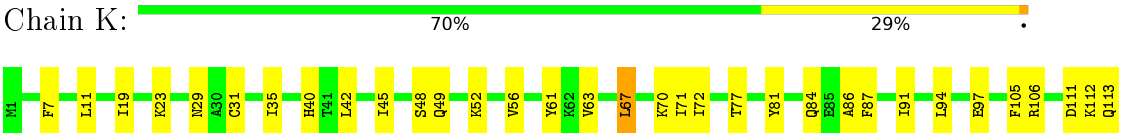
- Molecule 10: DNA-directed RNA polymerase II subunit RPB10

Chain J:



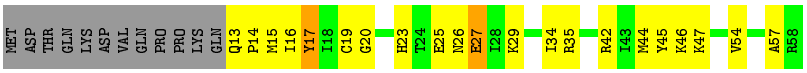
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a

Chain K:



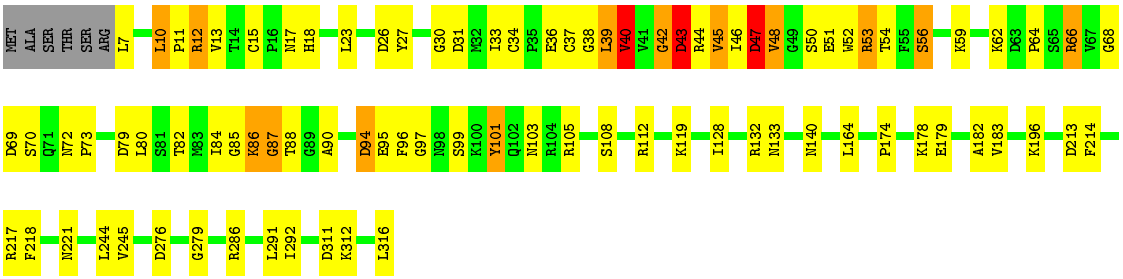
• Molecule 12: DNA-directed RNA polymerase II subunit RPB12

Chain L:



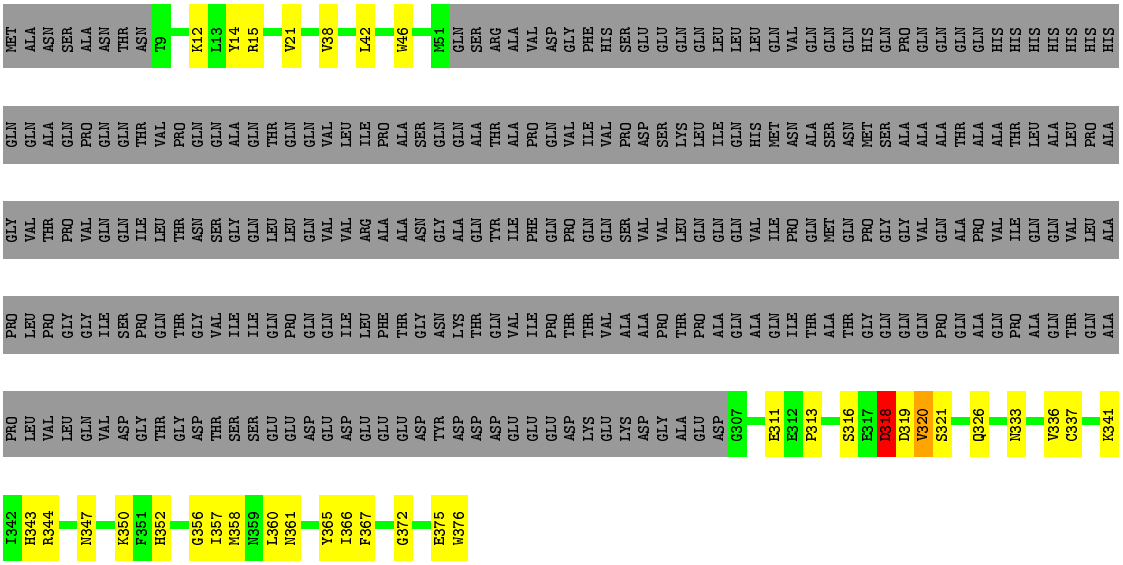
• Molecule 13: Transcription initiation factor IIB

Chain M:



• Molecule 14: Transcription initiation factor IIA subunit 1

Chain N:

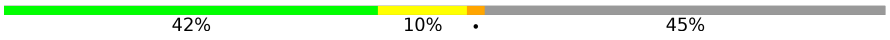


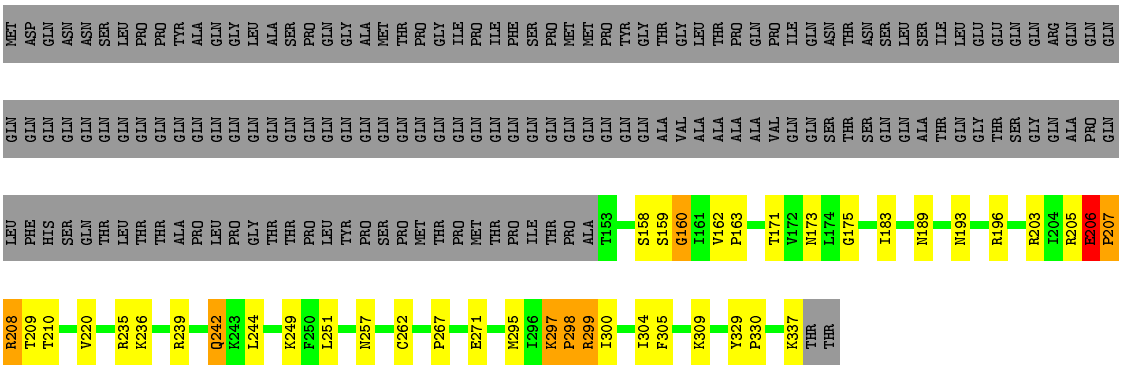
• Molecule 15: Transcription initiation factor IIA subunit 2

Chain O:

- Molecule 16: TATA-box-binding protein

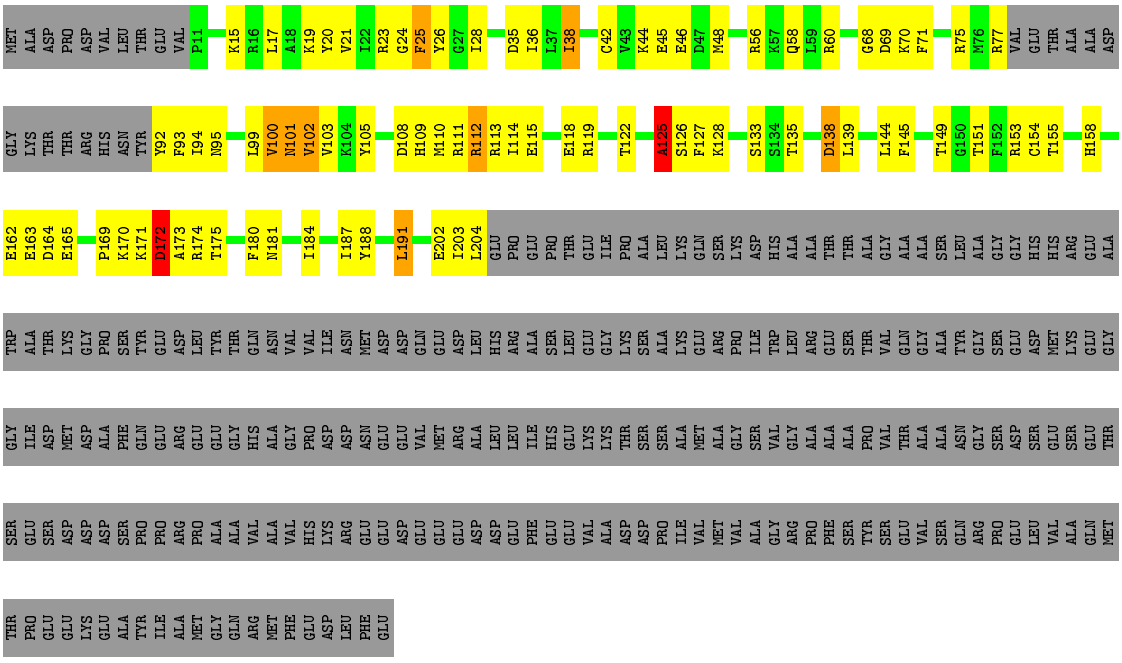
Chain P:





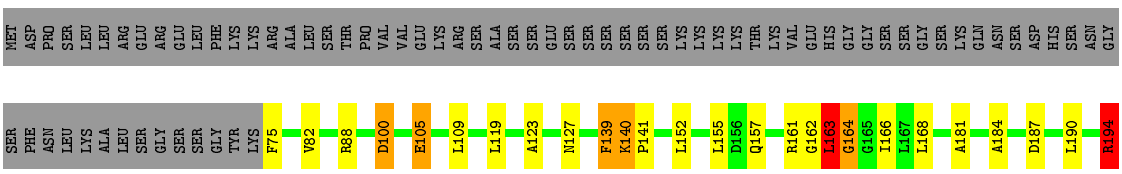
- Molecule 17: General transcription factor IIE subunit 1

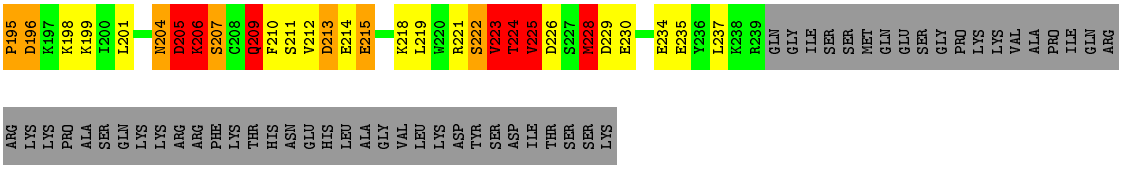
Chain Q:



- Molecule 18: Transcription initiation factor IIE subunit beta

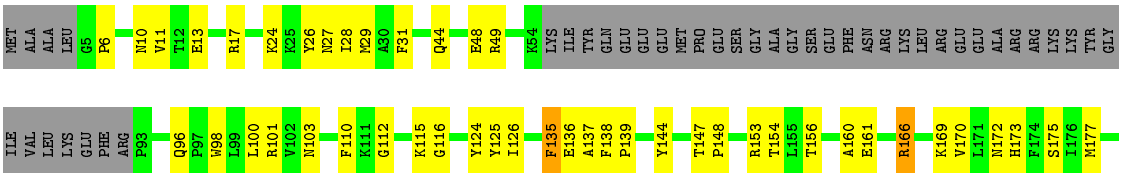
Chain R:

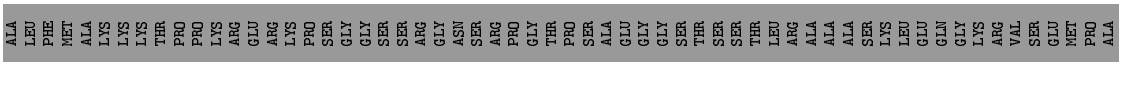




• Molecule 19: General transcription factor IIF subunit 1

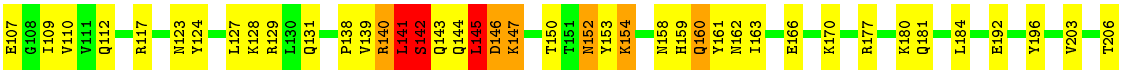
Chain S:





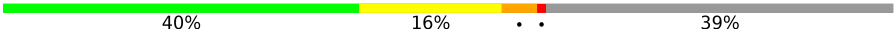
• Molecule 20: General transcription factor IIF subunit 2

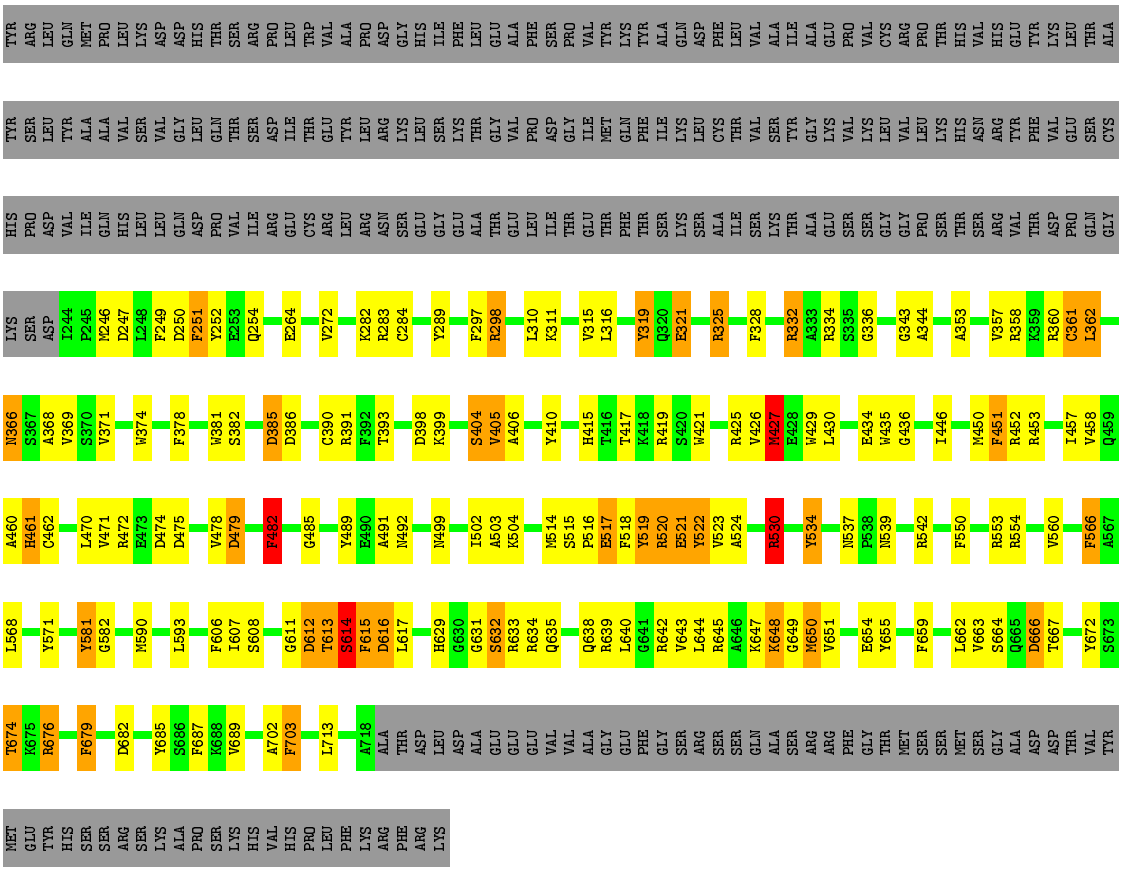
Chain T:



• Molecule 21: TFIIH basal transcription factor complex helicase XPB subunit

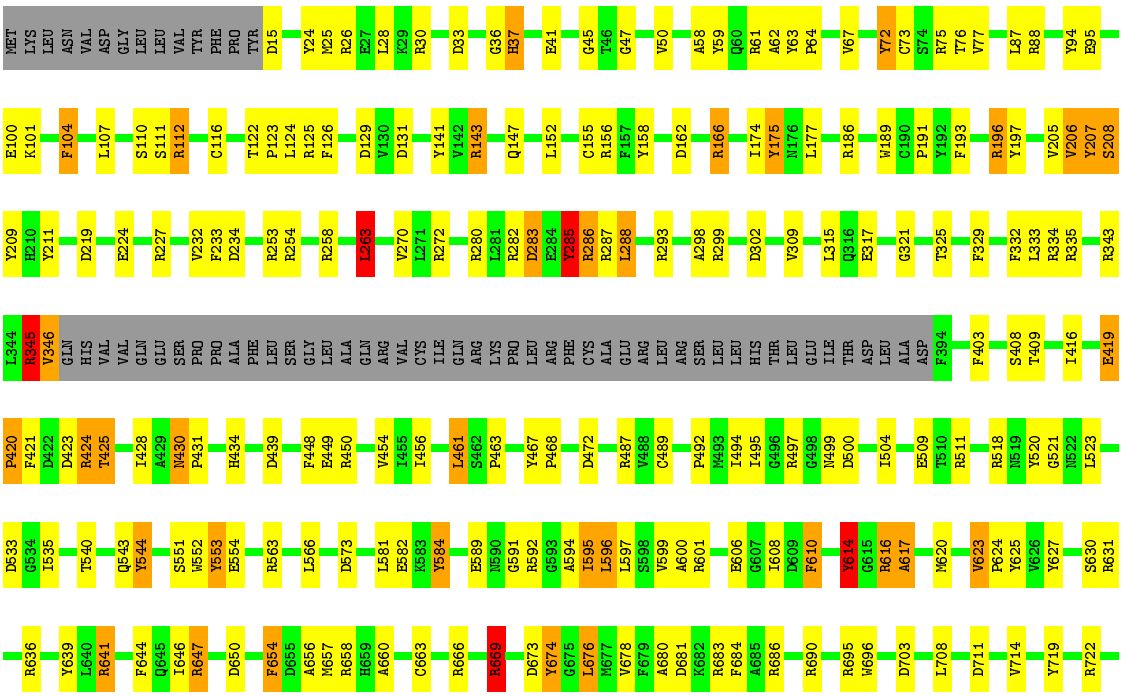
Chain V:





• Molecule 22: TFIIH basal transcription factor complex helicase XPD subunit

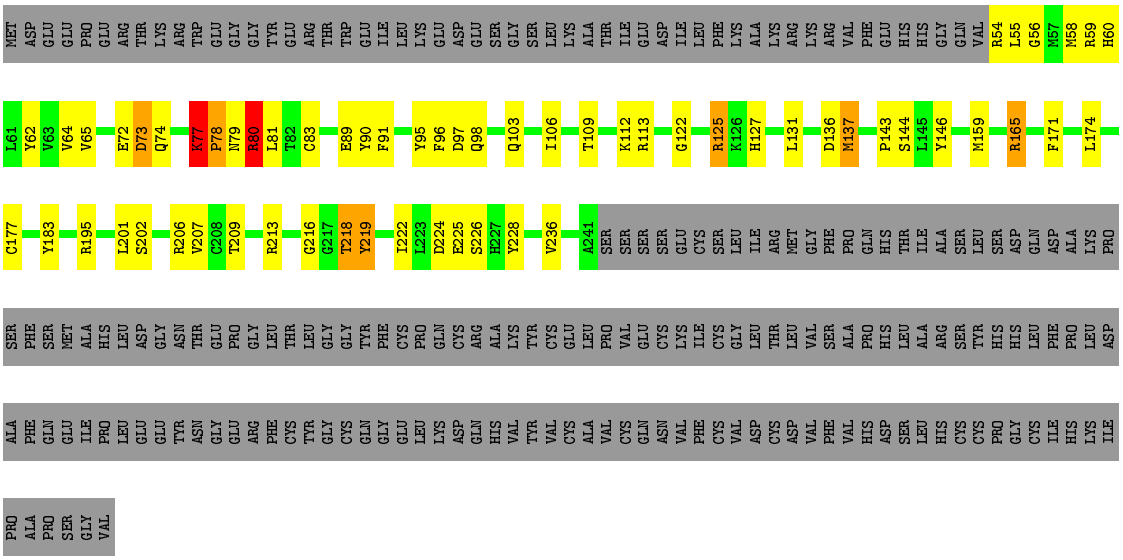
Chain W:



WORLDWIDE PDB PROTEIN DATA BANK
EMDataBank Unified Data Resource for 3DEM

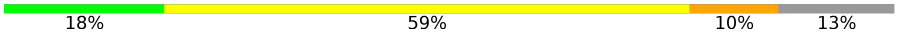
• Molecule 23: General transcription factor IIH subunit 2

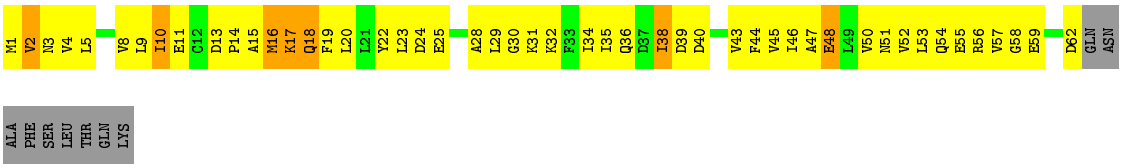
Chain 0:



• Molecule 24: General transcription factor IIH subunit 5

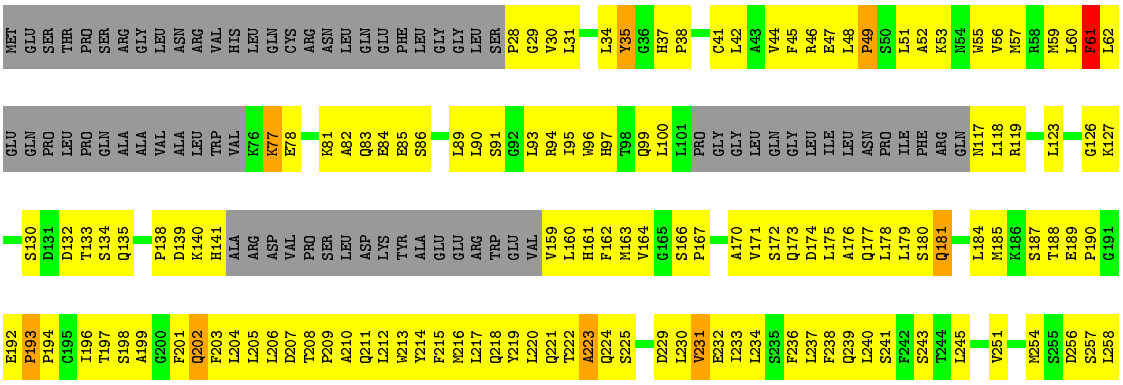
Chain 1:





• Molecule 25: General transcription factor IIH subunit 4

Chain 2:



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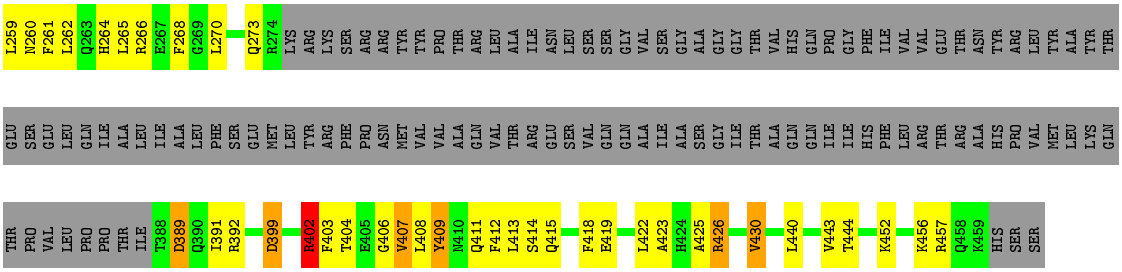
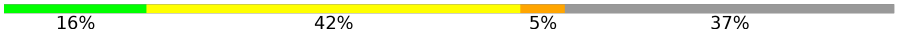
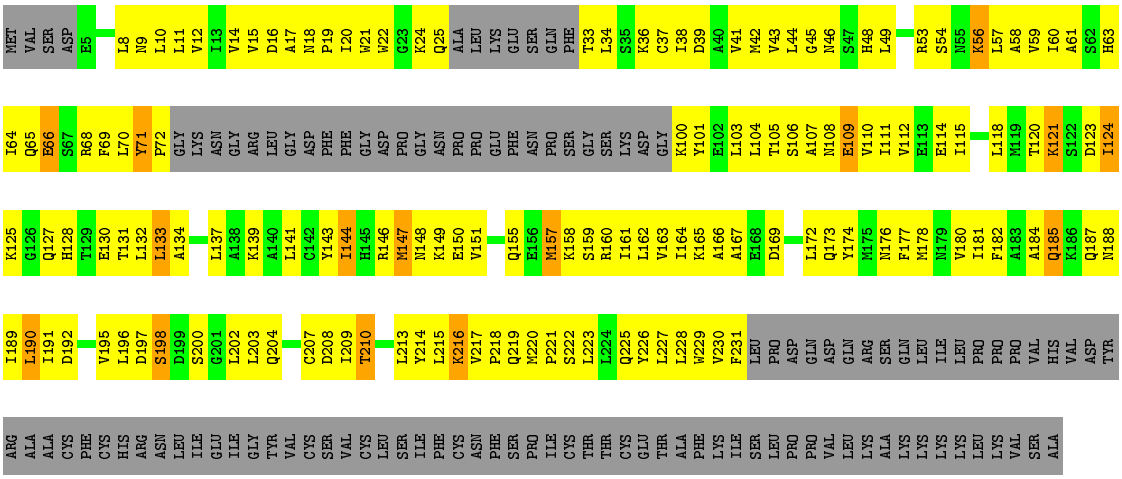
EMDataBank Unified Data Resource for 3DEM



• Molecule 26: General transcription factor IIH subunit 3

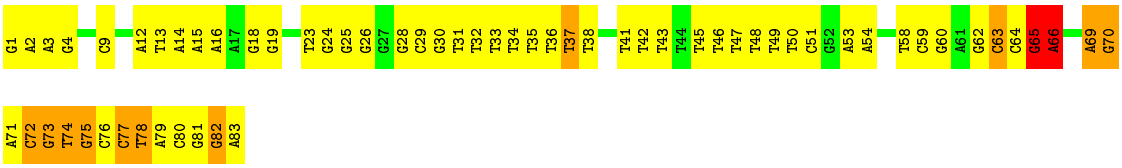
Chain 3:





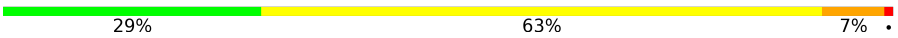
• Molecule 27: SCP-X

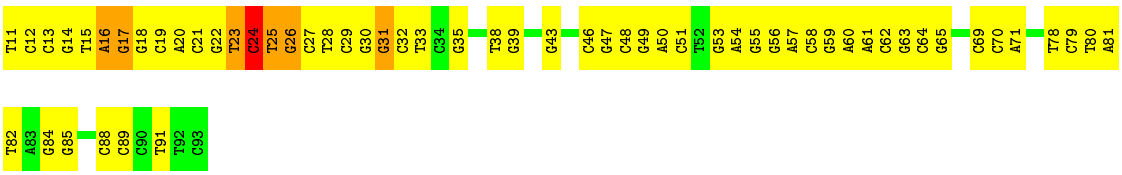
Chain X:



• Molecule 28: SCP-Y

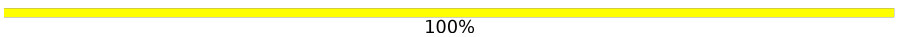
Chain Y:

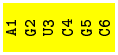




• Molecule 29: RNA

Chain Z:




A1
G2
U3
C4
G5
C6

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	91642	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	27500	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.56	1/11727 (0.0%)	0.81	15/15833 (0.1%)
10	J	0.66	1/542 (0.2%)	0.89	0/730
11	K	0.50	0/956	0.72	1/1294 (0.1%)
12	L	0.56	0/394	0.73	0/524
13	M	0.42	0/2429	0.73	3/3281 (0.1%)
14	N	0.24	0/945	0.52	0/1274
15	O	0.34	0/816	0.53	0/1105
16	P	0.29	0/1489	0.54	0/2005
17	Q	0.29	0/1507	0.63	1/2023 (0.0%)
18	R	0.67	4/1380 (0.3%)	1.13	6/1854 (0.3%)
19	S	0.27	0/1167	0.54	0/1576
2	B	0.67	3/9503 (0.0%)	0.87	8/12831 (0.1%)
20	T	0.28	0/1817	0.66	2/2445 (0.1%)
21	V	1.46	15/3931 (0.4%)	1.96	111/5298 (2.1%)
22	W	1.55	24/5460 (0.4%)	2.05	161/7390 (2.2%)
23	0	1.49	5/1506 (0.3%)	1.98	45/2038 (2.2%)
24	1	0.84	0/496	1.16	0/669
25	2	0.88	0/2243	1.18	8/3024 (0.3%)
26	3	0.85	0/1548	1.14	2/2090 (0.1%)
27	X	1.17	20/1917 (1.0%)	1.52	41/2962 (1.4%)
28	Y	1.16	13/1880 (0.7%)	1.48	43/2896 (1.5%)
29	Z	0.37	0/139	0.84	0/215
3	C	0.54	0/2259	0.76	1/3073 (0.0%)
4	D	0.27	0/1077	0.52	0/1446
5	E	0.43	0/1753	0.85	1/2368 (0.0%)
6	F	0.44	0/700	0.71	0/946
7	G	0.32	0/1382	0.58	0/1874
8	H	0.45	0/1227	0.71	1/1654 (0.1%)
9	I	0.38	0/1038	1.06	4/1407 (0.3%)
All	All	0.85	86/63228 (0.1%)	1.17	454/86125 (0.5%)

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
1	A	0	2
15	O	0	1
16	P	0	1
17	Q	0	2
18	R	0	20
20	T	0	1
21	V	0	16
22	W	0	18
23	0	0	2
24	1	0	1
25	2	0	8
27	X	0	3
28	Y	0	3
8	H	0	1
All	All	0	79

The worst 5 of 86 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Y	25	DT	O3'-P	10.60	1.73	1.61
27	X	71	DA	P-O5'	-9.87	1.49	1.59
28	Y	31	DG	O3'-P	-9.02	1.50	1.61
27	X	79	DA	C5'-C4'	8.68	1.60	1.51
27	X	69	DA	C4'-C3'	8.62	1.61	1.53

The worst 5 of 454 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	84	HIS	C-N-CD	-28.48	57.95	120.60
5	E	52	ARG	C-N-CD	-22.65	70.76	120.60
23	0	77	LYS	C-N-CD	-22.15	71.87	120.60
26	3	71	TYR	C-N-CD	-20.77	74.91	120.60
1	A	622	SER	C-N-CD	-20.67	75.13	120.60

There are no chirality outliers.

5 of 79 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1291	ASN	Sidechain
1	A	210	GLN	Mainchain
8	H	99	ILE	Peptide
15	O	86	GLU	Sidechain
16	P	242	GLN	Sidechain

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	A	11515	0	11608	512	0
2	B	9317	0	9307	414	0
3	C	2213	0	2153	98	0
4	D	1062	0	1042	15	0
5	E	1723	0	1745	65	0
6	F	689	0	715	11	0
7	G	1351	0	1358	42	0
8	H	1205	0	1167	48	0
9	I	1013	0	930	78	0
10	J	533	0	553	39	0
11	K	937	0	959	25	0
12	L	388	0	393	24	0
13	M	2391	0	2410	164	0
14	N	930	0	888	34	0
15	O	806	0	818	25	0
16	P	1462	0	1548	53	0
17	Q	1484	0	1498	212	0
18	R	1357	0	1381	224	0
19	S	1138	0	1103	42	0
20	T	1788	0	1819	92	0
21	V	3855	0	3871	131	0
22	W	5348	0	5373	122	0
23	0	1479	0	1524	43	0
24	1	491	0	507	228	0
25	2	2196	0	2206	571	0
26	3	1526	0	1561	461	0
27	X	1710	0	941	67	0
28	Y	1681	0	932	56	0
29	Z	125	0	67	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	A	2	0	0	0	0
31	A	2	0	0	0	0
31	B	1	0	0	0	0
31	C	1	0	0	0	0
31	I	2	0	0	0	0
31	J	1	0	0	0	0
31	L	1	0	0	0	0
31	M	1	0	0	0	0
31	Q	1	0	0	0	0
All	All	61725	0	60377	3159	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 26.

The worst 5 of 3159 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)
26:3:59:VAL:HG12	26:3:71:TYR:CD1	1.24	1.66
21:V:516:PRO:CG	24:1:15:ALA:HB3	1.21	1.65
1:A:1171:ALA:CB	9:I:59:THR:HG21	1.18	1.59
18:R:223:VAL:CG2	18:R:224:THR:HG21	1.29	1.59
21:V:315:VAL:HG13	22:W:500:ASP:CB	1.21	1.57

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	A	1450/1970 (74%)	1268 (87%)	120 (8%)	62 (4%)	3 34
2	B	1163/1174 (99%)	996 (86%)	116 (10%)	51 (4%)	3 33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	273/275 (99%)	239 (88%)	25 (9%)	9 (3%)	5 40
4	D	127/142 (89%)	119 (94%)	8 (6%)	0	100 100
5	E	208/210 (99%)	191 (92%)	11 (5%)	6 (3%)	6 43
6	F	84/127 (66%)	82 (98%)	2 (2%)	0	100 100
7	G	169/172 (98%)	158 (94%)	10 (6%)	1 (1%)	30 74
8	H	148/150 (99%)	118 (80%)	20 (14%)	10 (7%)	1 23
9	I	123/125 (98%)	92 (75%)	16 (13%)	15 (12%)	0 8
10	J	65/67 (97%)	51 (78%)	9 (14%)	5 (8%)	1 20
11	K	115/117 (98%)	109 (95%)	4 (4%)	2 (2%)	11 55
12	L	44/58 (76%)	33 (75%)	9 (20%)	2 (4%)	3 33
13	M	308/316 (98%)	263 (85%)	32 (10%)	13 (4%)	3 34
14	N	109/376 (29%)	101 (93%)	6 (6%)	2 (2%)	11 53
15	O	97/109 (89%)	95 (98%)	2 (2%)	0	100 100
16	P	183/339 (54%)	170 (93%)	6 (3%)	7 (4%)	4 37
17	Q	176/439 (40%)	158 (90%)	10 (6%)	8 (4%)	3 33
18	R	163/291 (56%)	140 (86%)	14 (9%)	9 (6%)	2 28
19	S	134/517 (26%)	120 (90%)	10 (8%)	4 (3%)	5 42
20	T	218/249 (88%)	190 (87%)	20 (9%)	8 (4%)	4 37
21	V	473/782 (60%)	398 (84%)	47 (10%)	28 (6%)	2 26
22	W	661/760 (87%)	570 (86%)	69 (10%)	22 (3%)	5 40
23	0	186/395 (47%)	168 (90%)	13 (7%)	5 (3%)	6 44
24	1	60/71 (84%)	53 (88%)	5 (8%)	2 (3%)	5 40
25	2	264/462 (57%)	246 (93%)	14 (5%)	4 (2%)	13 57
26	3	187/308 (61%)	176 (94%)	9 (5%)	2 (1%)	17 63
All	All	7188/10001 (72%)	6304 (88%)	607 (8%)	277 (4%)	7 36

5 of 277 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	LYS
1	A	153	ILE
1	A	204	HIS
1	A	205	VAL
1	A	207	GLU

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	
1	A	1279/1748 (73%)	1235 (97%)	44 (3%)	44	75
2	B	1020/1028 (99%)	985 (97%)	35 (3%)	44	75
3	C	252/252 (100%)	244 (97%)	8 (3%)	46	76
4	D	119/126 (94%)	118 (99%)	1 (1%)	86	94
5	E	192/192 (100%)	186 (97%)	6 (3%)	47	77
6	F	74/111 (67%)	74 (100%)	0	100	100
7	G	152/153 (99%)	151 (99%)	1 (1%)	88	94
8	H	131/131 (100%)	126 (96%)	5 (4%)	40	73
9	I	112/112 (100%)	108 (96%)	4 (4%)	42	74
10	J	56/56 (100%)	53 (95%)	3 (5%)	27	64
11	K	106/106 (100%)	105 (99%)	1 (1%)	84	93
12	L	43/55 (78%)	42 (98%)	1 (2%)	58	82
13	M	263/268 (98%)	256 (97%)	7 (3%)	52	79
14	N	105/324 (32%)	104 (99%)	1 (1%)	82	92
15	O	90/98 (92%)	89 (99%)	1 (1%)	80	91
16	P	159/293 (54%)	157 (99%)	2 (1%)	76	89
17	Q	164/373 (44%)	158 (96%)	6 (4%)	41	73
18	R	150/261 (58%)	139 (93%)	11 (7%)	17	54
19	S	121/448 (27%)	118 (98%)	3 (2%)	55	81
20	T	196/218 (90%)	190 (97%)	6 (3%)	47	77
21	V	422/688 (61%)	403 (96%)	19 (4%)	34	69
22	W	577/664 (87%)	543 (94%)	34 (6%)	24	61
23	0	171/352 (49%)	163 (95%)	8 (5%)	32	68
24	1	56/64 (88%)	52 (93%)	4 (7%)	18	55
25	2	238/399 (60%)	229 (96%)	9 (4%)	40	73
26	3	171/272 (63%)	159 (93%)	12 (7%)	19	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	6419/8792 (73%)	6187 (96%)	232 (4%)	46 74

5 of 232 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	7	CYS
18	R	163	LEU
25	2	202	GLN
12	L	27	GLU
15	O	21	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
21	V	281	GLN
22	W	430	ASN
26	3	155	GLN
21	V	366	ASN
21	V	677	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	Z	5/6 (83%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.