Full wwPDB EM Validation Report ⓘ

Nov 5, 2024 – 06:02 AM EST

PDB ID	:	8UMH
EMDB ID	:	EMD-42379
Title	:	Consensus map of PICdeltaTFIIK form2
Authors	:	Yang, C.; Murakami, K.
Deposited on	:	2023-10-17
Resolution	:	4.10 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:

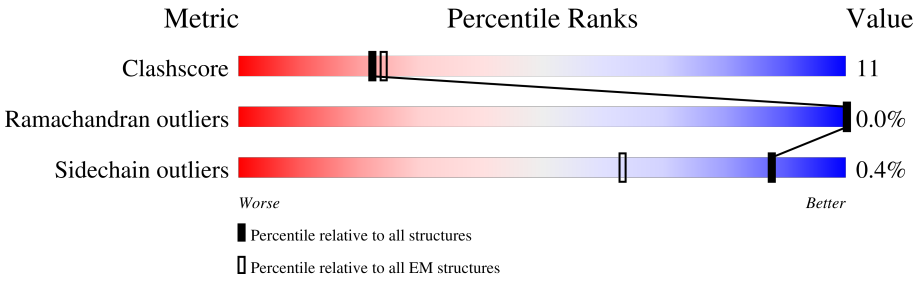
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.10 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	M	345	27% 63% 18% 19%
2	A	1733	• 59% 23% 18%
3	B	1224	6% 67% 27% 5%
4	C	318	19% 56% 27% 17%
5	E	215	84% 15%
6	F	155	6% 43% 13% 44%
7	H	146	8% 57% 35% • 8%
8	I	122	• 61% 33% 7%

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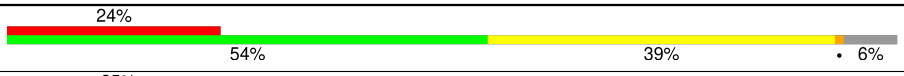
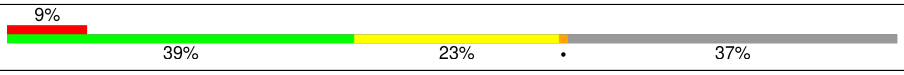
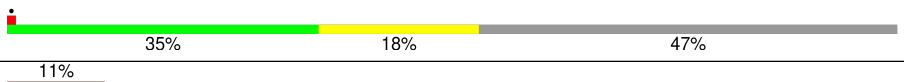
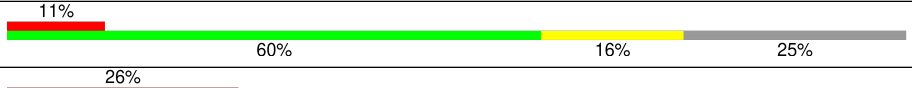
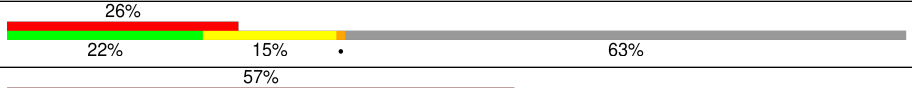
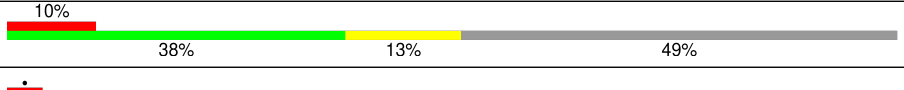
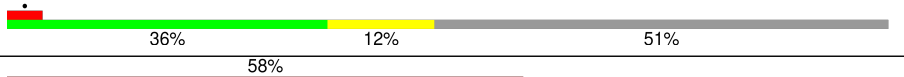
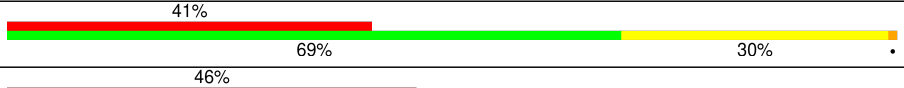
Mol	Chain	Length	Quality of chain
9	J	70	
10	K	120	
11	L	70	
12	Q	735	
13	P	400	
14	S	309	
15	O	240	
16	U	286	
17	V	122	
18	W	482	
19	X	328	
20	D	221	
21	G	171	
22	0	778	
23	1	642	
24	4	338	
25	6	461	
26	7	843	
27	2	513	
28	5	72	
29	N	64	
30	T	64	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	SF4	0	801	-	-	X	-

2 Entry composition (i)

There are 33 unique types of molecules in this entry. The entry contains 70481 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 Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	M	279	2175	1382	373	403	17	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	1425	11167	7036	1948	2121	62	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	1166	9227	5823	1619	1729	56	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	265	2086	1312	347	414	13	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	214	1752	1111	309	321	11	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	87	705	451	119	132	3	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	135	Total	C	N	O	S	0	0
			1080	679	182	214	5		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	114	Total	C	N	O	S	0	0
			927	571	168	178	10		

- Molecule 9 is a protein called DNA-directed RNA polymerases II subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	66	Total	C	N	O	S	0	0
			540	345	94	95	6		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	115	Total	C	N	O	S	0	0
			924	593	157	172	2		

- Molecule 11 is a protein called DNA-directed RNA polymerases II subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	44	Total	C	N	O	S	0	0
			352	217	70	61	4		

- Molecule 12 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	214	Total	C	N	O	S	0	0
			1619	1017	297	299	6		

- Molecule 13 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	179	Total	C	N	O	S	0	0
			1484	941	258	279	6		

- Molecule 14 is a protein called Transcription elongation factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	164	Total	C	N	O	S	0	0
			1294	809	230	247	8		

- Molecule 15 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	181	Total	C	N	O	S	0	0
			1422	925	243	248	6		

- Molecule 16 is a protein called Transcription initiation factor IIA large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	107	Total	C	N	O	S	0	0
			885	559	147	176	3		

- Molecule 17 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	104	Total	C	N	O	S	0	0
			815	511	136	164	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	247	Total	C	N	O	S	0	0
			2010	1275	347	381	7		

- Molecule 19 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	160	Total	C	N	O	S	0	0
			1288	826	212	245	5		

- Molecule 20 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	D	168	Total	C	N	O	S	0	0
			1331	822	237	270	2		

- Molecule 21 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	G	171	Total	C	N	O	S	0	0
			1335	858	221	248	8		

- Molecule 22 is a protein called General transcription and DNA repair factor IIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	0	752	Total	C	N	O	S	0	0
			6091	3882	1029	1142	38		

- Molecule 23 is a protein called TFB1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1	417	Total	C	N	O	S	0	0
			3382	2139	587	640	16		

- Molecule 24 is a protein called General transcription and DNA repair factor IIH subunit TFB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	4	292	Total	C	N	O	S	0	0
			2267	1449	376	428	14		

- Molecule 25 is a protein called General transcription and DNA repair factor IIH.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	6	355	Total	C	N	O	S	0	0
			2786	1765	481	512	28		

- Molecule 26 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	7	608	Total	C	N	O	S	0	0
			4889	3110	847	906	26		

- Molecule 27 is a protein called RNA polymerase II transcription factor B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	445	Total	C	N	O	S	0	0
			3546	2291	585	654	16		

- Molecule 28 is a protein called General transcription and DNA repair factor IIH subunit

TFB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	5	66	Total	C	N	O	S	0	0
			498	314	89	93	2		

- Molecule 29 is a DNA chain called DNA (63-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
29	N	63	Total	C	N	O	P	0	0
			1288	621	225	380	62		

- Molecule 30 is a DNA chain called DNA (63-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
30	T	63	Total	C	N	O	P	0	0
			1291	619	236	373	63		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	-10	DC	DT	conflict	GB 2567904391

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

Mol	Chain	Residues	Atoms		AltConf
31	M	1	Total	Zn	0
			1	1	
31	A	2	Total	Zn	0
			2	2	
31	B	1	Total	Zn	0
			1	1	
31	C	1	Total	Zn	0
			1	1	
31	I	2	Total	Zn	0
			2	2	
31	J	1	Total	Zn	0
			1	1	
31	L	1	Total	Zn	0
			1	1	
31	S	1	Total	Zn	0
			1	1	
31	4	1	Total	Zn	0
			1	1	

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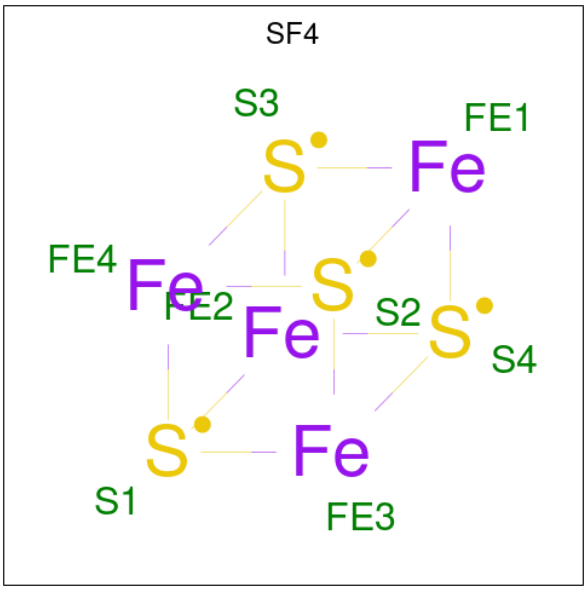
Mol	Chain	Residues	Atoms	AltConf
31	6	4	Total Zn 4 4	0

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
32	A	1	Total Mg 1 1	0
32	7	1	Total Mg 1 1	0

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



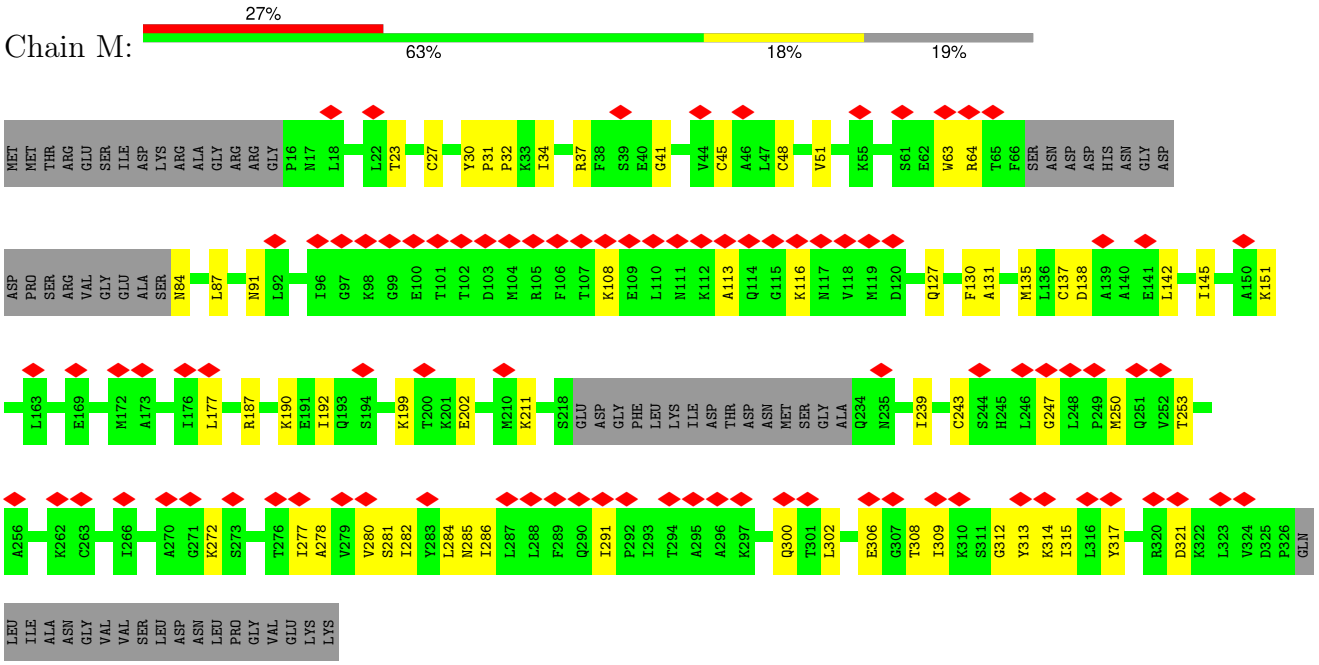
Mol	Chain	Residues	Atoms	AltConf
33	0	1	Total Fe S 8 4 4	0

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.

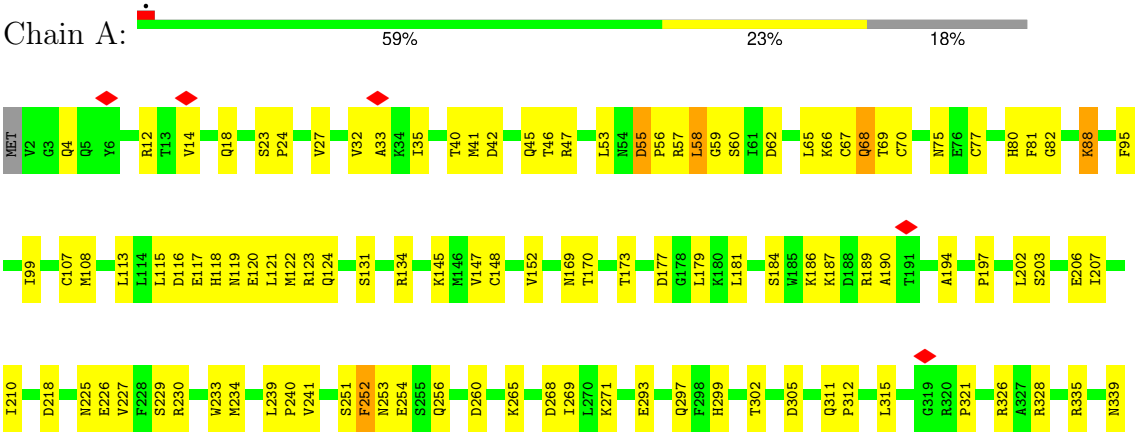
• Molecule 1: Transcription initiation factor IIB

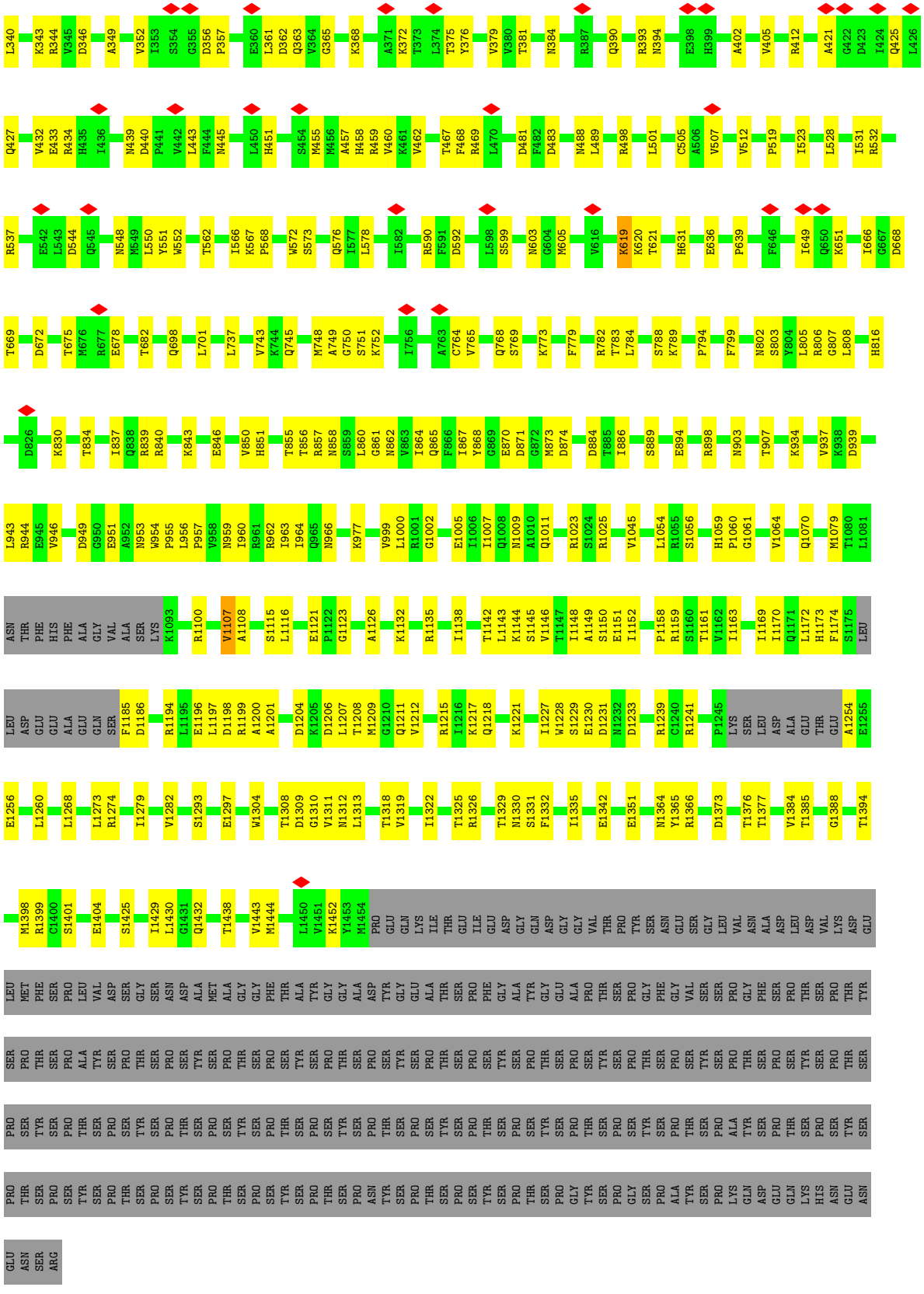
Chain M:



• Molecule 2: DNA-directed RNA polymerase subunit

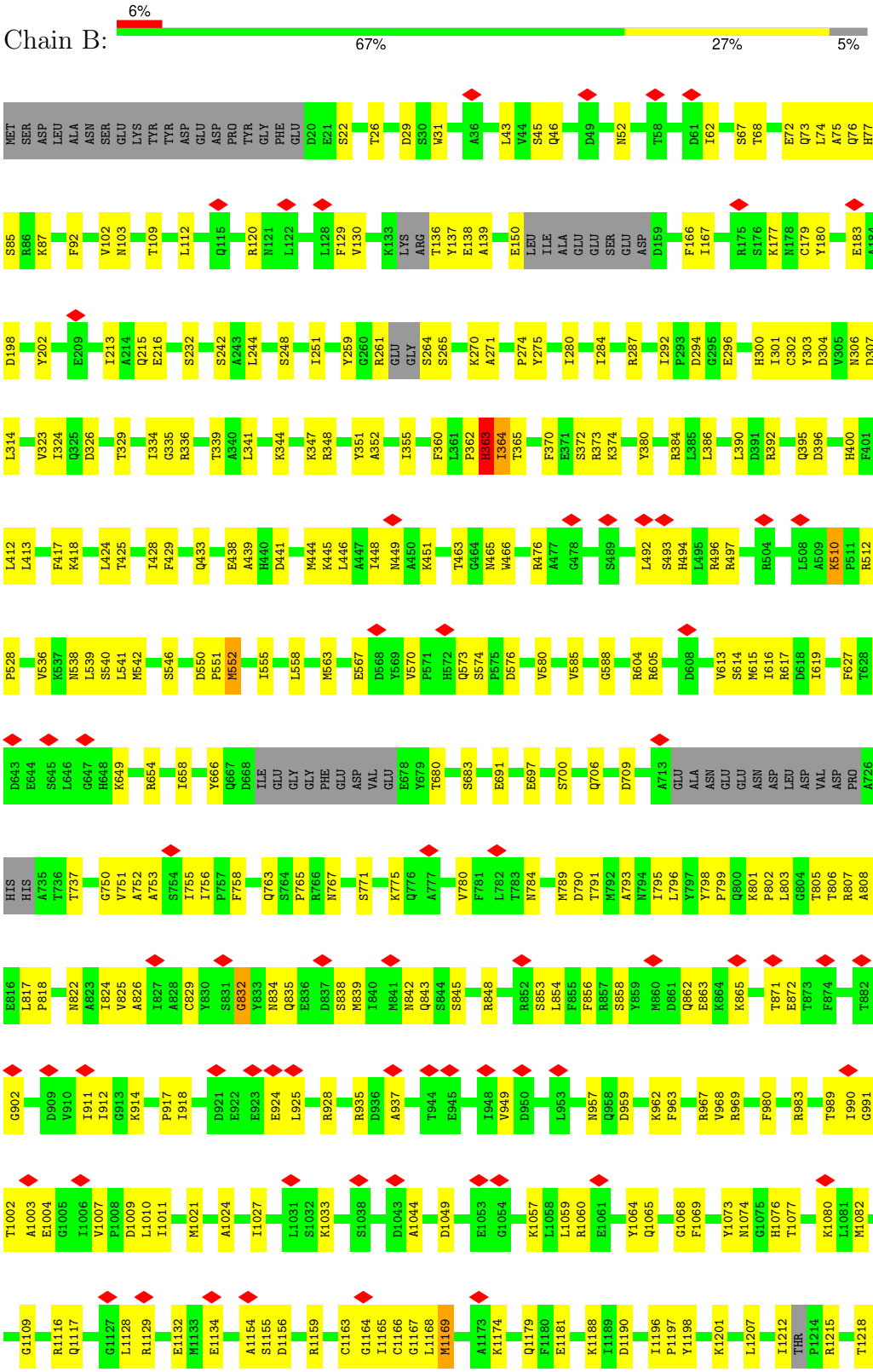
Chain A:





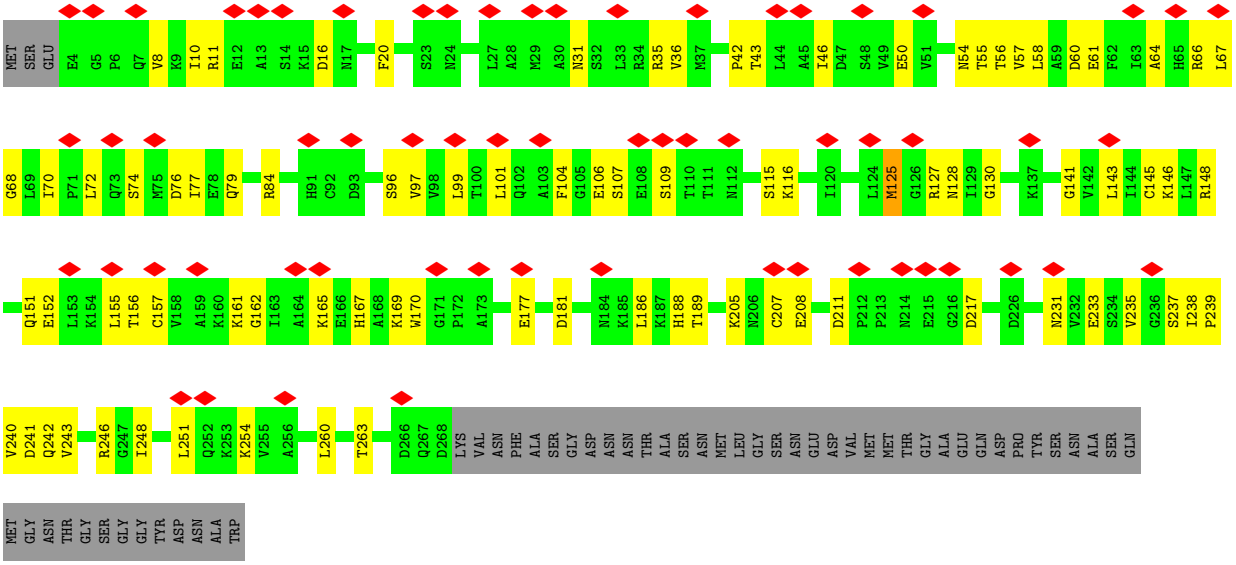
• Molecule 3: DNA-directed RNA polymerase subunit beta

Chain B:



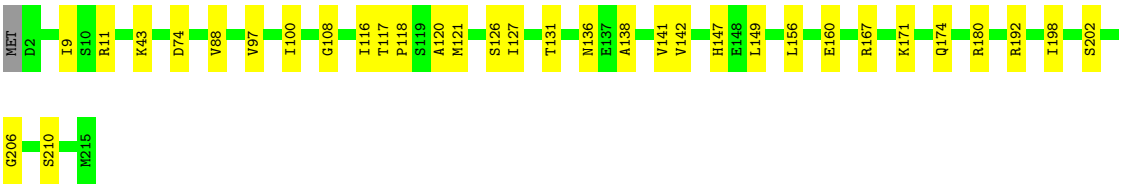
• Molecule 4: DNA-directed RNA polymerase II subunit RPB3

Chain C:



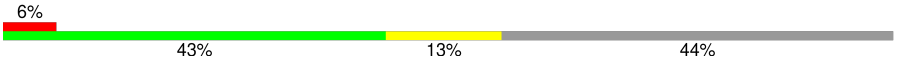
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

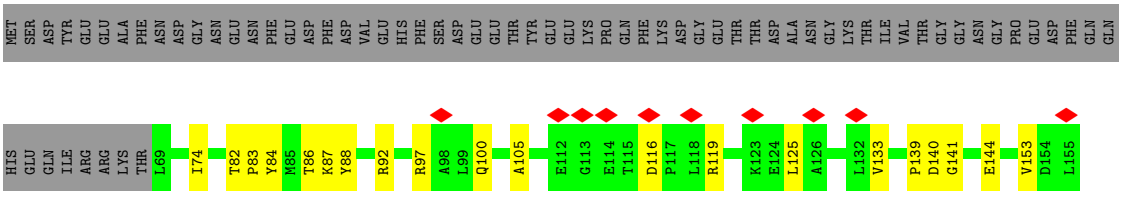
Chain E:



• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

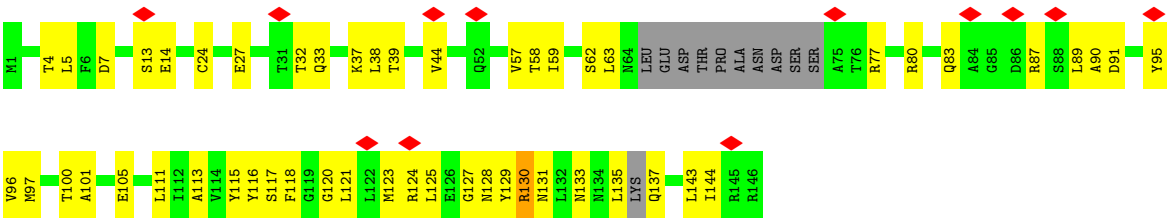
Chain F:





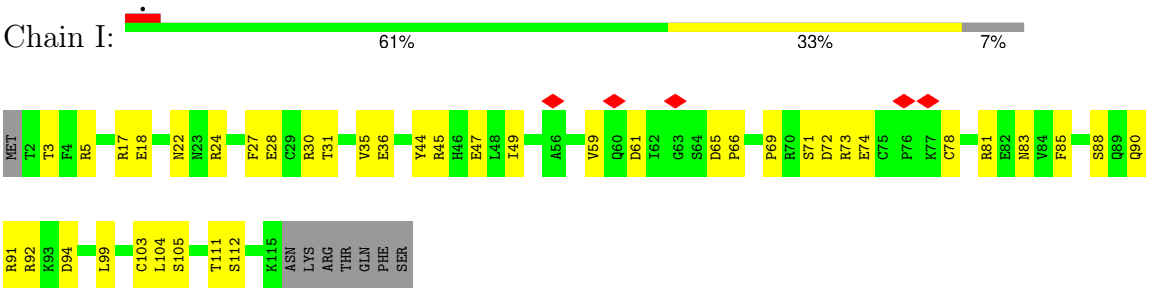
• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



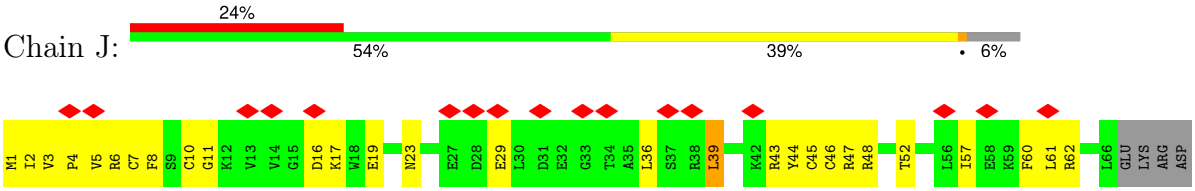
• Molecule 8: DNA-directed RNA polymerase II subunit RPB9

Chain I:



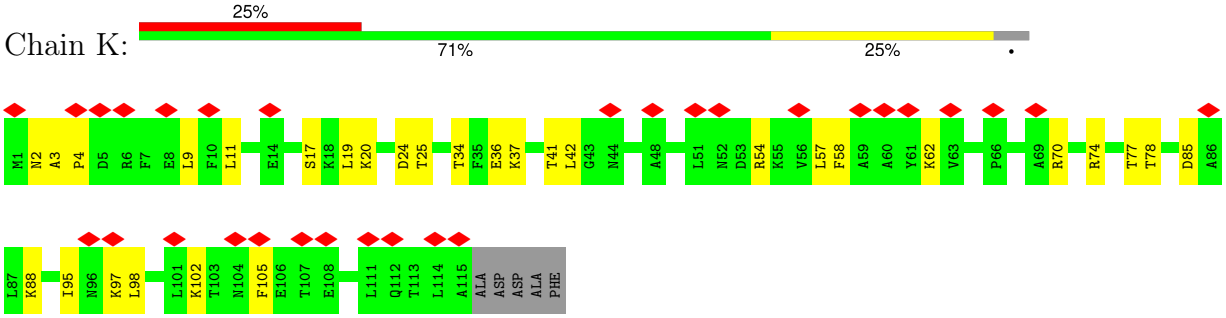
• Molecule 9: DNA-directed RNA polymerases II subunit RPABC5

Chain J:



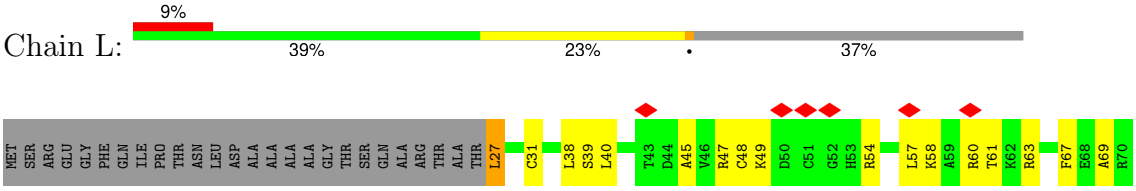
• Molecule 10: DNA-directed RNA polymerase II subunit RPB11

Chain K:



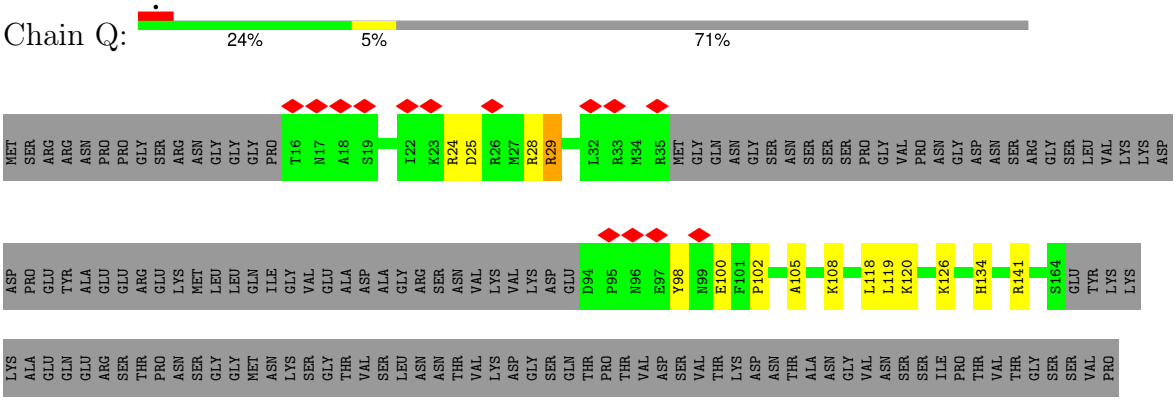
• Molecule 11: DNA-directed RNA polymerases II subunit RPABC4

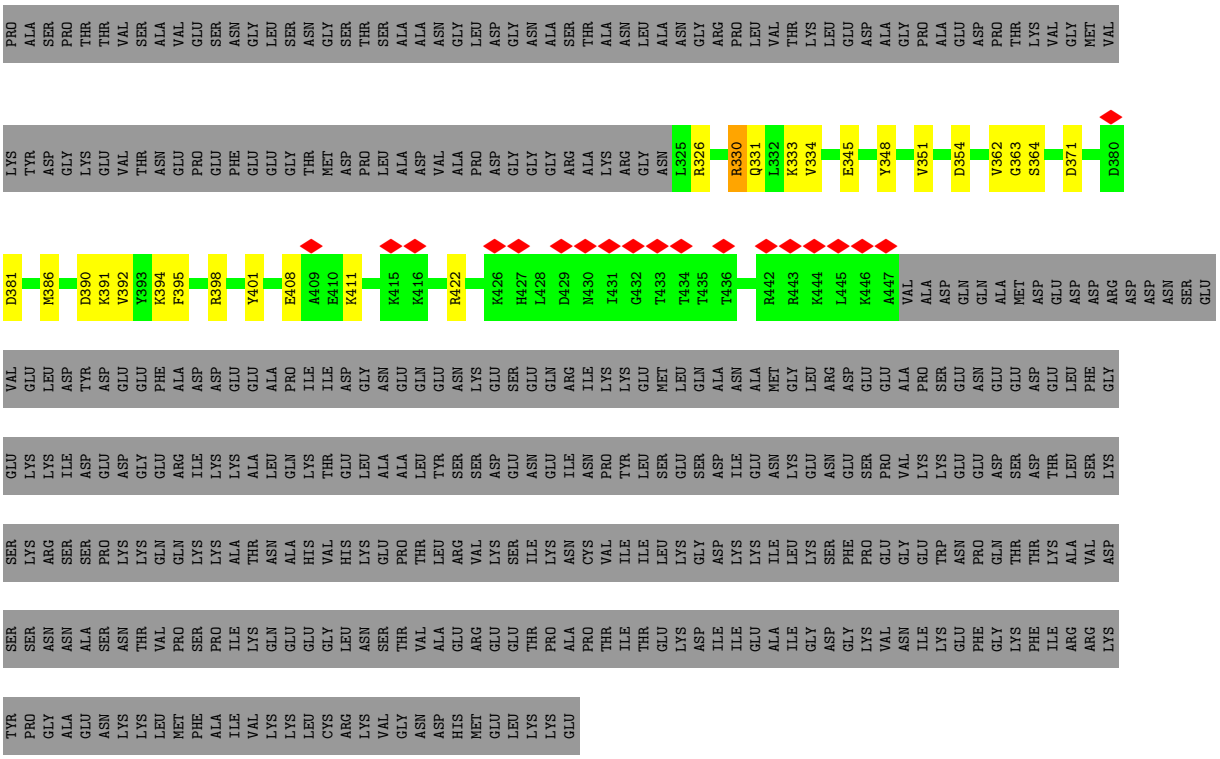
Chain L:



• Molecule 12: Transcription initiation factor IIF subunit alpha

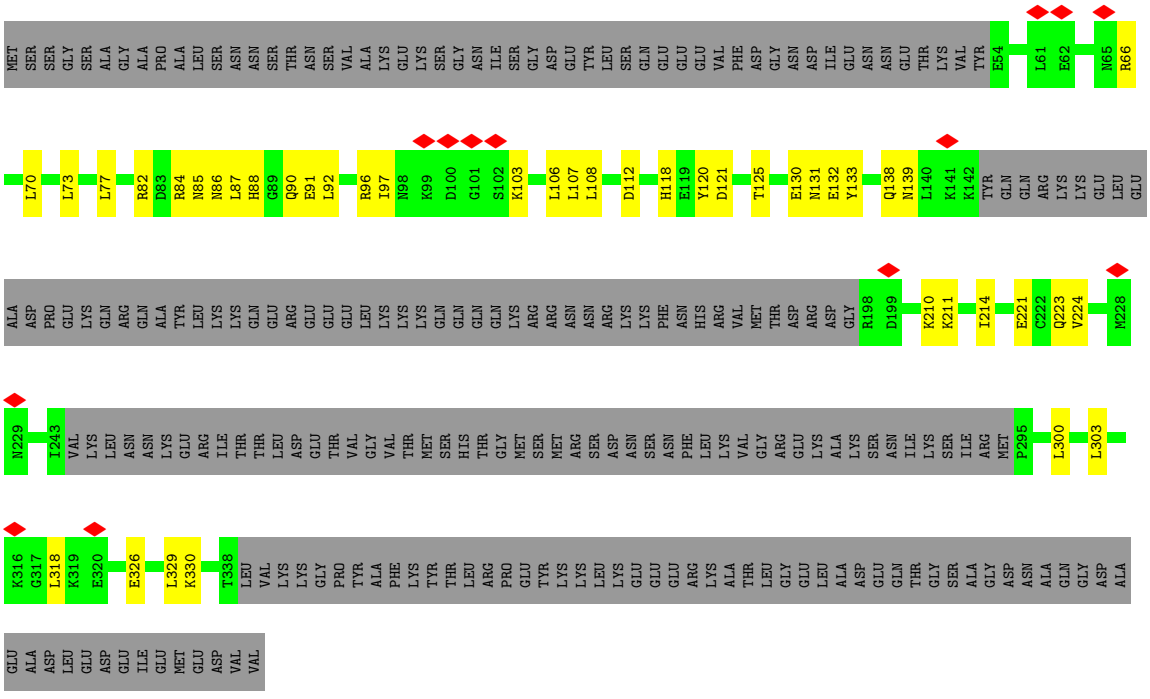
Chain Q:





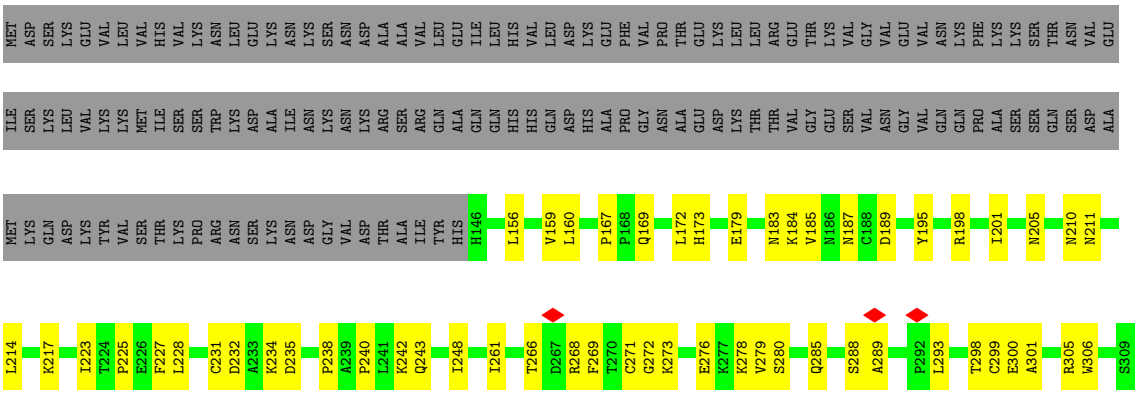
• Molecule 13: Transcription initiation factor IIF subunit beta

Chain P:



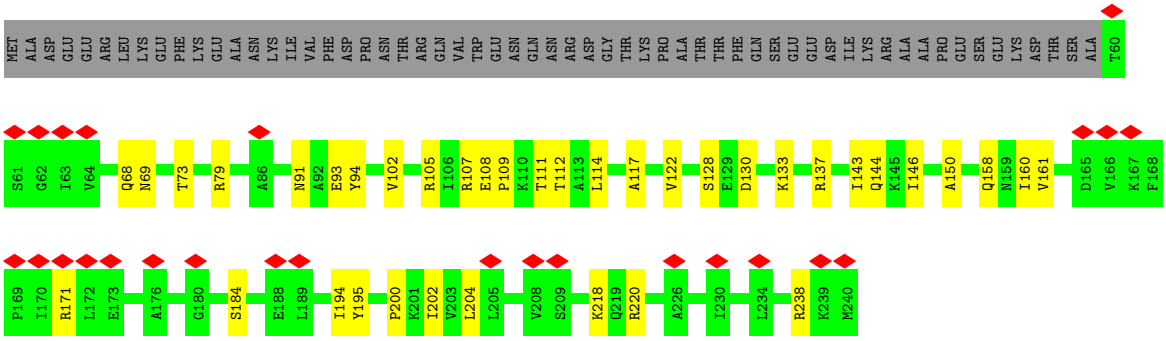
• Molecule 14: Transcription elongation factor

Chain S:



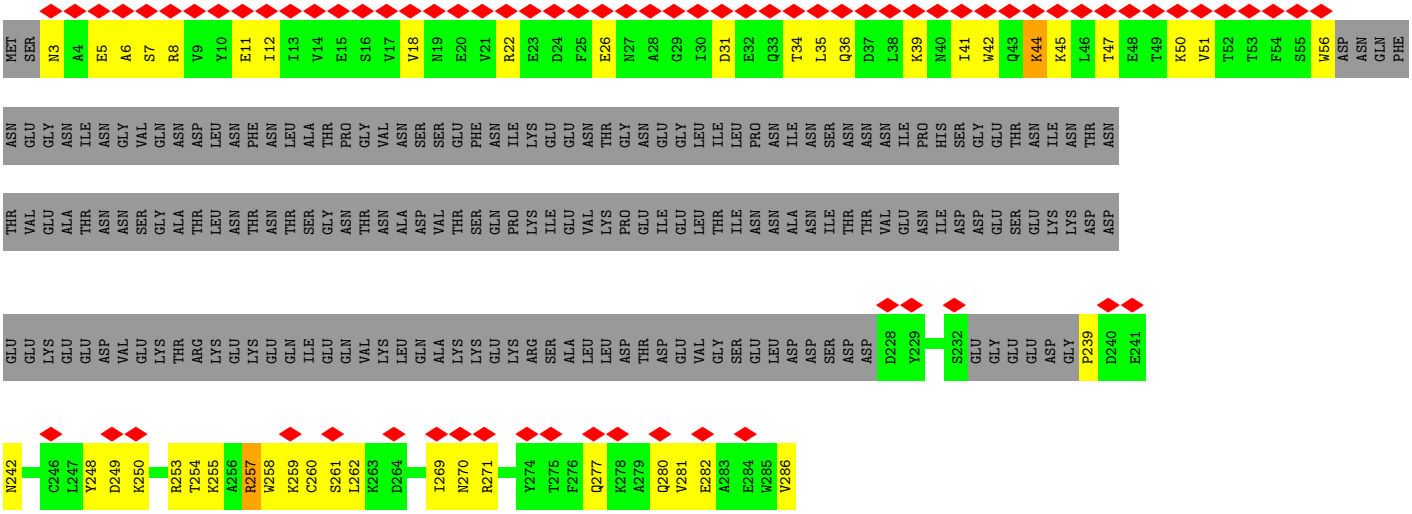
• Molecule 15: TATA-box-binding protein

Chain O:



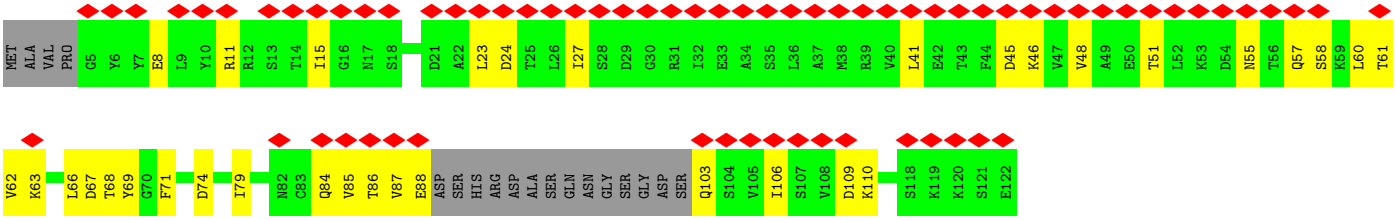
• Molecule 16: Transcription initiation factor IIA large subunit

Chain U:



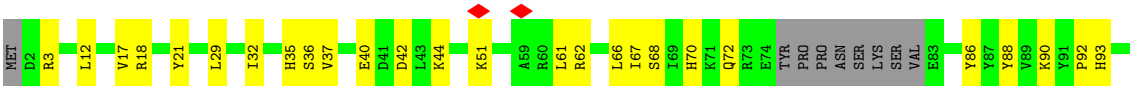
• Molecule 17: Transcription initiation factor IIA subunit 2

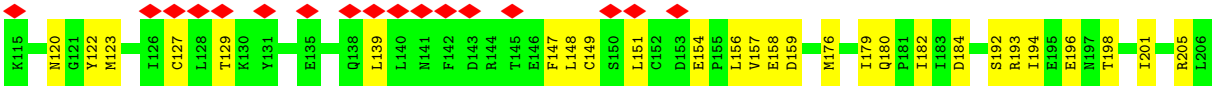
Chain V:

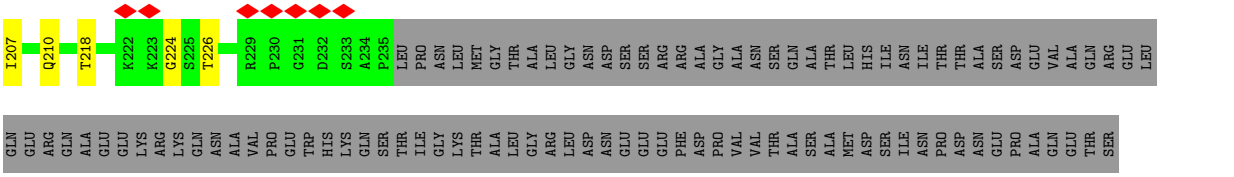


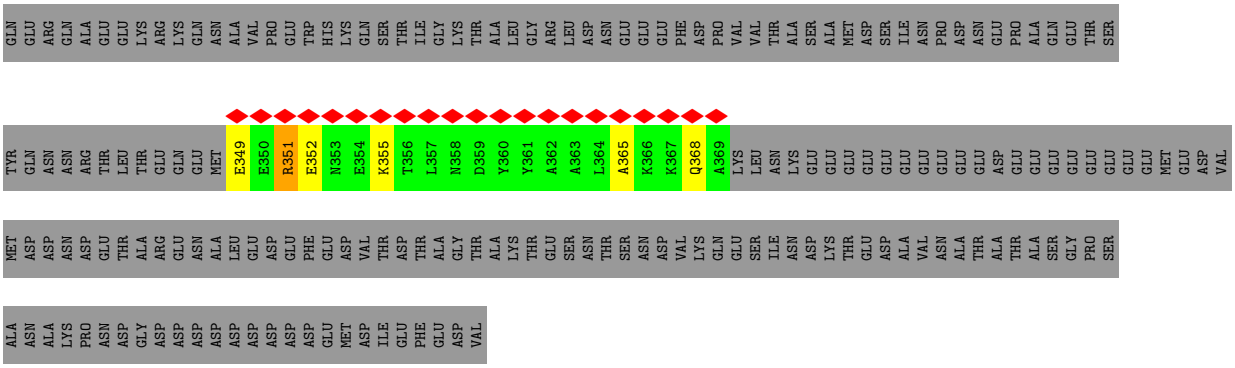
• Molecule 18: Transcription initiation factor IIE subunit alpha

Chain W:



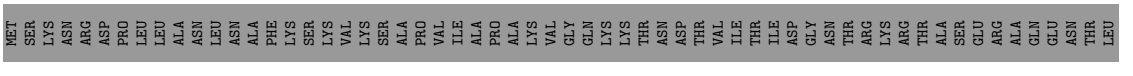


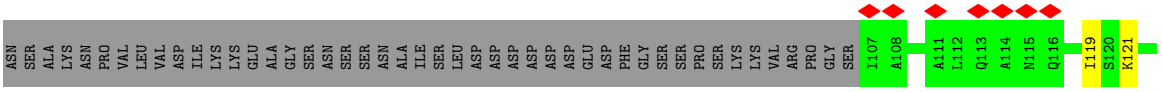


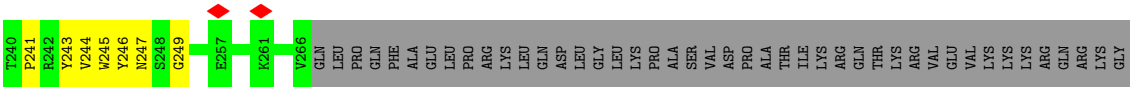


• Molecule 19: Transcription initiation factor IIE subunit beta

Chain X:

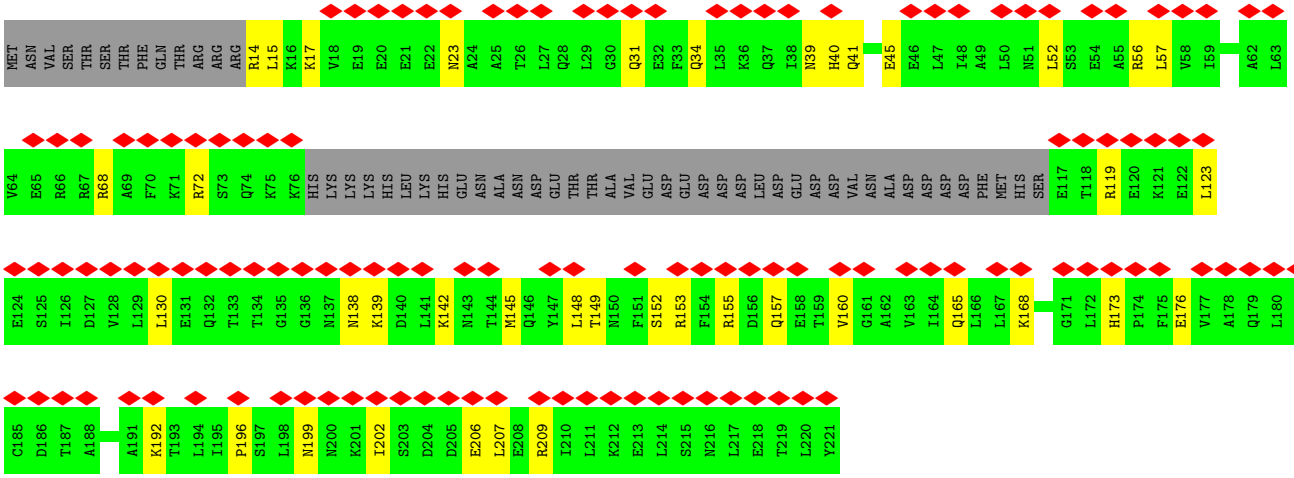






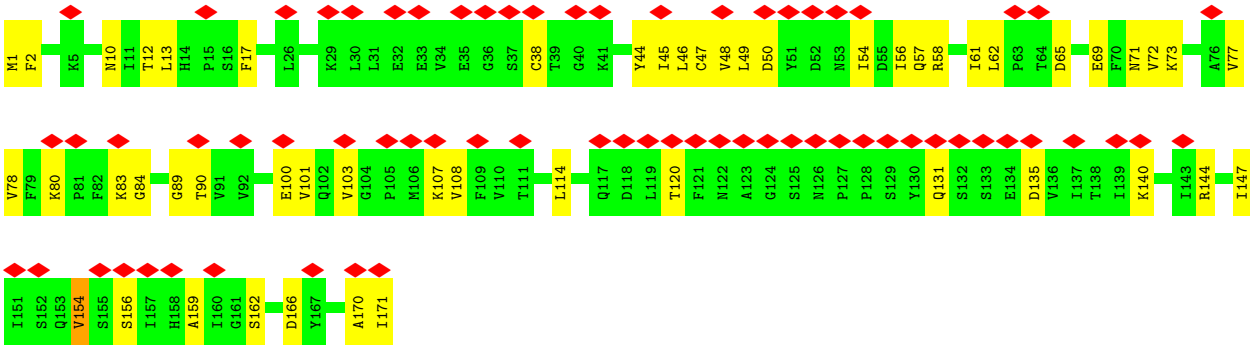
• Molecule 20: DNA-directed RNA polymerase II subunit RPB4

Chain D:



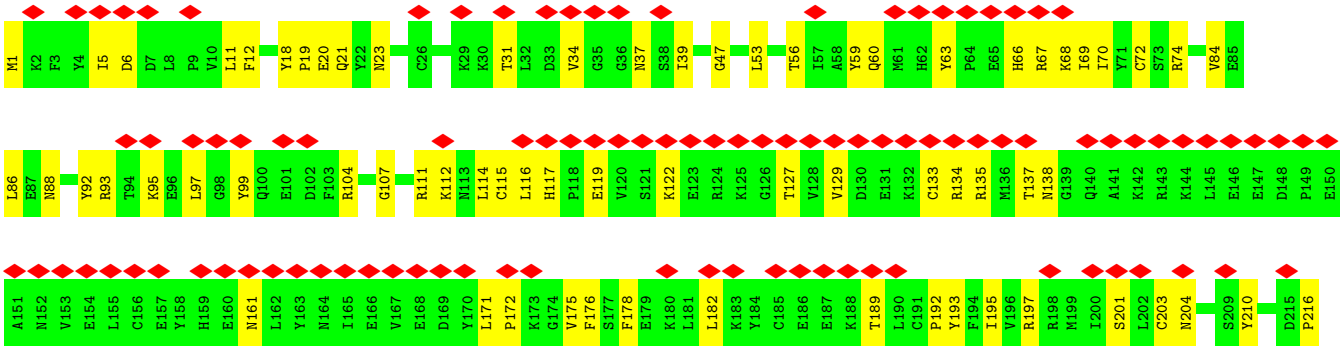
• Molecule 21: DNA-directed RNA polymerase II subunit RPB7

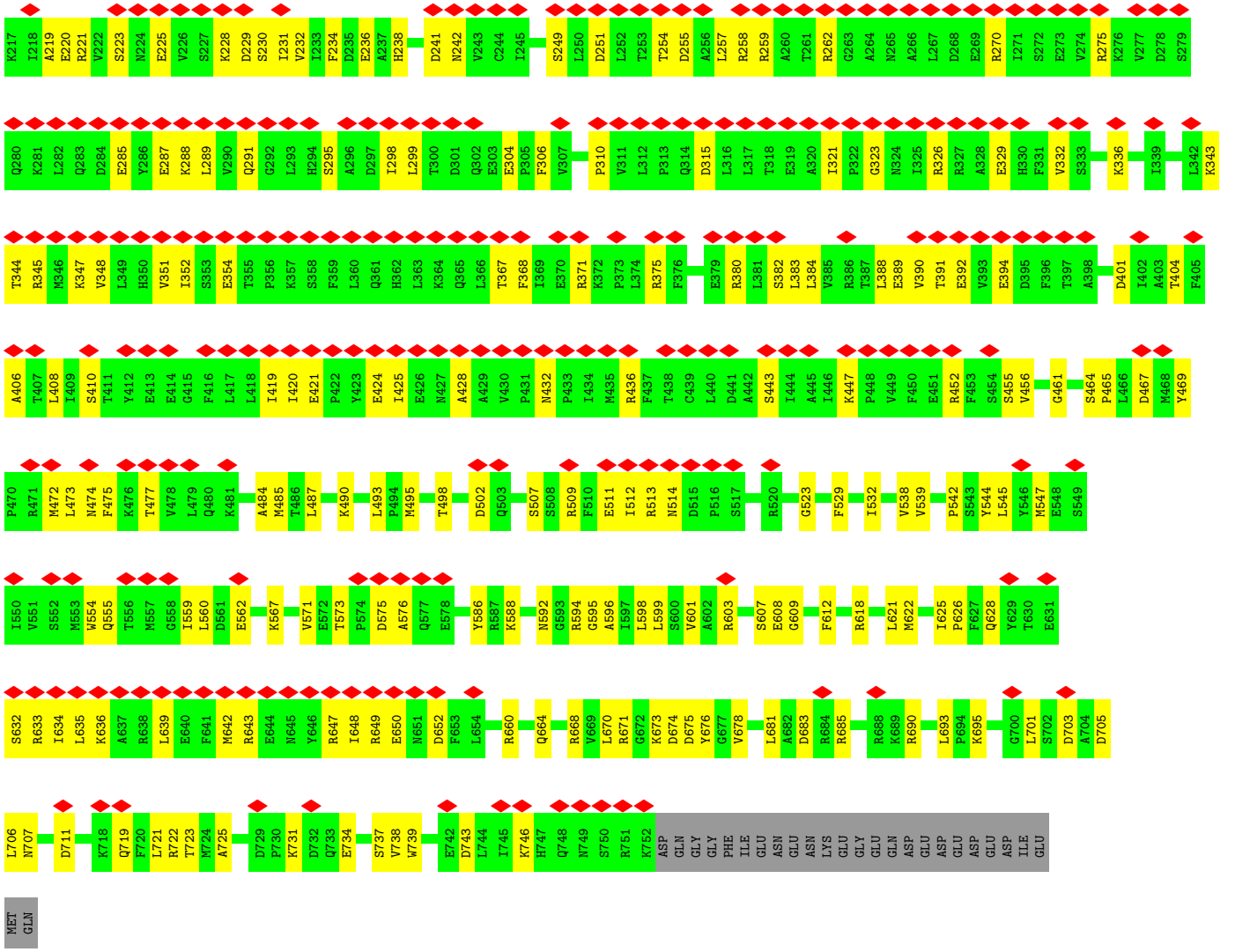
Chain G:



• Molecule 22: General transcription and DNA repair factor IIH helicase subunit XPD

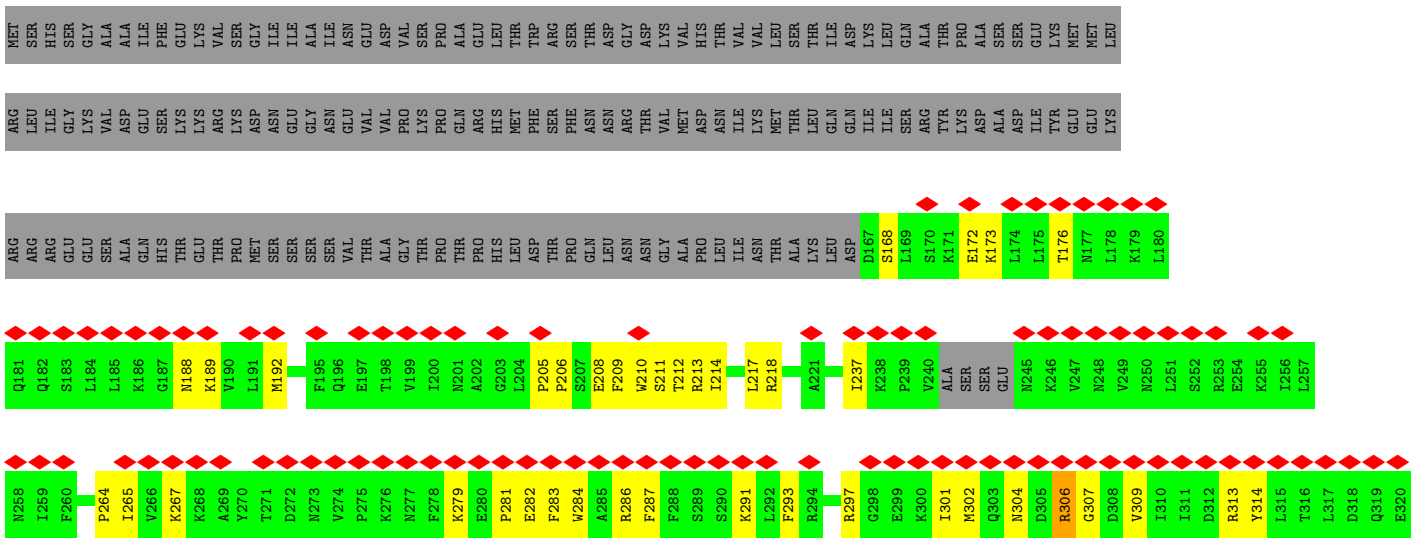
Chain 0:

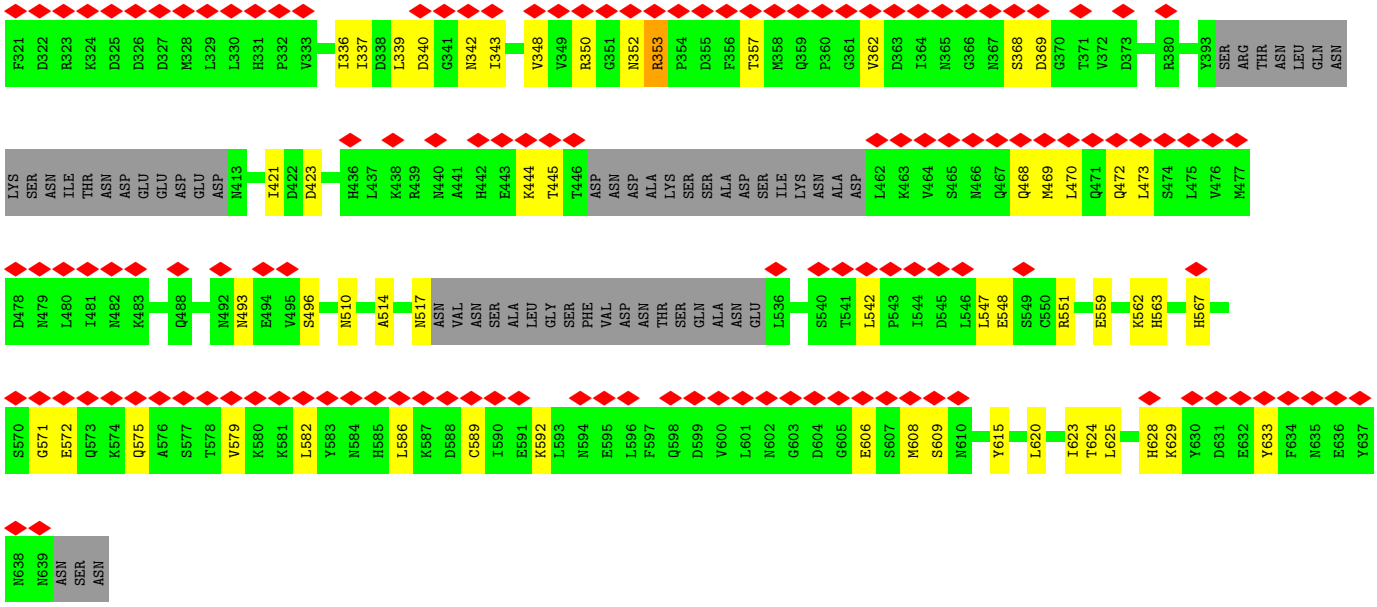




• Molecule 23: TFB1 isoform 1

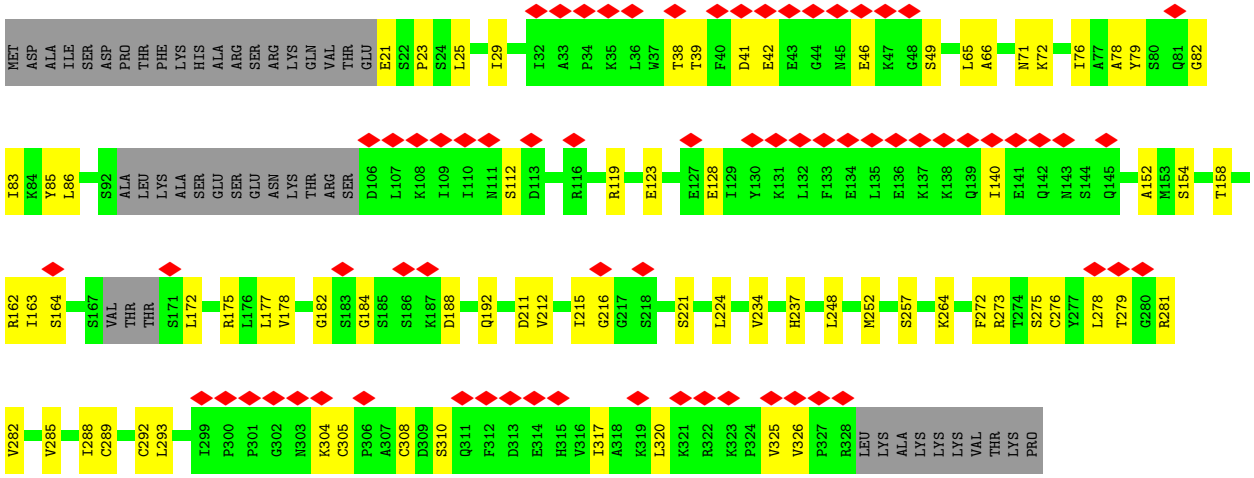
Chain 1:





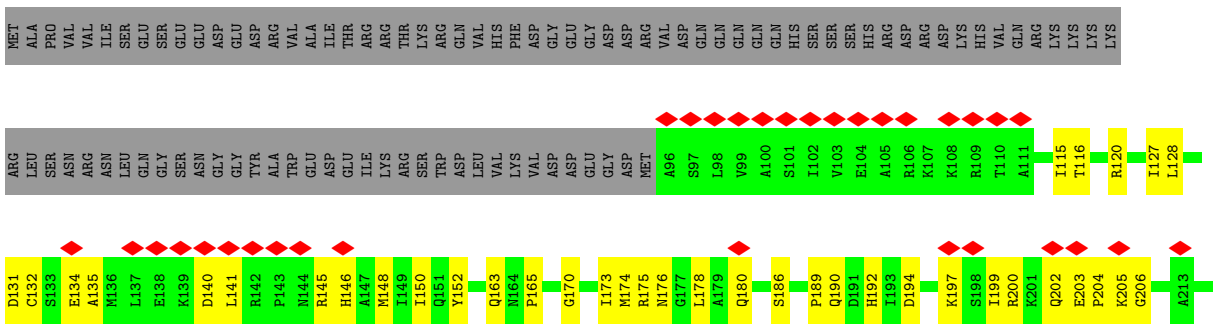
• Molecule 24: General transcription and DNA repair factor IIH subunit TFB4

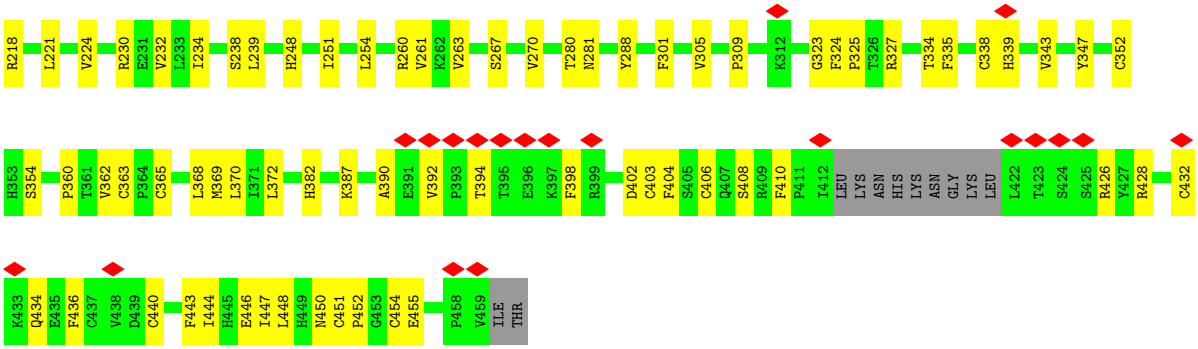
Chain 4:



• Molecule 25: General transcription and DNA repair factor IIH

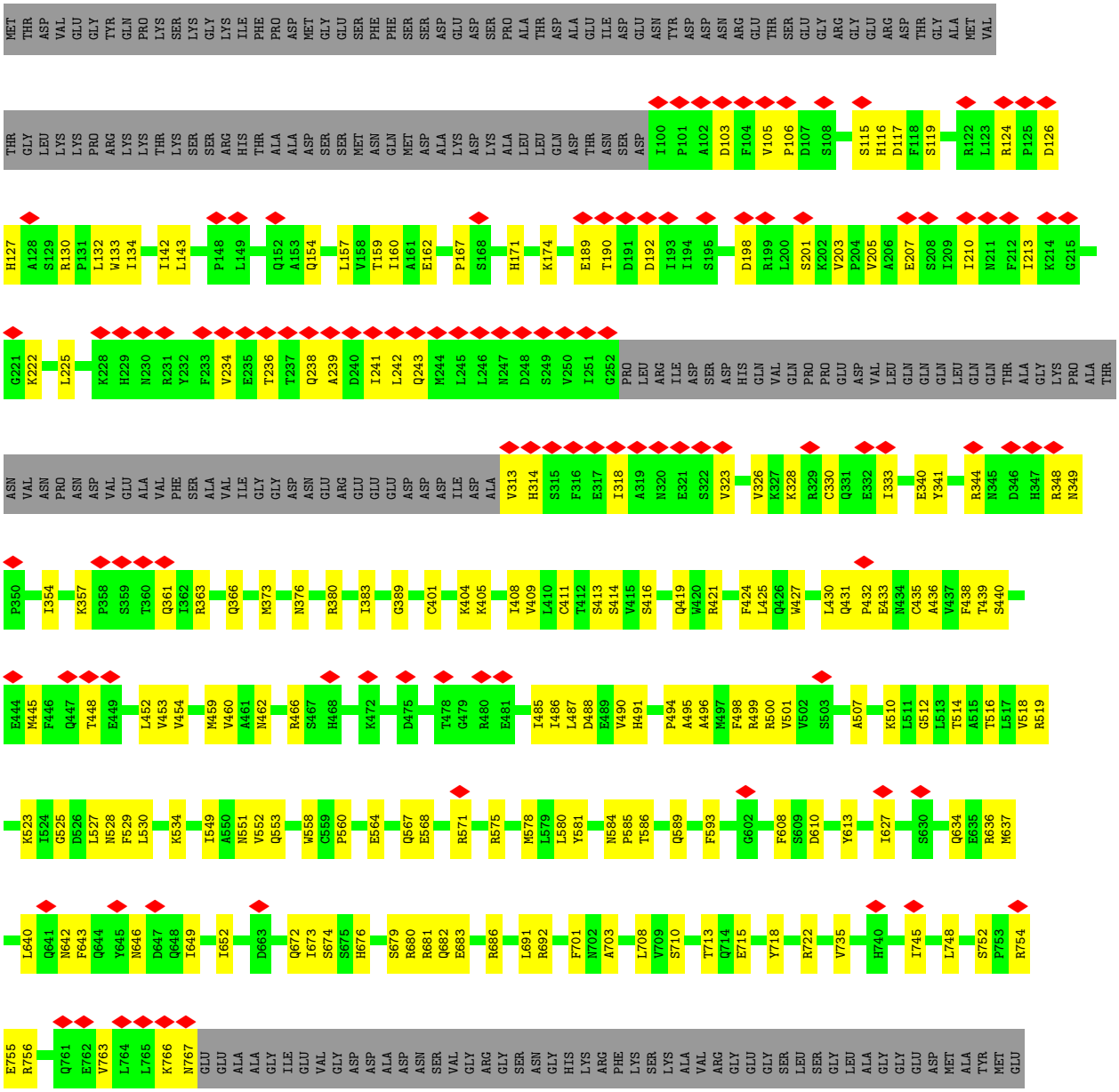
Chain 6:





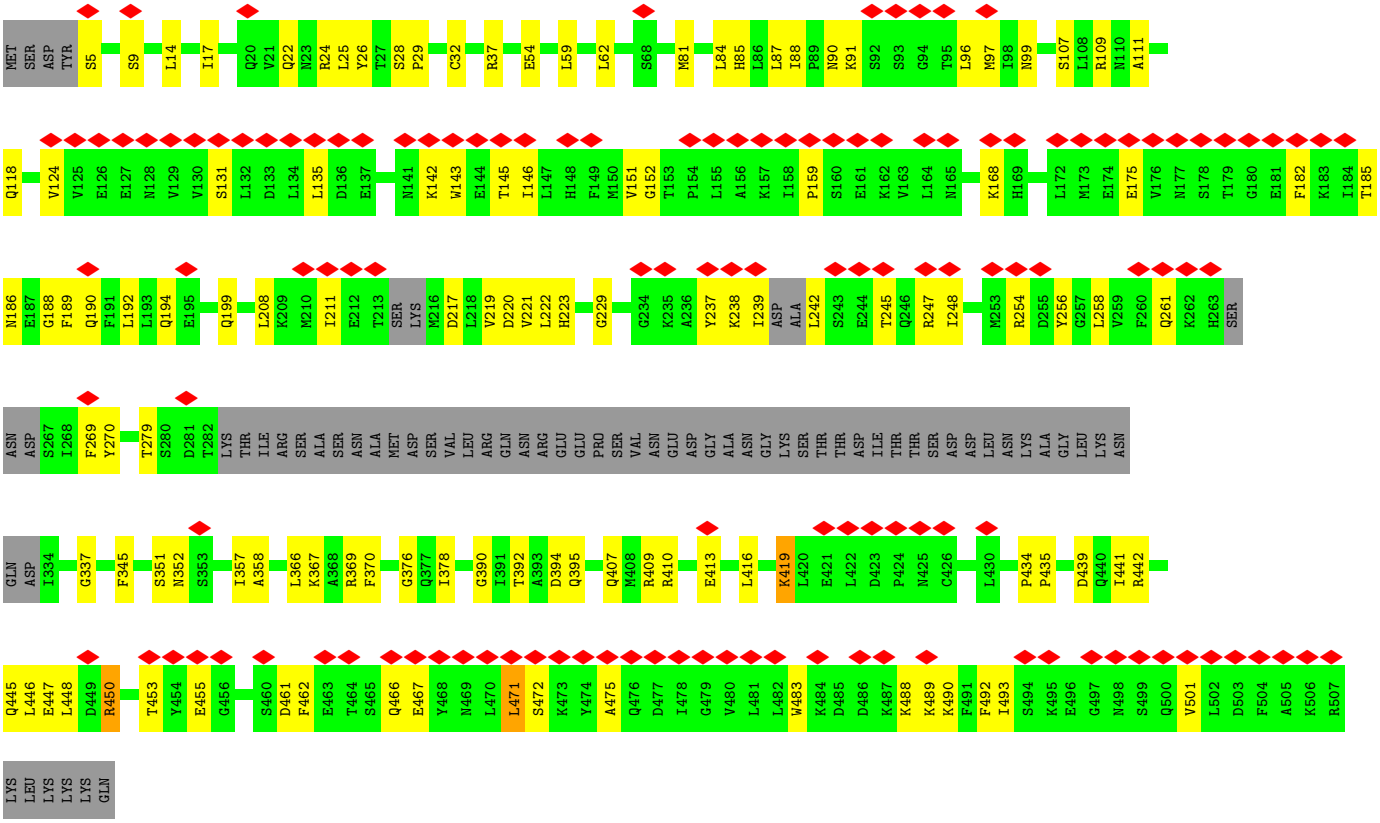
• Molecule 26: General transcription and DNA repair factor IIH helicase subunit XPB

Chain 7:



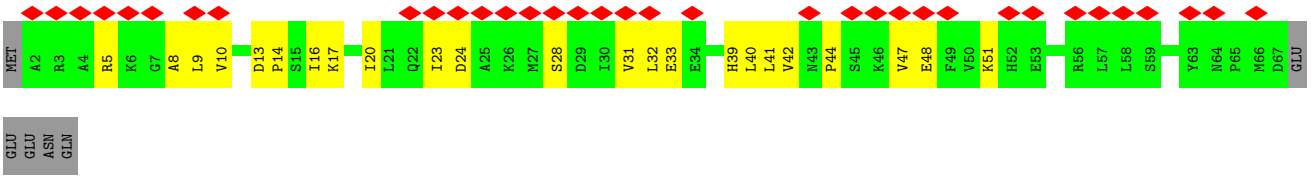
• Molecule 27: RNA polymerase II transcription factor B subunit 2

Chain 2:



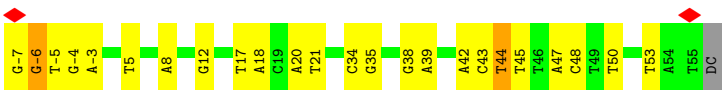
• Molecule 28: General transcription and DNA repair factor IIH subunit TFB5

Chain 5:



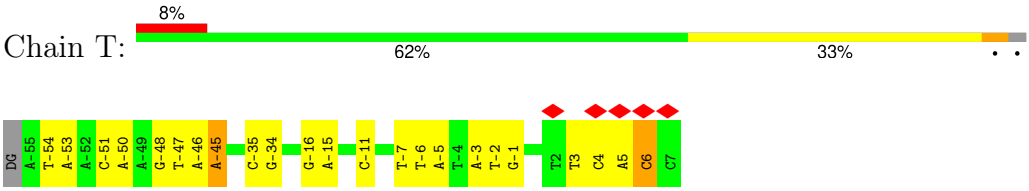
• Molecule 29: DNA (63-MER)

Chain N:



• Molecule 30: DNA (63-MER)

Chain T:


8%
62%
33%
DG
A-55
T-54
A-53
A-52
C-51
A-50
A-49
G-48
T-47
A-46
A-45
C-35
G-34
G-16
A-15
C-11
T-7
T-6
A-5
T-4
A-3
T-2
G-1
T2
T3
C4
A5
C6
C7

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90136	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.25	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	1750	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.078	Depositor
Minimum map value	-0.023	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0098	Depositor
Map size (Å)	414.72003, 414.72003, 414.72003	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	M	0.29	0/2204	0.60	0/2963
2	A	0.40	0/11368	0.65	4/15383 (0.0%)
3	B	0.43	0/9402	0.66	4/12680 (0.0%)
4	C	0.43	0/2124	0.64	1/2879 (0.0%)
5	E	0.38	0/1788	0.60	0/2406
6	F	0.41	0/717	0.64	0/967
7	H	0.41	0/1097	0.67	0/1484
8	I	0.36	0/945	0.56	0/1273
9	J	0.58	0/549	0.83	2/738 (0.3%)
10	K	0.39	0/942	0.59	0/1272
11	L	0.41	0/354	0.84	1/468 (0.2%)
12	Q	0.31	0/1648	0.54	0/2226
13	P	0.28	0/1511	0.54	0/2035
14	S	0.31	0/1317	0.61	0/1778
15	O	0.30	0/1449	0.53	0/1952
16	U	0.29	0/898	0.59	0/1212
17	V	0.31	0/822	0.63	0/1109
18	W	0.27	0/2045	0.49	0/2757
19	X	0.27	0/1312	0.49	0/1767
20	D	0.27	0/1339	0.52	0/1793
21	G	0.32	0/1363	0.63	0/1840
22	0	0.30	0/6209	0.52	0/8384
23	1	0.28	0/3434	0.51	0/4624
24	4	0.29	0/2305	0.50	0/3117
25	6	0.29	0/2843	0.53	0/3845
26	7	0.30	0/4992	0.56	0/6754
27	2	0.29	0/3611	0.56	1/4881 (0.0%)
28	5	0.30	0/502	0.72	0/677
29	N	0.84	0/1443	1.20	10/2226 (0.4%)
30	T	0.85	1/1449 (0.1%)	1.18	6/2233 (0.3%)
All	All	0.38	1/71982 (0.0%)	0.63	29/97723 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	M	0	3
2	A	0	7
3	B	0	5
5	E	0	1
11	L	0	1
14	S	0	2
21	G	0	1
All	All	0	20

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	T	-47	DT	C3'-O3'	-5.19	1.37	1.44

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	N	8	DA	O4'-C4'-C3'	-6.91	101.73	104.50
29	N	-6	DG	O4'-C4'-C3'	-6.28	101.99	104.50
2	A	58	LEU	CA-CB-CG	5.96	129.00	115.30
9	J	29	GLU	CA-CB-CG	5.90	126.38	113.40
2	A	234	MET	CA-CB-CG	5.80	123.17	113.30
29	N	45	DT	N3-C4-O4	5.69	123.32	119.90
9	J	39	LEU	CA-CB-CG	5.64	128.28	115.30
27	2	471	LEU	CA-CB-CG	5.59	128.16	115.30
29	N	50	DT	C3'-C2'-C1'	-5.59	95.80	102.50
2	A	701	LEU	CA-CB-CG	5.56	128.09	115.30
11	L	27	LEU	CA-CB-CG	5.55	128.08	115.30
2	A	1107	VAL	C-N-CA	5.52	135.50	121.70
29	N	45	DT	O4'-C1'-N1	5.47	111.83	108.00
29	N	44	DT	N3-C4-O4	5.47	123.18	119.90
3	B	1169	MET	CB-CG-SD	5.43	128.69	112.40
3	B	552	MET	CA-CB-CG	5.42	122.51	113.30
30	T	-45	DA	O4'-C4'-C3'	-5.41	102.33	104.50
3	B	79	THR	C-N-CA	5.39	135.18	121.70
4	C	125	MET	CA-CB-CG	5.36	122.42	113.30
30	T	-48	DG	O4'-C1'-N9	5.18	111.62	108.00
29	N	45	DT	C5-C4-O4	-5.14	121.30	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	918	ILE	C-N-CA	5.12	134.51	121.70
29	N	-7	DG	O4'-C1'-N9	5.12	111.58	108.00
30	T	6	DC	O4'-C4'-C3'	-5.05	102.48	104.50
30	T	-51	DC	C3'-C2'-C1'	-5.04	96.45	102.50
30	T	-50	DA	C4'-C3'-C2'	-5.04	98.56	103.10
29	N	44	DT	C5-C4-O4	-5.03	121.38	124.90
29	N	8	DA	C4'-C3'-C2'	-5.03	98.57	103.10
30	T	-50	DA	O4'-C4'-C3'	-5.00	102.50	104.50

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	1404	GLU	Peptide
2	A	152	VAL	Peptide
2	A	252	PHE	Peptide
2	A	55	ASP	Peptide
2	A	639	PRO	Peptide
2	A	65	LEU	Peptide
2	A	750	GLY	Peptide
3	B	1169	MET	Peptide
3	B	137	TYR	Peptide
3	B	363	HIS	Peptide
3	B	510	LYS	Peptide
3	B	832	GLY	Peptide
5	E	171	LYS	Peptide
21	G	154	VAL	Peptide
11	L	58	LYS	Peptide
1	M	272	LYS	Peptide
1	M	30	TYR	Peptide
1	M	31	PRO	Peptide
14	S	227	PHE	Peptide
14	S	261	ILE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	2175	0	2283	39	0
2	A	11167	0	11189	284	0
3	B	9227	0	9200	246	0
4	C	2086	0	2045	61	0
5	E	1752	0	1776	23	0
6	F	705	0	731	17	0
7	H	1080	0	1049	42	0
8	I	927	0	880	32	0
9	J	540	0	553	21	0
10	K	924	0	934	28	0
11	L	352	0	375	12	0
12	Q	1619	0	1452	35	0
13	P	1484	0	1480	35	0
14	S	1294	0	1289	31	0
15	O	1422	0	1500	28	0
16	U	885	0	866	33	0
17	V	815	0	822	31	0
18	W	2010	0	2026	44	0
19	X	1288	0	1307	24	0
20	D	1331	0	1345	27	0
21	G	1335	0	1346	31	0
22	0	6091	0	6155	178	0
23	1	3382	0	3436	66	0
24	4	2267	0	2323	52	0
25	6	2786	0	2804	68	0
26	7	4889	0	4876	125	0
27	2	3546	0	3593	82	0
28	5	498	0	506	13	0
29	N	1288	0	719	16	0
30	T	1291	0	713	16	0
31	4	1	0	0	0	0
31	6	4	0	0	0	0
31	A	2	0	0	0	0
31	B	1	0	0	0	0
31	C	1	0	0	0	0
31	I	2	0	0	0	0
31	J	1	0	0	0	0
31	L	1	0	0	0	0
31	M	1	0	0	0	0
31	S	1	0	0	0	0
32	7	1	0	0	0	0
32	A	1	0	0	0	0
33	0	8	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	70481	0	69573	1575	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 11.

All (1575) 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)
11:L:27:LEU:N	11:L:39:SER:HG	1.59	1.01
25:6:406:CYS:HB3	25:6:440:CYS:SG	2.01	0.99
22:0:134:ARG:O	22:0:138:ASN:HB2	1.72	0.88
11:L:31:CYS:SG	11:L:48:CYS:HB3	2.16	0.84
2:A:107:CYS:SG	2:A:148:CYS:HB2	2.18	0.82
25:6:338:CYS:SG	25:6:339:HIS:CE1	2.72	0.82
2:A:1170:ILE:O	2:A:1174:PHE:HB2	1.79	0.82
3:B:364:ILE:HG22	3:B:585:VAL:HG13	1.64	0.80
2:A:344:ARG:HH12	3:B:1129:ARG:HH11	1.31	0.79
26:7:642:ASN:O	26:7:646:ASN:HB3	1.82	0.79
2:A:88:LYS:HE2	2:A:293:GLU:HB2	1.65	0.78
29:N:-6:DG:N2	30:T:6:DC:O2	2.19	0.76
3:B:842:ASN:HA	3:B:999:MET:HE1	1.68	0.76
2:A:1149:ALA:HB3	2:A:1196:GLU:HB2	1.68	0.75
3:B:680:THR:H	3:B:683:SER:HB2	1.51	0.75
2:A:567:LYS:HD3	7:H:95:TYR:HA	1.68	0.75
21:G:89:GLY:HA3	21:G:103:VAL:HG22	1.69	0.73
9:J:10:CYS:SG	9:J:11:GLY:N	2.62	0.72
27:2:190:GLN:HG3	27:2:395:GLN:HE21	1.55	0.71
2:A:532:ARG:NH2	2:A:748:MET:SD	2.63	0.71
13:P:133:TYR:HB3	13:P:214:ILE:HD11	1.73	0.70
16:U:257:ARG:HH22	16:U:282:GLU:HA	1.57	0.70
11:L:31:CYS:HA	11:L:57:LEU:H	1.57	0.69
18:W:17:VAL:HG21	18:W:29:LEU:HD13	1.74	0.69
2:A:1329:THR:HB	2:A:1335:ILE:HD11	1.74	0.69
26:7:330:CYS:HA	26:7:333:ILE:HG12	1.74	0.69
22:0:544:TYR:HA	22:0:547:MET:HG3	1.74	0.69
26:7:459:MET:SD	26:7:466:ARG:NH2	2.65	0.69
8:I:45:ARG:HH21	8:I:47:GLU:H	1.37	0.69
27:2:461:ASP:HA	27:2:489:LYS:HE2	1.74	0.69
3:B:336:ARG:NH2	3:B:339:THR:O	2.26	0.69
3:B:75:ALA:HB2	3:B:83:ASN:H	1.58	0.69
28:5:24:ASP:O	28:5:28:SER:HA	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:2:462:PHE:H	27:2:489:LYS:HB3	1.57	0.68
2:A:18:GLN:HB3	3:B:1215:ARG:HB2	1.74	0.68
2:A:1060:PRO:HD2	6:F:86:THR:HG21	1.74	0.68
3:B:806:THR:HG23	3:B:808:ALA:H	1.59	0.68
11:L:61:THR:HG22	11:L:63:ARG:H	1.58	0.68
22:0:111:ARG:HH12	22:0:134:ARG:HG3	1.58	0.68
22:0:721:LEU:O	22:0:725:ALA:HB2	1.94	0.68
3:B:73:GLN:HA	12:Q:330:ARG:HH22	1.59	0.67
10:K:36:GLU:HG2	10:K:37:LYS:HG2	1.76	0.67
26:7:132:LEU:HB3	26:7:201:SER:HA	1.77	0.67
7:H:80:ARG:HH22	10:K:57:LEU:HD13	1.57	0.67
26:7:676:HIS:HB3	26:7:679:SER:HB3	1.77	0.67
24:4:65:LEU:HA	24:4:71:ASN:HD21	1.59	0.67
2:A:856:THR:HB	2:A:865:GLN:H	1.60	0.67
4:C:235:VAL:HG13	4:C:237:SER:H	1.60	0.66
3:B:323:VAL:HG13	3:B:324:ILE:HG13	1.75	0.66
3:B:801:LYS:O	9:J:52:THR:OG1	2.14	0.66
4:C:56:THR:HG23	4:C:58:LEU:H	1.60	0.66
24:4:162:ARG:NH2	25:6:406:CYS:O	2.29	0.66
3:B:805:THR:OG1	3:B:809:MET:SD	2.53	0.66
23:1:210:TRP:HB3	23:1:217:LEU:HD11	1.76	0.66
27:2:14:LEU:O	27:2:22:GLN:NE2	2.26	0.66
2:A:566:ILE:HB	7:H:96:VAL:HG13	1.78	0.66
2:A:1329:THR:HG22	2:A:1331:SER:H	1.59	0.66
22:0:134:ARG:HH12	22:0:304:GLU:HB2	1.60	0.66
7:H:115:TYR:OH	7:H:124:ARG:NH1	2.27	0.66
3:B:1174:LYS:HB2	3:B:1179:GLN:HB2	1.78	0.65
3:B:995:ARG:NH1	4:C:165:LYS:O	2.29	0.65
23:1:559:GLU:O	23:1:563:HIS:ND1	2.29	0.65
25:6:134:GLU:HG3	25:6:206:GLY:H	1.61	0.65
15:O:94:TYR:HB2	15:O:102:VAL:HG23	1.79	0.65
2:A:184:SER:HB2	2:A:197:PRO:HB2	1.79	0.65
3:B:310:MET:SD	3:B:310:MET:N	2.69	0.65
3:B:829:CYS:HA	3:B:834:ASN:HD21	1.62	0.65
2:A:393:ARG:NH2	2:A:421:ALA:O	2.29	0.65
3:B:1076:HIS:O	4:C:31:ASN:ND2	2.28	0.65
26:7:589:GLN:HE22	26:7:756:ARG:HH21	1.45	0.65
2:A:311:GLN:HG2	2:A:312:PRO:HD3	1.79	0.64
22:0:289:LEU:HD22	22:0:321:ILE:HG13	1.79	0.64
26:7:527:LEU:HA	26:7:530:LEU:HB2	1.79	0.64
13:P:90:GLN:HE21	13:P:92:LEU:HD11	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:54:ASN:ND2	4:C:60:ASP:OD1	2.28	0.64
18:W:122:TYR:HB3	18:W:156:LEU:HB3	1.80	0.64
2:A:840:ARG:NH1	2:A:1384:VAL:O	2.30	0.64
24:4:305:CYS:HB3	24:4:310:SER:H	1.63	0.64
7:H:90:ALA:HB1	7:H:143:LEU:HD11	1.80	0.64
25:6:363:CYS:HB3	25:6:368:LEU:H	1.62	0.64
2:A:60:SER:HB3	2:A:67:CYS:H	1.63	0.64
3:B:771:SER:O	3:B:775:LYS:NZ	2.31	0.64
2:A:764:CYS:SG	2:A:765:VAL:N	2.71	0.64
3:B:756:ILE:HD13	3:B:767:ASN:HD22	1.62	0.64
2:A:592:ASP:O	2:A:603:ASN:ND2	2.31	0.63
2:A:1229:SER:OG	2:A:1230:GLU:N	2.30	0.63
23:1:606:GLU:HA	23:1:609:SER:HB3	1.78	0.63
27:2:151:VAL:HG11	27:2:358:ALA:HB1	1.79	0.63
16:U:257:ARG:NH1	16:U:258:TRP:O	2.31	0.63
22:0:1:MET:N	22:0:12:PHE:O	2.30	0.63
2:A:42:ASP:O	2:A:45:GLN:NE2	2.32	0.63
2:A:365:GLY:HA3	2:A:469:ARG:HB3	1.80	0.63
2:A:108:MET:HA	2:A:210:ILE:HG12	1.80	0.63
12:Q:102:PRO:HB2	13:P:91:GLU:HB3	1.80	0.63
27:2:175:GLU:HA	27:2:182:PHE:HA	1.81	0.63
11:L:31:CYS:H	11:L:57:LEU:HB2	1.64	0.63
22:0:443:SER:HB3	22:0:473:LEU:HA	1.79	0.63
27:2:32:CYS:SG	27:2:107:SER:OG	2.54	0.63
2:A:439:ASN:HA	2:A:460:VAL:H	1.64	0.62
8:I:78:CYS:SG	8:I:105:SER:OG	2.57	0.62
14:S:271:CYS:HB3	14:S:276:GLU:H	1.63	0.62
2:A:173:THR:HG1	2:A:184:SER:HG	1.46	0.62
9:J:5:VAL:HG12	9:J:6:ARG:HG2	1.80	0.62
19:X:232:VAL:HA	19:X:244:VAL:HG12	1.82	0.62
22:0:60:GLN:O	22:0:66:HIS:ND1	2.31	0.62
3:B:129:PHE:HB3	3:B:166:PHE:HA	1.81	0.62
7:H:105:GLU:HB3	7:H:113:ALA:HB3	1.81	0.62
20:D:139:LYS:HD2	20:D:142:LYS:HD2	1.81	0.62
25:6:221:LEU:O	25:6:230:ARG:NH1	2.32	0.62
2:A:1199:ARG:NH1	2:A:1231:ASP:O	2.31	0.62
23:1:209:PHE:O	23:1:213:ARG:NH1	2.32	0.62
1:M:281:SER:O	1:M:285:ASN:ND2	2.31	0.62
3:B:552:MET:HA	3:B:555:ILE:HG22	1.82	0.62
22:0:288:LYS:HE2	22:0:298:ILE:HG12	1.80	0.62
25:6:176:ASN:HD21	25:6:205:LYS:HG3	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:7:589:GLN:HB3	26:7:748:LEU:HD22	1.82	0.62
22:0:127:THR:HG22	23:1:348:VAL:HG12	1.82	0.62
2:A:1207:LEU:HD21	2:A:1274:ARG:HE	1.64	0.61
27:2:29:PRO:HB3	27:2:111:ALA:HB2	1.81	0.61
3:B:302:CYS:SG	3:B:303:TYR:N	2.74	0.61
14:S:271:CYS:SG	14:S:272:GLY:N	2.73	0.61
3:B:326:ASP:OD1	12:Q:398:ARG:NH1	2.32	0.61
3:B:341:LEU:HD22	3:B:344:LYS:HD2	1.82	0.61
2:A:855:THR:OG1	2:A:857:ARG:NH1	2.33	0.61
4:C:74:SER:HB2	4:C:238:ILE:HB	1.81	0.61
2:A:425:GLN:HE22	2:A:427:GLN:HB2	1.64	0.61
3:B:793:ALA:HB3	3:B:856:PHE:HB2	1.82	0.61
2:A:379:VAL:O	2:A:384:ASN:ND2	2.34	0.61
20:D:165:GLN:HA	20:D:168:LYS:HE3	1.82	0.61
22:0:232:VAL:HB	22:0:456:VAL:HA	1.81	0.61
23:1:633:TYR:HB3	24:4:326:VAL:HG21	1.82	0.61
13:P:106:LEU:HB3	13:P:120:TYR:HB2	1.83	0.61
18:W:40:GLU:HG2	18:W:44:LYS:HE2	1.83	0.61
18:W:70:HIS:HB3	18:W:86:TYR:HB2	1.82	0.61
25:6:175:ARG:NH1	25:6:203:GLU:O	2.34	0.61
2:A:1293:SER:HB3	2:A:1297:GLU:H	1.66	0.61
3:B:287:ARG:NH2	3:B:294:ASP:OD1	2.34	0.61
22:0:1:MET:N	22:0:92:TYR:OH	2.34	0.61
25:6:444:ILE:HG12	25:6:448:LEU:HD12	1.83	0.61
2:A:860:LEU:O	5:E:174:GLN:NE2	2.33	0.60
11:L:38:LEU:HB3	11:L:40:LEU:HD23	1.83	0.60
23:1:470:LEU:HD13	24:4:140:ILE:HG12	1.83	0.60
7:H:83:GLN:O	7:H:87:ARG:NH1	2.34	0.60
8:I:103:CYS:SG	8:I:104:LEU:N	2.74	0.60
15:O:107:ARG:NH1	16:U:286:VAL:OXT	2.34	0.60
2:A:226:GLU:OE2	2:A:230:ARG:NH2	2.34	0.60
2:A:802:ASN:ND2	2:A:803:SER:O	2.35	0.60
4:C:177:GLU:OE2	4:C:231:ASN:ND2	2.35	0.60
8:I:71:SER:OG	8:I:72:ASP:N	2.34	0.60
8:I:88:SER:O	8:I:91:ARG:NH1	2.33	0.60
14:S:156:LEU:HA	14:S:159:VAL:HG22	1.83	0.60
26:7:496:ALA:O	26:7:500:ARG:NH2	2.33	0.60
3:B:80:GLU:HG2	3:B:83:ASN:HB2	1.84	0.60
15:O:91:ASN:ND2	15:O:105:ARG:O	2.35	0.60
22:0:642:MET:HB2	22:0:648:ILE:HD12	1.83	0.60
23:1:309:VAL:O	23:1:313:ARG:NH1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:1:510:ASN:ND2	24:4:264:LYS:O	2.35	0.60
3:B:313:MET:HG3	3:B:386:LEU:HD11	1.84	0.60
22:0:419:ILE:HB	22:0:436:ARG:HB2	1.82	0.60
1:M:284:LEU:HD21	1:M:313:TYR:HA	1.82	0.60
9:J:36:LEU:HD23	9:J:47:ARG:HG2	1.83	0.60
3:B:72:GLU:O	12:Q:330:ARG:NH2	2.34	0.60
3:B:179:CYS:SG	3:B:180:TYR:N	2.75	0.60
2:A:567:LYS:HB2	2:A:568:PRO:HD3	1.83	0.59
16:U:262:LEU:HD11	16:U:281:VAL:HG23	1.84	0.59
22:0:636:LYS:HA	22:0:639:LEU:HD12	1.83	0.59
25:6:327:ARG:HA	25:6:347:TYR:HA	1.84	0.59
21:G:47:CYS:SG	21:G:48:VAL:N	2.75	0.59
22:0:270:ARG:HG2	22:0:390:VAL:HG12	1.83	0.59
22:0:306:PHE:HB3	22:0:382:SER:HA	1.84	0.59
26:7:236:THR:O	26:7:313:VAL:N	2.35	0.59
2:A:874:ASP:O	2:A:1366:ARG:NH1	2.35	0.59
12:Q:141:ARG:NH1	12:Q:345:GLU:O	2.35	0.59
16:U:254:THR:OG1	16:U:259:LYS:NZ	2.34	0.59
27:2:467:GLU:HG2	27:2:471:LEU:HD21	1.83	0.59
22:0:59:TYR:O	22:0:63:TYR:HB2	2.03	0.59
22:0:542:PRO:HB3	22:0:626:PRO:HA	1.83	0.59
24:4:78:ALA:HA	24:4:83:ILE:HA	1.85	0.59
25:6:224:VAL:O	25:6:230:ARG:NH2	2.36	0.59
27:2:88:ILE:HB	27:2:99:ASN:HB3	1.84	0.59
2:A:1115:SER:OG	2:A:1330:ASN:ND2	2.35	0.59
22:0:67:ARG:NE	22:0:229:ASP:O	2.34	0.59
22:0:670:LEU:HD13	22:0:675:ASP:HB3	1.84	0.59
27:2:238:LYS:NZ	27:2:239:ILE:O	2.34	0.59
3:B:43:LEU:O	3:B:496:ARG:NH2	2.35	0.59
3:B:799:PRO:HB2	3:B:818:PRO:HG2	1.84	0.59
15:O:108:GLU:HG2	15:O:109:PRO:HD3	1.85	0.59
17:V:11:ARG:NH1	17:V:45:ASP:OD2	2.36	0.59
22:0:310:PRO:HB3	22:0:404:THR:HG23	1.84	0.59
2:A:1159:ARG:NH2	2:A:1186:ASP:OD1	2.36	0.59
2:A:1173:HIS:NE2	2:A:1228:TRP:O	2.30	0.59
3:B:445:LYS:HG3	3:B:446:LEU:HD22	1.84	0.59
27:2:81:MET:HG3	27:2:87:LEU:HB2	1.83	0.59
30:T:-46:DA:H2'	30:T:-45:DA:C8	2.37	0.59
2:A:939:ASP:OD2	2:A:1023:ARG:NH1	2.35	0.59
4:C:56:THR:OG1	4:C:57:VAL:N	2.36	0.59
16:U:282:GLU:HB3	17:V:63:LYS:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:27:CYS:SG	1:M:48:CYS:HB3	2.43	0.59
2:A:70:CYS:SG	2:A:80:HIS:CE1	2.96	0.59
2:A:119:ASN:HB3	2:A:122:MET:HG3	1.85	0.58
2:A:75:ASN:HA	3:B:1116:ARG:HH22	1.68	0.58
2:A:512:VAL:HA	2:A:519:PRO:HA	1.85	0.58
4:C:254:LYS:HD3	10:K:42:LEU:HD11	1.84	0.58
24:4:292:CYS:HB3	24:4:308:CYS:SG	2.43	0.58
26:7:487:LEU:HB2	26:7:512:GLY:HA2	1.84	0.58
1:M:84:ASN:OD1	1:M:151:LYS:NZ	2.37	0.58
26:7:424:PHE:HE2	26:7:430:LEU:HD22	1.68	0.58
4:C:242:GLN:HB3	4:C:246:ARG:HH12	1.66	0.58
11:L:47:ARG:HB2	11:L:54:ARG:HE	1.68	0.58
26:7:354:ILE:HG13	26:7:430:LEU:HD12	1.84	0.58
2:A:949:ASP:OD1	2:A:949:ASP:N	2.37	0.58
6:F:86:THR:OG1	6:F:87:LYS:N	2.36	0.58
23:1:624:THR:O	23:1:628:HIS:ND1	2.31	0.58
13:P:139:ASN:HA	13:P:210:LYS:HD2	1.84	0.58
22:0:251:ASP:OD2	23:1:353:ARG:NH1	2.37	0.58
26:7:421:ARG:NH2	26:7:435:CYS:SG	2.76	0.58
2:A:1398:MET:SD	2:A:1425:SER:OG	2.61	0.58
4:C:76:ASP:OD2	4:C:128:ASN:N	2.37	0.58
8:I:94:ASP:OD1	8:I:94:ASP:N	2.35	0.58
22:0:11:LEU:HD22	22:0:93:ARG:HG2	1.84	0.58
22:0:238:HIS:HB2	22:0:660:ARG:HD2	1.84	0.58
23:1:293:PHE:O	23:1:297:ARG:HB2	2.03	0.58
25:6:260:ARG:HH21	25:6:281:ASN:HB3	1.69	0.58
3:B:136:THR:N	3:B:138:GLU:OE2	2.37	0.58
8:I:17:ARG:NH1	8:I:18:GLU:O	2.37	0.58
26:7:340:GLU:OE2	26:7:380:ARG:NH1	2.36	0.58
28:5:14:PRO:HA	28:5:17:LYS:HE2	1.86	0.57
2:A:1100:ARG:NH2	2:A:1351:GLU:OE2	2.37	0.57
3:B:826:ALA:HB3	3:B:1011:ILE:HG13	1.85	0.57
5:E:141:VAL:HG13	5:E:142:VAL:HG23	1.85	0.57
23:1:563:HIS:O	23:1:567:HIS:ND1	2.31	0.57
26:7:130:ARG:NH1	26:7:198:ASP:O	2.37	0.57
27:2:435:PRO:O	27:2:439:ASP:N	2.37	0.57
3:B:102:VAL:H	3:B:112:LEU:HD23	1.69	0.57
15:O:68:GLN:HE21	30:T:-5:DA:H4'	1.69	0.57
22:0:588:LYS:O	22:0:592:ASN:ND2	2.37	0.57
27:2:352:ASN:ND2	27:2:370:PHE:O	2.38	0.57
3:B:911:ILE:HG13	3:B:912:ILE:HG12	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:35:ARG:HH21	10:K:41:THR:H	1.53	0.57
10:K:95:ILE:HD12	10:K:98:LEU:HD11	1.85	0.57
22:0:509:ARG:NH2	22:0:511:GLU:OE1	2.38	0.57
1:M:190:LYS:NZ	1:M:302:LEU:O	2.36	0.57
2:A:1208:THR:OG1	2:A:1211:GLN:OE1	2.21	0.57
3:B:750:GLY:H	3:B:753:ALA:HB3	1.69	0.57
22:0:472:MET:HG3	22:0:473:LEU:HG	1.86	0.57
3:B:706:GLN:HB2	3:B:709:ASP:HB3	1.85	0.57
9:J:1:MET:SD	9:J:2:ILE:N	2.68	0.57
16:U:51:VAL:HG12	16:U:271:ARG:HA	1.86	0.57
3:B:1002:THR:OG1	3:B:1003:ALA:N	2.36	0.57
20:D:39:ASN:ND2	20:D:41:GLN:OE1	2.38	0.57
22:0:507:SER:OG	22:0:685:ARG:NH1	2.38	0.57
5:E:136:ASN:HD21	5:E:138:ALA:HB3	1.70	0.57
13:P:87:LEU:H	13:P:90:GLN:HE22	1.51	0.57
22:0:287:GLU:OE1	22:0:291:GLN:NE2	2.38	0.57
26:7:222:LYS:HB3	26:7:241:ILE:HG12	1.86	0.57
7:H:13:SER:OG	7:H:27:GLU:OE2	2.23	0.57
14:S:185:VAL:O	14:S:189:ASP:N	2.35	0.57
19:X:163:LEU:HG	19:X:169:ILE:HG21	1.87	0.57
22:0:601:VAL:HG12	22:0:603:ARG:H	1.70	0.57
23:1:339:LEU:HD12	23:1:342:ASN:HD22	1.69	0.57
2:A:523:ILE:HG21	2:A:649:ILE:HD11	1.86	0.56
3:B:604:ARG:NH2	3:B:613:VAL:O	2.38	0.56
22:0:223:SER:O	22:0:452:ARG:NH2	2.38	0.56
26:7:491:HIS:O	26:7:519:ARG:NH2	2.38	0.56
2:A:1373:ASP:HA	2:A:1376:THR:HG22	1.86	0.56
22:0:401:ASP:OD1	23:1:350:ARG:NH1	2.38	0.56
27:2:25:LEU:HD22	27:2:222:LEU:HD13	1.87	0.56
1:M:91:ASN:OD1	2:A:271:LYS:NZ	2.28	0.56
1:M:239:ILE:HG23	1:M:282:ILE:HD11	1.88	0.56
2:A:108:MET:SD	2:A:108:MET:N	2.78	0.56
2:A:802:ASN:HD21	2:A:806:ARG:HB2	1.71	0.56
3:B:402:GLY:O	3:B:405:ARG:NH1	2.39	0.56
3:B:546:SER:OG	3:B:631:GLY:N	2.37	0.56
8:I:3:THR:O	8:I:5:ARG:NH1	2.39	0.56
14:S:232:ASP:HB3	14:S:235:ASP:HB3	1.87	0.56
18:W:62:ARG:NH1	18:W:67:ILE:O	2.38	0.56
20:D:68:ARG:HD2	20:D:72:ARG:HH12	1.70	0.56
23:1:340:ASP:HA	23:1:343:ILE:HG12	1.88	0.56
24:4:76:ILE:HG12	24:4:85:TYR:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:4:308:CYS:SG	24:4:310:SER:OG	2.63	0.56
26:7:239:ALA:O	26:7:243:GLN:NE2	2.38	0.56
2:A:769:SER:OG	2:A:773:LYS:O	2.24	0.56
2:A:783:THR:OG1	2:A:784:LEU:N	2.39	0.56
7:H:62:SER:OG	7:H:63:LEU:N	2.38	0.56
14:S:179:GLU:O	14:S:183:ASN:ND2	2.38	0.56
22:0:554:TRP:HZ3	22:0:559:ILE:HD12	1.71	0.56
23:1:473:LEU:HD22	24:4:140:ILE:HD13	1.87	0.56
26:7:239:ALA:HA	26:7:242:LEU:HD23	1.88	0.56
26:7:676:HIS:O	26:7:722:ARG:NH1	2.39	0.56
27:2:208:LEU:HD13	27:2:221:VAL:HG11	1.87	0.56
2:A:390:GLN:NE2	2:A:394:ASN:OD1	2.39	0.56
3:B:352:ALA:HA	3:B:355:ILE:HD12	1.87	0.56
3:B:1198:TYR:HA	3:B:1201:LYS:HG2	1.87	0.56
2:A:368:LYS:HE2	10:K:4:PRO:HD3	1.88	0.56
2:A:745:GLN:O	2:A:749:ALA:CB	2.54	0.56
2:A:873:MET:O	2:A:1366:ARG:NH1	2.39	0.56
2:A:1132:LYS:HA	2:A:1135:ARG:HG2	1.87	0.56
17:V:87:VAL:HG12	17:V:88:GLU:HG3	1.86	0.56
20:D:152:SER:O	20:D:155:ARG:NH2	2.38	0.56
21:G:38:CYS:HA	21:G:44:TYR:HA	1.87	0.56
25:6:135:ALA:O	25:6:145:ARG:NH1	2.38	0.56
27:2:194:GLN:O	27:2:199:GLN:NE2	2.39	0.56
2:A:802:ASN:ND2	2:A:807:GLY:O	2.39	0.56
19:X:228:SER:O	19:X:247:ASN:ND2	2.36	0.56
2:A:202:LEU:HB3	2:A:207:ILE:HD11	1.87	0.56
3:B:296:GLU:O	3:B:300:HIS:ND1	2.28	0.56
26:7:672:GLN:NE2	26:7:683:GLU:OE2	2.39	0.56
2:A:187:LYS:NZ	18:W:226:THR:O	2.37	0.56
2:A:363:GLN:O	2:A:458:HIS:ND1	2.38	0.56
3:B:428:ILE:HA	3:B:445:LYS:HE3	1.87	0.56
6:F:100:GLN:HB3	6:F:105:ALA:HB3	1.86	0.56
18:W:147:PHE:HB2	18:W:156:LEU:HB2	1.88	0.56
22:0:509:ARG:HB2	22:0:512:ILE:HG12	1.87	0.56
26:7:494:PRO:HG2	26:7:523:LYS:HE3	1.87	0.56
1:M:313:TYR:O	1:M:317:TYR:HB2	2.05	0.55
2:A:1318:THR:HG22	5:E:141:VAL:HG11	1.88	0.55
3:B:924:GLU:HG2	3:B:925:LEU:HD12	1.88	0.55
21:G:114:LEU:HD23	21:G:162:SER:HB2	1.87	0.55
23:1:562:LYS:HG2	25:6:365:CYS:HA	1.88	0.55
3:B:755:ILE:O	3:B:983:ARG:NH2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S:266:THR:HG23	14:S:268:ARG:H	1.71	0.55
7:H:5:LEU:H	7:H:59:ILE:HB	1.71	0.55
22:0:571:VAL:HG13	22:0:599:LEU:HB2	1.88	0.55
25:6:190:GLN:NE2	25:6:194:ASP:OD1	2.40	0.55
25:6:394:THR:HA	25:6:398:PHE:HZ	1.71	0.55
2:A:862:ASN:HA	5:E:174:GLN:HB3	1.88	0.55
2:A:1430:LEU:HB3	2:A:1432:GLN:HE22	1.71	0.55
3:B:194:GLU:HA	3:B:784:ASN:HD22	1.71	0.55
3:B:576:ASP:OD1	3:B:576:ASP:N	2.39	0.55
26:7:613:TYR:CZ	26:7:766:LYS:HE3	2.42	0.55
3:B:883:LEU:HD21	3:B:928:ARG:HD3	1.87	0.55
20:D:196:PRO:HA	20:D:199:ASN:HB2	1.87	0.55
7:H:32:THR:OG1	7:H:33:GLN:OE1	2.25	0.55
14:S:285:GLN:HB3	14:S:293:LEU:HD23	1.89	0.55
3:B:1065:GLN:OE1	3:B:1068:GLY:N	2.39	0.55
16:U:8:ARG:NH1	17:V:55:ASN:OD1	2.40	0.55
26:7:234:VAL:HG21	26:7:318:ILE:HD12	1.89	0.55
2:A:1002:GLY:HA3	2:A:1007:ILE:HG21	1.89	0.55
13:P:96:ARG:NH2	13:P:103:LYS:O	2.40	0.55
16:U:249:ASP:N	16:U:261:SER:O	2.39	0.55
26:7:383:ILE:HB	26:7:534:LYS:HA	1.88	0.55
2:A:405:VAL:HG23	2:A:432:VAL:HG12	1.89	0.55
18:W:3:ARG:NH2	18:W:192:SER:OG	2.36	0.55
27:2:453:THR:HG23	28:5:10:VAL:HG22	1.87	0.55
3:B:796:LEU:HA	3:B:853:SER:HA	1.89	0.55
4:C:79:GLN:HB3	4:C:127:ARG:HH11	1.72	0.55
5:E:118:PRO:HA	5:E:121:MET:HB2	1.89	0.55
14:S:187:ASN:HB2	14:S:228:LEU:HD11	1.88	0.55
2:A:376:TYR:OH	2:A:498:ARG:NH1	2.40	0.54
2:A:528:LEU:HD11	2:A:619:LYS:HB3	1.88	0.54
2:A:698:GLN:HG2	8:I:99:LEU:HD21	1.89	0.54
2:A:1199:ARG:NH2	2:A:1233:ASP:O	2.41	0.54
5:E:97:VAL:HA	5:E:100:ILE:HD12	1.89	0.54
10:K:17:SER:OG	10:K:19:LEU:O	2.24	0.54
26:7:401:CYS:O	26:7:404:LYS:NZ	2.35	0.54
16:U:22:ARG:HE	16:U:26:GLU:HG2	1.72	0.54
22:0:270:ARG:NH1	22:0:389:GLU:O	2.40	0.54
26:7:425:LEU:HD13	26:7:432:PRO:HG3	1.89	0.54
29:N:17:DT:H2"	29:N:18:DA:H5"	1.89	0.54
7:H:128:ASN:OD1	7:H:131:ASN:ND2	2.39	0.54
18:W:42:ASP:OD1	18:W:210:GLN:NE2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:D:192:LYS:O	20:D:199:ASN:ND2	2.41	0.54
26:7:117:ASP:OD2	27:2:369:ARG:NH1	2.40	0.54
26:7:132:LEU:HD23	26:7:201:SER:HB2	1.88	0.54
27:2:466:GLN:HG2	27:2:467:GLU:HG3	1.89	0.54
2:A:537:ARG:NH2	2:A:599:SER:OG	2.40	0.54
18:W:68:SER:N	18:W:88:TYR:O	2.41	0.54
24:4:29:ILE:HB	24:4:178:VAL:HA	1.88	0.54
3:B:1060:ARG:O	3:B:1060:ARG:NH1	2.39	0.54
14:S:240:PRO:O	14:S:243:GLN:NE2	2.40	0.54
19:X:186:VAL:HG13	19:X:191:GLU:HB2	1.90	0.54
22:0:315:ASP:O	22:0:375:ARG:NH1	2.41	0.54
27:2:409:ARG:HE	27:2:413:GLU:HG2	1.73	0.54
2:A:745:GLN:O	2:A:749:ALA:HB2	2.08	0.54
7:H:123:MET:SD	7:H:123:MET:N	2.80	0.54
22:0:135:ARG:NH1	22:0:392:GLU:OE2	2.40	0.54
23:1:282:GLU:OE2	23:1:286:ARG:NH1	2.38	0.54
24:4:273:ARG:HE	25:6:324:PHE:HB2	1.73	0.54
3:B:62:ILE:HD11	3:B:418:LYS:HB2	1.90	0.54
4:C:125:MET:SD	4:C:127:ARG:NE	2.81	0.54
14:S:201:ILE:O	14:S:205:ASN:ND2	2.39	0.54
22:0:639:LEU:HD23	22:0:642:MET:HE1	1.89	0.54
3:B:363:HIS:O	3:B:365:THR:N	2.41	0.54
3:B:428:ILE:HG12	3:B:445:LYS:HZ1	1.73	0.54
3:B:558:LEU:HD21	3:B:580:VAL:HG11	1.89	0.54
7:H:118:PHE:O	7:H:120:GLY:N	2.41	0.54
21:G:10:ASN:HA	21:G:71:ASN:HA	1.90	0.54
22:0:56:THR:HB	22:0:69:ILE:HD13	1.90	0.54
23:1:265:ILE:HD11	23:1:314:TYR:HB3	1.90	0.54
25:6:446:GLU:HG3	25:6:447:ILE:HG12	1.90	0.54
27:2:217:ASP:HB3	27:2:220:ASP:HB2	1.90	0.54
18:W:179:ILE:HG13	18:W:182:ILE:HD12	1.89	0.54
7:H:95:TYR:HB3	7:H:144:ILE:HB	1.90	0.54
13:P:318:LEU:HG	13:P:329:LEU:HD21	1.90	0.54
22:0:18:TYR:OH	23:1:423:ASP:OD2	2.26	0.54
22:0:618:ARG:NH1	22:0:676:TYR:O	2.41	0.54
26:7:610:ASP:H	26:7:674:SER:HB3	1.73	0.54
2:A:346:ASP:H	3:B:1154:ALA:HB1	1.73	0.53
4:C:145:CYS:SG	4:C:146:LYS:N	2.80	0.53
17:V:66:LEU:HD11	17:V:69:TYR:HB3	1.90	0.53
2:A:46:THR:O	2:A:47:ARG:NE	2.36	0.53
2:A:788:SER:HB2	8:I:69:PRO:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1219:ASP:OD1	3:B:1219:ASP:N	2.42	0.53
25:6:390:ALA:N	25:6:428:ARG:O	2.36	0.53
2:A:668:ASP:OD2	2:A:743:VAL:N	2.41	0.53
3:B:1004:GLU:OE1	3:B:1064:TYR:OH	2.20	0.53
12:Q:126:LYS:HE3	13:P:131:ASN:H	1.72	0.53
22:0:539:VAL:HG22	22:0:621:LEU:HB2	1.90	0.53
23:1:571:GLY:HA2	24:4:325:VAL:H	1.73	0.53
25:6:178:LEU:O	25:6:180:GLN:NE2	2.40	0.53
2:A:1150:SER:H	8:I:45:ARG:NH2	2.05	0.53
3:B:1074:ASN:ND2	3:B:1077:THR:H	2.06	0.53
17:V:48:VAL:HA	17:V:51:THR:HG22	1.91	0.53
2:A:254:GLU:OE2	2:A:256:GLN:NE2	2.42	0.53
4:C:148:ARG:O	4:C:151:GLN:NE2	2.32	0.53
5:E:126:SER:OG	5:E:127:ILE:N	2.39	0.53
18:W:90:LYS:HB3	18:W:93:HIS:HB2	1.89	0.53
23:1:493:ASN:HA	23:1:496:SER:HB3	1.91	0.53
25:6:115:ILE:O	25:6:387:LYS:NZ	2.42	0.53
17:V:60:LEU:HB3	17:V:87:VAL:HG13	1.90	0.53
22:0:84:VAL:O	22:0:88:ASN:ND2	2.41	0.53
22:0:111:ARG:O	22:0:115:CYS:N	2.40	0.53
22:0:607:SER:O	22:0:668:ARG:NH2	2.42	0.53
26:7:551:ASN:H	26:7:701:PHE:HE2	1.55	0.53
2:A:14:VAL:HG21	2:A:1430:LEU:HD12	1.91	0.53
3:B:1163:CYS:O	3:B:1167:GLY:N	2.33	0.53
16:U:42:TRP:HZ2	17:V:15:ILE:HG23	1.73	0.53
23:1:237:ILE:O	23:1:297:ARG:NH2	2.41	0.53
23:1:589:CYS:HA	23:1:592:LYS:HE3	1.91	0.53
28:5:13:ASP:HB3	28:5:16:ILE:HG12	1.91	0.53
18:W:180:GLN:NE2	18:W:184:ASP:OD1	2.39	0.53
22:0:388:LEU:HB3	22:0:390:VAL:HG13	1.91	0.53
23:1:212:THR:OG1	23:1:213:ARG:NH1	2.42	0.53
23:1:214:ILE:HA	23:1:217:LEU:HD12	1.90	0.53
23:1:572:GLU:OE1	23:1:575:GLN:NE2	2.41	0.53
24:4:317:ILE:HA	24:4:320:LEU:HD12	1.91	0.53
3:B:617:ARG:HE	3:B:619:ILE:HD13	1.74	0.53
23:1:214:ILE:HG22	23:1:218:ARG:HH12	1.74	0.53
24:4:29:ILE:N	24:4:177:LEU:O	2.37	0.53
3:B:425:THR:HA	3:B:428:ILE:HD12	1.91	0.53
3:B:1082:MET:O	4:C:189:THR:OG1	2.27	0.53
14:S:185:VAL:HB	14:S:189:ASP:HA	1.90	0.53
16:U:47:THR:HB	16:U:56:TRP:HD1	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:18:ARG:HE	19:X:249:GLY:HA2	1.73	0.53
26:7:340:GLU:OE1	26:7:376:ASN:ND2	2.42	0.53
2:A:131:SER:O	2:A:134:ARG:NH2	2.43	0.52
2:A:871:ASP:OD2	2:A:1366:ARG:NH2	2.42	0.52
3:B:364:ILE:HD11	3:B:374:LYS:HD3	1.90	0.52
3:B:803:LEU:HD11	3:B:822:ASN:HD22	1.73	0.52
4:C:143:LEU:HD21	4:C:146:LYS:HE3	1.91	0.52
7:H:4:THR:HG21	7:H:7:ASP:HB2	1.91	0.52
21:G:56:ILE:HG22	21:G:72:VAL:HG22	1.91	0.52
27:2:186:ASN:ND2	27:2:390:GLY:O	2.42	0.52
1:M:45:CYS:HB3	1:M:48:CYS:SG	2.49	0.52
3:B:666:TYR:CD2	12:Q:28:ARG:HD2	2.44	0.52
3:B:1166:CYS:HB3	3:B:1168:LEU:HD23	1.91	0.52
18:W:72:GLN:NE2	18:W:218:THR:O	2.41	0.52
22:0:117:HIS:N	33:0:801:SF4:S3	2.80	0.52
22:0:469:TYR:HA	22:0:472:MET:HG2	1.91	0.52
22:0:586:TYR:HD1	22:0:596:ALA:HB3	1.75	0.52
25:6:338:CYS:SG	25:6:339:HIS:N	2.83	0.52
2:A:265:LYS:HZ1	2:A:302:THR:HG22	1.74	0.52
3:B:996:ARG:HD3	3:B:1007:VAL:HG21	1.90	0.52
19:X:204:GLY:HA3	19:X:243:TYR:HB3	1.91	0.52
2:A:1159:ARG:NH1	2:A:1185:PHE:O	2.41	0.52
4:C:72:LEU:HB3	4:C:130:GLY:HA2	1.91	0.52
19:X:163:LEU:HD12	19:X:166:LEU:HD12	1.92	0.52
24:4:66:ALA:O	27:2:37:ARG:NH2	2.42	0.52
2:A:830:LYS:NZ	2:A:1079:MET:O	2.28	0.52
2:A:1158:PRO:O	2:A:1241:ARG:NH1	2.38	0.52
2:A:1217:LYS:HE3	2:A:1221:LYS:HE2	1.91	0.52
5:E:108:GLY:N	5:E:131:THR:O	2.35	0.52
15:O:128:SER:OG	15:O:130:ASP:OD1	2.24	0.52
22:0:285:GLU:OE2	22:0:380:ARG:NH2	2.42	0.52
22:0:674:ASP:N	22:0:674:ASP:OD1	2.42	0.52
23:1:468:GLN:NE2	24:4:42:GLU:OE1	2.42	0.52
25:6:234:ILE:HB	25:6:263:VAL:HA	1.91	0.52
2:A:782:ARG:HD3	2:A:789:LYS:HD3	1.90	0.52
2:A:1121:GLU:HG3	2:A:1123:GLY:H	1.72	0.52
4:C:162:GLY:HA3	4:C:170:TRP:CE2	2.45	0.52
28:5:31:VAL:HG22	28:5:42:VAL:HG23	1.91	0.52
3:B:1165:ILE:N	3:B:1190:ASP:OD2	2.34	0.52
5:E:88:VAL:HB	5:E:116:ILE:HG23	1.91	0.52
16:U:280:GLN:HB2	17:V:61:THR:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:120:ASN:ND2	18:W:159:ASP:O	2.42	0.52
22:0:310:PRO:HB2	22:0:408:LEU:HG	1.92	0.52
23:1:567:HIS:HB3	23:1:579:VAL:HG22	1.91	0.52
2:A:368:LYS:HG2	2:A:462:VAL:HG22	1.91	0.52
3:B:709:ASP:N	3:B:709:ASP:OD1	2.42	0.52
22:0:20:GLU:HG2	22:0:485:MET:HA	1.92	0.52
22:0:275:ARG:NH1	22:0:329:GLU:OE2	2.43	0.52
22:0:467:ASP:N	22:0:467:ASP:OD1	2.41	0.52
25:6:238:SER:OG	25:6:239:LEU:N	2.43	0.52
25:6:325:PRO:HD3	25:6:370:LEU:HB3	1.91	0.52
12:Q:371:ASP:OD1	12:Q:371:ASP:N	2.43	0.52
13:P:85:ASN:O	13:P:88:HIS:NE2	2.38	0.52
17:V:87:VAL:O	17:V:103:GLN:N	2.43	0.52
2:A:66:LYS:HE2	2:A:68:GLN:HA	1.90	0.52
3:B:304:ASP:OD1	3:B:306:ASN:ND2	2.40	0.52
3:B:334:ILE:HA	3:B:347:LYS:HG3	1.91	0.52
7:H:130:ARG:H	7:H:130:ARG:HD3	1.74	0.52
26:7:411:CYS:HB2	26:7:488:ASP:HB2	1.92	0.52
26:7:433:GLU:OE2	26:7:448:THR:OG1	2.23	0.52
3:B:809:MET:HG3	3:B:814:PHE:HD2	1.75	0.51
4:C:36:VAL:HG11	4:C:251:LEU:HD12	1.92	0.51
4:C:107:SER:OG	4:C:109:SER:O	2.28	0.51
15:O:105:ARG:NH2	30:T:-7:DT:OP1	2.43	0.51
21:G:83:LYS:HG2	21:G:149:GLY:HA2	1.93	0.51
24:4:46:GLU:HB3	24:4:49:SER:HB3	1.91	0.51
26:7:167:PRO:HD2	26:7:171:HIS:HA	1.92	0.51
26:7:564:GLU:O	26:7:567:GLN:NE2	2.42	0.51
26:7:752:SER:HB2	26:7:755:GLU:HB2	1.92	0.51
1:M:138:ASP:HB3	3:B:451:LYS:HG3	1.90	0.51
2:A:1142:THR:O	2:A:1145:SER:OG	2.24	0.51
3:B:74:LEU:HA	3:B:85:SER:HA	1.93	0.51
4:C:101:LEU:HB3	4:C:155:LEU:HB2	1.91	0.51
16:U:12:ILE:HD13	17:V:55:ASN:HD21	1.75	0.51
16:U:41:ILE:HG13	16:U:44:LYS:HE3	1.92	0.51
26:7:567:GLN:HB2	26:7:571:ARG:HH11	1.75	0.51
26:7:679:SER:HB2	26:7:682:GLN:HB3	1.92	0.51
2:A:951:GLU:OE2	2:A:953:ASN:N	2.39	0.51
3:B:232:SER:O	3:B:261:ARG:NH1	2.44	0.51
6:F:116:ASP:OD2	6:F:119:ARG:N	2.40	0.51
10:K:57:LEU:HG	10:K:77:THR:HA	1.92	0.51
14:S:238:PRO:HB2	14:S:240:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:144:GLN:NE2	15:O:150:ALA:O	2.43	0.51
26:7:349:ASN:O	26:7:405:LYS:NZ	2.44	0.51
28:5:9:LEU:HD21	28:5:39:HIS:HD2	1.74	0.51
2:A:239:LEU:HD12	2:A:240:PRO:HD2	1.93	0.51
2:A:590:ARG:NH1	2:A:621:THR:OG1	2.43	0.51
2:A:1144:LYS:NZ	2:A:1268:LEU:O	2.36	0.51
2:A:1385:THR:OG1	2:A:1388:GLY:N	2.37	0.51
11:L:60:ARG:HE	11:L:61:THR:H	1.56	0.51
23:1:444:LYS:HE2	24:4:282:VAL:HG13	1.92	0.51
2:A:227:VAL:HG23	20:D:15:LEU:HB2	1.92	0.51
3:B:983:ARG:HD2	3:B:1091:TYR:HD1	1.76	0.51
22:0:513:ARG:NH1	22:0:514:ASN:OD1	2.44	0.51
22:0:573:THR:OG1	22:0:575:ASP:O	2.27	0.51
27:2:239:ILE:HG12	27:2:247:ARG:HG2	1.92	0.51
27:2:337:GLY:H	27:2:351:SER:HB3	1.76	0.51
2:A:551:TYR:O	10:K:62:LYS:NZ	2.44	0.51
2:A:636:GLU:HB2	2:A:962:ARG:HH21	1.75	0.51
21:G:135:ASP:HB3	21:G:170:ALA:HA	1.92	0.51
22:0:104:ARG:O	22:0:204:ASN:N	2.44	0.51
2:A:33:ALA:HB3	2:A:82:GLY:HA3	1.92	0.51
2:A:789:LYS:HB2	8:I:69:PRO:HD3	1.92	0.51
22:0:447:LYS:NZ	22:0:474:ASN:O	2.44	0.51
24:4:188:ASP:O	24:4:192:GLN:NE2	2.43	0.51
2:A:177:ASP:OD1	2:A:177:ASP:N	2.43	0.51
2:A:254:GLU:O	3:B:935:ARG:NH1	2.44	0.51
2:A:1005:GLU:OE2	2:A:1009:ASN:ND2	2.43	0.51
3:B:248:SER:H	3:B:418:LYS:HZ1	1.59	0.51
4:C:42:PRO:HB2	4:C:161:LYS:HE2	1.93	0.51
25:6:362:VAL:HA	25:6:369:MET:HA	1.93	0.51
26:7:134:ILE:HD13	26:7:205:VAL:HG13	1.93	0.51
2:A:116:ASP:O	2:A:118:HIS:ND1	2.43	0.51
3:B:809:MET:HB2	3:B:814:PHE:HB3	1.93	0.51
15:O:133:LYS:HB3	15:O:137:ARG:HH12	1.75	0.51
22:0:133:CYS:O	22:0:137:THR:OG1	2.19	0.51
27:2:441:ILE:O	27:2:445:GLN:N	2.41	0.51
3:B:493:SER:HA	3:B:751:VAL:HG21	1.93	0.50
3:B:838:SER:OG	3:B:839:MET:N	2.44	0.50
17:V:109:ASP:OD2	17:V:110:LYS:N	2.45	0.50
22:0:380:ARG:HH12	22:0:384:LEU:HD13	1.76	0.50
25:6:120:ARG:HA	25:6:309:PRO:HA	1.93	0.50
26:7:409:VAL:HG22	26:7:486:ILE:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:N:38:DG:H2"	29:N:39:DA:C8	2.46	0.50
1:M:34:ILE:HG22	1:M:45:CYS:HA	1.93	0.50
2:A:343:LYS:HE3	3:B:1117:GLN:HE21	1.77	0.50
3:B:629:ASP:N	3:B:629:ASP:OD1	2.42	0.50
3:B:914:LYS:HD2	3:B:937:ALA:HB3	1.94	0.50
8:I:73:ARG:O	8:I:83:ASN:ND2	2.44	0.50
22:0:238:HIS:O	22:0:660:ARG:NH1	2.44	0.50
26:7:225:LEU:HD12	26:7:234:VAL:HG22	1.93	0.50
30:T:-46:DA:H2'	30:T:-45:DA:H8	1.74	0.50
2:A:1254:ALA:N	2:A:1256:GLU:OE2	2.44	0.50
3:B:998:ASP:N	3:B:998:ASP:OD1	2.45	0.50
17:V:51:THR:O	17:V:55:ASN:CB	2.60	0.50
25:6:248:HIS:HA	25:6:251:ILE:HD12	1.93	0.50
27:2:131:SER:HA	27:2:135:LEU:HD13	1.94	0.50
2:A:457:ALA:N	2:A:505:CYS:O	2.44	0.50
2:A:605:MET:HG2	2:A:621:THR:HG21	1.92	0.50
2:A:751:SER:OG	2:A:752:LYS:N	2.44	0.50
2:A:1308:THR:OG1	2:A:1309:ASP:N	2.44	0.50
4:C:8:VAL:HG21	10:K:105:PHE:HD1	1.75	0.50
10:K:58:PHE:HE2	10:K:74:ARG:HH11	1.59	0.50
22:0:332:VAL:HG12	22:0:336:LYS:HE2	1.93	0.50
23:1:208:GLU:HA	23:1:211:SER:HB3	1.92	0.50
27:2:256:TYR:HB3	27:2:258:LEU:HD23	1.93	0.50
22:0:639:LEU:HB3	22:0:650:GLU:HG3	1.92	0.50
26:7:124:ARG:O	26:7:127:HIS:ND1	2.31	0.50
2:A:55:ASP:HA	2:A:58:LEU:HD23	1.93	0.50
2:A:362:ASP:N	2:A:362:ASP:OD1	2.44	0.50
4:C:16:ASP:OD1	4:C:16:ASP:N	2.41	0.50
4:C:99:LEU:HB2	4:C:157:CYS:HB2	1.94	0.50
19:X:234:ARG:HD3	19:X:239:LYS:HB3	1.92	0.50
22:0:119:GLU:HA	22:0:122:LYS:HE2	1.93	0.50
26:7:718:TYR:HB3	26:7:722:ARG:HH12	1.76	0.50
27:2:24:ARG:HE	27:2:219:VAL:HG21	1.76	0.50
1:M:113:ALA:HA	1:M:116:LYS:HG3	1.94	0.50
3:B:304:ASP:OD2	3:B:307:ASP:N	2.39	0.50
4:C:241:ASP:N	4:C:241:ASP:OD1	2.45	0.50
23:1:514:ALA:HA	23:1:517:ASN:HB3	1.93	0.50
2:A:884:ASP:OD2	2:A:1025:ARG:NE	2.37	0.50
2:A:894:GLU:O	2:A:898:ARG:HB3	2.12	0.50
3:B:242:SER:OG	3:B:251:ILE:O	2.30	0.50
3:B:567:GLU:OE1	3:B:567:GLU:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:883:LEU:HB2	3:B:935:ARG:HA	1.93	0.50
7:H:100:THR:O	7:H:117:SER:N	2.45	0.50
10:K:11:LEU:O	10:K:37:LYS:NZ	2.28	0.50
13:P:112:ASP:OD1	13:P:118:HIS:NE2	2.45	0.50
22:0:690:ARG:NH2	22:0:701:LEU:O	2.42	0.50
25:6:131:ASP:HA	25:6:174:MET:HB3	1.93	0.50
30:T:-16:DG:H2'	30:T:-15:DA:C8	2.47	0.50
16:U:248:TYR:OH	17:V:74:ASP:O	2.30	0.50
17:V:51:THR:O	17:V:55:ASN:HB3	2.12	0.50
18:W:90:LYS:HG3	18:W:92:PRO:HD2	1.93	0.50
21:G:56:ILE:HG13	21:G:57:GLN:H	1.76	0.50
22:0:37:ASN:HB2	22:0:477:THR:HA	1.94	0.50
23:1:586:LEU:HD21	23:1:623:ILE:HG23	1.93	0.50
26:7:494:PRO:HA	26:7:499:ARG:HD2	1.94	0.50
26:7:575:ARG:NH1	29:N:53:DT:H2'	2.25	0.50
27:2:448:LEU:O	27:2:450:ARG:NH2	2.42	0.50
8:I:27:PHE:N	8:I:36:GLU:O	2.43	0.49
18:W:139:LEU:O	18:W:148:LEU:N	2.45	0.49
19:X:196:LEU:HB3	19:X:246:TYR:HB2	1.94	0.49
23:1:444:LYS:NZ	23:1:445:THR:O	2.38	0.49
26:7:634:GLN:HA	26:7:637:MET:HG3	1.94	0.49
27:2:357:ILE:HD11	27:2:369:ARG:HD3	1.94	0.49
3:B:344:LYS:HD3	3:B:348:ARG:H	1.76	0.49
7:H:127:GLY:O	7:H:130:ARG:NH1	2.45	0.49
12:Q:119:LEU:HD23	13:P:133:TYR:HB2	1.94	0.49
18:W:149:CYS:HB3	18:W:154:GLU:H	1.77	0.49
26:7:431:GLN:NE2	26:7:433:GLU:OE1	2.46	0.49
27:2:168:LYS:HD2	27:2:175:GLU:HB2	1.94	0.49
1:M:63:TRP:HD1	1:M:64:ARG:HH12	1.60	0.49
3:B:45:SER:OG	3:B:46:GLN:NE2	2.45	0.49
3:B:546:SER:OG	3:B:632:ARG:N	2.38	0.49
22:0:114:LEU:HD13	22:0:193:TYR:HA	1.94	0.49
22:0:201:SER:HB3	22:0:225:GLU:HB3	1.94	0.49
22:0:703:ASP:N	22:0:703:ASP:OD1	2.45	0.49
2:A:40:THR:OG1	2:A:41:MET:N	2.46	0.49
3:B:213:ILE:O	3:B:215:GLN:NE2	2.44	0.49
5:E:117:THR:HG23	5:E:120:ALA:H	1.76	0.49
19:X:211:LYS:NZ	19:X:215:PRO:O	2.40	0.49
22:0:53:LEU:HD22	22:0:86:LEU:HD12	1.92	0.49
22:0:436:ARG:HD3	22:0:634:ILE:HD11	1.94	0.49
22:0:643:ARG:O	22:0:647:ARG:NH1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:2:54:GLU:OE2	27:2:109:ARG:NH2	2.45	0.49
27:2:152:GLY:HA2	27:2:182:PHE:HE2	1.77	0.49
27:2:208:LEU:HA	27:2:211:ILE:HG22	1.93	0.49
3:B:76:GLN:HB2	12:Q:326:ARG:HE	1.77	0.49
3:B:271:ALA:O	3:B:280:ILE:N	2.44	0.49
14:S:280:SER:HB3	14:S:300:GLU:HB2	1.94	0.49
2:A:903:ASN:O	2:A:907:THR:OG1	2.30	0.49
2:A:1135:ARG:HE	2:A:1282:VAL:HG23	1.76	0.49
3:B:139:ALA:N	3:B:150:GLU:O	2.45	0.49
7:H:118:PHE:HB2	7:H:121:LEU:HB2	1.94	0.49
7:H:135:LEU:HB3	7:H:137:GLN:HB3	1.94	0.49
25:6:352:CYS:SG	25:6:354:SER:OG	2.69	0.49
2:A:839:ARG:NE	3:B:1132:GLU:OE1	2.42	0.49
3:B:616:ILE:HG12	3:B:697:GLU:HA	1.95	0.49
13:P:125:THR:OG1	13:P:221:GLU:OE1	2.30	0.49
15:O:114:LEU:HB2	15:O:122:VAL:HB	1.95	0.49
22:0:295:SER:O	22:0:299:LEU:HB2	2.13	0.49
26:7:495:ALA:HB3	26:7:498:PHE:HD2	1.77	0.49
2:A:562:THR:O	2:A:572:TRP:NE1	2.37	0.49
3:B:563:MET:SD	3:B:588:GLY:HA3	2.53	0.49
3:B:825:VAL:HG23	3:B:1010:LEU:HG	1.95	0.49
4:C:11:ARG:HG3	4:C:20:PHE:HA	1.95	0.49
7:H:101:ALA:HA	7:H:116:TYR:HA	1.93	0.49
16:U:22:ARG:HD2	16:U:35:LEU:HD11	1.95	0.49
16:U:36:GLN:HA	16:U:36:GLN:NE2	2.28	0.49
22:0:112:LYS:HD3	22:0:129:VAL:HG21	1.95	0.49
22:0:135:ARG:NH1	22:0:391:THR:OG1	2.45	0.49
22:0:259:ARG:NH1	22:0:394:GLU:O	2.44	0.49
22:0:502:ASP:O	26:7:361:GLN:NE2	2.39	0.49
23:1:625:LEU:HG	23:1:629:LYS:HE2	1.93	0.49
24:4:182:GLY:N	24:4:215:ILE:O	2.46	0.49
26:7:642:ASN:HB3	26:7:649:ILE:HG13	1.93	0.49
1:M:277:ILE:HA	1:M:280:VAL:HG22	1.94	0.49
9:J:19:GLU:O	9:J:23:ASN:ND2	2.46	0.49
17:V:67:ASP:HB3	17:V:79:ILE:HG22	1.94	0.49
26:7:608:PHE:HB2	26:7:672:GLN:HG2	1.94	0.49
2:A:1394:THR:HB	2:A:1399:ARG:HD3	1.95	0.49
3:B:412:LEU:HB3	3:B:466:TRP:HZ2	1.78	0.49
22:0:197:ARG:HH12	22:0:221:ARG:HB3	1.78	0.49
22:0:567:LYS:HE3	22:0:595:GLY:HA3	1.95	0.49
26:7:323:VAL:HA	26:7:326:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:252:PHE:HB3	2:A:256:GLN:HB2	1.94	0.48
2:A:794:PRO:O	2:A:799:PHE:N	2.46	0.48
2:A:858:ASN:OD1	2:A:861:GLY:N	2.46	0.48
3:B:780:VAL:HG21	3:B:817:LEU:HD12	1.95	0.48
18:W:29:LEU:HA	18:W:32:ILE:HG12	1.94	0.48
22:0:352:ILE:HB	22:0:420:ILE:HB	1.95	0.48
2:A:77:CYS:SG	2:A:80:HIS:CD2	3.05	0.48
2:A:147:VAL:HA	2:A:170:THR:HA	1.94	0.48
9:J:52:THR:OG1	9:J:52:THR:O	2.31	0.48
12:Q:134:HIS:ND1	12:Q:354:ASP:OD2	2.41	0.48
22:0:161:ASN:ND2	22:0:189:THR:O	2.47	0.48
22:0:424:GLU:OE2	22:0:432:ASN:ND2	2.46	0.48
22:0:612:PHE:O	22:0:671:ARG:NH2	2.45	0.48
23:1:615:TYR:HB3	25:6:335:PHE:HE2	1.78	0.48
24:4:216:GLY:O	24:4:237:HIS:NE2	2.39	0.48
2:A:170:THR:HG21	2:A:187:LYS:HA	1.94	0.48
2:A:1194:ARG:NE	2:A:1196:GLU:OE2	2.46	0.48
3:B:441:ASP:OD2	3:B:444:MET:N	2.41	0.48
3:B:52:ASN:OD1	3:B:177:LYS:N	2.46	0.48
3:B:862:GLN:HB3	3:B:963:PHE:HD1	1.78	0.48
26:7:643:PHE:HB2	26:7:652:ILE:HD11	1.94	0.48
2:A:56:PRO:O	2:A:66:LYS:NZ	2.39	0.48
3:B:542:MET:SD	3:B:542:MET:N	2.87	0.48
3:B:763:GLN:HG2	3:B:765:PRO:HD2	1.96	0.48
4:C:104:PHE:HD2	4:C:106:GLU:HB3	1.79	0.48
15:O:171:ARG:NH2	15:O:238:ARG:O	2.45	0.48
17:V:85:VAL:O	17:V:106:ILE:N	2.44	0.48
21:G:46:LEU:HB2	21:G:77:VAL:HG13	1.95	0.48
21:G:62:LEU:HD23	21:G:65:ASP:HB2	1.95	0.48
22:0:690:ARG:HD2	22:0:706:LEU:HD11	1.96	0.48
24:4:119:ARG:NH2	24:4:123:GLU:OE1	2.46	0.48
26:7:525:GLY:O	26:7:528:ASN:ND2	2.40	0.48
26:7:637:MET:HA	26:7:640:LEU:HG	1.95	0.48
27:2:22:GLN:OE1	27:2:85:HIS:ND1	2.34	0.48
2:A:864:ILE:HD12	2:A:1377:THR:HG21	1.96	0.48
3:B:463:THR:HG22	3:B:465:ASN:H	1.78	0.48
3:B:871:THR:OG1	3:B:872:GLU:N	2.45	0.48
5:E:198:ILE:O	5:E:210:SER:OG	2.29	0.48
12:Q:25:ASP:O	12:Q:29:ARG:NE	2.34	0.48
15:O:195:TYR:HB3	15:O:204:LEU:HB2	1.94	0.48
18:W:61:LEU:HD23	18:W:66:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:0:67:ARG:NH1	22:0:230:SER:O	2.47	0.48
25:6:116:THR:O	25:6:120:ARG:NH2	2.47	0.48
2:A:18:GLN:O	3:B:1215:ARG:N	2.47	0.48
3:B:198:ASP:OD2	3:B:202:TYR:OH	2.30	0.48
3:B:341:LEU:HA	3:B:344:LYS:HE2	1.96	0.48
3:B:980:PHE:CE1	3:B:1094:ARG:HG3	2.48	0.48
4:C:148:ARG:HG2	9:J:61:LEU:HG	1.95	0.48
15:O:160:ILE:HD13	15:O:220:ARG:HH21	1.78	0.48
26:7:124:ARG:NH1	26:7:203:VAL:O	2.47	0.48
26:7:460:VAL:HB	26:7:501:VAL:HG12	1.96	0.48
26:7:560:PRO:HG2	26:7:586:THR:HG21	1.96	0.48
26:7:575:ARG:HH11	29:N:53:DT:H2'	1.77	0.48
3:B:842:ASN:OD1	3:B:845:SER:N	2.46	0.48
3:B:1065:GLN:OE1	3:B:1069:PHE:N	2.39	0.48
7:H:83:GLN:HA	10:K:54:ARG:HH22	1.79	0.48
19:X:119:ILE:HG21	19:X:151:LEU:HB2	1.95	0.48
22:0:731:LYS:HA	22:0:734:GLU:HB2	1.96	0.48
24:4:23:PRO:HB2	24:4:172:LEU:HD22	1.95	0.48
24:4:288:ILE:HB	24:4:293:LEU:HA	1.96	0.48
25:6:141:LEU:HD13	25:6:145:ARG:HG2	1.96	0.48
26:7:578:MET:HA	26:7:581:TYR:CE1	2.49	0.48
2:A:603:ASN:OD1	2:A:603:ASN:N	2.47	0.48
3:B:540:SER:OG	3:B:541:LEU:N	2.47	0.48
3:B:795:ILE:O	3:B:854:LEU:N	2.35	0.48
26:7:159:THR:HB	26:7:160:ILE:HD12	1.96	0.48
26:7:341:TYR:OH	26:7:349:ASN:OD1	2.32	0.48
1:M:23:THR:HA	1:M:32:PRO:HG3	1.94	0.48
2:A:1132:LYS:NZ	2:A:1206:ASP:OD2	2.47	0.48
3:B:883:LEU:HD23	3:B:935:ARG:H	1.79	0.48
5:E:202:SER:OG	5:E:206:GLY:N	2.47	0.48
7:H:135:LEU:O	7:H:137:GLN:N	2.47	0.48
18:W:198:THR:H	18:W:201:ILE:HB	1.79	0.48
22:0:39:ILE:HD11	22:0:475:PHE:HZ	1.78	0.48
22:0:67:ARG:NH1	22:0:455:SER:OG	2.47	0.48
26:7:354:ILE:HG21	26:7:430:LEU:HB2	1.96	0.48
26:7:485:ILE:HD11	26:7:510:LYS:HD2	1.95	0.48
2:A:260:ASP:OD1	2:A:260:ASP:N	2.40	0.47
2:A:531:ILE:HD11	2:A:578:LEU:HD22	1.95	0.47
2:A:573:SER:OG	2:A:576:GLN:N	2.41	0.47
13:P:70:LEU:HB3	13:P:221:GLU:HG2	1.96	0.47
16:U:253:ARG:HB3	16:U:258:TRP:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1143:LEU:HD12	2:A:1273:LEU:HD21	1.96	0.47
3:B:824:ILE:N	3:B:1009:ASP:OD2	2.37	0.47
17:V:11:ARG:HD2	17:V:41:LEU:HD12	1.95	0.47
20:D:14:ARG:HE	20:D:17:LYS:HD2	1.77	0.47
21:G:154:VAL:O	21:G:156:SER:N	2.46	0.47
22:0:576:ALA:HB3	23:1:343:ILE:HD13	1.95	0.47
22:0:625:ILE:HD11	22:0:685:ARG:HB2	1.96	0.47
26:7:357:LYS:NZ	26:7:427:TRP:O	2.47	0.47
26:7:436:ALA:HB3	26:7:453:VAL:HG22	1.95	0.47
2:A:999:VAL:H	2:A:1011:GLN:HE22	1.63	0.47
5:E:74:ASP:N	5:E:74:ASP:OD1	2.47	0.47
20:D:145:MET:HA	20:D:148:LEU:HD12	1.95	0.47
28:5:20:ILE:HA	28:5:23:ILE:HD12	1.96	0.47
2:A:964:ILE:HG22	2:A:1045:VAL:HG21	1.96	0.47
3:B:989:THR:OG1	3:B:990:ILE:N	2.47	0.47
20:D:56:ARG:HD3	20:D:149:THR:HA	1.96	0.47
20:D:202:ILE:HD13	20:D:207:LEU:HD13	1.96	0.47
21:G:100:GLU:HB3	21:G:107:LYS:HD2	1.95	0.47
24:4:221:SER:HB3	24:4:224:LEU:HD13	1.94	0.47
25:6:128:LEU:N	25:6:170:GLY:O	2.44	0.47
26:7:679:SER:O	26:7:683:GLU:HB2	2.13	0.47
2:A:352:VAL:O	2:A:467:THR:OG1	2.32	0.47
2:A:1332:PHE:HA	2:A:1335:ILE:HD13	1.97	0.47
5:E:147:HIS:HE1	5:E:149:LEU:HD13	1.79	0.47
12:Q:386:MET:HB2	13:P:87:LEU:HD11	1.95	0.47
21:G:150:CYS:HA	21:G:159:ALA:HA	1.96	0.47
22:0:68:LYS:NZ	22:0:203:CYS:O	2.40	0.47
22:0:406:ALA:O	22:0:410:SER:OG	2.30	0.47
22:0:618:ARG:HA	22:0:618:ARG:HD3	1.73	0.47
26:7:389:GLY:HA3	26:7:692:ARG:HB3	1.95	0.47
2:A:1198:ASP:HB3	2:A:1201:ALA:HB3	1.96	0.47
21:G:120:THR:OG1	21:G:131:GLN:O	2.32	0.47
22:0:618:ARG:HH12	22:0:676:TYR:H	1.60	0.47
1:M:308:THR:OG1	30:T:-1:DG:OP2	2.27	0.47
3:B:570:VAL:O	3:B:574:SER:OG	2.31	0.47
3:B:983:ARG:HD2	3:B:1091:TYR:HB3	1.96	0.47
4:C:46:ILE:HG23	4:C:68:GLY:HA2	1.95	0.47
4:C:96:SER:OG	4:C:97:VAL:N	2.48	0.47
22:0:498:THR:OG1	22:0:707:ASN:OD1	2.32	0.47
22:0:608:GLU:OE1	22:0:664:GLN:NE2	2.44	0.47
22:0:721:LEU:O	22:0:725:ALA:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:4:276:CYS:N	24:4:281:ARG:O	2.47	0.47
26:7:642:ASN:O	26:7:646:ASN:CB	2.58	0.47
2:A:519:PRO:HG3	2:A:631:HIS:HB2	1.96	0.47
2:A:1444:MET:HB2	6:F:133:VAL:HG23	1.97	0.47
15:O:79:ARG:NE	15:O:117:ALA:O	2.38	0.47
21:G:1:MET:SD	21:G:2:PHE:N	2.87	0.47
22:0:559:ILE:HA	22:0:562:GLU:HG3	1.97	0.47
24:4:21:GLU:OE1	24:4:257:SER:OG	2.30	0.47
26:7:143:LEU:HB3	26:7:171:HIS:HB2	1.96	0.47
26:7:438:PHE:HB2	26:7:445:MET:HE3	1.95	0.47
27:2:91:LYS:HA	27:2:96:LEU:HA	1.96	0.47
27:2:242:LEU:HD23	27:2:247:ARG:HG3	1.97	0.47
30:T:4:DC:N3	30:T:5:DA:N6	2.63	0.47
2:A:357:PRO:HG3	3:B:832:GLY:HA2	1.97	0.47
2:A:375:THR:OG1	2:A:433:GLU:OE1	2.23	0.47
2:A:1149:ALA:HA	8:I:45:ARG:HH12	1.80	0.47
3:B:872:GLU:HG2	3:B:917:PRO:HD3	1.97	0.47
20:D:130:LEU:HB3	20:D:138:ASN:HD21	1.80	0.47
22:0:618:ARG:NH1	22:0:675:ASP:OD1	2.48	0.47
23:1:172:GLU:O	23:1:176:THR:OG1	2.25	0.47
25:6:334:THR:N	25:6:343:VAL:O	2.46	0.47
26:7:207:GLU:HA	26:7:210:ILE:HB	1.97	0.47
27:2:189:PHE:HA	27:2:192:LEU:HD12	1.97	0.47
2:A:346:ASP:OD2	3:B:1106:ARG:NH1	2.48	0.47
2:A:1161:THR:HG22	2:A:1163:ILE:H	1.80	0.47
25:6:150:ILE:HG21	25:6:200:ARG:HB2	1.97	0.47
26:7:507:ALA:O	26:7:510:LYS:NZ	2.33	0.47
27:2:392:THR:HG22	27:2:394:ASP:H	1.80	0.47
27:2:442:ARG:O	27:2:446:LEU:N	2.42	0.47
1:M:87:LEU:HD13	1:M:151:LYS:HD3	1.96	0.46
1:M:211:LYS:NZ	15:O:184:SER:OG	2.41	0.46
2:A:1364:ASN:OD1	2:A:1365:TYR:N	2.48	0.46
3:B:1049:ASP:OD1	3:B:1049:ASP:N	2.42	0.46
7:H:91:ASP:OD1	7:H:91:ASP:N	2.46	0.46
12:Q:363:GLY:HA2	12:Q:395:PHE:HA	1.96	0.46
16:U:7:SER:O	16:U:11:GLU:HG2	2.15	0.46
19:X:195:LEU:O	19:X:199:GLN:NE2	2.34	0.46
25:6:127:ILE:HB	25:6:232:VAL:HG22	1.96	0.46
25:6:146:HIS:CG	25:6:204:PRO:HG3	2.49	0.46
26:7:462:ASN:O	26:7:466:ARG:NH1	2.42	0.46
27:2:219:VAL:HA	27:2:222:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:24:PRO:HA	2:A:27:VAL:HG12	1.96	0.46
2:A:95:PHE:O	2:A:99:ILE:HG13	2.15	0.46
2:A:445:ASN:HA	2:A:455:MET:HE1	1.96	0.46
2:A:1312:ASN:OD1	2:A:1313:LEU:N	2.48	0.46
4:C:35:ARG:HH21	10:K:41:THR:HG23	1.78	0.46
12:Q:105:ALA:HB1	13:P:87:LEU:HG	1.98	0.46
15:O:107:ARG:HH22	17:V:66:LEU:HD21	1.81	0.46
15:O:184:SER:N	15:O:194:ILE:O	2.48	0.46
16:U:255:LYS:NZ	30:T:-6:DT:O5'	2.40	0.46
22:0:545:LEU:N	23:1:357:THR:O	2.47	0.46
28:5:5:ARG:HH12	28:5:32:LEU:HD13	1.80	0.46
2:A:1054:LEU:HB3	6:F:84:TYR:HE1	1.79	0.46
3:B:43:LEU:HD22	3:B:492:LEU:HD12	1.98	0.46
3:B:758:PHE:H	3:B:1044:ALA:HB1	1.80	0.46
7:H:63:LEU:HB3	7:H:89:LEU:HD13	1.97	0.46
13:P:108:LEU:HB3	13:P:118:HIS:HA	1.96	0.46
17:V:68:THR:O	17:V:79:ILE:N	2.41	0.46
18:W:18:ARG:NE	19:X:249:GLY:HA2	2.29	0.46
22:0:255:ASP:OD1	22:0:258:ARG:NH2	2.35	0.46
22:0:690:ARG:HA	22:0:693:LEU:HD12	1.97	0.46
26:7:354:ILE:O	26:7:404:LYS:NZ	2.45	0.46
27:2:146:ILE:HD13	27:2:159:PRO:HB3	1.97	0.46
29:N:-4:DG:H1'	29:N:-3:DA:H5'	1.97	0.46
2:A:1146:VAL:HG23	2:A:1197:LEU:HD22	1.97	0.46
3:B:614:SER:OG	3:B:632:ARG:NH1	2.48	0.46
4:C:207:CYS:SG	4:C:208:GLU:N	2.88	0.46
5:E:11:ARG:HH22	5:E:138:ALA:HB2	1.81	0.46
9:J:7:CYS:HB3	9:J:11:GLY:H	1.81	0.46
25:6:363:CYS:N	25:6:368:LEU:O	2.42	0.46
2:A:1152:ILE:HD11	2:A:1260:LEU:HD23	1.97	0.46
3:B:301:ILE:HG21	3:B:314:LEU:HD11	1.98	0.46
3:B:526:GLU:OE2	3:B:752:ALA:N	2.49	0.46
4:C:167:HIS:CE1	4:C:169:LYS:HG3	2.50	0.46
8:I:22:ASN:HB3	8:I:24:ARG:HH11	1.81	0.46
12:Q:126:LYS:HD3	13:P:130:GLU:HB2	1.98	0.46
13:P:223:GLN:NE2	13:P:224:VAL:O	2.49	0.46
16:U:239:PRO:O	16:U:270:ASN:N	2.49	0.46
16:U:250:LYS:H	16:U:261:SER:HB2	1.80	0.46
22:0:295:SER:HA	22:0:383:LEU:HD21	1.98	0.46
25:6:261:VAL:HB	25:6:280:THR:HG21	1.97	0.46
2:A:672:ASP:O	2:A:675:THR:OG1	2.26	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1135:ARG:HA	2:A:1138:ILE:HG22	1.97	0.46
3:B:521:LEU:O	3:B:540:SER:N	2.49	0.46
5:E:202:SER:N	5:E:206:GLY:O	2.41	0.46
12:Q:98:TYR:HB3	13:P:97:ILE:HG12	1.97	0.46
18:W:37:VAL:HG12	18:W:88:TYR:HB3	1.97	0.46
20:D:119:ARG:HH21	20:D:149:THR:HG23	1.80	0.46
23:1:188:ASN:OD1	23:1:189:LYS:N	2.47	0.46
23:1:472:GLN:NE2	24:4:41:ASP:OD2	2.48	0.46
27:2:87:LEU:HD12	27:2:87:LEU:HA	1.79	0.46
2:A:328:ARG:HH11	2:A:335:ARG:HH12	1.62	0.46
2:A:666:ILE:O	2:A:669:THR:N	2.47	0.46
4:C:8:VAL:HG11	10:K:105:PHE:HA	1.98	0.46
4:C:217:ASP:OD1	4:C:217:ASP:N	2.49	0.46
6:F:125:LEU:HD11	6:F:153:VAL:HG11	1.96	0.46
7:H:83:GLN:HA	10:K:54:ARG:NH2	2.30	0.46
16:U:260:CYS:HB3	16:U:281:VAL:HB	1.98	0.46
19:X:209:ASP:OD1	19:X:209:ASP:N	2.49	0.46
20:D:153:ARG:HH22	20:D:160:VAL:HA	1.80	0.46
22:0:673:LYS:NZ	22:0:737:SER:O	2.47	0.46
23:1:284:TRP:HA	23:1:287:PHE:HB2	1.98	0.46
27:2:152:GLY:HA2	27:2:182:PHE:CE2	2.51	0.46
1:M:321:ASP:OD1	1:M:321:ASP:N	2.47	0.46
2:A:402:ALA:HA	2:A:434:ARG:HA	1.98	0.46
2:A:1000:LEU:N	2:A:1011:GLN:OE1	2.49	0.46
2:A:1229:SER:OG	2:A:1233:ASP:OD2	2.30	0.46
4:C:10:ILE:HD12	4:C:20:PHE:HB3	1.97	0.46
14:S:298:THR:HA	14:S:305:ARG:HA	1.97	0.46
15:O:69:ASN:ND2	30:T:-7:DT:H2”	2.31	0.46
20:D:123:LEU:HD11	20:D:149:THR:HG21	1.98	0.46
22:0:19:PRO:HG3	22:0:739:TRP:CE2	2.51	0.46
22:0:743:ASP:OD1	22:0:746:LYS:NZ	2.45	0.46
23:1:542:LEU:HB2	23:1:547:LEU:HD12	1.97	0.46
25:6:165:PRO:HB2	25:6:360:PRO:HG3	1.96	0.46
26:7:154:GLN:HA	26:7:157:LEU:HB2	1.98	0.46
26:7:584:ASN:ND2	26:7:710:SER:OG	2.49	0.46
27:2:17:ILE:O	27:2:22:GLN:NE2	2.49	0.46
2:A:807:GLY:HA3	3:B:728:ARG:HH22	1.81	0.46
3:B:380:TYR:CZ	3:B:384:ARG:HD2	2.51	0.46
8:I:74:GLU:HB3	8:I:81:ARG:HD3	1.98	0.46
10:K:57:LEU:HD21	10:K:78:THR:HG23	1.97	0.46
13:P:84:ARG:NE	13:P:84:ARG:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S:299:CYS:HB2	14:S:306:TRP:HZ3	1.79	0.46
21:G:166:ASP:N	21:G:166:ASP:OD1	2.49	0.46
22:0:18:TYR:HE1	22:0:738:VAL:HG22	1.81	0.46
22:0:683:ASP:OD2	22:0:685:ARG:NH1	2.40	0.46
25:6:402:ASP:OD1	25:6:402:ASP:N	2.49	0.46
1:M:286:ILE:HD11	1:M:291:ILE:HB	1.98	0.46
9:J:16:ASP:OD1	9:J:16:ASP:N	2.47	0.46
12:Q:326:ARG:HH12	12:Q:330:ARG:HB3	1.81	0.46
26:7:236:THR:OG1	26:7:238:GLN:O	2.25	0.46
2:A:190:ALA:HB3	2:A:194:ALA:HB2	1.98	0.45
2:A:1215:ARG:O	2:A:1218:GLN:NE2	2.42	0.45
3:B:244:LEU:HD23	3:B:362:PRO:HB2	1.97	0.45
20:D:52:LEU:HD12	20:D:148:LEU:HD23	1.98	0.45
20:D:173:HIS:HD2	20:D:176:GLU:H	1.64	0.45
23:1:168:SER:HA	23:1:173:LYS:HG3	1.98	0.45
25:6:132:CYS:N	25:6:174:MET:O	2.36	0.45
26:7:413:SER:OG	26:7:414:SER:N	2.49	0.45
27:2:239:ILE:HG23	27:2:247:ARG:HD3	1.97	0.45
29:N:42:DA:H2"	29:N:43:DC:H5"	1.98	0.45
2:A:75:ASN:OD1	2:A:75:ASN:N	2.50	0.45
2:A:1279:ILE:HA	2:A:1310:GLY:HA3	1.97	0.45
4:C:61:GLU:HB3	11:L:67:PHE:CE1	2.52	0.45
13:P:300:LEU:HD23	13:P:303:LEU:HD21	1.98	0.45
23:1:291:LYS:HG3	23:1:307:GLY:HA3	1.97	0.45
26:7:549:ILE:HD12	26:7:691:LEU:HD11	1.99	0.45
26:7:568:GLU:HA	26:7:571:ARG:HG2	1.98	0.45
4:C:46:ILE:HD13	4:C:67:LEU:HB3	1.97	0.45
4:C:186:LEU:HB3	4:C:188:HIS:CD2	2.51	0.45
5:E:9:ILE:HG21	5:E:43:LYS:HD3	1.98	0.45
5:E:167:ARG:HD3	5:E:167:ARG:HA	1.80	0.45
12:Q:141:ARG:NH1	12:Q:348:TYR:O	2.47	0.45
14:S:269:PHE:HB2	14:S:279:VAL:HG21	1.98	0.45
16:U:242:ASN:HB3	16:U:269:ILE:HG22	1.97	0.45
18:W:17:VAL:HA	18:W:21:TYR:HD2	1.81	0.45
21:G:12:THR:HA	21:G:69:GLU:HA	1.99	0.45
22:0:424:GLU:HB3	22:0:432:ASN:HB3	1.99	0.45
27:2:493:ILE:HG21	27:2:501:VAL:HG11	1.98	0.45
28:5:17:LYS:HG3	28:5:40:LEU:HD11	1.99	0.45
30:T:3:DT:H2'	30:T:4:DC:C2	2.52	0.45
3:B:843:GLN:HB2	3:B:993:THR:HB	1.98	0.45
16:U:5:GLU:OE1	17:V:57:GLN:NE2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:X:193:LEU:HD21	19:X:229:LYS:HD2	1.98	0.45
22:0:719:GLN:O	22:0:723:THR:OG1	2.23	0.45
24:4:164:SER:HA	24:4:172:LEU:HD12	1.99	0.45
24:4:175:ARG:HE	24:4:177:LEU:HD21	1.82	0.45
25:6:260:ARG:HA	25:6:280:THR:HG22	1.98	0.45
1:M:199:LYS:HE3	1:M:202:GLU:HB2	1.98	0.45
2:A:678:GLU:O	2:A:682:THR:OG1	2.28	0.45
2:A:1150:SER:H	8:I:45:ARG:HH22	1.65	0.45
2:A:1152:ILE:HG22	8:I:44:TYR:H	1.81	0.45
2:A:1173:HIS:CE1	2:A:1228:TRP:H	2.34	0.45
14:S:235:ASP:HA	14:S:242:LYS:HD3	1.99	0.45
19:X:202:PHE:O	19:X:245:TRP:NE1	2.45	0.45
21:G:45:ILE:HA	21:G:78:VAL:HG12	1.98	0.45
22:0:220:GLU:HA	22:0:223:SER:HB3	1.98	0.45
22:0:351:VAL:HG13	22:0:421:GLU:HG2	1.99	0.45
22:0:722:ARG:NH2	25:6:267:SER:O	2.50	0.45
23:1:302:MET:HG3	23:1:304:ASN:H	1.81	0.45
2:A:443:LEU:HD22	2:A:501:LEU:HD11	1.99	0.45
2:A:544:ASP:O	2:A:548:ASN:ND2	2.34	0.45
2:A:1059:HIS:ND1	6:F:86:THR:OG1	2.31	0.45
3:B:1134:GLU:OE1	3:B:1134:GLU:N	2.42	0.45
10:K:85:ASP:HA	10:K:88:LYS:HG2	1.97	0.45
12:Q:98:TYR:CE2	12:Q:100:GLU:HB2	2.52	0.45
14:S:198:ARG:NH2	14:S:231:CYS:H	2.14	0.45
22:0:31:THR:HA	22:0:34:VAL:HG12	1.99	0.45
22:0:86:LEU:HD22	22:0:175:VAL:HG11	1.99	0.45
22:0:107:GLY:HA3	22:0:178:PHE:HZ	1.82	0.45
26:7:408:ILE:HG22	26:7:453:VAL:H	1.80	0.45
27:2:434:PRO:HA	27:2:435:PRO:HD3	1.83	0.45
27:2:455:GLU:HG2	28:5:8:ALA:HB1	1.99	0.45
1:M:312:GLY:HA2	1:M:315:ILE:HG22	1.98	0.45
2:A:857:ARG:HB3	2:A:861:GLY:HA2	1.98	0.45
2:A:858:ASN:OD1	2:A:862:ASN:N	2.41	0.45
3:B:120:ARG:NH2	3:B:957:ASN:O	2.49	0.45
3:B:274:PRO:HA	3:B:275:TYR:HA	1.73	0.45
3:B:326:ASP:O	3:B:329:THR:OG1	2.32	0.45
3:B:372:SER:OG	3:B:373:ARG:NH1	2.50	0.45
3:B:980:PHE:HE1	3:B:1094:ARG:HG3	1.82	0.45
3:B:1207:LEU:HD22	3:B:1212:ILE:HG13	1.97	0.45
4:C:233:GLU:OE1	9:J:43:ARG:NH2	2.46	0.45
12:Q:108:LYS:HE2	13:P:84:ARG:HE	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:12:LEU:HD11	18:W:182:ILE:HG23	1.98	0.45
21:G:101:VAL:HB	21:G:108:VAL:HG13	1.99	0.45
25:6:392:VAL:HG22	25:6:426:ARG:HB2	1.99	0.45
26:7:558:TRP:HZ3	26:7:735:VAL:HA	1.82	0.45
2:A:843:LYS:NZ	2:A:1401:SER:O	2.43	0.45
3:B:1164:GLY:N	3:B:1190:ASP:OD2	2.50	0.45
4:C:181:ASP:OD1	4:C:186:LEU:N	2.42	0.45
23:1:205:PRO:HA	23:1:206:PRO:HD3	1.88	0.45
25:6:403:CYS:HB3	25:6:408:SER:H	1.82	0.45
2:A:1204:ASP:OD1	2:A:1204:ASP:N	2.50	0.45
3:B:902:GLY:HA3	11:L:60:ARG:HH22	1.80	0.45
3:B:1073:TYR:HE1	3:B:1080:LYS:HD2	1.82	0.45
7:H:111:LEU:HA	7:H:128:ASN:HB2	1.99	0.45
19:X:168:ARG:HA	19:X:181:LEU:HB3	1.99	0.45
22:0:609:GLY:H	22:0:668:ARG:NH1	2.14	0.45
22:0:633:ARG:HH21	22:0:636:LYS:HE2	1.81	0.45
25:6:163:GLN:HE21	25:6:382:HIS:CE1	2.34	0.45
26:7:673:ILE:HG22	26:7:708:LEU:HB2	1.99	0.45
29:N:43:DC:H2"	29:N:44:DT:H5"	1.99	0.45
2:A:115:LEU:HD21	2:A:145:LYS:HD3	1.98	0.45
2:A:590:ARG:NH1	2:A:620:LYS:O	2.43	0.45
3:B:26:THR:N	3:B:29:ASP:OD2	2.50	0.45
3:B:526:GLU:O	3:B:538:ASN:ND2	2.50	0.45
4:C:43:THR:HA	4:C:77:ILE:HG12	1.99	0.45
10:K:36:GLU:HA	10:K:70:ARG:HA	1.99	0.45
18:W:120:ASN:HD22	18:W:158:GLU:HG2	1.81	0.45
19:X:168:ARG:O	19:X:181:LEU:N	2.50	0.45
22:0:19:PRO:O	22:0:23:ASN:ND2	2.34	0.45
27:2:447:GLU:O	27:2:450:ARG:NH2	2.50	0.45
1:M:84:ASN:HB3	1:M:87:LEU:HD12	1.99	0.44
1:M:314:LYS:HE2	1:M:314:LYS:HB2	1.83	0.44
3:B:822:ASN:ND2	9:J:48:ARG:HE	2.16	0.44
3:B:863:GLU:OE2	3:B:962:LYS:N	2.38	0.44
9:J:44:TYR:HA	9:J:47:ARG:HB2	1.99	0.44
18:W:35:HIS:HA	18:W:207:ILE:HB	1.99	0.44
18:W:349:GLU:HB2	18:W:351:ARG:HH11	1.82	0.44
20:D:23:ASN:HB2	21:G:83:LYS:HZ3	1.81	0.44
22:0:567:LYS:HA	22:0:594:ARG:HE	1.82	0.44
26:7:189:GLU:OE2	26:7:192:ASP:N	2.49	0.44
27:2:261:GLN:HA	27:2:269:PHE:HA	1.99	0.44
27:2:366:LEU:HA	27:2:376:GLY:HA3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:179:LEU:HB3	2:A:297:GLN:HE22	1.82	0.44
2:A:203:SER:O	2:A:206:GLU:HG2	2.17	0.44
1:M:243:CYS:O	1:M:247:GLY:N	2.47	0.44
3:B:801:LYS:HD3	3:B:815:ARG:HG3	2.00	0.44
8:I:69:PRO:HB2	8:I:85:PHE:CE1	2.52	0.44
8:I:90:GLN:HE22	8:I:92:ARG:HG3	1.83	0.44
15:O:143:ILE:HA	15:O:146:ILE:HD12	1.99	0.44
18:W:365:ALA:O	18:W:368:GLN:NE2	2.50	0.44
22:0:72:CYS:HB3	22:0:210:TYR:HE1	1.83	0.44
24:4:39:THR:HG21	24:4:184:GLY:HA2	1.99	0.44
26:7:518:VAL:HG13	26:7:681:ARG:HB2	1.98	0.44
27:2:219:VAL:O	27:2:223:HIS:ND1	2.36	0.44
3:B:77:HIS:CE1	3:B:80:GLU:HB2	2.53	0.44
3:B:789:MET:SD	3:B:967:ARG:HD3	2.57	0.44
5:E:147:HIS:CE1	5:E:149:LEU:HB2	2.53	0.44
16:U:41:ILE:HG12	16:U:45:LYS:HE2	1.99	0.44
24:4:72:LYS:HB2	24:4:72:LYS:HE2	1.79	0.44
25:6:194:ASP:HA	25:6:197:LYS:HE3	2.00	0.44
25:6:270:VAL:N	25:6:288:TYR:OH	2.48	0.44
26:7:585:PRO:HG3	26:7:756:ARG:HG2	1.99	0.44
27:2:254:ARG:NH1	27:2:261:GLN:O	2.47	0.44
2:A:481:ASP:OD1	2:A:481:ASP:N	2.51	0.44
2:A:488:ASN:HB3	3:B:1128:LEU:HD21	2.00	0.44
2:A:552:TRP:CD1	2:A:651:LYS:HB3	2.52	0.44
2:A:1452:LYS:HE3	2:A:1452:LYS:HB3	1.89	0.44
3:B:22:SER:O	3:B:654:ARG:NH1	2.51	0.44
4:C:50:GLU:HB2	4:C:156:THR:HB	2.00	0.44
17:V:63:LYS:N	17:V:84:GLN:O	2.50	0.44
19:X:142:VAL:HB	19:X:146:GLU:HG3	1.99	0.44
22:0:257:LEU:HD13	22:0:343:LYS:HG2	1.98	0.44
22:0:721:LEU:HD12	22:0:722:ARG:HD2	1.99	0.44
26:7:490:VAL:HG12	26:7:514:THR:HB	1.99	0.44
27:2:143:TRP:HA	27:2:146:ILE:HG22	1.98	0.44
3:B:627:PHE:O	3:B:632:ARG:NH1	2.51	0.44
3:B:957:ASN:ND2	3:B:959:ASP:OD1	2.46	0.44
4:C:54:ASN:OD1	4:C:56:THR:HG22	2.18	0.44
12:Q:351:VAL:HG22	12:Q:362:VAL:HA	1.99	0.44
15:O:158:GLN:O	15:O:218:LYS:NZ	2.40	0.44
20:D:57:LEU:HD22	20:D:157:GLN:HB3	2.00	0.44
23:1:567:HIS:CE1	23:1:582:LEU:HG	2.53	0.44
24:4:25:LEU:HD13	24:4:163:ILE:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:4:79:TYR:N	24:4:82:GLY:O	2.51	0.44
24:4:112:SER:HA	24:4:119:ARG:HE	1.82	0.44
26:7:643:PHE:HA	26:7:649:ILE:HB	1.99	0.44
27:2:135:LEU:HD21	27:2:270:TYR:HB3	1.98	0.44
2:A:12:ARG:NH2	3:B:1218:THR:OG1	2.50	0.44
2:A:1148:ILE:HG13	8:I:49:ILE:HD13	1.99	0.44
3:B:996:ARG:HG2	3:B:1007:VAL:HG11	1.98	0.44
8:I:45:ARG:NH2	8:I:47:GLU:H	2.11	0.44
13:P:73:LEU:HG	13:P:77:LEU:HB3	1.98	0.44
16:U:3:ASN:HB3	16:U:6:ALA:HB3	2.00	0.44
18:W:36:SER:OG	18:W:205:ARG:O	2.28	0.44
22:0:104:ARG:NH1	22:0:171:LEU:O	2.50	0.44
25:6:452:PRO:HA	25:6:455:GLU:HG2	1.99	0.44
26:7:115:SER:O	26:7:115:SER:OG	2.35	0.44
26:7:763:VAL:O	26:7:767:ASN:ND2	2.47	0.44
2:A:362:ASP:O	2:A:459:ARG:N	2.31	0.44
2:A:599:SER:OG	2:A:599:SER:O	2.36	0.44
3:B:264:SER:OG	3:B:265:SER:N	2.50	0.44
3:B:287:ARG:HD3	3:B:292:ILE:HA	2.00	0.44
3:B:1021:MET:SD	3:B:1021:MET:N	2.90	0.44
9:J:57:ILE:HA	9:J:60:PHE:HB2	2.00	0.44
16:U:277:GLN:N	17:V:58:SER:O	2.47	0.44
22:0:5:ILE:HG13	22:0:6:ASP:H	1.82	0.44
23:1:469:MET:HA	24:4:38:THR:HG21	1.99	0.44
24:4:304:LYS:HE2	24:4:304:LYS:HB3	1.86	0.44
26:7:416:SER:O	26:7:419:GLN:HG2	2.17	0.44
2:A:834:THR:HA	2:A:837:ILE:HG22	2.00	0.44
2:A:857:ARG:CZ	6:F:139:PRO:HG2	2.47	0.44
6:F:140:ASP:OD1	6:F:141:GLY:N	2.51	0.44
21:G:49:LEU:HD23	21:G:50:ASP:HB2	1.99	0.44
22:0:70:ILE:N	22:0:231:ILE:O	2.36	0.44
22:0:228:LYS:HZ3	22:0:452:ARG:HG3	1.83	0.44
22:0:258:ARG:HD2	22:0:262:ARG:HH21	1.83	0.44
22:0:344:THR:HA	22:0:347:LYS:HE2	1.99	0.44
26:7:119:SER:OG	27:2:369:ARG:O	2.36	0.44
26:7:363:ARG:N	26:7:366:GLN:OE1	2.47	0.44
26:7:373:MET:HA	26:7:380:ARG:HD2	1.98	0.44
27:2:90:ASN:O	27:2:97:MET:N	2.50	0.44
27:2:242:LEU:O	27:2:247:ARG:NH1	2.51	0.44
27:2:483:TRP:HE3	27:2:492:PHE:HB2	1.83	0.44
2:A:843:LYS:HA	2:A:846:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1438:THR:HA	6:F:88:TYR:HB3	2.00	0.43
3:B:271:ALA:N	3:B:280:ILE:O	2.39	0.43
3:B:526:GLU:OE2	3:B:753:ALA:N	2.36	0.43
3:B:805:THR:O	3:B:1044:ALA:N	2.51	0.43
3:B:995:ARG:HH22	10:K:9:LEU:HD11	1.82	0.43
3:B:1181:GLU:HA	3:B:1188:LYS:HE3	1.98	0.43
14:S:271:CYS:SG	14:S:273:LYS:N	2.90	0.43
22:0:259:ARG:HG2	22:0:262:ARG:HH12	1.83	0.43
25:6:173:ILE:HG23	25:6:180:GLN:HB2	1.99	0.43
26:7:408:ILE:HA	26:7:452:LEU:HD12	2.00	0.43
3:B:130:VAL:HG23	3:B:167:ILE:HD13	2.00	0.43
8:I:31:THR:HG23	12:Q:401:TYR:CG	2.53	0.43
12:Q:364:SER:N	12:Q:394:LYS:O	2.48	0.43
1:M:250:MET:O	1:M:253:THR:OG1	2.25	0.43
2:A:32:VAL:N	2:A:81:PHE:O	2.51	0.43
3:B:497:ARG:NH2	3:B:775:LYS:HD3	2.34	0.43
6:F:74:ILE:HG21	6:F:144:GLU:HG2	2.00	0.43
17:V:68:THR:HB	17:V:79:ILE:HB	2.00	0.43
19:X:119:ILE:HA	19:X:121:LYS:HE3	2.00	0.43
22:0:722:ARG:HH22	25:6:267:SER:HA	1.82	0.43
24:4:275:SER:HA	24:4:282:VAL:HA	2.00	0.43
1:M:135:MET:SD	3:B:448:ILE:HG12	2.58	0.43
2:A:445:ASN:HB3	2:A:488:ASN:HB2	2.00	0.43
2:A:737:LEU:HD12	2:A:737:LEU:HA	1.84	0.43
3:B:550:ASP:HA	3:B:551:PRO:HD3	1.77	0.43
7:H:130:ARG:HB2	7:H:133:ASN:HB3	2.00	0.43
8:I:30:ARG:NE	12:Q:422:ARG:O	2.47	0.43
18:W:44:LYS:HD3	18:W:51:LYS:HG3	2.00	0.43
18:W:127:CYS:SG	18:W:129:THR:OG1	2.68	0.43
22:0:484:ALA:HB2	22:0:695:LYS:HE3	2.01	0.43
24:4:212:VAL:HG21	24:4:224:LEU:HB3	2.00	0.43
1:M:37:ARG:O	1:M:41:GLY:N	2.51	0.43
3:B:395:GLN:OE1	3:B:396:ASP:N	2.51	0.43
3:B:510:LYS:O	3:B:512:ARG:N	2.51	0.43
9:J:17:LYS:HD2	9:J:39:LEU:HG	1.99	0.43
13:P:121:ASP:OD1	13:P:121:ASP:N	2.50	0.43
22:0:711:ASP:N	22:0:711:ASP:OD1	2.50	0.43
2:A:340:LEU:HB3	2:A:1429:ILE:HG22	1.99	0.43
3:B:307:ASP:OD1	3:B:308:TRP:N	2.50	0.43
3:B:802:PRO:HB3	3:B:1091:TYR:CD1	2.54	0.43
3:B:848:ARG:NH1	9:J:8:PHE:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:43:THR:HG23	4:C:170:TRP:HD1	1.83	0.43
22:0:554:TRP:HB3	22:0:560:LEU:HG	2.00	0.43
1:M:51:VAL:HG11	2:A:412:ARG:HB2	2.01	0.43
2:A:483:ASP:N	2:A:483:ASP:OD1	2.52	0.43
3:B:496:ARG:HB2	3:B:539:LEU:HD13	2.00	0.43
5:E:180:ARG:HH21	5:E:192:ARG:HB2	1.83	0.43
13:P:138:GLN:HB2	13:P:211:LYS:HB3	2.00	0.43
21:G:84:GLY:N	21:G:147:ILE:O	2.41	0.43
21:G:90:THR:OG1	21:G:140:LYS:O	2.35	0.43
21:G:144:ARG:HG2	21:G:171:ILE:HG22	2.00	0.43
22:0:114:LEU:HD22	22:0:192:PRO:HB2	2.00	0.43
22:0:523:GLY:HA3	22:0:554:TRP:CH2	2.54	0.43
1:M:306:GLU:HA	1:M:309:ILE:HD12	1.99	0.43
2:A:528:LEU:HD22	2:A:751:SER:HB3	2.00	0.43
2:A:1126:ALA:HA	2:A:1304:TRP:HD1	1.84	0.43
3:B:1033:LYS:HD2	3:B:1059:LEU:HD11	2.00	0.43
4:C:55:THR:HB	4:C:152:GLU:H	1.83	0.43
9:J:3:VAL:HA	9:J:4:PRO:HD3	1.83	0.43
22:0:249:SER:HB3	23:1:352:ASN:HD21	1.84	0.43
23:1:369:ASP:OD1	23:1:369:ASP:N	2.51	0.43
23:1:548:GLU:HG2	23:1:551:ARG:HH11	1.83	0.43
27:2:416:LEU:HD12	27:2:419:LYS:HE3	2.00	0.43
2:A:1209:MET:HA	2:A:1212:VAL:HG22	2.00	0.43
3:B:438:GLU:HA	3:B:439:ALA:HA	1.81	0.43
3:B:497:ARG:HH22	3:B:775:LYS:HD3	1.84	0.43
3:B:839:MET:O	3:B:991:GLY:N	2.41	0.43
8:I:59:VAL:HG13	8:I:61:ASP:H	1.83	0.43
14:S:223:ILE:HG13	14:S:225:PRO:HD2	1.99	0.43
16:U:18:VAL:HG11	16:U:39:LYS:HD3	2.00	0.43
24:4:86:LEU:HA	24:4:128:GLU:HG2	2.00	0.43
25:6:218:ARG:HB2	25:6:254:LEU:HD21	2.01	0.43
26:7:126:ASP:OD2	26:7:130:ARG:NE	2.50	0.43
2:A:186:LYS:NZ	30:T:-34:DG:OP2	2.52	0.43
2:A:225:ASN:N	2:A:229:SER:OG	2.52	0.43
2:A:339:ASN:ND2	3:B:1117:GLN:OE1	2.52	0.43
2:A:959:ASN:OD1	2:A:960:ILE:N	2.51	0.43
2:A:1443:VAL:HG12	21:G:61:ILE:HD13	2.00	0.43
3:B:68:THR:HG21	12:Q:334:VAL:HG21	2.01	0.43
3:B:429:PHE:CZ	12:Q:331:GLN:HB2	2.54	0.43
3:B:494:HIS:HA	3:B:497:ARG:HE	1.83	0.43
3:B:1155:SER:OG	3:B:1156:ASP:N	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:62:VAL:HA	17:V:85:VAL:HG22	2.01	0.43
18:W:192:SER:OG	18:W:193:ARG:N	2.50	0.43
20:D:139:LYS:HZ3	20:D:142:LYS:HB2	1.83	0.43
22:0:424:GLU:N	22:0:432:ASN:O	2.32	0.43
23:1:264:PRO:HA	23:1:267:LYS:HB3	2.01	0.43
23:1:362:VAL:HA	23:1:368:SER:HA	1.99	0.43
24:4:71:ASN:OD1	24:4:71:ASN:N	2.52	0.43
26:7:103:ASP:N	26:7:103:ASP:OD1	2.52	0.43
26:7:682:GLN:HE22	26:7:686:ARG:NE	2.17	0.43
2:A:35:ILE:HD13	2:A:241:VAL:HG11	2.01	0.42
2:A:181:LEU:HD23	2:A:181:LEU:HA	1.89	0.42
2:A:349:ALA:HB3	2:A:489:LEU:HB3	1.99	0.42
2:A:567:LYS:HG2	7:H:96:VAL:H	1.83	0.42
2:A:636:GLU:HB2	2:A:962:ARG:NH2	2.34	0.42
3:B:605:ARG:NH2	3:B:691:GLU:OE1	2.52	0.42
3:B:835:GLN:OE1	3:B:835:GLN:N	2.45	0.42
7:H:37:LYS:HD2	7:H:37:LYS:HA	1.78	0.42
7:H:38:LEU:HD11	7:H:57:VAL:HG11	2.01	0.42
15:O:73:THR:OG1	15:O:158:GLN:NE2	2.52	0.42
17:V:61:THR:O	17:V:63:LYS:NZ	2.44	0.42
20:D:206:GLU:HA	20:D:209:ARG:HG2	2.00	0.42
22:0:345:ARG:NH2	22:0:354:GLU:OE2	2.52	0.42
26:7:627:ILE:HA	26:7:636:ARG:CZ	2.49	0.42
29:N:47:DA:H2"	29:N:48:DC:H5'	2.01	0.42
1:M:187:ARG:HA	1:M:187:ARG:HD3	1.74	0.42
2:A:69:THR:HG21	18:W:151:LEU:HD22	2.01	0.42
4:C:248:ILE:HG21	10:K:102:LYS:HB2	2.00	0.42
10:K:24:ASP:OD1	10:K:25:THR:N	2.51	0.42
11:L:45:ALA:HB3	11:L:49:LYS:HD2	2.01	0.42
16:U:44:LYS:HA	16:U:47:THR:HG22	2.01	0.42
17:V:24:ASP:HA	17:V:27:ILE:HB	2.00	0.42
18:W:92:PRO:HB3	18:W:194:ILE:HD11	2.00	0.42
18:W:352:GLU:HA	18:W:355:LYS:HE2	2.01	0.42
22:0:348:VAL:HG21	22:0:420:ILE:HG22	2.01	0.42
22:0:529:PHE:HA	22:0:532:ILE:HG12	2.01	0.42
27:2:245:THR:HA	27:2:248:ILE:HG22	2.01	0.42
29:N:20:DA:C8	29:N:21:DT:H72	2.54	0.42
1:M:108:LYS:HD3	1:M:108:LYS:HA	1.76	0.42
1:M:239:ILE:HD12	1:M:282:ILE:HD11	2.02	0.42
2:A:33:ALA:H	2:A:82:GLY:HA2	1.85	0.42
3:B:351:TYR:CZ	3:B:355:ILE:HD11	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:791:THR:HA	3:B:858:SER:HB2	2.01	0.42
3:B:1106:ARG:CZ	3:B:1109:GLY:H	2.32	0.42
3:B:1196:ILE:HD12	3:B:1197:PRO:HD2	2.00	0.42
4:C:115:SER:HB3	4:C:141:GLY:HA3	2.01	0.42
21:G:54:ILE:HD12	21:G:54:ILE:HA	1.93	0.42
21:G:58:ARG:HD3	21:G:58:ARG:HA	1.78	0.42
26:7:116:HIS:HB3	27:2:367:LYS:O	2.19	0.42
26:7:553:GLN:N	26:7:703:ALA:O	2.48	0.42
2:A:190:ALA:HB2	18:W:224:GLY:HA2	2.01	0.42
2:A:1169:ILE:HA	2:A:1172:LEU:HB2	2.00	0.42
2:A:1173:HIS:CG	2:A:1227:ILE:HG23	2.54	0.42
3:B:700:SER:O	3:B:700:SER:OG	2.34	0.42
8:I:90:GLN:NE2	8:I:92:ARG:HG3	2.34	0.42
10:K:97:LYS:HB3	10:K:97:LYS:HE2	1.85	0.42
15:O:68:GLN:HB2	15:O:161:VAL:HG12	2.01	0.42
16:U:22:ARG:NH2	16:U:26:GLU:OE2	2.52	0.42
22:0:74:ARG:NH1	22:0:236:GLU:O	2.52	0.42
22:0:216:PRO:HA	22:0:219:ALA:HB3	2.00	0.42
22:0:228:LYS:HZ3	22:0:452:ARG:HH11	1.68	0.42
23:1:281:PRO:HA	23:1:284:TRP:CE2	2.54	0.42
23:1:291:LYS:NZ	23:1:306:ARG:O	2.51	0.42
23:1:620:LEU:HA	23:1:623:ILE:HB	2.01	0.42
25:6:301:PHE:O	25:6:305:VAL:HG23	2.19	0.42
25:6:451:CYS:HB3	25:6:454:CYS:SG	2.59	0.42
2:A:62:ASP:OD1	2:A:62:ASP:N	2.52	0.42
2:A:315:LEU:HB2	2:A:321:PRO:HA	2.01	0.42
2:A:381:THR:HG1	2:A:384:ASN:H	1.67	0.42
2:A:440:ASP:H	2:A:460:VAL:HG12	1.83	0.42
2:A:954:TRP:HE3	2:A:955:PRO:HD2	1.84	0.42
3:B:29:ASP:HB3	3:B:658:ILE:HD13	2.02	0.42
3:B:400:HIS:CE1	3:B:402:GLY:H	2.38	0.42
9:J:45:CYS:SG	9:J:46:CYS:N	2.93	0.42
14:S:169:GLN:HG3	14:S:172:LEU:HD22	2.00	0.42
18:W:198:THR:HG23	18:W:201:ILE:HD12	2.01	0.42
18:W:352:GLU:HG2	23:1:192:MET:SD	2.60	0.42
22:0:72:CYS:HB2	22:0:234:PHE:HA	2.00	0.42
22:0:254:THR:OG1	22:0:432:ASN:OD1	2.32	0.42
22:0:632:SER:HB3	22:0:635:LEU:HB3	2.01	0.42
24:4:158:THR:HG22	25:6:443:PHE:HE2	1.83	0.42
26:7:190:THR:HG23	26:7:213:ILE:HG22	2.01	0.42
1:M:127:GLN:HA	1:M:130:PHE:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:768:GLN:OE1	2:A:816:HIS:ND1	2.40	0.42
3:B:365:THR:HG21	3:B:370:PHE:HB2	2.00	0.42
3:B:448:ILE:HD12	3:B:448:ILE:HA	1.79	0.42
8:I:111:THR:OG1	8:I:112:SER:N	2.52	0.42
13:P:66:ARG:HD3	13:P:66:ARG:HA	1.84	0.42
15:O:79:ARG:HH21	15:O:117:ALA:HB1	1.83	0.42
20:D:173:HIS:CD2	20:D:176:GLU:H	2.38	0.42
27:2:407:GLN:OE1	27:2:410:ARG:NH2	2.53	0.42
1:M:131:ALA:O	1:M:135:MET:HG2	2.19	0.42
2:A:120:GLU:OE1	2:A:123:ARG:NH1	2.53	0.42
2:A:807:GLY:HA3	3:B:728:ARG:NH2	2.35	0.42
2:A:1325:THR:OG1	2:A:1326:ARG:N	2.53	0.42
8:I:65:ASP:HA	8:I:66:PRO:HD3	1.92	0.42
17:V:63:LYS:HZ1	17:V:86:THR:HG22	1.85	0.42
24:4:272:PHE:HB2	25:6:372:LEU:HD22	2.02	0.42
28:5:44:PRO:HA	28:5:47:VAL:HG13	2.01	0.42
1:M:137:CYS:HB2	1:M:142:LEU:HB2	2.00	0.42
2:A:851:HIS:CE1	6:F:139:PRO:HG3	2.55	0.42
2:A:1319:VAL:HG23	2:A:1322:ILE:HG13	2.02	0.42
3:B:103:ASN:HB3	3:B:109:THR:HA	2.02	0.42
3:B:604:ARG:NH2	3:B:614:SER:HA	2.35	0.42
4:C:260:LEU:HA	4:C:263:THR:HG22	2.01	0.42
7:H:63:LEU:HB3	7:H:89:LEU:HB3	2.01	0.42
12:Q:390:ASP:OD1	12:Q:391:LYS:N	2.51	0.42
22:0:182:LEU:HD23	22:0:182:LEU:HA	1.95	0.42
24:4:154:SER:OG	25:6:450:ASN:ND2	2.36	0.42
26:7:157:LEU:HD23	26:7:157:LEU:HA	1.89	0.42
26:7:490:VAL:H	26:7:514:THR:HB	1.84	0.42
27:2:59:LEU:HB2	27:2:96:LEU:HB3	2.00	0.42
27:2:185:THR:OG1	27:2:188:GLY:N	2.47	0.42
2:A:269:ILE:HD13	2:A:269:ILE:HA	1.92	0.42
2:A:361:LEU:HB3	2:A:507:VAL:HG21	2.02	0.42
2:A:368:LYS:HD3	10:K:3:ALA:HA	2.00	0.42
3:B:183:GLU:N	3:B:183:GLU:OE1	2.53	0.42
3:B:334:ILE:HB	3:B:347:LYS:HE2	2.00	0.42
3:B:1024:ALA:HA	3:B:1027:ILE:HG22	2.01	0.42
3:B:1196:ILE:HD12	3:B:1196:ILE:HA	1.85	0.42
7:H:129:TYR:CZ	7:H:130:ARG:HD2	2.53	0.42
9:J:48:ARG:O	9:J:52:THR:HG22	2.20	0.42
14:S:278:LYS:HD2	14:S:301:ALA:HB2	2.01	0.42
22:0:425:ILE:HB	22:0:428:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:1:421:ILE:HG22	23:1:423:ASP:H	1.84	0.42
26:7:516:THR:HB	26:7:518:VAL:HG12	2.01	0.42
27:2:124:VAL:HA	27:2:237:TYR:HD2	1.85	0.42
2:A:451:HIS:HA	2:A:1070:GLN:HB3	2.02	0.42
3:B:129:PHE:HA	3:B:167:ILE:HG23	2.02	0.42
3:B:424:LEU:HD13	3:B:449:ASN:HB3	2.02	0.42
3:B:802:PRO:HB3	3:B:1091:TYR:CG	2.55	0.42
7:H:58:THR:HB	7:H:143:LEU:HB2	2.02	0.42
12:Q:408:GLU:HA	12:Q:411:LYS:HE2	2.02	0.42
13:P:86:ASN:OD1	13:P:90:GLN:NE2	2.53	0.42
14:S:288:SER:OG	14:S:289:ALA:N	2.53	0.42
18:W:123:MET:N	18:W:157:VAL:O	2.42	0.42
26:7:439:THR:OG1	26:7:440:SER:N	2.51	0.42
27:2:26:TYR:OH	27:2:84:LEU:O	2.27	0.42
27:2:29:PRO:HD2	27:2:118:GLN:HE22	1.85	0.42
27:2:59:LEU:HA	27:2:62:LEU:HD12	2.02	0.42
27:2:229:GLY:O	27:2:279:THR:OG1	2.33	0.42
29:N:-5:DT:H6	29:N:-5:DT:H2'	1.66	0.42
1:M:177:LEU:HD13	1:M:192:ILE:HD11	2.02	0.41
2:A:23:SER:HA	2:A:233:TRP:CD1	2.55	0.41
2:A:117:GLU:H	2:A:122:MET:HE3	1.85	0.41
2:A:372:LYS:HD2	10:K:2:ASN:HB2	2.02	0.41
2:A:1116:LEU:HD23	2:A:1311:VAL:HA	2.02	0.41
3:B:433:GLN:H	3:B:433:GLN:HG3	1.70	0.41
21:G:13:LEU:HD21	21:G:17:PHE:HB2	2.02	0.41
22:0:241:ASP:OD1	22:0:242:ASN:N	2.53	0.41
22:0:352:ILE:O	22:0:420:ILE:N	2.39	0.41
22:0:622:MET:HB3	22:0:681:LEU:HD13	2.02	0.41
23:1:336:ILE:HG23	23:1:337:ILE:HD12	2.02	0.41
25:6:432:CYS:O	25:6:434:GLN:NE2	2.47	0.41
26:7:710:SER:N	26:7:715:GLU:OE1	2.53	0.41
26:7:748:LEU:HD23	26:7:748:LEU:HA	1.88	0.41
2:A:956:LEU:HD23	2:A:956:LEU:HA	1.90	0.41
3:B:216:GLU:HB3	3:B:406:LEU:HD13	2.02	0.41
3:B:528:PRO:HG3	3:B:536:VAL:HB	2.02	0.41
13:P:96:ARG:HB2	13:P:107:LEU:HD11	2.02	0.41
14:S:159:VAL:HG23	14:S:160:LEU:HD12	2.02	0.41
15:O:93:GLU:HA	17:V:71:PHE:HD2	1.85	0.41
19:X:214:TRP:HB3	19:X:217:CYS:HB3	2.02	0.41
19:X:218:ASP:HB3	19:X:241:PRO:HG3	2.02	0.41
22:0:21:GLN:NE2	22:0:47:GLY:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:0:487:LEU:HD11	22:0:490:LYS:HA	2.02	0.41
28:5:33:GLU:HG3	28:5:41:LEU:HB3	2.01	0.41
1:M:145:ILE:HD12	3:B:865:LYS:HB2	2.02	0.41
2:A:33:ALA:HA	2:A:57:ARG:HH21	1.85	0.41
2:A:808:LEU:N	3:B:728:ARG:HH12	2.18	0.41
2:A:1227:ILE:HB	2:A:1239:ARG:HB2	2.01	0.41
3:B:649:LYS:HZ3	3:B:737:THR:HA	1.85	0.41
3:B:790:ASP:OD1	3:B:791:THR:N	2.49	0.41
12:Q:371:ASP:O	13:P:82:ARG:NH1	2.53	0.41
22:0:538:VAL:HG22	22:0:598:LEU:HB2	2.02	0.41
25:6:404:PHE:HB3	25:6:436:PHE:CD2	2.56	0.41
2:A:121:LEU:O	2:A:124:GLN:NE2	2.53	0.41
2:A:1313:LEU:HD23	2:A:1313:LEU:HA	1.87	0.41
3:B:284:ILE:H	3:B:284:ILE:HG13	1.60	0.41
3:B:809:MET:SD	3:B:809:MET:N	2.93	0.41
3:B:949:VAL:HA	3:B:968:VAL:HA	2.03	0.41
3:B:969:ARG:NH2	4:C:60:ASP:H	2.18	0.41
4:C:64:ALA:HB1	11:L:69:ALA:HB2	2.03	0.41
13:P:326:GLU:O	13:P:330:LYS:N	2.47	0.41
18:W:92:PRO:HD3	18:W:196:GLU:HA	2.01	0.41
22:0:380:ARG:NH2	22:0:380:ARG:O	2.53	0.41
22:0:493:LEU:HB3	22:0:678:VAL:HA	2.03	0.41
26:7:105:VAL:HA	26:7:106:PRO:HD3	1.90	0.41
26:7:593:PHE:HB2	26:7:745:ILE:HG21	2.02	0.41
29:N:12:DG:N2	30:T:-11:DC:O2	2.53	0.41
2:A:356:ASP:HB2	2:A:469:ARG:HD2	2.01	0.41
2:A:590:ARG:HH22	2:A:620:LYS:HB3	1.84	0.41
3:B:67:SER:HG	3:B:92:PHE:H	1.63	0.41
3:B:360:PHE:CE2	3:B:374:LYS:HD2	2.56	0.41
3:B:615:MET:SD	3:B:615:MET:N	2.94	0.41
4:C:77:ILE:HG13	4:C:161:LYS:HE3	2.03	0.41
4:C:84:ARG:HD2	10:K:11:LEU:HD21	2.02	0.41
4:C:211:ASP:OD1	4:C:211:ASP:N	2.53	0.41
12:Q:118:LEU:HB3	12:Q:392:VAL:HG13	2.03	0.41
12:Q:120:LYS:HD3	13:P:132:GLU:HG2	2.03	0.41
17:V:23:LEU:HD23	17:V:23:LEU:HA	1.91	0.41
24:4:78:ALA:HB2	24:4:152:ALA:HB2	2.02	0.41
25:6:148:MET:O	25:6:152:TYR:HB2	2.20	0.41
27:2:239:ILE:HA	27:2:269:PHE:HE1	1.84	0.41
2:A:566:ILE:HD13	7:H:96:VAL:HG22	2.03	0.41
2:A:1107:VAL:HA	2:A:1108:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1116:LEU:HG	2:A:1308:THR:HG21	2.03	0.41
2:A:1342:GLU:HG3	5:E:198:ILE:HD13	2.02	0.41
3:B:31:TRP:CD2	3:B:807:ARG:HG2	2.55	0.41
3:B:604:ARG:NH1	3:B:691:GLU:OE2	2.53	0.41
4:C:70:ILE:HD13	4:C:70:ILE:HA	1.95	0.41
15:O:105:ARG:HG2	15:O:112:THR:HG23	2.01	0.41
22:0:116:LEU:N	33:0:801:SF4:S3	2.94	0.41
24:4:278:LEU:HG	24:4:279:THR:HG23	2.03	0.41
25:6:140:ASP:OD1	25:6:140:ASP:N	2.52	0.41
25:6:186:SER:HB3	25:6:192:HIS:CE1	2.55	0.41
26:7:491:HIS:ND1	26:7:514:THR:OG1	2.41	0.41
2:A:187:LYS:HZ3	2:A:189:ARG:HD2	1.85	0.41
2:A:1151:GLU:HG2	8:I:45:ARG:HD2	2.02	0.41
3:B:334:ILE:HG13	3:B:335:GLY:H	1.86	0.41
3:B:617:ARG:NE	3:B:619:ILE:HD13	2.35	0.41
3:B:798:TYR:OH	4:C:66:ARG:NH2	2.53	0.41
12:Q:381:ASP:OD1	12:Q:381:ASP:N	2.53	0.41
14:S:214:LEU:HD12	14:S:217:LYS:HD3	2.03	0.41
15:O:200:PRO:HG2	15:O:202:ILE:HD12	2.03	0.41
17:V:8:GLU:HA	17:V:11:ARG:HH12	1.85	0.41
18:W:62:ARG:HA	18:W:62:ARG:HD3	1.90	0.41
18:W:176:MET:HA	18:W:179:ILE:HG22	2.03	0.41
20:D:31:GLN:O	20:D:34:GLN:NE2	2.54	0.41
22:0:367:THR:OG1	22:0:368:PHE:N	2.53	0.41
24:4:248:LEU:HD23	24:4:252:MET:HG3	2.03	0.41
24:4:289:CYS:O	24:4:293:LEU:N	2.39	0.41
25:6:189:PRO:HA	25:6:192:HIS:CD2	2.55	0.41
25:6:410:PHE:CG	25:6:426:ARG:HG2	2.55	0.41
27:2:142:LYS:O	27:2:145:THR:OG1	2.33	0.41
27:2:472:SER:HA	27:2:475:ALA:HB3	2.03	0.41
27:2:488:LYS:HG2	27:2:490:LYS:HE3	2.03	0.41
29:N:34:DC:H2"	29:N:35:DG:N7	2.35	0.41
3:B:259:TYR:HE1	3:B:270:LYS:HD2	1.85	0.41
6:F:82:THR:HA	6:F:83:PRO:HD3	1.93	0.41
22:0:74:ARG:HG2	22:0:210:TYR:CE2	2.56	0.41
29:N:35:DG:H22	30:T:-35:DC:H42	1.68	0.41
2:A:4:GLN:O	3:B:1159:ARG:NH2	2.44	0.41
2:A:40:THR:HG22	2:A:53:LEU:HB2	2.02	0.41
2:A:169:ASN:OD1	2:A:170:THR:N	2.52	0.41
2:A:467:THR:OG1	2:A:468:PHE:N	2.54	0.41
2:A:867:ILE:HG23	2:A:870:GLU:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:886:ILE:O	2:A:944:ARG:NH2	2.54	0.41
2:A:963:ILE:HA	2:A:966:ASN:HD21	1.86	0.41
2:A:1054:LEU:HB3	6:F:84:TYR:CE1	2.56	0.41
3:B:72:GLU:HB3	3:B:87:LYS:HA	2.03	0.41
3:B:190:TYR:CE1	9:J:62:ARG:HG3	2.55	0.41
3:B:194:GLU:N	3:B:194:GLU:OE1	2.53	0.41
3:B:336:ARG:HH12	3:B:341:LEU:H	1.67	0.41
3:B:570:VAL:HG13	3:B:573:GLN:HB2	2.03	0.41
3:B:1057:LYS:HA	3:B:1057:LYS:HD2	1.91	0.41
7:H:13:SER:OG	7:H:14:GLU:N	2.54	0.41
10:K:20:LYS:O	10:K:34:THR:OG1	2.35	0.41
12:Q:126:LYS:HA	13:P:131:ASN:HD21	1.86	0.41
13:P:84:ARG:NH2	13:P:87:LEU:O	2.47	0.41
14:S:184:LYS:NZ	14:S:195:TYR:O	2.35	0.41
20:D:39:ASN:HB2	20:D:45:GLU:HB2	2.01	0.41
20:D:40:HIS:CG	21:G:73:LYS:HD2	2.56	0.41
21:G:1:MET:N	21:G:80:LYS:O	2.40	0.41
22:0:95:LYS:HE3	22:0:95:LYS:HB3	1.95	0.41
22:0:236:GLU:OE1	22:0:461:GLY:N	2.51	0.41
26:7:328:LYS:HB2	26:7:529:PHE:CG	2.56	0.41
26:7:552:VAL:HG22	26:7:703:ALA:HB3	2.03	0.41
27:2:5:SER:O	27:2:9:SER:N	2.47	0.41
27:2:131:SER:HB2	27:2:135:LEU:HD22	2.03	0.41
29:N:38:DG:H2"	29:N:39:DA:N7	2.36	0.41
1:M:278:ALA:O	1:M:282:ILE:HD12	2.21	0.41
2:A:805:LEU:HA	2:A:805:LEU:HD12	1.87	0.41
2:A:943:LEU:HA	2:A:946:VAL:HG22	2.02	0.41
4:C:239:PRO:HB2	4:C:242:GLN:HG2	2.03	0.41
22:0:172:PRO:HG2	22:0:176:PHE:HZ	1.86	0.41
22:0:371:ARG:NE	22:0:410:SER:O	2.54	0.41
23:1:444:LYS:HA	23:1:444:LYS:HD2	1.88	0.41
26:7:242:LEU:HD21	26:7:314:HIS:HB2	2.03	0.41
26:7:710:SER:O	26:7:713:THR:OG1	2.38	0.41
29:N:5:DT:H6	29:N:5:DT:H2'	1.64	0.41
2:A:118:HIS:HA	2:A:123:ARG:NH2	2.36	0.40
2:A:251:SER:O	2:A:253:ASN:N	2.52	0.40
2:A:889:SER:HA	2:A:1297:GLU:HG3	2.02	0.40
2:A:999:VAL:H	2:A:1011:GLN:NE2	2.19	0.40
6:F:92:ARG:HD2	6:F:92:ARG:HA	1.82	0.40
7:H:97:MET:HG3	7:H:118:PHE:CD1	2.56	0.40
12:Q:25:ASP:OD1	12:Q:25:ASP:N	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:P:112:ASP:OD1	13:P:112:ASP:N	2.52	0.40
14:S:169:GLN:HG2	14:S:173:HIS:CE1	2.56	0.40
14:S:184:LYS:HA	14:S:228:LEU:HD12	2.03	0.40
14:S:210:ASN:HA	14:S:211:ASN:HA	1.61	0.40
19:X:124:ASP:OD1	19:X:124:ASP:N	2.54	0.40
22:0:39:ILE:HG13	22:0:477:THR:HG21	2.03	0.40
22:0:97:LEU:HB3	22:0:99:TYR:CE1	2.56	0.40
22:0:192:PRO:HA	22:0:195:ILE:HB	2.02	0.40
22:0:628:GLN:HG3	22:0:635:LEU:HD22	2.03	0.40
23:1:542:LEU:HG	23:1:608:MET:HE2	2.02	0.40
26:7:222:LYS:HD2	26:7:241:ILE:HD11	2.02	0.40
26:7:568:GLU:HG3	26:7:580:LEU:HD21	2.02	0.40
27:2:483:TRP:HB3	27:2:492:PHE:HB3	2.03	0.40
2:A:59:GLY:HA2	2:A:80:HIS:HD2	1.85	0.40
2:A:268:ASP:OD2	2:A:299:HIS:ND1	2.55	0.40
2:A:550:LEU:HD12	2:A:550:LEU:HA	1.80	0.40
2:A:779:PHE:CZ	3:B:517:THR:HA	2.56	0.40
2:A:850:VAL:HG13	2:A:1061:GLY:H	1.86	0.40
2:A:868:TYR:CE1	2:A:1064:VAL:HG11	2.56	0.40
2:A:977:LYS:HA	2:A:977:LYS:HD3	1.81	0.40
3:B:848:ARG:NH2	9:J:11:GLY:HA3	2.36	0.40
5:E:156:LEU:HD12	5:E:160:GLU:HB3	2.02	0.40
7:H:125:LEU:HD12	7:H:125:LEU:HA	1.87	0.40
19:X:134:TYR:HD1	19:X:137:LYS:HD3	1.85	0.40
22:0:555:GLN:HB2	22:0:560:LEU:HD12	2.03	0.40
22:0:649:ARG:HB2	22:0:652:ASP:HB2	2.03	0.40
26:7:409:VAL:HB	26:7:454:VAL:HG23	2.03	0.40
27:2:28:SER:HA	27:2:29:PRO:HD3	1.98	0.40
27:2:345:PHE:HD2	27:2:378:ILE:HB	1.87	0.40
2:A:113:LEU:HD21	2:A:218:ASP:HB3	2.02	0.40
2:A:305:ASP:OD1	2:A:326:ARG:N	2.42	0.40
2:A:1200:ALA:HB2	14:S:248:ILE:HD12	2.04	0.40
3:B:22:SER:H	3:B:22:SER:HG	1.61	0.40
3:B:413:LEU:O	3:B:417:PHE:HB2	2.21	0.40
3:B:808:ALA:O	3:B:811:TYR:N	2.52	0.40
6:F:97:ARG:HA	6:F:97:ARG:HD2	1.81	0.40
15:O:133:LYS:HB3	15:O:137:ARG:NH1	2.36	0.40
26:7:133:TRP:HB2	26:7:142:ILE:HB	2.03	0.40
26:7:680:ARG:HG3	26:7:722:ARG:HA	2.02	0.40
30:T:-3:DA:H2'	30:T:-2:DT:C6	2.56	0.40
2:A:934:LYS:HA	2:A:937:VAL:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:956:LEU:HD22	2:A:957:PRO:HD2	2.04	0.40
4:C:240:VAL:HA	4:C:243:VAL:HG22	2.02	0.40
7:H:27:GLU:HA	7:H:39:THR:HA	2.03	0.40
8:I:28:GLU:HB3	8:I:35:VAL:HG23	2.03	0.40
8:I:103:CYS:SG	8:I:105:SER:N	2.94	0.40
10:K:41:THR:OG1	10:K:42:LEU:N	2.54	0.40
15:O:109:PRO:HB2	15:O:111:THR:HG23	2.04	0.40
16:U:31:ASP:O	16:U:34:THR:OG1	2.34	0.40
22:0:323:GLY:HA2	22:0:326:ARG:HB2	2.03	0.40
22:0:464:SER:HA	22:0:465:PRO:HA	1.85	0.40
22:0:495:MET:HA	22:0:705:ASP:HB3	2.03	0.40
22:0:609:GLY:H	22:0:668:ARG:HH12	1.70	0.40
23:1:279:LYS:O	23:1:283:PHE:CB	2.69	0.40
24:4:211:ASP:OD1	24:4:234:VAL:N	2.51	0.40
25:6:199:ILE:HA	25:6:202:GLN:HG2	2.04	0.40
26:7:162:GLU:N	26:7:174:LYS:O	2.47	0.40
30:T:-54:DT:H2"	30:T:-53:DA:O4'	2.22	0.40
2:A:1056:SER:O	2:A:1056:SER:OG	2.40	0.40
3:B:390:LEU:HD23	3:B:392:ARG:HE	1.87	0.40
7:H:5:LEU:HB2	7:H:59:ILE:HG21	2.02	0.40
7:H:24:CYS:HB2	7:H:44:VAL:HB	2.03	0.40
20:D:56:ARG:HH12	20:D:155:ARG:HA	1.86	0.40
23:1:291:LYS:HG2	23:1:301:ILE:HD11	2.04	0.40
24:4:285:VAL:HG23	25:6:323:GLY:HA3	2.04	0.40
28:5:48:GLU:HA	28:5:51:LYS:HB2	2.03	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	M	273/345 (79%)	239 (88%)	34 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	1417/1733 (82%)	1240 (88%)	177 (12%)	0	100	100
3	B	1150/1224 (94%)	990 (86%)	158 (14%)	2 (0%)	44	77
4	C	263/318 (83%)	225 (86%)	38 (14%)	0	100	100
5	E	212/215 (99%)	193 (91%)	19 (9%)	0	100	100
6	F	85/155 (55%)	76 (89%)	9 (11%)	0	100	100
7	H	129/146 (88%)	108 (84%)	21 (16%)	0	100	100
8	I	112/122 (92%)	98 (88%)	14 (12%)	0	100	100
9	J	64/70 (91%)	53 (83%)	11 (17%)	0	100	100
10	K	113/120 (94%)	106 (94%)	7 (6%)	0	100	100
11	L	42/70 (60%)	31 (74%)	11 (26%)	0	100	100
12	Q	208/735 (28%)	201 (97%)	7 (3%)	0	100	100
13	P	173/400 (43%)	163 (94%)	10 (6%)	0	100	100
14	S	162/309 (52%)	143 (88%)	18 (11%)	1 (1%)	22	59
15	O	179/240 (75%)	168 (94%)	11 (6%)	0	100	100
16	U	101/286 (35%)	96 (95%)	5 (5%)	0	100	100
17	V	100/122 (82%)	99 (99%)	1 (1%)	0	100	100
18	W	241/482 (50%)	229 (95%)	12 (5%)	0	100	100
19	X	158/328 (48%)	147 (93%)	11 (7%)	0	100	100
20	D	164/221 (74%)	159 (97%)	5 (3%)	0	100	100
21	G	169/171 (99%)	155 (92%)	14 (8%)	0	100	100
22	0	750/778 (96%)	709 (94%)	41 (6%)	0	100	100
23	1	407/642 (63%)	393 (97%)	14 (3%)	0	100	100
24	4	286/338 (85%)	276 (96%)	10 (4%)	0	100	100
25	6	351/461 (76%)	337 (96%)	14 (4%)	0	100	100
26	7	604/843 (72%)	564 (93%)	40 (7%)	0	100	100
27	2	435/513 (85%)	412 (95%)	23 (5%)	0	100	100
28	5	64/72 (89%)	56 (88%)	8 (12%)	0	100	100
All	All	8412/11459 (73%)	7666 (91%)	743 (9%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	364	ILE

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Mol	Chain	Res	Type
3	B	363	HIS
14	S	167	PRO

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	M	245/299 (82%)	244 (100%)	1 (0%)	89 91
2	A	1235/1520 (81%)	1232 (100%)	3 (0%)	92 94
3	B	1000/1061 (94%)	997 (100%)	3 (0%)	91 92
4	C	233/274 (85%)	231 (99%)	2 (1%)	75 83
5	E	196/197 (100%)	196 (100%)	0	100 100
6	F	77/137 (56%)	77 (100%)	0	100 100
7	H	118/128 (92%)	116 (98%)	2 (2%)	56 72
8	I	108/116 (93%)	108 (100%)	0	100 100
9	J	61/65 (94%)	61 (100%)	0	100 100
10	K	99/102 (97%)	99 (100%)	0	100 100
11	L	39/57 (68%)	39 (100%)	0	100 100
12	Q	147/641 (23%)	143 (97%)	4 (3%)	40 61
13	P	166/363 (46%)	166 (100%)	0	100 100
14	S	141/274 (52%)	140 (99%)	1 (1%)	81 86
15	O	153/205 (75%)	153 (100%)	0	100 100
16	U	99/260 (38%)	96 (97%)	3 (3%)	36 57
17	V	94/108 (87%)	93 (99%)	1 (1%)	70 80
18	W	224/429 (52%)	223 (100%)	1 (0%)	89 91
19	X	144/295 (49%)	142 (99%)	2 (1%)	62 76
20	D	146/200 (73%)	146 (100%)	0	100 100
21	G	151/152 (99%)	151 (100%)	0	100 100
22	0	684/707 (97%)	684 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	1	389/589 (66%)	387 (100%)	2 (0%)	86 90
24	4	259/300 (86%)	259 (100%)	0	100 100
25	6	322/418 (77%)	322 (100%)	0	100 100
26	7	540/737 (73%)	537 (99%)	3 (1%)	84 88
27	2	394/468 (84%)	392 (100%)	2 (0%)	86 90
28	5	53/66 (80%)	53 (100%)	0	100 100
All	All	7517/10168 (74%)	7487 (100%)	30 (0%)	88 91

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	300	GLN
2	A	68	GLN
2	A	88	LYS
2	A	619	LYS
3	B	310	MET
3	B	476	ARG
3	B	884	ARG
4	C	116	LYS
4	C	205	LYS
7	H	77	ARG
7	H	130	ARG
12	Q	24	ARG
12	Q	29	ARG
12	Q	330	ARG
12	Q	333	LYS
14	S	234	LYS
16	U	44	LYS
16	U	50	LYS
16	U	257	ARG
17	V	46	LYS
18	W	351	ARG
19	X	155	LYS
19	X	208	LYS
23	1	306	ARG
23	1	353	ARG
26	7	344	ARG
26	7	348	ARG
26	7	754	ARG
27	2	419	LYS

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Mol	Chain	Res	Type
27	2	450	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	45	GLN
2	A	445	ASN
2	A	966	ASN
2	A	1330	ASN
9	J	23	ASN
13	P	90	GLN
14	S	183	ASN
16	U	36	GLN
20	D	138	ASN
20	D	173	HIS
24	4	71	ASN
25	6	163	GLN
26	7	589	GLN
26	7	672	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 17 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
33	SF4	0	801	22	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	SF4	0	801	22	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	0	801	SF4	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

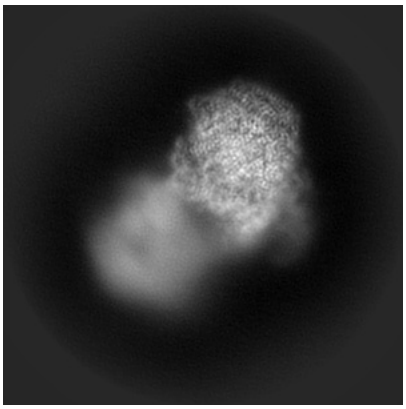
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42379. These allow visual inspection of the internal detail of the map and identification of artifacts.

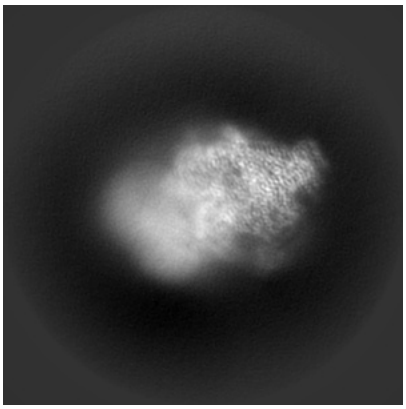
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

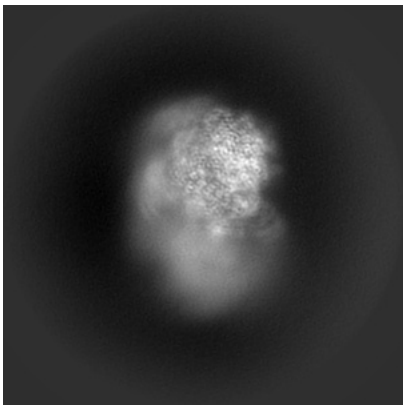
6.1.1 Primary map



X

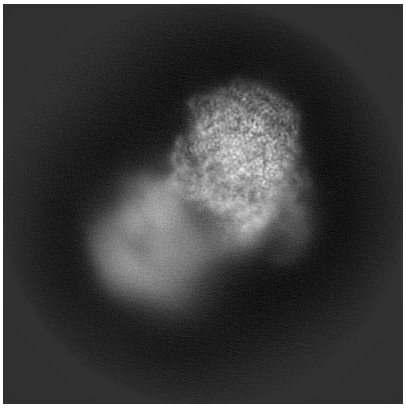


Y

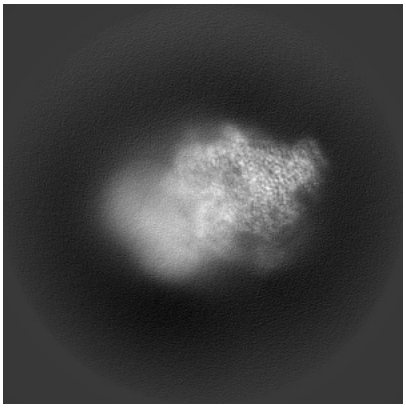


Z

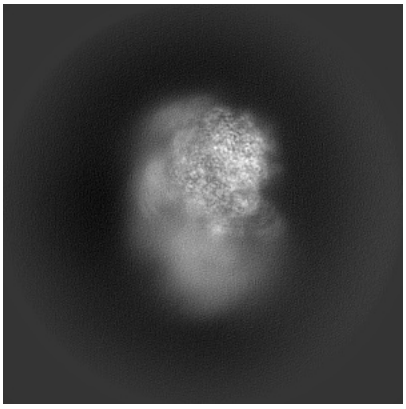
6.1.2 Raw map



X



Y

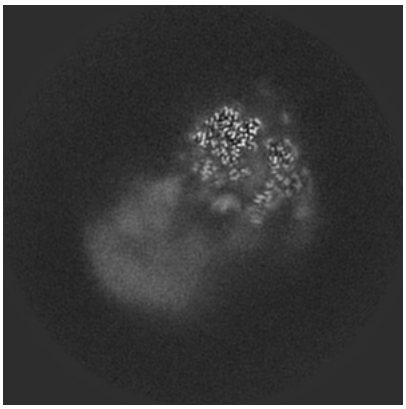


Z

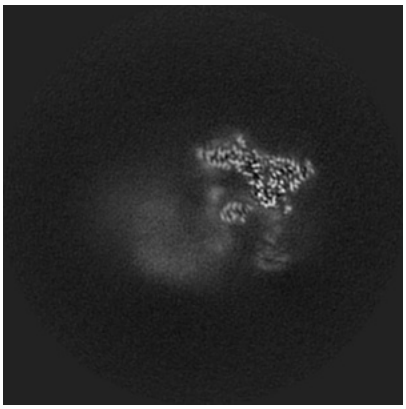
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

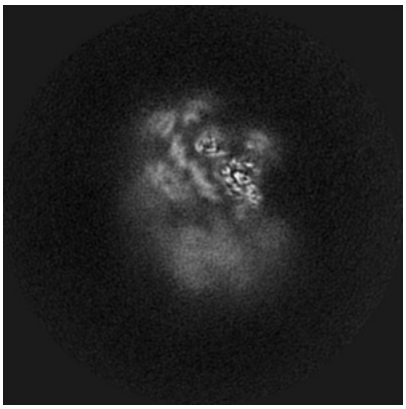
6.2.1 Primary map



X Index: 192

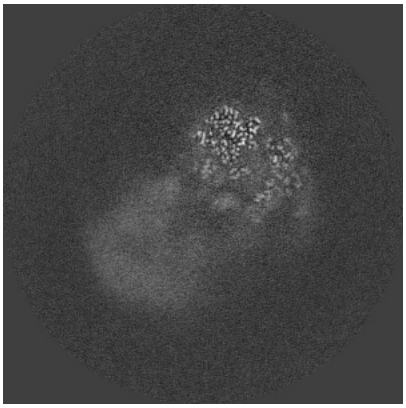


Y Index: 192

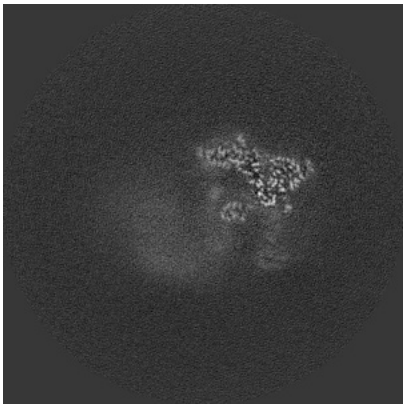


Z Index: 192

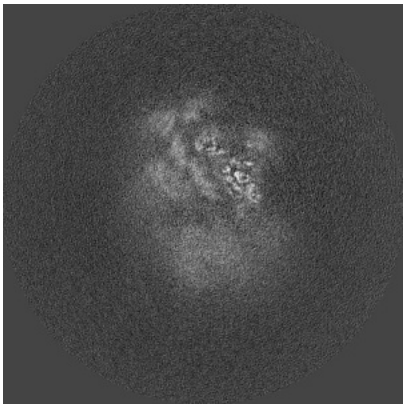
6.2.2 Raw map



X Index: 192



Y Index: 192

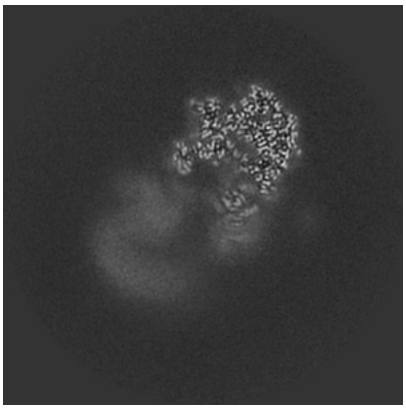


Z Index: 192

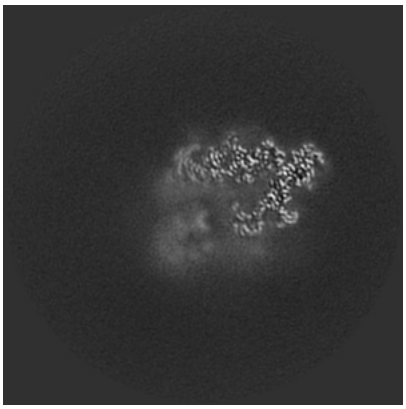
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

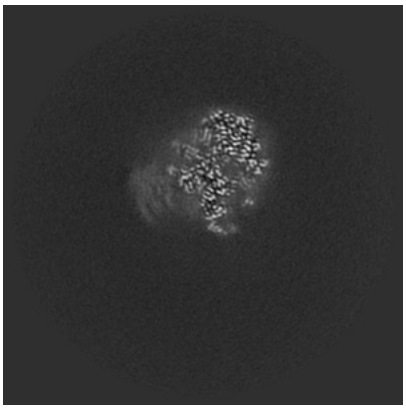
6.3.1 Primary map



X Index: 215

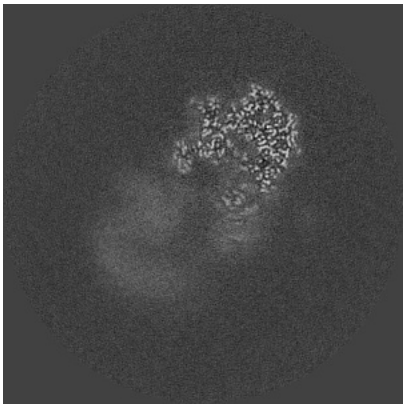


Y Index: 232

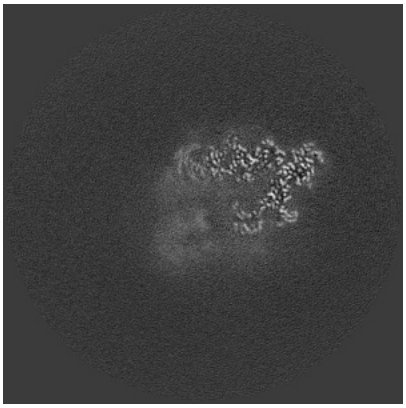


Z Index: 253

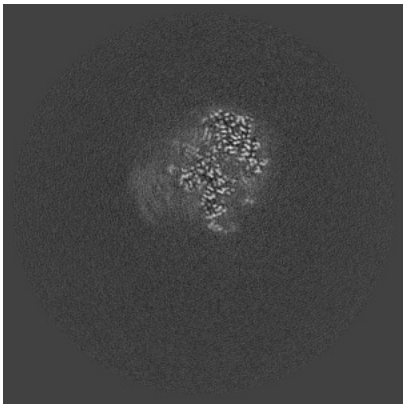
6.3.2 Raw map



X Index: 215



Y Index: 232

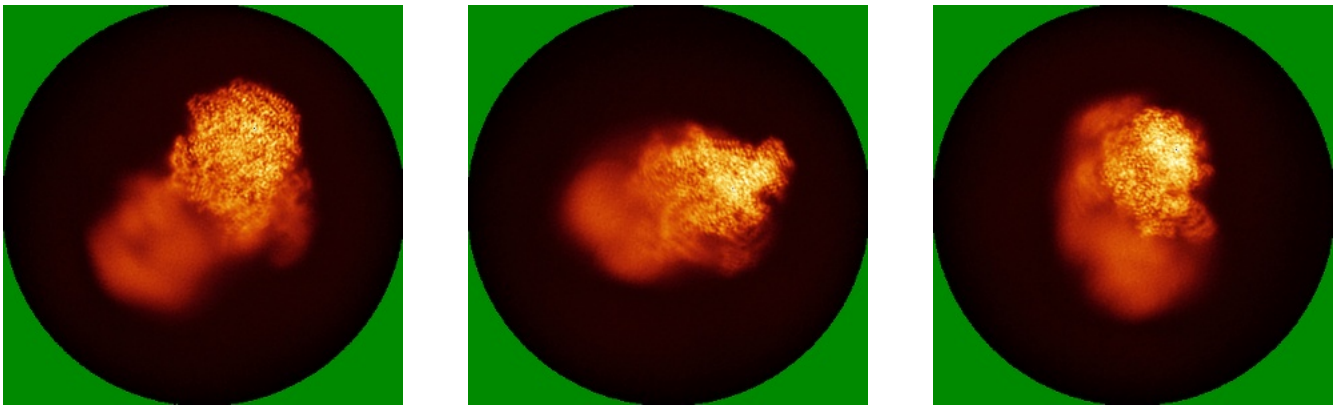


Z Index: 253

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

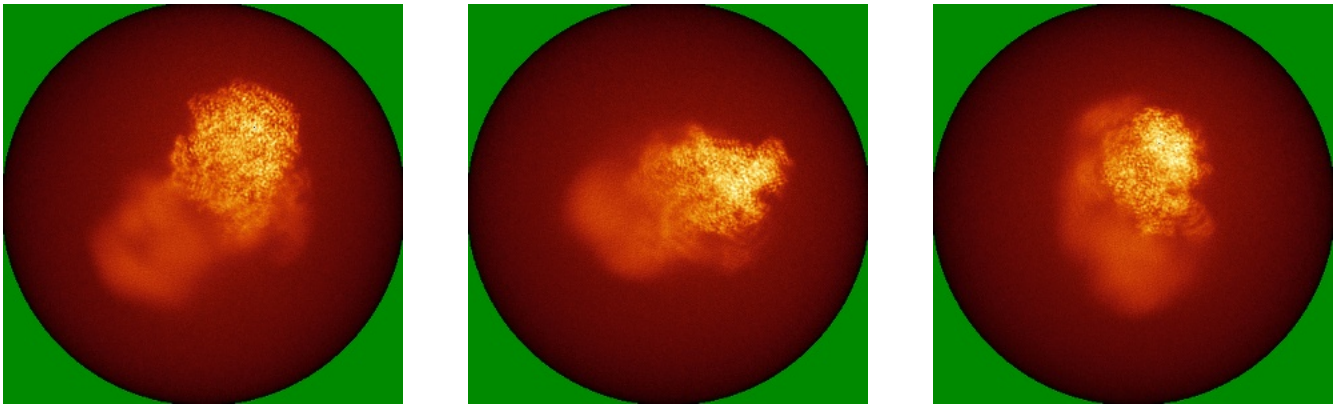
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw 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.

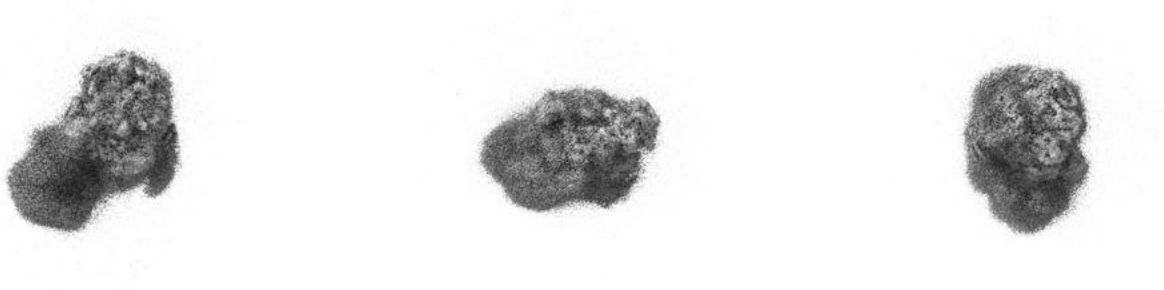
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0098. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

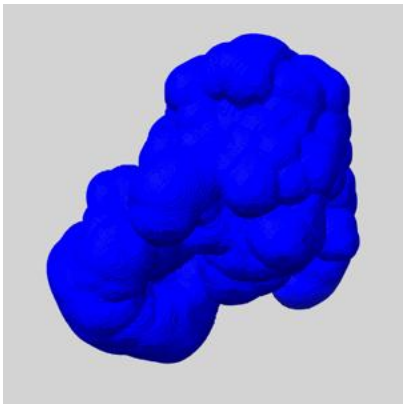
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

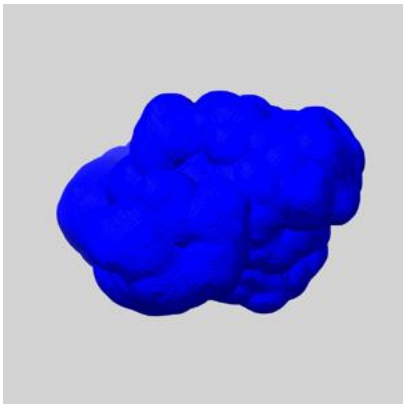
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

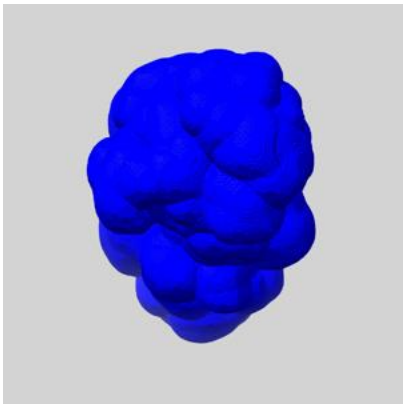
6.6.1 emd_42379_msk_1.map



X



Y

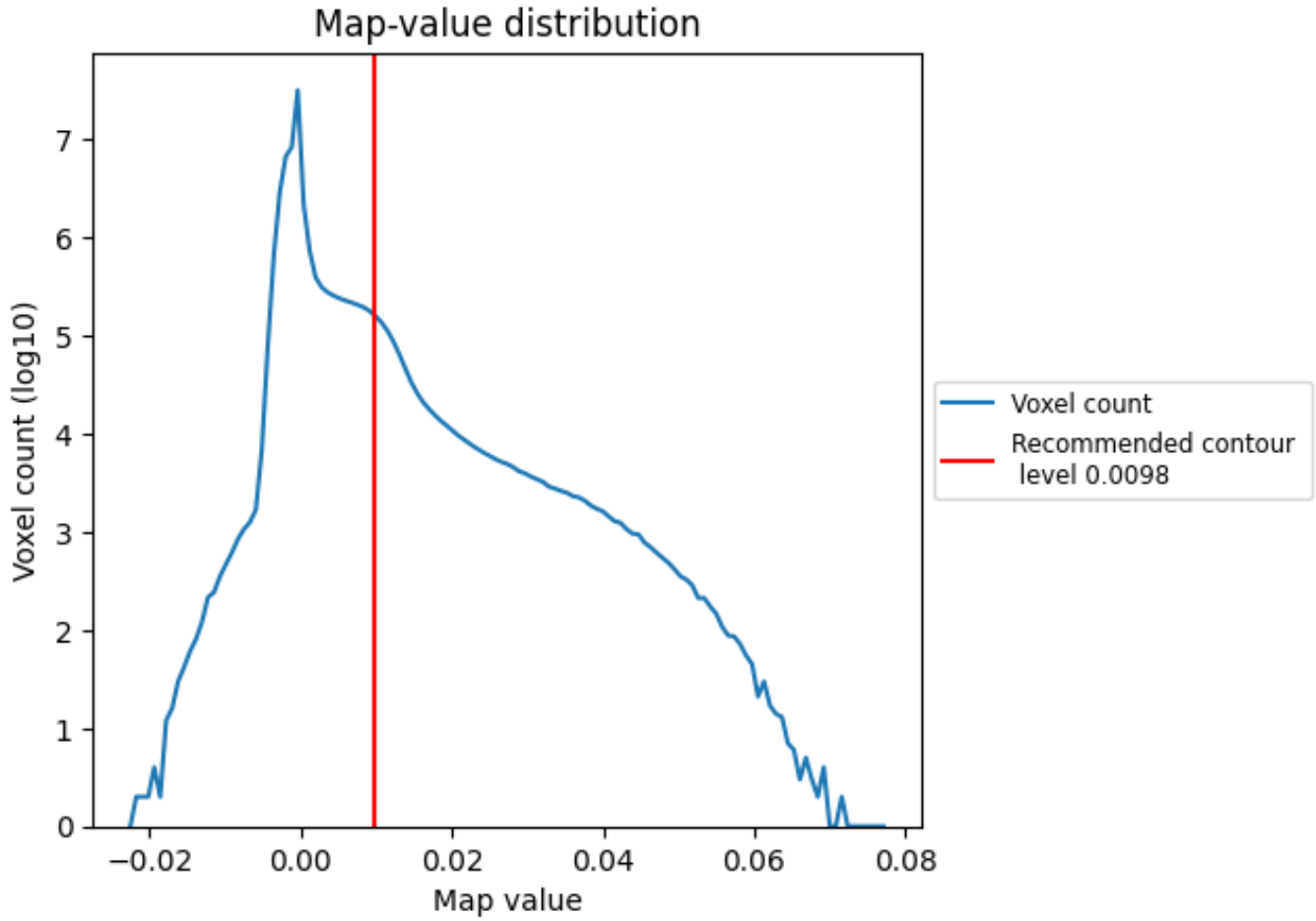


Z

7 Map analysis

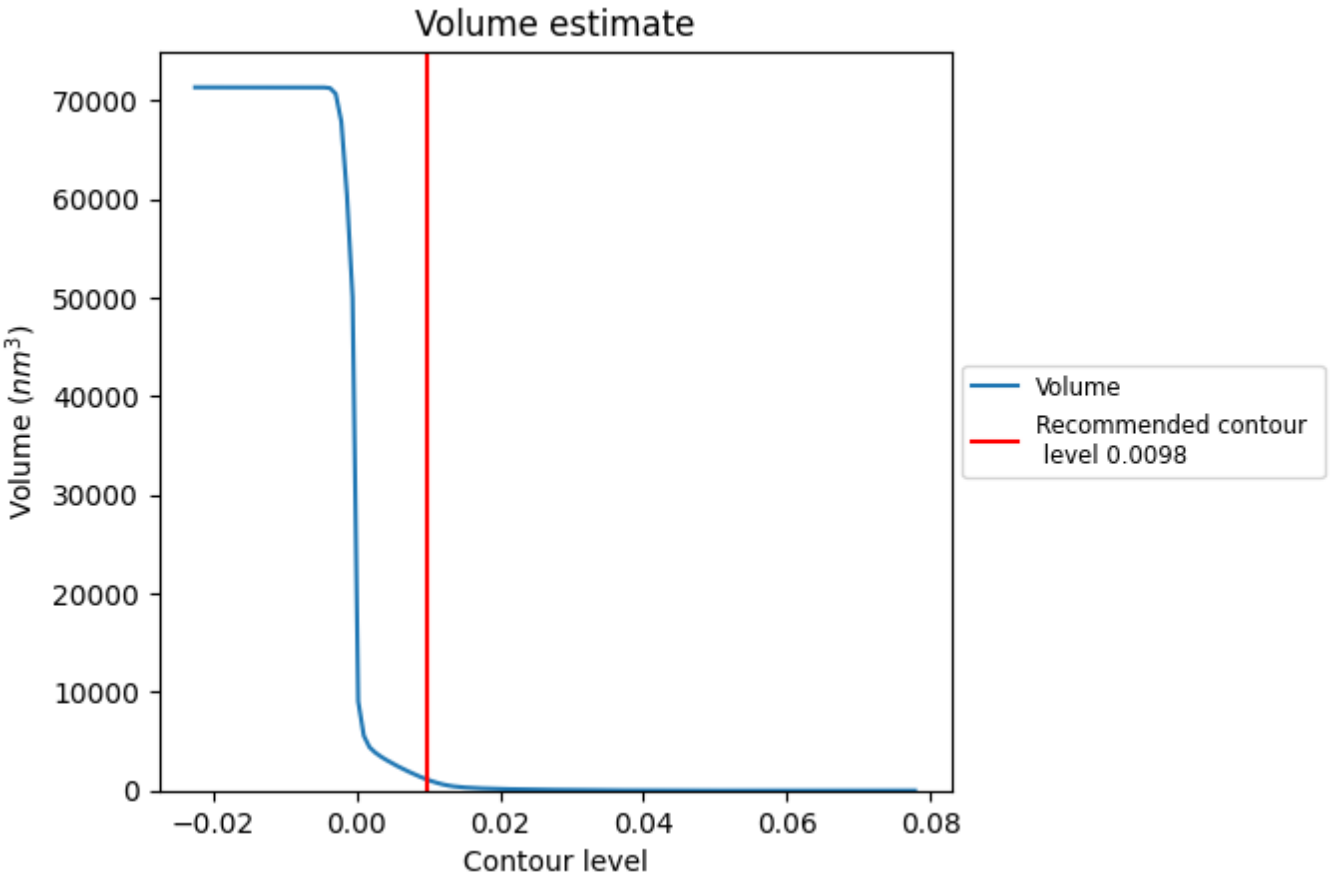
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

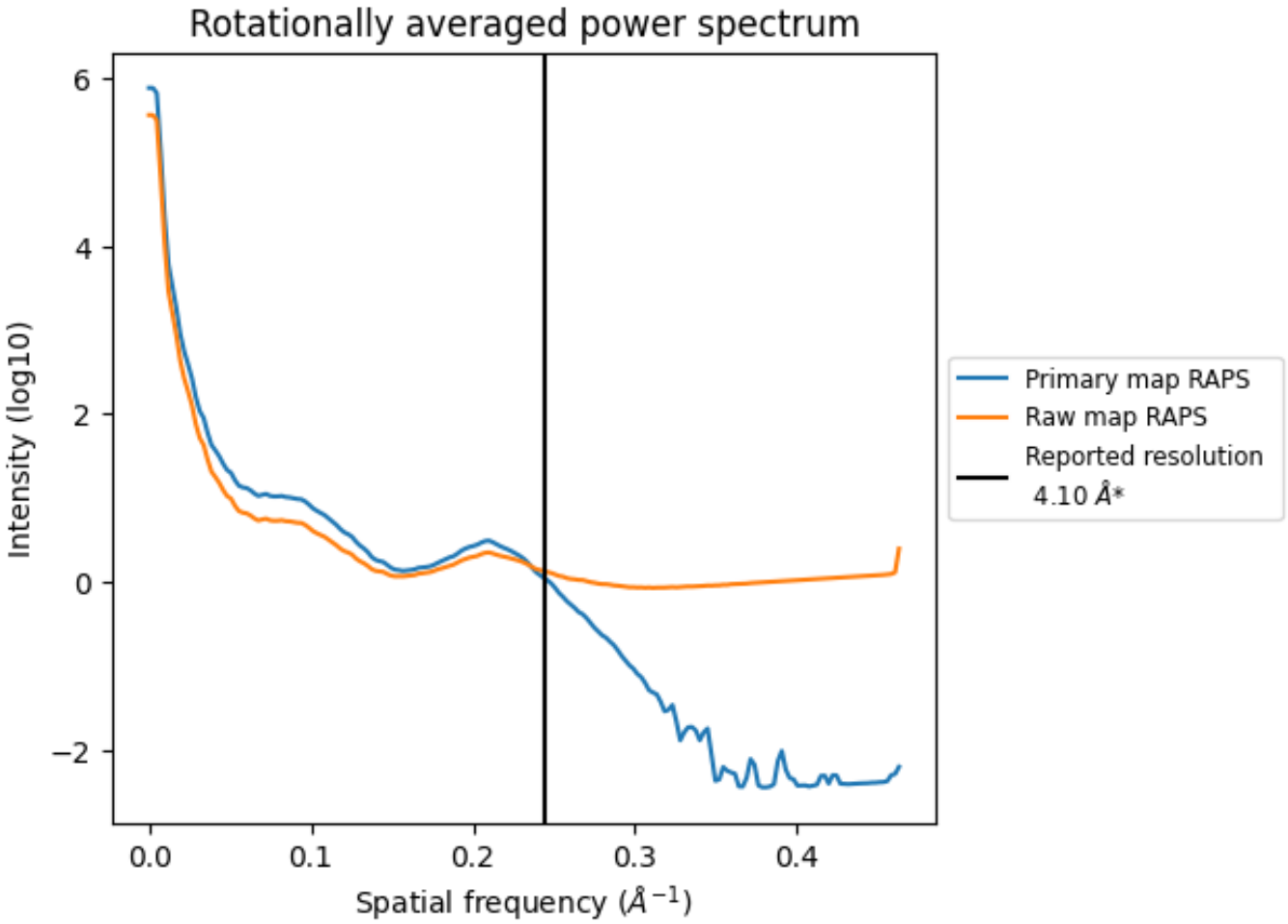
7.2 Volume estimate



The volume at the recommended contour level is 1130 nm^3; this corresponds to an approximate mass of 1021 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)

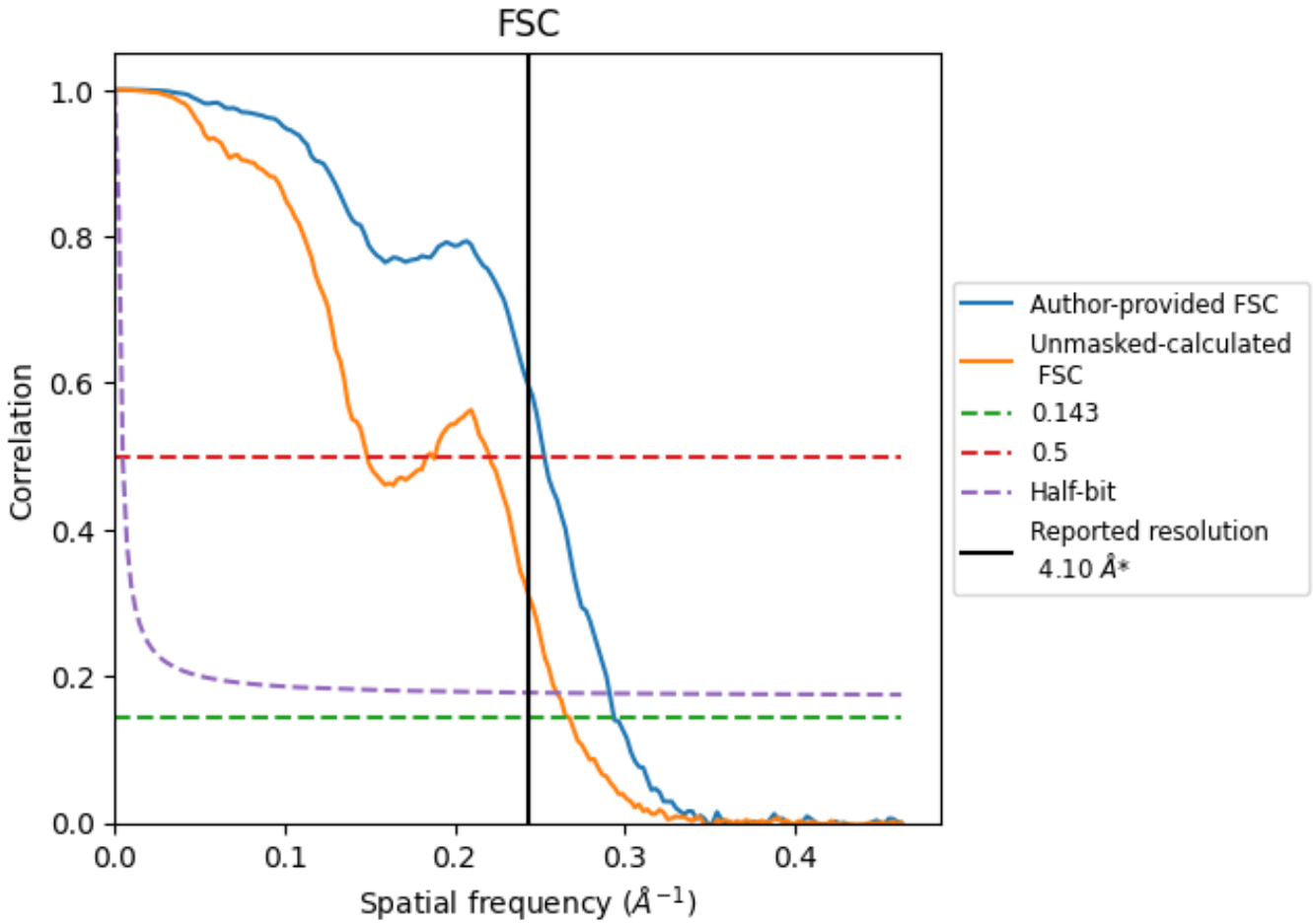


*Reported resolution corresponds to spatial frequency of 0.244 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.244 Å^{-1}

8.2 Resolution estimates (i)

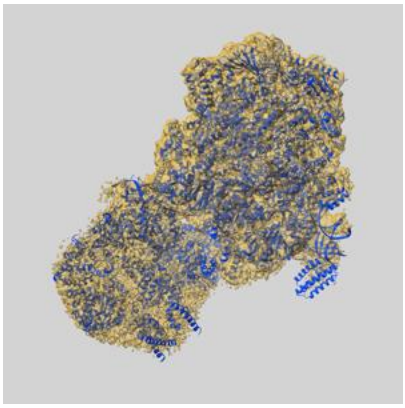
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	3.40	3.96	3.43
Unmasked-calculated*	3.74	6.73	3.84

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.40 differs from the reported value 4.1 by more than 10 %

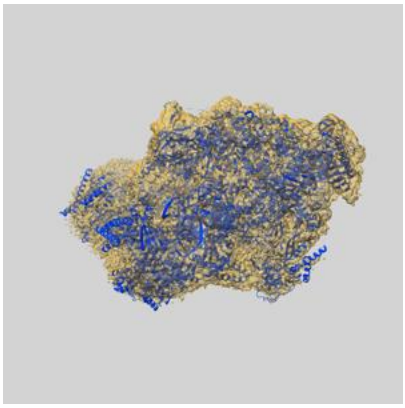
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42379 and PDB model 8UMH. Per-residue inclusion information can be found in section 3 on page 11.

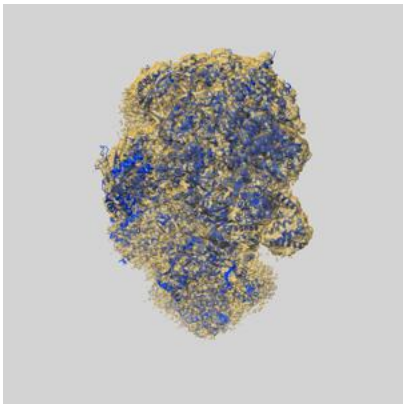
9.1 Map-model overlay



X



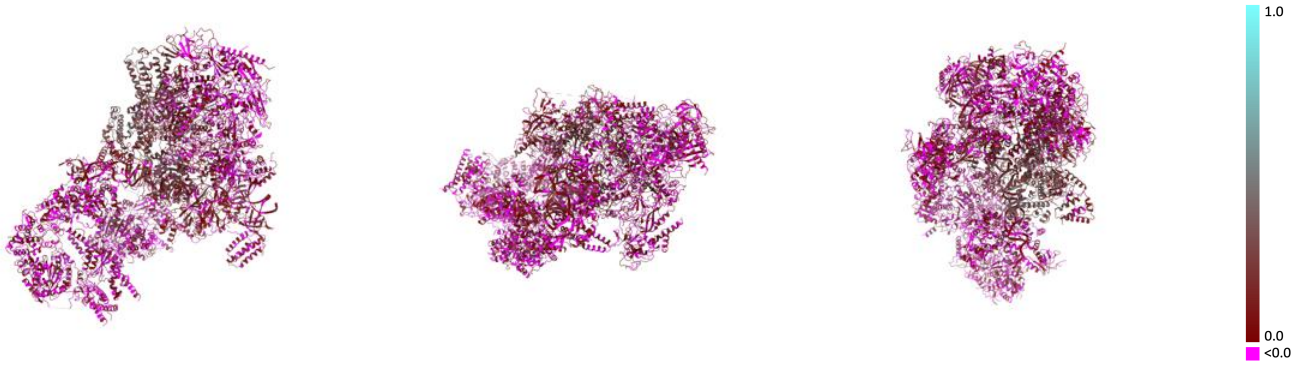
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0098 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.

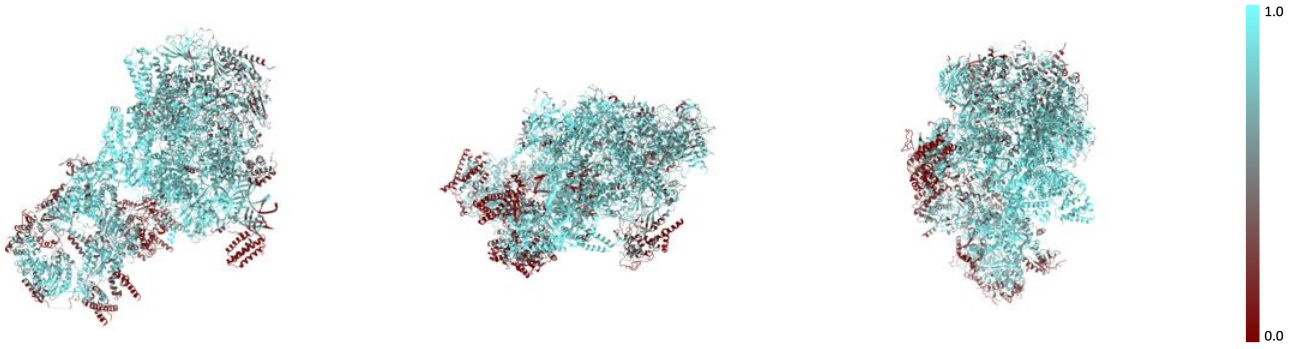
9.2 Q-score mapped to coordinate model



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.

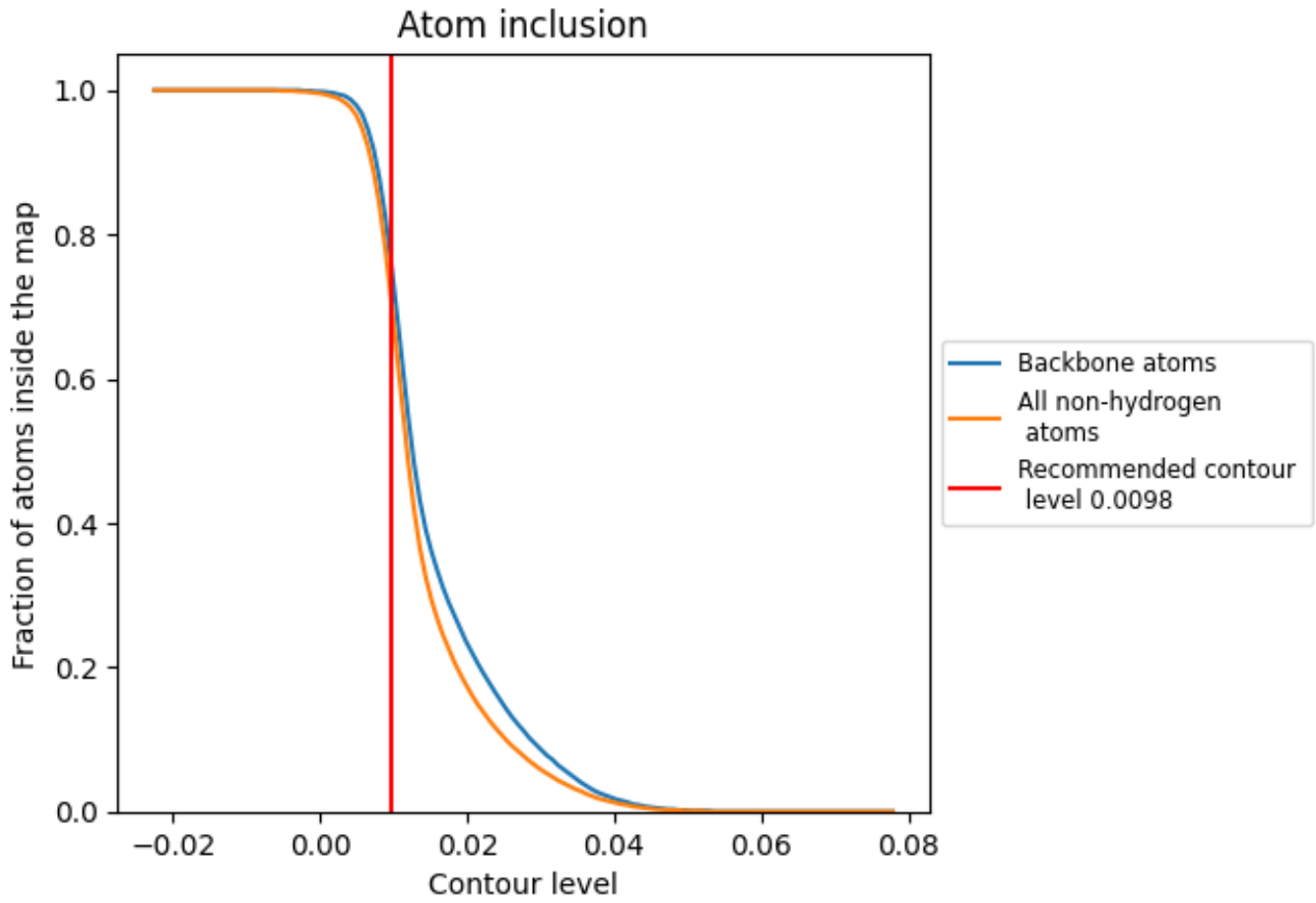
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0098).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0098) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6980	0.0810
0	0.4800	0.0170
1	0.3720	-0.0050
2	0.6150	0.0270
4	0.6940	0.0080
5	0.3900	0.0130
6	0.8040	0.0050
7	0.7630	0.0210
A	0.8460	0.1840
B	0.7780	0.0990
C	0.6130	-0.0030
D	0.2250	0.0310
E	0.9600	0.3580
F	0.7700	0.1480
G	0.4540	0.0510
H	0.7480	0.0840
I	0.8470	0.1730
J	0.6040	-0.0140
K	0.6420	0.0220
L	0.7380	0.0420
M	0.5740	0.0270
N	0.8830	0.1380
O	0.7930	0.0210
P	0.8560	0.1120
Q	0.7570	0.1470
S	0.8770	0.1340
T	0.8120	0.1040
U	0.2700	0.0460
V	0.3060	0.0670
W	0.7430	0.0810
X	0.8720	0.0790