Full wwPDB EM Validation Report

Jun 5, 2021 – 06:38 am BST

PDB ID	:	7NVY
EMDB ID	:	EMD-12617
Title	:	RNA polymerase II pre-initiation complex with closed promoter DNA in proximal position
Authors	:	Aibara, S.; Schilbach, S.; Cramer, P.
Deposited on	:	2021-03-16
Resolution	:	7.30 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 following versions of software and data (see references ⓘ) were used in the production of this report:

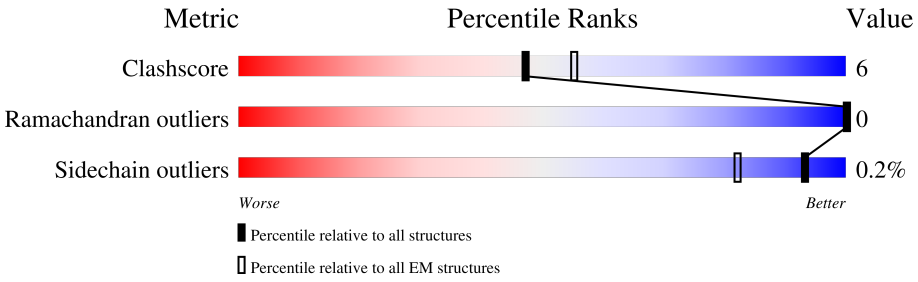
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.19

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 7.30 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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%

Mol	Chain	Length	Quality of chain
1	0	760	72% 21% 6%
2	1	548	40% 8% 52%
3	2	462	71% 13% 16%
4	3	309	33% 15% 52%
5	4	308	66% 19% 15%
6	5	71	82% 11% 7%
7	6	395	73% 15% 12%
8	7	782	64% 13% 23%
9	A	1970	60% 12% 28%

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Mol	Chain	Length	Quality of chain
10	B	1174	85% 11%
11	C	275	83% 10% 7%
12	D	142	77% 13% 10%
13	E	210	88% 11%
14	F	127	54% 8% 38%
15	G	172	90% 10%
16	H	150	90% 9%
17	I	125	87% 9%
18	J	67	78% 18%
19	K	117	89% 9%
20	L	58	64% 12% 24%
21	M	316	70% 10% 20%
22	N	106	42% 19% 40%
23	O	339	48% 5% 47%
24	Q	517	24% 73%
25	R	249	77% 12% 11%
26	T	106	51% 9% 40%
27	U	376	26% 5% 70%
28	V	109	74% 16% 9%
29	W	439	35% 11% 54%
30	X	291	48% 11% 41%
31	Y	19	100%
32	Z	8	100%

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 67474 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 TFIIH basal transcription factor complex helicase XPD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	714	5751	3683	999	1040	29	0	0

- Molecule 2 is a protein called General transcription factor IIH subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	265	2167	1382	378	395	12	0	0

- Molecule 3 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	390	3158	2050	545	551	12	0	0

- Molecule 4 is a protein called CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	149	1225	763	212	240	10	0	0

- Molecule 5 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	263	2066	1323	344	380	19	0	0

- Molecule 6 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	66	523	337	83	100	3	0	0

- Molecule 7 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	347	Total	C	N	O	S	0	0
			2732	1726	471	508	27		

- Molecule 8 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	605	Total	C	N	O	S	0	0
			4890	3127	848	885	30		

- Molecule 9 is a protein called RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	1423	Total	C	N	O	S	0	0
			11274	7092	2016	2094	72		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	1136	Total	C	N	O	S	0	0
			9076	5739	1597	1676	64		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	257	Total	C	N	O	S	0	0
			2059	1294	351	408	6		

- Molecule 12 is a protein called RPOL4c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	128	Total	C	N	O	S	0	0
			1050	656	178	212	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	209	Total	C	N	O	S	0	0
			1721	1089	300	324	8		

- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	79	Total	C	N	O	S	0	0
			636	406	108	117	5		

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 17 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	114	Total	C	N	O	S	0	0
			928	571	166	180	11		

- Molecule 18 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	64	Total	C	N	O	S	0	0
			507	328	86	87	6		

- Molecule 19 is a protein called RNA_pol_L_2 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 20 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	44	Total	C	N	O	S	0	0
			373	231	72	64	6		

- Molecule 21 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	252	Total	C	N	O	S	0	0
			1953	1224	346	366	17		

- Molecule 22 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	64	Total	C	N	O	P	0	0
			1318	624	243	388	63		

- Molecule 23 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	179	Total	C	N	O	S	0	0
			1422	923	251	241	7		

- Molecule 24 is a protein called General transcription factor IIF subunit 1.

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

- Molecule 25 is a protein called General transcription factor IIF subunit 2.

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

- Molecule 26 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	64	Total	C	N	O	P	0	0
			1303	616	245	378	64		

- Molecule 27 is a protein called Transcription initiation factor IIA subunit 1.

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

- Molecule 28 is a protein called Transcription initiation factor IIA subunit 2.

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

- Molecule 29 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	202	Total	C	N	O	S	0	0
			1659	1042	299	307	11		

- Molecule 30 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	171	Total	C	N	O	S	0	0
			1403	895	243	261	4		

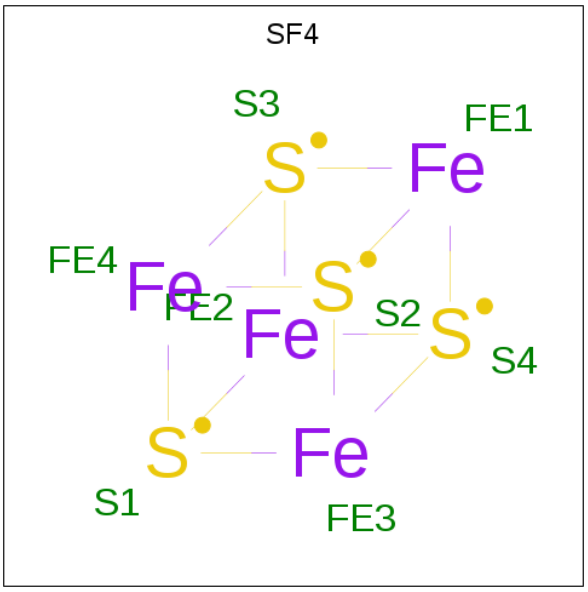
- Molecule 31 is a protein called Unassigned peptide, likely TFIIE-beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	Y	19	Total	C	N	O	0	0
			95	57	19	19		

- Molecule 32 is a protein called Unassigned peptide, likely XPB.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Z	8	Total	C	N	O	0	0
			40	24	8	8		

- Molecule 33 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
33	0	1	Total Fe S 8 4 4	0

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
34	3	2	Total Zn 2 2	0
34	4	2	Total Zn 2 2	0
34	6	3	Total Zn 3 3	0
34	A	2	Total Zn 2 2	0
34	B	1	Total Zn 1 1	0
34	C	1	Total Zn 1 1	0
34	I	2	Total Zn 2 2	0
34	J	1	Total Zn 1 1	0
34	L	1	Total Zn 1 1	0
34	M	1	Total Zn 1 1	0
34	W	1	Total Zn 1 1	0

- Molecule 35 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

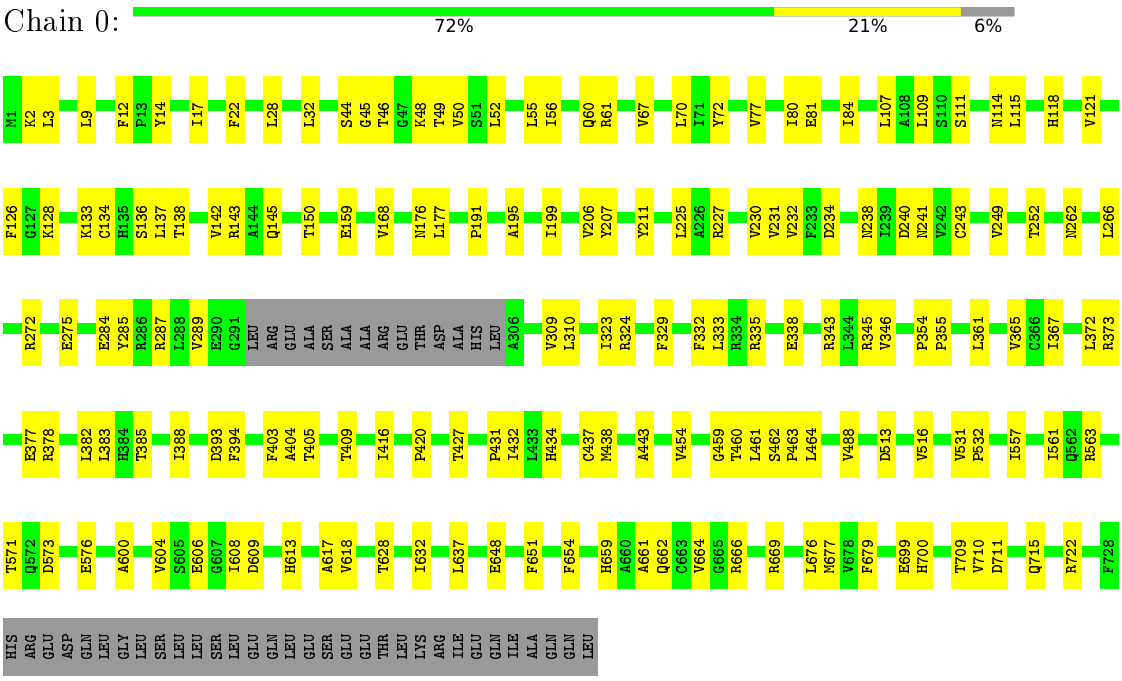
Mol	Chain	Residues	Atoms	AltConf
35	A	1	Total Mg 1 1	0

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. 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.

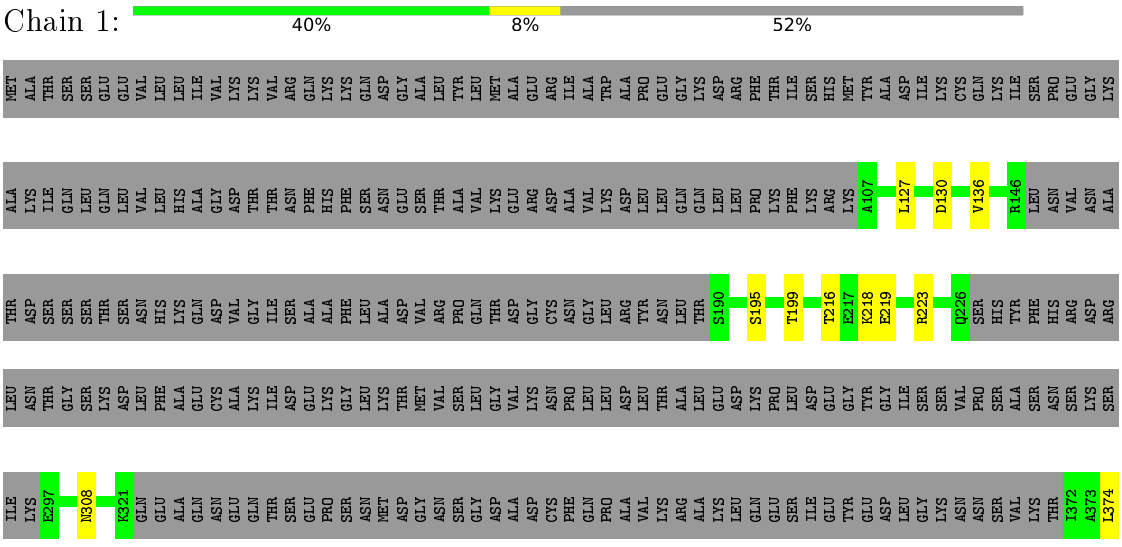
- Molecule 1: TFIIH basal transcription factor complex helicase XPD subunit

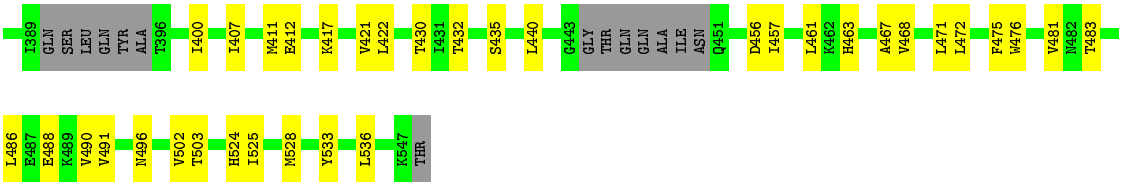
Chain 0:



- Molecule 2: General transcription factor IIH subunit 1

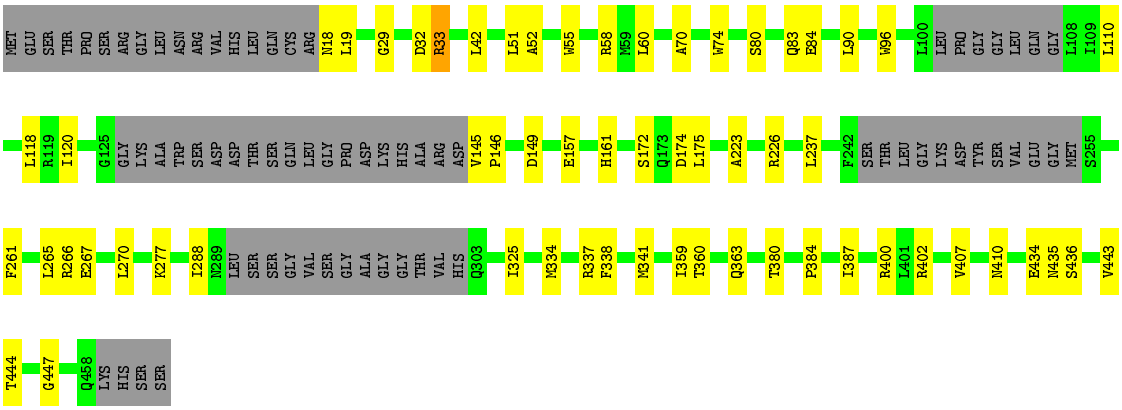
Chain 1:





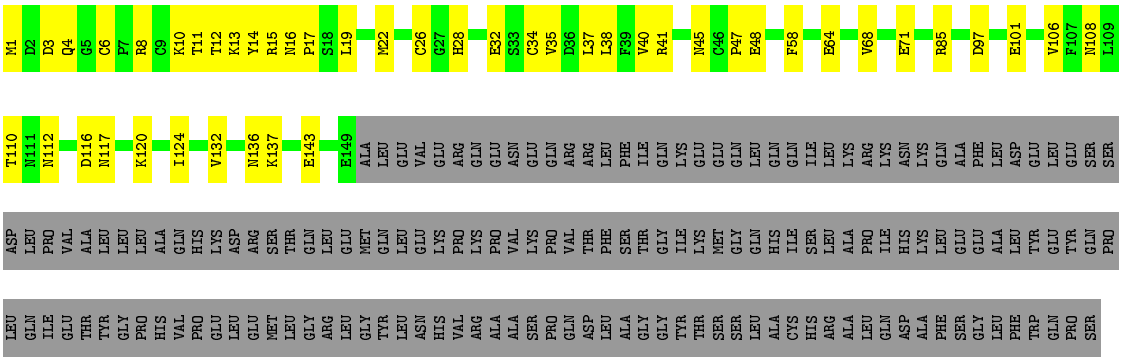
- Molecule 3: General transcription factor IIH subunit 4

Chain 2:



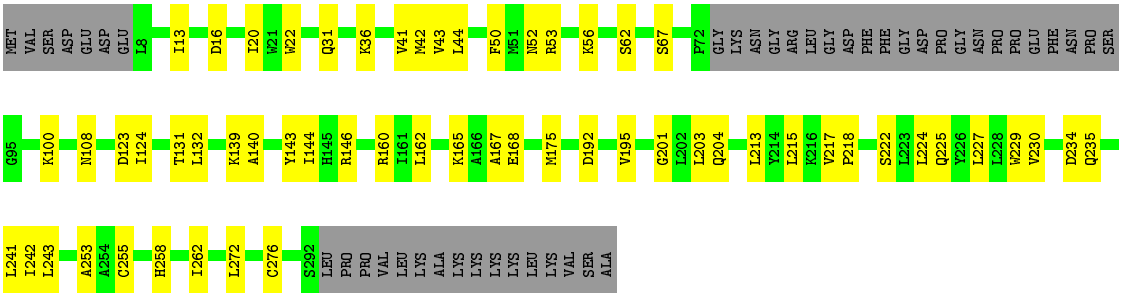
- Molecule 4: CDK-activating kinase assembly factor MAT1

Chain 3:



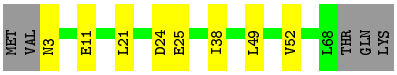
- Molecule 5: General transcription factor IIH subunit 3

Chain 4:



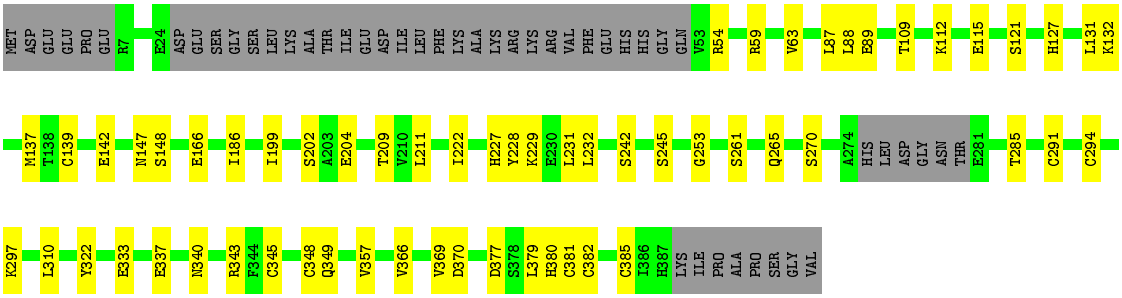
• Molecule 6: General transcription factor IIH subunit 5

Chain 5:



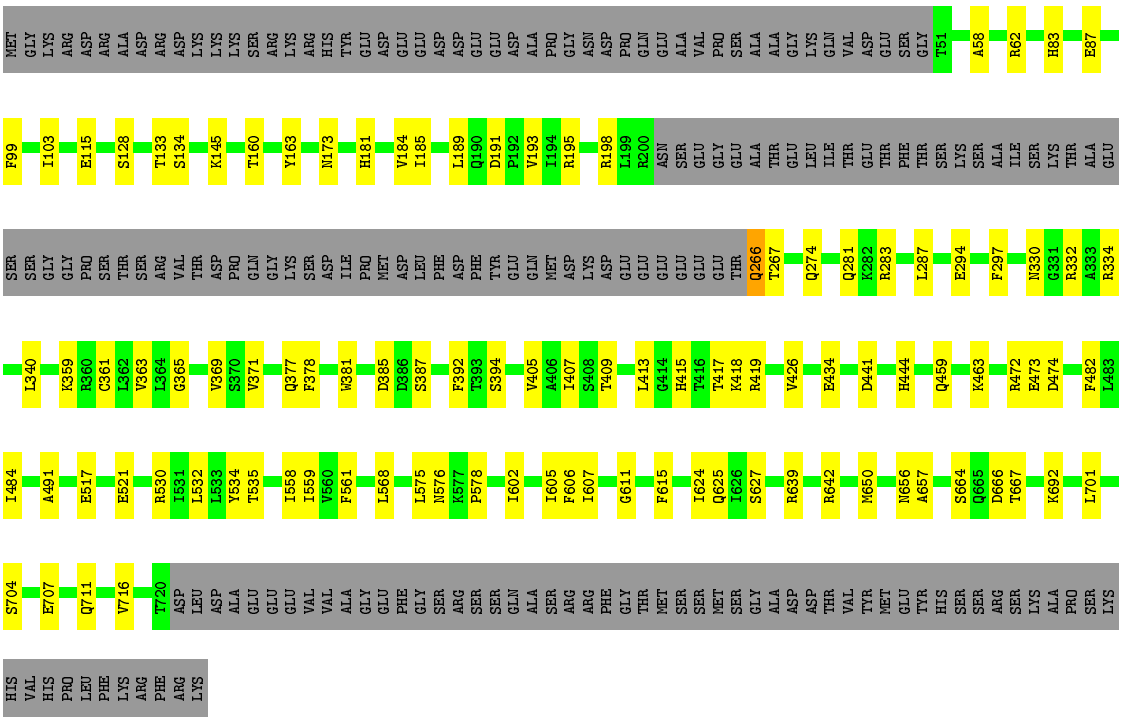
• Molecule 7: General transcription factor IIH subunit 2

Chain 6:



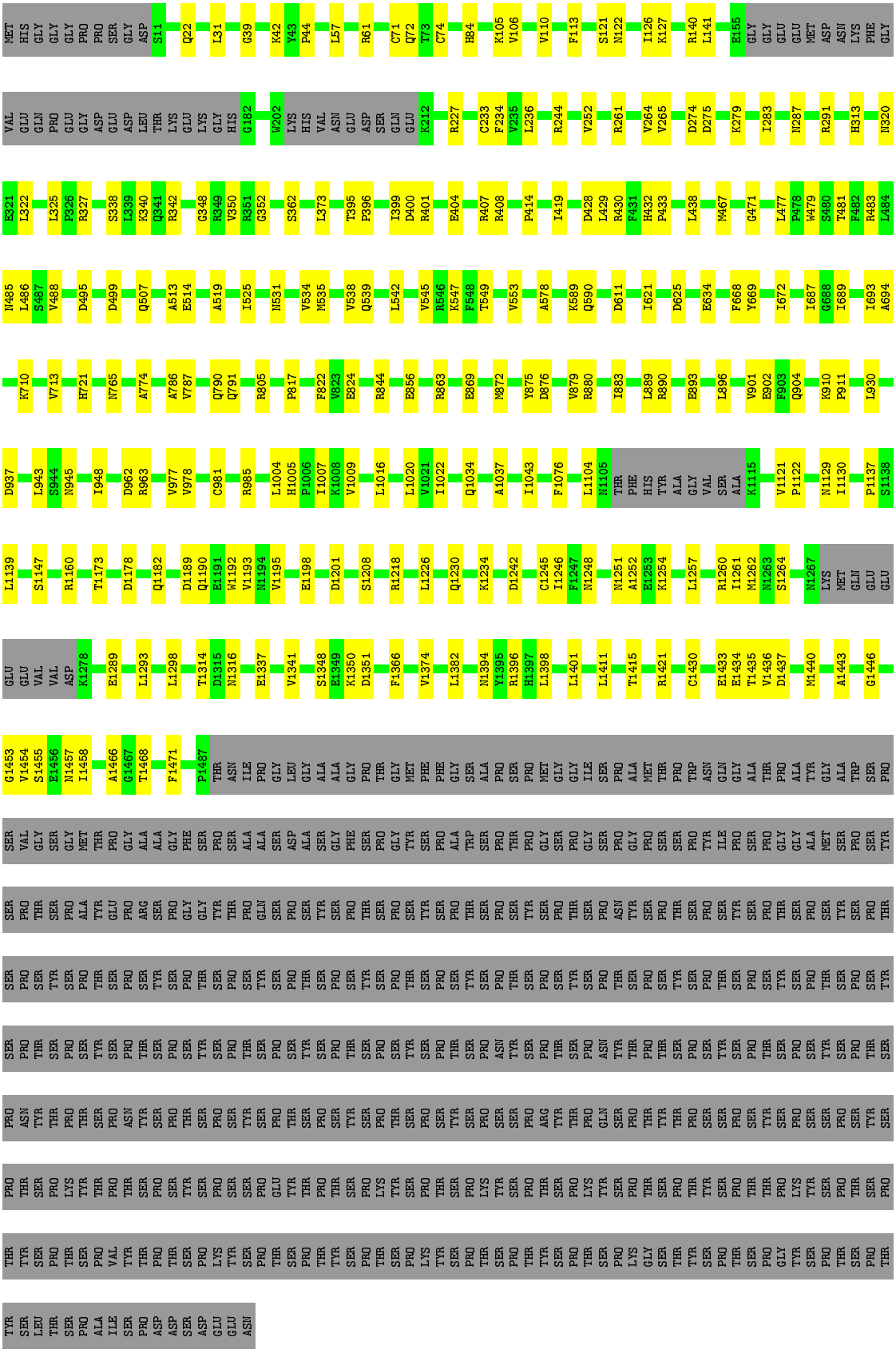
• Molecule 8: General transcription and DNA repair factor IIH helicase subunit XPB

Chain 7:



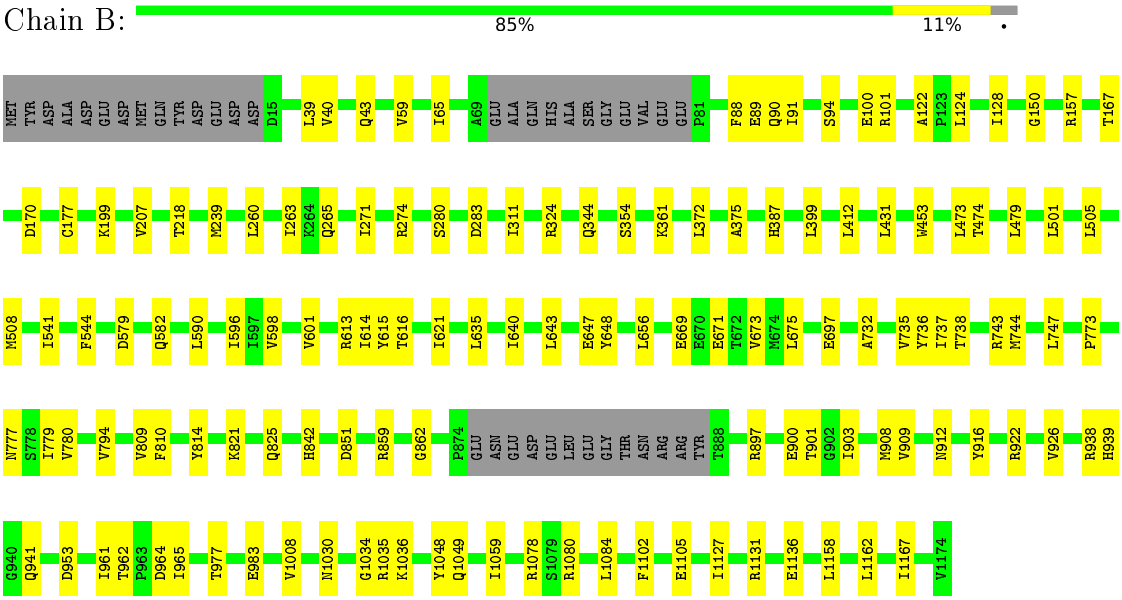
• Molecule 9: RPB1

Chain A:



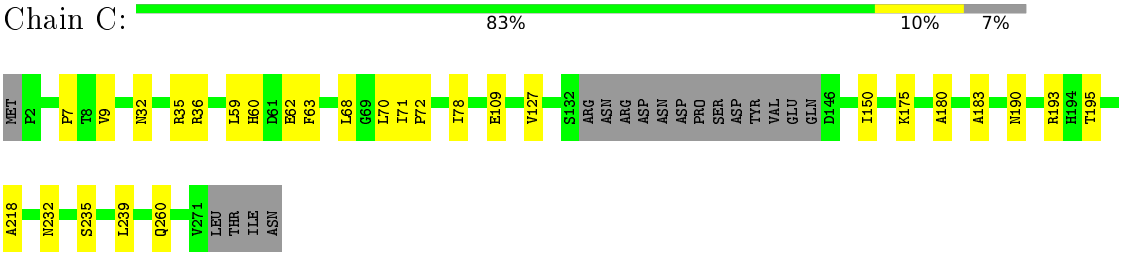
- Molecule 10: DNA-directed RNA polymerase subunit beta

Chain B:



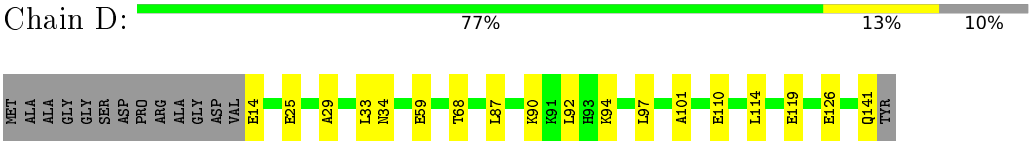
• Molecule 11: DNA-directed RNA polymerase II subunit RPB3

Chain C:



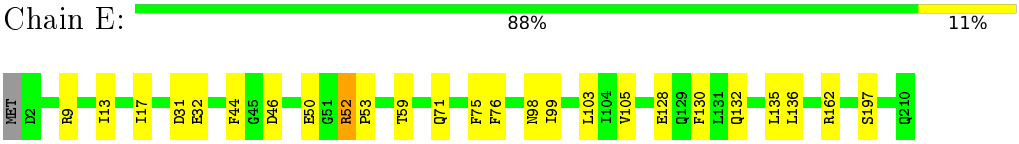
• Molecule 12: RPOL4c domain-containing protein

Chain D:



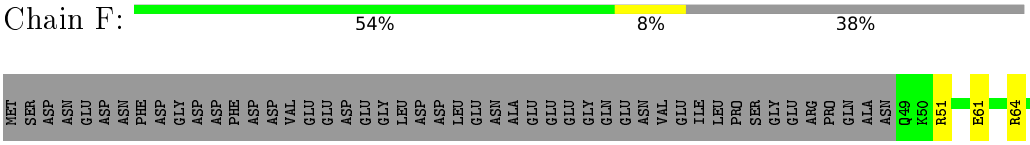
• Molecule 13: DNA-directed RNA polymerase II subunit E

Chain E:



• Molecule 14: DNA-directed RNA polymerase II subunit F

Chain F:

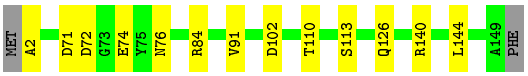


• Molecule 15: DNA-directed RNA polymerase II subunit RPB7

Chain G:

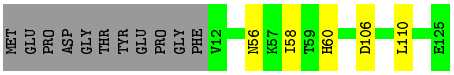
• Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



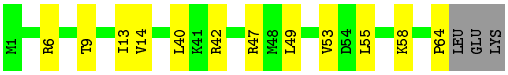
• Molecule 17: DNA-directed RNA polymerase II subunit RPB9

Chain I:



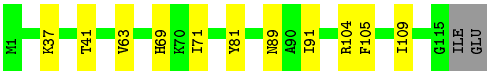
• Molecule 18: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



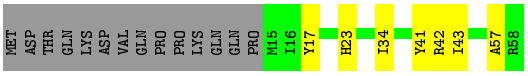
• Molecule 19: RNA_pol_L_2 domain-containing protein

Chain K:



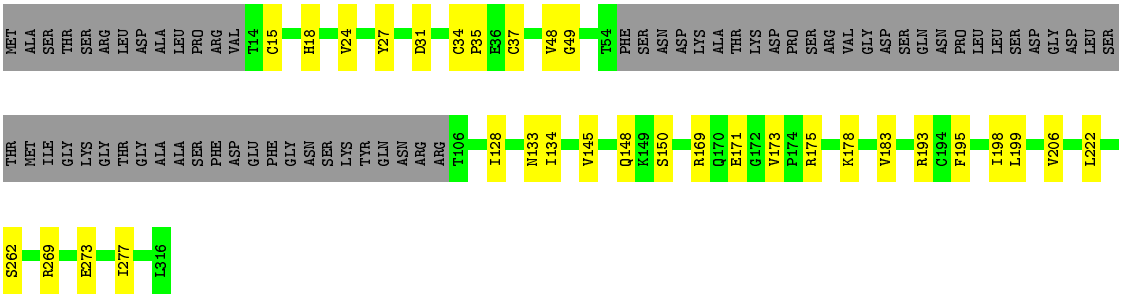
• Molecule 20: RNA polymerase II subunit K

Chain L:



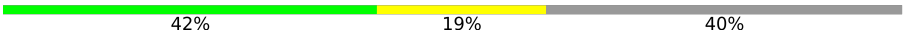
• Molecule 21: Transcription initiation factor IIB

Chain M:



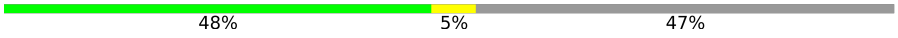
• Molecule 22: Non-template DNA

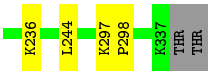
Chain N:



• Molecule 23: TATA-box-binding protein

Chain O:



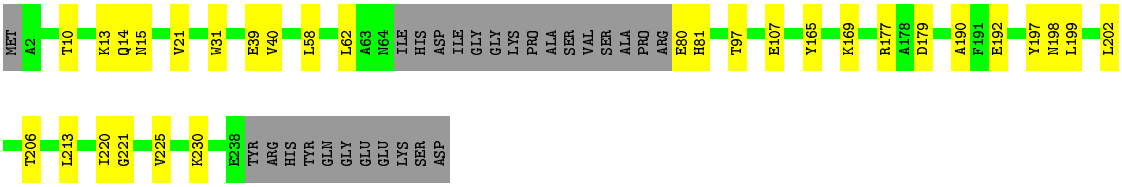


• Molecule 24: General transcription factor IIF subunit 1

Chain Q:

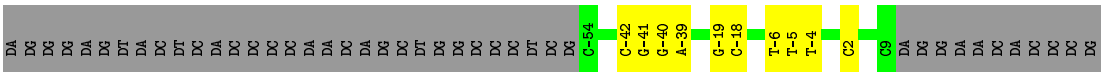
• Molecule 25: General transcription factor IIF subunit 2

Chain R:



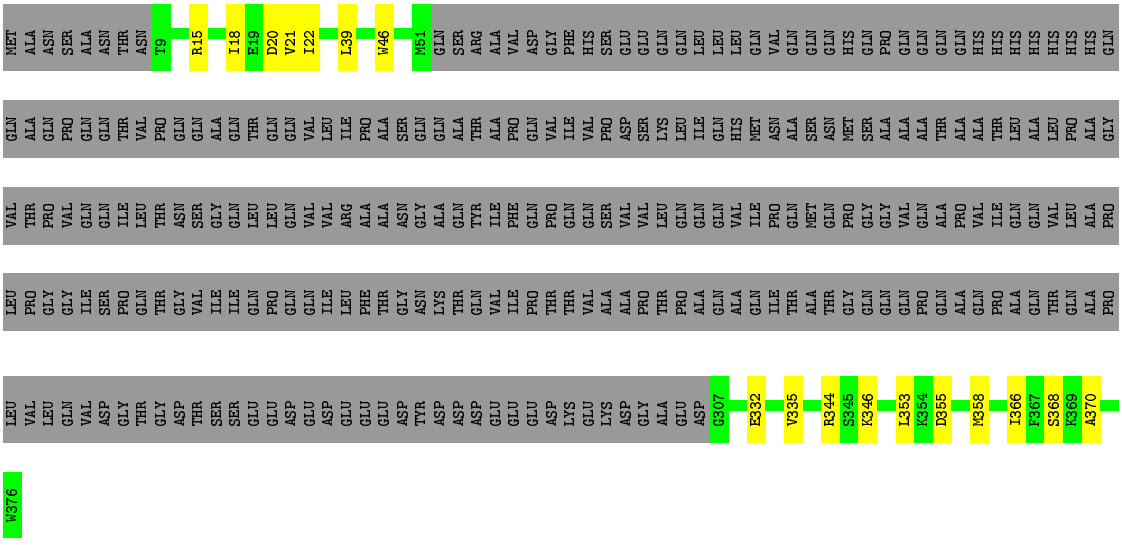
• Molecule 26: Template DNA

Chain T:



• Molecule 27: Transcription initiation factor IIA subunit 1

Chain U:

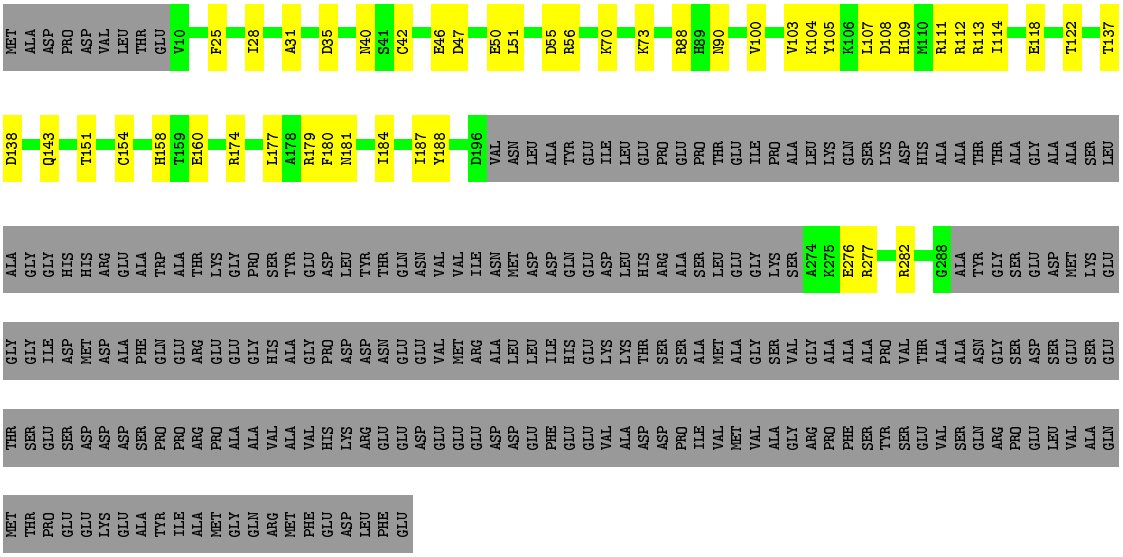


• Molecule 28: Transcription initiation factor IIA subunit 2

Chain V:

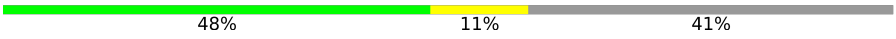
• Molecule 29: General transcription factor IIE subunit 1

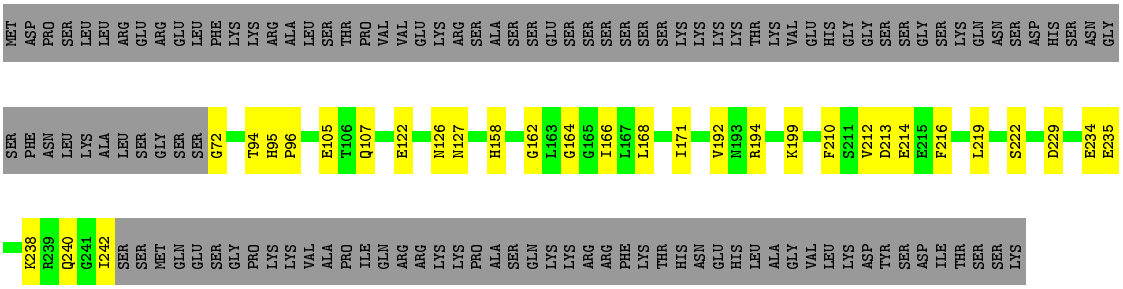
Chain W:



• Molecule 30: Transcription initiation factor IIE subunit beta

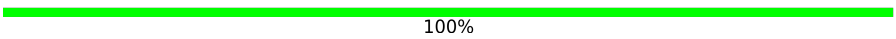
Chain X:





• Molecule 31: Unassigned peptide, likely TFIIE-beta

Chain Y:



There are no outlier residues recorded for this chain.

• Molecule 32: Unassigned peptide, likely XPB

Chain Z:

There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15226	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 ($e^-/Å^2$)	41.1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, SF4

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	0	0.25	0/5875	0.41	0/7955
2	1	0.25	0/2210	0.40	0/2975
3	2	0.26	0/3230	0.42	0/4376
4	3	0.27	0/1241	0.44	0/1665
5	4	0.28	0/2103	0.46	0/2846
6	5	0.24	0/529	0.40	0/714
7	6	0.24	0/2793	0.41	0/3780
8	7	0.24	0/4994	0.40	0/6745
9	A	0.24	0/11479	0.41	0/15496
10	B	0.24	0/9257	0.41	0/12493
11	C	0.24	0/2102	0.42	0/2857
12	D	0.24	0/1064	0.37	0/1428
13	E	0.24	0/1752	0.41	0/2366
14	F	0.23	0/646	0.40	0/871
15	G	0.25	0/1382	0.41	0/1874
16	H	0.24	0/1207	0.44	0/1628
17	I	0.23	0/949	0.44	0/1284
18	J	0.25	0/516	0.40	0/696
19	K	0.25	0/939	0.39	0/1271
20	L	0.30	0/378	0.42	0/500
21	M	0.24	0/1983	0.41	0/2679
22	N	0.52	0/1478	0.89	0/2283
23	O	0.25	0/1448	0.42	0/1948
24	Q	0.24	0/1167	0.40	0/1576
25	R	0.24	0/1817	0.41	0/2445
26	T	0.53	0/1461	0.85	0/2249
27	U	0.23	0/945	0.42	0/1274
28	V	0.24	0/816	0.41	0/1105
29	W	0.27	0/1686	0.46	0/2266
30	X	0.25	0/1427	0.41	0/1916
All	All	0.26	0/68874	0.45	0/93561

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	5751	0	5794	109	0
2	1	2167	0	2175	36	0
3	2	3158	0	3213	45	0
4	3	1225	0	1224	48	0
5	4	2066	0	2098	50	0
6	5	523	0	530	8	0
7	6	2732	0	2698	45	0
8	7	4890	0	4949	68	0
9	A	11274	0	11406	160	0
10	B	9076	0	9116	90	0
11	C	2059	0	2007	25	0
12	D	1050	0	1033	12	0
13	E	1721	0	1737	20	0
14	F	636	0	665	10	0
15	G	1351	0	1358	11	0
16	H	1186	0	1147	8	0
17	I	928	0	859	5	0
18	J	507	0	523	15	0
19	K	920	0	942	11	0
20	L	373	0	378	7	0
21	M	1953	0	1987	20	0
22	N	1318	0	721	12	0
23	O	1422	0	1514	12	0
24	Q	1138	0	1103	6	0
25	R	1788	0	1819	19	0
26	T	1303	0	714	10	0
27	U	930	0	888	16	0
28	V	806	0	818	13	0
29	W	1659	0	1665	60	0
30	X	1403	0	1428	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	Y	95	0	24	0	0
32	Z	40	0	10	0	0
33	0	8	0	0	0	0
34	3	2	0	0	0	0
34	4	2	0	0	0	0
34	6	3	0	0	0	0
34	A	2	0	0	0	0
34	B	1	0	0	0	0
34	C	1	0	0	0	0
34	I	2	0	0	0	0
34	J	1	0	0	0	0
34	L	1	0	0	0	0
34	M	1	0	0	0	0
34	W	1	0	0	0	0
35	A	1	0	0	0	0
All	All	67474	0	66543	854	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (854) 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)
5:4:255:CYS:SG	5:4:258:HIS:ND1	2.34	1.00
4:3:11:THR:HA	29:W:111:ARG:CZ	1.92	0.99
3:2:120:ILE:O	5:4:100:LYS:NZ	2.06	0.87
1:0:571:THR:OG1	1:0:573:ASP:OD1	1.93	0.86
5:4:62:SER:OG	5:4:132:LEU:O	1.95	0.84
13:E:46:ASP:O	13:E:52:ARG:NH1	2.10	0.84
29:W:100:VAL:HG22	29:W:104:LYS:NZ	1.93	0.83
29:W:100:VAL:HG22	29:W:104:LYS:HZ3	1.43	0.82
10:B:274:ARG:NH1	10:B:311:ILE:O	2.12	0.82
2:1:430:THR:OG1	5:4:222:SER:OG	1.98	0.82
5:4:255:CYS:HG	5:4:258:HIS:HD1	1.24	0.81
4:3:85:ARG:NH2	4:3:143:GLU:OE1	2.14	0.81
9:A:911:PRO:O	9:A:963:ARG:NH2	2.13	0.81
11:C:193:ARG:NH2	11:C:218:ALA:O	2.15	0.80
30:X:240:GLN:NE2	30:X:242:ILE:HG23	1.97	0.79
9:A:113:PHE:O	9:A:227:ARG:NH1	2.15	0.79
8:7:266:GLN:HE21	8:7:266:GLN:N	1.79	0.79
11:C:36:ARG:NH1	19:K:41:THR:OG1	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:722:ARG:NH2	7:6:202:SER:OG	2.16	0.78
9:A:535:MET:O	9:A:669:TYR:OH	1.99	0.78
10:B:953:ASP:OD1	11:C:36:ARG:NH2	2.17	0.77
10:B:344:GLN:NE2	10:B:354:SER:O	2.17	0.77
10:B:777:ASN:O	18:J:47:ARG:NH1	2.17	0.77
15:G:30:LEU:HD22	15:G:70:VAL:HG11	1.67	0.77
5:4:56:LYS:NZ	5:4:143:TYR:OH	2.18	0.76
9:A:39:GLY:O	9:A:42:LYS:NZ	2.18	0.76
5:4:140:ALA:O	5:4:144:ILE:HD12	1.85	0.76
1:0:711:ASP:OD1	1:0:715:GLN:NE2	2.17	0.75
2:1:503:THR:HG1	2:1:533:TYR:HH	1.23	0.75
14:F:100:ARG:NH2	14:F:121:ASP:O	2.19	0.75
9:A:513:ALA:HB2	14:F:90:LEU:HD21	1.68	0.75
23:O:191:GLU:OE2	23:O:203:ARG:NH2	2.18	0.75
9:A:373:LEU:O	9:A:485:ASN:ND2	2.19	0.75
16:H:102:ASP:OD2	16:H:110:THR:OG1	2.04	0.75
9:A:481:THR:O	9:A:483:ARG:NH1	2.20	0.75
4:3:8:ARG:O	29:W:181:ASN:ND2	2.19	0.74
6:5:24:ASP:OD1	6:5:25:GLU:N	2.20	0.74
9:A:1005:HIS:CD2	9:A:1007:ILE:HG22	2.22	0.74
9:A:322:LEU:O	9:A:327:ARG:NH2	2.20	0.74
2:1:195:SER:O	2:1:199:THR:OG1	2.04	0.74
10:B:814:TYR:OH	10:B:900:GLU:OE1	2.06	0.74
5:4:67:SER:O	5:4:139:LYS:NZ	2.19	0.74
8:7:371:VAL:HG23	8:7:407:ILE:HG22	1.68	0.73
10:B:821:LYS:O	10:B:825:GLN:NE2	2.21	0.73
10:B:794:VAL:HG13	10:B:965:ILE:HG23	1.69	0.73
13:E:9:ARG:O	13:E:13:ILE:HD12	1.89	0.73
1:0:571:THR:OG1	1:0:576:GLU:OE1	2.07	0.73
1:0:252:THR:HG22	1:0:432:ILE:HG22	1.72	0.72
29:W:108:ASP:OD1	29:W:109:HIS:N	2.22	0.72
3:2:29:GLY:O	3:2:33:ARG:NE	2.21	0.72
9:A:1411:LEU:O	9:A:1421:ARG:NH2	2.22	0.72
4:3:15:ARG:O	30:X:240:GLN:NE2	2.21	0.72
29:W:51:LEU:HD22	30:X:162:GLY:O	1.88	0.71
9:A:22:GLN:NE2	9:A:1446:GLY:O	2.23	0.71
1:0:231:VAL:HG13	1:0:454:VAL:HG23	1.71	0.71
10:B:613:ARG:NH1	10:B:615:TYR:OH	2.24	0.71
9:A:1234:LYS:NZ	9:A:1298:LEU:O	2.24	0.70
10:B:909:VAL:HG12	20:L:34:ILE:HD13	1.73	0.70
23:O:186:ARG:NH1	23:O:244:LEU:O	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:120:LYS:O	4:3:124:ILE:HD12	1.91	0.70
9:A:1178:ASP:OD2	9:A:1260:ARG:NH2	2.24	0.70
4:3:38:LEU:HD21	4:3:47:PRO:HD3	1.72	0.70
8:7:611:GLY:O	8:7:642:ARG:NH2	2.25	0.70
15:G:153:ASP:OD2	29:W:143:GLN:NE2	2.25	0.70
5:4:272:LEU:O	5:4:272:LEU:HD23	1.90	0.69
10:B:387:HIS:NE2	10:B:671:GLU:OE2	2.26	0.69
1:0:637:LEU:HD11	1:0:648:GLU:HA	1.74	0.69
2:1:468:VAL:HG21	2:1:525:ILE:HD11	1.74	0.69
8:7:394:SER:OG	26:T:-41:DG:OP2	2.04	0.69
12:D:90:LYS:NZ	12:D:126:GLU:OE2	2.26	0.69
4:3:40:VAL:HG22	29:W:122:THR:CB	2.23	0.69
5:4:160:ARG:NH2	5:4:234:ASP:OD1	2.24	0.69
9:A:227:ARG:NH2	30:X:229:ASP:OD2	2.26	0.68
16:H:74:GLU:OE1	16:H:76:ASN:ND2	2.26	0.68
1:0:60:GLN:OE1	1:0:61:ARG:NH1	2.26	0.68
8:7:191:ASP:O	8:7:195:ARG:NH1	2.25	0.68
9:A:1182:GLN:O	9:A:1190:GLN:NE2	2.26	0.68
3:2:400:ARG:NH2	8:7:666:ASP:OD2	2.27	0.68
29:W:118:GLU:OE1	29:W:174:ARG:NH1	2.25	0.68
19:K:81:TYR:OH	19:K:89:ASN:OD1	2.11	0.68
9:A:869:GLU:OE1	9:A:1455:SER:OG	2.12	0.68
1:0:72:TYR:OH	1:0:234:ASP:OD2	2.12	0.68
10:B:128:ILE:HG21	10:B:431:LEU:HD21	1.75	0.68
4:3:40:VAL:HG22	29:W:122:THR:HB	1.76	0.68
11:C:180:ALA:O	18:J:42:ARG:NH2	2.27	0.67
3:2:410:ASN:O	6:5:3:ASN:N	2.28	0.67
9:A:122:ASN:O	9:A:127:LYS:NZ	2.27	0.67
7:6:377:ASP:O	7:6:380:HIS:NE2	2.27	0.67
8:7:419:ARG:NH2	26:T:-42:DC:O3'	2.26	0.67
9:A:408:ARG:NH1	9:A:414:PRO:O	2.28	0.66
13:E:52:ARG:HD3	13:E:53:PRO:HD3	1.76	0.66
3:2:60:LEU:HD13	3:2:118:LEU:HD23	1.78	0.66
9:A:710:LYS:NZ	9:A:824:GLU:OE1	2.22	0.66
7:6:137:MET:SD	7:6:139:CYS:N	2.68	0.66
7:6:63:VAL:HG11	7:6:88:LEU:HD11	1.78	0.66
23:O:206:GLU:OE1	23:O:236:LYS:NZ	2.28	0.66
1:0:382:LEU:O	1:0:385:THR:OG1	2.11	0.66
9:A:233:CYS:SG	9:A:244:ARG:NH1	2.69	0.66
4:3:106:VAL:O	4:3:110:THR:HG23	1.95	0.65
8:7:701:LEU:O	8:7:704:SER:OG	2.13	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:O:185:LEU:O	28:V:66:ARG:NH2	2.29	0.65
29:W:114:ILE:O	29:W:118:GLU:HG2	1.96	0.65
1:0:238:ASN:ND2	1:0:662:GLN:OE1	2.28	0.65
5:4:43:VAL:HG11	5:4:224:LEU:HD21	1.79	0.65
8:7:287:LEU:HD23	8:7:287:LEU:O	1.97	0.65
8:7:330:ASN:OD1	8:7:334:ARG:NH2	2.30	0.65
9:A:893:GLU:OE1	13:E:197:SER:OG	2.05	0.65
2:1:432:THR:O	2:1:435:SER:OG	2.11	0.65
10:B:101:ARG:NH2	21:M:171:GLU:O	2.30	0.65
29:W:100:VAL:HA	29:W:103:VAL:HG22	1.79	0.65
29:W:107:LEU:HD13	29:W:188:TYR:CE1	2.32	0.65
29:W:276:GLU:OE2	29:W:282:ARG:NH1	2.29	0.64
30:X:158:HIS:ND1	30:X:164:GLY:O	2.31	0.64
5:4:168:GLU:N	5:4:168:GLU:OE1	2.30	0.64
8:7:266:GLN:HG2	8:7:267:THR:HG23	1.80	0.64
9:A:348:GLY:O	9:A:352:GLY:N	2.30	0.64
1:0:44:SER:OG	1:0:46:THR:O	2.12	0.64
8:7:128:SER:HG	8:7:163:TYR:HH	1.43	0.64
3:2:172:SER:OG	3:2:174:ASP:OD1	2.14	0.64
4:3:11:THR:O	29:W:111:ARG:NE	2.30	0.64
29:W:113:ARG:NE	30:X:219:LEU:HD11	2.13	0.64
18:J:64:PRO:O	20:L:23:HIS:NE2	2.31	0.64
24:Q:142:ASN:OD1	24:Q:143:TRP:N	2.31	0.64
7:6:242:SER:O	7:6:245:SER:OG	2.15	0.64
23:O:208:ARG:NH2	27:U:346:LYS:O	2.31	0.64
29:W:105:TYR:O	29:W:108:ASP:OD1	2.15	0.64
10:B:643:LEU:HD11	10:B:656:LEU:HD11	1.80	0.64
4:3:11:THR:HA	29:W:111:ARG:NE	2.12	0.63
8:7:371:VAL:HG23	8:7:407:ILE:CG2	2.29	0.63
15:G:54:ILE:HD13	15:G:70:VAL:HG13	1.80	0.63
18:J:14:VAL:HG13	18:J:49:LEU:HD11	1.81	0.63
1:0:343:ARG:O	1:0:346:VAL:HG12	1.99	0.63
1:0:2:LYS:HB3	1:0:9:LEU:HD11	1.80	0.62
9:A:1248:ASN:ND2	9:A:1254:LYS:O	2.31	0.62
9:A:1173:THR:OG1	17:I:56:ASN:OD1	2.15	0.62
28:V:57:ASN:OD1	28:V:58:PHE:N	2.33	0.62
6:5:49:LEU:HD12	6:5:52:VAL:CG1	2.29	0.62
7:6:87:LEU:HD22	7:6:232:LEU:HD12	1.81	0.62
8:7:281:GLN:NE2	8:7:482:PHE:O	2.33	0.62
9:A:621:ILE:HG23	9:A:621:ILE:O	2.00	0.62
8:7:473:GLU:N	8:7:473:GLU:OE1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:851:ASP:OD2	20:L:17:TYR:OH	2.17	0.61
2:1:130:ASP:OD2	2:1:463:HIS:NE2	2.33	0.61
1:0:335:ARG:NH1	4:3:71:GLU:OE2	2.33	0.61
1:0:609:ASP:OD1	1:0:669:ARG:NH2	2.34	0.61
7:6:112:LYS:O	7:6:147:ASN:ND2	2.33	0.61
13:E:71:GLN:HB2	13:E:99:ILE:HD12	1.81	0.61
12:D:34:ASN:O	12:D:68:THR:OG1	2.18	0.61
10:B:601:VAL:HG22	10:B:616:THR:HG23	1.82	0.61
9:A:31:LEU:HD22	9:A:252:VAL:HG13	1.83	0.61
9:A:261:ARG:HD2	9:A:261:ARG:O	2.01	0.61
28:V:62:LEU:HA	28:V:76:LEU:HD23	1.83	0.61
1:0:628:THR:O	1:0:628:THR:HG22	2.01	0.60
1:0:461:LEU:HD23	1:0:464:LEU:CD2	2.32	0.60
10:B:1035:ARG:NH1	10:B:1036:LYS:O	2.34	0.60
9:A:668:PHE:CZ	9:A:672:ILE:HD11	2.36	0.60
7:6:379:LEU:HD22	7:6:381:CYS:O	2.01	0.60
1:0:664:VAL:HG22	1:0:677:MET:HG2	1.84	0.60
9:A:350:VAL:HG21	9:A:1435:THR:HG21	1.84	0.60
10:B:862:GLY:O	10:B:1078:ARG:NH2	2.34	0.60
9:A:904:GLN:N	9:A:977:VAL:O	2.32	0.60
1:0:405:THR:O	1:0:409:THR:OG1	2.15	0.60
10:B:747:LEU:HD22	10:B:810:PHE:HZ	1.66	0.60
21:M:273:GLU:O	21:M:277:ILE:HD12	2.02	0.60
30:X:234:GLU:OE1	30:X:238:LYS:NZ	2.29	0.60
8:7:415:HIS:NE2	8:7:417:THR:OG1	2.33	0.60
3:2:265:LEU:CD1	3:2:270:LEU:HD12	2.31	0.60
10:B:669:GLU:O	10:B:673:VAL:HG23	2.01	0.60
1:0:462:SER:OG	1:0:463:PRO:HD2	2.02	0.60
9:A:1005:HIS:HD2	9:A:1007:ILE:HG22	1.66	0.60
9:A:1382:LEU:HD23	9:A:1398:LEU:HD13	1.84	0.60
10:B:157:ARG:NH2	10:B:177:CYS:O	2.34	0.60
1:0:372:LEU:HD11	1:0:404:ALA:HB1	1.84	0.59
3:2:18:ASN:OD1	3:2:19:LEU:N	2.35	0.59
9:A:668:PHE:CE1	9:A:672:ILE:HD11	2.36	0.59
10:B:100:GLU:OE1	20:L:42:ARG:NH1	2.35	0.59
2:1:422:LEU:HD22	5:4:225:GLN:HE22	1.66	0.59
2:1:471:LEU:HD12	2:1:472:LEU:HD22	1.84	0.59
9:A:57:LEU:O	9:A:261:ARG:NH2	2.36	0.59
25:R:192:GLU:OE2	30:X:72:GLY:N	2.36	0.59
8:7:625:GLN:OE1	8:7:639:ARG:NH1	2.34	0.59
10:B:65:ILE:HD11	10:B:412:LEU:HG	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:103:LEU:HD11	13:E:130:PHE:CD2	2.37	0.59
4:3:15:ARG:NH1	29:W:108:ASP:O	2.35	0.59
4:3:37:LEU:HD12	29:W:118:GLU:HB3	1.85	0.59
11:C:7:PRO:O	19:K:104:ARG:NH1	2.35	0.59
5:4:195:VAL:HG12	5:4:203:LEU:HD23	1.85	0.59
2:1:417:LYS:HA	2:1:421:VAL:HG23	1.84	0.59
5:4:52:ASN:OD1	5:4:53:ARG:N	2.36	0.59
7:6:357:VAL:HG13	7:6:366:VAL:HG23	1.83	0.58
17:I:60:HIS:O	17:I:60:HIS:ND1	2.36	0.58
29:W:151:THR:OG1	29:W:160:GLU:OE2	2.18	0.58
4:3:19:LEU:HD22	4:3:32:GLU:HB2	1.86	0.58
1:0:262:ASN:O	1:0:266:LEU:HD23	2.04	0.58
8:7:189:LEU:O	8:7:195:ARG:NH1	2.36	0.58
3:2:58:ARG:HD2	5:4:229:TRP:CE3	2.38	0.58
4:3:4:GLN:HE22	4:3:10:LYS:HE3	1.68	0.58
7:6:345:CYS:O	7:6:349:GLN:N	2.35	0.58
30:X:166:ILE:HG21	30:X:171:ILE:HD11	1.85	0.58
3:2:55:TRP:CZ2	3:2:83:GLN:NE2	2.72	0.58
11:C:78:ILE:HG21	11:C:127:VAL:HG22	1.85	0.58
1:0:606:GLU:O	1:0:666:ARG:NH2	2.37	0.58
9:A:1314:THR:OG1	9:A:1316:ASN:OD1	2.07	0.58
2:1:422:LEU:HD22	5:4:225:GLN:NE2	2.19	0.58
8:7:266:GLN:N	8:7:266:GLN:NE2	2.50	0.58
14:F:51:ARG:NH2	14:F:117:ASP:O	2.33	0.58
26:T:-5:DT:H73	26:T:-4:DT:H72	1.86	0.58
1:0:513:ASP:OD1	1:0:516:VAL:N	2.29	0.57
9:A:1443:ALA:HB2	10:B:1167:ILE:HG23	1.86	0.57
13:E:31:ASP:OD1	13:E:32:GLU:N	2.37	0.57
25:R:190:ALA:O	25:R:197:TYR:OH	2.10	0.57
7:6:337:GLU:O	7:6:340:ASN:ND2	2.36	0.57
12:D:14:GLU:N	12:D:14:GLU:OE1	2.37	0.57
27:U:20:ASP:OD2	28:V:51:ARG:NH2	2.37	0.57
3:2:266:ARG:HE	3:2:277:LYS:HZ2	1.53	0.57
4:3:8:ARG:NE	4:3:48:GLU:OE2	2.37	0.57
1:0:240:ASP:OD1	1:0:241:ASN:N	2.36	0.57
5:4:241:LEU:HD23	5:4:243:LEU:HD11	1.86	0.57
8:7:707:GLU:O	8:7:711:GLN:OE1	2.23	0.57
9:A:477:LEU:HD12	9:A:483:ARG:HD3	1.87	0.57
7:6:261:SER:OG	7:6:265:GLN:O	2.22	0.57
10:B:265:GLN:OE1	10:B:324:ARG:NH1	2.38	0.57
29:W:107:LEU:HD13	29:W:188:TYR:HE1	1.66	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:926:VAL:HG21	11:C:62:GLU:HG3	1.87	0.57
7:6:121:SER:OG	7:6:127:HIS:NE2	2.34	0.57
21:M:133:ASN:OD1	21:M:134:ILE:N	2.37	0.57
27:U:18:ILE:HD11	27:U:46:TRP:CZ3	2.40	0.57
28:V:29:THR:HG23	28:V:32:LEU:H	1.70	0.57
4:3:15:ARG:HH12	29:W:108:ASP:HB2	1.69	0.56
12:D:110:GLU:O	12:D:114:LEU:HD23	2.05	0.56
21:M:128:ILE:HG23	21:M:183:VAL:HG11	1.86	0.56
9:A:72:GLN:N	9:A:72:GLN:OE1	2.37	0.56
9:A:549:THR:O	9:A:589:LYS:NZ	2.35	0.56
7:6:227:HIS:CE1	7:6:231:LEU:HD11	2.40	0.56
9:A:1382:LEU:HD23	9:A:1398:LEU:CD1	2.35	0.56
9:A:902:GLU:OE2	9:A:985:ARG:NH2	2.38	0.56
5:4:16:ASP:OD1	5:4:131:THR:OG1	2.16	0.56
10:B:901:THR:HG23	10:B:901:THR:O	2.06	0.56
4:3:15:ARG:HH11	29:W:112:ARG:HG3	1.71	0.56
25:R:10:THR:O	25:R:14:GLN:OE1	2.24	0.56
2:1:486:LEU:O	2:1:490:VAL:HG23	2.05	0.56
8:7:87:GLU:OE2	8:7:145:LYS:NZ	2.38	0.56
8:7:361:CYS:SG	8:7:405:VAL:HG13	2.46	0.56
9:A:287:ASN:OD1	9:A:291:ARG:NH2	2.39	0.56
11:C:68:LEU:HA	11:C:71:ILE:HD12	1.87	0.56
12:D:87:LEU:HB3	12:D:97:LEU:HD22	1.88	0.56
1:0:420:PRO:HA	1:0:431:PRO:HB3	1.88	0.55
1:0:462:SER:HG	1:0:654:PHE:HD1	1.54	0.55
11:C:9:VAL:HG11	19:K:105:PHE:CD1	2.41	0.55
5:4:215:LEU:HD22	5:4:230:VAL:HG21	1.88	0.55
7:6:59:ARG:NH2	7:6:166:GLU:OE1	2.39	0.55
11:C:9:VAL:HG11	19:K:105:PHE:HD1	1.70	0.55
8:7:444:HIS:O	8:7:472:ARG:NH1	2.39	0.55
30:X:105:GLU:O	30:X:107:GLN:NE2	2.39	0.55
9:A:395:THR:HG22	9:A:396:PRO:HD2	1.88	0.55
22:N:5:DA:H2	23:O:169:VAL:HG21	1.72	0.55
2:1:456:ASP:OD1	2:1:457:ILE:HD12	2.05	0.55
21:M:262:SER:OG	21:M:269:ARG:N	2.38	0.55
23:O:169:VAL:HG22	23:O:222:THR:HG22	1.89	0.55
29:W:25:PHE:CE2	30:X:212:VAL:HG21	2.42	0.55
1:0:17:ILE:HD11	1:0:22:PHE:CZ	2.42	0.55
10:B:598:VAL:CG2	10:B:601:VAL:HG23	2.37	0.55
10:B:735:VAL:HG21	18:J:55:LEU:CD1	2.37	0.55
15:G:30:LEU:O	15:G:34:VAL:HG22	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Q:43:ASN:OD1	24:Q:44:GLN:N	2.40	0.55
3:2:265:LEU:HD12	3:2:270:LEU:HD12	1.89	0.54
1:0:365:VAL:HG22	1:0:365:VAL:O	2.07	0.54
1:0:664:VAL:HG21	1:0:679:PHE:CE1	2.40	0.54
21:M:173:VAL:O	21:M:175:ARG:NH1	2.41	0.54
27:U:332:GLU:N	27:U:332:GLU:OE1	2.40	0.54
4:3:38:LEU:HD22	4:3:45:ASN:O	2.06	0.54
10:B:40:VAL:O	10:B:40:VAL:HG22	2.07	0.54
3:2:42:LEU:HD13	5:4:50:PHE:CE1	2.42	0.54
3:2:402:ARG:NH1	6:5:11:GLU:OE2	2.41	0.54
27:U:355:ASP:N	27:U:368:SER:O	2.40	0.54
1:0:309:VAL:HG12	1:0:309:VAL:O	2.07	0.54
9:A:106:VAL:O	9:A:110:VAL:HG12	2.07	0.54
13:E:103:LEU:HD11	13:E:130:PHE:CE2	2.43	0.54
22:N:10:DG:OP1	25:R:177:ARG:NE	2.40	0.54
5:4:44:LEU:HD21	5:4:162:LEU:HD13	1.89	0.54
7:6:54:ARG:NH2	7:6:245:SER:O	2.41	0.54
8:7:377:GLN:OE1	8:7:381:TRP:NE1	2.41	0.54
11:C:175:LYS:NZ	20:L:57:ALA:O	2.39	0.54
19:K:105:PHE:CD2	19:K:109:ILE:HD11	2.43	0.54
9:A:1226:LEU:HD23	9:A:1230:GLN:HE21	1.72	0.54
12:D:59:GLU:OE1	12:D:59:GLU:N	2.38	0.54
3:2:80:SER:O	3:2:84:GLU:OE1	2.26	0.53
2:1:127:LEU:HD12	2:1:467:ALA:HA	1.90	0.53
19:K:63:VAL:HG23	19:K:63:VAL:O	2.09	0.53
8:7:418:LYS:NZ	26:T:-40:DG:OP2	2.40	0.53
10:B:738:THR:HG21	18:J:58:LYS:HG3	1.88	0.53
1:0:80:ILE:HD11	1:0:206:VAL:HB	1.89	0.53
5:4:195:VAL:CG1	5:4:203:LEU:HD23	2.39	0.53
9:A:467:MET:HG2	9:A:534:VAL:HG11	1.90	0.53
29:W:154:CYS:O	29:W:158:HIS:N	2.40	0.53
30:X:240:GLN:HE21	30:X:242:ILE:HG23	1.70	0.53
1:0:488:VAL:HG23	1:0:488:VAL:O	2.09	0.53
5:4:258:HIS:HE1	5:4:276:CYS:SG	2.31	0.53
7:6:88:LEU:CD2	7:6:131:LEU:HD21	2.38	0.53
10:B:344:GLN:O	10:B:361:LYS:NZ	2.41	0.53
5:4:44:LEU:HD22	5:4:227:LEU:HB3	1.90	0.53
8:7:181:HIS:O	8:7:184:VAL:HG12	2.09	0.53
8:7:664:SER:O	8:7:667:THR:OG1	2.27	0.53
9:A:1382:LEU:HD21	9:A:1401:LEU:HD23	1.91	0.53
20:L:41:TYR:CE2	20:L:43:ILE:HB	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R:97:THR:OG1	25:R:107:GLU:OE2	2.17	0.53
2:1:412:GLU:N	2:1:412:GLU:OE1	2.42	0.53
8:7:568:LEU:HD11	8:7:606:PHE:HB3	1.90	0.53
9:A:805:ARG:NH2	10:B:671:GLU:O	2.42	0.53
1:0:289:VAL:HG22	1:0:324:ARG:NH1	2.23	0.53
1:0:393:ASP:OD1	1:0:394:PHE:N	2.42	0.53
3:2:32:ASP:OD1	3:2:33:ARG:N	2.42	0.53
1:0:28:LEU:HD22	1:0:55:LEU:HD23	1.90	0.53
4:3:35:VAL:HG13	4:3:58:PHE:CE2	2.43	0.53
29:W:100:VAL:C	29:W:104:LYS:HZ3	2.13	0.53
29:W:277:ARG:O	29:W:282:ARG:NH1	2.41	0.52
1:0:77:VAL:HG11	1:0:114:ASN:ND2	2.24	0.52
9:A:1289:GLU:OE2	9:A:1293:LEU:HD11	2.09	0.52
9:A:1208:SER:O	9:A:1260:ARG:NH1	2.43	0.52
9:A:1454:VAL:HG12	9:A:1458:ILE:HD12	1.91	0.52
10:B:280:SER:OG	10:B:283:ASP:OD2	2.27	0.52
24:Q:173:HIS:O	24:Q:176:ILE:HG22	2.10	0.52
1:0:709:THR:HG22	1:0:710:VAL:N	2.25	0.52
8:7:463:LYS:O	8:7:484:ILE:HG23	2.09	0.52
11:C:72:PRO:HG3	18:J:13:ILE:HD11	1.92	0.52
9:A:141:LEU:HD12	9:A:236:LEU:O	2.10	0.52
9:A:945:ASN:HD21	9:A:948:ILE:HD12	1.75	0.52
9:A:1218:ARG:NH2	9:A:1252:ALA:O	2.43	0.52
2:1:136:VAL:HG11	2:1:502:VAL:HG12	1.92	0.52
4:3:34:CYS:O	4:3:37:LEU:HB3	2.10	0.52
8:7:363:VAL:HG21	8:7:378:PHE:HE2	1.75	0.52
10:B:842:HIS:CD2	21:M:24:VAL:HG13	2.45	0.51
10:B:938:ARG:NH2	10:B:983:GLU:OE2	2.41	0.51
4:3:32:GLU:OE1	4:3:32:GLU:N	2.41	0.51
9:A:400:ASP:OD1	9:A:401:ARG:N	2.42	0.51
9:A:634:GLU:OE2	16:H:140:ARG:NH2	2.40	0.51
10:B:501:LEU:HD12	10:B:505:LEU:HD12	1.93	0.51
21:M:178:LYS:NZ	26:T:2:DC:OP1	2.42	0.51
4:3:6:CYS:O	4:3:10:LYS:HB3	2.10	0.51
8:7:340:LEU:HD23	8:7:491:ALA:HB2	1.92	0.51
9:A:105:LYS:HD3	9:A:141:LEU:HD22	1.92	0.51
16:H:91:VAL:HG22	16:H:144:LEU:HD23	1.92	0.51
5:4:242:ILE:C	5:4:243:LEU:HD12	2.31	0.51
8:7:578:PRO:HG3	8:7:602:ILE:HD11	1.93	0.51
9:A:875:TYR:OH	14:F:61:GLU:OE2	2.15	0.51
27:U:353:LEU:HD21	27:U:370:ALA:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:83:HIS:ND1	8:7:115:GLU:OE2	2.44	0.51
9:A:1020:LEU:HD22	9:A:1076:PHE:CG	2.45	0.51
10:B:735:VAL:HG21	18:J:55:LEU:HD13	1.93	0.51
19:K:105:PHE:CE2	19:K:109:ILE:HD11	2.46	0.51
21:M:27:TYR:HA	21:M:48:VAL:HG11	1.93	0.51
7:6:87:LEU:HD11	7:6:229:LYS:CG	2.41	0.51
16:H:2:ALA:O	16:H:84:ARG:NH2	2.43	0.51
24:Q:153:ARG:NH1	24:Q:180:ARG:O	2.44	0.51
1:0:377:GLU:N	1:0:377:GLU:OE1	2.45	0.50
7:6:87:LEU:HD11	7:6:229:LYS:HG2	1.91	0.50
9:A:578:ALA:N	9:A:590:GLN:OE1	2.43	0.50
13:E:103:LEU:HD12	13:E:128:GLU:HB2	1.93	0.50
29:W:40:ASN:ND2	29:W:42:CYS:O	2.44	0.50
9:A:507:GLN:N	10:B:1105:GLU:OE2	2.42	0.50
8:7:363:VAL:HG21	8:7:378:PHE:CE2	2.47	0.50
9:A:432:HIS:NE2	21:M:35:PRO:O	2.40	0.50
9:A:1192:TRP:HZ3	9:A:1246:ILE:HG22	1.76	0.50
10:B:736:TYR:CE2	10:B:737:ILE:HG22	2.46	0.50
12:D:119:GLU:N	12:D:119:GLU:OE1	2.44	0.50
3:2:435:ASN:ND2	6:5:38:ILE:O	2.44	0.50
1:0:3:LEU:O	1:0:9:LEU:HD12	2.11	0.50
1:0:115:LEU:HD13	1:0:191:PRO:HB2	1.94	0.50
9:A:1160:ARG:NH2	9:A:1350:LYS:O	2.45	0.50
2:1:503:THR:OG1	2:1:533:TYR:OH	2.01	0.50
7:6:112:LYS:N	7:6:142:GLU:O	2.40	0.50
10:B:743:ARG:O	10:B:922:ARG:NH1	2.45	0.50
18:J:40:LEU:CD1	18:J:49:LEU:HD13	2.41	0.50
2:1:524:HIS:ND1	7:6:270:SER:OG	2.39	0.50
7:6:87:LEU:HD13	7:6:228:TYR:HD2	1.77	0.50
10:B:635:LEU:HD21	10:B:640:ILE:HD11	1.94	0.50
2:1:471:LEU:HD13	2:1:475:PHE:HE2	1.76	0.50
2:1:481:VAL:HG23	2:1:483:THR:HG23	1.94	0.50
3:2:174:ASP:OD1	3:2:175:LEU:N	2.45	0.50
4:3:11:THR:HA	29:W:111:ARG:NH2	2.26	0.50
12:D:29:ALA:O	12:D:94:LYS:NZ	2.22	0.50
1:0:437:CYS:SG	1:0:438:MET:N	2.85	0.49
4:3:12:THR:HG22	4:3:19:LEU:HD12	1.93	0.49
9:A:1189:ASP:O	9:A:1193:VAL:HG23	2.11	0.49
12:D:25:GLU:OE2	15:G:78:ARG:NH2	2.45	0.49
7:6:204:GLU:OE1	7:6:209:THR:OG1	2.30	0.49
2:1:374:LEU:HD12	2:1:374:LEU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:369:VAL:HG11	8:7:615:PHE:HA	1.94	0.49
9:A:1251:ASN:OD1	9:A:1252:ALA:N	2.45	0.49
27:U:21:VAL:HG21	28:V:40:PHE:CD1	2.47	0.49
11:C:190:ASN:ND2	11:C:195:THR:O	2.42	0.49
29:W:88:ARG:NH1	29:W:90:ASN:OD1	2.45	0.49
29:W:187:ILE:HD11	30:X:210:PHE:CZ	2.47	0.49
4:3:15:ARG:HH22	29:W:108:ASP:HB2	1.77	0.49
5:4:146:ARG:NH2	7:6:348:CYS:O	2.46	0.49
8:7:274:GLN:OE1	8:7:459:GLN:NE2	2.46	0.49
1:0:310:LEU:HG	1:0:409:THR:HG21	1.95	0.49
2:1:471:LEU:HD13	2:1:475:PHE:CE2	2.48	0.49
10:B:1059:ILE:O	10:B:1080:ARG:NH2	2.46	0.49
13:E:44:PHE:HB3	13:E:52:ARG:HG3	1.94	0.49
3:2:58:ARG:HD2	5:4:229:TRP:HE3	1.76	0.49
3:2:338:PHE:N	3:2:341:MET:O	2.45	0.49
4:3:12:THR:CG2	4:3:19:LEU:HD12	2.43	0.49
9:A:44:PRO:O	9:A:57:LEU:HD12	2.13	0.49
9:A:362:SER:HB2	10:B:1084:LEU:HD12	1.94	0.49
11:C:70:LEU:O	18:J:6:ARG:NE	2.43	0.49
15:G:39:THR:O	15:G:43:GLY:N	2.43	0.49
1:0:81:GLU:O	1:0:84:ILE:HG22	2.12	0.49
5:4:31:GLN:OE1	5:4:36:LYS:NZ	2.42	0.49
1:0:126:PHE:CE2	1:0:128:LYS:HB2	2.48	0.49
1:0:637:LEU:HD13	1:0:651:PHE:CD2	2.48	0.49
8:7:650:MET:SD	8:7:656:ASN:ND2	2.83	0.49
11:C:59:LEU:HD13	11:C:63:PHE:CE2	2.48	0.49
1:0:284:GLU:HA	1:0:287:ARG:HG2	1.94	0.48
1:0:284:GLU:HG2	1:0:385:THR:HG21	1.94	0.48
3:2:172:SER:OG	3:2:267:GLU:OE2	2.14	0.48
1:0:52:LEU:HD21	1:0:232:VAL:HG11	1.95	0.48
9:A:141:LEU:O	9:A:141:LEU:HD23	2.13	0.48
25:R:198:ASN:OD1	25:R:199:LEU:N	2.46	0.48
21:M:34:CYS:HB3	21:M:37:CYS:HB3	1.95	0.48
7:6:253:GLY:N	7:6:310:LEU:HD21	2.28	0.48
8:7:418:LYS:HD2	26:T:-40:DG:P	2.54	0.48
9:A:872:MET:HE2	9:A:1466:ALA:HA	1.95	0.48
25:R:179:ASP:OD1	25:R:179:ASP:N	2.45	0.48
11:C:235:SER:OG	11:C:239:LEU:O	2.25	0.48
25:R:13:LYS:O	25:R:15:ASN:ND2	2.46	0.48
1:0:136:SER:O	1:0:142:VAL:HG21	2.13	0.48
5:4:13:ILE:HD13	5:4:41:VAL:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:192:ASP:OD1	5:4:213:LEU:N	2.45	0.48
29:W:70:LYS:O	29:W:73:LYS:NZ	2.45	0.48
1:0:118:HIS:HB3	1:0:121:VAL:HG22	1.94	0.48
1:0:243:CYS:SG	1:0:443:ALA:HB3	2.54	0.48
7:6:285:THR:O	7:6:297:LYS:NZ	2.46	0.48
9:A:930:LEU:HD12	9:A:943:LEU:HD21	1.96	0.48
1:0:115:LEU:HD12	1:0:115:LEU:O	2.14	0.48
6:5:49:LEU:HD12	6:5:52:VAL:HG11	1.95	0.48
22:N:52:DC:H4'	22:N:53:DT:OP1	2.13	0.48
3:2:261:PHE:O	3:2:265:LEU:HD23	2.13	0.48
3:2:360:THR:HG22	3:2:363:GLN:OE1	2.13	0.48
9:A:404:GLU:O	9:A:407:ARG:HG2	2.14	0.48
27:U:18:ILE:HD11	27:U:46:TRP:CH2	2.48	0.48
30:X:235:GLU:HA	30:X:238:LYS:HZ3	1.78	0.48
4:3:37:LEU:O	4:3:40:VAL:HG12	2.14	0.48
9:A:479:TRP:HB2	9:A:483:ARG:NH2	2.29	0.48
21:M:169:ARG:NH2	21:M:206:VAL:HG23	2.29	0.48
2:1:440:LEU:HD11	5:4:218:PRO:CD	2.43	0.47
5:4:20:ILE:HD12	5:4:20:ILE:H	1.79	0.47
8:7:575:LEU:O	8:7:576:ASN:OD1	2.32	0.47
1:0:28:LEU:O	1:0:32:LEU:HD23	2.14	0.47
4:3:132:VAL:O	4:3:136:ASN:ND2	2.47	0.47
29:W:118:GLU:OE2	29:W:177:LEU:CD1	2.61	0.47
9:A:549:THR:O	9:A:549:THR:HG22	2.15	0.47
8:7:605:ILE:HD12	8:7:607:ILE:HD11	1.96	0.47
2:1:422:LEU:HD13	5:4:225:GLN:NE2	2.29	0.47
9:A:395:THR:CG2	9:A:396:PRO:HD2	2.44	0.47
10:B:59:VAL:HG21	10:B:91:ILE:HD11	1.97	0.47
27:U:353:LEU:HD23	27:U:353:LEU:H	1.79	0.47
1:0:45:GLY:O	1:0:48:LYS:NZ	2.48	0.47
1:0:563:ARG:NH2	7:6:142:GLU:OE1	2.48	0.47
4:3:14:TYR:CD1	29:W:111:ARG:NH2	2.83	0.47
5:4:255:CYS:SG	5:4:258:HIS:CE1	3.05	0.47
9:A:471:GLY:N	9:A:519:ALA:O	2.42	0.47
9:A:611:ASP:N	9:A:611:ASP:OD1	2.48	0.47
9:A:1016:LEU:O	9:A:1020:LEU:HG	2.14	0.47
13:E:59:THR:HG22	13:E:75:PHE:HA	1.96	0.47
22:N:45:DT:C2	22:N:46:DC:C5	3.02	0.47
25:R:97:THR:HG23	25:R:107:GLU:CG	2.45	0.47
29:W:113:ARG:CD	30:X:219:LEU:HD11	2.43	0.47
1:0:460:THR:HB	1:0:661:ALA:HB1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:121:SER:HA	9:A:126:ILE:HG21	1.97	0.47
9:A:279:LYS:O	9:A:283:ILE:HG12	2.15	0.47
9:A:514:GLU:OE1	10:B:1102:PHE:N	2.44	0.47
9:A:904:GLN:NE2	9:A:981:CYS:O	2.44	0.47
5:4:123:ASP:OD1	5:4:124:ILE:N	2.45	0.47
11:C:260:GLN:HB2	19:K:91:ILE:HG21	1.97	0.47
22:N:23:DT:H2'	22:N:24:DT:H72	1.97	0.47
9:A:429:LEU:CD2	9:A:438:LEU:HD22	2.45	0.47
30:X:168:LEU:N	30:X:199:LYS:O	2.45	0.47
30:X:240:GLN:HE22	30:X:242:ILE:HG23	1.74	0.47
8:7:173:ASN:N	8:7:434:GLU:OE2	2.47	0.46
10:B:473:LEU:HD23	10:B:474:THR:HG23	1.96	0.46
29:W:100:VAL:CG2	29:W:104:LYS:HZ3	2.19	0.46
29:W:113:ARG:HE	30:X:219:LEU:HD11	1.80	0.46
3:2:337:ARG:O	8:7:62:ARG:NH1	2.47	0.46
9:A:1139:LEU:CD1	9:A:1341:VAL:HA	2.45	0.46
9:A:1262:MET:SD	9:A:1264:SER:OG	2.72	0.46
10:B:747:LEU:HD22	10:B:810:PHE:CZ	2.48	0.46
11:C:78:ILE:HG21	11:C:127:VAL:CG2	2.44	0.46
5:4:255:CYS:HG	5:4:258:HIS:CE1	2.34	0.46
9:A:689:ILE:O	9:A:693:ILE:HG12	2.15	0.46
1:0:77:VAL:HA	1:0:80:ILE:HG22	1.96	0.46
1:0:137:LEU:O	1:0:142:VAL:HG11	2.15	0.46
3:2:334:MET:HB3	8:7:58:ALA:HB2	1.98	0.46
3:2:444:THR:HG23	3:2:447:GLY:H	1.80	0.46
9:A:340:LYS:HE2	9:A:1436:VAL:HG11	1.95	0.46
10:B:779:ILE:O	10:B:964:ASP:N	2.48	0.46
2:1:472:LEU:HD12	2:1:476:TRP:CD1	2.51	0.46
23:O:206:GLU:HB3	23:O:207:PRO:HD3	1.98	0.46
29:W:118:GLU:OE2	29:W:177:LEU:HD13	2.14	0.46
4:3:97:ASP:O	4:3:101:GLU:OE1	2.34	0.46
7:6:357:VAL:CG1	7:6:366:VAL:HG23	2.45	0.46
1:0:613:HIS:O	1:0:613:HIS:ND1	2.49	0.46
4:3:4:GLN:HE22	4:3:10:LYS:CE	2.29	0.46
6:5:38:ILE:HD12	6:5:38:ILE:H	1.80	0.46
7:6:88:LEU:HD22	7:6:131:LEU:HD21	1.98	0.46
9:A:1147:SER:OG	9:A:1351:ASP:OD2	2.17	0.46
10:B:738:THR:HG21	18:J:58:LYS:CG	2.46	0.46
9:A:320:ASN:N	9:A:338:SER:OG	2.49	0.46
9:A:486:LEU:HB3	9:A:538:VAL:HG21	1.98	0.46
29:W:55:ASP:OD1	30:X:194:ARG:NE	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:140:ARG:NH1	9:A:234:PHE:O	2.47	0.45
9:A:1137:PRO:HB2	9:A:1341:VAL:HG13	1.99	0.45
1:0:134:CYS:O	1:0:138:THR:HG22	2.15	0.45
1:0:361:LEU:O	1:0:365:VAL:HG12	2.16	0.45
9:A:1139:LEU:HD11	9:A:1341:VAL:HA	1.98	0.45
10:B:596:ILE:HG22	10:B:596:ILE:O	2.17	0.45
1:0:434:HIS:CB	1:0:632:ILE:HD11	2.47	0.45
8:7:656:ASN:OD1	8:7:657:ALA:N	2.50	0.45
12:D:141:GLN:OE1	12:D:141:GLN:N	2.49	0.45
29:W:28:ILE:HD11	30:X:192:VAL:HG22	1.98	0.45
1:0:111:SER:N	1:0:211:TYR:OH	2.49	0.45
3:2:52:ALA:HB1	3:2:90:LEU:HD21	1.98	0.45
5:4:42:MET:SD	5:4:108:ASN:ND2	2.89	0.45
5:4:44:LEU:HD21	5:4:162:LEU:CD1	2.46	0.45
9:A:863:ARG:NH2	9:A:1415:THR:HG23	2.31	0.45
10:B:961:ILE:HG23	18:J:9:THR:HG21	1.97	0.45
13:E:17:ILE:HD11	13:E:135:LEU:HD21	1.97	0.45
21:M:15:CYS:HB3	21:M:18:HIS:HB2	1.98	0.45
25:R:39:GLU:OE1	25:R:40:VAL:N	2.49	0.45
27:U:15:ARG:HA	27:U:18:ILE:HD12	1.99	0.45
1:0:617:ALA:HB2	1:0:676:LEU:HD21	1.98	0.45
3:2:407:VAL:N	3:2:443:VAL:O	2.48	0.45
7:6:199:ILE:CG2	7:6:222:ILE:HD11	2.47	0.45
9:A:1261:ILE:HG22	9:A:1262:MET:N	2.31	0.45
10:B:239:MET:HB2	10:B:372:LEU:HD21	1.98	0.45
10:B:271:ILE:HD11	10:B:311:ILE:HD13	1.97	0.45
10:B:1127:ILE:HD11	10:B:1136:GLU:OE2	2.17	0.45
1:0:107:LEU:HD12	1:0:195:ALA:HB1	1.99	0.45
5:4:13:ILE:HG21	5:4:41:VAL:HG13	1.98	0.45
5:4:201:GLY:O	5:4:204:GLN:HG2	2.17	0.45
8:7:294:GLU:OE2	8:7:334:ARG:NH1	2.49	0.45
9:A:1020:LEU:O	9:A:1034:GLN:NE2	2.50	0.45
9:A:1104:LEU:HD22	9:A:1122:PRO:HD2	1.98	0.45
10:B:39:LEU:HD13	10:B:479:LEU:HD13	1.98	0.45
10:B:780:VAL:HG11	10:B:1048:TYR:OH	2.16	0.45
22:N:38:DT:C6	22:N:39:DT:H72	2.51	0.45
29:W:100:VAL:HG22	29:W:104:LYS:HZ2	1.77	0.45
1:0:576:GLU:OE2	2:1:308:ASN:ND2	2.48	0.45
4:3:11:THR:CA	29:W:111:ARG:NE	2.80	0.45
26:T:-40:DG:H2"	26:T:-39:DA:C8	2.52	0.45
3:2:288:ILE:H	3:2:288:ILE:HD12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:15:ARG:NH1	29:W:112:ARG:NE	2.65	0.45
28:V:56:VAL:HG22	28:V:57:ASN:H	1.81	0.45
30:X:122:GLU:OE1	30:X:126:ASN:ND2	2.50	0.45
1:0:143:ARG:NH1	1:0:159:GLU:OE1	2.47	0.45
1:0:600:ALA:HB1	1:0:659:HIS:HD2	1.81	0.45
1:0:722:ARG:NH1	7:6:222:ILE:O	2.47	0.45
2:1:488:GLU:O	2:1:491:VAL:HG22	2.16	0.45
5:4:165:LYS:NZ	5:4:167:ALA:O	2.36	0.45
7:6:63:VAL:CG1	7:6:88:LEU:HD11	2.44	0.45
7:6:369:VAL:HG13	7:6:370:ASP:N	2.32	0.45
4:3:136:ASN:OD1	4:3:137:LYS:N	2.50	0.45
5:4:235:GLN:O	5:4:235:GLN:NE2	2.47	0.45
9:A:274:ASP:OD1	9:A:275:ASP:N	2.50	0.45
25:R:80:GLU:OE2	25:R:81:HIS:N	2.50	0.45
1:0:323:ILE:O	1:0:378:ARG:NH1	2.50	0.44
2:1:400:ILE:HD12	2:1:400:ILE:H	1.82	0.44
8:7:133:THR:HG23	8:7:134:SER:N	2.33	0.44
9:A:896:LEU:O	9:A:1396:ARG:NH1	2.50	0.44
9:A:962:ASP:HB3	9:A:1043:ILE:HG23	1.98	0.44
9:A:1468:THR:HG22	14:F:64:ARG:HD2	1.98	0.44
1:0:373:ARG:O	1:0:405:THR:OG1	2.28	0.44
2:1:457:ILE:HG22	2:1:461:LEU:HD13	1.99	0.44
4:3:1:MET:HB2	4:3:17:PRO:HB3	1.99	0.44
10:B:40:VAL:HG22	10:B:43:GLN:HB2	1.99	0.44
10:B:541:ILE:HG21	10:B:614:ILE:HG21	1.99	0.44
10:B:544:PHE:CZ	10:B:590:LEU:HD11	2.52	0.44
11:C:32:ASN:HA	11:C:35:ARG:HG2	1.98	0.44
29:W:184:ILE:HD12	29:W:187:ILE:HD13	2.00	0.44
1:0:285:TYR:O	1:0:289:VAL:HG23	2.17	0.44
8:7:185:ILE:HG22	8:7:189:LEU:HD13	1.98	0.44
9:A:786:ALA:O	9:A:787:VAL:HG23	2.17	0.44
10:B:207:VAL:HG11	10:B:375:ALA:CB	2.47	0.44
18:J:40:LEU:HD13	18:J:49:LEU:HD13	2.00	0.44
29:W:180:PHE:HB2	30:X:216:PHE:CE1	2.52	0.44
7:6:242:SER:N	7:6:245:SER:OG	2.50	0.44
9:A:713:VAL:HG11	9:A:817:PRO:HD3	1.99	0.44
9:A:1366:PHE:HB2	9:A:1374:VAL:HG21	1.98	0.44
7:6:89:GLU:OE2	7:6:132:LYS:NZ	2.38	0.44
10:B:88:PHE:CE1	10:B:128:ILE:HG23	2.51	0.44
10:B:94:SER:O	10:B:122:ALA:HB1	2.18	0.44
10:B:399:LEU:HB3	10:B:453:TRP:CZ3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:50:GLU:OE1	13:E:50:GLU:N	2.51	0.44
17:I:58:ILE:HD12	17:I:58:ILE:H	1.81	0.44
28:V:73:THR:HG22	28:V:73:THR:O	2.17	0.44
1:0:176:ASN:OD1	1:0:177:LEU:N	2.49	0.44
2:1:456:ASP:OD1	2:1:456:ASP:N	2.47	0.44
9:A:790:GLN:NE2	9:A:791:GLN:O	2.45	0.44
10:B:675:LEU:HD21	10:B:697:GLU:OE2	2.18	0.44
21:M:193:ARG:NE	22:N:2:DA:OP1	2.51	0.44
25:R:165:TYR:OH	25:R:169:LYS:NZ	2.44	0.44
27:U:366:ILE:HD11	28:V:48:LEU:HG	1.99	0.44
30:X:126:ASN:OD1	30:X:127:ASN:N	2.51	0.44
1:0:329:PHE:O	1:0:333:LEU:HD23	2.17	0.44
9:A:428:ASP:OD2	9:A:430:ARG:NH1	2.51	0.44
9:A:467:MET:SD	9:A:467:MET:N	2.91	0.44
9:A:693:ILE:HD11	10:B:1008:VAL:HG11	2.00	0.44
10:B:579:ASP:OD2	10:B:582:GLN:NE2	2.39	0.44
8:7:133:THR:HB	8:7:160:THR:HG21	2.00	0.44
1:0:225:LEU:O	1:0:227:ARG:NH1	2.51	0.43
9:A:872:MET:O	9:A:879:VAL:HA	2.18	0.43
10:B:780:VAL:HG21	10:B:1048:TYR:CZ	2.52	0.43
26:T:-19:DG:H2'	26:T:-18:DC:C5	2.54	0.43
30:X:95:HIS:ND1	30:X:96:PRO:O	2.46	0.43
1:0:109:LEU:HD12	1:0:207:TYR:CD2	2.53	0.43
5:4:253:ALA:O	5:4:262:ILE:N	2.43	0.43
29:W:113:ARG:NH2	30:X:222:SER:OG	2.51	0.43
1:0:345:ARG:NH2	4:3:64:GLU:OE1	2.52	0.43
7:6:382:CYS:HB3	7:6:385:CYS:HB3	1.99	0.43
8:7:184:VAL:HG13	8:7:185:ILE:N	2.33	0.43
9:A:721:HIS:ND1	17:I:110:LEU:HD11	2.33	0.43
13:E:52:ARG:CD	13:E:53:PRO:HD3	2.45	0.43
1:0:168:VAL:O	1:0:168:VAL:HG13	2.18	0.43
3:2:157:GLU:O	3:2:161:HIS:ND1	2.51	0.43
4:3:26:CYS:SG	4:3:28:HIS:HB2	2.59	0.43
9:A:547:LYS:O	9:A:553:VAL:HG21	2.18	0.43
9:A:693:ILE:HG22	9:A:694:ALA:N	2.33	0.43
9:A:1430:CYS:HB3	9:A:1435:THR:HG23	1.99	0.43
10:B:809:VAL:HG21	11:C:60:HIS:CE1	2.53	0.43
14:F:84:GLU:N	14:F:84:GLU:OE1	2.52	0.43
22:N:-1:DG:C4	22:N:0:DC:C5	3.06	0.43
22:N:35:DC:H2'	22:N:36:DT:H72	1.99	0.43
27:U:335:VAL:HG13	27:U:358:MET:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:U:353:LEU:CD2	27:U:370:ALA:HB3	2.48	0.43
3:2:51:LEU:HB3	3:2:55:TRP:CZ3	2.53	0.43
10:B:941:GLN:NE2	10:B:977:THR:OG1	2.47	0.43
13:E:44:PHE:HB3	13:E:52:ARG:HE	1.84	0.43
1:0:459:GLY:O	1:0:460:THR:OG1	2.24	0.43
1:0:462:SER:OG	1:0:463:PRO:CD	2.66	0.43
7:6:87:LEU:HD23	7:6:87:LEU:O	2.19	0.43
8:7:409:THR:O	8:7:413:LEU:HD13	2.19	0.43
9:A:1453:GLY:O	9:A:1457:ASN:ND2	2.43	0.43
10:B:89:GLU:HG2	10:B:90:GLN:N	2.33	0.43
10:B:263:ILE:HG23	10:B:324:ARG:O	2.18	0.43
13:E:44:PHE:CB	13:E:52:ARG:HE	2.31	0.43
21:M:31:ASP:N	21:M:31:ASP:OD1	2.49	0.43
25:R:220:ILE:HG13	25:R:221:GLY:H	1.83	0.43
29:W:137:THR:HG22	29:W:138:ASP:N	2.32	0.43
1:0:67:VAL:HG23	1:0:67:VAL:O	2.19	0.43
7:6:291:CYS:SG	7:6:294:CYS:N	2.81	0.43
9:A:325:LEU:O	9:A:327:ARG:NH2	2.51	0.43
23:O:212:LEU:HD11	26:T:-6:DT:O2	2.19	0.43
23:O:297:LYS:HB3	23:O:298:PRO:HD3	2.01	0.43
1:0:557:ILE:HG22	1:0:561:ILE:HD12	2.01	0.43
4:3:13:LYS:HD3	4:3:14:TYR:HD2	1.84	0.43
8:7:99:PHE:CZ	8:7:103:ILE:HD13	2.54	0.43
8:7:532:LEU:CD2	8:7:716:VAL:HG13	2.49	0.43
9:A:274:ASP:OD2	9:A:342:ARG:NH2	2.51	0.43
9:A:433:PRO:HA	9:A:438:LEU:HD11	1.99	0.43
12:D:33:LEU:HD22	12:D:101:ALA:HB3	2.00	0.43
24:Q:15:VAL:HG12	24:Q:16:VAL:N	2.33	0.43
2:1:524:HIS:NE2	2:1:528:MET:SD	2.92	0.43
8:7:532:LEU:HD23	8:7:532:LEU:O	2.19	0.43
10:B:773:PRO:CG	18:J:53:VAL:HG21	2.49	0.43
11:C:62:GLU:OE1	11:C:62:GLU:N	2.51	0.43
14:F:84:GLU:O	14:F:84:GLU:HG2	2.19	0.43
21:M:148:GLN:OE1	21:M:150:SER:OG	2.32	0.43
4:3:22:MET:HG3	4:3:35:VAL:HG21	2.01	0.43
6:5:21:LEU:O	6:5:24:ASP:OD1	2.37	0.43
9:A:876:ASP:OD2	9:A:880:ARG:NH2	2.52	0.43
9:A:1436:VAL:O	9:A:1440:MET:HG2	2.18	0.43
11:C:71:ILE:HD11	11:C:150:ILE:HG12	2.01	0.43
25:R:225:VAL:HG13	25:R:225:VAL:O	2.19	0.43
28:V:16:GLN:NE2	28:V:20:ASP:OD2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:354:PRO:HB2	1:0:355:PRO:HD3	2.00	0.42
9:A:485:ASN:O	9:A:488:VAL:HG22	2.18	0.42
17:I:106:ASP:N	17:I:106:ASP:OD1	2.51	0.42
4:3:11:THR:HB	29:W:111:ARG:HA	2.00	0.42
8:7:559:ILE:HG22	8:7:561:PHE:CE1	2.54	0.42
9:A:399:ILE:HG23	9:A:400:ASP:N	2.34	0.42
9:A:1436:VAL:HG13	9:A:1437:ASP:N	2.34	0.42
10:B:647:GLU:O	10:B:648:TYR:CG	2.72	0.42
14:F:69:ARG:NE	14:F:96:GLU:OE1	2.38	0.42
21:M:195:PHE:CZ	21:M:199:LEU:HD11	2.55	0.42
28:V:64:THR:HG22	28:V:65:TYR:N	2.33	0.42
1:0:133:LYS:O	1:0:137:LEU:HD23	2.19	0.42
1:0:332:PHE:CZ	1:0:367:ILE:HG23	2.54	0.42
1:0:338:GLU:HG2	4:3:68:VAL:HG11	2.01	0.42
19:K:37:LYS:N	19:K:69:HIS:O	2.51	0.42
29:W:47:ASP:O	29:W:51:LEU:HG	2.19	0.42
3:2:325:ILE:HD12	3:2:325:ILE:H	1.83	0.42
5:4:217:VAL:HG23	5:4:217:VAL:O	2.19	0.42
8:7:535:THR:HG23	8:7:627:SER:HB2	2.01	0.42
9:A:687:ILE:HD12	9:A:765:ASN:HB2	2.01	0.42
9:A:883:ILE:O	9:A:883:ILE:HG22	2.19	0.42
29:W:113:ARG:HD2	30:X:219:LEU:HD11	2.00	0.42
30:X:94:THR:HG22	30:X:94:THR:O	2.19	0.42
8:7:517:GLU:O	8:7:521:GLU:OE1	2.37	0.42
9:A:84:HIS:HD1	10:B:1127:ILE:HG22	1.85	0.42
10:B:218:THR:O	10:B:218:THR:HG23	2.20	0.42
13:E:76:PHE:CE2	13:E:105:VAL:HG21	2.54	0.42
30:X:213:ASP:OD2	30:X:214:GLU:N	2.52	0.42
1:0:49:THR:HG23	1:0:50:VAL:N	2.35	0.42
1:0:109:LEU:HD11	1:0:199:ILE:HD11	2.02	0.42
1:0:722:ARG:NH2	7:6:202:SER:HG	2.12	0.42
3:2:359:ILE:HG22	3:2:360:THR:N	2.35	0.42
4:3:116:ASP:OD1	4:3:117:ASN:N	2.51	0.42
9:A:1471:PHE:O	14:F:64:ARG:NH1	2.46	0.42
16:H:72:ASP:OD1	16:H:72:ASP:C	2.57	0.42
23:O:204:ILE:HD12	23:O:207:PRO:HG2	2.02	0.42
29:W:31:ALA:O	29:W:35:ASP:OD1	2.38	0.42
29:W:51:LEU:O	30:X:164:GLY:HA3	2.19	0.42
1:0:354:PRO:HA	1:0:416:ILE:HD12	2.02	0.42
1:0:531:VAL:HG12	1:0:532:PRO:O	2.20	0.42
3:2:261:PHE:CZ	3:2:265:LEU:HD21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:889:LEU:O	9:A:890:ARG:NH1	2.49	0.42
10:B:1162:LEU:HB3	10:B:1167:ILE:HB	2.02	0.42
24:Q:127:PHE:CE2	25:R:21:VAL:HG21	2.54	0.42
7:6:115:GLU:N	7:6:115:GLU:OE1	2.53	0.42
7:6:379:LEU:O	7:6:379:LEU:HD23	2.20	0.42
8:7:297:PHE:O	8:7:359:LYS:NZ	2.37	0.42
13:E:132:GLN:O	13:E:136:LEU:HG	2.19	0.42
15:G:43:GLY:HA2	15:G:157:ILE:HD12	2.02	0.42
16:H:113:SER:OG	16:H:126:GLN:HG2	2.19	0.42
29:W:184:ILE:HG23	29:W:188:TYR:CE2	2.55	0.42
3:2:380:THR:HG23	3:2:380:THR:O	2.19	0.42
3:2:434:GLU:OE2	3:2:436:SER:N	2.53	0.42
4:3:108:ASN:OD1	4:3:112:ASN:HB3	2.20	0.42
8:7:193:VAL:HG11	8:7:283:ARG:HD3	2.02	0.42
9:A:264:VAL:HG12	9:A:265:VAL:N	2.35	0.42
9:A:817:PRO:HB2	9:A:822:PHE:HB3	2.01	0.42
10:B:909:VAL:HG12	20:L:34:ILE:CD1	2.47	0.42
3:2:384:PRO:HB2	3:2:387:ILE:HG12	2.02	0.42
8:7:385:ASP:OD2	8:7:387:SER:OG	2.28	0.42
9:A:1195:VAL:HA	9:A:1198:GLU:OE1	2.20	0.42
10:B:1030:ASN:O	10:B:1034:GLY:N	2.45	0.42
15:G:18:PHE:HA	15:G:22:LEU:HD12	2.01	0.42
15:G:34:VAL:HG21	15:G:48:VAL:CG2	2.50	0.42
23:O:168:ILE:N	23:O:224:ALA:O	2.53	0.42
10:B:167:THR:HG23	10:B:170:ASP:H	1.85	0.41
10:B:939:HIS:NE2	10:B:983:GLU:OE1	2.42	0.41
25:R:206:THR:HG21	25:R:213:LEU:HD13	2.01	0.41
29:W:46:GLU:O	29:W:50:GLU:HG2	2.20	0.41
29:W:109:HIS:O	29:W:109:HIS:ND1	2.53	0.41
1:0:28:LEU:HD22	1:0:55:LEU:CD2	2.49	0.41
9:A:1245:CYS:HB3	9:A:1257:LEU:HD21	2.02	0.41
1:0:195:ALA:O	1:0:199:ILE:HG12	2.20	0.41
3:2:96:TRP:HB3	3:2:110:LEU:HD23	2.03	0.41
7:6:333:GLU:HG2	7:6:333:GLU:O	2.20	0.41
9:A:531:ASN:ND2	9:A:531:ASN:O	2.53	0.41
16:H:71:ASP:OD1	16:H:72:ASP:N	2.53	0.41
28:V:82:ARG:NH1	28:V:83:GLU:O	2.54	0.41
29:W:179:ARG:HD2	30:X:216:PHE:CE2	2.55	0.41
3:2:70:ALA:HB1	3:2:74:TRP:CZ2	2.55	0.41
8:7:332:ARG:O	8:7:334:ARG:NH1	2.53	0.41
8:7:365:GLY:HA2	8:7:441:ASP:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:495:ASP:OD1	9:A:499:ASP:CG	2.58	0.41
13:E:98:ASN:O	13:E:99:ILE:HD13	2.20	0.41
25:R:31:TRP:CD1	25:R:62:LEU:HD21	2.55	0.41
4:3:15:ARG:O	4:3:16:ASN:HB3	2.20	0.41
9:A:589:LYS:NZ	9:A:625:ASP:OD2	2.33	0.41
9:A:1242:ASP:O	9:A:1262:MET:N	2.53	0.41
11:C:109:GLU:OE1	11:C:109:GLU:N	2.53	0.41
29:W:100:VAL:CG2	29:W:104:LYS:NZ	2.75	0.41
1:0:329:PHE:CZ	1:0:333:LEU:HD21	2.56	0.41
3:2:146:PRO:HA	3:2:149:ASP:OD2	2.20	0.41
9:A:542:LEU:O	9:A:545:VAL:HG12	2.19	0.41
9:A:937:ASP:N	9:A:937:ASP:OD1	2.54	0.41
9:A:1022:ILE:HD11	9:A:1076:PHE:CZ	2.55	0.41
9:A:1433:GLU:HG2	9:A:1434:GLU:N	2.36	0.41
9:A:1468:THR:HG23	14:F:64:ARG:HB2	2.03	0.41
22:N:43:DC:C2	22:N:44:DA:C8	3.09	0.41
1:0:12:PHE:CE2	1:0:14:TYR:HB2	2.56	0.41
1:0:56:ILE:HG21	1:0:70:LEU:HD22	2.01	0.41
2:1:496:ASN:HB3	2:1:536:LEU:HD11	2.02	0.41
3:2:237:LEU:HD21	3:2:261:PHE:HZ	1.86	0.41
4:3:3:ASP:O	4:3:13:LYS:HG3	2.21	0.41
9:A:1394:ASN:O	9:A:1398:LEU:HD23	2.21	0.41
10:B:744:MET:SD	10:B:908:MET:HG2	2.61	0.41
1:0:573:ASP:OD1	1:0:573:ASP:N	2.53	0.41
2:1:216:THR:HG22	2:1:218:LYS:H	1.86	0.41
2:1:422:LEU:HD21	5:4:224:LEU:HB3	2.02	0.41
3:2:223:ALA:HA	3:2:226:ARG:HG2	2.02	0.41
8:7:558:ILE:HG23	8:7:624:ILE:HD13	2.03	0.41
9:A:910:LYS:N	9:A:911:PRO:HD2	2.36	0.41
9:A:1337:GLU:N	9:A:1337:GLU:OE1	2.53	0.41
11:C:32:ASN:O	11:C:36:ARG:HG3	2.21	0.41
19:K:63:VAL:HG12	19:K:71:ILE:HG22	2.03	0.41
27:U:344:ARG:HD2	27:U:346:LYS:H	1.85	0.41
1:0:661:ALA:HA	1:0:664:VAL:HG12	2.02	0.41
7:6:109:THR:OG1	7:6:148:SER:OG	2.05	0.41
9:A:71:CYS:SG	9:A:74:CYS:HB2	2.61	0.41
9:A:350:VAL:HG22	10:B:1158:LEU:HD22	2.02	0.41
10:B:962:THR:O	18:J:9:THR:HG23	2.21	0.41
15:G:92:VAL:HG23	15:G:139:GLN:HG2	2.03	0.41
28:V:56:VAL:HG22	28:V:57:ASN:N	2.36	0.41
29:W:105:TYR:O	29:W:105:TYR:CD2	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:618:VAL:HG11	1:0:664:VAL:HA	2.02	0.41
3:2:118:LEU:HD11	5:4:50:PHE:CZ	2.56	0.41
8:7:193:VAL:HG11	8:7:283:ARG:CD	2.51	0.41
9:A:283:ILE:HD13	9:A:313:HIS:HB3	2.01	0.41
9:A:1004:LEU:HD21	9:A:1009:VAL:HG22	2.03	0.41
9:A:1201:ASP:OD1	9:A:1201:ASP:N	2.51	0.41
22:N:50:DG:H2'	22:N:51:DT:H72	2.03	0.41
25:R:202:LEU:O	25:R:206:THR:HG22	2.21	0.41
26:T:-5:DT:OP1	27:U:344:ARG:NH1	2.52	0.41
1:0:56:ILE:HD12	1:0:230:VAL:HG11	2.03	0.40
1:0:145:GLN:HG2	1:0:150:THR:HG22	2.03	0.40
1:0:604:VAL:O	1:0:608:ILE:HG22	2.20	0.40
2:1:219:GLU:O	2:1:223:ARG:HG2	2.21	0.40
2:1:411:MET:HG2	2:1:411:MET:O	2.21	0.40
9:A:483:ARG:HD2	9:A:483:ARG:N	2.36	0.40
9:A:525:ILE:O	9:A:534:VAL:HG12	2.21	0.40
9:A:539:GLN:HA	9:A:774:ALA:HB1	2.03	0.40
9:A:856:GLU:OE1	9:A:1121:VAL:HG11	2.21	0.40
10:B:912:ASN:OD1	10:B:916:TYR:N	2.50	0.40
3:2:145:VAL:HB	3:2:146:PRO:HD3	2.02	0.40
5:4:175:MET:HE1	7:6:322:TYR:HB2	2.03	0.40
5:4:213:LEU:HD22	5:4:230:VAL:HG12	2.04	0.40
7:6:186:ILE:HG12	7:6:211:LEU:HD12	2.04	0.40
8:7:392:PHE:CE1	8:7:426:VAL:HG11	2.55	0.40
9:A:1022:ILE:HG21	9:A:1037:ALA:HB1	2.02	0.40
9:A:1129:ASN:O	9:A:1130:ILE:C	2.59	0.40
9:A:1348:SER:HB3	13:E:136:LEU:HD13	2.01	0.40
11:C:183:ALA:HB3	11:C:232:ASN:HB3	2.03	0.40
25:R:58:LEU:HD11	25:R:62:LEU:HD23	2.03	0.40
27:U:22:ILE:HG22	27:U:39:LEU:HD11	2.03	0.40
1:0:272:ARG:HA	1:0:275:GLU:HG2	2.02	0.40
1:0:427:THR:O	1:0:427:THR:HG23	2.21	0.40
8:7:392:PHE:CD1	8:7:426:VAL:HG11	2.56	0.40
8:7:530:ARG:O	8:7:534:TYR:CD2	2.74	0.40
10:B:260:LEU:HB2	10:B:263:ILE:HD12	2.02	0.40
10:B:732:ALA:HB1	10:B:1049:GLN:HB3	2.02	0.40
21:M:48:VAL:HG23	21:M:49:GLY:N	2.37	0.40
1:0:249:VAL:HG21	1:0:403:PHE:HB2	2.02	0.40
1:0:383:LEU:HD21	1:0:388:ILE:HD11	2.03	0.40
1:0:699:GLU:OE2	1:0:700:HIS:ND1	2.54	0.40
2:1:407:ILE:HD12	5:4:22:TRP:CB	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:337:ARG:O	8:7:62:ARG:NH2	2.55	0.40
4:3:6:CYS:N	4:3:10:LYS:HA	2.36	0.40
8:7:474:ASP:OD1	8:7:474:ASP:N	2.53	0.40
9:A:419:ILE:HD12	9:A:429:LEU:HD21	2.03	0.40
9:A:945:ASN:OD1	9:A:945:ASN:O	2.39	0.40
10:B:124:LEU:N	10:B:150:GLY:O	2.44	0.40
15:G:120:ASP:OD1	15:G:122:ASN:ND2	2.55	0.40
21:M:222:LEU:CD2	21:M:277:ILE:HD13	2.51	0.40
9:A:141:LEU:HD23	9:A:141:LEU:C	2.42	0.40
9:A:844:ARG:NH2	10:B:501:LEU:HD13	2.37	0.40
9:A:901:VAL:HB	9:A:978:VAL:HG12	2.04	0.40
10:B:508:MET:HB3	10:B:621:ILE:HD13	2.03	0.40
10:B:859:ARG:NH1	10:B:903:ILE:HD11	2.37	0.40
12:D:92:LEU:HB2	12:D:97:LEU:HD21	2.03	0.40
21:M:145:VAL:HG21	21:M:198:ILE:HG12	2.04	0.40
22:N:-2:DG:C2	22:N:-1:DG:C5	3.10	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	710/760 (93%)	682 (96%)	28 (4%)	0	100	100
2	1	253/548 (46%)	245 (97%)	8 (3%)	0	100	100
3	2	380/462 (82%)	365 (96%)	15 (4%)	0	100	100
4	3	147/309 (48%)	136 (92%)	11 (8%)	0	100	100
5	4	259/308 (84%)	255 (98%)	4 (2%)	0	100	100
6	5	64/71 (90%)	63 (98%)	1 (2%)	0	100	100
7	6	341/395 (86%)	329 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	7	601/782 (77%)	577 (96%)	24 (4%)	0	100	100
9	A	1413/1970 (72%)	1378 (98%)	35 (2%)	0	100	100
10	B	1130/1174 (96%)	1097 (97%)	33 (3%)	0	100	100
11	C	253/275 (92%)	248 (98%)	5 (2%)	0	100	100
12	D	126/142 (89%)	125 (99%)	1 (1%)	0	100	100
13	E	207/210 (99%)	201 (97%)	6 (3%)	0	100	100
14	F	77/127 (61%)	76 (99%)	1 (1%)	0	100	100
15	G	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
16	H	146/150 (97%)	143 (98%)	3 (2%)	0	100	100
17	I	112/125 (90%)	107 (96%)	5 (4%)	0	100	100
18	J	62/67 (92%)	60 (97%)	2 (3%)	0	100	100
19	K	113/117 (97%)	112 (99%)	1 (1%)	0	100	100
20	L	42/58 (72%)	42 (100%)	0	0	100	100
21	M	248/316 (78%)	242 (98%)	6 (2%)	0	100	100
23	O	177/339 (52%)	174 (98%)	3 (2%)	0	100	100
24	Q	134/517 (26%)	130 (97%)	4 (3%)	0	100	100
25	R	218/249 (88%)	213 (98%)	5 (2%)	0	100	100
27	U	109/376 (29%)	102 (94%)	7 (6%)	0	100	100
28	V	97/109 (89%)	95 (98%)	2 (2%)	0	100	100
29	W	198/439 (45%)	195 (98%)	3 (2%)	0	100	100
30	X	169/291 (58%)	163 (96%)	6 (4%)	0	100	100
All	All	7955/10858 (73%)	7720 (97%)	235 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	0	624/664 (94%)	624 (100%)	0	100	100
2	1	241/484 (50%)	241 (100%)	0	100	100
3	2	342/399 (86%)	341 (100%)	1 (0%)	92	95
4	3	143/283 (50%)	142 (99%)	1 (1%)	84	90
5	4	234/272 (86%)	234 (100%)	0	100	100
6	5	59/64 (92%)	59 (100%)	0	100	100
7	6	311/352 (88%)	310 (100%)	1 (0%)	92	95
8	7	536/688 (78%)	533 (99%)	3 (1%)	86	92
9	A	1254/1749 (72%)	1253 (100%)	1 (0%)	93	97
10	B	994/1027 (97%)	991 (100%)	3 (0%)	92	95
11	C	234/252 (93%)	234 (100%)	0	100	100
12	D	118/126 (94%)	118 (100%)	0	100	100
13	E	191/192 (100%)	189 (99%)	2 (1%)	76	86
14	F	69/111 (62%)	69 (100%)	0	100	100
15	G	152/153 (99%)	151 (99%)	1 (1%)	84	90
16	H	129/131 (98%)	129 (100%)	0	100	100
17	I	103/112 (92%)	103 (100%)	0	100	100
18	J	53/56 (95%)	53 (100%)	0	100	100
19	K	104/106 (98%)	104 (100%)	0	100	100
20	L	41/55 (74%)	41 (100%)	0	100	100
21	M	215/268 (80%)	215 (100%)	0	100	100
23	O	154/293 (53%)	154 (100%)	0	100	100
24	Q	121/448 (27%)	120 (99%)	1 (1%)	81	89
25	R	196/218 (90%)	195 (100%)	1 (0%)	88	93
27	U	105/324 (32%)	105 (100%)	0	100	100
28	V	90/98 (92%)	89 (99%)	1 (1%)	73	84
29	W	182/373 (49%)	181 (100%)	1 (0%)	88	93
30	X	154/261 (59%)	154 (100%)	0	100	100
All	All	7149/9559 (75%)	7132 (100%)	17 (0%)	93	96

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	2	33	ARG
4	3	41	ARG
7	6	343	ARG
8	7	198	ARG
8	7	266	GLN
8	7	692	LYS
9	A	61	ARG
10	B	199	LYS
10	B	897	ARG
10	B	1131	ARG
13	E	52	ARG
13	E	162	ARG
15	G	81	LYS
24	Q	151	ARG
25	R	230	LYS
28	V	82	ARG
29	W	56	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	114	ASN
4	3	16	ASN
4	3	24	ASN
7	6	227	HIS
9	A	945	ASN
9	A	1005	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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 19 ligands modelled in this entry, 18 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
33	SF4	0	1000	1	0,12,12	0.00	-	-		

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
33	SF4	0	1000	1	-	-	0/6/5/5

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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.