Full wwPDB EM Validation Report ⓘ

Oct 22, 2024 – 05:34 AM JST

PDB ID	:	8XGC
EMDB ID	:	EMD-38317
Title	:	Structure of yeast replisome associated with FACT and histone hexamer, Composite map
Authors	:	Li, N.; Gao, Y.; Yu, D.; Gao, N.; Zhai, Y.
Deposited on	:	2023-12-15
Resolution	:	3.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

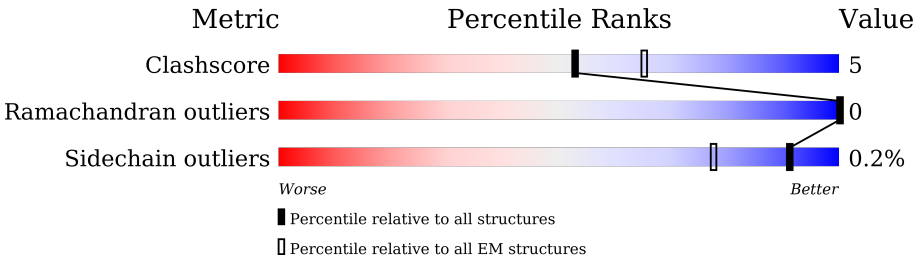
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	2	868	16% 75% 14% 10%
2	3	971	10% 54% 9% 37%
3	4	933	24% 61% 12% 27%
4	5	775	13% 75% 13% 13%
5	6	1017	9% 54% 9% 38%
6	7	845	32% 65% 10% 25%
7	8	2222	33% 6% 61%
8	9	689	13% 69% 14% 17%

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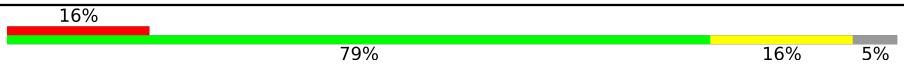
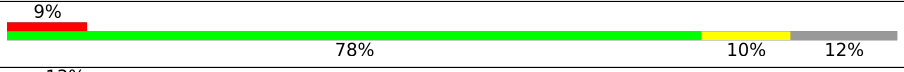
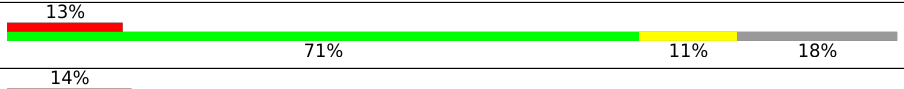
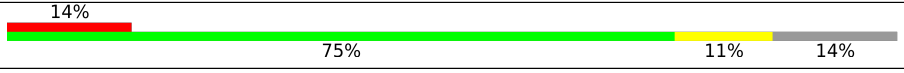
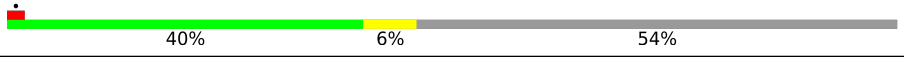
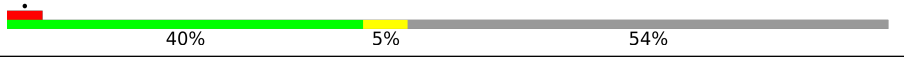
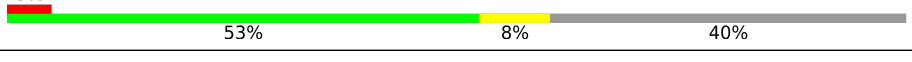
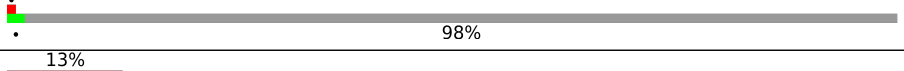
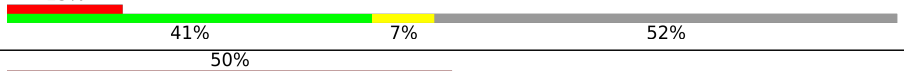
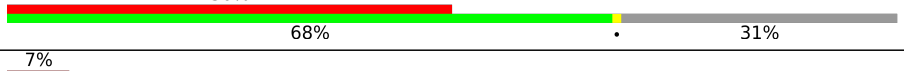
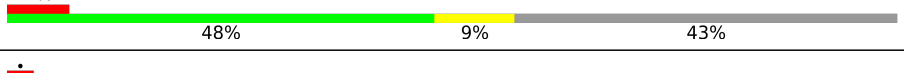
Mol	Chain	Length	Quality of chain
9	A	208	
10	B	251	
11	C	194	
12	D	294	
13	E	650	
14	F	927	
14	G	927	
14	H	927	
15	I	1238	
16	J	317	
17	K	1096	
18	L	1035	
19	M	552	
20	N	136	
20	R	136	
21	O	103	
21	S	103	
22	P	132	
23	Q	131	
24	X	51	
25	Y	39	

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 82765 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 replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	2	778	6161	3835	1105	1198	23	0	0

- Molecule 2 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3	613	4795	3026	854	902	13	0	0

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	4	679	5269	3313	922	1005	29	0	0

- Molecule 4 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	5	678	5376	3379	937	1036	24	0	0

- Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	6	634	4991	3151	875	940	25	0	0

- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	7	635	4919	3112	860	923	24	0	0

- Molecule 7 is a protein called DNA polymerase epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	857	Total	C	N	O	S	0	0
			6945	4496	1137	1274	38		

- Molecule 8 is a protein called DNA polymerase epsilon subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	573	Total	C	N	O	S	0	0
			4594	2947	788	840	19		

- Molecule 9 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	197	Total	C	N	O	S	0	0
			1611	1012	277	313	9		

- Molecule 10 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	192	Total	C	N	O	S	0	0
			1609	1034	285	286	4		

- Molecule 11 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	171	Total	C	N	O	S	0	0
			1379	899	222	252	6		

- Molecule 12 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	241	Total	C	N	O	S	0	0
			1988	1266	325	385	12		

- Molecule 13 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	562	Total	C	N	O	S	0	0
			4550	2906	766	864	14		

- Molecule 14 is a protein called DNA polymerase alpha-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	424	Total 3404	C 2188	N 564	O 637	S 15	0	0
14	G	422	Total 3380	C 2172	N 557	O 636	S 15	0	0
14	H	425	Total 3411	C 2193	N 565	O 638	S 15	0	0

- Molecule 15 is a protein called Topoisomerase 1-associated factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	745	Total 6057	C 3897	N 1027	O 1114	S 19	0	0

- Molecule 16 is a protein called Chromosome segregation in meiosis protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	94	Total 788	C 507	N 144	O 133	S 4	0	0

- Molecule 17 is a protein called Mediator of replication checkpoint protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	K	20	Total 163	C 102	N 23	O 38	0	0

- Molecule 18 is a protein called FACT complex subunit SPT16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	493	Total 3474	C 2177	N 616	O 671	S 10	0	0

- Molecule 19 is a protein called FACT complex subunit POB3.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	M	379	Total 1876	C 1118	N 379	O 379	0	0

- Molecule 20 is a protein called Histone H3.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	N	77	Total 629	C 399	N 118	O 112	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
20	R	90	Total 741	C 469	N 142	O 130	0	0

- Molecule 21 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	O	73	Total 583	C 365	N 114	O 104	0	0
21	S	85	Total 684	C 431	N 135	O 118	0	0

- Molecule 22 is a protein called Histone H2A.1.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	P	91	Total 703	C 439	N 139	O 125	0	0

- Molecule 23 is a protein called Histone H2B.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	91	Total 706	C 444	N 121	O 140	S 1	0	0

- Molecule 24 is a DNA chain called DNA (51-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	51	Total 1041	C 507	N 156	O 327	P 51	0	0

- Molecule 25 is a DNA chain called DNA (39-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	39	Total 796	C 382	N 149	O 226	P 39	0	0

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
26	2	1	Total 1	Zn 1	0

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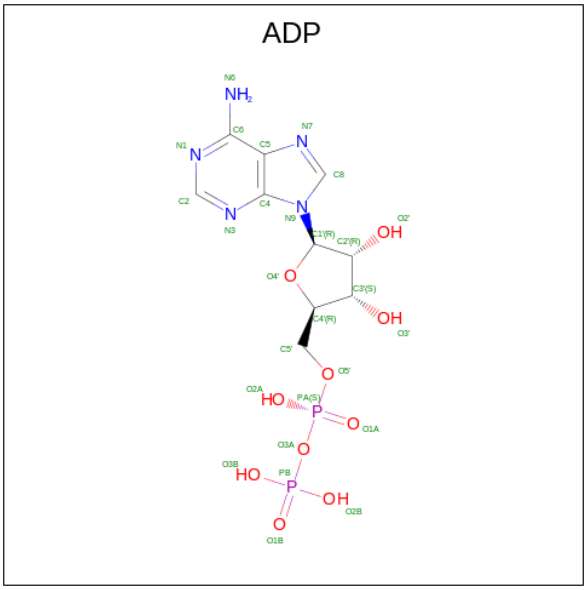
Mol	Chain	Residues	Atoms	AltConf
26	4	1	Total Zn 1 1	0
26	5	1	Total Zn 1 1	0
26	6	1	Total Zn 1 1	0
26	7	1	Total Zn 1 1	0
26	8	2	Total Zn 2 2	0

- Molecule 27 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



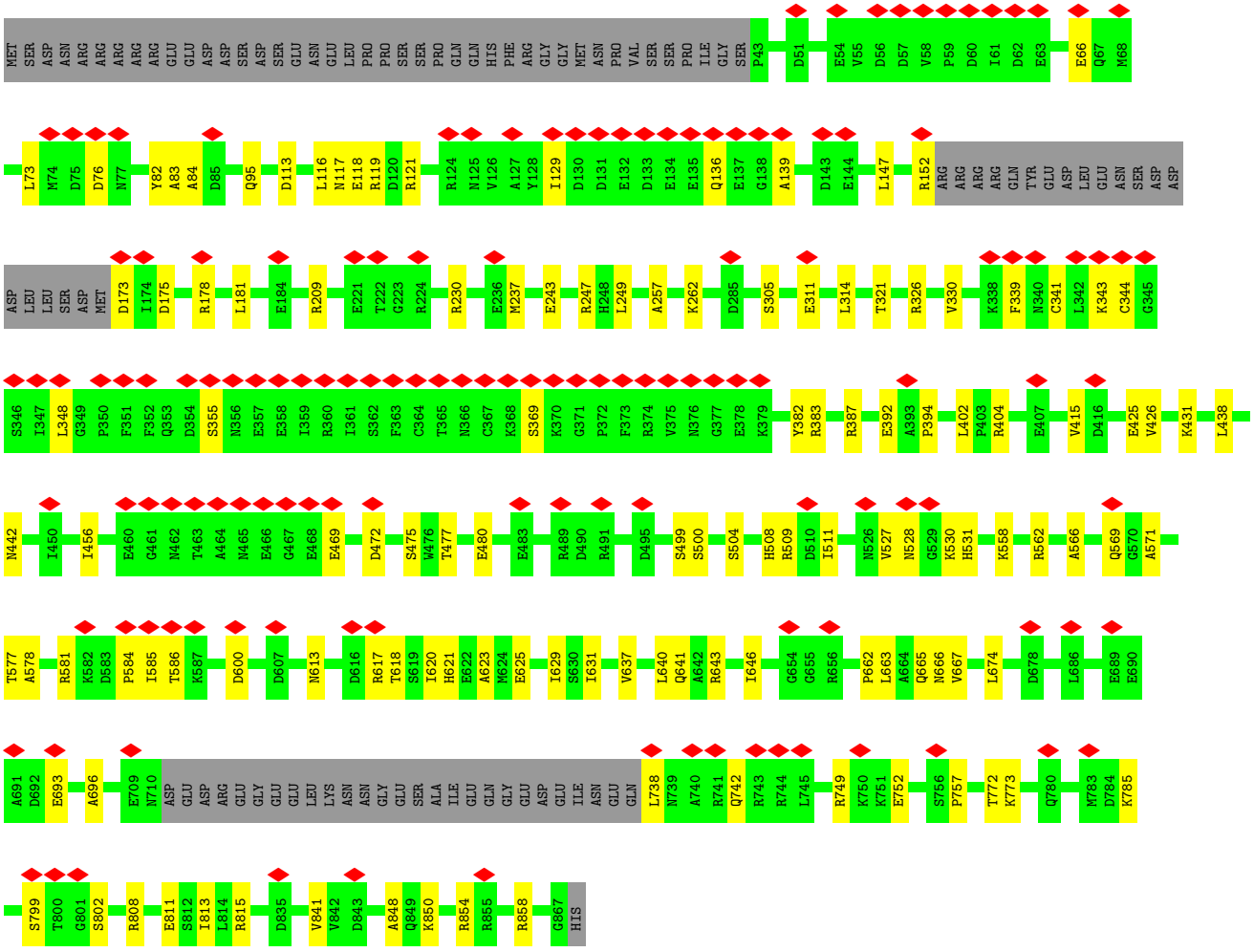
Mol	Chain	Residues	Atoms	AltConf
27	2	1	Total C N O P 27 10 5 10 2	0
27	3	1	Total C N O P 27 10 5 10 2	0
27	5	1	Total C N O P 27 10 5 10 2	0
27	6	1	Total C N O P 27 10 5 10 2	0
27	7	1	Total C N O P 27 10 5 10 2	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

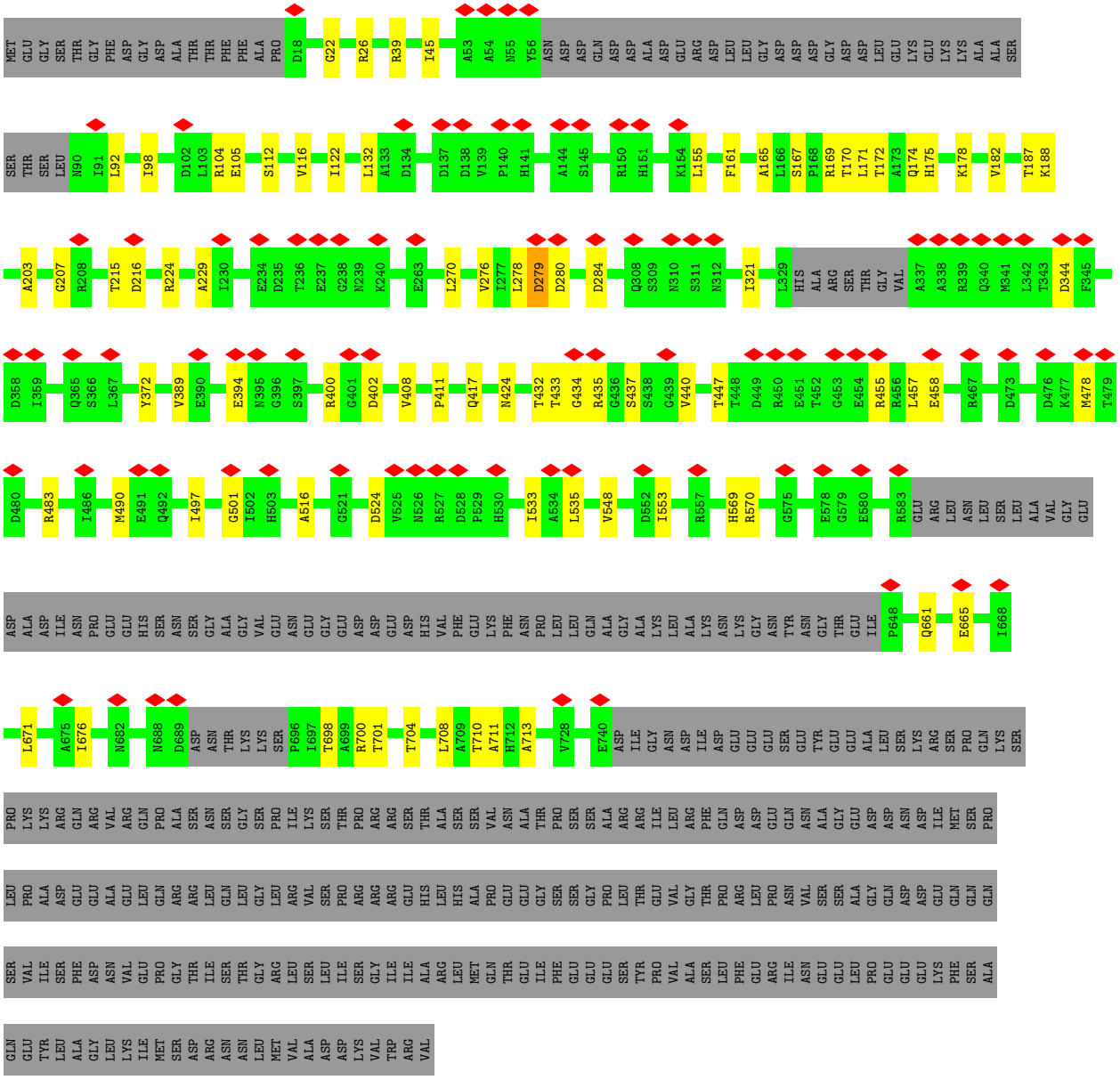
• Molecule 1: DNA replication licensing factor MCM2

Chain 2:



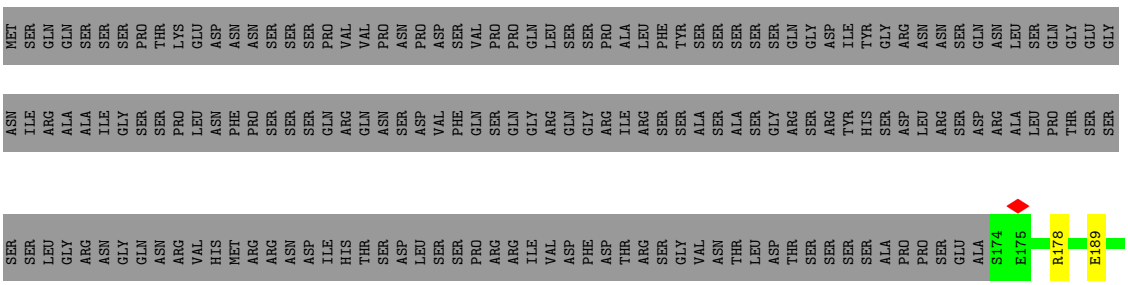
• Molecule 2: DNA replication licensing factor MCM3

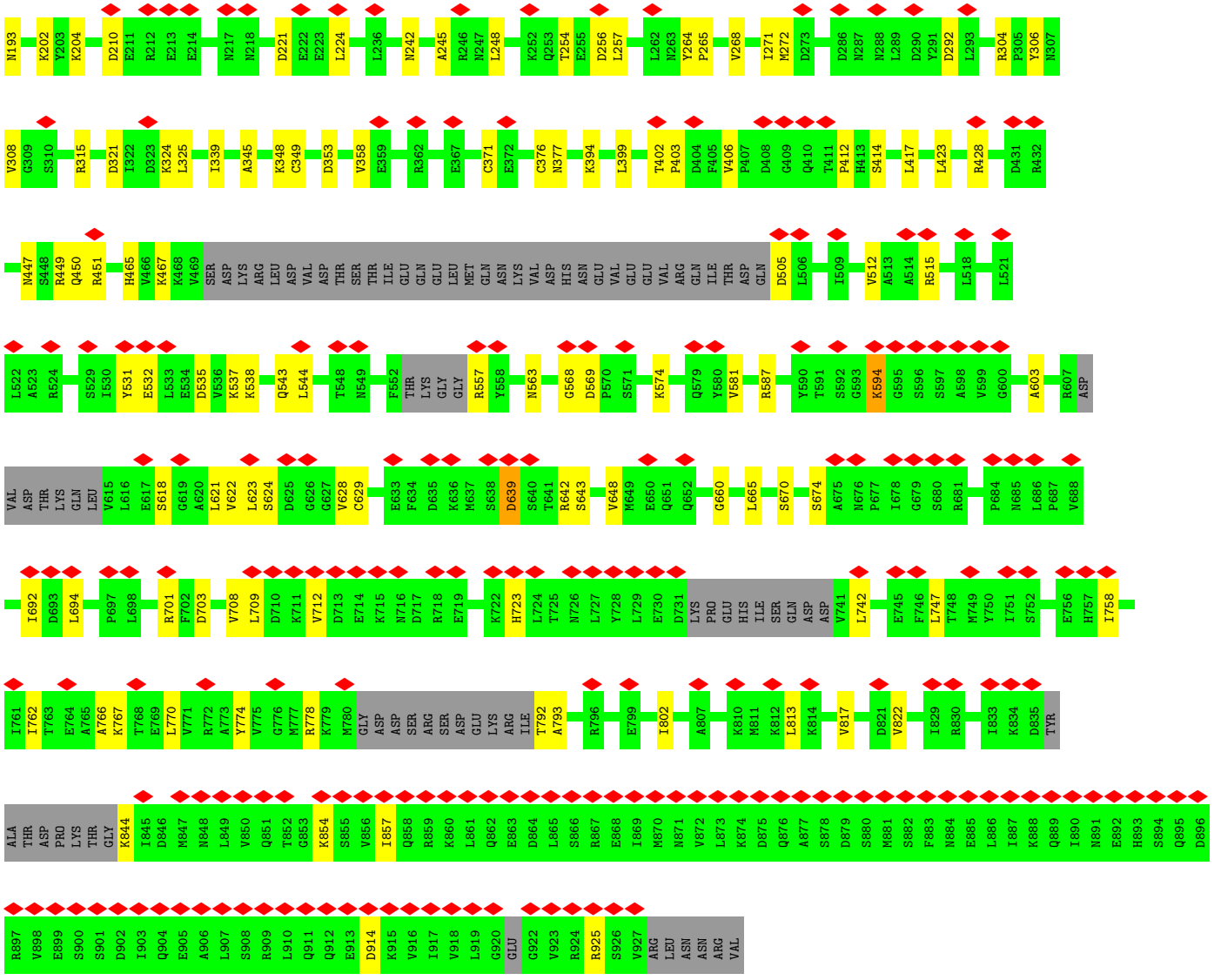
Chain 3:



• Molecule 3: DNA replication licensing factor MCM4

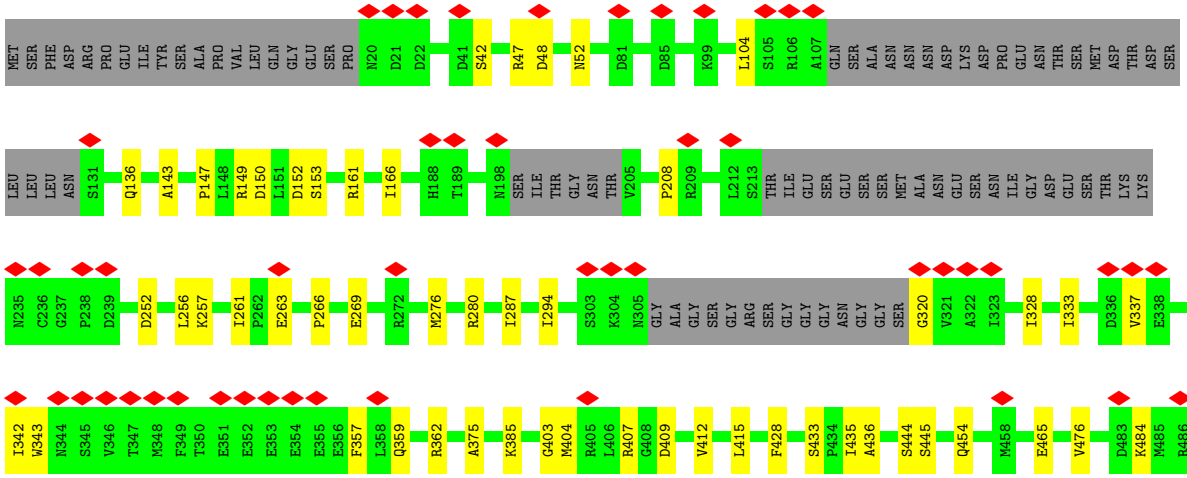
Chain 4:

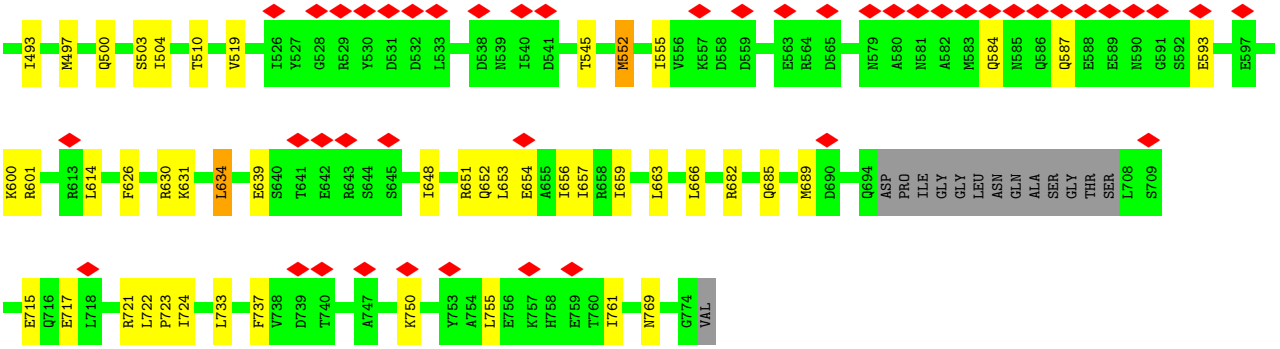




• Molecule 4: Minichromosome maintenance protein 5

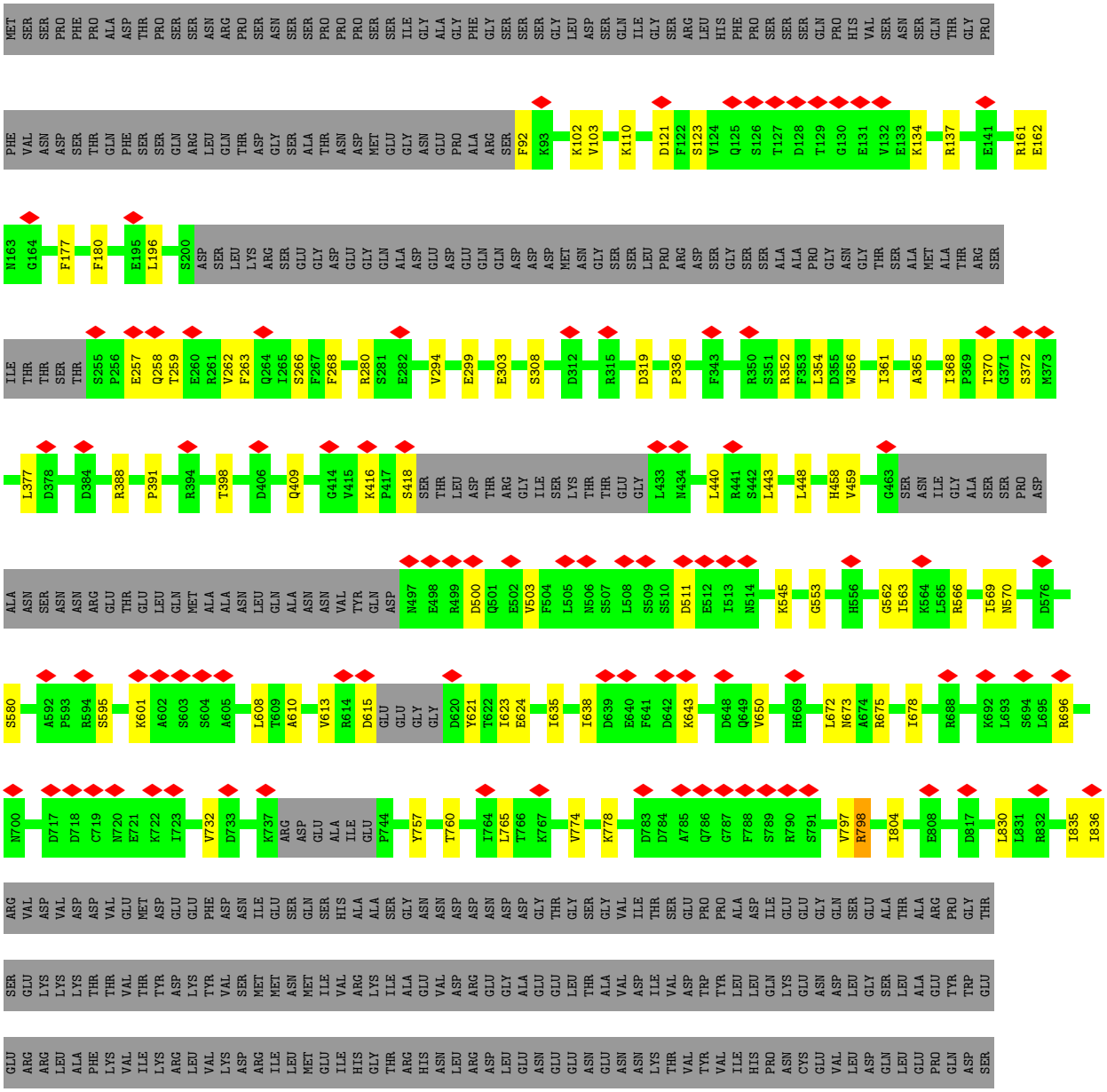
Chain 5:





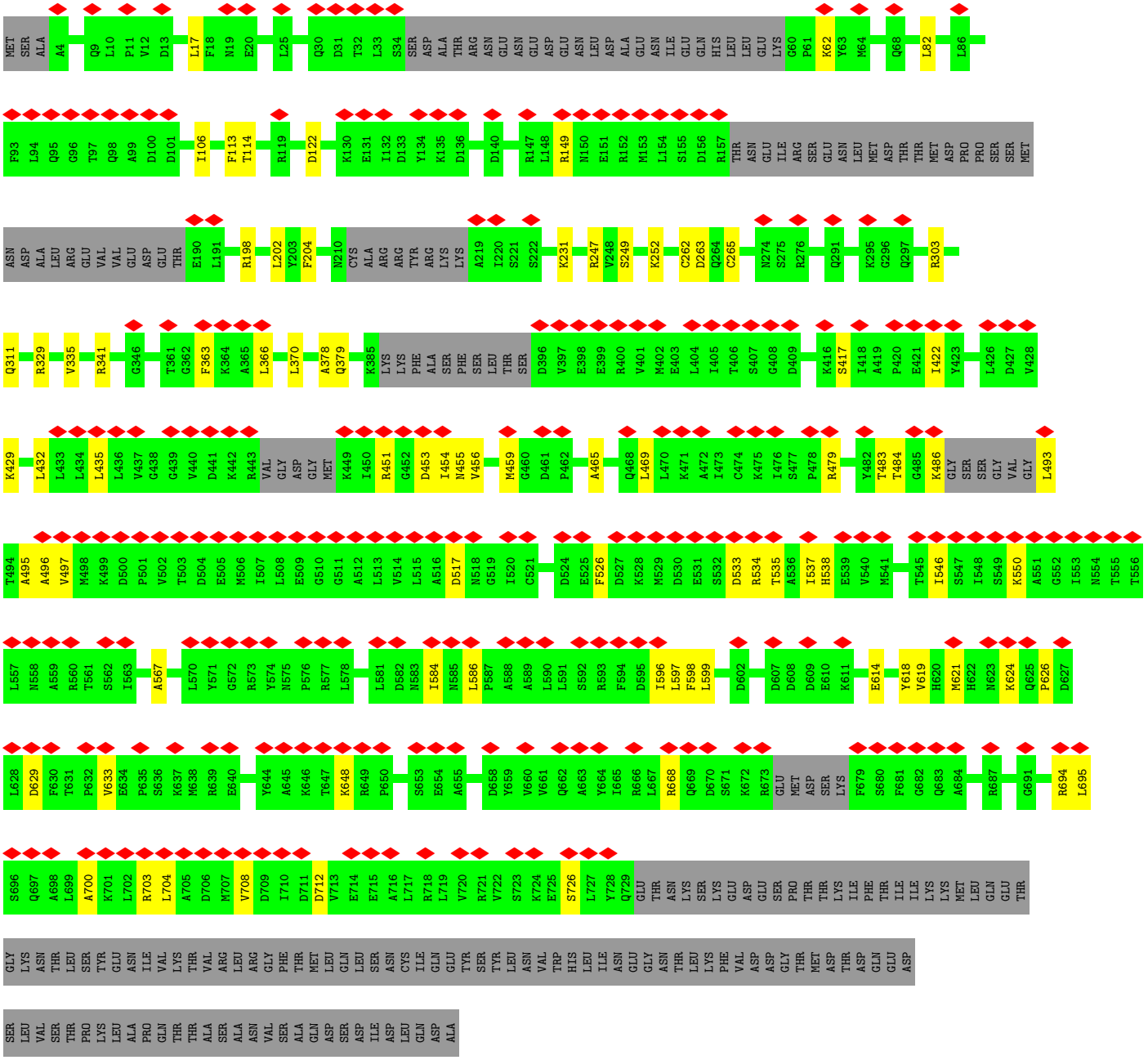
• Molecule 5: DNA replication licensing factor MCM6

Chain 6:



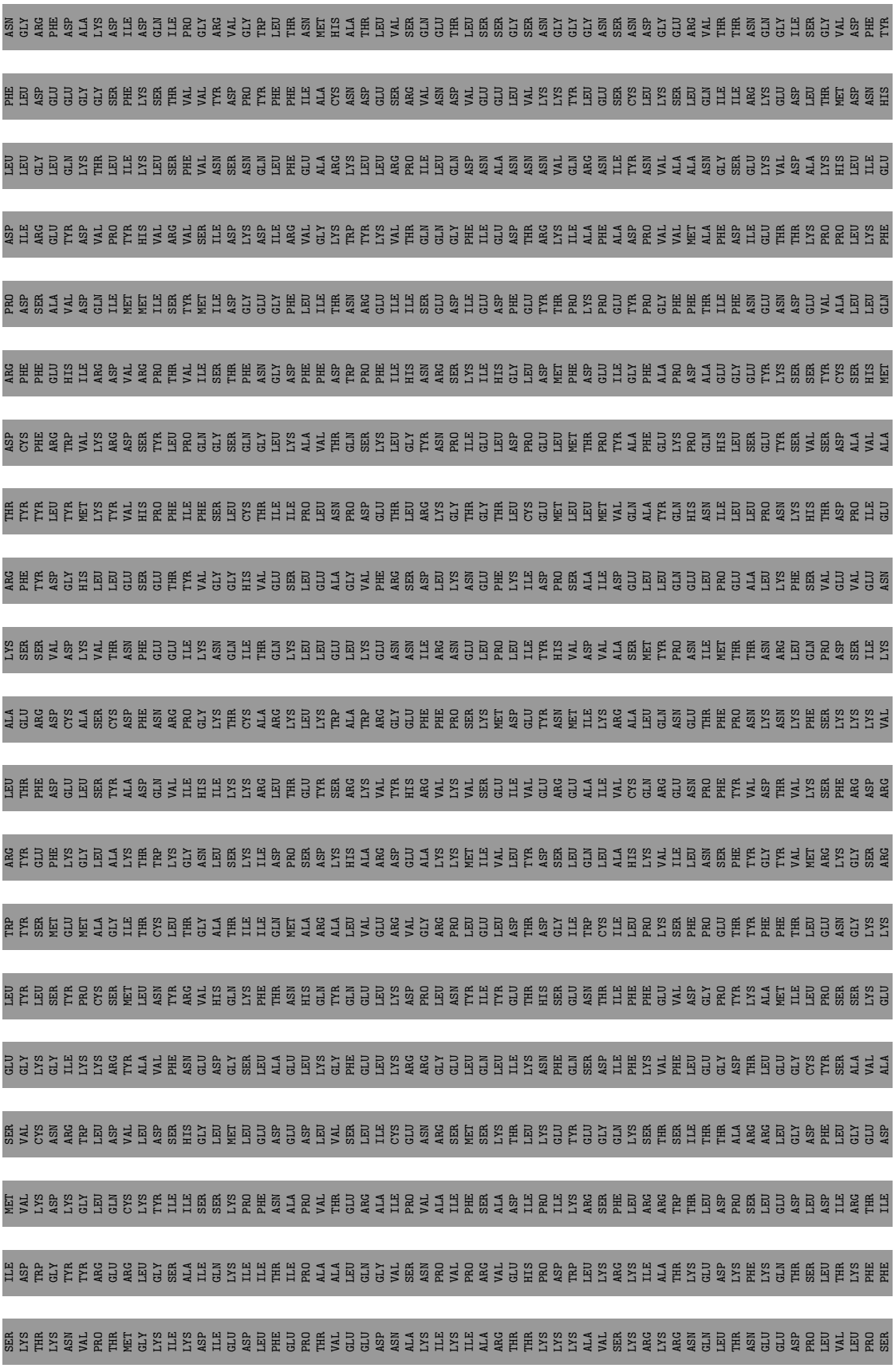
• Molecule 6: DNA replication licensing factor MCM7

Chain 7:



• Molecule 7: DNA polymerase epsilon catalytic subunit A

Chain 8:


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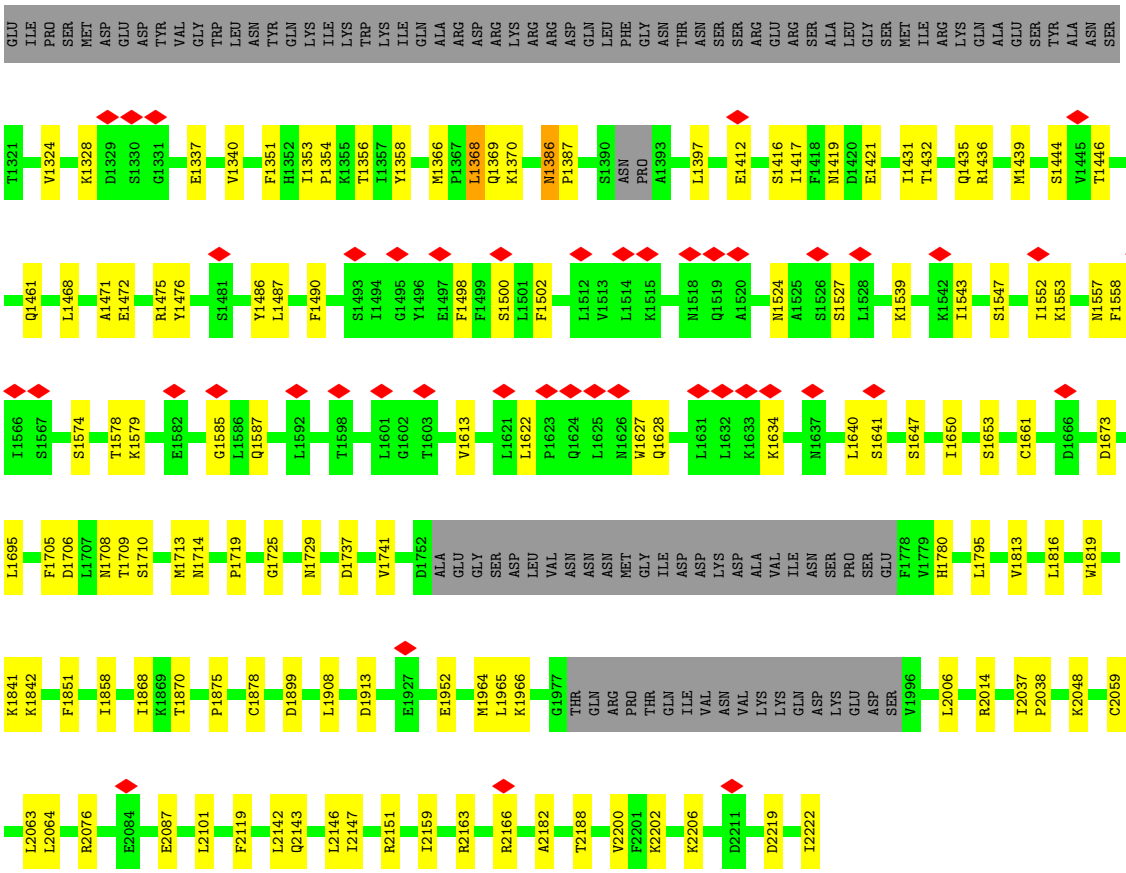
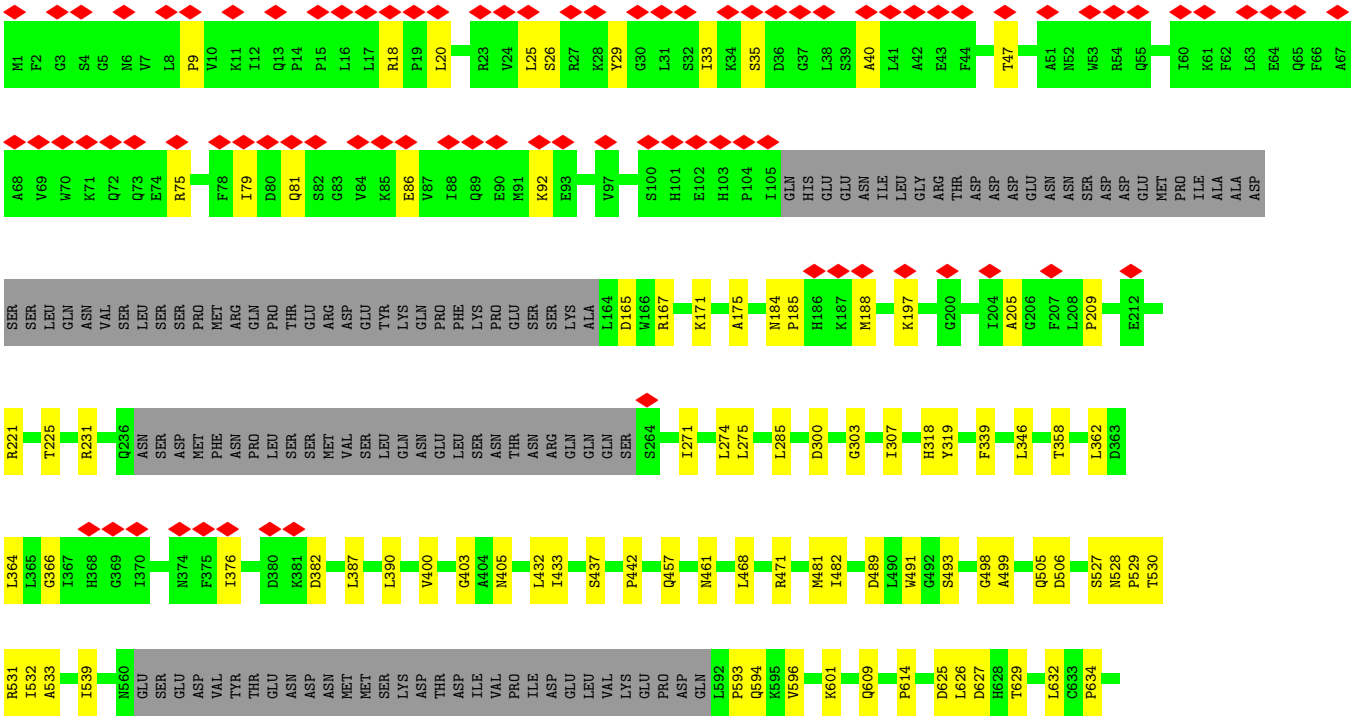
ARG TYR GLU PHE LYS GLY ASN LEU SER ASP LYS HIS ALA ARG ASP GLU ALA LYS LYS MET ILE VAL LEU TYR ASP SER LEU GLN LEU ALA ILE VAL CYS GLN ARG GLU ASN PRO PHE TYR VAL ASP THR VAL LYS SER PHE PRO LYS VAL ILE LEU ASN SER PHE TYR GLY TYR VAL MET ARG ALA LYS GLY SER ARG
TRP TYR SER MET GLU MET ALA GLY ILE THR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

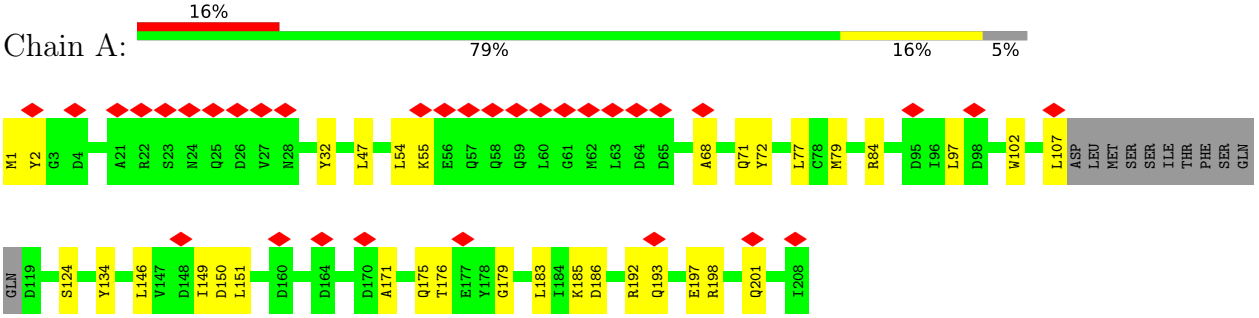


• Molecule 8: DNA polymerase epsilon subunit B

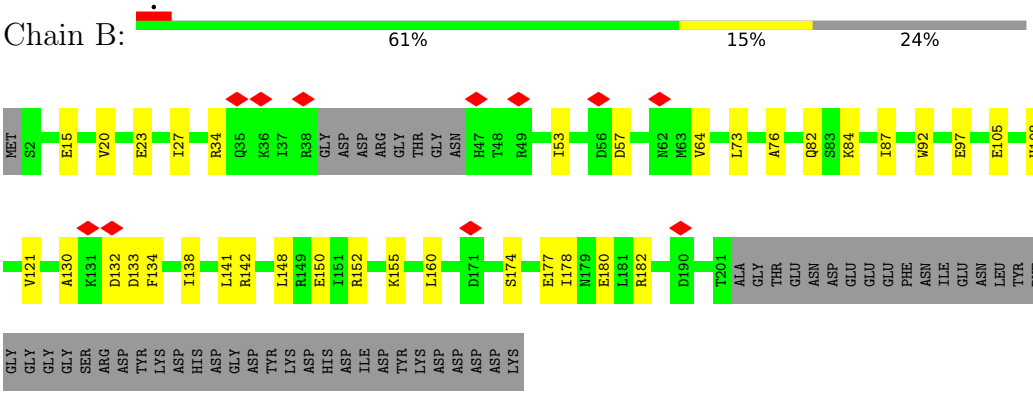
Chain 9:



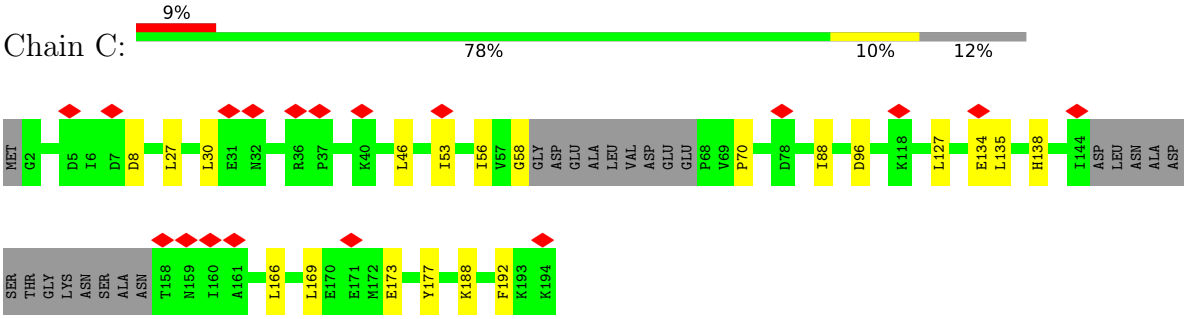
• Molecule 9: DNA replication complex GINS protein PSF1



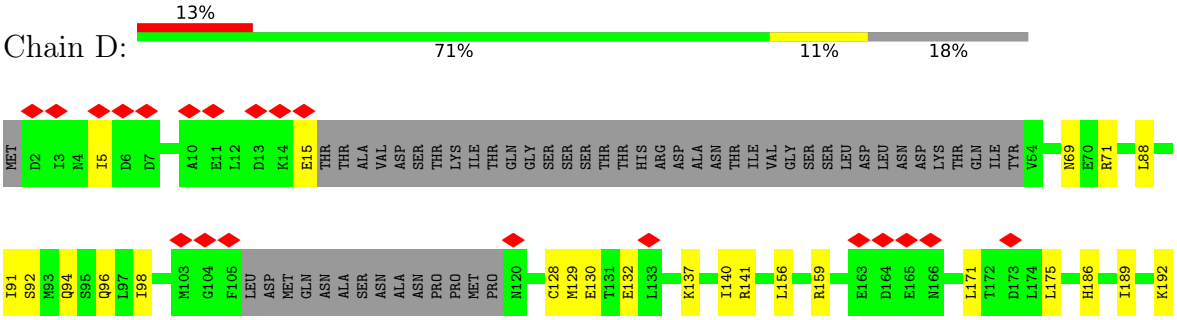
• Molecule 10: DNA replication complex GINS protein PSF2

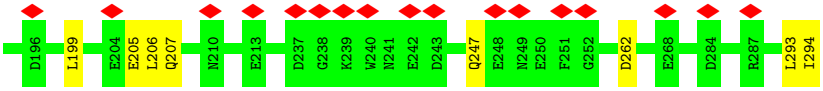


• Molecule 11: DNA replication complex GINS protein PSF3



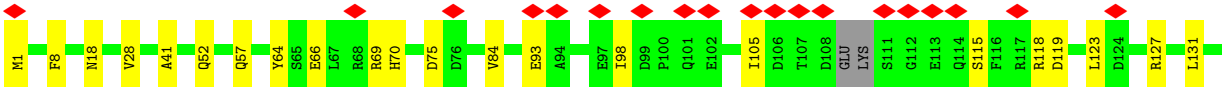
• Molecule 12: DNA replication complex GINS protein SLD5

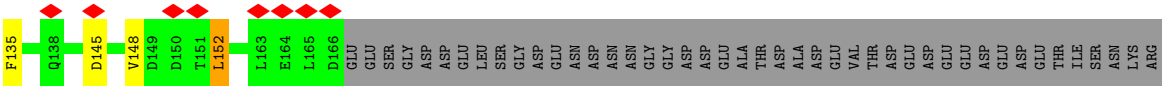


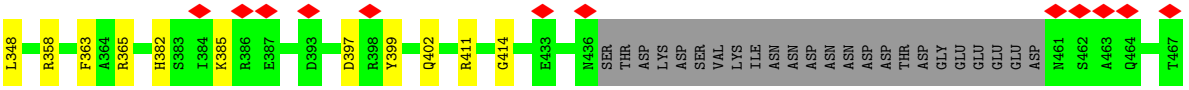


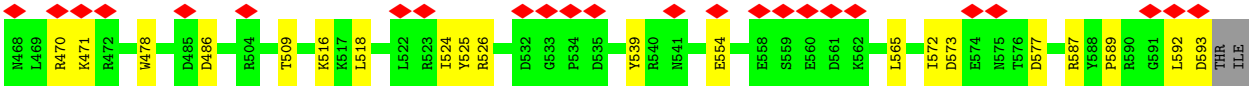
• Molecule 13: Cell division control protein 45

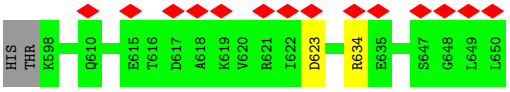
Chain E:





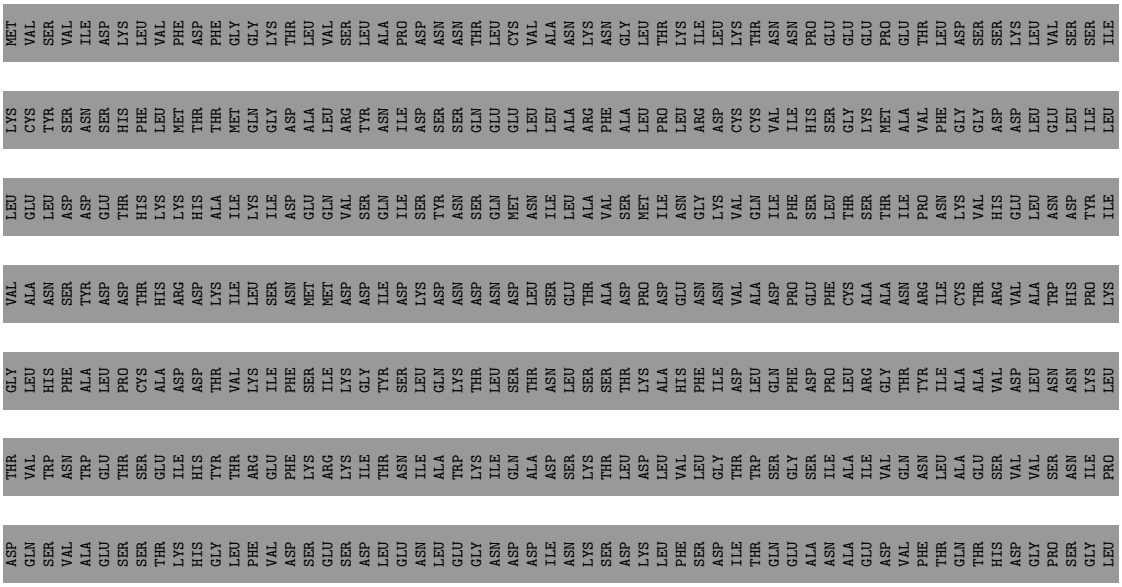


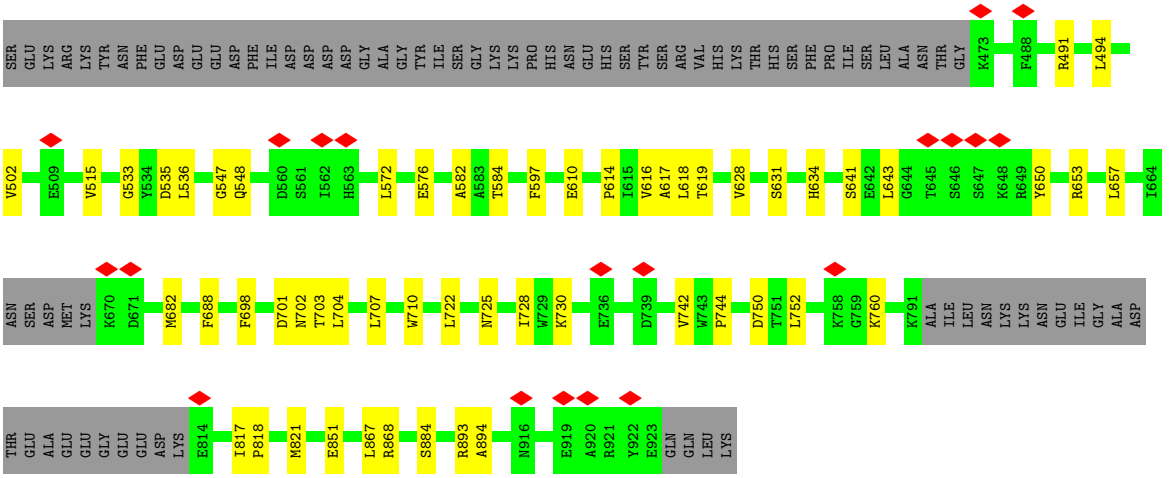




• Molecule 14: DNA polymerase alpha-binding protein

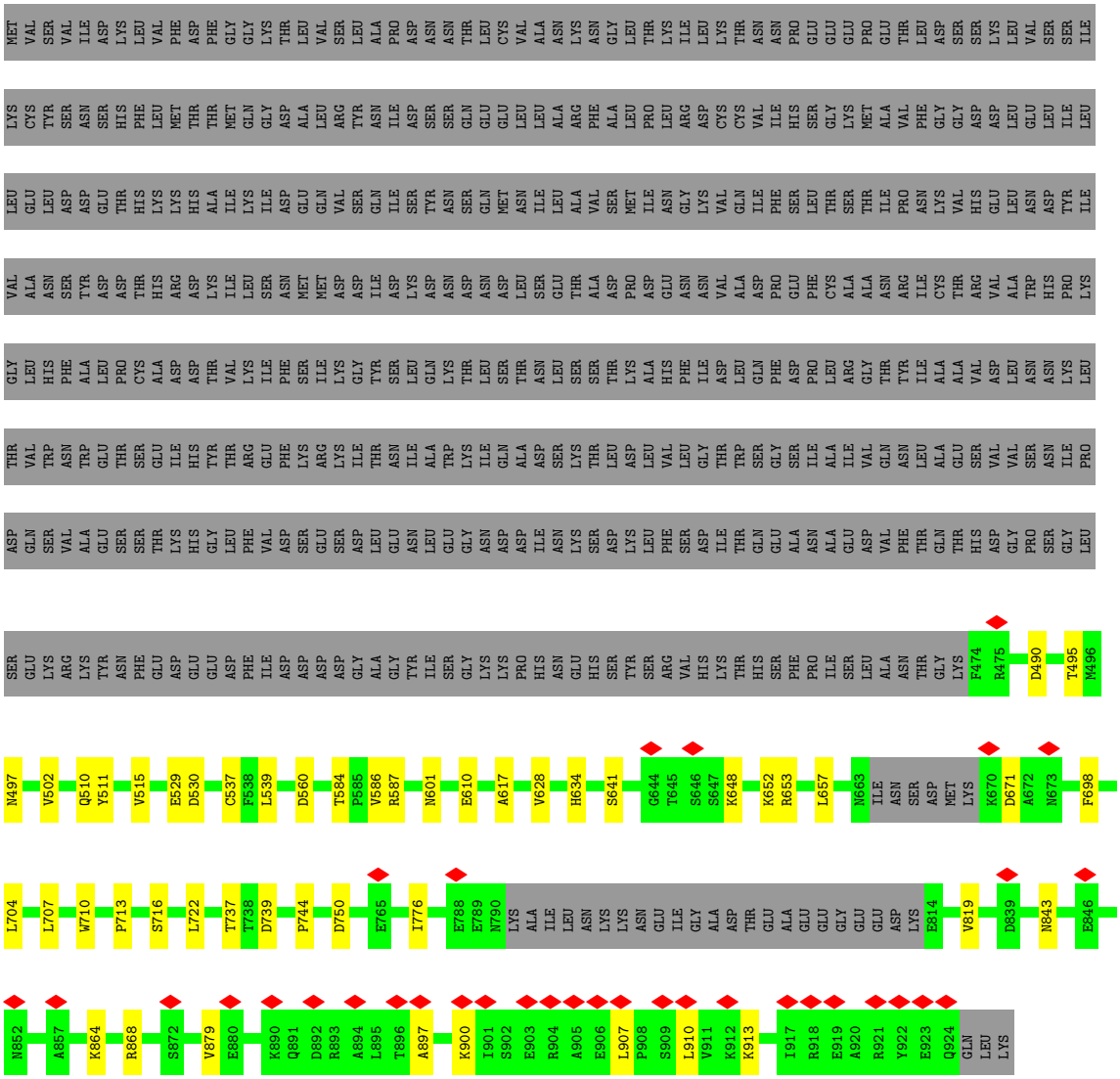
Chain F:





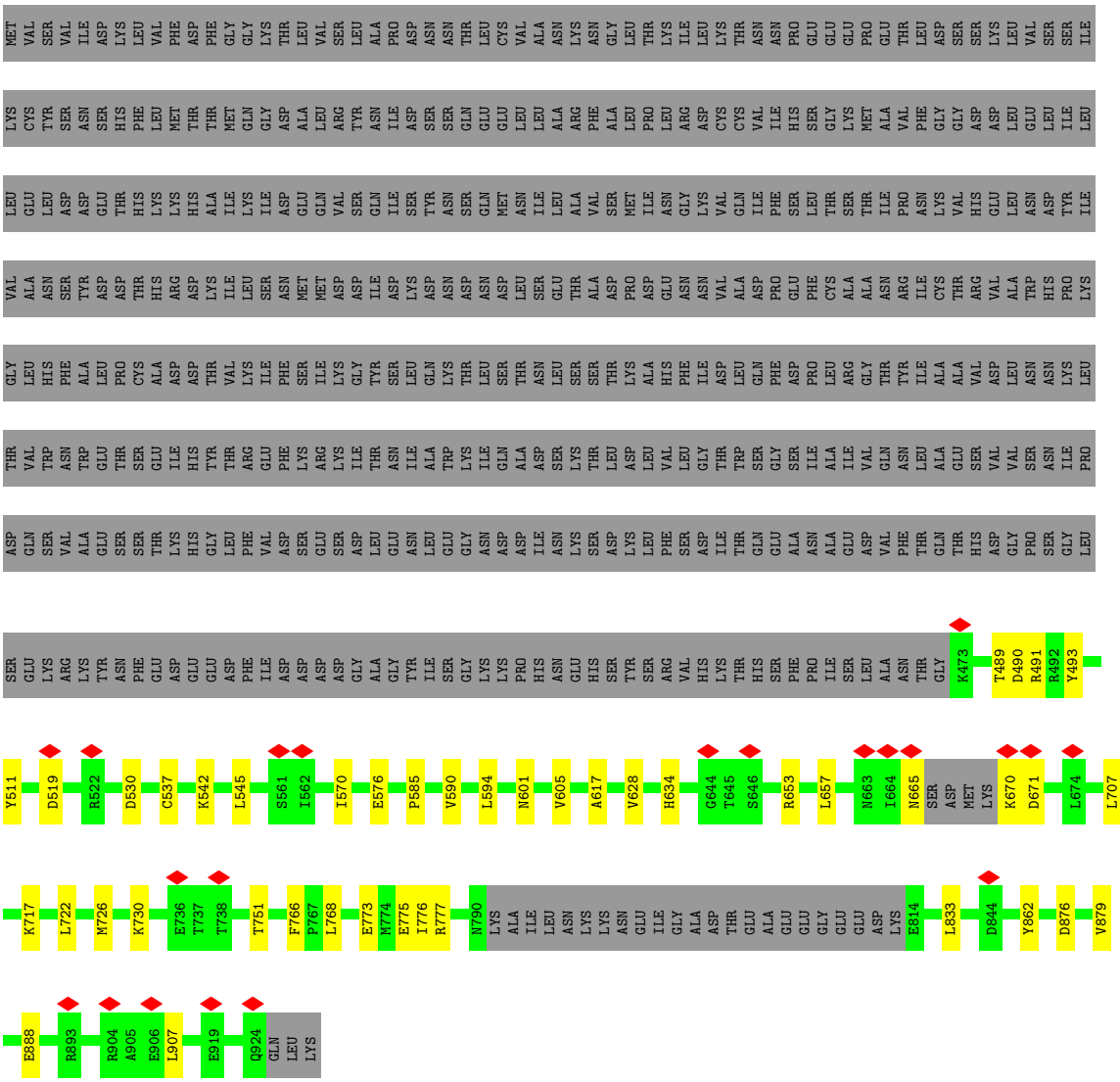
• Molecule 14: DNA polymerase alpha-binding protein

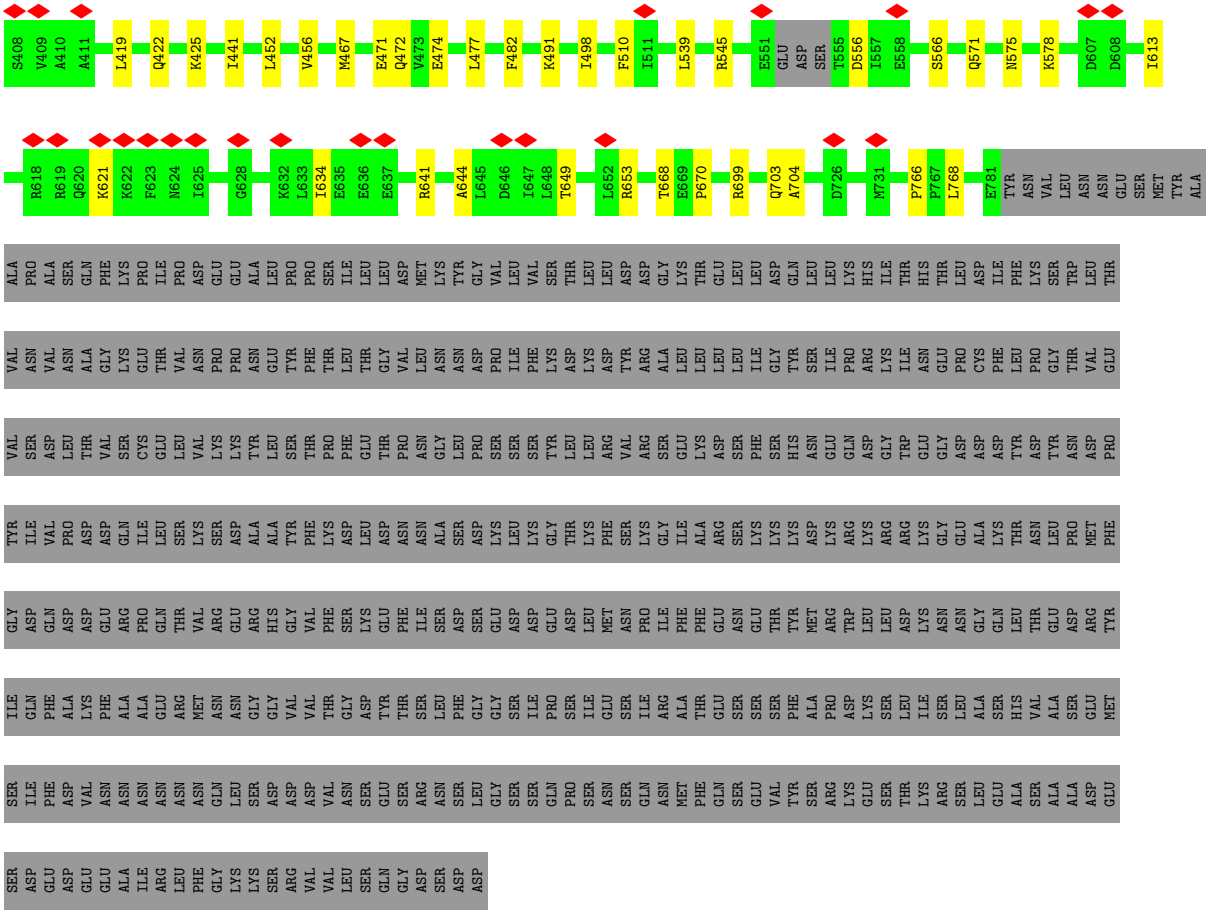
Chain G:



• Molecule 14: DNA polymerase alpha-binding protein

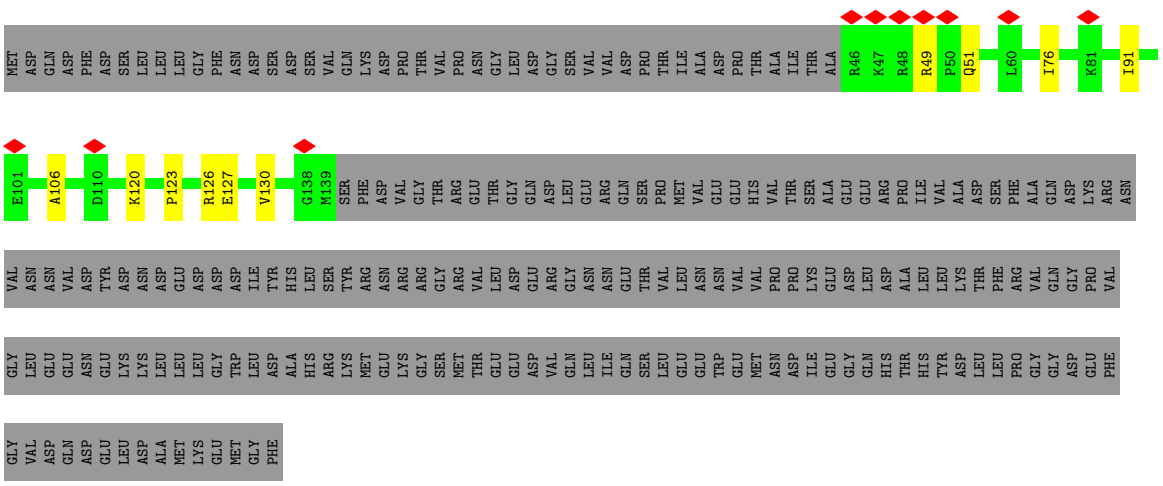
Chain H:


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



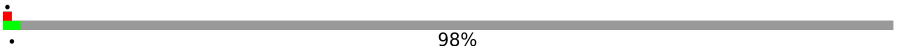
• Molecule 16: Chromosome segregation in meiosis protein 3

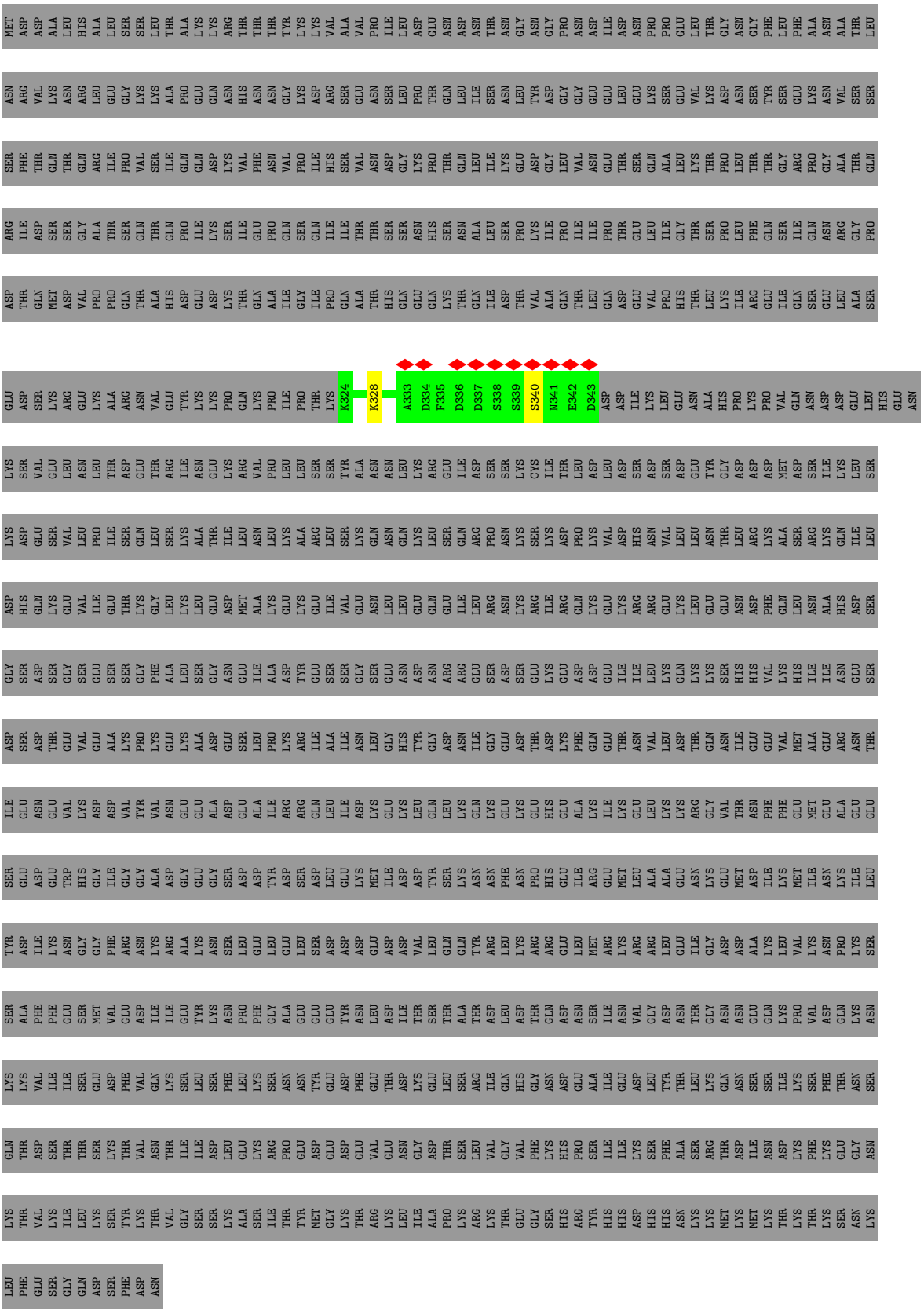
Chain J:



• Molecule 17: Mediator of replication checkpoint protein 1

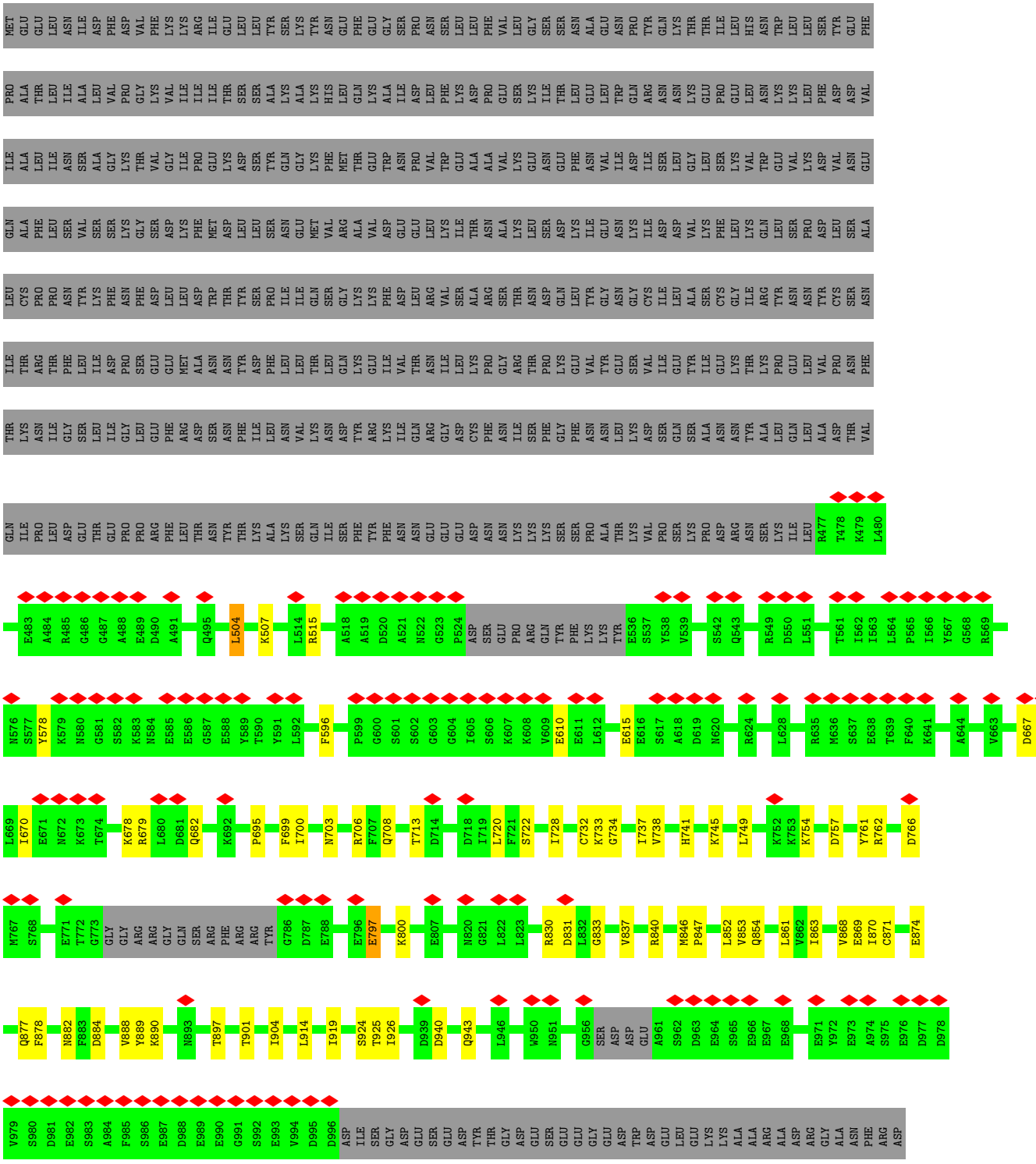
Chain K:





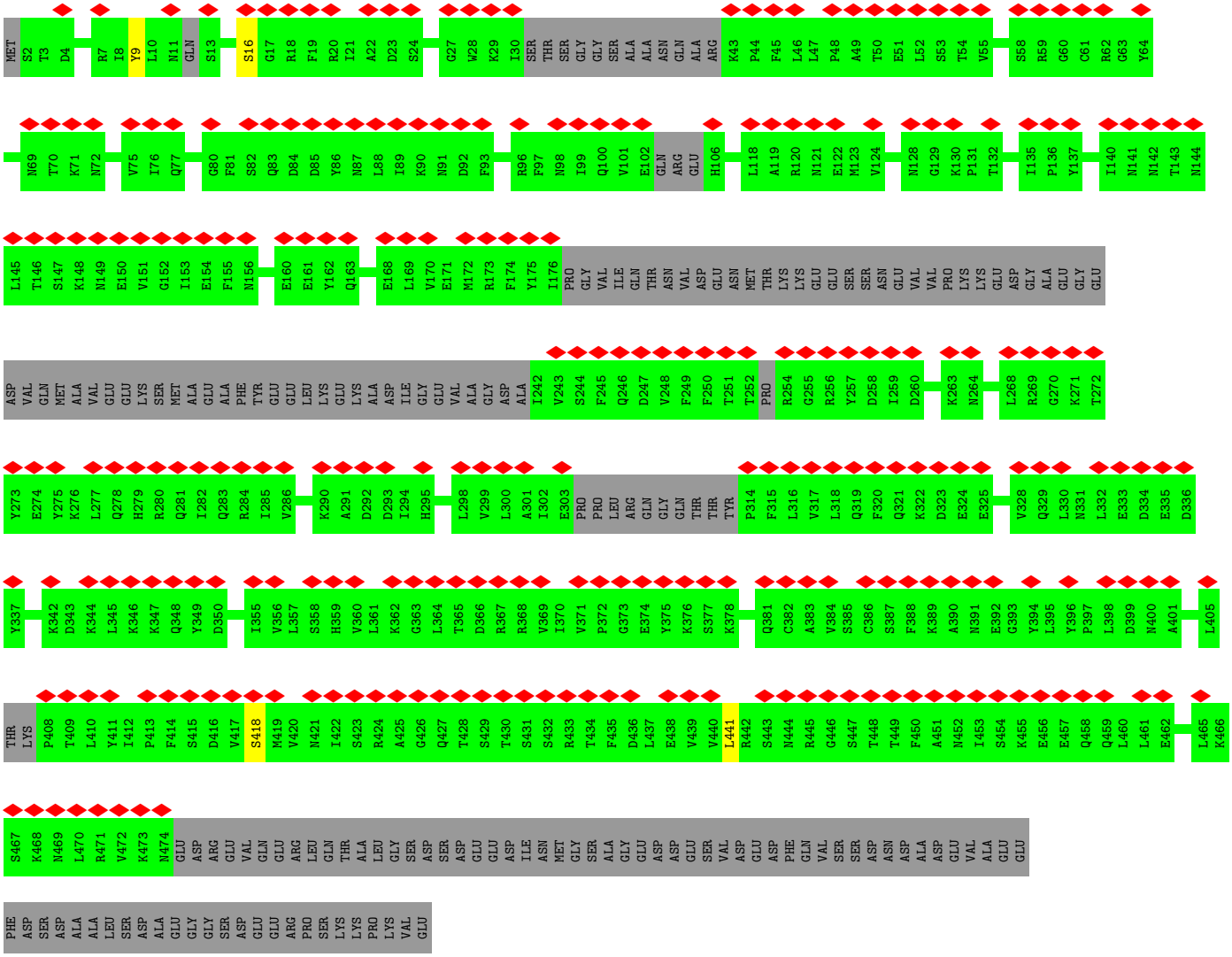
• Molecule 18: FACT complex subunit SPT16

Chain L:



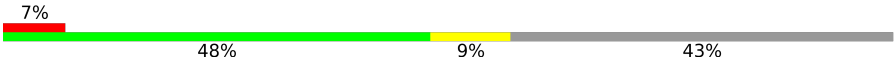
• Molecule 19: FACT complex subunit POB3

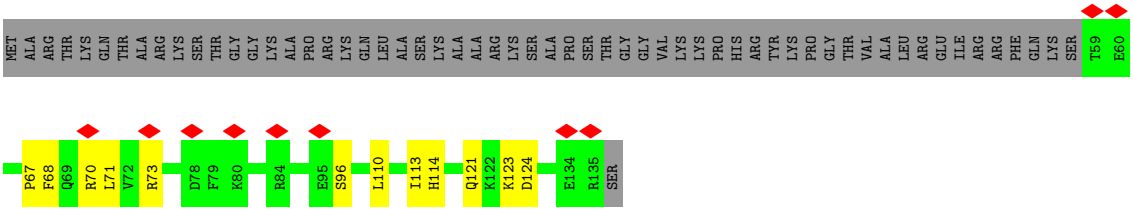
Chain M:



• Molecule 20: Histone H3

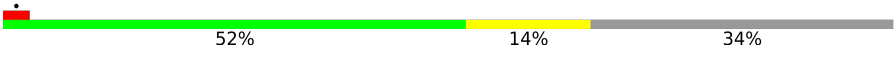
Chain N:





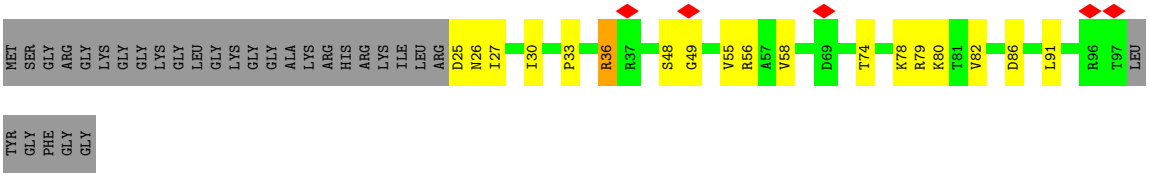
• Molecule 20: Histone H3

Chain R:



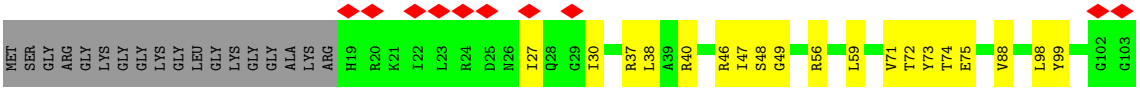
• Molecule 21: Histone H4

Chain O:



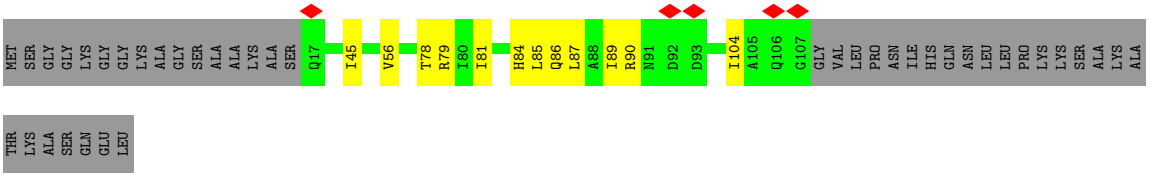
• Molecule 21: Histone H4

Chain S:



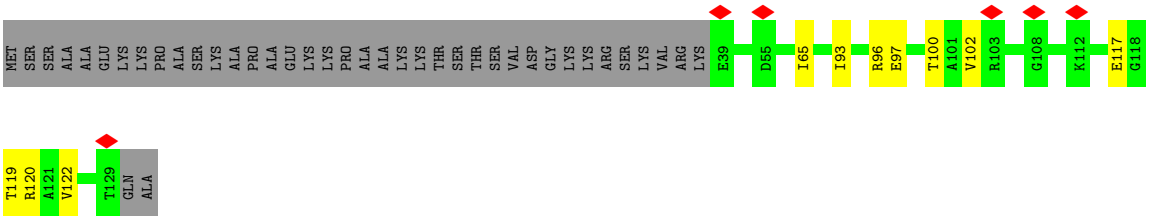
• Molecule 22: Histone H2A.1

Chain P:



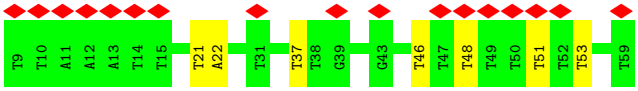
• Molecule 23: Histone H2B.2

Chain Q:



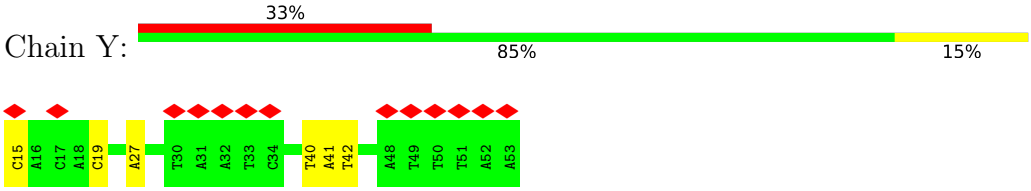
• Molecule 24: DNA (51-MER)

Chain X:



• Molecule 25: DNA (39-MER)

Chain Y:


33%
85%
15%
C15
A16
C17
A18
C19
A27
T30
A31
A32
T33
C34
T40
A41
T42
A48
T49
T50
T51
A52
A53

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	524000	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	84.549	Depositor
Minimum map value	-59.011	Depositor
Average map value	0.090	Depositor
Map value standard deviation	1.797	Depositor
Recommended contour level	10	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	2	0.28	0/6259	0.61	0/8458
2	3	0.27	0/4880	0.60	1/6619 (0.0%)
3	4	0.28	0/5337	0.65	3/7213 (0.0%)
4	5	0.31	1/5454 (0.0%)	0.61	4/7365 (0.1%)
5	6	0.28	0/5073	0.62	2/6846 (0.0%)
6	7	0.28	0/4993	0.62	2/6757 (0.0%)
7	8	0.30	0/7097	0.60	2/9594 (0.0%)
8	9	0.29	0/4699	0.64	5/6360 (0.1%)
9	A	0.29	0/1631	0.61	0/2194
10	B	0.28	0/1642	0.58	0/2221
11	C	0.28	0/1412	0.57	1/1908 (0.1%)
12	D	0.29	0/2024	0.63	2/2733 (0.1%)
13	E	0.27	0/4633	0.58	2/6269 (0.0%)
14	F	0.29	0/3489	0.58	1/4724 (0.0%)
14	G	0.29	0/3465	0.59	1/4696 (0.0%)
14	H	0.28	0/3496	0.56	1/4735 (0.0%)
15	I	0.29	0/6171	0.59	3/8321 (0.0%)
16	J	0.31	0/804	0.61	0/1074
17	K	0.33	0/166	0.52	0/220
18	L	0.29	0/3522	0.62	3/4786 (0.1%)
19	M	0.24	0/1868	0.47	0/2591
20	N	0.30	0/635	0.78	0/850
20	R	0.37	0/748	0.81	0/1000
21	O	0.36	0/588	0.83	0/788
21	S	0.31	0/692	0.69	0/924
22	P	0.35	0/711	0.68	0/959
23	Q	0.33	0/716	0.68	0/966
24	X	0.62	1/1159 (0.1%)	1.19	2/1789 (0.1%)
25	Y	0.56	0/894	0.96	0/1375
All	All	0.30	2/84258 (0.0%)	0.63	35/114335 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	208	PRO	CG-CD	-7.15	1.27	1.50
24	X	37	DT	C3'-O3'	5.43	1.51	1.44

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	F	750	ASP	CB-CG-OD2	9.38	126.75	118.30
4	5	208	PRO	N-CD-CG	-9.33	89.21	103.20
7	8	1680	LEU	CA-CB-CG	7.60	132.78	115.30
8	9	632	LEU	CA-CB-CG	7.50	132.55	115.30
8	9	650	ASP	CB-CG-OD2	7.41	124.97	118.30
12	D	262	ASP	CB-CG-OD1	7.32	124.89	118.30
6	7	629	ASP	CB-CG-OD1	7.24	124.82	118.30
11	C	96	ASP	CB-CG-OD1	6.50	124.15	118.30
4	5	208	PRO	CA-N-CD	-6.48	102.42	111.50
18	L	504	LEU	CB-CG-CD1	6.22	121.58	111.00
3	4	639	ASP	CB-CG-OD2	6.16	123.84	118.30
8	9	275	LEU	CA-CB-CG	6.13	129.41	115.30
14	G	530	ASP	CB-CG-OD2	6.10	123.79	118.30
7	8	1368	LEU	CA-CB-CG	6.00	129.11	115.30
13	E	152	LEU	CA-CB-CG	6.00	129.11	115.30
8	9	20	LEU	CA-CB-CG	5.99	129.06	115.30
8	9	626	LEU	CA-CB-CG	5.91	128.90	115.30
2	3	279	ASP	CB-CG-OD1	5.73	123.46	118.30
18	L	797	GLU	CA-CB-CG	5.66	125.85	113.40
18	L	797	GLU	N-CA-CB	5.66	120.78	110.60
4	5	634	LEU	CA-CB-CG	5.61	128.21	115.30
15	I	704	ALA	C-N-CA	5.51	135.47	121.70
15	I	556	ASP	CB-CG-OD1	5.36	123.12	118.30
3	4	210	ASP	CB-CG-OD1	5.32	123.09	118.30
6	7	695	LEU	CA-CB-CG	5.25	127.38	115.30
24	X	37	DT	P-O3'-C3'	5.25	126.00	119.70
5	6	162	GLU	CA-CB-CG	5.24	124.92	113.40
13	E	316	LEU	CA-CB-CG	5.24	127.34	115.30
3	4	272	MET	CB-CG-SD	5.18	127.95	112.40
12	D	129	MET	CA-CB-CG	5.16	122.07	113.30
5	6	798	ARG	NE-CZ-NH1	5.15	122.88	120.30
14	H	876	ASP	CB-CG-OD1	5.12	122.91	118.30
15	I	67	ASP	CB-CG-OD1	5.09	122.89	118.30
24	X	48	DT	O4'-C1'-N1	5.09	111.56	108.00
4	5	552	MET	CA-CB-CG	5.01	121.82	113.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	6161	0	6082	85	0
2	3	4795	0	4858	61	0
3	4	5269	0	5238	75	0
4	5	5376	0	5440	65	0
5	6	4991	0	5001	59	0
6	7	4919	0	4913	54	0
7	8	6945	0	7025	82	0
8	9	4594	0	4631	55	0
9	A	1611	0	1615	26	0
10	B	1609	0	1662	25	0
11	C	1379	0	1393	13	0
12	D	1988	0	1986	19	0
13	E	4550	0	4536	48	0
14	F	3404	0	3352	34	0
14	G	3380	0	3310	30	0
14	H	3411	0	3355	28	0
15	I	6057	0	6200	66	0
16	J	788	0	827	7	0
17	K	163	0	136	1	0
18	L	3474	0	3005	46	0
19	M	1876	0	802	2	0
20	N	629	0	668	12	0
20	R	741	0	791	20	0
21	O	583	0	626	14	0
21	S	684	0	732	16	0
22	P	703	0	737	10	0
23	Q	706	0	722	7	0
24	X	1041	0	593	4	0
25	Y	796	0	440	6	0
26	2	1	0	0	0	0
26	4	1	0	0	0	0
26	5	1	0	0	0	0
26	6	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	7	1	0	0	0	0
26	8	2	0	0	0	0
27	2	27	0	12	1	0
27	3	27	0	12	3	0
27	5	27	0	12	0	0
27	6	27	0	12	2	0
27	7	27	0	12	2	0
All	All	82765	0	80736	838	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 5.

All (838) 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)
18:L:874:GLU:HB3	18:L:884:ASP:O	1.83	0.78
7:8:2059:CYS:O	7:8:2063:LEU:HB2	1.89	0.71
7:8:1490:PHE:HB2	7:8:1498:PHE:HB2	1.73	0.68
3:4:563:ASN:H	3:4:703:ASP:HB2	1.60	0.67
6:7:614:GLU:O	6:7:618:TYR:HB2	1.93	0.67
1:2:129:ILE:HG21	15:I:204:LEU:HB2	1.78	0.66
4:5:717:GLU:O	4:5:721:ARG:HB2	1.95	0.66
14:F:730:LYS:HD3	14:F:817:ILE:HD11	1.77	0.66
18:L:515:ARG:HH12	18:L:890:LYS:HB3	1.61	0.66
5:6:601:LYS:HD3	5:6:643:LYS:HE3	1.79	0.65
14:F:619:THR:HG21	14:F:688:PHE:HA	1.78	0.64
8:9:362:LEU:HD11	8:9:376:ILE:HD12	1.80	0.64
1:2:341:CYS:HB3	1:2:344:CYS:SG	2.36	0.64
5:6:610:ALA:HA	5:6:624:GLU:O	1.99	0.63
7:8:2151:ARG:NH1	8:9:491:TRP:O	2.31	0.63
14:G:704:LEU:HB3	14:G:722:LEU:HB3	1.81	0.63
1:2:581:ARG:HH22	1:2:584:PRO:HD3	1.62	0.63
8:9:648:GLN:HA	8:9:660:ASN:O	1.99	0.63
3:4:304:ARG:HD3	3:4:423:LEU:HD11	1.81	0.62
21:O:78:LYS:HG3	23:Q:96:ARG:HH12	1.65	0.62
10:B:27:ILE:HG13	10:B:87:ILE:HA	1.82	0.62
18:L:678:LYS:HB2	18:L:700:ILE:HD12	1.80	0.62
2:3:457:LEU:HD21	2:3:497:ILE:HG21	1.81	0.62
4:5:769:ASN:ND2	7:8:1708:ASN:OD1	2.32	0.61
7:8:1457:LYS:O	7:8:1461:GLN:HB2	2.01	0.61
8:9:9:PRO:HB3	8:9:47:THR:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:L:797:GLU:HA	18:L:800:LYS:HG2	1.83	0.61
1:2:629:ILE:HB	1:2:640:LEU:HB2	1.82	0.60
7:8:1386:ASN:C	7:8:1386:ASN:HD22	2.04	0.60
18:L:667:ASP:H	18:L:720:LEU:HD11	1.65	0.60
6:7:465:ALA:HA	27:7:902:ADP:H5'2	1.83	0.60
5:6:570:ASN:HD22	5:6:678:ILE:H	1.50	0.60
1:2:136:GLN:HB3	1:2:139:ALA:HB2	1.84	0.60
8:9:673:MET:SD	8:9:684:GLN:NE2	2.74	0.60
8:9:307:ILE:HG22	8:9:339:PHE:HB3	1.84	0.60
15:I:768:LEU:HD21	16:J:130:VAL:HG12	1.83	0.60
20:R:121:GLN:H	20:R:124:ASP:HB2	1.65	0.60
15:I:634:ILE:HD11	15:I:641:ARG:HB3	1.84	0.60
7:8:1431:ILE:HG12	7:8:1436:ARG:HE	1.67	0.59
18:L:833:GLY:HA2	18:L:847:PRO:HD2	1.83	0.59
7:8:1673:ASP:OD1	7:8:1819:TRP:NE1	2.35	0.59
20:N:70:ARG:HH12	21:O:25:ASP:HA	1.67	0.59
3:4:178:ARG:NH1	15:I:383:VAL:O	2.34	0.59
23:Q:117:GLU:HG3	23:Q:120:ARG:HH12	1.66	0.59
3:4:428:ARG:HH22	5:6:372:SER:HB3	1.68	0.59
13:E:84:VAL:HG22	13:E:123:LEU:HD12	1.84	0.59
9:A:47:LEU:HD13	9:A:79:MET:HG2	1.85	0.59
15:I:40:ILE:HG22	15:I:42:PRO:HD2	1.85	0.59
1:2:569:GLN:OE1	1:2:613:ASN:ND2	2.35	0.59
1:2:618:THR:OG1	4:5:484:LYS:NZ	2.34	0.59
4:5:136:GLN:HB2	4:5:280:ARG:HE	1.68	0.59
7:8:1486:TYR:HB3	7:8:1502:PHE:HB3	1.84	0.59
18:L:837:VAL:HG11	20:R:113:ILE:HD13	1.85	0.59
20:R:121:GLN:HB2	20:R:124:ASP:H	1.68	0.58
1:2:662:PRO:HG3	1:2:850:LYS:HD2	1.85	0.58
6:7:584:ILE:HG23	6:7:586:LEU:H	1.66	0.58
20:N:110:LEU:HA	20:N:113:ILE:HG12	1.84	0.58
1:2:785:LYS:NZ	7:8:2087:GLU:OE1	2.36	0.58
13:E:526:ARG:HE	13:E:565:LEU:HB2	1.68	0.58
3:4:531:TYR:OH	3:4:723:HIS:ND1	2.37	0.58
18:L:871:CYS:HB3	18:L:914:LEU:HD11	1.85	0.58
7:8:2163:ARG:HE	7:8:2188:THR:HG22	1.66	0.58
18:L:868:VAL:HA	18:L:889:TYR:HA	1.85	0.58
18:L:722:SER:O	18:L:745:LYS:NZ	2.36	0.58
7:8:1421:GLU:OE1	8:9:594:GLN:NE2	2.37	0.58
21:S:27:ILE:HB	21:S:56:ARG:HD3	1.85	0.58
10:B:23:GLU:OE1	10:B:118:ASN:ND2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:489:THR:HG22	14:H:491:ARG:H	1.68	0.58
1:2:577:THR:HG23	1:2:629:ILE:HD12	1.86	0.57
1:2:341:CYS:CB	1:2:344:CYS:SG	2.92	0.57
7:8:1431:ILE:HG21	7:8:1436:ARG:HH21	1.69	0.57
2:3:417:GLN:HG2	27:3:1001:ADP:H5'2	1.86	0.57
8:9:493:SER:HB2	8:9:498:GLY:H	1.70	0.57
8:9:531:ARG:NH1	8:9:629:THR:O	2.37	0.57
15:I:422:GLN:HB3	15:I:425:LYS:HG2	1.86	0.57
18:L:854:GLN:HB3	18:L:861:LEU:HB3	1.85	0.57
27:3:1001:ADP:O2A	4:5:651:ARG:NH2	2.38	0.57
13:E:8:PHE:HB3	13:E:258:LEU:HD12	1.87	0.57
5:6:123:SER:HA	5:6:134:LYS:H	1.70	0.57
8:9:505:GLN:HB2	8:9:528:ASN:HB2	1.86	0.57
6:7:262:CYS:HB3	6:7:265:CYS:SG	2.44	0.57
6:7:422:ILE:HD13	6:7:469:LEU:HD21	1.86	0.57
10:B:34:ARG:HG3	10:B:64:VAL:HG22	1.87	0.56
11:C:166:LEU:HD13	11:C:169:LEU:HD12	1.87	0.56
11:C:188:LYS:O	11:C:192:PHE:HB2	2.05	0.56
6:7:451:ARG:HH12	6:7:455:ASN:HD21	1.53	0.56
14:G:510:GLN:NE2	14:G:511:TYR:O	2.38	0.56
1:2:631:ILE:O	1:2:637:VAL:HA	2.06	0.56
1:2:641:GLN:OE1	1:2:643:ARG:NH2	2.39	0.56
2:3:533:ILE:HD12	2:3:535:LEU:HB2	1.86	0.56
8:9:432:LEU:HB3	8:9:481:MET:HG2	1.88	0.56
20:R:62:LEU:O	21:S:37:ARG:NH1	2.38	0.56
9:A:150:ASP:OD1	12:D:141:ARG:NH1	2.38	0.56
14:H:493:TYR:HE2	14:H:768:LEU:HD13	1.69	0.56
3:4:204:LYS:HB3	3:4:221:ASP:HB3	1.88	0.56
8:9:221:ARG:NH2	8:9:627:ASP:OD2	2.38	0.56
1:2:119:ARG:NH1	15:I:278:ASP:OD2	2.39	0.56
5:6:443:LEU:HD21	5:6:448:LEU:HB2	1.88	0.56
20:R:62:LEU:HD22	21:S:38:LEU:HD23	1.88	0.56
1:2:426:VAL:HG22	1:2:456:ILE:HG12	1.88	0.56
1:2:438:LEU:O	1:2:442:ASN:HB2	2.06	0.56
1:2:613:ASN:O	1:2:617:ARG:N	2.36	0.56
2:3:45:ILE:HG12	2:3:92:LEU:HD13	1.88	0.56
16:J:123:PRO:HA	16:J:126:ARG:HD3	1.87	0.56
1:2:500:SER:HB2	1:2:757:PRO:HD2	1.88	0.55
2:3:216:ASP:HB2	6:7:370:LEU:HD12	1.88	0.55
3:4:349:CYS:HB2	3:4:371:CYS:SG	2.45	0.55
8:9:209:PRO:HB3	8:9:625:ASP:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:343:LYS:NZ	1:2:369:SER:OG	2.39	0.55
4:5:493:ILE:HG22	4:5:497:MET:HG3	1.87	0.55
4:5:497:MET:HG2	4:5:519:VAL:HG21	1.88	0.55
4:5:656:ILE:HA	4:5:659:ILE:HD12	1.87	0.55
14:H:601:ASN:HD21	14:H:605:VAL:HB	1.70	0.55
14:H:751:THR:HB	14:H:773:GLU:HB2	1.86	0.55
7:8:2101:LEU:HD22	7:8:2119:PHE:HB2	1.88	0.55
15:I:365:SER:HB3	15:I:373:ARG:HE	1.71	0.55
4:5:149:ARG:NH1	4:5:269:GLU:OE1	2.40	0.55
4:5:436:ALA:HA	4:5:476:VAL:O	2.07	0.55
13:E:303:THR:O	14:F:491:ARG:NH1	2.40	0.55
18:L:728:ILE:HG12	18:L:853:VAL:HG11	1.89	0.55
1:2:665:GLN:HG3	3:4:925:ARG:HH12	1.71	0.55
1:2:83:ALA:O	15:I:641:ARG:NH2	2.39	0.55
6:7:483:THR:HG1	6:7:493:LEU:N	2.05	0.55
7:8:1358:TYR:HB3	7:8:1397:LEU:HD11	1.87	0.55
14:G:716:SER:O	14:H:653:ARG:NH2	2.40	0.55
1:2:116:LEU:HD11	21:S:72:THR:HG21	1.87	0.55
7:8:2101:LEU:HD12	7:8:2200:VAL:HG12	1.88	0.55
22:P:104:ILE:HG22	21:S:99:TYR:HB2	1.89	0.55
14:G:584:THR:HB	14:G:587:ARG:H	1.71	0.55
20:R:130:ARG:HA	20:R:135:ARG:HD3	1.88	0.55
14:G:641:SER:HB3	14:G:648:LYS:HE2	1.88	0.54
2:3:455:ARG:HH12	24:X:51:DT:H1'	1.71	0.54
14:H:511:TYR:HB2	14:H:530:ASP:HB3	1.89	0.54
21:S:27:ILE:O	21:S:56:ARG:NH1	2.41	0.54
1:2:247:ARG:NH1	1:2:469:GLU:OE1	2.40	0.54
18:L:699:PHE:HB2	18:L:706:ARG:HB3	1.88	0.54
3:4:447:ASN:HB3	3:4:450:GLN:HB2	1.89	0.54
3:4:543:GLN:HE21	3:4:670:SER:HB2	1.73	0.54
3:4:594:LYS:NZ	6:7:535:THR:O	2.40	0.54
13:E:248:VAL:O	13:E:290:ARG:NH2	2.41	0.54
13:E:572:ILE:HD11	13:E:634:ARG:HH21	1.72	0.54
14:F:641:SER:OG	14:F:653:ARG:NH1	2.41	0.54
15:I:256:SER:O	15:I:260:ASN:ND2	2.41	0.54
2:3:433:THR:OG1	4:5:503:SER:OG	2.24	0.54
5:6:294:VAL:HB	5:6:391:PRO:HA	1.90	0.54
7:8:1524:ASN:ND2	7:8:1628:GLN:OE1	2.37	0.54
14:G:610:GLU:OE2	14:G:653:ARG:NH2	2.41	0.54
14:G:879:VAL:HG22	14:G:907:LEU:HD21	1.90	0.54
13:E:348:LEU:O	13:E:358:ARG:NH1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:412:VAL:HG13	4:5:552:MET:HB2	1.90	0.53
10:B:130:ALA:HB1	10:B:133:ASP:HB2	1.90	0.53
21:O:79:ARG:NH2	21:O:86:ASP:OD2	2.41	0.53
3:4:406:VAL:HG11	3:4:412:PRO:HG3	1.90	0.53
7:8:1353:ILE:HD12	7:8:1354:PRO:HD2	1.89	0.53
13:E:226:ARG:HG3	13:E:230:ILE:HD12	1.88	0.53
14:G:657:LEU:O	14:H:634:HIS:NE2	2.42	0.53
15:I:571:GLN:O	15:I:575:ASN:ND2	2.39	0.53
6:7:599:LEU:H	6:7:726:SER:HB3	1.73	0.53
7:8:1875:PRO:HA	7:8:1878:CYS:HB3	1.90	0.53
1:2:527:VAL:HB	1:2:531:HIS:HB3	1.90	0.53
3:4:914:ASP:OD2	5:6:696:ARG:NH1	2.38	0.53
11:C:169:LEU:HD22	11:C:173:GLU:HB3	1.91	0.53
21:O:27:ILE:O	21:O:56:ARG:NE	2.41	0.53
6:7:249:SER:O	6:7:311:GLN:NE2	2.40	0.53
7:8:1552:ILE:HG22	7:8:1553:LYS:HG2	1.91	0.53
5:6:336:PRO:O	15:I:223:ASN:ND2	2.41	0.53
7:8:1622:LEU:HD13	7:8:1627:TRP:HB2	1.91	0.53
1:2:321:THR:HG22	1:2:425:GLU:HG2	1.90	0.53
3:4:264:TYR:HE1	6:7:303:ARG:HD3	1.74	0.53
8:9:457:GLN:OE1	8:9:461:ASN:ND2	2.42	0.53
13:E:18:ASN:ND2	13:E:119:ASP:OD2	2.42	0.53
13:E:411:ARG:NH2	13:E:486:ASP:OD1	2.41	0.53
13:E:573:ASP:O	13:E:577:ASP:HA	2.08	0.53
1:2:113:ASP:O	1:2:117:ASN:ND2	2.42	0.53
5:6:103:VAL:HG22	15:I:422:GLN:HE22	1.74	0.53
14:G:617:ALA:HB3	14:G:628:VAL:HB	1.90	0.53
1:2:404:ARG:HD2	5:6:299:GLU:HG3	1.91	0.53
3:4:265:PRO:HB3	3:4:325:LEU:HD12	1.91	0.53
7:8:1613:VAL:HG12	7:8:1661:CYS:HA	1.91	0.53
15:I:93:ILE:HG12	15:I:174:LYS:HB3	1.91	0.53
2:3:104:ARG:NH2	2:3:105:GLU:OE2	2.40	0.52
2:3:447:THR:OG1	2:3:458:GLU:OE2	2.24	0.52
2:3:553:ILE:HG23	4:5:630:ARG:HE	1.73	0.52
5:6:258:GLN:O	15:I:242:ASN:ND2	2.41	0.52
3:4:854:LYS:HA	3:4:857:ILE:HG22	1.91	0.52
18:L:840:ARG:NH2	20:R:116:LYS:O	2.42	0.52
2:3:39:ARG:HG2	2:3:132:LEU:HD21	1.91	0.52
3:4:569:ASP:O	3:4:574:LYS:NZ	2.40	0.52
8:9:489:ASP:O	8:9:493:SER:OG	2.27	0.52
9:A:1:MET:SD	9:A:2:TYR:N	2.82	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:575:ASN:HA	15:I:578:LYS:HD3	1.91	0.52
4:5:454:GLN:NE2	4:5:465:GLU:OE1	2.43	0.52
8:9:319:TYR:HE2	8:9:601:LYS:HE2	1.74	0.52
13:E:52:GLN:NE2	13:E:264:GLU:OE2	2.42	0.52
13:E:123:LEU:HD13	13:E:255:ILE:HD11	1.90	0.52
1:2:528:ASN:ND2	4:5:584:GLN:OE1	2.42	0.52
3:4:315:ARG:HH22	3:4:412:PRO:HA	1.74	0.52
7:8:1543:ILE:HG22	7:8:1547:SER:HB2	1.92	0.52
11:C:30:LEU:HD12	11:C:46:LEU:HD22	1.92	0.52
15:I:566:SER:HA	15:I:613:ILE:HG23	1.92	0.52
4:5:654:GLU:HA	4:5:657:ILE:HD12	1.92	0.52
6:7:429:LYS:HD2	6:7:432:LEU:HD12	1.91	0.52
13:E:313:PRO:HA	13:E:414:GLY:HA2	1.90	0.52
23:Q:119:THR:HA	23:Q:122:VAL:HG12	1.91	0.52
1:2:558:LYS:HD2	5:6:562:GLY:HA3	1.91	0.52
5:6:409:GLN:NE2	5:6:418:SER:O	2.43	0.52
8:9:165:ASP:OD2	8:9:167:ARG:NH1	2.43	0.52
14:H:617:ALA:HB3	14:H:628:VAL:HB	1.91	0.52
13:E:145:ASP:OD1	13:E:249:ASN:ND2	2.42	0.52
20:R:107:ASP:OD2	20:R:132:ARG:NH1	2.43	0.52
10:B:115:LEU:HD11	10:B:148:LEU:HD13	1.91	0.51
14:F:617:ALA:HB3	14:F:628:VAL:HB	1.92	0.51
5:6:266:SER:HB3	5:6:458:HIS:HB2	1.93	0.51
11:C:135:LEU:HD11	11:C:177:TYR:HB2	1.92	0.51
14:H:489:THR:HG23	14:H:491:ARG:HH21	1.75	0.51
15:I:161:LEU:HD22	15:I:248:ILE:HD13	1.90	0.51
1:2:113:ASP:OD1	21:S:73:TYR:OH	2.25	0.51
1:2:230:ARG:NH1	1:2:243:GLU:O	2.43	0.51
3:4:802:ILE:HD11	5:6:732:VAL:HG12	1.92	0.51
13:E:554:GLU:HG2	13:E:587:ARG:HH21	1.75	0.51
16:J:76:ILE:HD12	16:J:91:ILE:HD13	1.92	0.51
1:2:262:LYS:NZ	5:6:257:GLU:OE2	2.43	0.51
5:6:303:GLU:HG3	5:6:356:TRP:HB2	1.92	0.51
7:8:1908:LEU:HD23	7:8:1965:LEU:HD22	1.92	0.51
13:E:75:ASP:O	13:E:118:ARG:NH2	2.43	0.51
13:E:365:ARG:NH1	13:E:399:TYR:OH	2.43	0.51
3:4:315:ARG:O	6:7:341:ARG:NH1	2.44	0.51
3:4:587:ARG:NH2	3:4:623:LEU:O	2.43	0.51
6:7:618:TYR:HA	6:7:621:MET:HG2	1.92	0.51
11:C:134:GLU:OE2	11:C:138:HIS:NE2	2.43	0.51
15:I:27:LEU:HD23	15:I:58:LEU:HD22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:401:ARG:NH1	15:I:402:ILE:O	2.44	0.51
18:L:940:ASP:HB3	18:L:943:GLN:HB3	1.92	0.51
20:N:70:ARG:HB2	20:N:73:ARG:HH21	1.75	0.51
2:3:203:ALA:O	2:3:207:GLY:N	2.44	0.51
2:3:501:GLY:O	6:7:247:ARG:NH2	2.44	0.51
15:I:192:LEU:HD21	21:S:75:GLU:HG3	1.93	0.51
15:I:467:MET:HG3	15:I:472:GLN:HE21	1.76	0.51
3:4:268:VAL:HA	3:4:271:ILE:HD12	1.93	0.51
7:8:1366:MET:HG3	7:8:1368:LEU:HD22	1.92	0.51
18:L:749:LEU:HA	18:L:754:LYS:HA	1.93	0.51
18:L:869:GLU:HB2	18:L:890:LYS:HA	1.93	0.51
21:S:71:VAL:HA	21:S:74:THR:HG22	1.93	0.51
1:2:578:ALA:HB3	1:2:631:ILE:HD11	1.93	0.51
7:8:1908:LEU:HD21	7:8:1964:MET:HB3	1.93	0.51
9:A:193:GLN:O	9:A:197:GLU:HB2	2.11	0.51
14:F:572:LEU:HD22	14:F:576:GLU:HG2	1.93	0.51
4:5:639:GLU:OE2	4:5:750:LYS:NZ	2.44	0.50
5:6:570:ASN:HA	5:6:678:ILE:O	2.11	0.50
7:8:1585:GLY:O	7:8:1587:GLN:NE2	2.44	0.50
18:L:874:GLU:OE1	18:L:924:SER:OG	2.29	0.50
2:3:483:ARG:HD3	2:3:535:LEU:HD22	1.92	0.50
3:4:292:ASP:OD1	3:4:292:ASP:N	2.44	0.50
3:4:348:LYS:NZ	3:4:353:ASP:OD1	2.41	0.50
4:5:143:ALA:O	4:5:161:ARG:NH1	2.42	0.50
9:A:77:LEU:HD21	11:C:53:ILE:HD11	1.93	0.50
14:F:728:ILE:HD11	14:F:742:VAL:HG23	1.93	0.50
18:L:504:LEU:HA	18:L:507:LYS:HG2	1.93	0.50
18:L:877:GLN:NE2	18:L:925:THR:O	2.43	0.50
7:8:1432:THR:OG1	7:8:1435:GLN:OE1	2.25	0.50
8:9:643:ASP:HB3	8:9:660:ASN:HD21	1.76	0.50
10:B:152:ARG:NH1	10:B:177:GLU:OE1	2.44	0.50
11:C:27:LEU:HB3	11:C:30:LEU:HD23	1.93	0.50
18:L:682:GLN:HA	18:L:695:PRO:HB3	1.94	0.50
4:5:685:GLN:HA	4:5:689:MET:HB2	1.93	0.50
7:8:1795:LEU:HD13	7:8:1816:LEU:HD13	1.93	0.50
21:O:74:THR:HG21	21:O:82:VAL:HA	1.92	0.50
2:3:279:ASP:OD1	2:3:280:ASP:N	2.42	0.50
5:6:613:VAL:O	5:6:621:TYR:HA	2.12	0.50
8:9:75:ARG:NH1	8:9:86:GLU:OE2	2.45	0.50
1:2:152:ARG:NH2	15:I:50:ASP:OD2	2.44	0.50
2:3:671:LEU:HG	2:3:676:ILE:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:108:HIS:O	10:B:155:LYS:NZ	2.38	0.50
1:2:738:LEU:N	1:2:742:GLN:OE1	2.45	0.50
2:3:175:HIS:HA	2:3:178:LYS:HD2	1.92	0.50
2:3:389:VAL:HG12	2:3:710:THR:HG21	1.93	0.50
10:B:82:GLN:HB3	10:B:84:LYS:HG2	1.94	0.50
12:D:171:LEU:HD23	12:D:175:LEU:HD22	1.93	0.50
13:E:589:PRO:HG2	13:E:592:LEU:HD23	1.94	0.50
1:2:618:THR:HB	1:2:621:HIS:HE1	1.77	0.50
2:3:394:GLU:HB2	6:7:624:LYS:HB2	1.93	0.50
8:9:26:SER:OG	9:A:198:ARG:NH1	2.44	0.50
18:L:578:TYR:HA	18:L:596:PHE:HA	1.94	0.50
18:L:682:GLN:OE1	18:L:762:ARG:NH2	2.44	0.50
1:2:772:THR:HG23	1:2:773:LYS:HG2	1.92	0.50
2:3:708:LEU:O	2:3:711:ALA:HB3	2.12	0.50
10:B:20:VAL:HG11	10:B:121:VAL:HG21	1.94	0.50
1:2:394:PRO:HB2	5:6:672:LEU:HD21	1.94	0.49
6:7:114:THR:HG23	6:7:202:LEU:HD23	1.95	0.49
6:7:262:CYS:CB	6:7:265:CYS:SG	3.00	0.49
13:E:224:LYS:O	13:E:228:LYS:HB2	2.12	0.49
2:3:39:ARG:HE	2:3:132:LEU:HD11	1.77	0.49
15:I:368:THR:OG1	15:I:370:ASP:O	2.25	0.49
1:2:84:ALA:HA	15:I:641:ARG:HH12	1.77	0.49
1:2:118:GLU:OE2	1:2:121:ARG:NH2	2.38	0.49
6:7:495:ALA:HB3	6:7:546:ILE:HG21	1.92	0.49
7:8:1647:SER:HA	7:8:1650:ILE:HD12	1.95	0.49
7:8:2076:ARG:NH2	7:8:2087:GLU:O	2.45	0.49
13:E:127:ARG:HD2	13:E:248:VAL:HG22	1.93	0.49
7:8:1476:TYR:HE2	7:8:1653:SER:HB3	1.77	0.49
7:8:2119:PHE:HZ	7:8:2142:LEU:HD22	1.77	0.49
9:A:146:LEU:HD23	9:A:151:LEU:HD21	1.93	0.49
15:I:104:LYS:HD3	17:K:340:SER:HA	1.94	0.49
8:9:185:PRO:HA	8:9:188:MET:HA	1.95	0.49
12:D:199:LEU:HD22	12:D:207:GLN:HA	1.94	0.49
7:8:1524:ASN:HB3	7:8:1527:SER:HB3	1.95	0.49
15:I:398:TRP:HD1	16:J:106:ALA:HA	1.77	0.49
15:I:649:THR:HB	15:I:653:ARG:HH12	1.77	0.49
2:3:411:PRO:HG3	4:5:545:THR:HG22	1.94	0.49
3:4:792:THR:N	3:4:844:LYS:O	2.45	0.49
4:5:375:ALA:HB3	4:5:385:LYS:HE2	1.94	0.49
6:7:700:ALA:HB2	6:7:708:VAL:HG22	1.94	0.49
8:9:271:ILE:HA	8:9:274:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:48:SER:OG	21:S:49:GLY:N	2.46	0.49
9:A:171:ALA:HB3	9:A:183:LEU:HG	1.94	0.49
14:H:665:ASN:O	14:H:670:LYS:NZ	2.46	0.49
1:2:147:LEU:HD11	15:I:20:LEU:HD12	1.94	0.49
3:4:202:LYS:HG2	3:4:224:LEU:HD23	1.95	0.49
3:4:449:ARG:NH2	24:X:46:DT:O5'	2.39	0.49
7:8:1858:ILE:HG22	7:8:1868:ILE:HG22	1.95	0.49
8:9:491:TRP:CD1	8:9:506:ASP:HB2	2.47	0.49
13:E:93:GLU:HA	13:E:98:ILE:HB	1.95	0.49
14:H:490:ASP:OD1	14:H:490:ASP:N	2.44	0.49
3:4:178:ARG:HD3	15:I:385:GLU:HG2	1.94	0.49
3:4:621:LEU:HD13	3:4:648:VAL:HG21	1.95	0.49
3:4:774:TYR:OH	3:4:778:ARG:NH1	2.45	0.49
6:7:479:ARG:NH2	6:7:517:ASP:OD1	2.46	0.49
8:9:609:GLN:HG3	8:9:614:PRO:HG3	1.95	0.49
3:4:304:ARG:HB3	3:4:465:HIS:HD2	1.78	0.48
14:F:533:GLY:O	14:F:548:GLN:NE2	2.46	0.48
1:2:181:LEU:O	1:2:209:ARG:NH2	2.44	0.48
7:8:1709:THR:O	7:8:1713:MET:HB3	2.13	0.48
8:9:171:LYS:HG2	8:9:533:ALA:HB3	1.96	0.48
18:L:882:ASN:HB2	18:L:901:THR:HA	1.94	0.48
5:6:262:VAL:HG21	5:6:354:LEU:HD21	1.95	0.48
7:8:1539:LYS:NZ	7:8:1641:SER:OG	2.43	0.48
18:L:733:LYS:O	18:L:830:ARG:NH1	2.46	0.48
1:2:811:GLU:HB3	1:2:815:ARG:NH1	2.28	0.48
3:4:465:HIS:HE1	3:4:467:LYS:HE2	1.79	0.48
4:5:343:TRP:HE1	4:5:435:ILE:HD11	1.78	0.48
4:5:407:ARG:HA	4:5:500:GLN:HE21	1.78	0.48
6:7:435:LEU:HD13	6:7:456:VAL:HG12	1.96	0.48
7:8:1356:THR:O	7:8:1436:ARG:NH2	2.47	0.48
1:2:237:MET:SD	1:2:237:MET:N	2.85	0.48
2:3:698:THR:HG22	2:3:700:ARG:H	1.78	0.48
3:4:254:THR:HA	3:4:257:LEU:HD13	1.96	0.48
6:7:619:VAL:HA	6:7:626:PRO:HG3	1.94	0.48
14:G:737:THR:OG1	14:G:739:ASP:OD1	2.32	0.48
18:L:757:ASP:N	18:L:757:ASP:OD1	2.46	0.48
2:3:203:ALA:O	2:3:207:GLY:CA	2.62	0.48
20:R:120:ILE:HD11	21:S:47:ILE:HG13	1.96	0.48
5:6:440:LEU:HB2	5:6:443:LEU:HB2	1.95	0.48
7:8:1966:LYS:HD2	7:8:2006:LEU:HD21	1.95	0.48
9:A:186:ASP:HB3	13:E:478:TRP:HD1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:335:TYR:HD1	13:E:363:PHE:HE2	1.60	0.48
15:I:287:LEU:HD13	15:I:456:VAL:HG11	1.96	0.48
1:2:667:VAL:HG21	1:2:674:LEU:HD11	1.94	0.48
4:5:663:LEU:HD23	4:5:666:LEU:HD11	1.96	0.48
9:A:84:ARG:NH2	11:C:8:ASP:OD2	2.46	0.48
14:G:560:ASP:OD1	14:G:560:ASP:N	2.45	0.48
14:H:671:ASP:OD1	14:H:671:ASP:N	2.47	0.48
7:8:1412:GLU:OE1	8:9:667:ASN:ND2	2.47	0.48
15:I:364:LEU:HB2	15:I:382:LEU:HD23	1.96	0.48
2:3:344:ASP:OD1	2:3:344:ASP:N	2.47	0.48
2:3:432:THR:OG1	2:3:437:SER:OG	2.29	0.48
3:4:568:GLY:HA2	3:4:709:LEU:HD12	1.95	0.48
5:6:259:THR:HB	5:6:352:ARG:HD2	1.96	0.48
9:A:102:TRP:NE1	9:A:134:TYR:OH	2.43	0.48
12:D:69:ASN:HA	12:D:293:LEU:HB2	1.96	0.48
1:2:618:THR:HB	1:2:621:HIS:CE1	2.48	0.47
3:4:544:LEU:HD21	3:4:581:VAL:HG23	1.97	0.47
7:8:1444:SER:HB2	7:8:1471:ALA:HB3	1.96	0.47
8:9:364:LEU:HD13	8:9:634:PRO:HG3	1.96	0.47
13:E:573:ASP:O	13:E:577:ASP:CA	2.62	0.47
14:H:726:MET:HG3	14:H:730:LYS:HE3	1.96	0.47
13:E:573:ASP:O	13:E:577:ASP:N	2.47	0.47
20:N:110:LEU:HD21	20:R:130:ARG:HH22	1.80	0.47
2:3:433:THR:HG1	4:5:503:SER:HG	1.57	0.47
5:6:177:PHE:HA	5:6:180:PHE:HD2	1.80	0.47
5:6:361:ILE:HD11	5:6:377:LEU:HD23	1.96	0.47
14:F:535:ASP:OD1	14:F:535:ASP:N	2.48	0.47
18:L:670:ILE:H	18:L:703:ASN:HD21	1.62	0.47
6:7:526:PHE:HB3	6:7:567:ALA:HB2	1.96	0.47
20:N:121:GLN:N	20:N:124:ASP:OD2	2.46	0.47
1:2:508:HIS:HB3	1:2:511:ILE:HB	1.97	0.47
2:3:187:THR:HG22	2:3:188:LYS:HG3	1.97	0.47
4:5:166:ILE:HD12	4:5:256:LEU:HD23	1.97	0.47
7:8:1705:PHE:HZ	7:8:2159:ILE:HD13	1.80	0.47
7:8:1795:LEU:HD11	7:8:1813:VAL:HG23	1.95	0.47
11:C:88:ILE:HG23	11:C:127:LEU:HD13	1.96	0.47
1:2:95:GLN:OE1	20:R:73:ARG:NH1	2.48	0.47
3:4:643:SER:HA	5:6:601:LYS:HE2	1.95	0.47
4:5:433:SER:HB3	4:5:436:ALA:HB2	1.97	0.47
7:8:2048:LYS:HA	7:8:2048:LYS:HD3	1.70	0.47
10:B:174:SER:HB3	10:B:177:GLU:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:53:ILE:HG22	11:C:56:ILE:HD12	1.97	0.47
1:2:562:ARG:HH21	1:2:600:ASP:H	1.62	0.47
2:3:569:HIS:NE2	4:5:654:GLU:OE1	2.43	0.47
3:4:254:THR:HG22	3:4:257:LEU:HD22	1.96	0.47
8:9:18:ARG:HH22	9:A:176:THR:H	1.63	0.47
15:I:441:ILE:HG23	15:I:482:PHE:HE1	1.80	0.47
3:4:532:GLU:O	3:4:537:LYS:NZ	2.37	0.47
14:H:775:GLU:OE1	14:H:777:ARG:NH2	2.48	0.47
18:L:852:LEU:HB3	18:L:863:ILE:HB	1.96	0.47
2:3:524:ASP:OD1	2:3:524:ASP:N	2.42	0.47
3:4:622:VAL:HG21	3:4:665:LEU:HB3	1.97	0.47
8:9:171:LYS:NZ	8:9:366:GLY:O	2.45	0.47
14:F:698:PHE:CG	14:F:744:PRO:HG3	2.50	0.47
18:L:831:ASP:OD1	18:L:831:ASP:N	2.47	0.47
1:2:696:ALA:HB3	5:6:774:VAL:HG23	1.98	0.46
2:3:122:ILE:HG23	2:3:155:LEU:HD12	1.97	0.46
7:8:1741:VAL:HG13	7:8:1795:LEU:HD21	1.96	0.46
12:D:205:GLU:HB3	12:D:206:LEU:HD12	1.97	0.46
15:I:184:LEU:HA	15:I:187:ILE:HB	1.97	0.46
22:P:78:THR:HG23	22:P:79:ARG:HG2	1.97	0.46
7:8:1356:THR:HB	7:8:1436:ARG:HH12	1.80	0.46
12:D:156:LEU:HA	12:D:159:ARG:HG2	1.98	0.46
14:F:818:PRO:HG2	14:F:821:MET:HG2	1.97	0.46
18:L:732:CYS:HB2	18:L:738:VAL:HB	1.96	0.46
6:7:335:VAL:HG12	6:7:378:ALA:HB3	1.96	0.46
7:8:1324:VAL:HA	7:8:1340:VAL:HG12	1.97	0.46
7:8:1557:ASN:OD1	7:8:1558:PHE:N	2.48	0.46
7:8:1719:PRO:HD3	7:8:1841:LYS:HE2	1.98	0.46
7:8:1729:ASN:ND2	7:8:1870:THR:O	2.48	0.46
12:D:92:SER:O	12:D:96:GLN:OE1	2.32	0.46
13:E:470:ARG:NH2	13:E:623:ASP:OD2	2.41	0.46
18:L:863:ILE:HD11	18:L:897:THR:HG21	1.97	0.46
1:2:305:SER:OG	1:2:392:GLU:OE2	2.31	0.46
3:4:639:ASP:HA	3:4:642:ARG:HE	1.79	0.46
4:5:48:ASP:OD2	4:5:52:ASN:ND2	2.47	0.46
5:6:835:ILE:HG23	5:6:836:ILE:HG23	1.97	0.46
6:7:17:LEU:HD13	6:7:113:PHE:HZ	1.81	0.46
7:8:1710:SER:O	7:8:1714:ASN:HB2	2.16	0.46
7:8:2202:LYS:HG2	7:8:2206:LYS:HE2	1.96	0.46
1:2:693:GLU:HB2	5:6:778:LYS:HE3	1.97	0.46
4:5:682:ARG:HG3	7:8:2182:ALA:HB1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:524:ILE:HG23	13:E:525:TYR:HD1	1.81	0.46
15:I:286:LEU:HD23	15:I:452:LEU:HD13	1.98	0.46
16:J:51:GLN:HE22	25:Y:27:DA:H4'	1.81	0.46
7:8:1706:ASP:HB3	7:8:1709:THR:HG22	1.98	0.46
7:8:1913:ASP:OD1	7:8:1913:ASP:N	2.48	0.46
14:G:584:THR:HG22	14:G:586:VAL:H	1.80	0.46
15:I:404:LYS:HG3	15:I:406:HIS:H	1.80	0.46
1:2:66:GLU:OE1	20:R:121:GLN:NE2	2.48	0.46
1:2:330:VAL:HG13	1:2:415:VAL:HG21	1.97	0.46
4:5:287:ILE:HD11	4:5:342:ILE:HA	1.97	0.46
4:5:715:GLU:HG2	4:5:755:LEU:HD21	1.98	0.46
5:6:610:ALA:HB1	5:6:623:ILE:HG23	1.97	0.46
8:9:400:VAL:HA	8:9:673:MET:O	2.16	0.46
15:I:164:LYS:HD2	15:I:215:ILE:HB	1.97	0.46
18:L:766:ASP:OD1	18:L:766:ASP:N	2.49	0.46
21:O:48:SER:OG	21:O:49:GLY:N	2.48	0.46
23:Q:97:GLU:HA	23:Q:100:THR:HG22	1.98	0.46
3:4:628:VAL:HA	3:4:670:SER:O	2.16	0.46
5:6:615:ASP:OD1	5:6:615:ASP:N	2.48	0.46
6:7:122:ASP:OD2	6:7:198:ARG:NH1	2.49	0.46
6:7:453:ASP:O	6:7:694:ARG:NH1	2.49	0.46
13:E:397:ASP:OD1	13:E:402:GLN:NE2	2.48	0.46
14:G:671:ASP:OD1	14:G:671:ASP:N	2.48	0.46
14:G:707:LEU:HG	14:G:710:TRP:HB3	1.96	0.46
14:H:862:TYR:OH	14:H:888:GLU:OE2	2.33	0.46
9:A:149:ILE:HD13	12:D:140:ILE:HG22	1.98	0.46
13:E:382:HIS:HA	13:E:385:LYS:HG2	1.98	0.46
14:H:707:LEU:HG	14:H:710:TRP:HB3	1.97	0.46
15:I:14:ASP:N	15:I:14:ASP:OD1	2.46	0.46
18:L:749:LEU:HB3	18:L:754:LYS:HG3	1.97	0.46
22:P:56:VAL:HG21	23:Q:102:VAL:HG21	1.97	0.46
6:7:496:ALA:HB1	6:7:550:LYS:HZ1	1.80	0.46
7:8:1737:ASP:HB3	7:8:1899:ASP:HB2	1.98	0.46
8:9:433:ILE:HG12	8:9:482:ILE:HB	1.97	0.46
12:D:128:CYS:O	12:D:132:GLU:HB2	2.16	0.46
13:E:66:GLU:OE2	13:E:70:HIS:NE2	2.48	0.46
21:S:30:ILE:HD11	21:S:59:LEU:HD22	1.98	0.46
5:6:511:ASP:OD1	5:6:511:ASP:N	2.47	0.45
7:8:1851:PHE:HD2	7:8:1868:ILE:HG21	1.81	0.45
3:4:535:ASP:HA	3:4:538:LYS:HG2	1.97	0.45
5:6:673:ASN:OD1	5:6:675:ARG:NE	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:149:ARG:NH2	15:I:372:THR:OG1	2.39	0.45
6:7:454:ILE:HG12	6:7:694:ARG:HB3	1.97	0.45
9:A:186:ASP:O	13:E:478:TRP:NE1	2.47	0.45
11:C:58:GLY:HA3	11:C:70:PRO:HA	1.98	0.45
13:E:84:VAL:HA	13:E:123:LEU:HB2	1.98	0.45
14:F:867:LEU:HD11	14:F:894:ALA:HB1	1.97	0.45
14:H:722:LEU:HD12	14:H:776:ILE:HA	1.96	0.45
2:3:440:VAL:HG11	24:X:53:DT:H3'	1.98	0.45
3:4:376:CYS:SG	3:4:377:ASN:N	2.89	0.45
4:5:47:ARG:NH2	10:B:150:GLU:OE1	2.44	0.45
8:9:25:LEU:HA	8:9:29:TYR:HD2	1.81	0.45
1:2:175:ASP:HB3	1:2:178:ARG:HB3	1.99	0.45
7:8:1710:SER:O	7:8:1714:ASN:CB	2.65	0.45
8:9:387:LEU:HD23	8:9:390:LEU:HD21	1.97	0.45
14:F:610:GLU:HG3	14:H:717:LYS:HB2	1.99	0.45
18:L:734:GLY:HA3	18:L:830:ARG:HH22	1.81	0.45
6:7:703:ARG:NH2	6:7:712:ASP:OD2	2.44	0.45
8:9:318:HIS:CE1	8:9:346:LEU:HB2	2.52	0.45
10:B:15:GLU:OE2	12:D:71:ARG:NH2	2.49	0.45
10:B:57:ASP:OD1	10:B:57:ASP:N	2.46	0.45
12:D:192:LYS:HE2	12:D:192:LYS:HB3	1.84	0.45
20:N:96:SER:HB2	21:O:91:LEU:HD11	1.98	0.45
1:2:173:ASP:OD1	1:2:173:ASP:N	2.49	0.45
3:4:254:THR:O	3:4:257:LEU:HB2	2.16	0.45
5:6:608:LEU:HD21	5:6:638:ILE:HD13	1.99	0.45
8:9:300:ASP:OD1	8:9:303:GLY:N	2.49	0.45
15:I:471:GLU:HA	15:I:474:GLU:HG2	1.97	0.45
20:N:123:LYS:HG3	20:R:114:HIS:HE1	1.82	0.45
1:2:387:ARG:HH12	4:5:320:GLY:HA3	1.82	0.45
9:A:185:LYS:HD3	13:E:471:LYS:HD2	1.97	0.45
14:G:502:VAL:HG13	14:G:515:VAL:HG12	1.98	0.45
18:L:830:ARG:HG2	18:L:846:MET:HE1	1.99	0.45
20:N:71:LEU:HD11	21:O:30:ILE:HD11	1.97	0.45
2:3:229:ALA:HB2	6:7:370:LEU:HD23	1.99	0.45
2:3:400:ARG:NH2	2:3:490:MET:O	2.50	0.45
3:4:256:ASP:N	3:4:256:ASP:OD1	2.49	0.45
3:4:345:ALA:HB3	3:4:358:VAL:HG23	1.98	0.45
3:4:603:ALA:HA	3:4:618:SER:HA	1.98	0.45
4:5:359:GLN:OE1	4:5:362:ARG:NH2	2.49	0.45
13:E:28:VAL:HG22	13:E:57:GLN:HB3	1.99	0.45
1:2:477:THR:HG23	1:2:480:GLU:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:172:THR:OG1	4:5:252:ASP:OD2	2.34	0.45
2:3:276:VAL:HG22	2:3:321:ILE:HB	1.99	0.45
2:3:434:GLY:HA2	2:3:478:MET:SD	2.57	0.45
9:A:107:LEU:HB3	9:A:201:GLN:HG2	1.97	0.45
12:D:15:GLU:O	14:F:893:ARG:NH1	2.50	0.45
14:H:542:LYS:HG3	14:H:585:PRO:HB3	1.99	0.45
20:R:118:VAL:HG12	21:S:46:ARG:HG2	1.98	0.45
1:2:431:LYS:HE3	1:2:431:LYS:HB2	1.82	0.45
3:4:399:LEU:O	3:4:414:SER:HA	2.17	0.45
4:5:337:VAL:HG23	4:5:600:LYS:HD3	1.99	0.45
4:5:407:ARG:HG2	4:5:409:ASP:H	1.82	0.45
5:6:798:ARG:HH11	5:6:798:ARG:HG2	1.81	0.45
7:8:1565:ASP:OD1	7:8:1565:ASP:N	2.49	0.45
13:E:509:THR:HG21	13:E:539:TYR:HE2	1.81	0.45
14:H:776:ILE:HD11	14:H:833:LEU:HD11	1.99	0.45
4:5:587:GLN:NE2	4:5:593:GLU:OE2	2.50	0.44
5:6:121:ASP:O	5:6:161:ARG:NH1	2.50	0.44
8:9:40:ALA:HB2	8:9:81:GLN:HG3	2.00	0.44
8:9:382:ASP:OD1	8:9:382:ASP:N	2.48	0.44
14:F:502:VAL:HG22	14:F:515:VAL:HG13	1.99	0.44
14:G:897:ALA:HA	14:G:900:LYS:HE3	1.99	0.44
18:L:926:ILE:HD12	20:R:59:THR:HG22	2.00	0.44
1:2:76:ASP:N	1:2:76:ASP:OD1	2.50	0.44
2:3:701:THR:O	2:3:704:THR:HB	2.17	0.44
3:4:189:GLU:O	3:4:193:ASN:ND2	2.50	0.44
5:6:102:LYS:HZ3	15:I:236:ILE:HD11	1.81	0.44
6:7:614:GLU:O	6:7:618:TYR:CB	2.65	0.44
7:8:1351:PHE:HE2	7:8:1468:LEU:HD11	1.81	0.44
8:9:197:LYS:HA	8:9:205:ALA:HB1	1.99	0.44
14:G:750:ASP:HA	14:G:776:ILE:HD12	1.99	0.44
22:P:104:ILE:HD12	23:Q:65:ILE:HD13	1.99	0.44
6:7:204:PHE:H	6:7:379:GLN:HB3	1.82	0.44
7:8:1387:PRO:HB3	7:8:1780:HIS:HB3	2.00	0.44
10:B:132:ASP:OD1	10:B:132:ASP:N	2.49	0.44
12:D:186:HIS:HA	12:D:189:ILE:HG22	1.98	0.44
14:G:495:THR:OG1	14:G:537:CYS:O	2.34	0.44
15:I:217:PRO:HD3	15:I:248:ILE:HG21	1.99	0.44
2:3:112:SER:O	2:3:116:VAL:HB	2.17	0.44
3:4:178:ARG:HG2	15:I:366:ILE:HG22	2.00	0.44
5:6:134:LYS:HB3	5:6:137:ARG:HG3	2.00	0.44
5:6:566:ARG:NH1	5:6:570:ASN:OD1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:9:225:THR:HG22	8:9:285:LEU:HD11	1.98	0.44
1:2:585:ILE:HG22	1:2:586:THR:HG23	2.00	0.44
1:2:620:ILE:HD12	1:2:646:ILE:HD13	1.99	0.44
5:6:545:LYS:HE3	5:6:830:LEU:HD21	1.99	0.44
7:8:1446:THR:HG23	7:8:1471:ALA:HB2	1.99	0.44
14:F:634:HIS:NE2	14:H:657:LEU:O	2.48	0.44
15:I:510:PHE:HE1	15:I:539:LEU:HD11	1.82	0.44
19:M:9:TYR:HA	19:M:16:SER:HA	1.99	0.44
1:2:311:GLU:HA	1:2:314:LEU:HD23	1.99	0.44
1:2:472:ASP:HB3	1:2:475:SER:HB2	1.98	0.44
2:3:215:THR:HG21	2:3:224:ARG:HD2	1.98	0.44
7:8:1416:SER:OG	7:8:1417:ILE:N	2.50	0.44
20:R:72:VAL:HG21	20:R:93:LEU:HD13	1.98	0.44
2:3:700:ARG:NH1	27:7:902:ADP:O3'	2.50	0.44
1:2:249:LEU:HB3	1:2:257:ALA:HB2	2.00	0.44
2:3:167:SER:HB3	2:3:170:THR:HG22	2.00	0.44
4:5:149:ARG:HG2	4:5:266:PRO:HG3	1.99	0.44
6:7:497:VAL:O	6:7:550:LYS:NZ	2.49	0.44
18:L:737:ILE:HD12	18:L:761:TYR:HB2	2.00	0.44
1:2:623:ALA:HB2	1:2:629:ILE:HD11	2.00	0.44
3:4:178:ARG:HB3	15:I:364:LEU:HD11	1.98	0.44
13:E:1:MET:HB2	13:E:148:VAL:HG21	2.00	0.44
19:M:418:SER:H	19:M:441:LEU:HA	1.83	0.44
4:5:724:ILE:HB	7:8:1842:LYS:HE2	2.00	0.43
5:6:500:ASP:HB3	5:6:503:VAL:HG22	2.00	0.43
5:6:595:SER:HA	5:6:635:ILE:O	2.18	0.43
10:B:92:TRP:HA	10:B:97:GLU:HG2	1.99	0.43
10:B:178:ILE:O	10:B:182:ARG:HB2	2.18	0.43
13:E:148:VAL:HG23	13:E:152:LEU:HD23	1.99	0.43
20:N:67:PRO:O	21:O:26:ASN:ND2	2.51	0.43
5:6:765:LEU:HD21	5:6:804:ILE:HD11	2.00	0.43
4:5:294:ILE:HG12	4:5:333:ILE:HD13	1.99	0.43
5:6:92:PHE:HE2	5:6:336:PRO:HB2	1.82	0.43
7:8:2037:ILE:HD12	7:8:2038:PRO:HD2	1.99	0.43
14:G:490:ASP:OD1	14:G:490:ASP:N	2.50	0.43
14:G:819:VAL:HG23	14:G:868:ARG:HH22	1.81	0.43
15:I:419:LEU:HD13	15:I:477:LEU:HD11	2.00	0.43
5:6:196:LEU:HG	5:6:263:PHE:HZ	1.84	0.43
8:9:657:LYS:HB2	8:9:680:LYS:HE2	1.99	0.43
9:A:54:LEU:HD11	9:A:71:GLN:HE21	1.84	0.43
13:E:64:TYR:N	13:E:623:ASP:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:131:LEU:HD21	13:E:152:LEU:HD11	2.00	0.43
1:2:663:LEU:HD22	1:2:848:ALA:HB1	2.00	0.43
2:3:284:ASP:OD2	6:7:329:ARG:NH2	2.52	0.43
3:4:399:LEU:HD22	3:4:417:LEU:HD22	1.99	0.43
3:4:742:LEU:HD23	3:4:747:LEU:HG	2.00	0.43
4:5:357:PHE:HZ	4:5:601:ARG:HB3	1.83	0.43
4:5:648:ILE:HA	4:5:652:GLN:HG3	2.00	0.43
6:7:263:ASP:OD1	6:7:263:ASP:N	2.50	0.43
8:9:593:PRO:HG2	8:9:596:VAL:HB	1.99	0.43
10:B:134:PHE:HD2	10:B:138:ILE:HG12	1.84	0.43
14:F:707:LEU:HG	14:F:710:TRP:HB3	1.99	0.43
18:L:870:ILE:HG22	18:L:888:VAL:HB	2.00	0.43
22:P:45:ILE:HA	23:Q:93:ILE:HB	1.99	0.43
1:2:355:SER:OG	1:2:383:ARG:NH2	2.52	0.43
2:3:400:ARG:HG2	2:3:402:ASP:H	1.83	0.43
2:3:435:ARG:HD2	2:3:435:ARG:HA	1.71	0.43
4:5:444:SER:OG	4:5:445:SER:N	2.51	0.43
9:A:55:LYS:HA	9:A:55:LYS:HD3	1.76	0.43
14:G:698:PHE:CG	14:G:744:PRO:HG3	2.54	0.43
18:L:878:PHE:CD2	22:P:86:GLN:HB3	2.53	0.43
3:4:451:ARG:NH1	25:Y:19:DC:OP2	2.51	0.43
6:7:366:LEU:HB3	25:Y:15:DC:H6	1.84	0.43
7:8:2166:ARG:NH2	7:8:2182:ALA:O	2.45	0.43
13:E:131:LEU:O	13:E:135:PHE:HB2	2.18	0.43
13:E:593:ASP:N	13:E:593:ASP:OD1	2.50	0.43
14:F:851:GLU:OE2	14:F:851:GLU:N	2.52	0.43
2:3:171:LEU:HD11	2:3:182:VAL:HG11	2.00	0.43
3:4:242:ASN:HB3	3:4:306:TYR:HE2	1.83	0.43
8:9:18:ARG:NH2	9:A:179:GLY:O	2.51	0.43
8:9:33:ILE:HG12	8:9:79:ILE:HD12	2.01	0.43
14:F:582:ALA:HB2	14:F:618:LEU:HB3	2.00	0.43
14:F:614:PRO:HD2	14:F:631:SER:HB2	1.99	0.43
14:F:650:TYR:HB3	14:F:653:ARG:HD3	2.01	0.43
14:F:703:THR:HA	14:F:722:LEU:O	2.18	0.43
14:H:570:ILE:HD13	14:H:590:VAL:HG11	2.01	0.43
20:R:94:GLN:O	20:R:98:GLU:HG3	2.19	0.43
2:3:161:PHE:HB2	2:3:165:ALA:HB2	2.00	0.43
4:5:504:ILE:O	4:5:510:THR:HA	2.18	0.43
4:5:626:PHE:HB2	4:5:653:LEU:HD13	2.00	0.43
5:6:110:LYS:HE2	15:I:334:GLU:HB3	2.01	0.43
7:8:1487:LEU:HA	7:8:1500:SER:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:9:527:SER:O	8:9:530:THR:OG1	2.37	0.43
14:G:497:ASN:ND2	14:G:539:LEU:O	2.51	0.43
15:I:78:VAL:HG22	15:I:83:ILE:HD12	2.00	0.43
21:O:74:THR:HG22	21:O:79:ARG:HH22	1.83	0.43
1:2:749:ARG:HA	1:2:752:GLU:HG2	2.00	0.43
1:2:854:ARG:O	1:2:858:ARG:HB2	2.19	0.43
13:E:66:GLU:OE1	13:E:69:ARG:NH1	2.51	0.43
13:E:296:GLN:HG2	13:E:320:ILE:HD13	2.00	0.43
14:F:657:LEU:O	14:G:634:HIS:NE2	2.49	0.43
18:L:904:ILE:HD11	22:P:90:ARG:HH11	1.83	0.43
1:2:339:PHE:HD2	1:2:348:LEU:HD23	1.84	0.42
2:3:169:ARG:NH2	2:3:270:LEU:O	2.46	0.42
3:4:512:VAL:HA	3:4:515:ARG:HD3	2.00	0.42
5:6:388:ARG:HD3	5:6:459:VAL:HB	2.00	0.42
6:7:82:LEU:HD21	6:7:106:ILE:HG21	2.00	0.42
7:8:1574:SER:O	7:8:1578:THR:OG1	2.31	0.42
8:9:184:ASN:O	8:9:188:MET:N	2.51	0.42
9:A:32:TYR:CD1	9:A:124:SER:HB2	2.54	0.42
10:B:177:GLU:HA	10:B:180:GLU:HG2	2.00	0.42
12:D:88:LEU:HA	12:D:91:ILE:HG22	2.01	0.42
14:F:760:LYS:HB2	14:F:760:LYS:HE2	1.89	0.42
21:S:88:VAL:HG23	21:S:98:LEU:HB3	2.01	0.42
2:3:372:TYR:H	27:3:1001:ADP:N6	2.17	0.42
3:4:568:GLY:HA3	3:4:708:VAL:HB	2.00	0.42
3:4:624:SER:OG	3:4:629:CYS:SG	2.76	0.42
3:4:766:ALA:HB1	3:4:822:VAL:HG21	2.01	0.42
13:E:105:ILE:O	13:E:115:SER:OG	2.36	0.42
14:F:702:ASN:HD22	14:F:725:ASN:HD21	1.67	0.42
15:I:184:LEU:HD23	15:I:187:ILE:HD12	2.01	0.42
15:I:766:PRO:HG3	16:J:120:LYS:HG3	2.00	0.42
20:R:117:ARG:NH1	20:R:124:ASP:OD1	2.51	0.42
1:2:625:GLU:OE1	1:2:808:ARG:NE	2.52	0.42
2:3:570:ARG:NH1	4:5:614:LEU:O	2.48	0.42
14:H:768:LEU:HD12	14:H:768:LEU:HA	1.92	0.42
18:L:914:LEU:HD13	18:L:919:ILE:HG23	2.01	0.42
20:N:110:LEU:HD21	20:R:130:ARG:NH2	2.34	0.42
2:3:661:GLN:O	2:3:665:GLU:HG2	2.19	0.42
3:4:245:ALA:HB3	3:4:308:VAL:HA	2.01	0.42
7:8:1472:GLU:HB3	7:8:1475:ARG:HD2	2.02	0.42
7:8:1695:LEU:HD11	8:9:499:ALA:HB2	2.01	0.42
9:A:186:ASP:HB3	13:E:478:TRP:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:F:597:PHE:HB3	14:F:610:GLU:HB3	2.01	0.42
1:2:499:SER:HB3	1:2:509:ARG:HH12	1.84	0.42
2:3:203:ALA:O	2:3:207:GLY:HA2	2.19	0.42
5:6:268:PHE:HA	5:6:398:THR:HG21	2.02	0.42
5:6:365:ALA:HA	5:6:368:ILE:HD12	2.02	0.42
6:7:459:MET:HB2	6:7:597:LEU:HD12	2.01	0.42
7:8:1694:PRO:HD2	8:9:442:PRO:HG2	2.01	0.42
14:H:576:GLU:HG3	14:H:594:LEU:HG	2.01	0.42
15:I:137:TRP:O	15:I:160:GLN:NE2	2.52	0.42
18:L:889:TYR:HH	18:L:897:THR:HG1	1.66	0.42
1:2:402:LEU:HG	3:4:660:GLY:HA3	2.00	0.42
5:6:553:GLY:HA2	5:6:569:ILE:HD12	2.01	0.42
14:G:864:LYS:O	14:G:868:ARG:HG3	2.20	0.42
5:6:757:TYR:O	5:6:760:THR:OG1	2.32	0.42
15:I:699:ARG:HA	15:I:703:GLN:HG3	2.00	0.42
2:3:424:ASN:HD22	4:5:403:GLY:HA3	1.85	0.42
3:4:505:ASP:OD1	3:4:505:ASP:N	2.52	0.42
3:4:778:ARG:NH1	3:4:793:ALA:O	2.53	0.42
4:5:261:ILE:HG22	4:5:263:GLU:H	1.84	0.42
6:7:252:LYS:HD2	6:7:252:LYS:HA	1.77	0.42
21:O:30:ILE:HD13	21:O:30:ILE:HA	1.93	0.42
21:O:33:PRO:HA	21:O:36:ARG:HB2	2.00	0.42
1:2:73:LEU:HD12	21:S:40:ARG:HG3	2.02	0.42
3:4:339:ILE:HB	3:4:394:LYS:O	2.20	0.42
7:8:1952:GLU:OE2	7:8:2014:ARG:NH2	2.45	0.42
8:9:92:LYS:HB2	8:9:92:LYS:HE2	1.88	0.42
11:C:166:LEU:HD21	11:C:177:TYR:CZ	2.55	0.42
13:E:41:ALA:HB1	13:E:255:ILE:HD12	2.02	0.42
16:J:127:GLU:HA	16:J:130:VAL:HG22	2.01	0.42
18:L:728:ILE:HD13	18:L:741:HIS:HD2	1.84	0.42
2:3:98:ILE:HG13	2:3:155:LEU:HD22	2.01	0.42
3:4:712:VAL:HG21	6:7:668:ARG:HB3	2.02	0.42
5:6:280:ARG:HA	5:6:280:ARG:HD3	1.87	0.42
8:9:532:ILE:HG13	8:9:539:ILE:HB	2.02	0.42
14:H:519:ASP:N	14:H:519:ASP:OD1	2.50	0.42
15:I:84:LEU:HD12	15:I:135:MET:HE3	2.01	0.42
1:2:530:LYS:HB3	4:5:428:PHE:HE1	1.84	0.41
3:4:701:ARG:NH2	27:6:1102:ADP:O2B	2.49	0.41
4:5:415:LEU:O	4:5:555:ILE:HA	2.19	0.41
6:7:451:ARG:HG2	6:7:453:ASP:H	1.84	0.41
6:7:596:ILE:HD12	6:7:598:PHE:HE2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:8:1369:GLN:HG2	7:8:1370:LYS:H	1.85	0.41
9:A:68:ALA:O	9:A:72:TYR:HB2	2.20	0.41
14:F:536:LEU:HB2	14:F:547:GLY:O	2.19	0.41
14:G:652:LYS:NZ	14:G:713:PRO:O	2.53	0.41
2:3:408:VAL:HA	2:3:516:ALA:O	2.20	0.41
8:9:468:LEU:HA	8:9:471:ARG:HH11	1.84	0.41
14:G:913:LYS:HE3	14:G:913:LYS:HB3	1.89	0.41
14:H:537:CYS:HA	14:H:545:LEU:O	2.20	0.41
2:3:22:GLY:O	2:3:26:ARG:HG2	2.21	0.41
3:4:402:THR:HA	3:4:403:PRO:HD3	1.94	0.41
3:4:692:ILE:HG22	3:4:694:LEU:H	1.85	0.41
4:5:722:LEU:HA	4:5:723:PRO:HD3	1.92	0.41
5:6:308:SER:HA	5:6:319:ASP:HA	2.03	0.41
7:8:2219:ASP:HA	7:8:2222:ILE:HG22	2.02	0.41
10:B:182:ARG:NH2	12:D:294:ILE:OXT	2.50	0.41
14:G:879:VAL:HG13	14:G:910:LEU:HG	2.02	0.41
10:B:73:LEU:HD12	10:B:76:ALA:HB3	2.02	0.41
12:D:5:ILE:HD11	14:F:868:ARG:HG3	2.01	0.41
12:D:98:ILE:HD11	12:D:130:GLU:HG3	2.02	0.41
14:F:704:LEU:HD22	14:F:752:LEU:HD13	2.01	0.41
15:I:161:LEU:HD11	15:I:217:PRO:HA	2.01	0.41
22:P:81:ILE:HG22	22:P:84:HIS:ND1	2.36	0.41
1:2:813:ILE:HG12	1:2:841:VAL:HG21	2.01	0.41
2:3:710:THR:O	2:3:713:ALA:HB3	2.20	0.41
3:4:245:ALA:O	3:4:248:LEU:HB2	2.21	0.41
3:4:428:ARG:NH2	5:6:370:THR:O	2.52	0.41
3:4:574:LYS:HD3	3:4:674:SER:HB2	2.02	0.41
4:5:104:LEU:HD23	4:5:104:LEU:HA	1.96	0.41
4:5:631:LYS:HA	4:5:634:LEU:HD23	2.01	0.41
6:7:484:THR:OG1	6:7:486:LYS:NZ	2.51	0.41
7:8:1328:LYS:HD3	7:8:1337:GLU:HB3	2.02	0.41
8:9:405:ASN:OD1	8:9:437:SER:OG	2.31	0.41
9:A:149:ILE:HG22	12:D:137:LYS:HG2	2.02	0.41
10:B:141:LEU:HD23	10:B:141:LEU:HA	1.94	0.41
15:I:621:LYS:NZ	25:Y:42:DT:OP1	2.54	0.41
25:Y:40:DT:H2"	25:Y:41:DA:C8	2.55	0.41
1:2:504:SER:HB3	5:6:563:ILE:HD12	2.03	0.41
1:2:799:SER:HB3	1:2:802:SER:HB3	2.03	0.41
6:7:534:ARG:O	6:7:538:HIS:CE1	2.74	0.41
7:8:1543:ILE:HD11	7:8:1640:LEU:HB3	2.03	0.41
9:A:97:LEU:HD23	9:A:97:LEU:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:569:GLN:H	5:6:650:VAL:HG21	1.85	0.41
1:2:662:PRO:O	1:2:666:ASN:ND2	2.52	0.41
2:3:278:LEU:HD23	2:3:278:LEU:HA	1.91	0.41
4:5:152:ASP:N	4:5:152:ASP:OD1	2.53	0.41
4:5:755:LEU:HD13	4:5:761:ILE:HD12	2.02	0.41
7:8:1858:ILE:HA	7:8:1868:ILE:HA	2.03	0.41
14:F:701:ASP:N	14:F:701:ASP:OD2	2.51	0.41
15:I:347:LYS:HE2	15:I:347:LYS:HB3	1.91	0.41
1:2:82:TYR:CZ	21:S:37:ARG:HG2	2.55	0.41
2:3:172:THR:HG23	2:3:174:GLN:HG2	2.03	0.41
2:3:408:VAL:O	2:3:548:VAL:HA	2.20	0.41
4:5:733:LEU:O	4:5:737:PHE:HB2	2.21	0.41
6:7:231:LYS:HE3	6:7:231:LYS:HB3	1.96	0.41
13:E:516:LYS:HG3	13:E:518:LEU:HG	2.03	0.41
15:I:275:LYS:HE2	15:I:275:LYS:HB2	1.82	0.41
15:I:329:THR:O	15:I:333:PHE:N	2.51	0.41
15:I:498:ILE:HD12	15:I:498:ILE:HA	1.93	0.41
1:2:382:TYR:HB3	4:5:153:SER:HB3	2.02	0.41
27:2:902:ADP:N3	5:6:797:VAL:HG21	2.36	0.41
3:4:758:ILE:HG13	3:4:813:LEU:HD22	2.02	0.41
4:5:42:SER:OG	10:B:142:ARG:NH1	2.53	0.41
4:5:717:GLU:O	4:5:721:ARG:CB	2.68	0.41
5:6:580:SER:HB3	27:6:1102:ADP:C8	2.55	0.41
7:8:1439:MET:HE1	7:8:1687:LEU:HD11	2.02	0.41
7:8:1634:LYS:HE3	7:8:1634:LYS:HB2	1.86	0.41
7:8:1725:GLY:HA2	7:8:2064:LEU:HB3	2.03	0.41
8:9:35:SER:HA	9:A:175:GLN:HE22	1.86	0.41
10:B:105:GLU:HG2	10:B:113:SER:HB3	2.02	0.41
14:F:584:THR:HG21	14:F:643:LEU:HD11	2.02	0.41
14:F:616:VAL:HG11	14:F:682:MET:HE3	2.03	0.41
14:G:510:GLN:HE21	14:G:529:GLU:HG3	1.86	0.41
18:L:610:GLU:O	18:L:615:GLU:N	2.50	0.41
18:L:878:PHE:HZ	22:P:87:LEU:HD23	1.86	0.41
3:4:767:LYS:HA	3:4:770:LEU:HD12	2.03	0.41
6:7:363:PHE:HE2	25:Y:15:DC:H5	1.69	0.41
6:7:648:LYS:NZ	6:7:704:LEU:HD22	2.35	0.41
9:A:192:ARG:HE	9:A:192:ARG:HB2	1.73	0.41
14:F:494:LEU:N	14:F:502:VAL:O	2.54	0.41
14:F:884:SER:OG	14:G:601:ASN:ND2	2.54	0.41
15:I:668:THR:HG22	15:I:670:PRO:HD2	2.02	0.41
20:N:68:PHE:HA	20:N:71:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:114:HIS:NE2	20:R:124:ASP:OD2	2.47	0.41
21:O:80:LYS:HA	21:O:80:LYS:HD2	1.94	0.41
3:4:321:ASP:HA	3:4:324:LYS:HD2	2.03	0.40
6:7:533:ASP:O	6:7:537:ILE:HG12	2.21	0.40
15:I:156:LEU:HD12	15:I:156:LEU:HA	1.87	0.40
18:L:708:GLN:HE21	18:L:713:THR:HA	1.86	0.40
21:O:55:VAL:HA	21:O:58:VAL:HG12	2.03	0.40
2:3:417:GLN:NE2	4:5:404:MET:SD	2.74	0.40
10:B:53:ILE:HD13	12:D:94:GLN:HG3	2.03	0.40
14:H:879:VAL:HG22	14:H:907:LEU:HD21	2.04	0.40
15:I:491:LYS:HB2	15:I:545:ARG:HH22	1.86	0.40
22:P:85:LEU:O	22:P:89:ILE:HG12	2.21	0.40
1:2:326:ARG:HH21	1:2:584:PRO:HD2	1.87	0.40
4:5:257:LYS:HE2	4:5:257:LYS:HB2	1.84	0.40
4:5:276:MET:HG2	4:5:328:ILE:HB	2.03	0.40
7:8:2101:LEU:HD21	7:8:2146:LEU:HD11	2.04	0.40
8:9:231:ARG:HD3	8:9:358:THR:HG21	2.02	0.40
8:9:403:GLY:HA2	8:9:661:PRO:HB2	2.02	0.40
10:B:160:LEU:HD23	10:B:160:LEU:HA	1.86	0.40
1:2:566:ALA:HB1	1:2:571:ALA:HB2	2.04	0.40
4:5:147:PRO:HG2	4:5:150:ASP:HB2	2.03	0.40
7:8:2143:GLN:O	7:8:2147:ILE:HG12	2.21	0.40
14:G:907:LEU:HD23	14:G:910:LEU:HD12	2.02	0.40
15:I:641:ARG:HA	15:I:644:ALA:HB3	2.02	0.40
24:X:21:DT:H2"	24:X:22:DA:C8	2.56	0.40
3:4:762:ILE:HD13	3:4:817:VAL:HG21	2.03	0.40
6:7:417:SER:HA	6:7:633:VAL:HG12	2.03	0.40
6:7:451:ARG:HH22	6:7:455:ASN:HD21	1.69	0.40
8:9:175:ALA:HB2	8:9:529:PRO:HG2	2.02	0.40
14:H:491:ARG:HD2	14:H:766:PHE:CG	2.55	0.40
15:I:78:VAL:HG13	15:I:83:ILE:HB	2.03	0.40
15:I:177:ARG:HA	15:I:180:ILE:HG12	2.04	0.40
15:I:477:LEU:HD23	15:I:477:LEU:HA	1.86	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	2	772/868 (89%)	753 (98%)	19 (2%)	0	100	100
2	3	603/971 (62%)	592 (98%)	11 (2%)	0	100	100
3	4	663/933 (71%)	646 (97%)	17 (3%)	0	100	100
4	5	666/775 (86%)	650 (98%)	16 (2%)	0	100	100
5	6	622/1017 (61%)	598 (96%)	24 (4%)	0	100	100
6	7	619/845 (73%)	596 (96%)	23 (4%)	0	100	100
7	8	849/2222 (38%)	829 (98%)	20 (2%)	0	100	100
8	9	565/689 (82%)	549 (97%)	16 (3%)	0	100	100
9	A	193/208 (93%)	187 (97%)	6 (3%)	0	100	100
10	B	188/251 (75%)	177 (94%)	11 (6%)	0	100	100
11	C	165/194 (85%)	160 (97%)	5 (3%)	0	100	100
12	D	235/294 (80%)	226 (96%)	9 (4%)	0	100	100
13	E	550/650 (85%)	532 (97%)	18 (3%)	0	100	100
14	F	418/927 (45%)	406 (97%)	12 (3%)	0	100	100
14	G	416/927 (45%)	402 (97%)	14 (3%)	0	100	100
14	H	419/927 (45%)	412 (98%)	7 (2%)	0	100	100
15	I	739/1238 (60%)	720 (97%)	19 (3%)	0	100	100
16	J	92/317 (29%)	89 (97%)	3 (3%)	0	100	100
17	K	18/1096 (2%)	16 (89%)	2 (11%)	0	100	100
18	L	485/1035 (47%)	464 (96%)	21 (4%)	0	100	100
19	M	363/552 (66%)	350 (96%)	13 (4%)	0	100	100
20	N	75/136 (55%)	75 (100%)	0	0	100	100
20	R	88/136 (65%)	84 (96%)	4 (4%)	0	100	100
21	O	71/103 (69%)	69 (97%)	2 (3%)	0	100	100
21	S	83/103 (81%)	80 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	P	89/132 (67%)	88 (99%)	1 (1%)	0	100	100
23	Q	89/131 (68%)	87 (98%)	2 (2%)	0	100	100
All	All	10135/17677 (57%)	9837 (97%)	298 (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	2	674/770 (88%)	674 (100%)	0	100	100
2	3	528/835 (63%)	528 (100%)	0	100	100
3	4	573/848 (68%)	571 (100%)	2 (0%)	91	94
4	5	609/688 (88%)	609 (100%)	0	100	100
5	6	547/886 (62%)	546 (100%)	1 (0%)	92	96
6	7	532/753 (71%)	531 (100%)	1 (0%)	92	96
7	8	786/2014 (39%)	783 (100%)	3 (0%)	89	93
8	9	517/629 (82%)	517 (100%)	0	100	100
9	A	182/193 (94%)	182 (100%)	0	100	100
10	B	182/228 (80%)	182 (100%)	0	100	100
11	C	154/173 (89%)	154 (100%)	0	100	100
12	D	232/279 (83%)	231 (100%)	1 (0%)	89	93
13	E	505/586 (86%)	505 (100%)	0	100	100
14	F	375/825 (46%)	375 (100%)	0	100	100
14	G	372/825 (45%)	371 (100%)	1 (0%)	91	94
14	H	375/825 (46%)	375 (100%)	0	100	100
15	I	681/1125 (60%)	681 (100%)	0	100	100
16	J	87/285 (30%)	86 (99%)	1 (1%)	70	80
17	K	19/1003 (2%)	18 (95%)	1 (5%)	19	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
18	L	297/935 (32%)	295 (99%)	2 (1%)	81 88
20	N	67/113 (59%)	67 (100%)	0	100 100
20	R	79/113 (70%)	79 (100%)	0	100 100
21	O	63/81 (78%)	62 (98%)	1 (2%)	58 74
21	S	72/81 (89%)	72 (100%)	0	100 100
22	P	71/99 (72%)	71 (100%)	0	100 100
23	Q	79/110 (72%)	79 (100%)	0	100 100
All	All	8658/15302 (57%)	8644 (100%)	14 (0%)	91 96

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	4	557	ARG
3	4	594	LYS
5	6	416	LYS
6	7	62	LYS
7	8	1386	ASN
7	8	1419	ASN
7	8	1579	LYS
12	D	247	GLN
14	G	843	ASN
16	J	49	ARG
17	K	328	LYS
18	L	668	LYS
18	L	679	ARG
21	O	36	ARG

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

Mol	Chain	Res	Type
2	3	164	HIS
3	4	465	HIS
4	5	769	ASN
7	8	1708	ASN
7	8	2060	HIS
14	G	510	GLN
18	L	741	HIS
20	R	114	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 7 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
27	ADP	6	1102	-	24,29,29	0.96	1 (4%)	29,45,45	1.48	4 (13%)
27	ADP	5	802	-	24,29,29	0.95	1 (4%)	29,45,45	1.54	4 (13%)
27	ADP	3	1001	-	24,29,29	0.94	1 (4%)	29,45,45	1.38	2 (6%)
27	ADP	7	902	-	24,29,29	0.95	1 (4%)	29,45,45	1.38	4 (13%)
27	ADP	2	902	-	24,29,29	0.92	1 (4%)	29,45,45	1.41	4 (13%)

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
27	ADP	6	1102	-	-	3/12/32/32	0/3/3/3
27	ADP	5	802	-	-	3/12/32/32	0/3/3/3
27	ADP	3	1001	-	-	4/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	ADP	7	902	-	-	2/12/32/32	0/3/3/3
27	ADP	2	902	-	-	2/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	6	1102	ADP	C5-C4	2.52	1.47	1.40
27	5	802	ADP	C5-C4	2.49	1.47	1.40
27	7	902	ADP	C5-C4	2.44	1.47	1.40
27	2	902	ADP	C5-C4	2.34	1.47	1.40
27	3	1001	ADP	C5-C4	2.22	1.46	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	5	802	ADP	PA-O3A-PB	-3.98	119.16	132.83
27	6	1102	ADP	C3'-C2'-C1'	3.86	106.78	100.98
27	5	802	ADP	C3'-C2'-C1'	3.66	106.48	100.98
27	2	902	ADP	PA-O3A-PB	-3.62	120.40	132.83
27	2	902	ADP	N3-C2-N1	-3.47	123.25	128.68
27	3	1001	ADP	PA-O3A-PB	-3.45	121.00	132.83
27	3	1001	ADP	N3-C2-N1	-3.32	123.49	128.68
27	6	1102	ADP	PA-O3A-PB	-3.26	121.64	132.83
27	7	902	ADP	N3-C2-N1	-3.26	123.59	128.68
27	7	902	ADP	PA-O3A-PB	-3.16	121.98	132.83
27	6	1102	ADP	N3-C2-N1	-3.11	123.82	128.68
27	5	802	ADP	N3-C2-N1	-3.07	123.88	128.68
27	7	902	ADP	C3'-C2'-C1'	2.90	105.35	100.98
27	2	902	ADP	C4-C5-N7	-2.70	106.59	109.40
27	7	902	ADP	C4-C5-N7	-2.68	106.61	109.40
27	2	902	ADP	C3'-C2'-C1'	2.59	104.88	100.98
27	6	1102	ADP	C4-C5-N7	-2.57	106.72	109.40
27	5	802	ADP	C4-C5-N7	-2.56	106.73	109.40

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	2	902	ADP	C5'-O5'-PA-O1A
27	3	1001	ADP	C5'-O5'-PA-O1A
27	3	1001	ADP	C5'-O5'-PA-O2A

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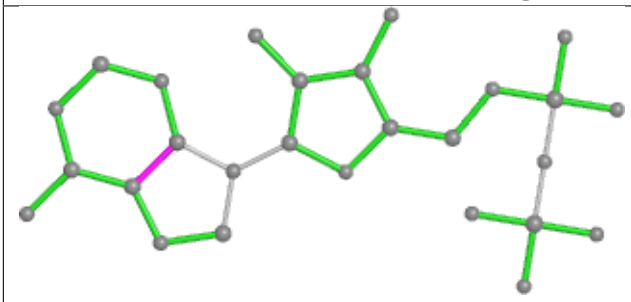
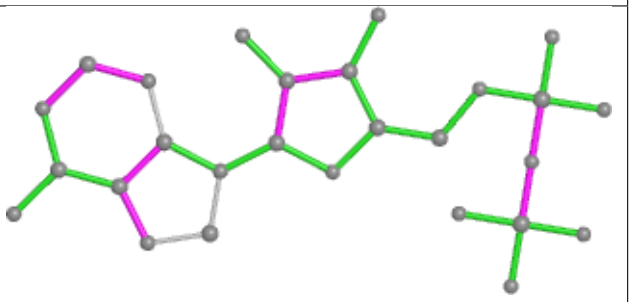
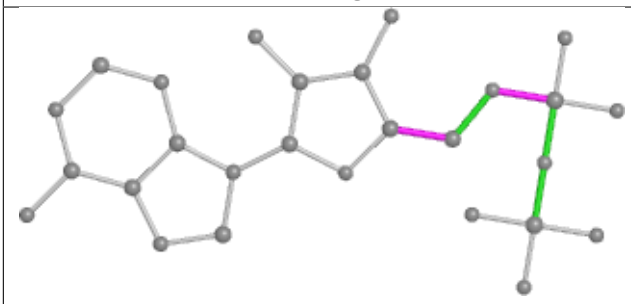
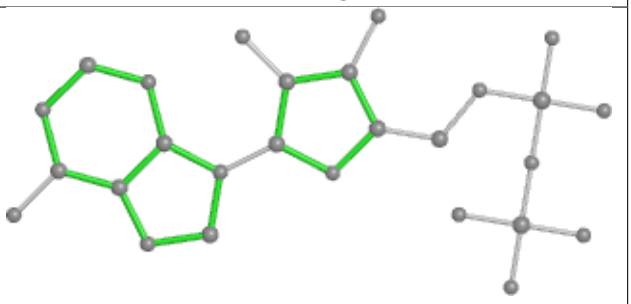
Mol	Chain	Res	Type	Atoms
27	5	802	ADP	C5'-O5'-PA-O3A
27	6	1102	ADP	C5'-O5'-PA-O3A
27	7	902	ADP	C3'-C4'-C5'-O5'
27	7	902	ADP	O4'-C4'-C5'-O5'
27	5	802	ADP	C5'-O5'-PA-O1A
27	6	1102	ADP	C5'-O5'-PA-O1A
27	6	1102	ADP	O4'-C4'-C5'-O5'
27	5	802	ADP	O4'-C4'-C5'-O5'
27	2	902	ADP	C5'-O5'-PA-O3A
27	3	1001	ADP	C5'-O5'-PA-O3A
27	3	1001	ADP	C4'-C5'-O5'-PA

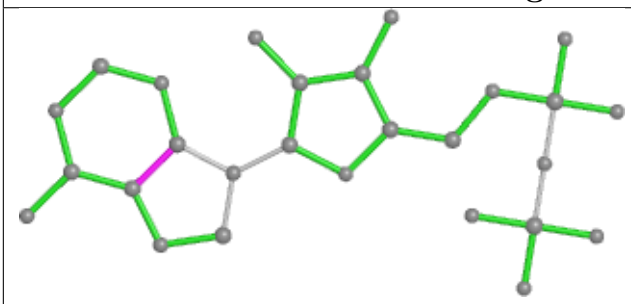
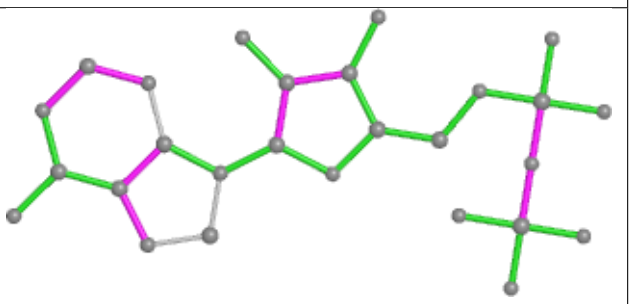
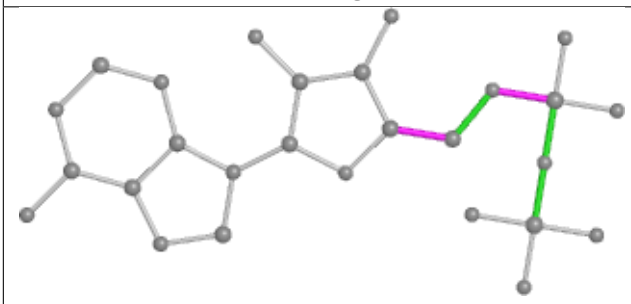
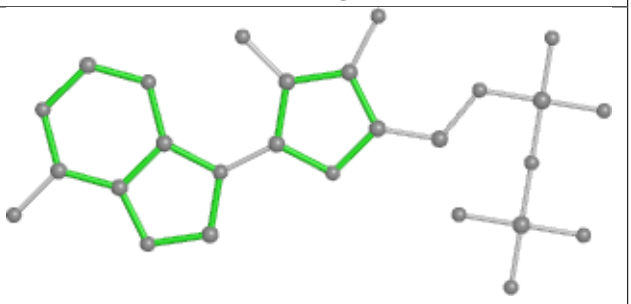
There are no ring outliers.

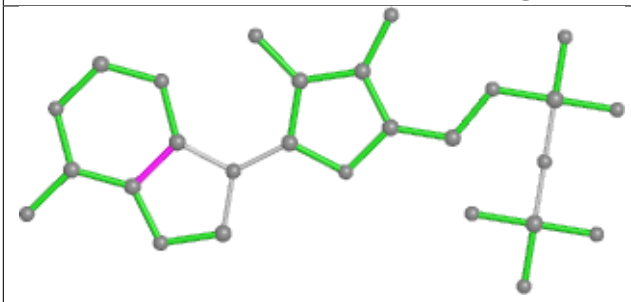
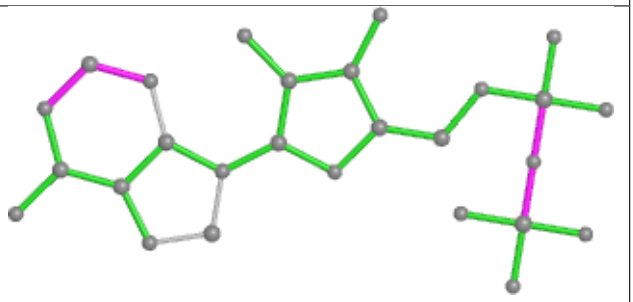
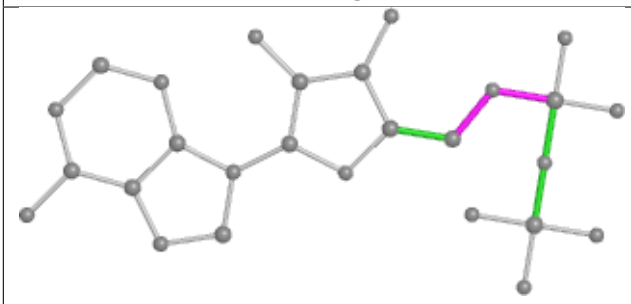
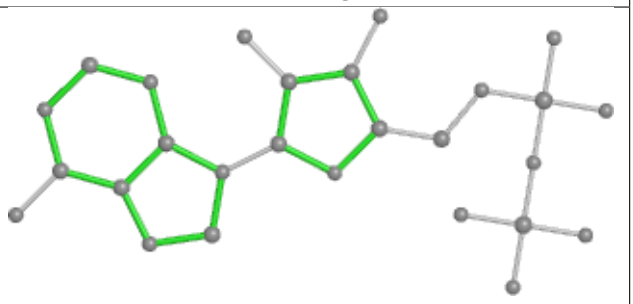
4 monomers are involved in 8 short contacts:

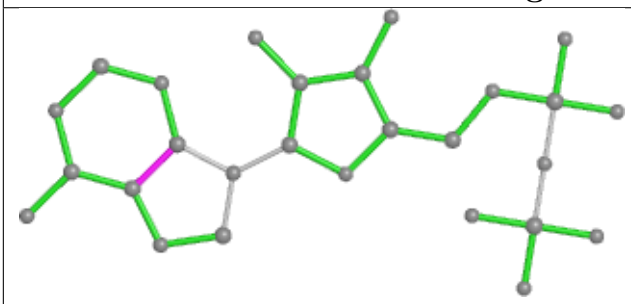
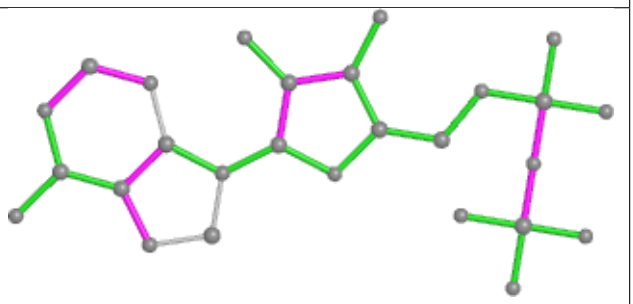
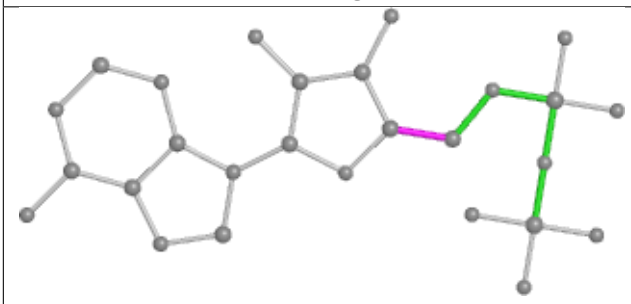
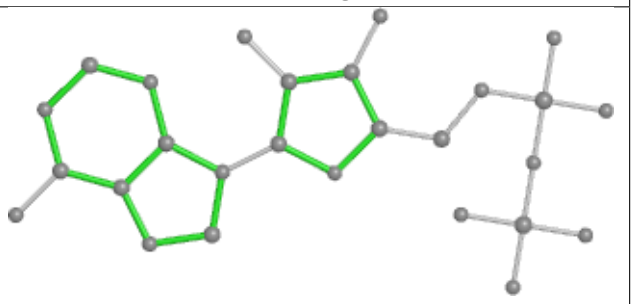
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	6	1102	ADP	2	0
27	3	1001	ADP	3	0
27	7	902	ADP	2	0
27	2	902	ADP	1	0

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

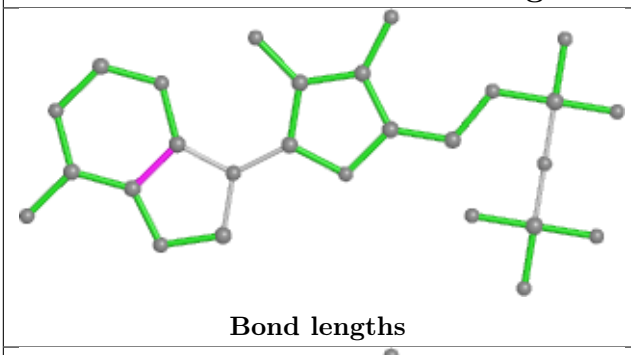
Ligand ADP 6 1102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP 5 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

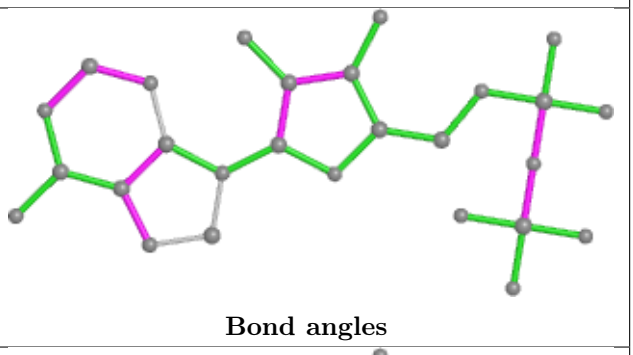
Ligand ADP 3 1001	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand ADP 7 902	
	
Bond lengths	Bond angles
	
Torsions	Rings

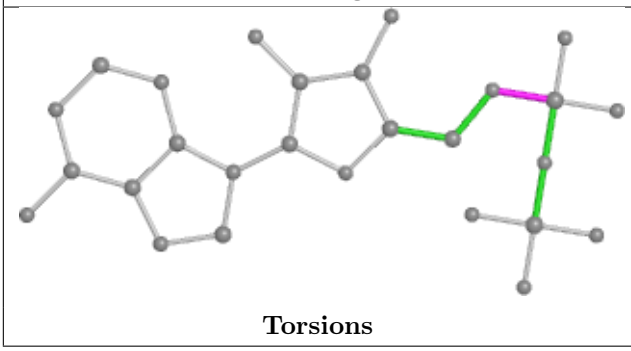
Ligand ADP 2 902



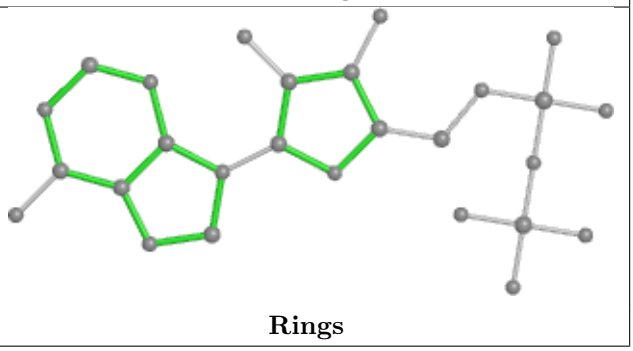
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

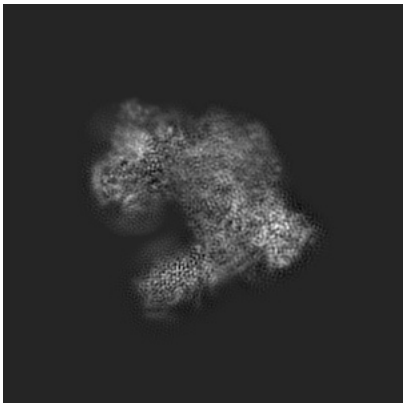
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38317. These allow visual inspection of the internal detail of the map and identification of artifacts.

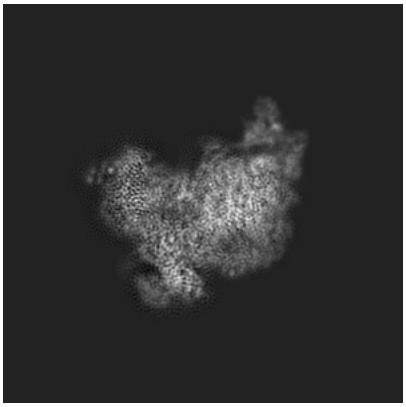
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

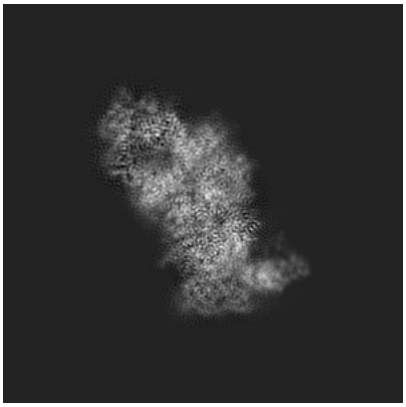
6.1.1 Primary map



X



Y

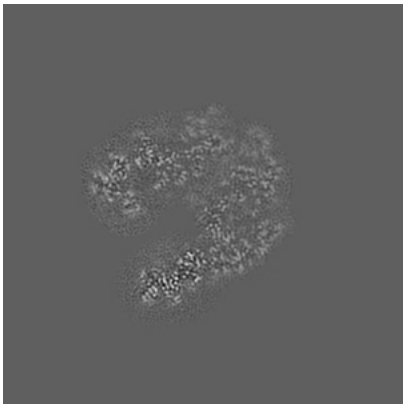


Z

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

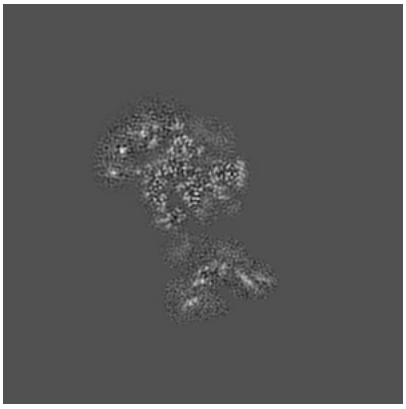
6.2 Central slices

6.2.1 Primary map



X Index: 200

Y Index: 200

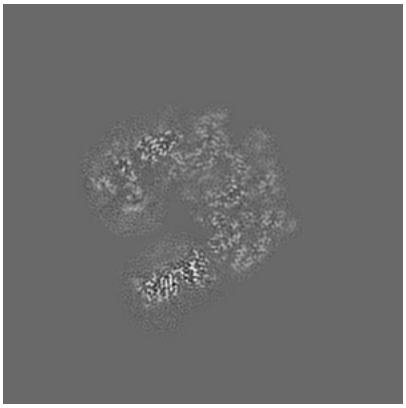


Z Index: 200

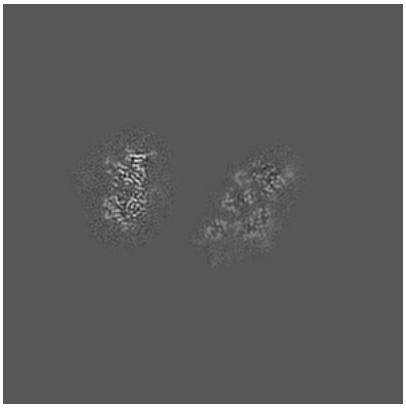
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

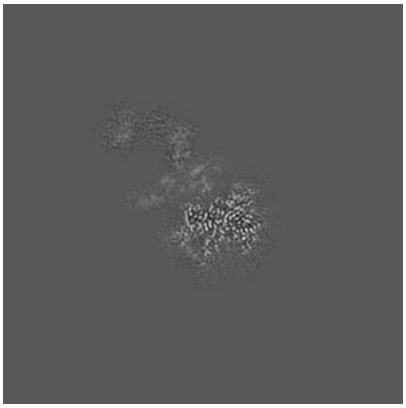
6.3.1 Primary map



X Index: 211



Y Index: 174

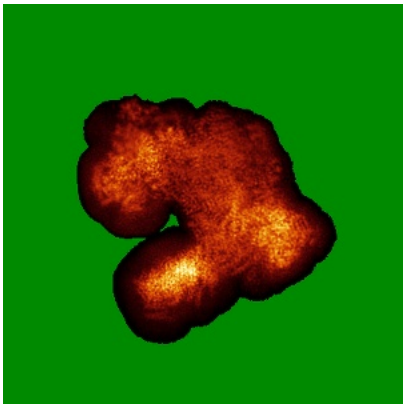


Z Index: 132

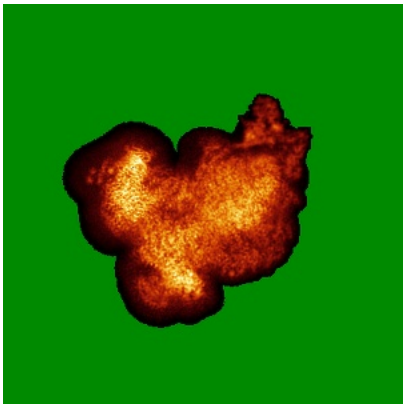
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

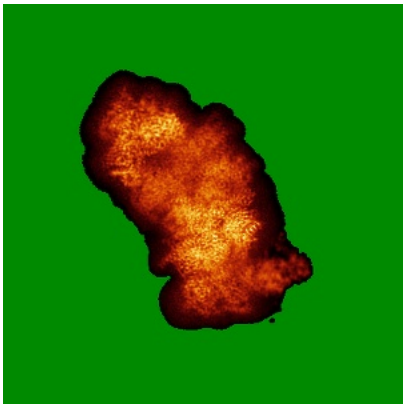
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 10.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

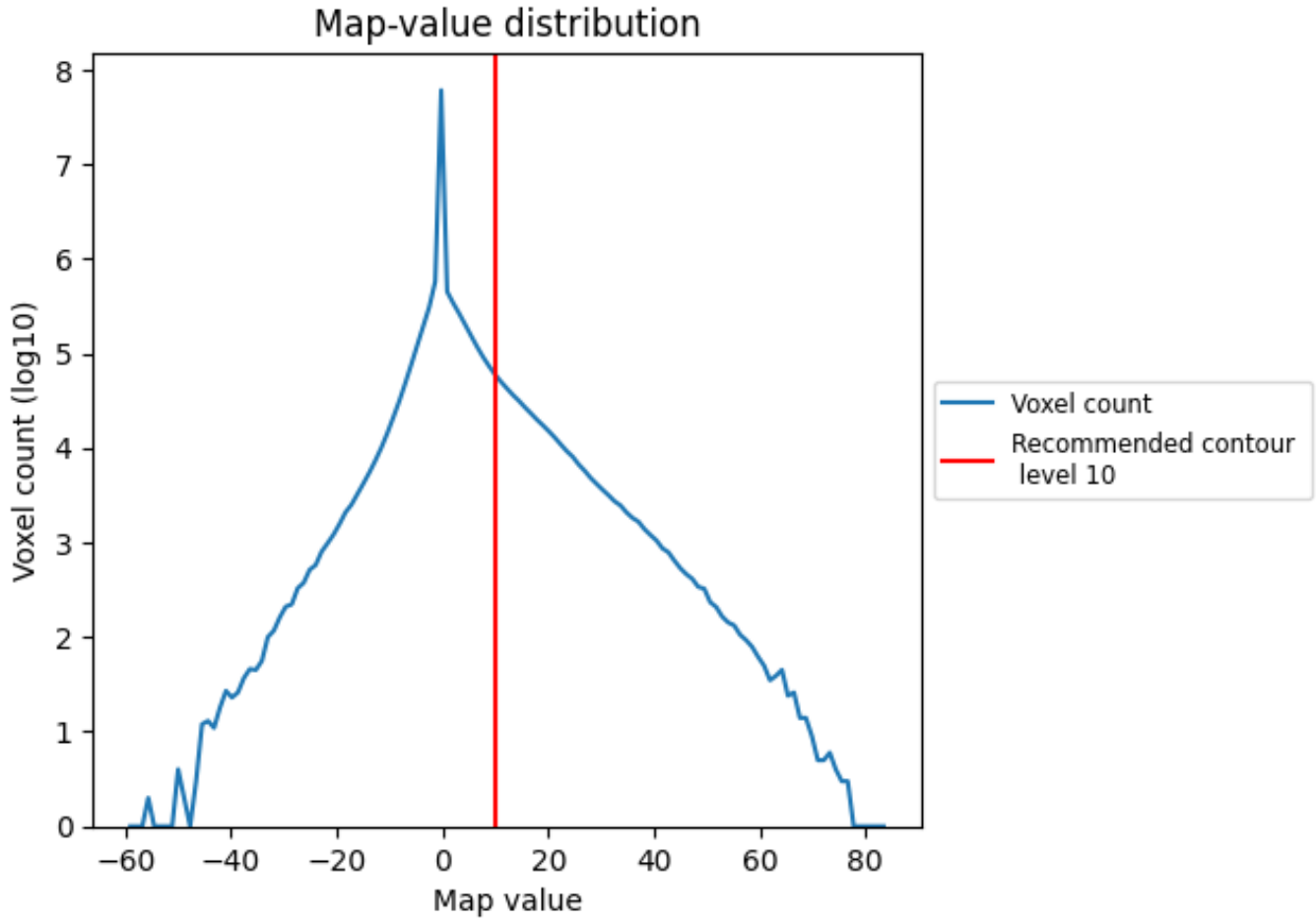
6.6 Mask visualisation (i)

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

7 Map analysis

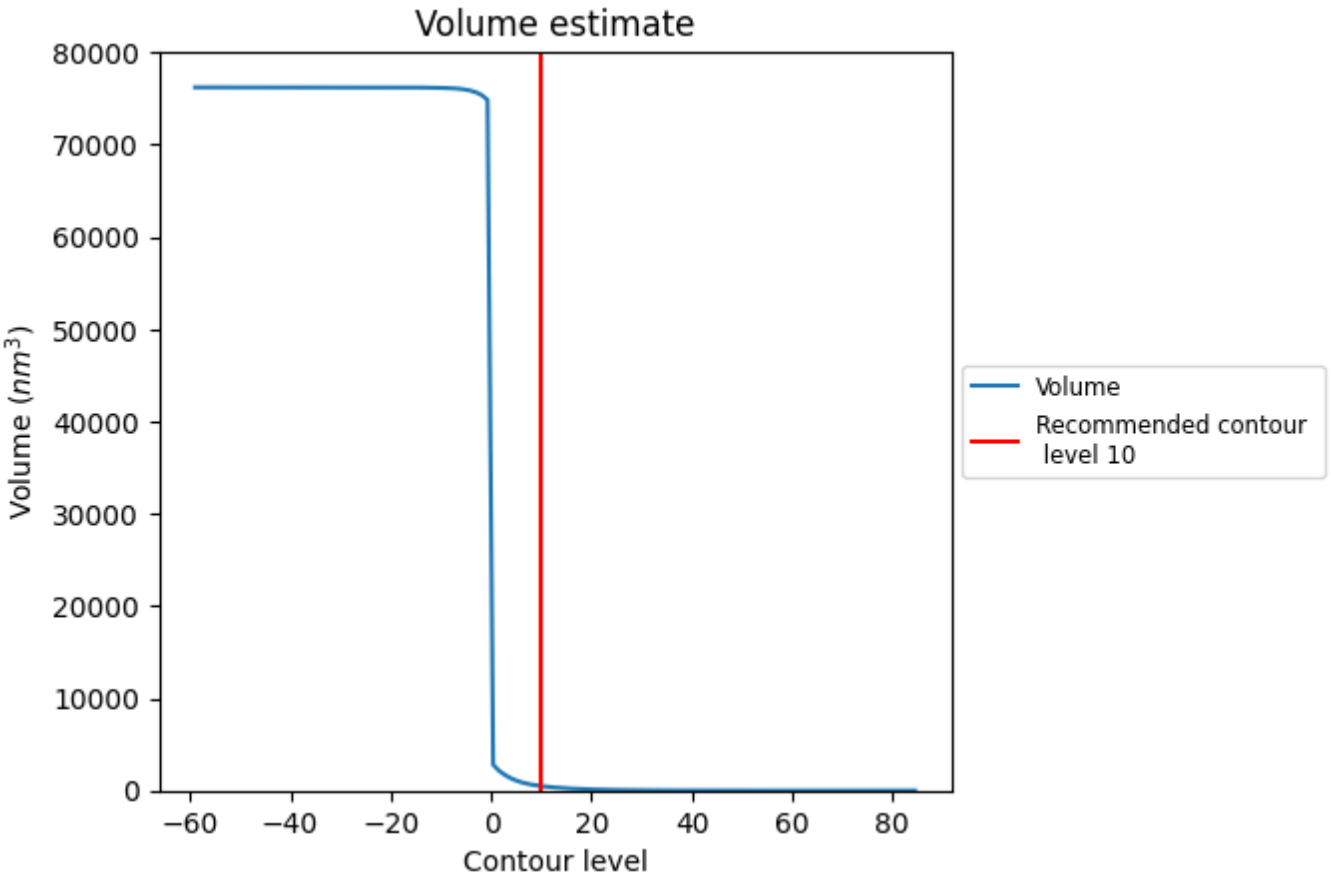
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

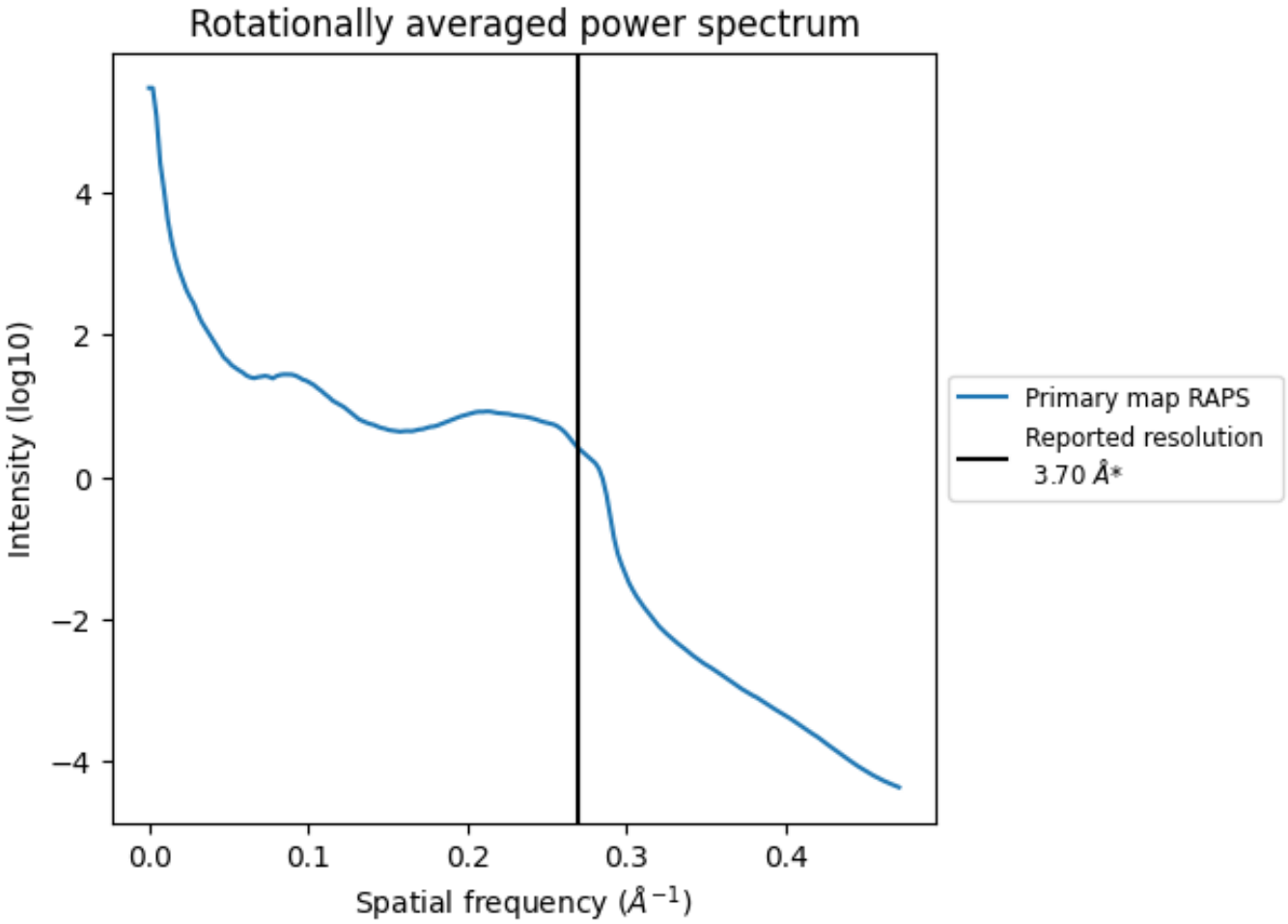
7.2 Volume estimate (i)



The volume at the recommended contour level is 489 nm^3; this corresponds to an approximate mass of 441 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.270 $Å^{-1}$

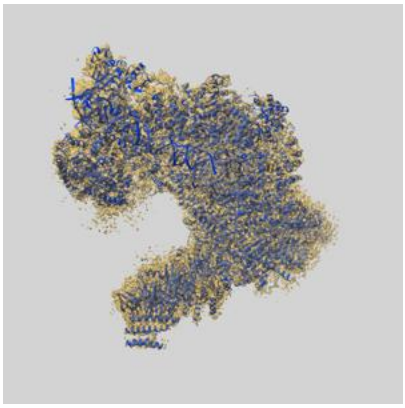
8 Fourier-Shell correlation (i)

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

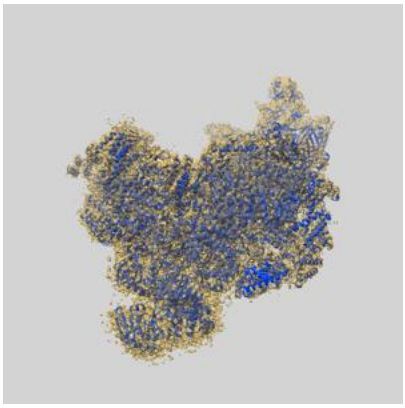
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38317 and PDB model 8XGC. Per-residue inclusion information can be found in section 3 on page 9.

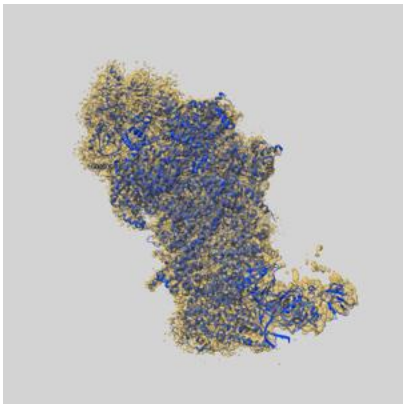
9.1 Map-model overlay



X



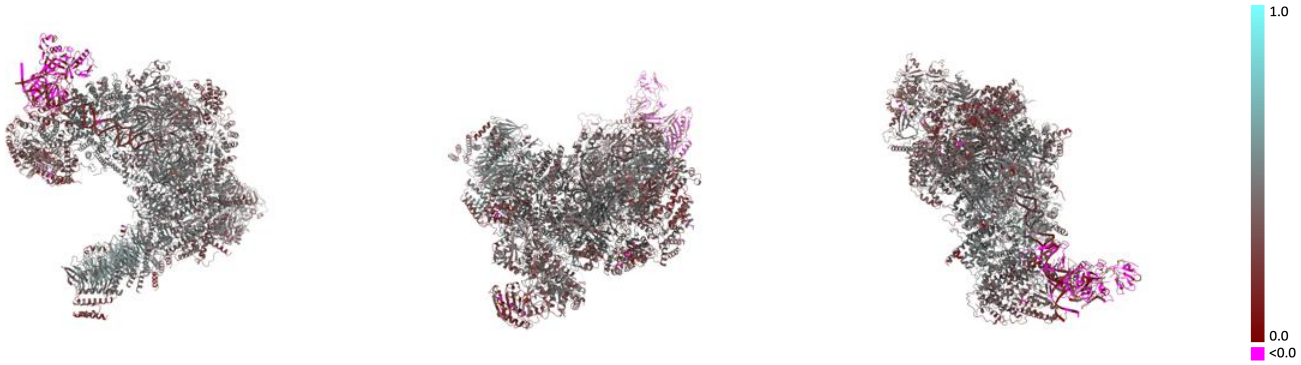
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 10.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

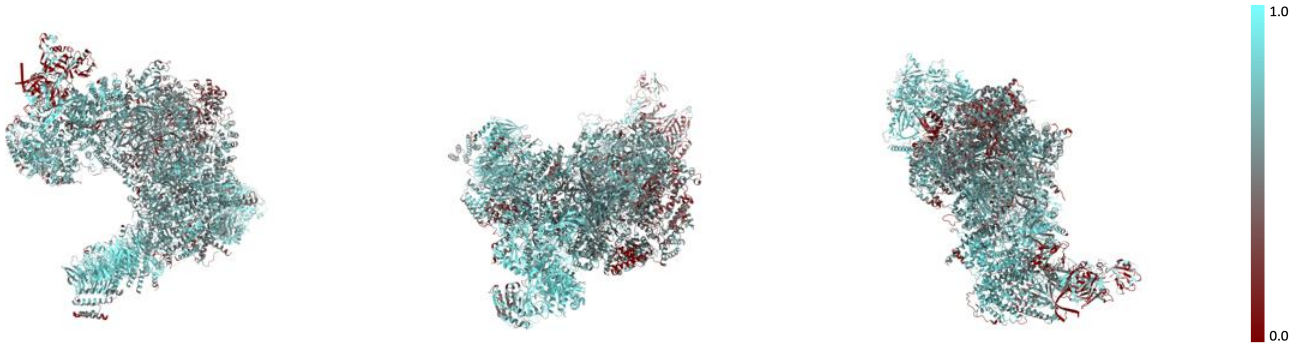
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

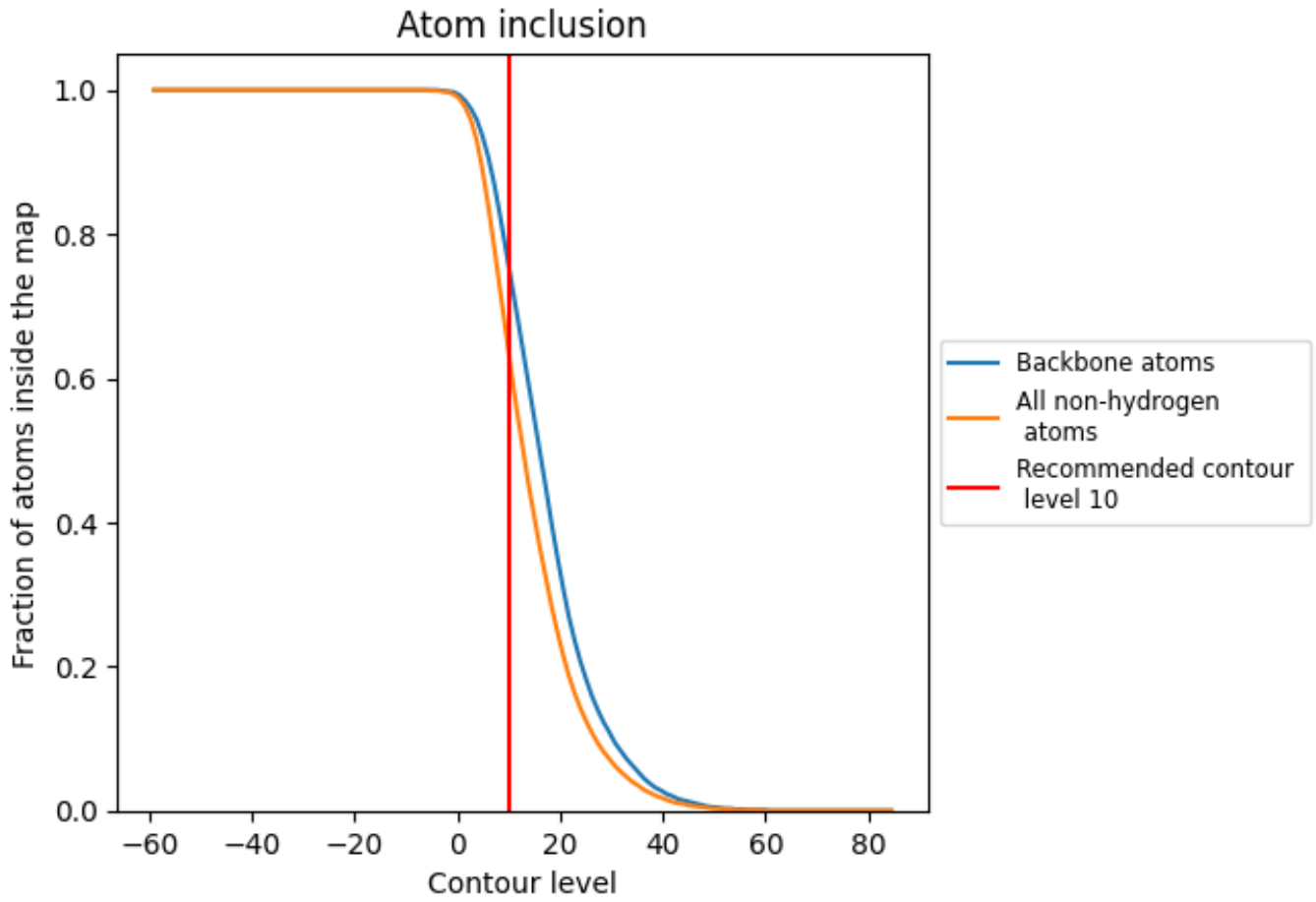
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (10).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (10) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6350	0.4070
2	0.6040	0.4400
3	0.6070	0.4410
4	0.4860	0.3860
5	0.6120	0.4410
6	0.6120	0.4360
7	0.4530	0.3750
8	0.7690	0.3780
9	0.7160	0.3940
A	0.5960	0.4030
B	0.6810	0.4620
C	0.6510	0.4430
D	0.6210	0.4240
E	0.6110	0.4400
F	0.7750	0.4910
G	0.7560	0.4550
H	0.7960	0.4740
I	0.7150	0.4640
J	0.6910	0.4390
K	0.4660	0.3630
L	0.5920	0.2970
M	0.2960	0.0490
N	0.6430	0.3600
O	0.6640	0.3510
P	0.7190	0.4000
Q	0.7140	0.3890
R	0.7400	0.4220
S	0.7320	0.4500
X	0.4680	0.1960
Y	0.4420	0.1650