Full wwPDB EM Validation Report ⓘ

May 1, 2024 – 12:03 am BST

PDB ID	:	5FYW
EMDB ID	:	EMD-3378
Title	:	Transcription initiation complex structures elucidate DNA opening (OC)
Authors	:	Plaschka, C.; Hantsche, M.; Dienemann, C.; Burzinski, C.; Plitzko, J.; Cramer, P.
Deposited on	:	2016-03-10
Resolution	:	4.35 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:

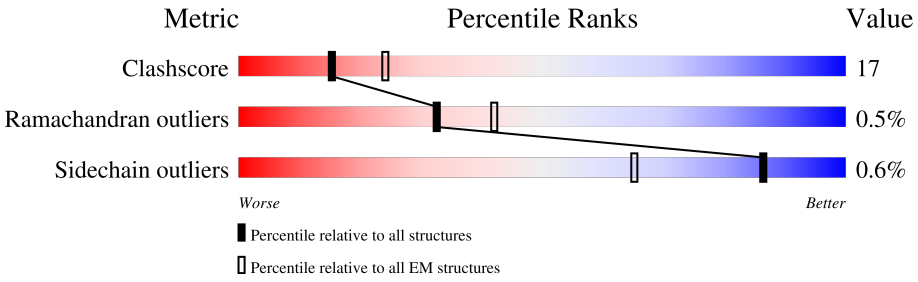
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 4.35 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	A	1733	14% 58% 23% 19%
2	B	1224	14% 62% 32% 5%
3	C	318	52% 31% 18%
4	D	221	57% 45% 26% 29%
5	E	215	20% 75% 24%
6	F	155	42% 12% 46%
7	G	171	49% 51% 48%
8	H	146	8% 52% 39% 7%

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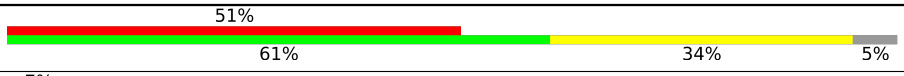
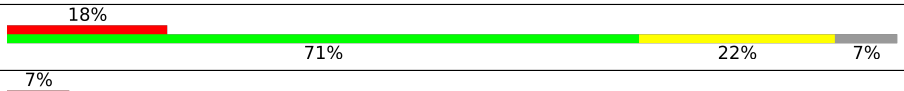
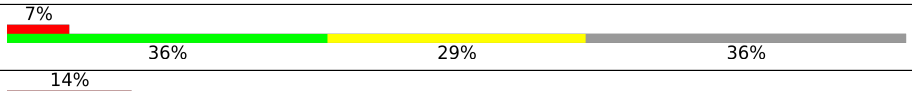
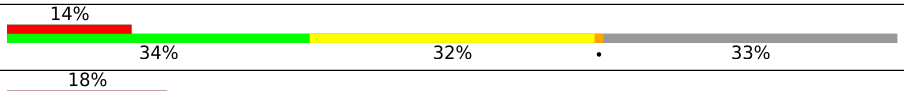
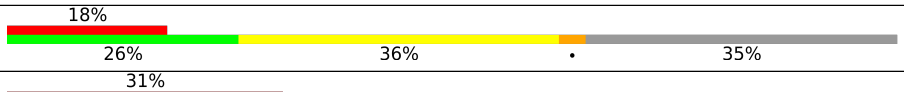
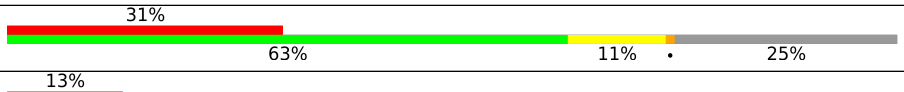
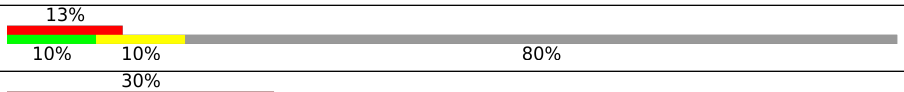
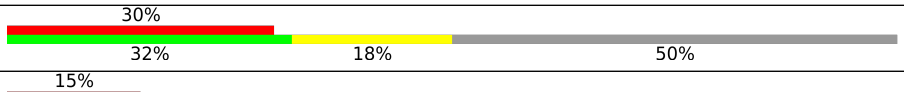
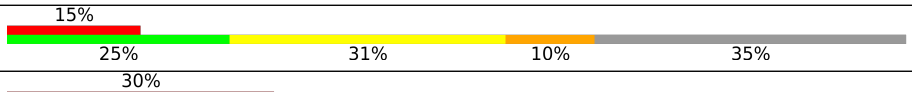
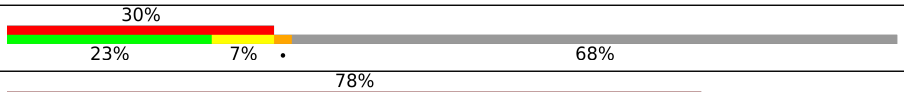
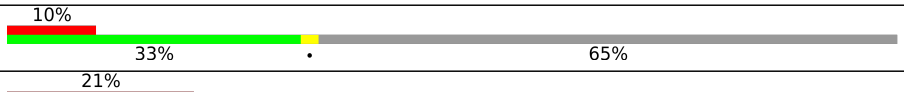
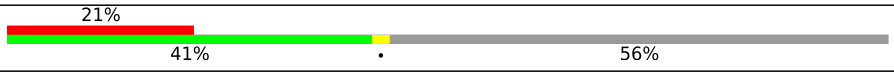
Mol	Chain	Length	Quality of chain
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	M	345	
14	N	72	
15	O	240	
16	Q	735	
17	R	400	
18	T	72	
19	U	286	
20	V	122	
21	W	482	
22	X	328	

2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 41710 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1398	10997	6931	1927	2078	61	0	0

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1157	9203	5822	1613	1713	55	0	0

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	262	2061	1299	343	406	13	0	0

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	157	1253	779	220	252	2	0	0

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	213	1744	1107	308	318	11	0	0

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	83	Total	C	N	O	S	0	0
			670	428	114	125	3		

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	136	Total	C	N	O	S	0	0
			1089	686	184	215	4		

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	116	Total	C	N	O	S	0	0
			944	581	172	181	10		

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	112	Total	C	N	O	S	0	0
			904	580	154	168	2		

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			358	221	71	62	4		

- Molecule 13 is a protein called TRANSCRIPTION INITIATION FACTOR IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	231	Total	C	N	O	S	0	0
			1785	1145	299	326	15		

- Molecule 14 is a DNA chain called NONTEMPLATE DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	47	Total	C	N	O	P	0	0
			919	461	178	234	46		

- Molecule 15 is a protein called TATA-BOX-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	180	Total	C	N	O	S	0	0
			1416	921	242	247	6		

- Molecule 16 is a protein called TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	148	Total	C	N	O	S	0	0
			1144	733	195	212	4		

- Molecule 17 is a protein called TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT BETA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	199	Total	C	N	O	S	0	0
			1347	838	247	255	7		

- Molecule 18 is a DNA chain called NONTEMPLATE DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	47	Total	C	N	O	P	0	0
			909	458	172	233	46		

- Molecule 19 is a protein called TRANSCRIPTION INITIATION FACTOR IIA LARGE SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	92	Total	C	N	O	S	0	0
			757	474	130	150	3		

- Molecule 20 is a protein called TRANSCRIPTION INITIATION FACTOR IIA SUBUNIT

2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	100	Total 782	C 492	N 130	O 156	S 4	0	0

- Molecule 21 is a protein called TRANSCRIPTION INITIATION FACTOR IIE SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	W	168	Total 835	C 499	N 168	O 168	0	0

- Molecule 22 is a protein called TRANSCRIPTION INITIATION FACTOR IIE SUBUNIT BETA.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	X	143	Total 710	C 424	N 143	O 143	0	0

- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

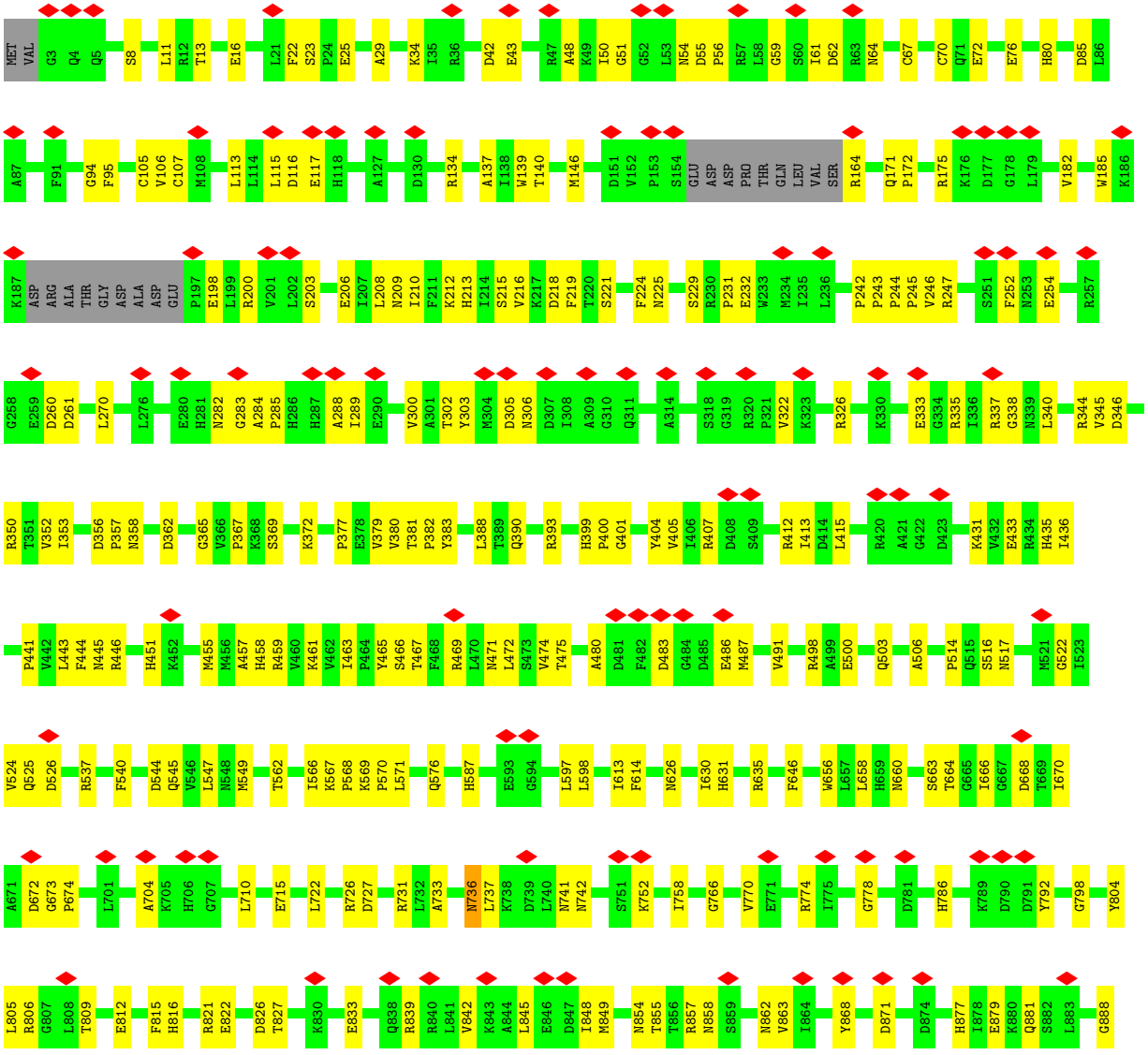
Mol	Chain	Residues	Atoms		AltConf
24	A	1	Total 1	Mg 1	0

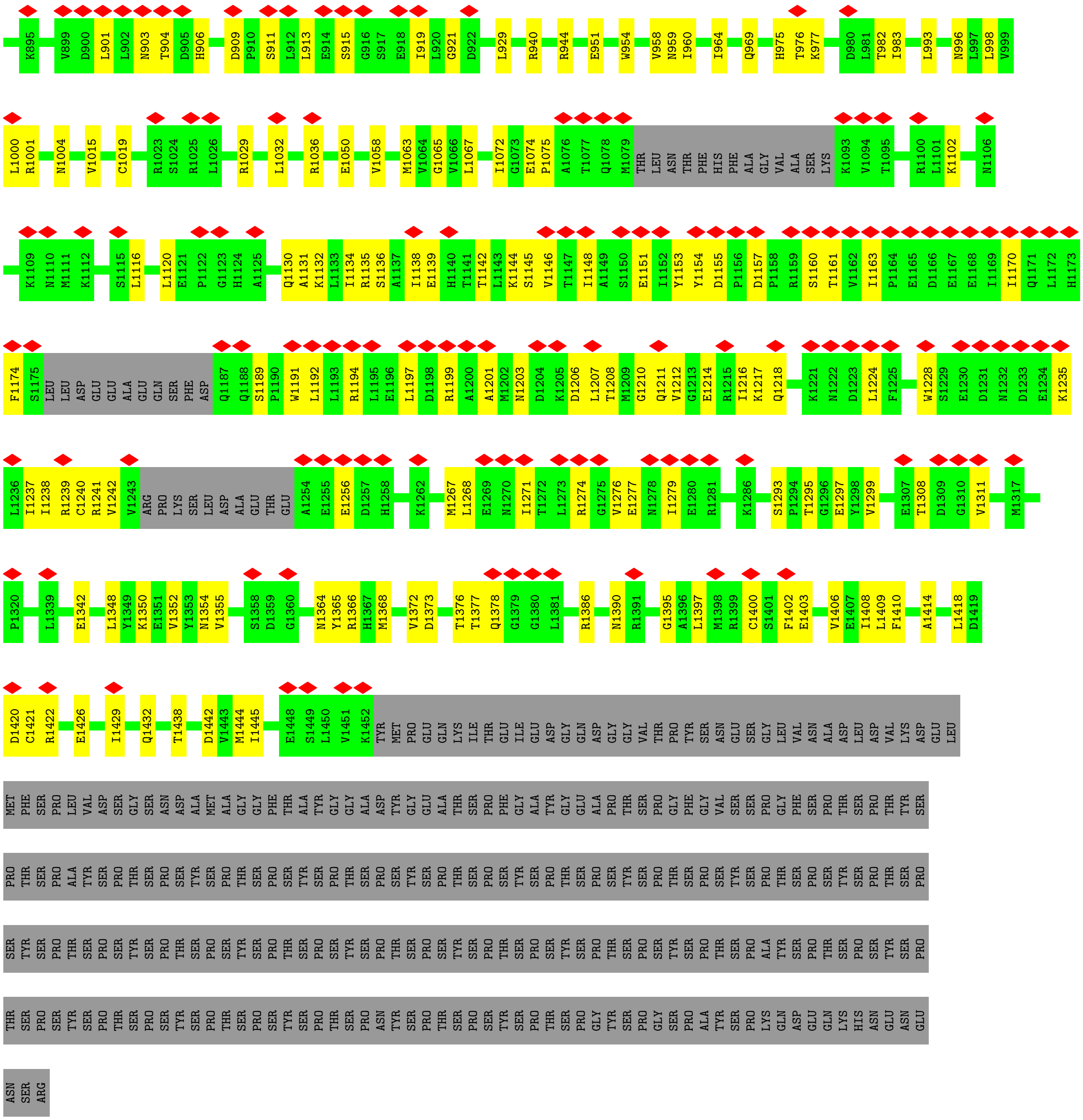
3 Residue-property plots (i)

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

• Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1

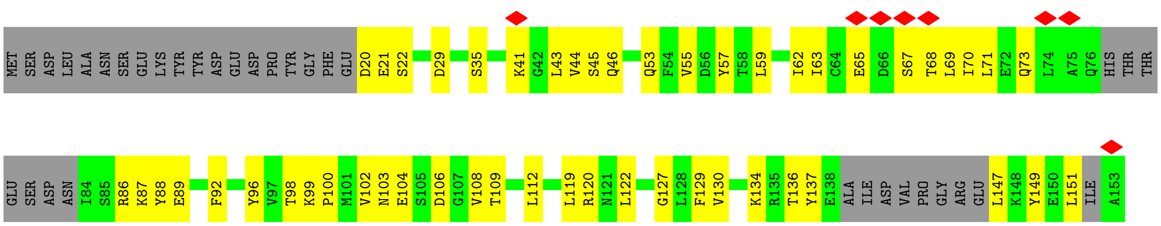
Chain A:

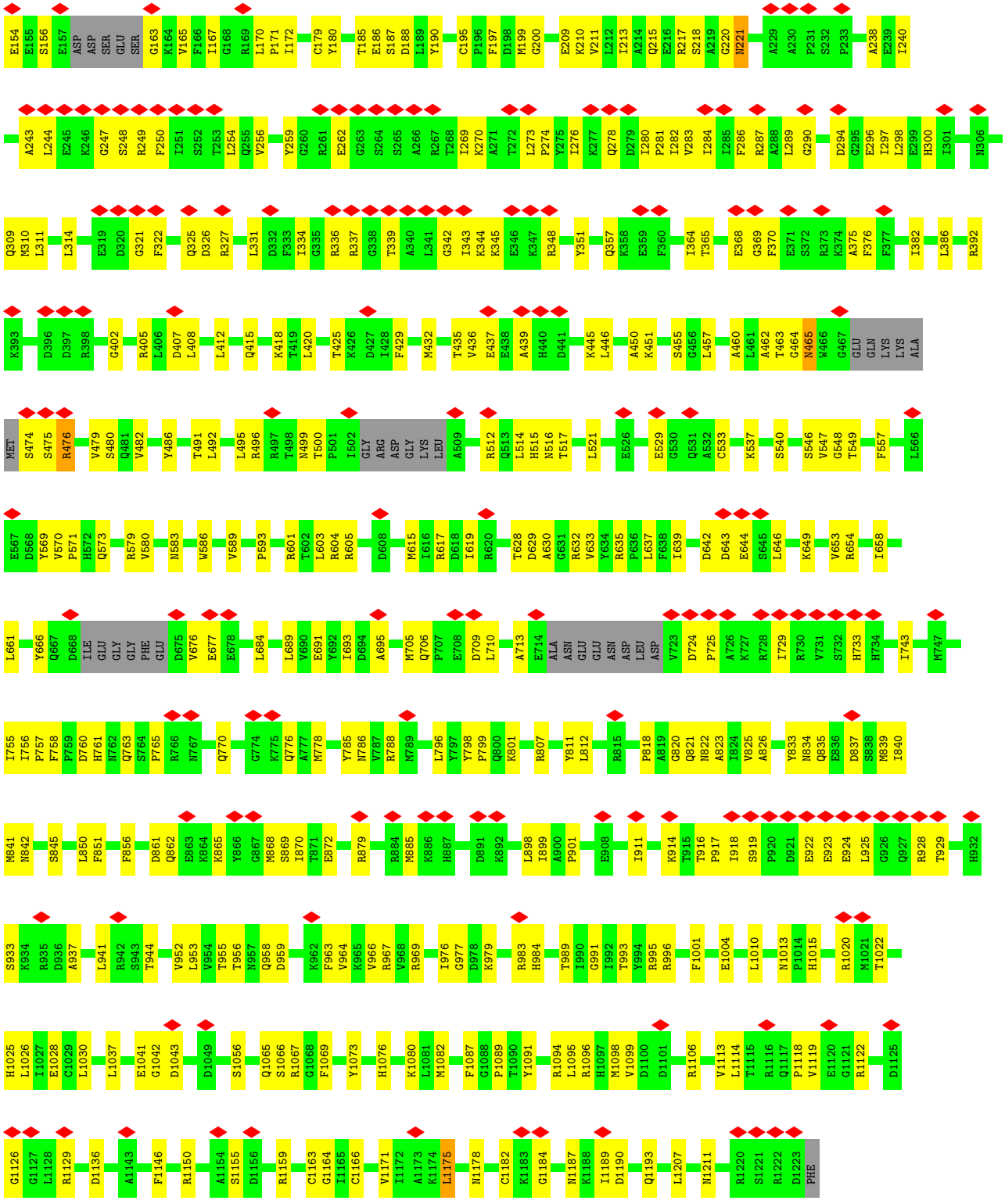




• Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2

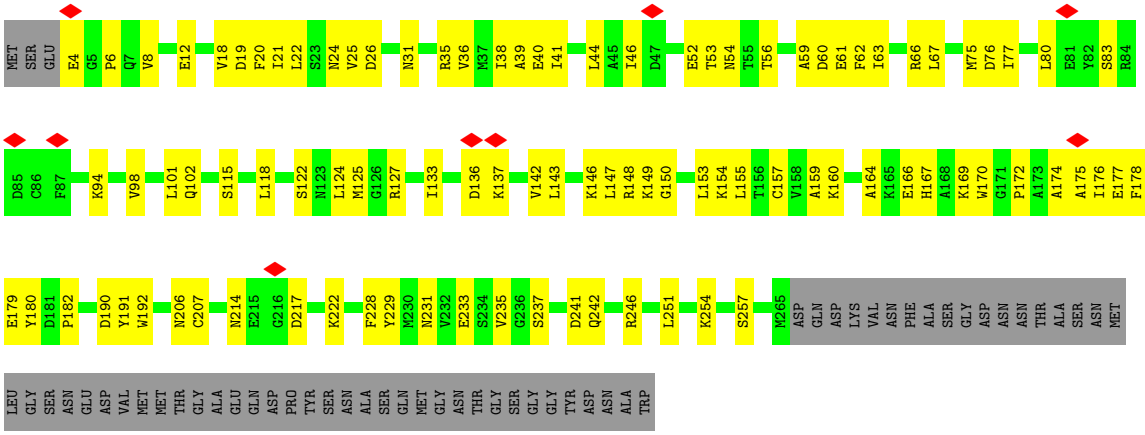
Chain B:





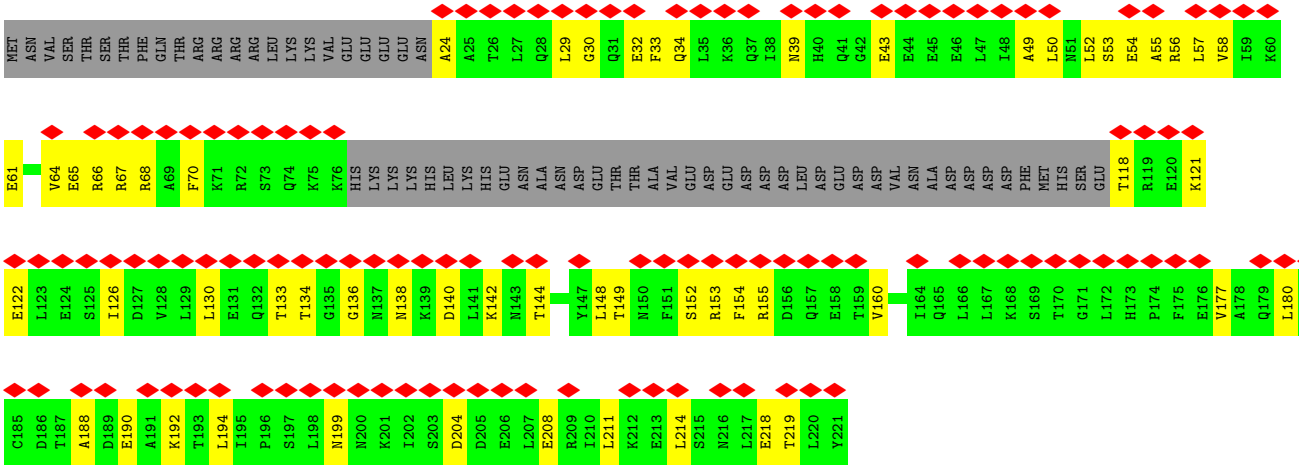
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

Chain C:



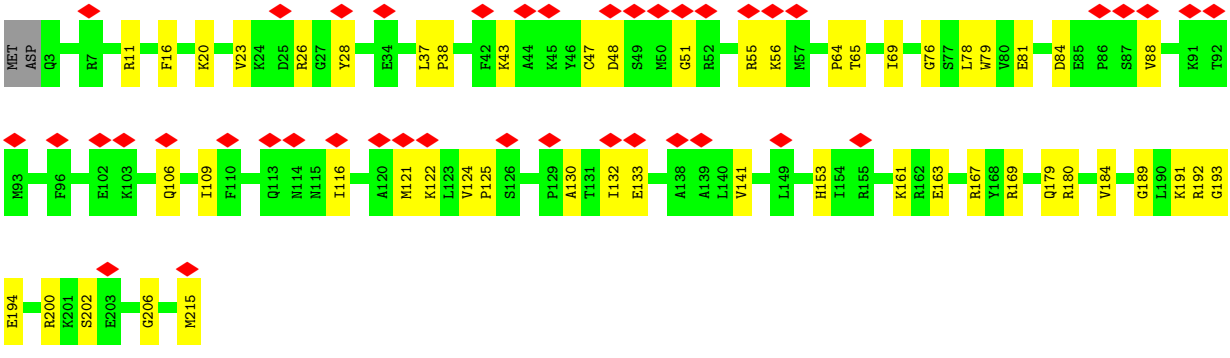
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4

Chain D:



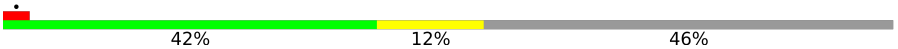
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1

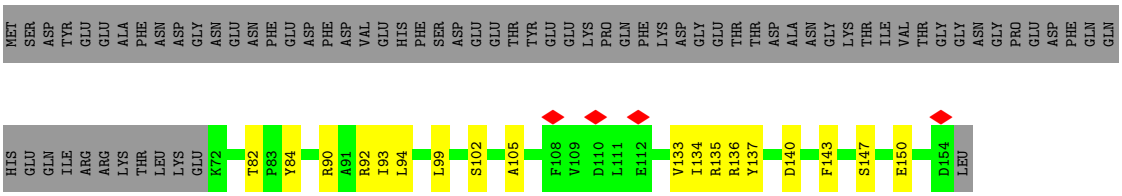
Chain E:



• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

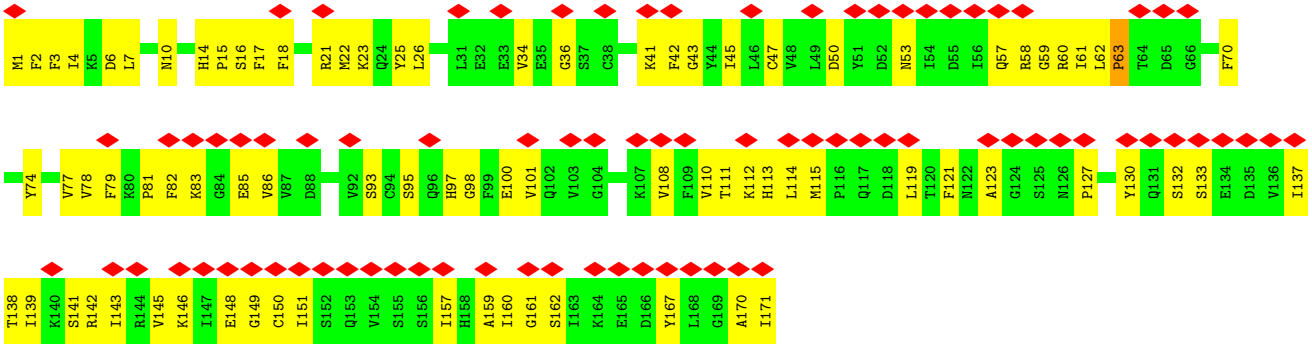
Chain F:





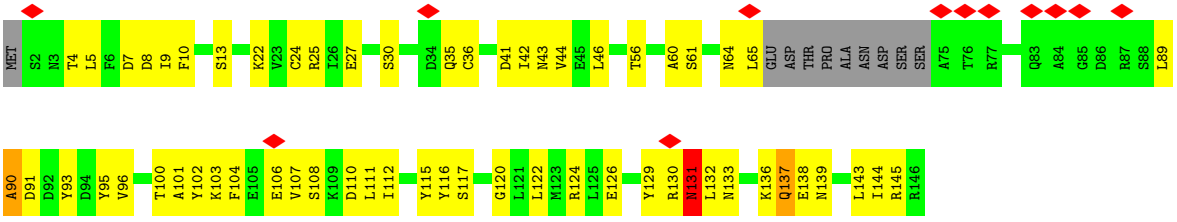
• Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

Chain G:



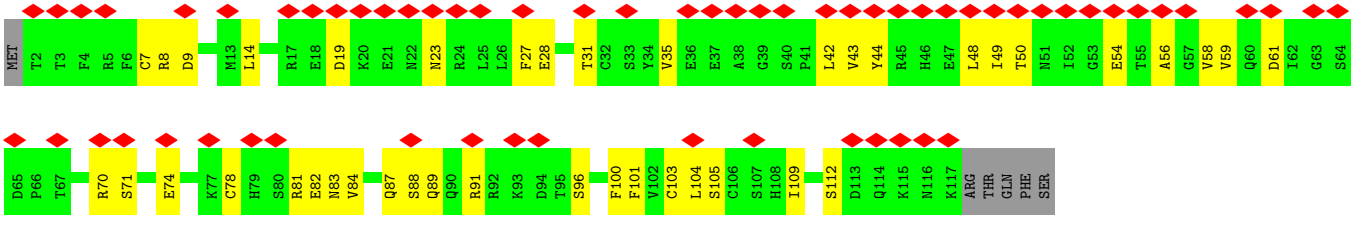
• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

Chain H:



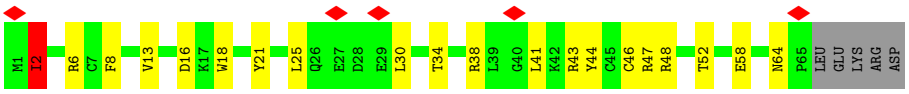
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9

Chain I:



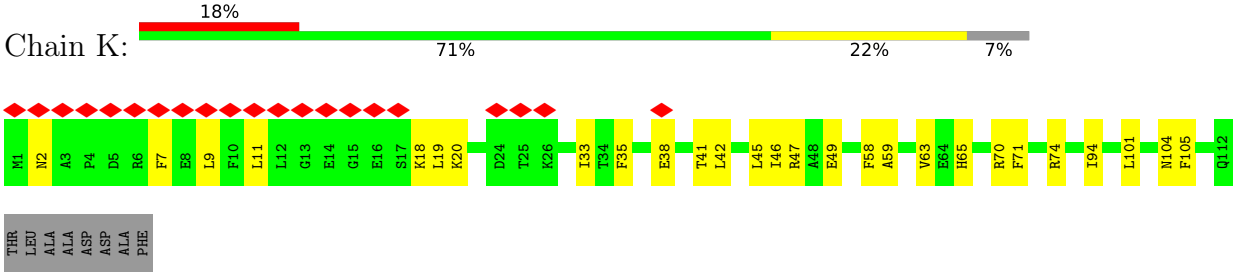
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

Chain J:



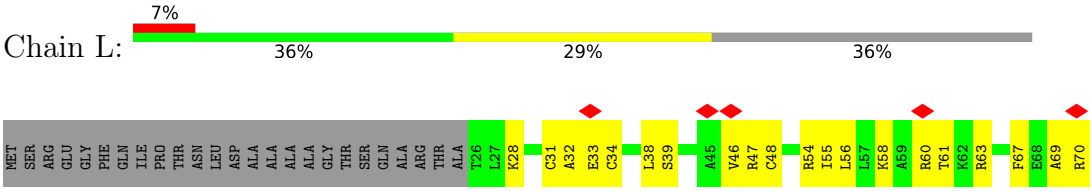
• Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

Chain K:



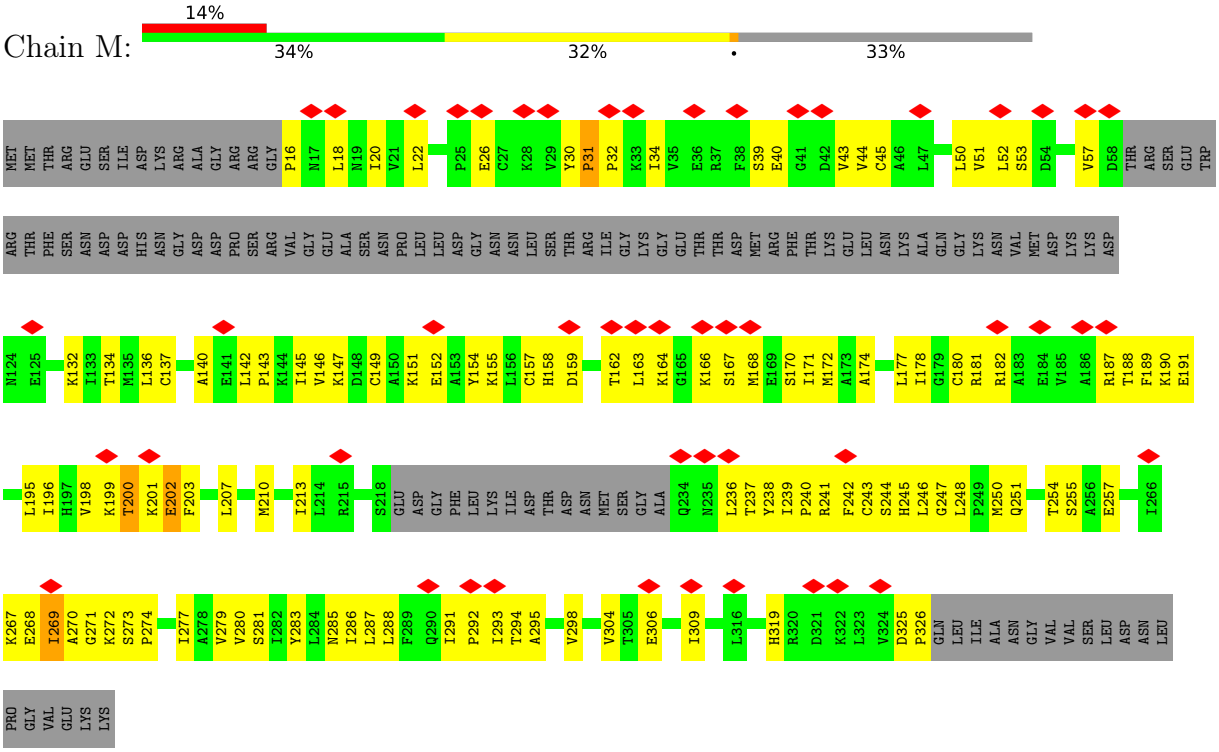
• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

Chain L:



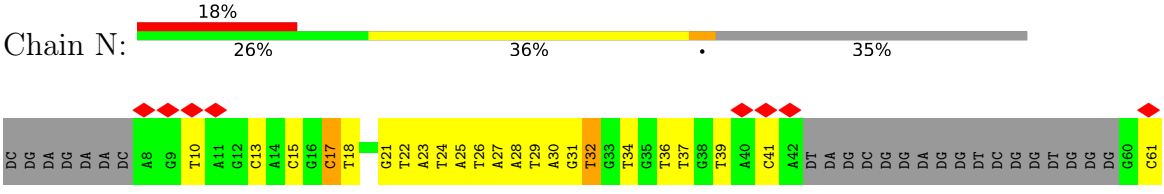
• Molecule 13: TRANSCRIPTION INITIATION FACTOR IIB

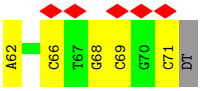
Chain M:



• Molecule 14: NONTEMPLATE DNA

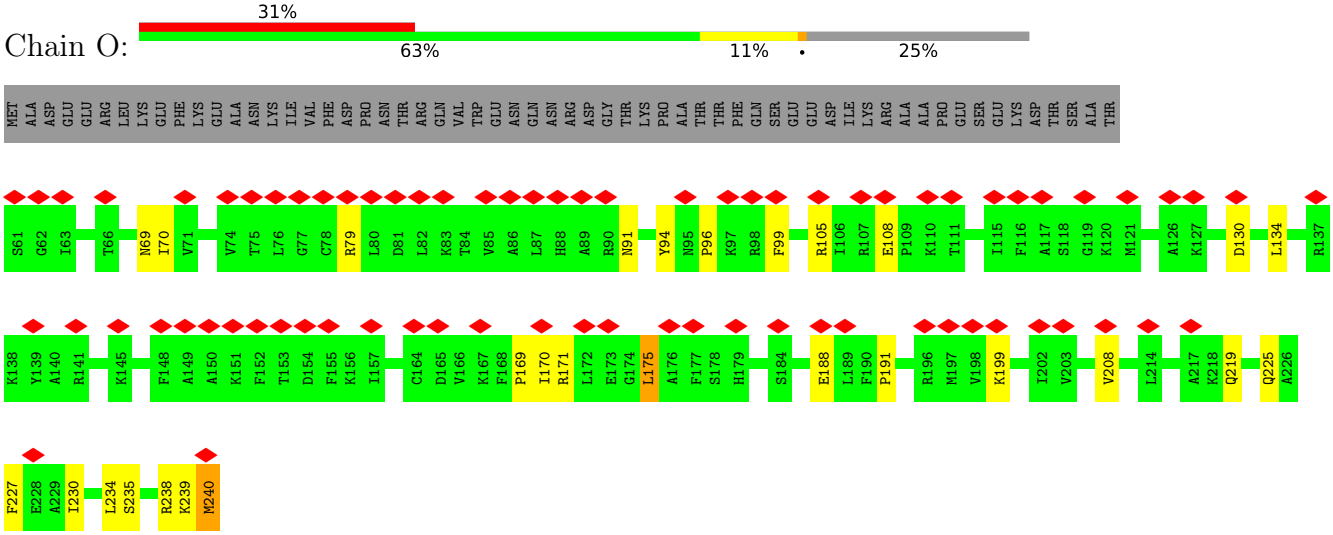
Chain N:





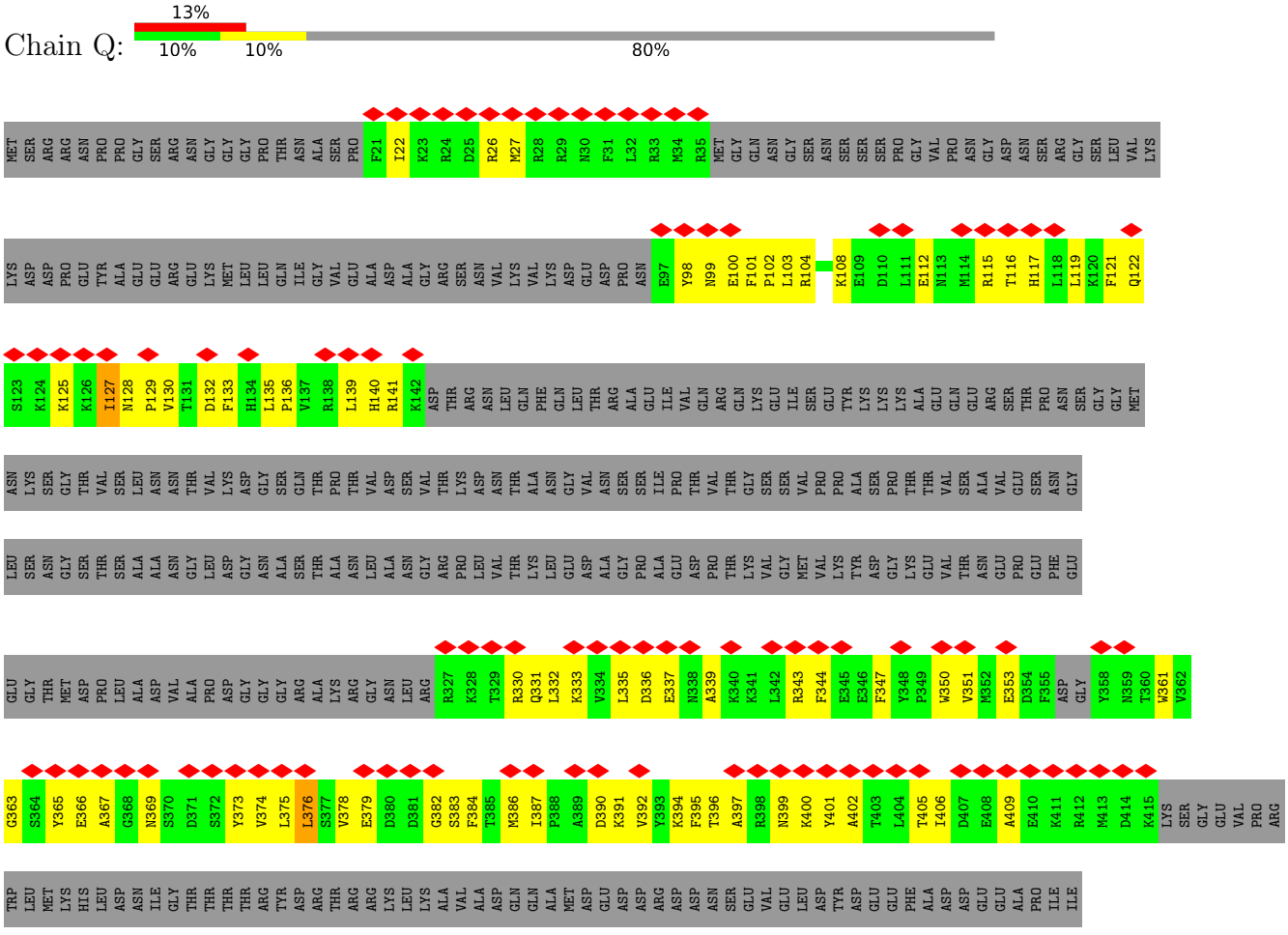
• Molecule 15: TATA-BOX-BINDING PROTEIN

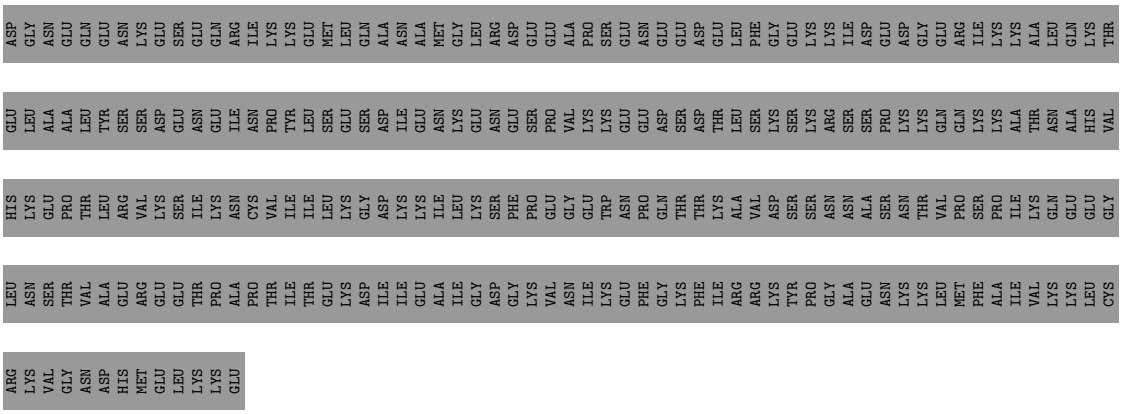
Chain O:



• Molecule 16: TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT ALPHA

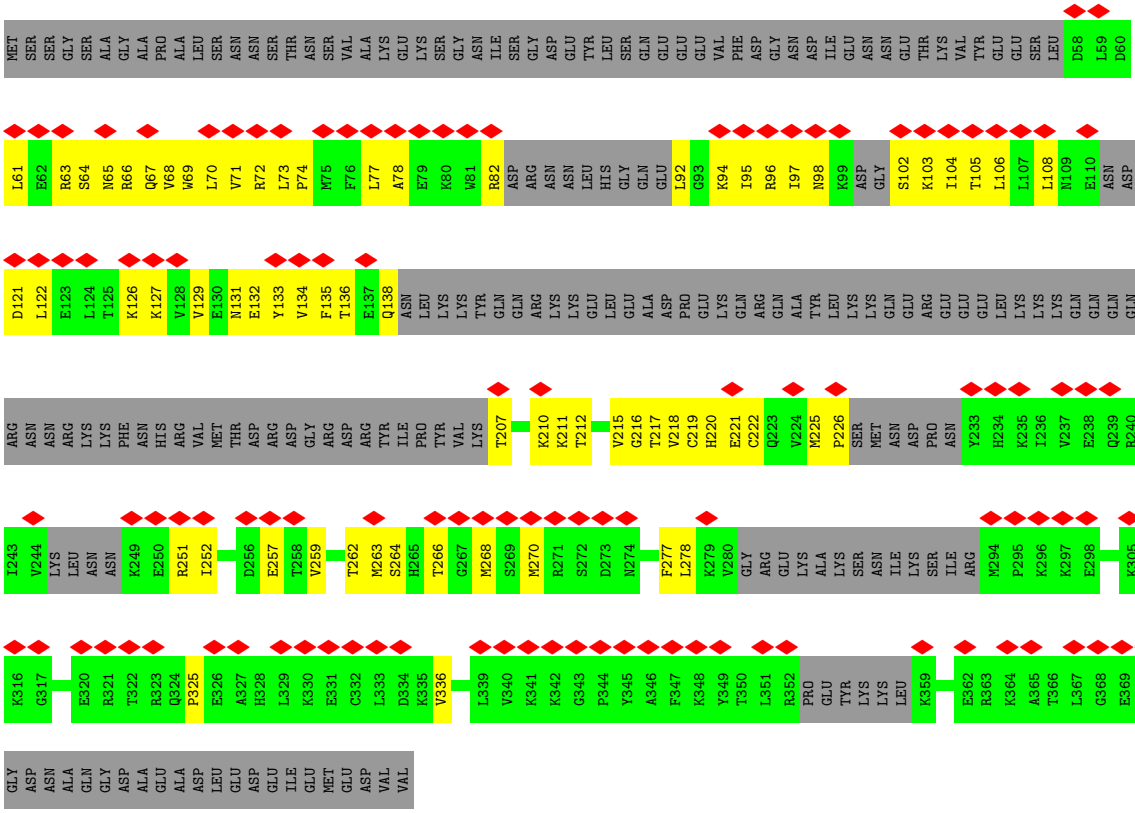
Chain Q:





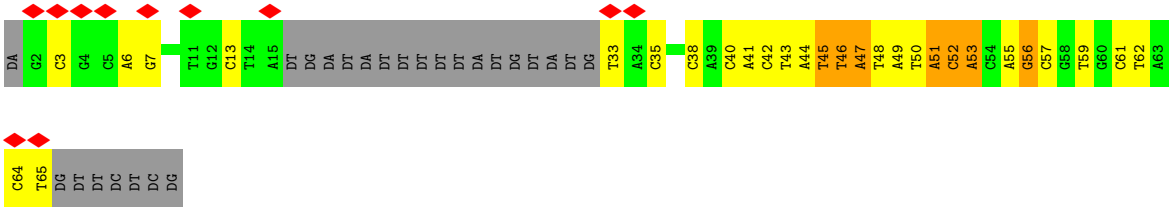
• Molecule 17: TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT BETA

Chain R:



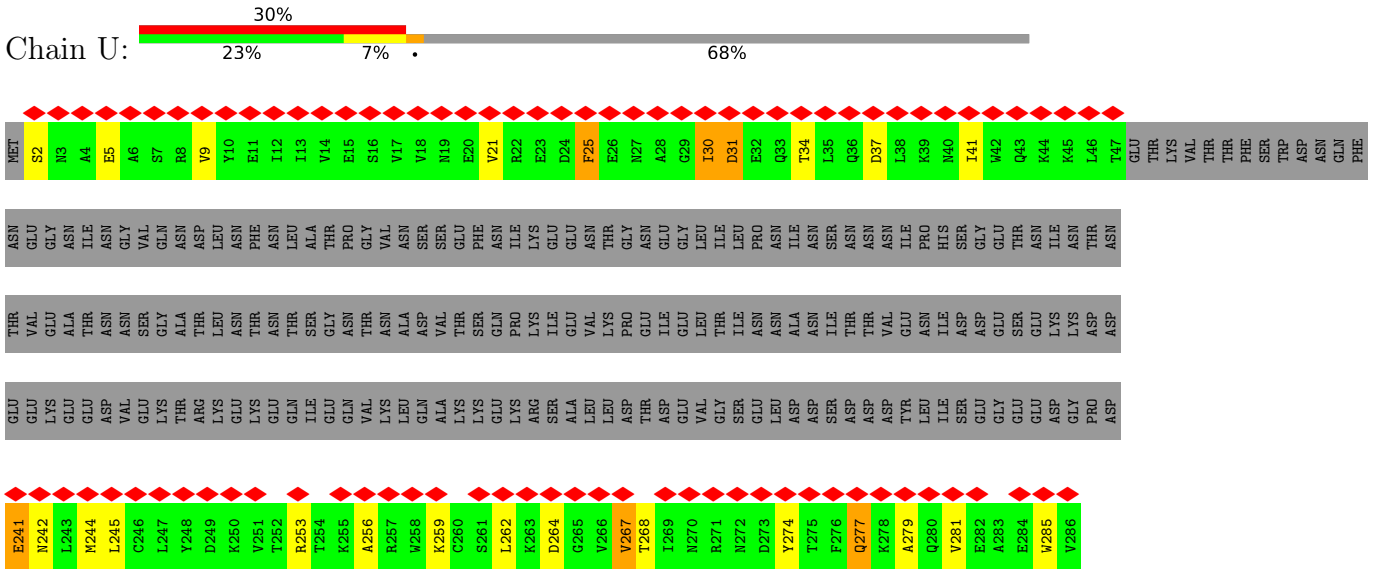
• Molecule 18: NONTEMPLATE DNA

Chain T:



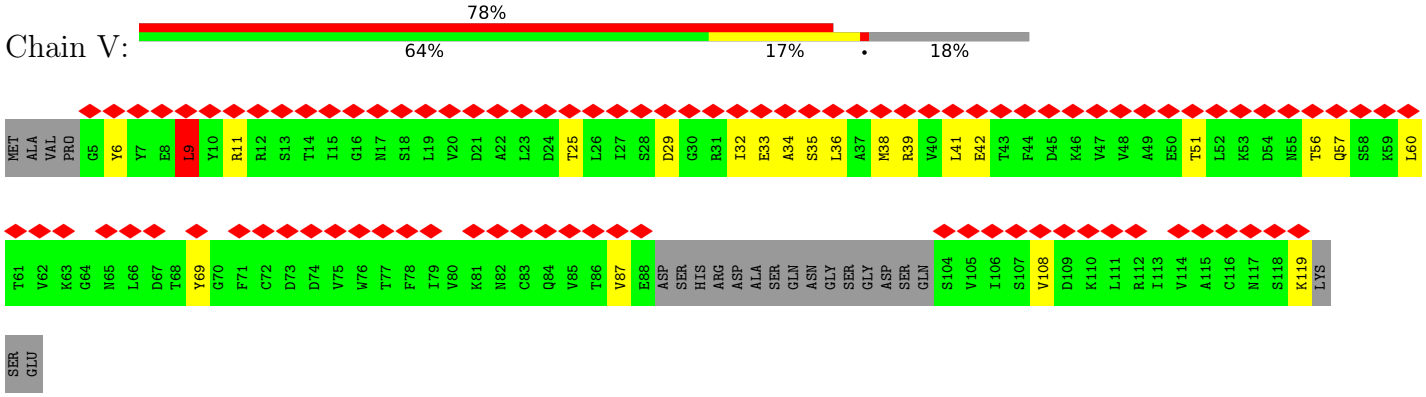
• Molecule 19: TRANSCRIPTION INITIATION FACTOR IIA LARGE SUBUNIT

Chain U:



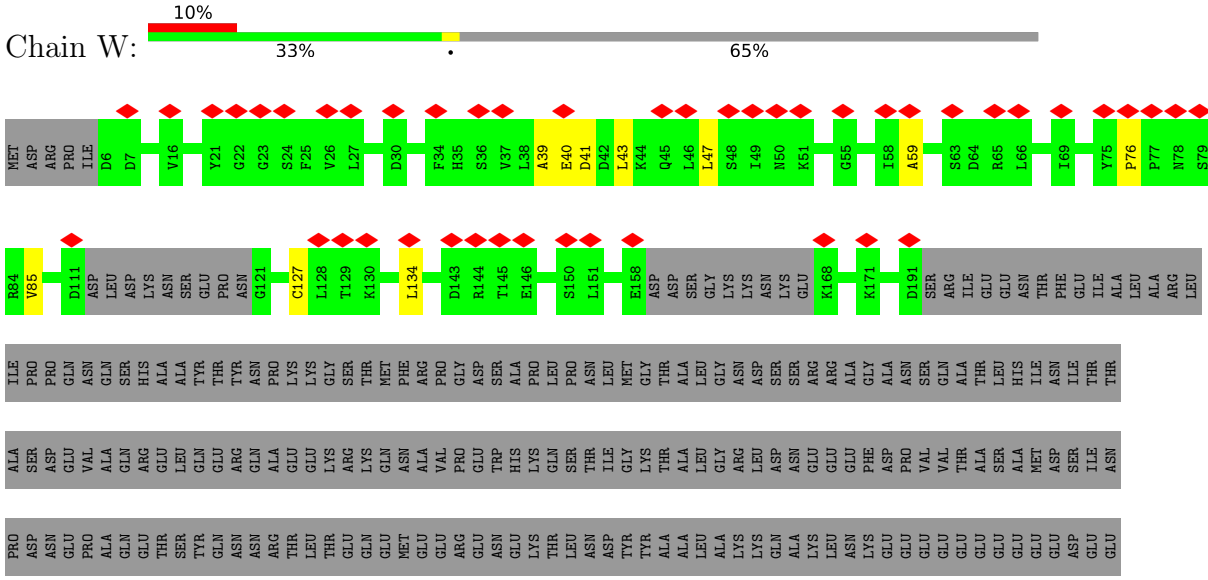
• Molecule 20: TRANSCRIPTION INITIATION FACTOR IIA SUBUNIT 2

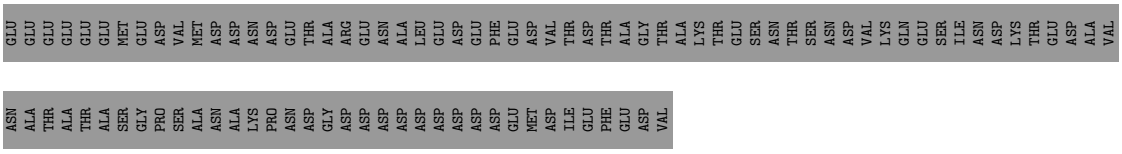
Chain V:



• Molecule 21: TRANSCRIPTION INITIATION FACTOR IIE SUBUNIT ALPHA

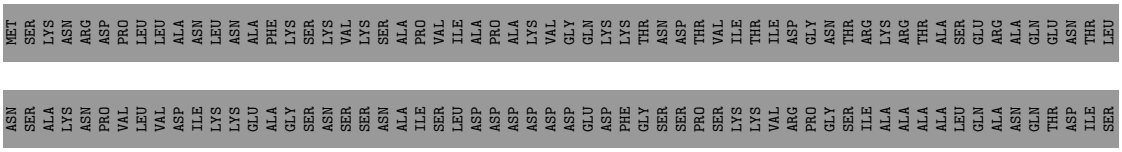
Chain W:

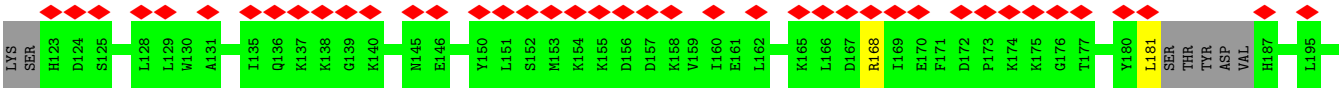


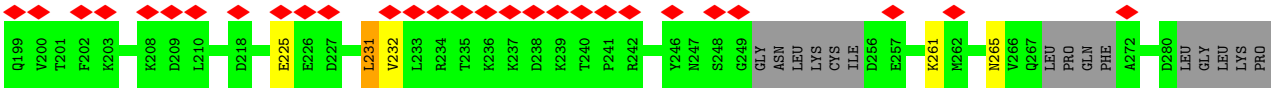


• Molecule 22: TRANSCRIPTION INITIATION FACTOR IIE SUBUNIT BETA

Chain X:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	11231	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	33	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	4200	Depositor
Magnification	37037	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.093	Depositor
Minimum map value	-0.039	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0325	Depositor
Map size (Å)	405.0, 405.0, 405.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	A	0.46	0/11192	0.55	1/15128 (0.0%)
2	B	0.51	0/9381	0.59	1/12650 (0.0%)
3	C	0.52	0/2099	0.57	0/2845
4	D	0.25	0/1262	0.44	0/1693
5	E	0.40	0/1780	0.49	0/2395
6	F	0.47	0/682	0.52	0/922
7	G	0.31	0/1368	0.50	0/1844
8	H	0.61	1/1107 (0.1%)	0.97	6/1499 (0.4%)
9	I	0.40	0/962	0.50	0/1295
10	J	0.53	0/541	0.56	0/727
11	K	0.43	0/922	0.53	0/1244
12	L	0.40	0/360	0.60	0/478
13	M	0.40	0/1809	0.60	0/2435
14	N	1.07	12/1036 (1.2%)	1.30	5/1530 (0.3%)
15	O	0.59	0/1443	0.78	1/1942 (0.1%)
16	Q	0.53	0/1168	0.68	1/1579 (0.1%)
17	R	0.43	0/1354	0.68	1/1832 (0.1%)
18	T	1.24	16/1023 (1.6%)	1.44	13/1507 (0.9%)
19	U	0.39	0/766	0.61	0/1032
20	V	0.38	0/789	0.62	1/1066 (0.1%)
21	W	0.33	1/832 (0.1%)	0.47	0/1157
22	X	0.26	0/706	0.47	0/979
All	All	0.52	30/42582 (0.1%)	0.65	30/57779 (0.1%)

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
2	B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	2
10	J	0	1
13	M	0	1
All	All	0	5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	131	ASN	C-N	-13.08	1.03	1.34
18	T	53	DA	P-O5'	-11.50	1.48	1.59
18	T	47	DA	C1'-N9	-10.28	1.32	1.47
18	T	56	DG	C1'-N9	-6.75	1.37	1.47
18	T	64	DC	C1'-N1	6.24	1.57	1.49
18	T	61	DC	C1'-N1	6.14	1.57	1.49
18	T	46	DT	C4'-C3'	-5.72	1.46	1.52
18	T	62	DT	C1'-N1	5.41	1.56	1.49
14	N	41	DC	C1'-N1	5.37	1.56	1.49
21	W	76	PRO	C-N	5.36	1.44	1.34
14	N	39	DT	C1'-N1	5.32	1.56	1.49
18	T	6	DA	O3'-P	-5.30	1.54	1.61
14	N	13	DC	C1'-N1	5.25	1.56	1.49
18	T	38	DC	C1'-N1	5.24	1.56	1.49
14	N	71	DC	C1'-N1	5.22	1.56	1.49
18	T	35	DC	C1'-N1	5.22	1.56	1.49
14	N	17	DC	C1'-N1	5.20	1.56	1.49
18	T	3	DC	C1'-N1	5.20	1.56	1.49
14	N	69	DC	C1'-N1	5.20	1.56	1.49
14	N	37	DT	C1'-N1	5.19	1.56	1.49
14	N	10	DT	C1'-N1	5.19	1.55	1.49
18	T	40	DC	C1'-N1	5.18	1.55	1.49
14	N	32	DT	C1'-N1	5.17	1.55	1.49
14	N	36	DT	C1'-N1	5.15	1.55	1.49
18	T	65	DT	C1'-N1	5.10	1.55	1.49
14	N	15	DC	C1'-N1	5.09	1.55	1.49
14	N	34	DT	C1'-N1	5.08	1.55	1.49
18	T	33	DT	C1'-N1	5.08	1.55	1.49
18	T	59	DT	C1'-N1	5.06	1.55	1.49
18	T	57	DC	C1'-N1	5.01	1.55	1.49

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	131	ASN	N-CA-C	16.18	154.67	111.00
8	H	131	ASN	O-C-N	-15.85	97.34	122.70
8	H	131	ASN	C-N-CA	15.68	160.91	121.70
18	T	46	DT	O4'-C4'-C3'	-11.75	98.95	106.00
17	R	336	VAL	CB-CA-C	-10.95	90.60	111.40
8	H	131	ASN	CA-C-N	9.74	138.63	117.20
14	N	26	DT	O4'-C4'-C3'	-9.39	100.37	106.00
18	T	6	DA	O3'-P-O5'	-9.07	86.76	104.00
14	N	66	DC	C2-N1-C1'	7.33	126.86	118.80
18	T	45	DT	O4'-C4'-C3'	-7.21	101.61	104.50
14	N	68	DG	P-O3'-C3'	7.16	128.29	119.70
8	H	131	ASN	N-CA-CB	-6.96	98.07	110.60
18	T	52	DC	N1-C1'-C2'	6.60	125.14	112.60
18	T	51	DA	O5'-P-OP1	-6.52	99.83	105.70
8	H	131	ASN	CB-CA-C	-6.38	97.65	110.40
18	T	46	DT	O4'-C1'-C2'	-6.25	100.90	105.90
18	T	46	DT	C4-C5-C6	6.00	121.60	118.00
14	N	66	DC	C6-N1-C1'	-5.85	113.78	120.80
18	T	53	DA	N1-C6-N6	-5.85	115.09	118.60
1	A	658	LEU	CA-CB-CG	5.66	128.31	115.30
18	T	47	DA	O4'-C1'-N9	-5.56	104.11	108.00
18	T	6	DA	P-O3'-C3'	5.51	126.31	119.70
15	O	175	LEU	CA-CB-CG	5.47	127.88	115.30
18	T	53	DA	P-O5'-C5'	5.41	129.56	120.90
18	T	7	DG	C5-C6-O6	-5.41	125.36	128.60
20	V	9	LEU	CA-CB-CG	5.40	127.73	115.30
14	N	26	DT	P-O3'-C3'	5.18	125.92	119.70
16	Q	376	LEU	CA-CB-CG	5.15	127.14	115.30
18	T	6	DA	O4'-C1'-N9	5.13	111.59	108.00
2	B	218	SER	CB-CA-C	-5.01	100.58	110.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1175	LEU	Peptide
8	H	131	ASN	Peptide,Mainchain
10	J	2	ILE	Peptide
13	M	292	PRO	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	A	10997	0	11082	291	0
2	B	9203	0	9203	371	0
3	C	2061	0	2029	72	0
4	D	1253	0	1273	62	0
5	E	1744	0	1772	32	0
6	F	670	0	690	15	0
7	G	1340	0	1356	95	0
8	H	1089	0	1061	40	0
9	I	944	0	899	30	0
10	J	532	0	543	22	0
11	K	904	0	911	20	0
12	L	358	0	380	24	0
13	M	1785	0	1891	170	0
14	N	919	0	533	33	0
15	O	1416	0	1493	69	0
16	Q	1144	0	1034	100	0
17	R	1347	0	1130	92	0
18	T	909	0	533	65	0
19	U	757	0	747	21	0
20	V	782	0	790	16	0
21	W	835	0	349	12	0
22	X	710	0	287	4	0
23	A	2	0	0	0	0
23	B	1	0	0	0	0
23	C	1	0	0	0	0
23	I	2	0	0	0	0
23	J	1	0	0	0	0
23	L	1	0	0	0	0
23	M	1	0	0	0	0
23	W	1	0	0	0	0
24	A	1	0	0	0	0
All	All	41710	0	39986	1351	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 17.

All (1351) 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)
2:B:865:LYS:CE	13:M:145:ILE:HD11	1.46	1.44
2:B:405:ARG:NH1	2:B:632:ARG:HG2	1.23	1.40
2:B:868:MET:HB2	13:M:149:CYS:SG	1.64	1.35
13:M:267:LYS:HE3	15:O:208:VAL:CG1	1.59	1.31
13:M:272:LYS:HB3	18:T:53:DA:P	1.71	1.29
13:M:272:LYS:HB3	18:T:53:DA:OP1	1.37	1.24
13:M:267:LYS:CE	15:O:208:VAL:CG1	2.16	1.24
13:M:272:LYS:HE2	18:T:52:DC:OP1	1.37	1.22
2:B:199:MET:CE	2:B:491:THR:HG22	1.69	1.21
2:B:865:LYS:HE2	13:M:145:ILE:CD1	1.70	1.19
2:B:405:ARG:NH1	2:B:632:ARG:CG	2.04	1.17
15:O:91:ASN:OD1	20:V:69:TYR:CZ	1.98	1.16
13:M:267:LYS:HE3	15:O:208:VAL:HG13	1.25	1.12
13:M:272:LYS:CB	18:T:53:DA:OP1	1.98	1.12
13:M:267:LYS:NZ	15:O:169:PRO:HB3	1.64	1.12
13:M:198:VAL:O	13:M:202:GLU:OE1	1.68	1.11
13:M:270:ALA:HB2	15:O:208:VAL:HG11	1.26	1.10
2:B:865:LYS:CE	13:M:145:ILE:CD1	2.27	1.09
14:N:24:DT:H2”	14:N:25:DA:H5’	1.25	1.09
2:B:865:LYS:HE2	13:M:145:ILE:HD11	1.09	1.08
2:B:199:MET:HE1	2:B:491:THR:CG2	1.82	1.07
15:O:191:PRO:CB	18:T:52:DC:H5”	1.83	1.07
2:B:199:MET:CE	2:B:491:THR:CG2	2.32	1.07
13:M:269:ILE:HG23	13:M:272:LYS:HE3	1.33	1.06
14:N:21:DG:H2”	14:N:22:DT:H5’	1.10	1.05
4:D:29:LEU:HD22	7:G:82:PHE:CZ	1.93	1.04
18:T:42:DC:H2”	18:T:43:DT:C5	1.93	1.04
2:B:868:MET:CB	13:M:149:CYS:SG	2.46	1.04
19:U:2:SER:N	19:U:274:TYR:HH	1.56	1.03
2:B:70:ILE:HD11	16:Q:333:LYS:HB2	1.42	1.02
15:O:91:ASN:ND2	19:U:285:TRP:CZ2	2.28	1.01
2:B:325:GLN:HB3	16:Q:401:TYR:OH	1.59	1.01
2:B:199:MET:HE1	2:B:491:THR:HG22	1.04	1.00
4:D:29:LEU:HD22	7:G:82:PHE:CE2	1.96	1.00
14:N:21:DG:C2’	14:N:22:DT:H5’	1.92	0.99
14:N:29:DT:H2”	14:N:30:DA:C8	1.97	0.99
2:B:475:SER:O	2:B:476:ARG:HG3	1.61	0.99
2:B:865:LYS:HE3	13:M:145:ILE:HD11	1.41	0.99
13:M:274:PRO:HD2	15:O:188:GLU:CG	1.92	0.98
12:L:47:ARG:NH1	13:M:250:MET:CE	2.27	0.98
7:G:151:ILE:CD1	21:W:134:LEU:CB	2.43	0.97
2:B:44:VAL:HG11	2:B:495:LEU:HD13	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:22:DT:H2"	14:N:23:DA:H5'	1.47	0.95
16:Q:127:ILE:HG22	16:Q:129:PRO:HD3	1.47	0.95
22:X:225:GLU:HA	22:X:231:LEU:HA	1.49	0.95
12:L:47:ARG:HH12	13:M:250:MET:HE3	1.31	0.95
13:M:269:ILE:CG2	13:M:272:LYS:HG3	1.96	0.95
2:B:44:VAL:HG11	2:B:495:LEU:CD1	1.98	0.94
2:B:249:ARG:NH1	2:B:415:GLN:O	1.89	0.94
7:G:79:PHE:HE2	7:G:81:PRO:HG3	1.31	0.94
2:B:405:ARG:HH12	2:B:632:ARG:HG2	1.17	0.94
14:N:21:DG:H2"	14:N:22:DT:C5'	1.97	0.94
1:A:70:CYS:SG	1:A:80:HIS:NE2	2.41	0.93
13:M:269:ILE:HG23	13:M:272:LYS:CE	1.99	0.92
7:G:79:PHE:CE2	7:G:81:PRO:HG3	2.05	0.92
15:O:191:PRO:HB3	18:T:52:DC:H5"	1.48	0.92
2:B:68:THR:HB	16:Q:335:LEU:CD1	2.00	0.92
13:M:272:LYS:CE	18:T:52:DC:OP1	2.18	0.91
13:M:269:ILE:HG22	13:M:272:LYS:HG3	1.50	0.91
2:B:405:ARG:HH11	2:B:632:ARG:HG2	1.08	0.91
12:L:47:ARG:HH12	13:M:250:MET:CE	1.84	0.90
2:B:914:LYS:HB3	2:B:937:ALA:O	1.73	0.89
4:D:49:ALA:HA	7:G:3:PHE:CD1	2.09	0.88
13:M:270:ALA:HB1	15:O:208:VAL:HG21	1.53	0.88
18:T:43:DT:H2"	18:T:44:DA:C8	2.09	0.87
12:L:47:ARG:NH1	13:M:250:MET:HE3	1.87	0.87
18:T:49:DA:C2'	18:T:50:DT:H5'	2.03	0.87
13:M:267:LYS:CE	15:O:208:VAL:HG11	2.03	0.87
13:M:267:LYS:HE3	15:O:208:VAL:HG11	1.52	0.87
2:B:868:MET:HB2	13:M:149:CYS:HG	1.34	0.87
2:B:199:MET:HE3	2:B:491:THR:CG2	2.05	0.87
14:N:22:DT:H2"	14:N:23:DA:C5'	2.04	0.87
13:M:274:PRO:HD2	15:O:188:GLU:HG3	1.55	0.86
17:R:98:ASN:HB3	17:R:103:LYS:O	1.75	0.86
1:A:326:ARG:HG3	1:A:1406:VAL:HG11	1.57	0.85
13:M:274:PRO:HD2	15:O:188:GLU:HG2	1.55	0.85
16:Q:336:ASP:OD1	16:Q:337:GLU:N	2.09	0.85
2:B:872:GLU:HG2	2:B:916:THR:HG22	1.57	0.85
2:B:405:ARG:HH11	2:B:632:ARG:CG	1.77	0.85
2:B:247:GLY:HA2	2:B:418:LYS:NZ	1.91	0.85
2:B:1041:GLU:O	16:Q:22:ILE:CB	2.23	0.85
2:B:247:GLY:N	2:B:418:LYS:HZ1	1.75	0.84
12:L:47:ARG:NH1	13:M:250:MET:HE1	1.92	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:373:TYR:CD1	17:R:70:LEU:HD21	2.13	0.84
2:B:644:GLU:HG3	2:B:646:LEU:H	1.43	0.84
4:D:32:GLU:HG3	7:G:42:PHE:CE1	2.11	0.84
13:M:267:LYS:HZ3	15:O:169:PRO:HB3	1.43	0.83
16:Q:141:ARG:HA	16:Q:350:TRP:HA	1.58	0.83
2:B:217:ARG:NH1	2:B:407:ASP:OD2	2.12	0.83
16:Q:366:GLU:HB3	16:Q:392:VAL:HG13	1.61	0.83
2:B:87:LYS:HB2	2:B:137:TYR:HB2	1.58	0.82
2:B:199:MET:HE3	2:B:491:THR:HG21	1.59	0.82
14:N:24:DT:C2'	14:N:25:DA:H5'	2.09	0.82
7:G:151:ILE:HD11	21:W:134:LEU:CB	2.08	0.82
13:M:267:LYS:CE	15:O:208:VAL:HG12	2.09	0.82
2:B:247:GLY:N	2:B:418:LYS:NZ	2.28	0.81
18:T:49:DA:H2"	18:T:50:DT:H5'	1.61	0.81
2:B:220:GLY:O	2:B:221:ASN:HB2	1.79	0.81
13:M:274:PRO:HG2	15:O:188:GLU:OE2	1.80	0.81
16:Q:104:ARG:HG2	17:R:92:LEU:HD22	1.62	0.81
17:R:138:GLN:HB2	17:R:211:LYS:HB3	1.64	0.80
2:B:68:THR:CB	16:Q:335:LEU:CD1	2.60	0.80
7:G:4:ILE:HG12	7:G:77:VAL:HG22	1.63	0.80
15:O:91:ASN:ND2	19:U:285:TRP:HZ2	1.77	0.80
2:B:757:PRO:HD3	2:B:983:ARG:HE	1.46	0.80
4:D:190:GLU:HA	7:G:167:TYR:CE2	2.16	0.80
15:O:91:ASN:OD1	20:V:69:TYR:CE2	2.35	0.79
2:B:365:THR:HG21	2:B:370:PHE:CD2	2.17	0.79
15:O:191:PRO:CB	18:T:52:DC:C5'	2.60	0.79
2:B:71:LEU:HD21	2:B:436:VAL:HG11	1.64	0.79
13:M:267:LYS:HE2	15:O:208:VAL:CG1	2.09	0.79
15:O:91:ASN:OD1	20:V:69:TYR:OH	2.01	0.79
18:T:52:DC:P	18:T:52:DC:H3'	2.23	0.78
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.65	0.78
2:B:53:GLN:OE1	2:B:547:VAL:HG22	1.84	0.78
8:H:129:TYR:O	8:H:133:ASN:ND2	2.17	0.78
17:R:129:VAL:HG11	17:R:221:GLU:HG2	1.66	0.77
13:M:268:GLU:OE1	13:M:319:HIS:NE2	2.12	0.77
8:H:89:LEU:HG	8:H:90:ALA:H	1.48	0.77
13:M:269:ILE:CG2	13:M:272:LYS:HE3	2.13	0.77
2:B:666:TYR:OH	16:Q:27:MET:HB3	1.84	0.77
9:I:82:GLU:HG2	9:I:104:LEU:HD12	1.65	0.77
16:Q:121:PHE:HB2	17:R:131:ASN:HB3	1.67	0.77
1:A:451:HIS:CE1	1:A:1074:GLU:HG3	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:GLY:CA	2:B:418:LYS:NZ	2.48	0.77
2:B:68:THR:OG1	16:Q:335:LEU:HD12	1.85	0.77
17:R:73:LEU:HD12	17:R:74:PRO:HD2	1.65	0.76
1:A:1397:LEU:HB2	1:A:1426:GLU:HG2	1.68	0.76
3:C:149:LYS:HG3	3:C:150:GLY:H	1.51	0.76
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.67	0.75
16:Q:102:PRO:HA	17:R:94:LYS:HA	1.67	0.75
2:B:247:GLY:H	2:B:418:LYS:NZ	1.83	0.75
16:Q:375:LEU:O	16:Q:386:MET:HA	1.87	0.75
18:T:48:DT:H2'	18:T:49:DA:C8	2.21	0.75
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.19	0.75
16:Q:376:LEU:HD23	16:Q:386:MET:HG2	1.68	0.75
2:B:369:GLY:HA3	16:Q:367:ALA:HB2	1.68	0.74
18:T:47:DA:N7	18:T:48:DT:O4	2.19	0.74
12:L:47:ARG:HH11	13:M:250:MET:HE1	1.51	0.74
18:T:42:DC:H2"	18:T:43:DT:C6	2.23	0.74
1:A:379:VAL:HG22	1:A:431:LYS:HG2	1.69	0.74
7:G:160:ILE:N	7:G:160:ILE:HD12	2.02	0.73
2:B:345:LYS:HA	2:B:348:ARG:HG2	1.70	0.73
2:B:287:ARG:NH2	2:B:294:ASP:OD1	2.20	0.73
18:T:52:DC:H1'	18:T:53:DA:H5'	1.69	0.73
4:D:56:ARG:NH1	4:D:122:GLU:OE2	2.21	0.73
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.69	0.73
13:M:238:TYR:HB3	13:M:242:PHE:HE2	1.54	0.73
17:R:120:TYR:HD1	17:R:226:PRO:HA	1.54	0.73
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.22	0.73
2:B:919:SER:HB2	2:B:922:GLU:HB2	1.72	0.72
1:A:362:ASP:OD2	1:A:459:ARG:NH1	2.21	0.72
12:L:32:ALA:HB2	12:L:55:ILE:HB	1.70	0.72
2:B:247:GLY:HA2	2:B:418:LYS:HZ3	1.53	0.72
13:M:236:LEU:HD11	13:M:257:GLU:HG3	1.72	0.72
16:Q:139:LEU:HB3	17:R:212:THR:HG21	1.71	0.72
1:A:1136:SER:O	1:A:1274:ARG:NH1	2.22	0.72
13:M:267:LYS:HZ2	15:O:239:LYS:HD2	1.55	0.72
5:E:56:LYS:NZ	5:E:84:ASP:OD2	2.22	0.72
5:E:116:ILE:HB	5:E:121:MET:HE2	1.72	0.72
13:M:157:CYS:HB2	13:M:163:LEU:HD11	1.72	0.72
13:M:270:ALA:CB	15:O:208:VAL:HG11	2.13	0.72
7:G:130:TYR:HB2	7:G:137:ILE:HB	1.72	0.72
1:A:405:VAL:HG23	1:A:415:LEU:HD11	1.71	0.71
13:M:166:LYS:HB3	13:M:170:SER:HB3	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:73:LEU:HD11	17:R:77:LEU:HD23	1.72	0.71
13:M:267:LYS:NZ	15:O:169:PRO:CB	2.51	0.71
13:M:274:PRO:CD	15:O:188:GLU:HG3	2.20	0.71
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.72	0.71
17:R:64:SER:HA	17:R:216:GLY:HA2	1.72	0.71
9:I:31:THR:O	16:Q:401:TYR:HB2	1.89	0.71
13:M:272:LYS:O	18:T:53:DA:OP1	2.08	0.71
17:R:104:ILE:HD11	17:R:122:LEU:HB3	1.73	0.71
2:B:220:GLY:O	2:B:221:ASN:CB	2.38	0.71
13:M:270:ALA:CB	15:O:208:VAL:HG21	2.20	0.71
1:A:61:ILE:HG22	1:A:62:ASP:H	1.55	0.71
2:B:475:SER:O	2:B:476:ARG:CG	2.38	0.71
4:D:54:GLU:HB2	4:D:160:VAL:HG11	1.73	0.71
13:M:267:LYS:NZ	15:O:239:LYS:HD2	2.06	0.71
1:A:881:GLN:NE2	1:A:959:ASN:HA	2.06	0.71
2:B:437:GLU:OE2	16:Q:330:ARG:O	2.09	0.71
1:A:107:CYS:SG	1:A:171:GLN:NE2	2.63	0.70
7:G:151:ILE:HG13	21:W:134:LEU:CB	2.21	0.70
7:G:159:ALA:C	7:G:160:ILE:HD12	2.11	0.70
4:D:24:ALA:HA	7:G:83:LYS:HB2	1.73	0.70
1:A:871:ASP:OD2	1:A:1366:ARG:NH2	2.24	0.70
2:B:73:GLN:HB3	2:B:86:ARG:HB3	1.73	0.70
2:B:549:THR:OG1	2:B:628:THR:OG1	2.09	0.70
2:B:984:HIS:NE2	2:B:1028:GLU:OE1	2.24	0.70
7:G:111:THR:HB	7:G:114:LEU:HD13	1.74	0.70
15:O:191:PRO:HB2	18:T:52:DC:H5"	1.68	0.70
2:B:1056:SER:OG	2:B:1067:ARG:NH1	2.24	0.70
18:T:46:DT:H2"	18:T:47:DA:O5'	1.91	0.70
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	1.73	0.70
7:G:79:PHE:CD2	7:G:81:PRO:HD3	2.26	0.70
17:R:67:GLN:HB3	17:R:219:CYS:HB2	1.73	0.70
4:D:192:LYS:NZ	4:D:204:ASP:OD1	2.23	0.70
2:B:1187:ASN:HD21	2:B:1190:ASP:HB3	1.56	0.69
1:A:441:PRO:HA	1:A:458:HIS:O	1.92	0.69
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.74	0.69
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.75	0.69
4:D:39:ASN:HD21	4:D:43:GLU:HB2	1.58	0.69
12:L:28:LYS:HA	12:L:39:SER:HA	1.74	0.69
1:A:598:LEU:HD21	8:H:124:ARG:HB2	1.73	0.69
1:A:1136:SER:HB3	1:A:1274:ARG:HH12	1.58	0.69
5:E:26:ARG:HH12	5:E:189:GLY:HA3	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:48:DT:H2'	18:T:49:DA:N7	2.08	0.69
1:A:626:ASN:O	1:A:631:HIS:ND1	2.23	0.69
2:B:463:THR:O	2:B:465:ASN:OD1	2.11	0.69
13:M:270:ALA:HB2	15:O:208:VAL:CG1	2.14	0.69
17:R:106:LEU:O	17:R:119:GLU:HA	1.93	0.68
2:B:593:PRO:HB2	2:B:617:ARG:HE	1.56	0.68
2:B:71:LEU:HD23	2:B:88:TYR:HD2	1.57	0.68
13:M:269:ILE:CG2	13:M:272:LYS:CG	2.72	0.68
2:B:53:GLN:OE1	2:B:547:VAL:CG2	2.42	0.68
17:R:63:ARG:NH1	17:R:66:ARG:HH22	1.92	0.68
1:A:906:HIS:O	1:A:1029:ARG:NH2	2.27	0.68
4:D:66:ARG:NH2	7:G:47:CYS:SG	2.67	0.67
13:M:267:LYS:HG3	13:M:268:GLU:H	1.59	0.67
3:C:66:ARG:NH2	3:C:143:LEU:O	2.26	0.67
4:D:32:GLU:HG3	7:G:41:LYS:HE2	1.76	0.67
2:B:758:PHE:HB3	2:B:761:HIS:HD2	1.59	0.67
4:D:32:GLU:CG	7:G:41:LYS:HE2	2.24	0.67
4:D:190:GLU:HA	7:G:167:TYR:CD2	2.28	0.67
1:A:524:VAL:HG12	1:A:525:GLN:HG2	1.77	0.67
17:R:105:THR:HA	17:R:120:TYR:O	1.95	0.67
1:A:407:ARG:HH11	1:A:413:ILE:HD11	1.60	0.67
16:Q:101:PHE:N	17:R:95:ILE:O	2.24	0.67
2:B:369:GLY:HA3	16:Q:367:ALA:CB	2.25	0.67
16:Q:397:ALA:HB3	16:Q:400:LYS:HE3	1.76	0.67
18:T:51:DA:H2'	18:T:52:DC:C6	2.29	0.67
2:B:215:GLN:NE2	2:B:479:VAL:HG22	2.09	0.67
16:Q:135:LEU:HB2	16:Q:136:PRO:HA	1.77	0.67
1:A:888:GLY:O	1:A:940:ARG:NH2	2.27	0.66
13:M:136:LEU:HD13	13:M:196:ILE:HD11	1.78	0.66
18:T:47:DA:C8	18:T:48:DT:O4	2.48	0.66
9:I:78:CYS:SG	9:I:105:SER:OG	2.54	0.66
15:O:191:PRO:HG3	18:T:52:DC:C5'	2.24	0.66
1:A:115:LEU:O	1:A:164:ARG:NH1	2.29	0.66
13:M:286:ILE:HG13	13:M:291:ILE:HG13	1.77	0.66
2:B:309:GLN:OE1	2:B:392:ARG:NH2	2.28	0.66
2:B:629:ASP:OD1	2:B:630:ALA:N	2.29	0.66
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.77	0.66
8:H:8:ASP:OD1	8:H:9:ILE:N	2.29	0.66
7:G:1:MET:HE3	7:G:85:GLU:OE2	1.96	0.66
1:A:362:ASP:O	1:A:458:HIS:ND1	2.28	0.66
2:B:92:PHE:HD2	2:B:130:VAL:HG11	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:22:LEU:HD11	11:K:101:LEU:HD11	1.77	0.66
2:B:68:THR:OG1	16:Q:335:LEU:CD1	2.44	0.65
13:M:272:LYS:HB3	18:T:52:DC:O3'	1.96	0.65
2:B:68:THR:HB	16:Q:335:LEU:HD11	1.76	0.65
16:Q:397:ALA:HB3	16:Q:400:LYS:CE	2.26	0.65
3:C:75:MET:O	3:C:246:ARG:NH2	2.23	0.65
2:B:247:GLY:CA	2:B:418:LYS:HZ3	2.06	0.65
3:C:54:ASN:ND2	3:C:60:ASP:OD1	2.29	0.65
13:M:272:LYS:HB2	18:T:53:DA:OP1	1.94	0.65
13:M:245:HIS:CD2	17:R:264:SER:HB2	2.32	0.65
14:N:31:DG:H3'	17:R:325:PRO:CB	2.26	0.65
7:G:151:ILE:CG1	21:W:134:LEU:CB	2.75	0.65
13:M:34:ILE:HG22	13:M:45:CYS:HA	1.79	0.65
4:D:32:GLU:HG3	7:G:42:PHE:CZ	2.30	0.65
13:M:22:LEU:HB3	13:M:52:LEU:HD23	1.77	0.65
16:Q:378:VAL:HG22	16:Q:384:PHE:HE1	1.61	0.65
19:U:30:ILE:HG23	19:U:31:ASP:H	1.60	0.65
1:A:821:ARG:HE	2:B:514:LEU:HB2	1.62	0.65
13:M:245:HIS:HA	17:R:264:SER:HB3	1.79	0.64
16:Q:373:TYR:HD1	17:R:70:LEU:HD21	1.59	0.64
1:A:198:GLU:OE2	1:A:200:ARG:NH2	2.27	0.64
2:B:835:GLN:HA	2:B:1013:ASN:HD22	1.62	0.64
2:B:837:ASP:OD2	2:B:1020:ARG:NH2	2.30	0.64
2:B:959:ASP:HB2	13:M:143:PRO:HB2	1.79	0.64
3:C:166:GLU:OE2	12:L:70:ARG:NH2	2.30	0.64
1:A:881:GLN:HE21	1:A:959:ASN:HA	1.62	0.64
13:M:188:THR:HG22	13:M:190:LYS:H	1.63	0.64
2:B:44:VAL:CG1	2:B:495:LEU:HD13	2.26	0.64
14:N:30:DA:O5'	14:N:30:DA:H8	1.81	0.64
15:O:191:PRO:HG3	18:T:52:DC:H5'	1.79	0.64
1:A:134:ARG:NH1	1:A:221:SER:O	2.31	0.64
1:A:537:ARG:NH1	8:H:120:GLY:O	2.31	0.64
7:G:111:THR:HG22	7:G:113:HIS:H	1.61	0.64
7:G:34:VAL:HG12	7:G:45:ILE:HG21	1.80	0.64
8:H:110:ASP:O	8:H:129:TYR:N	2.30	0.64
2:B:798:TYR:O	2:B:821:GLN:NE2	2.20	0.63
2:B:44:VAL:HG11	2:B:495:LEU:HD12	1.80	0.63
4:D:49:ALA:CB	7:G:3:PHE:CE1	2.82	0.63
9:I:9:ASP:OD2	16:Q:125:LYS:CE	2.47	0.63
13:M:200:THR:O	13:M:203:PHE:HB3	1.97	0.63
16:Q:141:ARG:O	17:R:207:THR:OG1	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ARG:HE	1:A:1406:VAL:HG21	1.62	0.63
1:A:806:ARG:HH22	2:B:729:ILE:HG13	1.63	0.63
18:T:49:DA:H2'	18:T:50:DT:H5'	1.79	0.63
5:E:76:GLY:N	5:E:106:GLN:OE1	2.31	0.63
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.80	0.63
2:B:278:GLN:HB2	2:B:337:ARG:HD2	1.79	0.63
17:R:98:ASN:HB3	17:R:103:LYS:HG3	1.79	0.63
18:T:44:DA:H2"	18:T:45:DT:O5'	1.99	0.63
2:B:102:VAL:HG23	2:B:112:LEU:HB2	1.81	0.62
9:I:58:VAL:HG21	9:I:109:ILE:HD11	1.80	0.62
1:A:1189:SER:N	1:A:1242:VAL:O	2.28	0.62
5:E:78:LEU:HD21	5:E:109:ILE:HD12	1.80	0.62
1:A:282:ASN:HA	21:W:59:ALA:CB	2.29	0.62
10:J:8:PHE:HB2	10:J:48:ARG:HH22	1.64	0.62
13:M:201:LYS:HA	14:N:23:DA:OP1	1.99	0.62
13:M:274:PRO:CD	15:O:188:GLU:CG	2.74	0.62
2:B:901:PRO:HG2	12:L:60:ARG:HA	1.80	0.62
3:C:146:LYS:NZ	10:J:58:GLU:OE2	2.24	0.62
13:M:267:LYS:CE	15:O:208:VAL:HG13	2.03	0.62
3:C:56:THR:HG22	3:C:147:LEU:HD21	1.81	0.62
5:E:55:ARG:HB2	5:E:84:ASP:OD1	1.99	0.62
1:A:352:VAL:HB	1:A:467:THR:HG22	1.81	0.62
2:B:41:LYS:O	2:B:45:SER:HB3	1.99	0.62
13:M:281:SER:O	13:M:285:ASN:ND2	2.31	0.62
7:G:151:ILE:HD12	21:W:134:LEU:CB	2.29	0.62
18:T:52:DC:H2"	18:T:53:DA:H5'	1.82	0.62
1:A:1146:VAL:HG12	1:A:1201:ALA:HB1	1.81	0.62
4:D:56:ARG:HA	4:D:148:LEU:HD13	1.81	0.62
18:T:42:DC:H2"	18:T:43:DT:C4	2.35	0.62
1:A:372:LYS:HA	1:A:435:HIS:CD2	2.35	0.62
3:C:153:LEU:HD11	3:C:155:LEU:HD23	1.82	0.62
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.82	0.61
3:C:179:GLU:OE1	3:C:206:ASN:ND2	2.32	0.61
9:I:14:LEU:HB3	9:I:27:PHE:HB3	1.81	0.61
3:C:254:LYS:HG2	11:K:42:LEU:HD12	1.82	0.61
7:G:1:MET:CE	7:G:85:GLU:OE2	2.49	0.61
15:O:170:ILE:O	15:O:239:LYS:HE2	2.00	0.61
1:A:587:HIS:CD2	1:A:969:GLN:HG3	2.35	0.61
2:B:870:ILE:HG23	2:B:917:PRO:HD2	1.83	0.61
1:A:335:ARG:NH2	2:B:1114:LEU:HD21	2.14	0.61
1:A:544:ASP:OD1	1:A:545:GLN:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:GLN:NE2	16:Q:401:TYR:OH	2.28	0.61
2:B:868:MET:HG2	13:M:182:ARG:HG3	1.83	0.61
4:D:32:GLU:CG	7:G:42:PHE:CE1	2.84	0.61
1:A:260:ASP:OD1	1:A:261:ASP:N	2.34	0.61
2:B:68:THR:CB	16:Q:335:LEU:HD12	2.30	0.61
2:B:865:LYS:NZ	13:M:145:ILE:CD1	2.63	0.61
2:B:865:LYS:HE2	13:M:145:ILE:HD12	1.76	0.61
16:Q:339:ALA:HB1	16:Q:343:ARG:HH12	1.65	0.61
19:U:37:ASP:O	19:U:41:ILE:HG13	2.01	0.61
1:A:929:LEU:HD11	1:A:983:ILE:HG21	1.83	0.60
13:M:43:VAL:HG12	13:M:53:SER:HB3	1.82	0.60
13:M:267:LYS:HD3	15:O:239:LYS:CD	2.31	0.60
2:B:119:LEU:HD22	2:B:953:LEU:HD21	1.82	0.60
2:B:199:MET:SD	2:B:492:LEU:HD23	2.42	0.60
21:W:39:ALA:HA	21:W:85:VAL:O	2.01	0.60
18:T:51:DA:C2'	18:T:52:DC:C6	2.83	0.60
1:A:261:ASP:HB3	1:A:322:VAL:HG13	1.83	0.60
8:H:104:PHE:HZ	8:H:137:GLN:H	1.48	0.60
18:T:50:DT:H2"	18:T:51:DA:H5'	1.82	0.60
1:A:1199:ARG:O	1:A:1203:ASN:ND2	2.35	0.60
2:B:465:ASN:OD1	2:B:465:ASN:N	2.33	0.60
3:C:115:SER:HB3	3:C:142:VAL:HB	1.83	0.60
16:Q:378:VAL:HG22	16:Q:384:PHE:CE1	2.36	0.60
18:T:43:DT:C6	18:T:43:DT:P	2.94	0.60
19:U:31:ASP:HB3	19:U:34:THR:OG1	2.02	0.60
1:A:22:PHE:HB2	2:B:1211:ASN:OD1	2.02	0.59
2:B:429:PHE:CZ	16:Q:332:LEU:HB2	2.37	0.59
5:E:88:VAL:HB	5:E:116:ILE:HG12	1.82	0.59
1:A:993:LEU:HD11	1:A:1050:GLU:HB2	1.84	0.59
2:B:247:GLY:CA	2:B:418:LYS:HZ1	2.13	0.59
2:B:283:VAL:HG11	2:B:321:GLY:HA3	1.82	0.59
18:T:47:DA:H2'	18:T:48:DT:C5	2.38	0.59
2:B:326:ASP:OD1	2:B:327:ARG:N	2.35	0.59
3:C:44:LEU:HB2	3:C:77:ILE:HD13	1.83	0.59
7:G:138:THR:HG22	7:G:139:ILE:H	1.67	0.59
1:A:95:PHE:HE1	1:A:1414:ALA:HB2	1.67	0.59
1:A:568:PRO:HG2	8:H:46:LEU:HD23	1.84	0.59
3:C:124:LEU:O	3:C:127:ARG:HG2	2.01	0.59
21:W:39:ALA:O	21:W:41:ASP:N	2.28	0.59
1:A:345:VAL:HG12	2:B:1155:SER:HB2	1.84	0.59
1:A:1116:LEU:HB2	1:A:1308:THR:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:GLU:HG2	2:B:190:TYR:HE2	1.67	0.59
2:B:62:ILE:O	2:B:65:GLU:HG2	2.01	0.59
2:B:71:LEU:HD12	16:Q:331:GLN:O	2.02	0.59
7:G:57:GLN:HG2	7:G:58:ARG:H	1.67	0.59
16:Q:373:TYR:OH	17:R:72:ARG:NH2	2.36	0.59
19:U:242:ASN:HA	19:U:268:THR:O	2.02	0.59
1:A:390:GLN:OE1	1:A:393:ARG:NH2	2.36	0.59
2:B:1042:GLY:HA2	16:Q:22:ILE:HA	1.83	0.59
15:O:191:PRO:CG	18:T:52:DC:C5'	2.80	0.59
7:G:148:GLU:H	7:G:161:GLY:HA2	1.67	0.59
12:L:33:GLU:HG3	12:L:34:CYS:N	2.18	0.59
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.84	0.58
2:B:1065:GLN:OE1	2:B:1066:SER:N	2.37	0.58
1:A:472:LEU:HD22	2:B:835:GLN:NE2	2.17	0.58
2:B:43:LEU:HD11	2:B:812:LEU:HD23	1.84	0.58
2:B:1037:LEU:O	10:J:47:ARG:NH2	2.36	0.58
16:Q:119:LEU:O	17:R:132:GLU:HA	2.03	0.58
13:M:267:LYS:HE2	15:O:208:VAL:HG11	1.79	0.58
17:R:138:GLN:HB2	17:R:211:LYS:CB	2.31	0.58
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.38	0.58
4:D:54:GLU:HG2	4:D:58:VAL:HG23	1.84	0.58
4:D:57:LEU:O	4:D:61:GLU:N	2.32	0.58
4:D:153:ARG:NH1	4:D:183:LEU:O	2.37	0.58
18:T:50:DT:H2'	18:T:51:DA:C8	2.38	0.58
1:A:1206:ASP:O	1:A:1274:ARG:NH2	2.37	0.58
2:B:835:GLN:HA	2:B:1013:ASN:ND2	2.19	0.58
12:L:33:GLU:HG3	12:L:34:CYS:H	1.69	0.58
2:B:109:THR:HG21	17:R:263:MET:HG3	1.86	0.58
17:R:306:LEU:O	17:R:310:TYR:N	2.37	0.58
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.39	0.58
1:A:381:THR:HG23	1:A:383:TYR:H	1.69	0.58
16:Q:373:TYR:HD1	17:R:70:LEU:HD11	1.68	0.58
16:Q:373:TYR:CE1	17:R:70:LEU:HD21	2.38	0.58
1:A:42:ASP:OD1	1:A:43:GLU:N	2.37	0.58
8:H:7:ASP:OD1	8:H:8:ASP:N	2.37	0.58
2:B:956:THR:HG23	12:L:46:VAL:HB	1.86	0.58
3:C:148:ARG:NH2	10:J:64:ASN:HA	2.19	0.58
4:D:148:LEU:O	4:D:152:SER:OG	2.15	0.57
15:O:105:ARG:HD2	20:V:69:TYR:OH	2.03	0.57
17:R:105:THR:OG1	17:R:120:TYR:O	2.18	0.57
18:T:48:DT:C2'	18:T:49:DA:C8	2.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:149:LYS:HG3	3:C:150:GLY:N	2.19	0.57
10:J:8:PHE:HB2	10:J:48:ARG:NH2	2.19	0.57
1:A:503:GLN:OE1	6:F:90:ARG:NH1	2.32	0.57
1:A:903:ASN:OD1	1:A:904:THR:N	2.37	0.57
2:B:911:ILE:HD11	2:B:941:LEU:HD12	1.86	0.57
2:B:1106:ARG:CZ	2:B:1118:PRO:HB3	2.34	0.57
2:B:1187:ASN:ND2	2:B:1190:ASP:O	2.38	0.57
2:B:156:SER:O	2:B:163:GLY:N	2.37	0.57
2:B:676:VAL:O	2:B:677:GLU:HG2	2.04	0.57
7:G:101:VAL:N	7:G:108:VAL:O	2.36	0.57
17:R:98:ASN:ND2	17:R:103:LYS:HE3	2.20	0.57
5:E:43:LYS:O	5:E:47:CYS:HB2	2.05	0.57
8:H:64:ASN:OD1	8:H:65:LEU:N	2.38	0.57
13:M:201:LYS:CA	14:N:23:DA:OP1	2.50	0.57
1:A:1445:ILE:HB	7:G:61:ILE:HD11	1.87	0.57
2:B:73:GLN:O	2:B:86:ARG:N	2.33	0.57
2:B:642:ASP:HA	2:B:649:LYS:HG2	1.86	0.57
5:E:65:THR:O	5:E:69:ILE:HD12	2.04	0.57
14:N:61:DC:H2'	14:N:62:DA:C8	2.40	0.57
1:A:34:LYS:NZ	1:A:85:ASP:OD2	2.38	0.57
1:A:365:GLY:HA2	1:A:461:LYS:O	2.05	0.57
1:A:471:ASN:OD1	1:A:472:LEU:N	2.37	0.57
2:B:209:GLU:OE2	2:B:788:ARG:NH2	2.37	0.57
17:R:120:TYR:CD1	17:R:226:PRO:HA	2.39	0.57
1:A:752:LYS:HG3	2:B:1015:HIS:HB3	1.85	0.56
2:B:217:ARG:NH1	2:B:407:ASP:CG	2.58	0.56
2:B:259:TYR:HE2	2:B:270:LYS:HB2	1.69	0.56
2:B:365:THR:HG21	2:B:370:PHE:CG	2.40	0.56
9:I:31:THR:O	16:Q:401:TYR:CB	2.53	0.56
1:A:367:PRO:HG2	1:A:466:SER:O	2.04	0.56
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.88	0.56
1:A:940:ARG:HH21	1:A:944:ARG:NH2	2.03	0.56
2:B:209:GLU:O	2:B:482:VAL:HA	2.06	0.56
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.19	0.56
8:H:56:THR:O	8:H:144:ILE:HA	2.06	0.56
13:M:177:LEU:HD22	13:M:207:LEU:HD11	1.85	0.56
17:R:64:SER:O	17:R:217:THR:HG23	2.06	0.56
18:T:52:DC:P	18:T:52:DC:C3'	2.94	0.56
5:E:179:GLN:HA	5:E:215:MET:HG2	1.86	0.56
15:O:91:ASN:HD22	19:U:285:TRP:HZ2	1.51	0.56
1:A:562:THR:O	1:A:576:GLN:NE2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:339:ALA:HB1	16:Q:343:ARG:NH1	2.20	0.56
1:A:29:ALA:HB1	2:B:1184:GLY:HA3	1.87	0.56
1:A:1146:VAL:HG23	1:A:1197:LEU:HD22	1.86	0.56
7:G:119:LEU:HD11	7:G:130:TYR:HB3	1.87	0.56
1:A:1138:ILE:O	1:A:1276:VAL:N	2.34	0.56
13:M:243:CYS:O	13:M:247:GLY:N	2.39	0.56
16:Q:100:GLU:HA	17:R:96:ARG:HA	1.86	0.56
1:A:146:MET:O	1:A:171:GLN:N	2.38	0.56
3:C:6:PRO:HB3	3:C:25:VAL:CG2	2.35	0.56
1:A:203:SER:N	1:A:206:GLU:OE2	2.39	0.56
1:A:491:VAL:O	2:B:1150:ARG:NH2	2.39	0.56
2:B:29:ASP:OD2	2:B:658:ILE:HG13	2.05	0.56
2:B:108:VAL:HA	13:M:244:SER:OG	2.06	0.56
3:C:60:ASP:HB3	12:L:67:PHE:HE2	1.70	0.56
7:G:79:PHE:CE2	7:G:81:PRO:CG	2.86	0.56
17:R:262:THR:O	17:R:266:THR:HG23	2.04	0.56
1:A:475:THR:OG1	1:A:480:ALA:O	2.21	0.56
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.41	0.56
1:A:1342:GLU:OE1	5:E:200:ARG:NH2	2.29	0.56
2:B:211:VAL:O	2:B:480:SER:HA	2.06	0.56
2:B:861:ASP:OD1	2:B:862:GLN:N	2.38	0.56
13:M:238:TYR:HB3	13:M:242:PHE:CE2	2.40	0.56
2:B:170:LEU:HD12	2:B:171:PRO:HD2	1.88	0.55
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.71	0.55
13:M:180:CYS:SG	13:M:187:ARG:HG2	2.46	0.55
17:R:127:LYS:HA	17:R:220:HIS:CE1	2.41	0.55
14:N:24:DT:H2"	14:N:25:DA:C5'	2.17	0.55
2:B:923:GLU:HB2	2:B:928:ARG:HD2	1.88	0.55
7:G:50:ASP:OD2	7:G:53:ASN:HB2	2.07	0.55
13:M:267:LYS:HD3	15:O:239:LYS:HD3	1.87	0.55
19:U:245:LEU:HB3	20:V:9:LEU:HD22	1.89	0.55
1:A:778:GLY:HA3	2:B:516:ASN:HB2	1.86	0.55
1:A:1224:LEU:HD12	1:A:1241:ARG:O	2.05	0.55
19:U:25:PHE:O	19:U:30:ILE:HG22	2.05	0.55
19:U:30:ILE:O	19:U:31:ASP:HB2	2.06	0.55
1:A:666:ILE:HG23	2:B:1026:LEU:HB3	1.87	0.55
1:A:833:GLU:OE2	1:A:1102:LYS:HD2	2.06	0.55
1:A:1148:ILE:HA	9:I:49:ILE:HD12	1.87	0.55
2:B:46:GLN:HG2	2:B:408:LEU:HD21	1.88	0.55
2:B:557:PHE:CZ	2:B:603:LEU:HD11	2.41	0.55
2:B:46:GLN:OE1	2:B:46:GLN:N	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296:GLU:HG2	2:B:300:HIS:NE2	2.22	0.55
14:N:28:DA:C8	14:N:29:DT:H73	2.42	0.55
16:Q:366:GLU:CB	16:Q:392:VAL:HG13	2.36	0.55
17:R:122:LEU:HD21	17:R:222:CYS:HB3	1.89	0.55
20:V:60:LEU:HD21	20:V:87:VAL:HG22	1.89	0.55
1:A:566:ILE:O	8:H:96:VAL:HB	2.07	0.55
1:A:1364:ASN:OD1	1:A:1365:TYR:N	2.40	0.55
2:B:104:GLU:OE2	12:L:54:ARG:HD2	2.07	0.55
14:N:22:DT:C2'	14:N:23:DA:O5'	2.54	0.55
16:Q:119:LEU:HD22	16:Q:395:PHE:CE2	2.41	0.55
2:B:44:VAL:CG1	2:B:495:LEU:CD1	2.81	0.54
14:N:29:DT:C2'	14:N:30:DA:C8	2.84	0.54
15:O:169:PRO:HG2	15:O:240:MET:SD	2.47	0.54
1:A:1386:ARG:HH21	18:T:13:DC:H4'	1.72	0.54
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.88	0.54
4:D:39:ASN:ND2	4:D:43:GLU:HB2	2.21	0.54
4:D:49:ALA:HB1	7:G:3:PHE:HE1	1.72	0.54
17:R:98:ASN:CB	17:R:103:LYS:O	2.53	0.54
3:C:46:ILE:HA	3:C:159:ALA:HA	1.89	0.54
13:M:267:LYS:HZ2	15:O:169:PRO:HB3	1.64	0.54
1:A:225:ASN:N	1:A:229:SER:OG	2.28	0.54
1:A:1144:LYS:HE3	9:I:48:LEU:HD22	1.89	0.54
1:A:1386:ARG:O	1:A:1390:ASN:HB3	2.07	0.54
9:I:9:ASP:OD2	16:Q:125:LYS:HE3	2.07	0.54
1:A:436:ILE:HD11	1:A:491:VAL:HG21	1.89	0.54
1:A:441:PRO:HD2	1:A:498:ARG:NH1	2.22	0.54
1:A:570:PRO:O	1:A:571:LEU:HD12	2.07	0.54
3:C:6:PRO:HB3	3:C:25:VAL:HG23	1.90	0.54
3:C:254:LYS:O	3:C:257:SER:OG	2.21	0.54
7:G:62:LEU:HD12	7:G:63:PRO:O	2.08	0.54
14:N:22:DT:H2"	14:N:23:DA:O5'	2.04	0.54
4:D:49:ALA:HA	7:G:3:PHE:CE1	2.43	0.54
2:B:86:ARG:HG3	2:B:137:TYR:O	2.08	0.54
2:B:1073:TYR:CE1	2:B:1080:LYS:HG2	2.43	0.54
3:C:136:ASP:OD1	3:C:137:LYS:N	2.41	0.54
17:R:122:LEU:HD21	17:R:222:CYS:SG	2.47	0.54
1:A:798:GLY:HA2	1:A:815:PHE:CD2	2.43	0.54
2:B:298:LEU:HD23	2:B:311:LEU:HD22	1.89	0.54
2:B:368:GLU:OE2	16:Q:344:PHE:HD1	1.90	0.54
1:A:285:PRO:HD2	1:A:288:ALA:HB3	1.89	0.53
2:B:756:ILE:HG12	2:B:770:GLN:HG2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1094:ARG:NH2	2:B:1098:MET:SD	2.82	0.53
13:M:177:LEU:HD11	13:M:189:PHE:CD1	2.43	0.53
1:A:821:ARG:HD2	2:B:514:LEU:H	1.73	0.53
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.88	0.53
4:D:134:THR:HG22	4:D:136:GLY:H	1.73	0.53
9:I:56:ALA:O	9:I:89:GLN:HG3	2.09	0.53
13:M:283:TYR:CZ	13:M:287:LEU:HD11	2.44	0.53
3:C:102:GLN:HG3	3:C:154:LYS:HG3	1.90	0.53
1:A:59:GLY:HA2	1:A:67:CYS:SG	2.48	0.53
1:A:284:ALA:HB1	1:A:289:ILE:HD11	1.90	0.53
2:B:129:PHE:HA	2:B:165:VAL:O	2.09	0.53
13:M:43:VAL:O	13:M:52:LEU:N	2.39	0.53
2:B:35:SER:OG	2:B:811:TYR:OH	2.18	0.53
4:D:183:LEU:HD11	7:G:86:VAL:O	2.08	0.53
13:M:273:SER:HB2	15:O:188:GLU:HA	1.89	0.53
16:Q:98:TYR:HA	17:R:97:ILE:O	2.08	0.53
2:B:104:GLU:OE2	12:L:54:ARG:CD	2.55	0.53
5:E:26:ARG:NH2	5:E:133:GLU:OE1	2.42	0.53
1:A:977:LYS:O	1:A:1036:ARG:NH2	2.38	0.53
2:B:969:ARG:HH22	3:C:60:ASP:HB2	1.74	0.53
1:A:13:THR:OG1	1:A:1432:GLN:OE1	2.27	0.53
8:H:136:LYS:O	8:H:138:GLU:N	2.41	0.53
2:B:283:VAL:O	2:B:287:ARG:HG2	2.09	0.53
2:B:369:GLY:C	16:Q:367:ALA:HB3	2.29	0.53
4:D:64:VAL:HG13	4:D:67:ARG:HH22	1.74	0.53
7:G:86:VAL:HA	7:G:146:LYS:HA	1.90	0.53
16:Q:99:ASN:O	17:R:97:ILE:N	2.37	0.53
1:A:806:ARG:NH2	2:B:729:ILE:HG13	2.24	0.53
17:R:63:ARG:HD2	17:R:66:ARG:CZ	2.39	0.53
1:A:839:ARG:NH2	1:A:1402:PHE:O	2.33	0.52
2:B:841:MET:O	2:B:993:THR:HA	2.09	0.52
13:M:255:SER:OG	13:M:285:ASN:OD1	2.17	0.52
1:A:208:LEU:HD21	1:A:212:LYS:HE3	1.90	0.52
2:B:451:LYS:O	2:B:455:SER:OG	2.17	0.52
3:C:8:VAL:HG11	11:K:105:PHE:HD1	1.74	0.52
2:B:499:ASN:OD1	2:B:500:THR:N	2.42	0.52
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.90	0.52
16:Q:365:TYR:CZ	16:Q:367:ALA:HA	2.45	0.52
1:A:826:ASP:OD1	1:A:827:THR:N	2.43	0.52
2:B:822:ASN:O	10:J:48:ARG:NH1	2.43	0.52
4:D:194:LEU:HD22	7:G:86:VAL:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:GLU:CG	1:A:1418:LEU:HD11	2.40	0.52
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.91	0.52
2:B:96:TYR:HB2	2:B:129:PHE:HB2	1.92	0.52
2:B:179:CYS:SG	2:B:180:TYR:N	2.82	0.52
2:B:296:GLU:OE2	16:Q:122:GLN:NE2	2.42	0.52
3:C:21:ILE:HG12	3:C:229:TYR:CD1	2.44	0.52
8:H:89:LEU:C	8:H:91:ASP:H	2.13	0.52
9:I:19:ASP:O	9:I:23:ASN:HA	2.10	0.52
9:I:28:GLU:HA	9:I:35:VAL:HG22	1.92	0.52
13:M:177:LEU:O	13:M:181:ARG:HG2	2.09	0.52
1:A:522:GLY:O	1:A:524:VAL:HG23	2.10	0.52
1:A:1350:LYS:O	1:A:1354:ASN:ND2	2.42	0.52
2:B:99:LYS:HB3	2:B:180:TYR:CE1	2.45	0.52
2:B:100:PRO:HD2	2:B:180:TYR:CZ	2.44	0.52
7:G:10:ASN:HA	7:G:70:PHE:O	2.10	0.52
1:A:367:PRO:HA	1:A:463:ILE:O	2.09	0.52
1:A:443:LEU:HD12	2:B:1146:PHE:CZ	2.44	0.52
13:M:174:ALA:O	13:M:178:ILE:HG12	2.10	0.52
2:B:637:LEU:HD12	2:B:693:ILE:HD13	1.91	0.52
7:G:95:SER:O	7:G:130:TYR:OH	2.27	0.52
8:H:130:ARG:O	8:H:133:ASN:ND2	2.41	0.52
15:O:191:PRO:HB3	18:T:52:DC:C5'	2.29	0.52
1:A:804:TYR:HH	1:A:816:HIS:CE1	2.27	0.52
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.93	0.52
5:E:122:LYS:O	5:E:125:PRO:HD2	2.10	0.52
1:A:1132:LYS:HG2	1:A:1135:ARG:HH22	1.75	0.51
1:A:1151:GLU:OE2	9:I:42:LEU:HD13	2.10	0.51
10:J:6:ARG:HA	10:J:13:VAL:HA	1.92	0.51
13:M:267:LYS:HE2	15:O:208:VAL:HG12	1.84	0.51
17:R:121:ASP:O	17:R:225:MET:HB2	2.10	0.51
17:R:126:LYS:HD2	17:R:129:VAL:HG12	1.91	0.51
19:U:259:LYS:HA	19:U:281:VAL:O	2.10	0.51
1:A:407:ARG:NH1	1:A:413:ILE:HD11	2.25	0.51
4:D:70:PHE:HE2	4:D:133:THR:HA	1.75	0.51
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.90	0.51
2:B:757:PRO:HG3	2:B:983:ARG:HH21	1.75	0.51
4:D:118:THR:HG21	4:D:121:LYS:HG2	1.91	0.51
13:M:154:TYR:CE1	13:M:171:ILE:HD13	2.45	0.51
16:Q:103:LEU:HD23	16:Q:384:PHE:HB2	1.92	0.51
14:N:21:DG:H2'	14:N:22:DT:H71	1.93	0.51
18:T:49:DA:C2'	18:T:50:DT:C5'	2.85	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:147:SER:O	6:F:150:GLU:HG2	2.11	0.51
8:H:100:THR:OG1	8:H:139:ASN:OD1	2.20	0.51
10:J:21:TYR:CZ	10:J:25:LEU:HD11	2.45	0.51
1:A:137:ALA:O	1:A:140:THR:OG1	2.19	0.51
2:B:405:ARG:HH12	2:B:632:ARG:CG	1.99	0.51
2:B:776:GLN:HG3	2:B:1095:LEU:HD22	1.91	0.51
7:G:21:ARG:HG3	7:G:25:TYR:HE1	1.75	0.51
1:A:407:ARG:NH2	13:M:26:GLU:OE2	2.44	0.51
1:A:996:ASN:HB3	1:A:1050:GLU:OE2	2.11	0.51
2:B:840:ILE:O	2:B:1010:LEU:HD12	2.10	0.51
4:D:49:ALA:HB1	7:G:3:PHE:CE1	2.45	0.51
8:H:36:CYS:HA	8:H:126:GLU:O	2.11	0.51
8:H:107:VAL:HG13	8:H:108:SER:H	1.75	0.51
13:M:191:GLU:HB3	17:R:268:MET:SD	2.51	0.51
1:A:613:ILE:HG22	1:A:614:PHE:HD1	1.76	0.51
1:A:663:SER:OG	1:A:664:THR:N	2.44	0.51
2:B:868:MET:CG	13:M:149:CYS:SG	2.99	0.51
2:B:1076:HIS:O	3:C:31:ASN:ND2	2.44	0.51
5:E:191:LYS:N	5:E:194:GLU:OE1	2.39	0.51
1:A:567:LYS:HZ2	8:H:91:ASP:HA	1.76	0.51
2:B:474:SER:O	2:B:475:SER:HB3	2.11	0.51
11:K:63:VAL:HG12	11:K:71:PHE:HB3	1.93	0.51
13:M:143:PRO:HG2	13:M:146:VAL:HG23	1.93	0.51
1:A:350:ARG:NE	1:A:486:GLU:OE1	2.44	0.51
7:G:151:ILE:HG13	21:W:134:LEU:CA	2.41	0.51
18:T:43:DT:H2"	18:T:44:DA:H8	1.67	0.51
1:A:209:ASN:OD1	1:A:213:HIS:NE2	2.44	0.50
1:A:597:LEU:HD13	8:H:103:LYS:HD3	1.93	0.50
16:Q:399:ASN:OD1	16:Q:402:ALA:HA	2.11	0.50
2:B:87:LYS:HE3	2:B:147:LEU:HD11	1.92	0.50
2:B:187:SER:HA	2:B:190:TYR:HD2	1.76	0.50
2:B:311:LEU:HA	2:B:314:LEU:HD12	1.93	0.50
2:B:706:GLN:HB2	2:B:709:ASP:HB2	1.93	0.50
6:F:99:LEU:O	6:F:102:SER:OG	2.19	0.50
1:A:23:SER:OG	1:A:25:GLU:OE1	2.28	0.50
1:A:225:ASN:H	1:A:229:SER:HG	1.55	0.50
1:A:549:MET:HE1	1:A:656:TRP:CD1	2.46	0.50
1:A:1138:ILE:HG13	1:A:1139:GLU:N	2.27	0.50
1:A:1442:ASP:OD2	7:G:60:ARG:HD2	2.12	0.50
4:D:32:GLU:HB3	7:G:42:PHE:HE1	1.77	0.50
4:D:39:ASN:HA	7:G:6:ASP:OD2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:306:GLU:O	13:M:309:ILE:HG12	2.11	0.50
13:M:325:ASP:HB3	13:M:326:PRO:HD3	1.92	0.50
1:A:1402:PHE:CD2	1:A:1403:GLU:HG2	2.45	0.50
7:G:101:VAL:HG21	7:G:145:VAL:HG21	1.93	0.50
13:M:134:THR:HG23	13:M:147:LYS:NZ	2.26	0.50
1:A:901:LEU:HB3	1:A:921:GLY:H	1.77	0.50
1:A:1402:PHE:CE2	1:A:1403:GLU:HG2	2.46	0.50
3:C:40:GLU:OE1	3:C:254:LYS:HE3	2.10	0.50
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.92	0.50
4:D:56:ARG:HB2	4:D:148:LEU:HB3	1.92	0.50
1:A:377:PRO:HB3	1:A:433:GLU:HG2	1.93	0.50
2:B:475:SER:O	2:B:476:ARG:CB	2.60	0.50
2:B:548:GLY:HA3	2:B:630:ALA:HB2	1.94	0.50
18:T:43:DT:P	18:T:43:DT:H6	2.33	0.50
2:B:55:VAL:O	17:R:252:ILE:HD12	2.12	0.50
2:B:496:ARG:NH2	2:B:540:SER:O	2.45	0.50
1:A:381:THR:OG1	1:A:382:PRO:HD2	2.11	0.50
2:B:368:GLU:OE2	16:Q:344:PHE:CD1	2.65	0.50
7:G:83:LYS:HE3	7:G:150:CYS:HB2	1.94	0.50
7:G:97:HIS:O	7:G:112:LYS:N	2.43	0.50
9:I:88:SER:O	9:I:91:ARG:NH1	2.45	0.50
15:O:169:PRO:HB2	15:O:239:LYS:HB2	1.93	0.50
8:H:35:GLN:HB3	8:H:111:LEU:HD21	1.94	0.50
13:M:30:TYR:CD1	13:M:31:PRO:HD2	2.47	0.50
13:M:272:LYS:O	13:M:273:SER:OG	2.24	0.50
1:A:1116:LEU:HD12	1:A:1311:VAL:HG22	1.93	0.49
1:A:1155:ASP:OD2	1:A:1161:THR:HA	2.12	0.49
2:B:486:TYR:HA	2:B:1096:ARG:HH21	1.76	0.49
16:Q:100:GLU:HG2	17:R:96:ARG:HB2	1.94	0.49
1:A:821:ARG:HD2	2:B:514:LEU:N	2.27	0.49
1:A:909:ASP:OD2	1:A:911:SER:OG	2.21	0.49
2:B:67:SER:HB2	2:B:92:PHE:HB2	1.94	0.49
2:B:149:TYR:HE2	2:B:151:LEU:HD23	1.78	0.49
3:C:25:VAL:HG12	3:C:26:ASP:O	2.13	0.49
3:C:125:MET:HB2	3:C:127:ARG:NH1	2.27	0.49
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	2.27	0.49
2:B:69:LEU:HD12	2:B:69:LEU:O	2.12	0.49
4:D:33:PHE:HZ	7:G:42:PHE:HA	1.77	0.49
5:E:202:SER:HB3	5:E:206:GLY:H	1.77	0.49
13:M:201:LYS:HE3	14:N:23:DA:O5'	2.12	0.49
1:A:51:GLY:H	1:A:55:ASP:HB3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:GLN:HG3	2:B:57:TYR:HD2	1.77	0.49
2:B:570:VAL:HG23	2:B:573:GLN:HB3	1.94	0.49
3:C:35:ARG:NE	11:K:41:THR:OG1	2.35	0.49
5:E:48:ASP:OD1	5:E:51:GLY:N	2.45	0.49
7:G:114:LEU:HD23	7:G:162:SER:HB3	1.94	0.49
1:A:733:ALA:O	1:A:737:LEU:HG	2.11	0.49
3:C:52:GLU:HG2	3:C:53:THR:HG23	1.94	0.49
4:D:52:LEU:HA	4:D:55:ALA:HB3	1.95	0.49
8:H:101:ALA:HB2	8:H:116:TYR:CE1	2.47	0.49
9:I:59:VAL:HG12	9:I:61:ASP:H	1.76	0.49
13:M:22:LEU:O	13:M:32:PRO:HB3	2.13	0.49
13:M:157:CYS:HB3	13:M:210:MET:SD	2.52	0.49
20:V:25:THR:O	20:V:29:ASP:HB3	2.13	0.49
1:A:848:ILE:HG12	1:A:858:ASN:HB3	1.94	0.49
2:B:106:ASP:OD1	2:B:108:VAL:HG12	2.12	0.49
2:B:601:ARG:HD3	2:B:605:ARG:NH2	2.28	0.49
11:K:45:LEU:HG	11:K:94:ILE:HD13	1.94	0.49
16:Q:133:PHE:HZ	16:Q:353:GLU:HA	1.77	0.49
2:B:1164:GLY:HA3	2:B:1190:ASP:OD2	2.13	0.49
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.95	0.49
3:C:169:LYS:NZ	12:L:69:ALA:HB3	2.28	0.49
5:E:16:PHE:CZ	5:E:20:LYS:HE3	2.46	0.49
9:I:71:SER:OG	9:I:83:ASN:OD1	2.25	0.49
16:Q:100:GLU:OE2	17:R:96:ARG:NH2	2.45	0.49
16:Q:139:LEU:HD12	16:Q:351:VAL:O	2.13	0.49
18:T:52:DC:H2"	18:T:53:DA:C5'	2.42	0.49
1:A:64:ASN:HA	13:M:20:ILE:HB	1.95	0.49
1:A:666:ILE:HD11	2:B:1030:LEU:HD22	1.94	0.49
2:B:778:MET:HA	2:B:1096:ARG:HH12	1.76	0.49
10:J:48:ARG:O	10:J:52:THR:OG1	2.10	0.49
14:N:23:DA:N6	18:T:51:DA:N6	2.60	0.49
1:A:8:SER:OG	2:B:1178:ASN:ND2	2.45	0.49
1:A:1420:ASP:OD2	1:A:1422:ARG:NE	2.36	0.49
2:B:856:PHE:CE1	2:B:969:ARG:HB3	2.48	0.49
7:G:83:LYS:HG2	7:G:149:GLY:HA2	1.94	0.49
2:B:22:SER:O	2:B:654:ARG:NH1	2.44	0.49
3:C:80:LEU:HD12	3:C:94:LYS:O	2.13	0.49
4:D:188:ALA:HB2	4:D:208:GLU:HG3	1.95	0.49
5:E:23:VAL:HG12	5:E:28:TYR:HB2	1.95	0.49
7:G:115:MET:HB3	7:G:119:LEU:HD23	1.94	0.49
13:M:277:ILE:HA	13:M:280:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:43:LEU:O	21:W:47:LEU:N	2.44	0.49
2:B:249:ARG:HH12	2:B:418:LYS:HB2	1.78	0.48
2:B:604:ARG:NH2	2:B:615:MET:HG2	2.28	0.48
2:B:619:ILE:O	9:I:59:VAL:HG21	2.12	0.48
2:B:807:ARG:HG2	2:B:1043:ASP:OD1	2.13	0.48
8:H:89:LEU:O	8:H:91:ASP:N	2.46	0.48
19:U:241:GLU:O	19:U:241:GLU:HG2	2.12	0.48
1:A:445:ASN:OD1	1:A:446:ARG:N	2.46	0.48
1:A:1444:MET:SD	6:F:135:ARG:NH2	2.84	0.48
2:B:217:ARG:NH1	2:B:407:ASP:OD1	2.45	0.48
2:B:569:TYR:CE2	2:B:571:PRO:HG3	2.48	0.48
3:C:59:ALA:O	3:C:62:PHE:HB3	2.13	0.48
4:D:194:LEU:HB3	7:G:86:VAL:HG21	1.95	0.48
13:M:199:LYS:O	13:M:200:THR:HB	2.13	0.48
13:M:267:LYS:HG3	13:M:268:GLU:N	2.27	0.48
1:A:1438:THR:HG23	6:F:92:ARG:HB2	1.95	0.48
8:H:13:SER:N	8:H:27:GLU:O	2.46	0.48
16:Q:121:PHE:CD1	16:Q:395:PHE:HB2	2.49	0.48
16:Q:344:PHE:O	16:Q:347:PHE:HD2	1.97	0.48
18:T:41:DA:H2"	18:T:42:DC:C6	2.47	0.48
22:X:261:LYS:O	22:X:265:ASN:N	2.47	0.48
1:A:113:LEU:HD11	1:A:218:ASP:HA	1.96	0.48
1:A:975:HIS:O	1:A:976:THR:OG1	2.24	0.48
2:B:856:PHE:CD1	2:B:969:ARG:HB3	2.47	0.48
2:B:1004:GLU:O	3:C:177:GLU:HG2	2.14	0.48
13:M:154:TYR:HE1	13:M:171:ILE:HD13	1.78	0.48
16:Q:121:PHE:HD1	16:Q:395:PHE:HB2	1.78	0.48
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.95	0.48
1:A:1130:GLN:O	1:A:1134:ILE:HD12	2.12	0.48
2:B:642:ASP:HB3	2:B:649:LYS:NZ	2.29	0.48
13:M:147:LYS:HE2	13:M:151:LYS:HE3	1.95	0.48
14:N:24:DT:H3'	14:N:24:DT:H6	1.79	0.48
1:A:630:ILE:HG12	1:A:646:PHE:HE1	1.78	0.48
2:B:210:LYS:NZ	2:B:462:ALA:HA	2.28	0.48
2:B:801:LYS:HG2	10:J:52:THR:O	2.13	0.48
2:B:869:SER:HB3	13:M:152:GLU:OE2	2.14	0.48
3:C:98:VAL:HB	3:C:122:SER:HB3	1.95	0.48
8:H:93:TYR:CD1	8:H:143:LEU:HD23	2.48	0.48
13:M:267:LYS:HD3	15:O:239:LYS:HE3	1.95	0.48
16:Q:119:LEU:HD21	17:R:135:PHE:CE1	2.48	0.48
1:A:337:ARG:HH12	1:A:839:ARG:NE	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:VAL:HG22	1:A:388:LEU:HD13	1.96	0.48
1:A:704:ALA:HB2	1:A:710:LEU:HA	1.95	0.48
2:B:336:ARG:HD2	2:B:348:ARG:NH1	2.28	0.48
5:E:106:GLN:O	5:E:130:ALA:HA	2.14	0.48
18:T:50:DT:H3'	18:T:50:DT:H6	1.79	0.48
1:A:1153:TYR:HB2	1:A:1192:LEU:HD23	1.96	0.48
2:B:995:ARG:NH1	11:K:9:LEU:HD13	2.29	0.48
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.96	0.48
5:E:79:TRP:HE1	5:E:81:GLU:HG3	1.79	0.48
13:M:137:CYS:SG	13:M:147:LYS:HB2	2.54	0.48
17:R:105:THR:HG1	17:R:106:LEU:H	1.62	0.48
1:A:11:LEU:HD12	2:B:1193:GLN:O	2.14	0.48
1:A:283:GLY:O	1:A:285:PRO:HD3	2.13	0.48
1:A:443:LEU:HD23	1:A:443:LEU:HA	1.73	0.48
1:A:471:ASN:O	1:A:474:VAL:HG12	2.13	0.48
1:A:670:ILE:HG12	1:A:805:LEU:HD21	1.96	0.48
2:B:983:ARG:NH2	2:B:1028:GLU:OE2	2.46	0.48
4:D:64:VAL:HG12	4:D:68:ARG:NH1	2.29	0.48
1:A:412:ARG:O	13:M:51:VAL:HG12	2.14	0.48
1:A:597:LEU:O	8:H:102:TYR:OH	2.32	0.48
1:A:1373:ASP:O	1:A:1377:THR:HG23	2.14	0.48
2:B:213:ILE:HG21	2:B:499:ASN:HB2	1.95	0.48
2:B:300:HIS:CE1	2:B:376:PHE:HE1	2.31	0.48
14:N:31:DG:H2"	14:N:32:DT:C6	2.49	0.48
2:B:70:ILE:HG21	16:Q:335:LEU:HD21	1.96	0.47
2:B:914:LYS:CB	2:B:937:ALA:O	2.53	0.47
7:G:143:ILE:HG13	7:G:170:ALA:HA	1.94	0.47
13:M:155:LYS:O	13:M:158:HIS:HB2	2.13	0.47
16:Q:405:THR:CB	16:Q:409:ALA:HB2	2.44	0.47
17:R:133:TYR:CE1	17:R:217:THR:HG22	2.49	0.47
19:U:277:GLN:HG2	20:V:56:THR:OG1	2.14	0.47
1:A:1072:ILE:O	1:A:1075:PRO:HD2	2.14	0.47
2:B:1089:PRO:HD3	10:J:44:TYR:HE2	1.78	0.47
13:M:241:ARG:O	13:M:245:HIS:ND1	2.45	0.47
15:O:171:ARG:HD3	15:O:238:ARG:O	2.14	0.47
2:B:167:ILE:O	2:B:450:ALA:HA	2.14	0.47
2:B:713:ALA:HA	2:B:733:HIS:CD2	2.50	0.47
3:C:60:ASP:HB3	12:L:67:PHE:CE2	2.47	0.47
3:C:180:TYR:HB3	3:C:228:PHE:HD1	1.80	0.47
5:E:64:PRO:HB2	5:E:69:ILE:HD11	1.95	0.47
5:E:161:LYS:NZ	5:E:193:GLY:O	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:22:LYS:O	8:H:43:ASN:HA	2.13	0.47
17:R:105:THR:CA	17:R:120:TYR:O	2.60	0.47
17:R:263:MET:O	17:R:266:THR:OG1	2.19	0.47
1:A:116:ASP:OD1	1:A:117:GLU:N	2.42	0.47
1:A:1032:LEU:O	1:A:1036:ARG:HD2	2.15	0.47
2:B:984:HIS:CD2	2:B:1025:HIS:HA	2.49	0.47
13:M:140:ALA:HB2	13:M:195:LEU:HD11	1.95	0.47
1:A:326:ARG:NE	1:A:1406:VAL:HG21	2.27	0.47
12:L:46:VAL:HG13	12:L:56:LEU:HD12	1.97	0.47
1:A:224:PHE:CE2	1:A:231:PRO:HG3	2.50	0.47
1:A:545:GLN:HG2	1:A:549:MET:HE3	1.97	0.47
2:B:799:PRO:HB2	2:B:818:PRO:HG2	1.96	0.47
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.95	0.47
2:B:839:MET:O	2:B:991:GLY:N	2.41	0.47
7:G:138:THR:O	7:G:141:SER:OG	2.23	0.47
13:M:16:PRO:HB3	21:W:127:CYS:HA	1.95	0.47
14:N:32:DT:P	17:R:325:PRO:CB	3.02	0.47
15:O:69:ASN:HB2	18:T:48:DT:O4'	2.14	0.47
16:Q:361:TRP:HA	16:Q:396:THR:O	2.15	0.47
18:T:47:DA:C8	18:T:48:DT:C4	3.02	0.47
1:A:792:TYR:HE2	9:I:87:GLN:HE22	1.63	0.47
1:A:1142:THR:O	1:A:1145:SER:OG	2.19	0.47
2:B:770:GLN:HG2	2:B:983:ARG:O	2.15	0.47
1:A:61:ILE:HG22	1:A:62:ASP:N	2.27	0.47
1:A:346:ASP:OD1	2:B:1106:ARG:NE	2.48	0.47
2:B:898:LEU:HD21	2:B:964:VAL:HG11	1.97	0.47
3:C:214:ASN:ND2	3:C:217:ASP:OD2	2.46	0.47
13:M:171:ILE:HD12	13:M:172:MET:HG3	1.96	0.47
13:M:269:ILE:CG2	13:M:272:LYS:CE	2.83	0.47
16:Q:99:ASN:O	17:R:96:ARG:HA	2.15	0.47
16:Q:117:HIS:HB2	17:R:135:PHE:CE1	2.50	0.47
18:T:50:DT:C2'	18:T:51:DA:H5'	2.45	0.47
1:A:567:LYS:NZ	8:H:91:ASP:HA	2.30	0.47
2:B:879:ARG:HG2	2:B:885:MET:SD	2.55	0.47
7:G:14:HIS:HB3	7:G:17:PHE:CE2	2.50	0.47
16:Q:140:HIS:O	16:Q:351:VAL:HG12	2.14	0.47
16:Q:376:LEU:O	17:R:69:TRP:N	2.39	0.47
1:A:879:GLU:OE1	1:A:959:ASN:HB2	2.15	0.46
2:B:617:ARG:NH1	2:B:619:ILE:HG12	2.30	0.46
2:B:923:GLU:HB3	2:B:925:LEU:HG	1.96	0.46
8:H:101:ALA:HA	8:H:115:TYR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:116:THR:O	16:Q:390:ASP:HB3	2.15	0.46
17:R:133:TYR:CD1	17:R:217:THR:HA	2.50	0.46
1:A:302:THR:HA	1:A:305:ASP:O	2.15	0.46
1:A:444:PHE:HE2	1:A:487:MET:SD	2.37	0.46
1:A:737:LEU:HD22	1:A:741:ASN:HD22	1.78	0.46
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.80	0.46
1:A:1208:THR:HB	1:A:1211:GLN:HG2	1.96	0.46
1:A:1444:MET:SD	6:F:135:ARG:NE	2.82	0.46
2:B:134:LYS:HD3	17:R:277:PHE:HB2	1.97	0.46
13:M:269:ILE:HG22	13:M:272:LYS:CG	2.34	0.46
15:O:170:ILE:HD13	15:O:234:LEU:HD22	1.96	0.46
16:Q:102:PRO:HB3	17:R:94:LYS:HG2	1.95	0.46
16:Q:375:LEU:HB2	16:Q:387:ILE:O	2.15	0.46
17:R:78:ALA:O	17:R:82:ARG:HG2	2.14	0.46
1:A:446:ARG:HB2	1:A:487:MET:HG2	1.96	0.46
2:B:642:ASP:N	2:B:649:LYS:HZ2	2.13	0.46
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.46	0.46
2:B:944:THR:HG21	2:B:1122:ARG:HH22	1.80	0.46
3:C:133:ILE:HD12	3:C:237:SER:HA	1.97	0.46
4:D:208:GLU:HA	4:D:211:LEU:HB2	1.98	0.46
11:K:20:LYS:O	11:K:33:ILE:HA	2.15	0.46
13:M:273:SER:CB	15:O:188:GLU:HA	2.46	0.46
16:Q:117:HIS:NE2	16:Q:390:ASP:OD2	2.49	0.46
2:B:289:LEU:HD13	2:B:375:ALA:HA	1.96	0.46
2:B:820:GLY:N	2:B:1091:TYR:OH	2.48	0.46
3:C:148:ARG:HH21	10:J:64:ASN:HA	1.79	0.46
4:D:52:LEU:HD12	4:D:52:LEU:O	2.15	0.46
7:G:22:MET:HA	7:G:25:TYR:HD1	1.80	0.46
7:G:101:VAL:O	7:G:108:VAL:N	2.43	0.46
15:O:191:PRO:CG	18:T:52:DC:H5'	2.45	0.46
19:U:30:ILE:HD11	20:V:32:ILE:HG13	1.98	0.46
1:A:216:VAL:HA	1:A:219:PHE:CE2	2.51	0.46
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.81	0.46
2:B:20:ASP:OD1	2:B:21:GLU:N	2.42	0.46
2:B:604:ARG:NH2	2:B:615:MET:H	2.13	0.46
7:G:93:SER:OG	7:G:100:GLU:OE1	2.33	0.46
17:R:108:LEU:HD11	17:R:120:TYR:HE2	1.80	0.46
20:V:32:ILE:HD12	20:V:32:ILE:N	2.30	0.46
1:A:465:TYR:CG	2:B:976:ILE:HD12	2.50	0.46
1:A:672:ASP:OD1	1:A:673:GLY:N	2.49	0.46
2:B:71:LEU:HB3	2:B:88:TYR:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:445:LYS:NZ	17:R:268:MET:HA	2.31	0.46
2:B:1163:CYS:HB3	2:B:1166:CYS:O	2.15	0.46
3:C:21:ILE:HG12	3:C:229:TYR:HD1	1.79	0.46
3:C:241:ASP:OD1	3:C:242:GLN:N	2.48	0.46
13:M:246:LEU:HD22	13:M:293:ILE:HD13	1.96	0.46
17:R:63:ARG:HD2	17:R:66:ARG:NH1	2.31	0.46
1:A:668:ASP:OD2	1:A:742:ASN:HB2	2.15	0.46
8:H:56:THR:HB	8:H:145:ARG:HG2	1.97	0.46
9:I:103:CYS:SG	9:I:105:SER:OG	2.62	0.46
1:A:1120:LEU:HD21	1:A:1131:ALA:HA	1.98	0.46
2:B:862:GLN:HA	2:B:963:PHE:HB2	1.98	0.46
2:B:952:VAL:HG22	2:B:966:VAL:HG22	1.96	0.46
3:C:76:ASP:OD2	3:C:127:ARG:HB2	2.16	0.46
4:D:50:LEU:HB2	7:G:2:PHE:O	2.16	0.46
9:I:70:ARG:HD3	9:I:84:VAL:HG22	1.97	0.46
13:M:267:LYS:HD3	15:O:239:LYS:CE	2.45	0.46
17:R:257:GLU:OE1	17:R:257:GLU:N	2.48	0.46
1:A:871:ASP:CG	1:A:1366:ARG:HH21	2.18	0.46
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.98	0.46
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.81	0.46
4:D:33:PHE:CZ	7:G:42:PHE:HA	2.50	0.46
17:R:68:VAL:O	17:R:69:TRP:HD1	1.99	0.46
2:B:280:ILE:HD13	2:B:334:ILE:HG13	1.97	0.46
3:C:66:ARG:NH1	10:J:2:ILE:O	2.48	0.46
8:H:5:LEU:HD11	8:H:61:SER:HB3	1.97	0.46
13:M:269:ILE:C	13:M:271:GLY:H	2.17	0.46
15:O:94:TYR:CZ	15:O:96:PRO:HG3	2.51	0.46
1:A:212:LYS:HA	1:A:232:GLU:OE2	2.16	0.45
1:A:483:ASP:HA	2:B:989:THR:HG23	1.97	0.45
4:D:53:SER:HB2	4:D:154:PHE:HB2	1.97	0.45
17:R:104:ILE:HD11	17:R:122:LEU:HD22	1.98	0.45
1:A:526:ASP:OD1	2:B:1015:HIS:ND1	2.49	0.45
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.80	0.45
2:B:286:PHE:CD2	2:B:297:ILE:HG23	2.51	0.45
2:B:300:HIS:CE1	2:B:376:PHE:CE1	3.04	0.45
4:D:32:GLU:HG2	7:G:41:LYS:HE2	1.98	0.45
4:D:49:ALA:HA	7:G:3:PHE:HD1	1.72	0.45
1:A:353:ILE:HG21	1:A:487:MET:SD	2.56	0.45
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.16	0.45
1:A:1390:ASN:HD21	1:A:1408:ILE:HD11	1.81	0.45
2:B:336:ARG:HD2	2:B:348:ARG:HH11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:11:ARG:NH1	20:V:41:LEU:HD13	2.31	0.45
20:V:34:ALA:O	20:V:35:SER:HB2	2.16	0.45
1:A:736:ASN:C	1:A:736:ASN:HD22	2.19	0.45
1:A:1132:LYS:HG2	1:A:1135:ARG:HH12	1.80	0.45
1:A:1170:ILE:HG23	1:A:1174:PHE:CE2	2.51	0.45
2:B:69:LEU:HD23	2:B:425:THR:HG23	1.99	0.45
2:B:865:LYS:HZ1	13:M:145:ILE:CD1	2.29	0.45
3:C:182:PRO:HB2	3:C:207:CYS:SG	2.56	0.45
7:G:149:GLY:O	7:G:159:ALA:HB1	2.16	0.45
8:H:122:LEU:HD23	8:H:122:LEU:HA	1.77	0.45
14:N:24:DT:H2'	14:N:25:DA:C8	2.51	0.45
1:A:358:ASN:OD1	2:B:833:TYR:OH	2.24	0.45
1:A:526:ASP:HB2	2:B:835:GLN:OE1	2.16	0.45
1:A:786:HIS:NE2	2:B:705:MET:SD	2.90	0.45
1:A:1277:GLU:O	1:A:1279:ILE:HD12	2.16	0.45
2:B:432:MET:O	2:B:436:VAL:HG12	2.17	0.45
2:B:569:TYR:CE1	2:B:589:VAL:HG11	2.51	0.45
2:B:923:GLU:HB2	2:B:928:ARG:CD	2.46	0.45
3:C:6:PRO:O	11:K:104:ASN:ND2	2.49	0.45
6:F:105:ALA:HA	7:G:16:SER:HA	1.98	0.45
13:M:137:CYS:SG	13:M:142:LEU:HB2	2.56	0.45
13:M:198:VAL:HG11	13:M:203:PHE:HD1	1.81	0.45
19:U:244:MET:HB2	19:U:267:VAL:HG13	1.99	0.45
2:B:776:GLN:O	2:B:1096:ARG:HG2	2.16	0.45
3:C:67:LEU:HD13	3:C:157:CYS:SG	2.56	0.45
6:F:82:THR:HG22	6:F:84:TYR:H	1.80	0.45
16:Q:117:HIS:HD2	16:Q:391:LYS:HB2	1.80	0.45
18:T:44:DA:C2'	18:T:45:DT:O5'	2.64	0.45
18:T:47:DA:C5	18:T:48:DT:O4	2.70	0.45
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.80	0.45
1:A:998:LEU:HD23	1:A:1001:ARG:HG2	1.98	0.45
1:A:1352:VAL:O	1:A:1355:VAL:HG12	2.16	0.45
2:B:460:ALA:O	2:B:464:GLY:N	2.38	0.45
18:T:52:DC:C2'	18:T:53:DA:H5'	2.45	0.45
1:A:660:ASN:OD1	2:B:1082:MET:HB3	2.16	0.45
2:B:463:THR:C	2:B:465:ASN:OD1	2.55	0.45
7:G:98:GLY:HA3	7:G:110:VAL:O	2.16	0.45
8:H:25:ARG:NH2	8:H:41:ASP:OD2	2.50	0.45
11:K:59:ALA:HA	11:K:74:ARG:O	2.17	0.45
13:M:267:LYS:NZ	15:O:208:VAL:CG1	2.78	0.45
13:M:295:ALA:O	13:M:298:VAL:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:239:LYS:O	15:O:240:MET:HG3	2.16	0.45
1:A:1295:THR:HG23	1:A:1297:GLU:OE1	2.17	0.45
2:B:331:LEU:HA	2:B:334:ILE:HG22	1.99	0.45
8:H:24:CYS:SG	8:H:44:VAL:HG21	2.57	0.45
11:K:7:PHE:HB2	11:K:11:LEU:HD13	1.98	0.45
13:M:134:THR:HA	13:M:147:LYS:HE3	1.99	0.45
16:Q:103:LEU:O	17:R:92:LEU:HB2	2.16	0.45
2:B:842:ASN:HB3	2:B:845:SER:HB2	1.99	0.45
4:D:56:ARG:HD3	4:D:149:THR:HA	1.99	0.45
16:Q:373:TYR:CD1	17:R:70:LEU:HD11	2.51	0.45
2:B:601:ARG:HD3	2:B:605:ARG:CZ	2.47	0.44
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.81	0.44
12:L:58:LYS:O	12:L:58:LYS:HG3	2.17	0.44
1:A:72:GLU:HB3	1:A:76:GLU:HB3	1.98	0.44
1:A:252:PHE:C	1:A:254:GLU:H	2.20	0.44
4:D:130:LEU:HD13	4:D:142:LYS:HG2	1.99	0.44
5:E:26:ARG:NH1	5:E:189:GLY:HA3	2.29	0.44
13:M:167:SER:O	13:M:168:MET:HB2	2.18	0.44
16:Q:405:THR:O	16:Q:409:ALA:N	2.44	0.44
20:V:34:ALA:C	20:V:36:LEU:H	2.21	0.44
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.57	0.44
2:B:244:LEU:HD13	2:B:250:PHE:CE2	2.52	0.44
4:D:24:ALA:CA	7:G:83:LYS:HB2	2.45	0.44
8:H:4:THR:HA	8:H:60:ALA:HA	1.99	0.44
14:N:25:DA:C8	14:N:25:DA:O5'	2.71	0.44
17:R:133:TYR:HD1	17:R:217:THR:HA	1.82	0.44
18:T:55:DA:H2"	18:T:56:DG:C8	2.52	0.44
2:B:446:LEU:HD23	2:B:446:LEU:HA	1.83	0.44
2:B:512:ARG:NH1	2:B:533:CYS:O	2.50	0.44
14:N:17:DC:H2"	14:N:18:DT:H71	1.98	0.44
1:A:469:ARG:HD3	1:A:469:ARG:HA	1.75	0.44
1:A:1217:LYS:HE2	1:A:1228:TRP:HZ3	1.82	0.44
1:A:1235:LYS:HG2	1:A:1237:ILE:HD11	1.99	0.44
2:B:322:PHE:HA	2:B:325:GLN:OE1	2.18	0.44
2:B:580:VAL:O	2:B:586:TRP:HD1	2.00	0.44
2:B:785:TYR:HA	2:B:788:ARG:HG2	1.99	0.44
6:F:133:VAL:HG11	7:G:58:ARG:NH2	2.33	0.44
7:G:7:LEU:HB2	7:G:74:TYR:CZ	2.53	0.44
13:M:199:LYS:O	13:M:199:LYS:HG3	2.17	0.44
14:N:28:DA:H8	14:N:29:DT:H73	1.81	0.44
16:Q:374:VAL:HB	17:R:71:VAL:HB	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:849:MET:HB3	1:A:1063:MET:SD	2.58	0.44
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	2.00	0.44
2:B:500:THR:OG1	2:B:537:LYS:NZ	2.48	0.44
3:C:148:ARG:NH2	10:J:64:ASN:OD1	2.51	0.44
7:G:160:ILE:HG22	7:G:161:GLY:N	2.33	0.44
14:N:27:DA:H2'	14:N:28:DA:C8	2.52	0.44
18:T:49:DA:H2'	18:T:50:DT:C5'	2.47	0.44
1:A:842:VAL:HG11	2:B:1136:ASP:OD2	2.18	0.44
1:A:1207:LEU:HA	1:A:1211:GLN:NE2	2.32	0.44
1:A:1444:MET:HB2	6:F:133:VAL:HG13	1.99	0.44
9:I:7:CYS:SG	9:I:8:ARG:N	2.90	0.44
16:Q:128:ASN:HB2	17:R:131:ASN:OD1	2.18	0.44
2:B:996:ARG:HH22	3:C:175:ALA:HA	1.82	0.44
2:B:1119:VAL:HG23	2:B:1126:GLY:HA2	1.99	0.44
2:B:1175:LEU:HD12	2:B:1175:LEU:O	2.16	0.44
4:D:177:VAL:HA	4:D:180:LEU:HD12	2.00	0.44
6:F:136:ARG:O	6:F:143:PHE:HA	2.18	0.44
7:G:15:PRO:HA	7:G:18:PHE:CZ	2.52	0.44
8:H:10:PHE:CD1	8:H:30:SER:HA	2.52	0.44
13:M:177:LEU:HD11	13:M:189:PHE:CE1	2.53	0.44
13:M:285:ASN:O	13:M:288:LEU:HB3	2.18	0.44
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.18	0.44
1:A:1189:SER:OG	1:A:1256:GLU:OE2	2.22	0.44
2:B:799:PRO:CB	2:B:818:PRO:HG2	2.48	0.44
10:J:30:LEU:HD13	10:J:38:ARG:NH1	2.32	0.44
2:B:273:LEU:HB2	2:B:276:ILE:HD13	2.00	0.43
4:D:65:GLU:HA	4:D:68:ARG:HH11	1.81	0.43
8:H:42:ILE:HG23	8:H:95:TYR:CZ	2.52	0.43
17:R:69:TRP:CD1	17:R:219:CYS:HB3	2.53	0.43
2:B:195:CYS:SG	2:B:197:PHE:HD2	2.41	0.43
2:B:274:PRO:O	2:B:276:ILE:HD12	2.18	0.43
2:B:839:MET:SD	2:B:1010:LEU:HD11	2.58	0.43
4:D:140:ASP:O	4:D:144:THR:N	2.46	0.43
5:E:43:LYS:HG3	5:E:47:CYS:SG	2.58	0.43
7:G:79:PHE:CE2	7:G:81:PRO:HD3	2.53	0.43
2:B:149:TYR:CE2	2:B:151:LEU:HD23	2.53	0.43
2:B:365:THR:HG21	2:B:370:PHE:CB	2.48	0.43
2:B:850:LEU:HG	2:B:851:PHE:HD2	1.83	0.43
2:B:924:GLU:HG3	2:B:929:THR:HB	2.00	0.43
2:B:1187:ASN:OD1	2:B:1190:ASP:N	2.51	0.43
7:G:127:PRO:HG3	7:G:139:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:21:VAL:HG12	19:U:25:PHE:CD1	2.54	0.43
1:A:372:LYS:HA	1:A:435:HIS:HD2	1.80	0.43
1:A:845:LEU:O	1:A:1065:GLY:HA3	2.19	0.43
2:B:850:LEU:HG	2:B:851:PHE:CD2	2.54	0.43
2:B:865:LYS:CE	13:M:145:ILE:HD12	2.38	0.43
3:C:4:GLU:O	3:C:24:ASN:ND2	2.51	0.43
3:C:56:THR:HG22	3:C:147:LEU:CD2	2.47	0.43
13:M:132:LYS:O	13:M:136:LEU:HG	2.18	0.43
1:A:857:ARG:HB2	1:A:862:ASN:O	2.17	0.43
1:A:1208:THR:O	1:A:1211:GLN:HG2	2.18	0.43
2:B:68:THR:CB	16:Q:335:LEU:HD13	2.46	0.43
2:B:839:MET:HG2	2:B:989:THR:O	2.18	0.43
6:F:137:TYR:HD1	6:F:143:PHE:HB3	1.83	0.43
2:B:310:MET:O	2:B:314:LEU:HG	2.19	0.43
2:B:635:ARG:NH1	2:B:637:LEU:HD21	2.34	0.43
3:C:133:ILE:CD1	3:C:237:SER:HA	2.48	0.43
4:D:194:LEU:HD22	7:G:86:VAL:HG11	2.00	0.43
11:K:46:ILE:O	11:K:49:GLU:N	2.51	0.43
15:O:99:PHE:CE1	18:T:45:DT:H1'	2.53	0.43
19:U:9:VAL:HG13	20:V:51:THR:HG22	1.99	0.43
22:X:168:ARG:O	22:X:181:LEU:N	2.48	0.43
1:A:737:LEU:HD11	1:A:758:ILE:HG21	2.00	0.43
1:A:915:SER:O	1:A:919:ILE:HG12	2.18	0.43
2:B:248:SER:HB3	2:B:250:PHE:CE2	2.54	0.43
2:B:282:ILE:HD12	2:B:382:ILE:HD13	1.99	0.43
2:B:1022:THR:HG23	2:B:1022:THR:O	2.18	0.43
9:I:54:GLU:HB3	9:I:100:PHE:HE2	1.84	0.43
12:L:38:LEU:HD21	12:L:48:CYS:HA	2.00	0.43
13:M:39:SER:OG	13:M:40:GLU:OE1	2.37	0.43
13:M:44:VAL:HG22	13:M:51:VAL:HA	2.01	0.43
17:R:129:VAL:HG21	17:R:218:VAL:HG12	2.01	0.43
19:U:262:LEU:HB2	19:U:279:ALA:HB3	2.01	0.43
2:B:103:ASN:O	2:B:958:GLN:OE1	2.36	0.43
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.47	0.43
3:C:18:VAL:HG12	3:C:20:PHE:HD1	1.83	0.43
3:C:41:ILE:HB	3:C:172:PRO:HG3	2.00	0.43
12:L:61:THR:CG2	12:L:63:ARG:HG2	2.49	0.43
13:M:158:HIS:CG	13:M:159:ASP:N	2.87	0.43
1:A:106:VAL:HG22	1:A:107:CYS:H	1.83	0.43
1:A:412:ARG:HB3	13:M:51:VAL:HG11	2.01	0.43
1:A:737:LEU:HD22	1:A:741:ASN:ND2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:VAL:HA	1:A:822:GLU:OE1	2.19	0.43
2:B:199:MET:CE	2:B:492:LEU:HD23	2.48	0.43
2:B:918:ILE:HG12	2:B:933:SER:O	2.18	0.43
2:B:979:LYS:HA	2:B:989:THR:HA	2.01	0.43
2:B:1187:ASN:OD1	2:B:1189:ILE:N	2.48	0.43
13:M:16:PRO:O	13:M:18:LEU:HG	2.19	0.43
13:M:239:ILE:HB	13:M:240:PRO:HD3	2.01	0.43
15:O:99:PHE:CZ	18:T:45:DT:O2	2.72	0.43
16:Q:108:LYS:O	16:Q:112:GLU:HG3	2.19	0.43
1:A:404:TYR:OH	13:M:40:GLU:HG2	2.19	0.43
1:A:547:LEU:HD22	11:K:58:PHE:CD1	2.53	0.43
2:B:457:LEU:HD23	2:B:457:LEU:HA	1.81	0.43
2:B:823:ALA:O	2:B:825:VAL:HG23	2.18	0.43
6:F:94:LEU:HD23	6:F:94:LEU:HA	1.66	0.43
1:A:105:CYS:SG	1:A:139:TRP:HD1	2.41	0.42
1:A:444:PHE:CE2	1:A:487:MET:SD	3.12	0.42
1:A:710:LEU:HD23	9:I:96:SER:HA	2.00	0.42
1:A:1144:LYS:HB2	1:A:1268:LEU:HB3	2.01	0.42
3:C:54:ASN:HD21	3:C:63:ILE:HD12	1.84	0.42
10:J:43:ARG:O	10:J:47:ARG:HG3	2.18	0.42
13:M:293:ILE:O	13:M:294:THR:OG1	2.28	0.42
17:R:63:ARG:C	17:R:65:ASN:H	2.21	0.42
1:A:48:ALA:HB3	1:A:56:PRO:HD3	2.01	0.42
1:A:1376:THR:O	1:A:1378:GLN:N	2.52	0.42
2:B:199:MET:CE	2:B:491:THR:HG21	2.21	0.42
3:C:190:ASP:OD1	3:C:191:TYR:N	2.52	0.42
11:K:18:LYS:NZ	11:K:38:GLU:OE2	2.47	0.42
13:M:279:VAL:HG11	13:M:304:VAL:HG21	2.01	0.42
15:O:171:ARG:HG3	15:O:239:LYS:HG2	2.00	0.42
16:Q:101:PHE:CD1	16:Q:382:GLY:HA3	2.54	0.42
16:Q:121:PHE:HE1	16:Q:395:PHE:HD2	1.66	0.42
17:R:94:LYS:O	17:R:106:LEU:HD12	2.19	0.42
1:A:206:GLU:O	1:A:210:ILE:HG12	2.18	0.42
1:A:982:THR:HG22	1:A:983:ILE:N	2.34	0.42
1:A:1144:LYS:NZ	2:B:262:GLU:OE2	2.51	0.42
2:B:44:VAL:HG11	2:B:199:MET:SD	2.59	0.42
2:B:106:ASP:OD1	2:B:106:ASP:N	2.52	0.42
2:B:199:MET:HG3	2:B:200:GLY:O	2.18	0.42
2:B:515:HIS:CE1	2:B:517:THR:HG23	2.54	0.42
2:B:755:ILE:HG22	2:B:983:ARG:HD2	2.00	0.42
3:C:12:GLU:HB2	3:C:19:ASP:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:138:THR:HG22	7:G:139:ILE:N	2.32	0.42
13:M:237:THR:O	13:M:240:PRO:HD2	2.18	0.42
17:R:135:PHE:HA	17:R:215:VAL:HG23	2.01	0.42
17:R:251:ARG:HG3	17:R:252:ILE:N	2.35	0.42
1:A:951:GLU:O	1:A:954:TRP:NE1	2.52	0.42
2:B:1067:ARG:HA	2:B:1067:ARG:HD3	1.87	0.42
5:E:153:HIS:CD2	5:E:184:VAL:HG11	2.55	0.42
9:I:27:PHE:O	9:I:35:VAL:HA	2.20	0.42
13:M:198:VAL:HG12	13:M:202:GLU:OE1	2.20	0.42
16:Q:130:VAL:O	16:Q:133:PHE:HB3	2.18	0.42
16:Q:363:GLY:HA2	16:Q:394:LYS:O	2.19	0.42
17:R:70:LEU:HD12	17:R:71:VAL:H	1.84	0.42
1:A:337:ARG:HH12	1:A:839:ARG:HE	1.67	0.42
1:A:344:ARG:HA	2:B:1129:ARG:HA	2.00	0.42
2:B:217:ARG:HH12	2:B:407:ASP:CG	2.22	0.42
2:B:1113:VAL:HG22	13:M:57:VAL:HB	2.02	0.42
3:C:174:ALA:N	3:C:233:GLU:O	2.52	0.42
11:K:19:LEU:HD22	11:K:35:PHE:CD1	2.54	0.42
13:M:187:ARG:NH1	13:M:241:ARG:HE	2.16	0.42
17:R:118:HIS:HB2	17:R:120:TYR:CE2	2.54	0.42
1:A:333:GLU:HA	1:A:338:GLY:HA3	2.01	0.42
1:A:356:ASP:OD2	11:K:65:HIS:NE2	2.28	0.42
1:A:673:GLY:N	1:A:674:PRO:HD2	2.34	0.42
1:A:854:ASN:HB2	1:A:1000:LEU:HD21	2.01	0.42
2:B:53:GLN:HG3	2:B:57:TYR:CD2	2.54	0.42
2:B:120:ARG:CG	12:L:55:ILE:HD11	2.50	0.42
2:B:309:GLN:HE22	9:I:50:THR:HG21	1.85	0.42
2:B:642:ASP:OD1	2:B:643:ASP:N	2.52	0.42
5:E:180:ARG:HH21	5:E:192:ARG:HG3	1.85	0.42
12:L:31:CYS:SG	12:L:32:ALA:N	2.93	0.42
1:A:94:GLY:HA3	1:A:1410:PHE:CE2	2.54	0.42
1:A:1210:GLY:HA2	1:A:1228:TRP:CE2	2.54	0.42
1:A:1395:GLY:HA3	1:A:1426:GLU:OE2	2.19	0.42
1:A:1418:LEU:HA	1:A:1418:LEU:HD12	1.85	0.42
2:B:435:THR:O	2:B:439:ALA:N	2.53	0.42
3:C:83:SER:OG	3:C:160:LYS:HD3	2.20	0.42
4:D:192:LYS:HB3	4:D:199:ASN:OD1	2.20	0.42
9:I:42:LEU:HD12	9:I:43:VAL:N	2.34	0.42
13:M:267:LYS:HZ1	15:O:169:PRO:HB3	1.70	0.42
20:V:38:MET:O	20:V:42:GLU:HG3	2.19	0.42
1:A:185:TRP:HB2	1:A:198:GLU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:HIS:O	1:A:401:GLY:N	2.53	0.42
1:A:1267:MET:HA	1:A:1271:ILE:HD12	2.01	0.42
1:A:1421:CYS:HA	1:A:1426:GLU:OE1	2.18	0.42
2:B:1094:ARG:HH21	2:B:1098:MET:HG2	1.84	0.42
17:R:68:VAL:HG21	17:R:134:VAL:HG21	2.01	0.42
1:A:300:VAL:O	1:A:303:TYR:HB3	2.20	0.42
1:A:1214:GLU:O	1:A:1218:GLN:HG2	2.19	0.42
2:B:59:LEU:O	2:B:63:ILE:HG12	2.19	0.42
2:B:134:LYS:HG2	2:B:154:GLU:O	2.20	0.42
2:B:213:ILE:CG2	2:B:499:ASN:HB2	2.49	0.42
3:C:167:HIS:HB3	3:C:170:TRP:CZ3	2.55	0.42
4:D:214:LEU:O	4:D:218:GLU:HG3	2.20	0.42
7:G:34:VAL:CG1	7:G:45:ILE:HG21	2.46	0.42
13:M:140:ALA:HB1	13:M:142:LEU:HD13	2.01	0.42
13:M:198:VAL:HG11	13:M:203:PHE:CD1	2.54	0.42
13:M:272:LYS:HD3	18:T:52:DC:H3'	2.01	0.42
18:T:48:DT:H2'	18:T:49:DA:C5	2.54	0.42
1:A:1293:SER:HB3	1:A:1299:VAL:HG23	2.02	0.42
2:B:120:ARG:HB2	2:B:122:LEU:HG	2.01	0.42
2:B:357:GLN:CD	2:B:368:GLU:HG2	2.40	0.42
3:C:222:LYS:HA	3:C:222:LYS:HD2	1.91	0.42
7:G:23:LYS:O	7:G:26:LEU:HB2	2.19	0.42
13:M:248:LEU:HD23	13:M:248:LEU:HA	1.79	0.42
15:O:191:PRO:HG3	18:T:52:DC:C4'	2.50	0.42
16:Q:119:LEU:HA	16:Q:119:LEU:HD23	1.76	0.42
1:A:635:ARG:NH2	1:A:877:HIS:HA	2.35	0.41
1:A:855:THR:HG21	1:A:863:VAL:HG22	2.01	0.41
1:A:1154:TYR:HB2	1:A:1191:TRP:CZ3	2.55	0.41
1:A:1212:VAL:O	1:A:1216:ILE:HD12	2.20	0.41
2:B:185:THR:O	2:B:188:ASP:HB3	2.19	0.41
4:D:194:LEU:CB	7:G:86:VAL:HG21	2.50	0.41
7:G:43:GLY:HA2	7:G:157:ILE:HD11	2.02	0.41
7:G:142:ARG:HB3	7:G:171:ILE:HD12	2.01	0.41
7:G:151:ILE:HG13	21:W:134:LEU:HA	2.00	0.41
9:I:101:PHE:CZ	9:I:112:SER:HB3	2.55	0.41
13:M:164:LYS:O	13:M:164:LYS:HG2	2.20	0.41
16:Q:115:ARG:HD3	16:Q:390:ASP:OD2	2.20	0.41
22:X:225:GLU:CB	22:X:232:VAL:H	2.33	0.41
2:B:136:THR:HB	2:B:151:LEU:HD12	2.01	0.41
2:B:369:GLY:O	16:Q:367:ALA:HB3	2.20	0.41
2:B:529:GLU:OE1	2:B:529:GLU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:171:ILE:CD1	13:M:172:MET:HG3	2.50	0.41
13:M:269:ILE:O	13:M:271:GLY:N	2.53	0.41
14:N:28:DA:H2'	14:N:29:DT:C6	2.55	0.41
16:Q:141:ARG:HD3	17:R:210:LYS:HZ3	1.85	0.41
16:Q:379:GLU:HG2	16:Q:383:SER:O	2.20	0.41
17:R:277:PHE:CE2	17:R:278:LEU:HD13	2.56	0.41
1:A:270:LEU:HD23	1:A:270:LEU:HA	1.82	0.41
2:B:760:ASP:OD1	2:B:760:ASP:N	2.53	0.41
2:B:1159:ARG:HD2	2:B:1193:GLN:OE1	2.19	0.41
17:R:63:ARG:O	17:R:64:SER:OG	2.27	0.41
1:A:80:HIS:H	1:A:243:PRO:HB3	1.85	0.41
1:A:215:SER:O	1:A:218:ASP:HB2	2.20	0.41
2:B:342:GLY:C	2:B:344:LYS:H	2.24	0.41
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.50	0.41
2:B:977:GLY:HA3	2:B:1099:VAL:HB	2.03	0.41
2:B:1069:PHE:HE2	3:C:192:TRP:CD2	2.38	0.41
4:D:155:ARG:HB3	4:D:219:THR:HG21	2.01	0.41
5:E:163:GLU:O	5:E:167:ARG:HG2	2.20	0.41
15:O:227:PHE:HA	15:O:230:ILE:HG22	2.01	0.41
1:A:1194:ARG:HA	1:A:1238:ILE:O	2.20	0.41
2:B:402:GLY:CA	2:B:695:ALA:HB3	2.50	0.41
2:B:1171:VAL:HG22	2:B:1182:CYS:HB2	2.02	0.41
11:K:35:PHE:CD2	11:K:71:PHE:CZ	3.07	0.41
13:M:200:THR:HG22	13:M:201:LYS:N	2.35	0.41
13:M:251:GLN:HA	13:M:254:THR:HG22	2.02	0.41
16:Q:115:ARG:O	17:R:136:THR:HA	2.20	0.41
18:T:51:DA:N3	18:T:52:DC:C2	2.89	0.41
2:B:796:LEU:HD11	2:B:851:PHE:HA	2.02	0.41
7:G:150:CYS:SG	7:G:159:ALA:HB2	2.61	0.41
9:I:74:GLU:HB3	9:I:81:ARG:HG2	2.01	0.41
10:J:2:ILE:O	10:J:2:ILE:HG23	2.21	0.41
14:N:28:DA:C8	14:N:29:DT:C7	3.04	0.41
16:Q:129:PRO:HG2	16:Q:132:ASP:HB2	2.03	0.41
1:A:913:LEU:HD23	1:A:1032:LEU:HD13	2.03	0.41
1:A:960:ILE:O	1:A:964:ILE:HD12	2.21	0.41
1:A:1397:LEU:HA	1:A:1400:CYS:SG	2.60	0.41
7:G:121:PHE:CE2	7:G:123:ALA:HB2	2.56	0.41
13:M:132:LYS:HB3	13:M:172:MET:HE3	2.03	0.41
16:Q:369:ASN:HB2	16:Q:392:VAL:HG11	2.02	0.41
1:A:353:ILE:H	1:A:353:ILE:HG13	1.66	0.41
1:A:516:SER:O	1:A:517:ASN:OD1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:238:ALA:HB3	2:B:256:VAL:HB	2.02	0.41
4:D:30:GLY:O	4:D:34:GLN:N	2.54	0.41
5:E:169:ARG:HD3	6:F:140:ASP:OD2	2.20	0.41
10:J:41:LEU:HD22	10:J:46:CYS:HB3	2.01	0.41
13:M:162:THR:HG23	13:M:213:ILE:HD11	2.03	0.41
14:N:25:DA:O5'	14:N:25:DA:H8	2.03	0.41
1:A:455:MET:HE2	1:A:455:MET:HB3	1.84	0.41
1:A:514:PRO:HG2	1:A:1067:LEU:HD11	2.01	0.41
1:A:722:LEU:HD23	1:A:722:LEU:HA	1.93	0.41
2:B:70:ILE:HG22	2:B:89:GLU:HG3	2.02	0.41
2:B:98:THR:OG1	2:B:127:GLY:N	2.54	0.41
2:B:171:PRO:O	2:B:172:ILE:HD13	2.21	0.41
2:B:339:THR:HG21	2:B:351:TYR:OH	2.20	0.41
2:B:412:LEU:HD23	2:B:476:ARG:HH12	1.85	0.41
2:B:705:MET:H	2:B:710:LEU:HD12	1.86	0.41
8:H:117:SER:HA	8:H:122:LEU:HD23	2.02	0.41
13:M:168:MET:HA	13:M:171:ILE:CG1	2.50	0.41
15:O:99:PHE:HB2	18:T:45:DT:H4'	2.01	0.41
16:Q:378:VAL:HA	16:Q:384:PHE:CD1	2.56	0.41
18:T:43:DT:P	18:T:43:DT:O4'	2.79	0.41
19:U:5:GLU:O	19:U:9:VAL:HG23	2.21	0.41
1:A:242:PRO:HB2	1:A:246:VAL:HB	2.01	0.41
1:A:306:ASN:ND2	1:A:322:VAL:O	2.49	0.41
1:A:369:SER:HB3	11:K:2:ASN:OD1	2.20	0.41
2:B:593:PRO:HB2	2:B:617:ARG:NE	2.32	0.41
2:B:724:ASP:OD1	2:B:725:PRO:HD2	2.21	0.41
10:J:18:TRP:O	10:J:21:TYR:HB3	2.21	0.41
16:Q:361:TRP:CH2	16:Q:397:ALA:HB2	2.56	0.41
17:R:61:LEU:HD21	17:R:63:ARG:O	2.20	0.41
17:R:118:HIS:HB2	17:R:120:TYR:CZ	2.56	0.41
20:V:119:LYS:N	20:V:119:LYS:HD3	2.36	0.41
2:B:243:ALA:HA	2:B:250:PHE:HB2	2.02	0.40
2:B:826:ALA:HB2	2:B:1087:PHE:HD1	1.86	0.40
3:C:101:LEU:HB2	3:C:118:LEU:HD23	2.02	0.40
9:I:43:VAL:HG23	9:I:44:TYR:H	1.86	0.40
11:K:35:PHE:O	11:K:70:ARG:HB2	2.21	0.40
17:R:73:LEU:HD12	17:R:74:PRO:CD	2.44	0.40
1:A:244:PRO:O	1:A:247:ARG:N	2.54	0.40
1:A:544:ASP:HB2	11:K:47:ARG:HH12	1.85	0.40
2:B:240:ILE:HG23	2:B:254:LEU:HB3	2.03	0.40
2:B:786:ASN:O	2:B:967:ARG:NH1	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:914:LYS:O	2:B:937:ALA:O	2.39	0.40
5:E:37:LEU:HA	5:E:38:PRO:HD3	1.93	0.40
7:G:59:GLY:HA2	7:G:70:PHE:HD1	1.85	0.40
13:M:44:VAL:HG13	13:M:50:LEU:O	2.21	0.40
13:M:157:CYS:SG	13:M:158:HIS:N	2.93	0.40
13:M:267:LYS:CE	15:O:239:LYS:HE3	2.52	0.40
14:N:24:DT:C2'	14:N:25:DA:C5'	2.90	0.40
15:O:171:ARG:HA	15:O:239:LYS:HZ3	1.87	0.40
16:Q:103:LEU:CD2	16:Q:384:PHE:HB2	2.51	0.40
17:R:270:MET:HB2	17:R:270:MET:HE3	1.93	0.40
1:A:175:ARG:O	1:A:182:VAL:HG12	2.20	0.40
2:B:290:GLY:HA2	2:B:327:ARG:HD2	2.03	0.40
2:B:420:LEU:HD23	2:B:420:LEU:HA	1.87	0.40
7:G:132:SER:OG	7:G:133:SER:N	2.54	0.40
8:H:106:GLU:HG2	8:H:112:ILE:HD13	2.04	0.40
13:M:267:LYS:CD	15:O:239:LYS:HE3	2.52	0.40
1:A:540:PHE:CG	1:A:571:LEU:HD23	2.56	0.40
1:A:1368:MET:O	1:A:1372:VAL:HG23	2.21	0.40
2:B:88:TYR:CD1	2:B:136:THR:HG23	2.56	0.40
2:B:546:SER:OG	2:B:632:ARG:N	2.54	0.40
2:B:604:ARG:HH22	2:B:615:MET:H	1.69	0.40
3:C:235:VAL:HG13	10:J:13:VAL:HG13	2.04	0.40
4:D:32:GLU:CB	7:G:42:PHE:HE1	2.34	0.40
4:D:126:ILE:O	4:D:130:LEU:HG	2.22	0.40
4:D:138:ASN:ND2	7:G:36:GLY:CA	2.84	0.40
5:E:11:ARG:NH2	5:E:141:VAL:HG21	2.36	0.40
10:J:34:THR:HG22	10:J:38:ARG:HH12	1.87	0.40
17:R:98:ASN:O	17:R:102:SER:N	2.54	0.40
19:U:256:ALA:HB1	19:U:285:TRP:O	2.21	0.40
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.57	0.40
1:A:727:ASP:HB3	1:A:731:ARG:HH12	1.85	0.40
1:A:809:THR:O	1:A:812:GLU:HB2	2.22	0.40
1:A:1132:LYS:HA	1:A:1135:ARG:NH1	2.35	0.40
1:A:1157:ASP:OD2	1:A:1160:SER:OG	2.27	0.40
8:H:10:PHE:HD1	8:H:30:SER:HA	1.86	0.40
10:J:16:ASP:OD1	10:J:16:ASP:N	2.54	0.40
13:M:162:THR:CG2	13:M:213:ILE:HD11	2.52	0.40
13:M:274:PRO:CG	15:O:188:GLU:OE2	2.61	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	A	1386/1733 (80%)	1306 (94%)	77 (6%)	3 (0%)	47 81
2	B	1139/1224 (93%)	1086 (95%)	48 (4%)	5 (0%)	34 72
3	C	260/318 (82%)	246 (95%)	14 (5%)	0	100 100
4	D	153/221 (69%)	145 (95%)	8 (5%)	0	100 100
5	E	211/215 (98%)	209 (99%)	2 (1%)	0	100 100
6	F	81/155 (52%)	76 (94%)	5 (6%)	0	100 100
7	G	169/171 (99%)	160 (95%)	8 (5%)	1 (1%)	25 65
8	H	132/146 (90%)	114 (86%)	14 (11%)	4 (3%)	4 32
9	I	114/122 (93%)	105 (92%)	9 (8%)	0	100 100
10	J	63/70 (90%)	57 (90%)	5 (8%)	1 (2%)	9 45
11	K	110/120 (92%)	107 (97%)	3 (3%)	0	100 100
12	L	43/70 (61%)	37 (86%)	6 (14%)	0	100 100
13	M	225/345 (65%)	202 (90%)	20 (9%)	3 (1%)	12 48
15	O	178/240 (74%)	174 (98%)	4 (2%)	0	100 100
16	Q	140/735 (19%)	124 (89%)	13 (9%)	3 (2%)	7 39
17	R	181/400 (45%)	171 (94%)	9 (5%)	1 (1%)	25 65
19	U	88/286 (31%)	82 (93%)	3 (3%)	3 (3%)	3 29
20	V	96/122 (79%)	87 (91%)	8 (8%)	1 (1%)	15 54
21	W	162/482 (34%)	154 (95%)	7 (4%)	1 (1%)	25 65
22	X	135/328 (41%)	125 (93%)	9 (7%)	1 (1%)	22 62
All	All	5066/7503 (68%)	4767 (94%)	272 (5%)	27 (0%)	32 68

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	343	ILE

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Mol	Chain	Res	Type
2	B	476	ARG
8	H	132	LEU
13	M	269	ILE
17	R	259	VAL
22	X	231	LEU
2	B	221	ASN
8	H	131	ASN
8	H	137	GLN
13	M	200	THR
19	U	31	ASP
19	U	264	ASP
20	V	6	TYR
21	W	40	GLU
2	B	364	ILE
7	G	63	PRO
8	H	90	ALA
16	Q	26	ARG
16	Q	406	ILE
2	B	743	ILE
13	M	31	PRO
1	A	958	VAL
1	A	50	ILE
16	Q	127	ILE
19	U	30	ILE
10	J	2	ILE
1	A	569	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1221/1520 (80%)	1219 (100%)	2 (0%)	93 96
2	B	1000/1061 (94%)	999 (100%)	1 (0%)	93 97
3	C	230/274 (84%)	230 (100%)	0	100 100
4	D	139/200 (70%)	139 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	E	195/197 (99%)	195 (100%)	0	100 100
6	F	73/137 (53%)	73 (100%)	0	100 100
7	G	152/152 (100%)	152 (100%)	0	100 100
8	H	119/128 (93%)	119 (100%)	0	100 100
9	I	110/116 (95%)	110 (100%)	0	100 100
10	J	60/65 (92%)	60 (100%)	0	100 100
11	K	97/102 (95%)	97 (100%)	0	100 100
12	L	40/57 (70%)	40 (100%)	0	100 100
13	M	201/299 (67%)	200 (100%)	1 (0%)	88 93
15	O	152/205 (74%)	141 (93%)	11 (7%)	14 41
16	Q	109/641 (17%)	109 (100%)	0	100 100
17	R	107/363 (30%)	107 (100%)	0	100 100
19	U	84/260 (32%)	79 (94%)	5 (6%)	19 46
20	V	90/108 (83%)	85 (94%)	5 (6%)	21 48
All	All	4179/5885 (71%)	4154 (99%)	25 (1%)	86 92

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	736	ASN
2	B	465	ASN
13	M	202	GLU
15	O	70	ILE
15	O	79	ARG
15	O	108	GLU
15	O	130	ASP
15	O	134	LEU
15	O	175	LEU
15	O	199	LYS
15	O	219	GLN
15	O	225	GLN
15	O	235	SER
15	O	240	MET
19	U	25	PHE
19	U	241	GLU
19	U	253	ARG

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Mol	Chain	Res	Type
19	U	267	VAL
19	U	277	GLN
20	V	9	LEU
20	V	33	GLU
20	V	39	ARG
20	V	57	GLN
20	V	108	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	60	GLN
2	B	215	GLN
2	B	325	GLN
4	D	143	ASN
4	D	173	HIS
15	O	95	ASN
15	O	158	GLN
15	O	219	GLN
16	Q	122	GLN
19	U	280	GLN
20	V	55	ASN
20	V	57	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	131:ASN	C	132:LEU	N	1.04

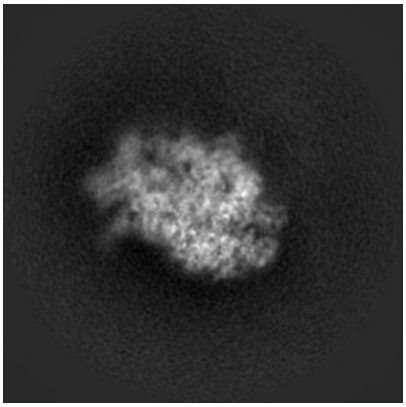
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3378. These allow visual inspection of the internal detail of the map and identification of artifacts.

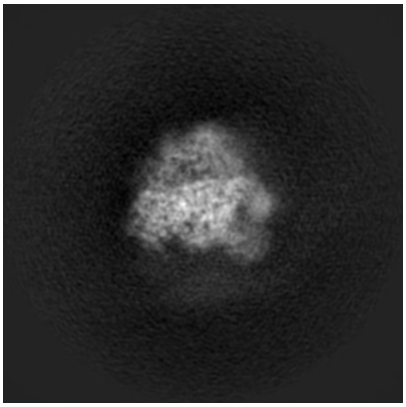
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

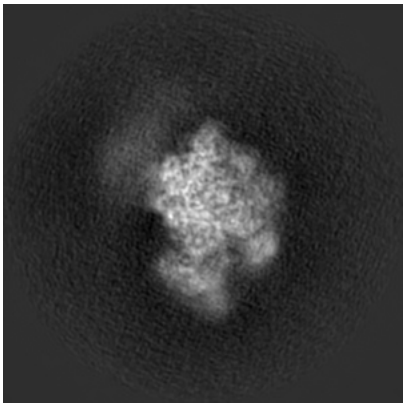
6.1.1 Primary map



X



Y

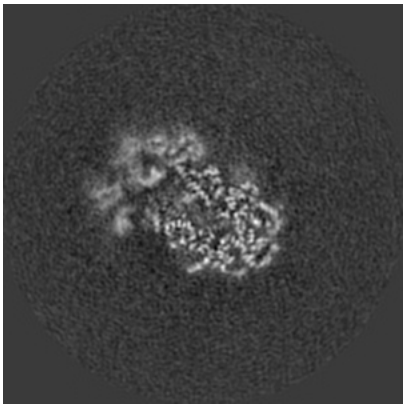


Z

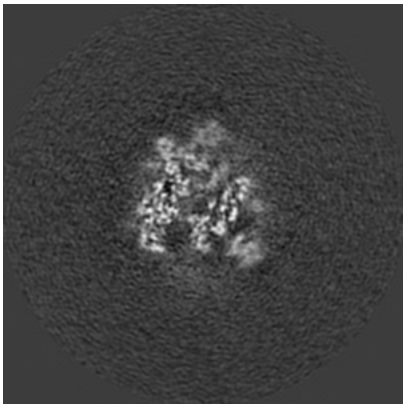
The images above show the map projected in three orthogonal directions.

6.2 Central slices

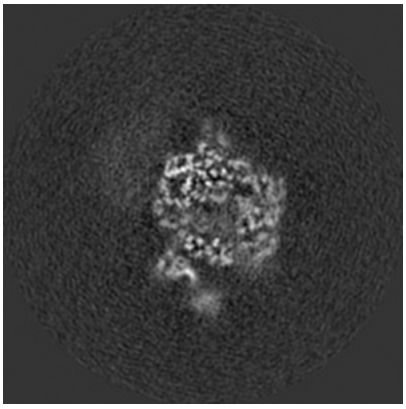
6.2.1 Primary map



X Index: 150



Y Index: 150

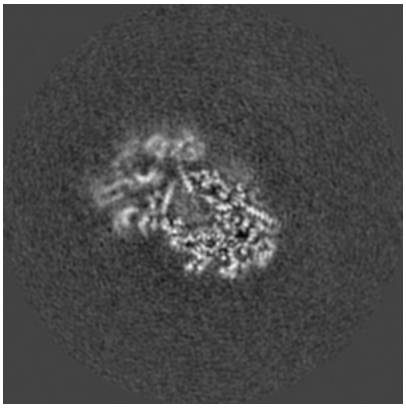


Z Index: 150

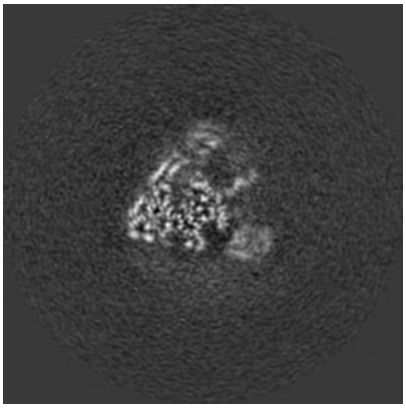
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

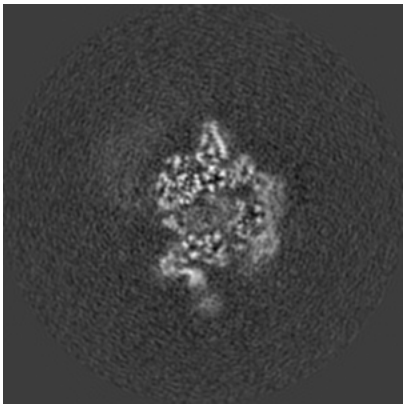
6.3.1 Primary map



X Index: 146



Y Index: 165

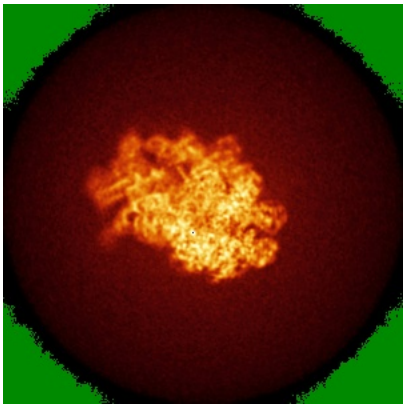


Z Index: 146

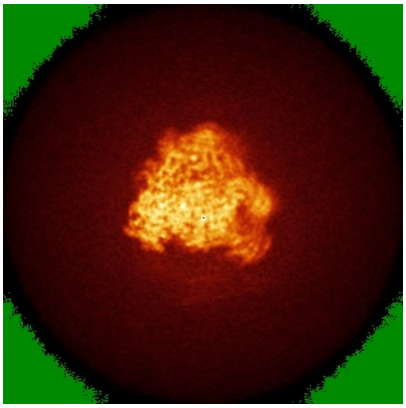
The images above show the largest variance slices of the map in three orthogonal directions.

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

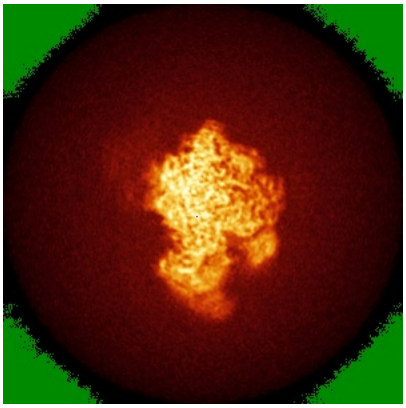
6.4.1 Primary map



X



Y

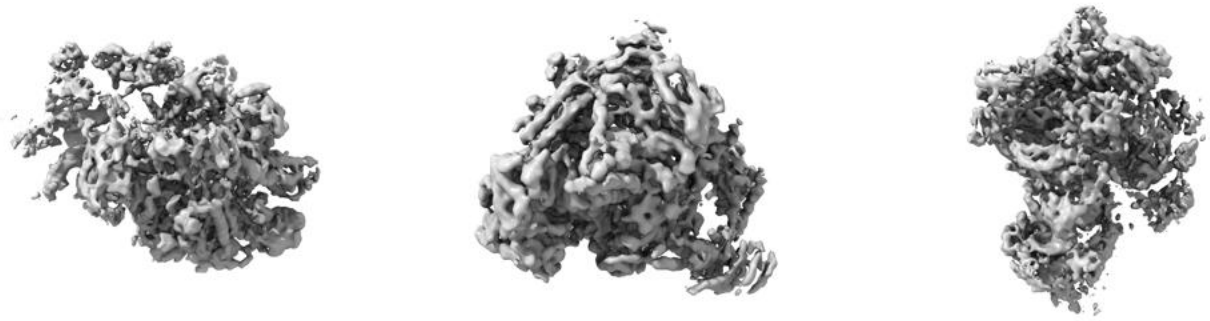


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0325. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

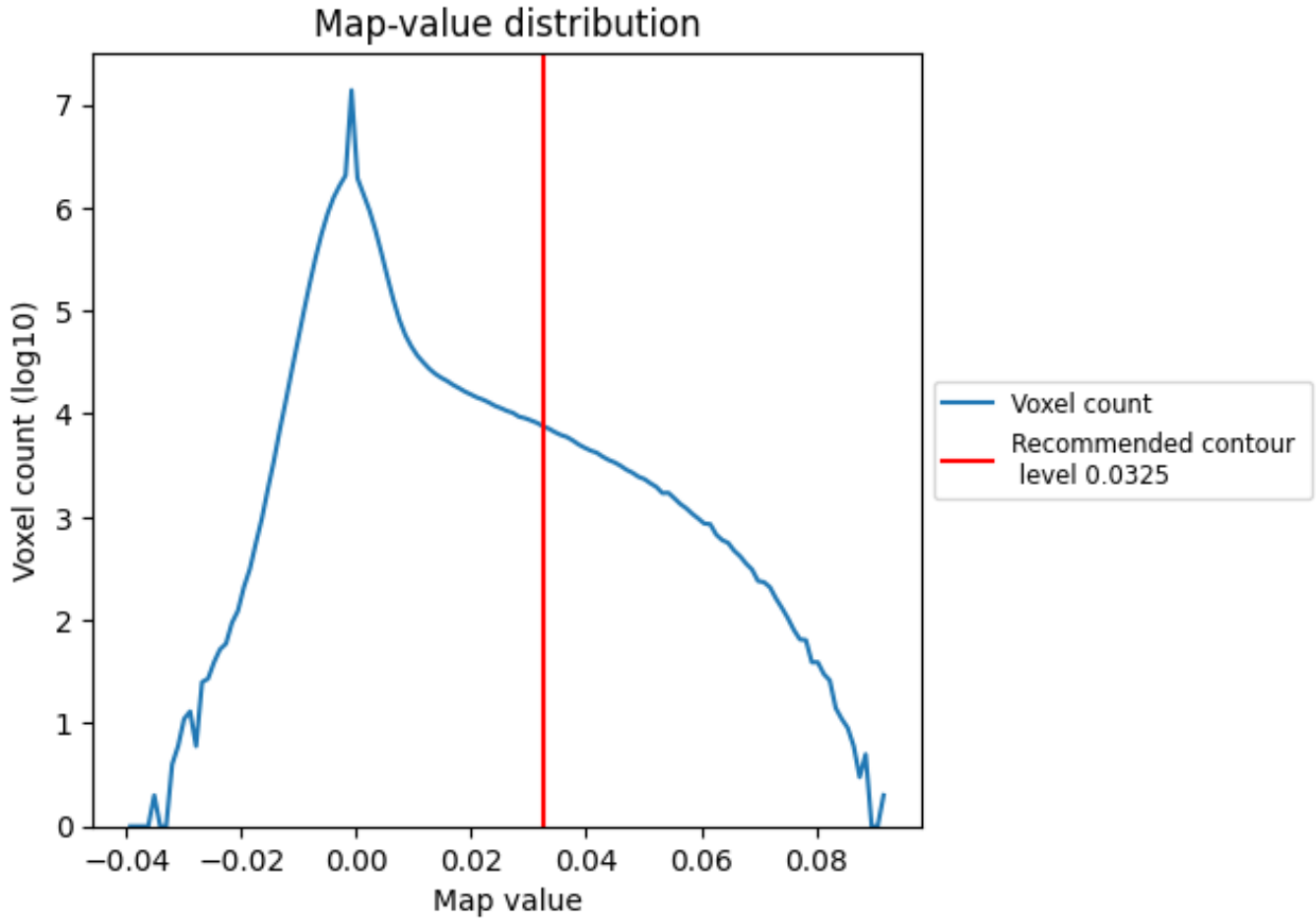
6.6 Mask visualisation (i)

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

7 Map analysis

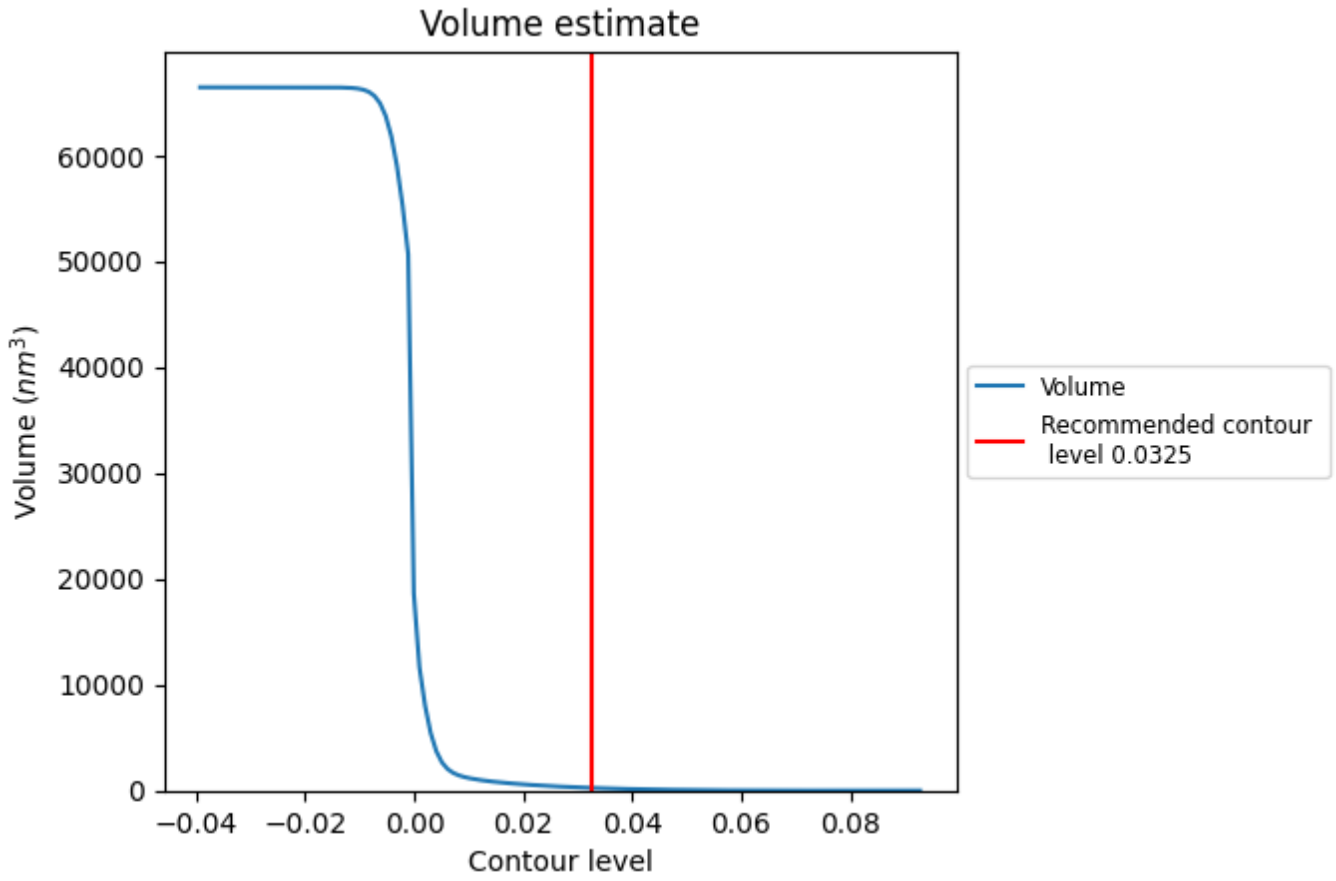
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

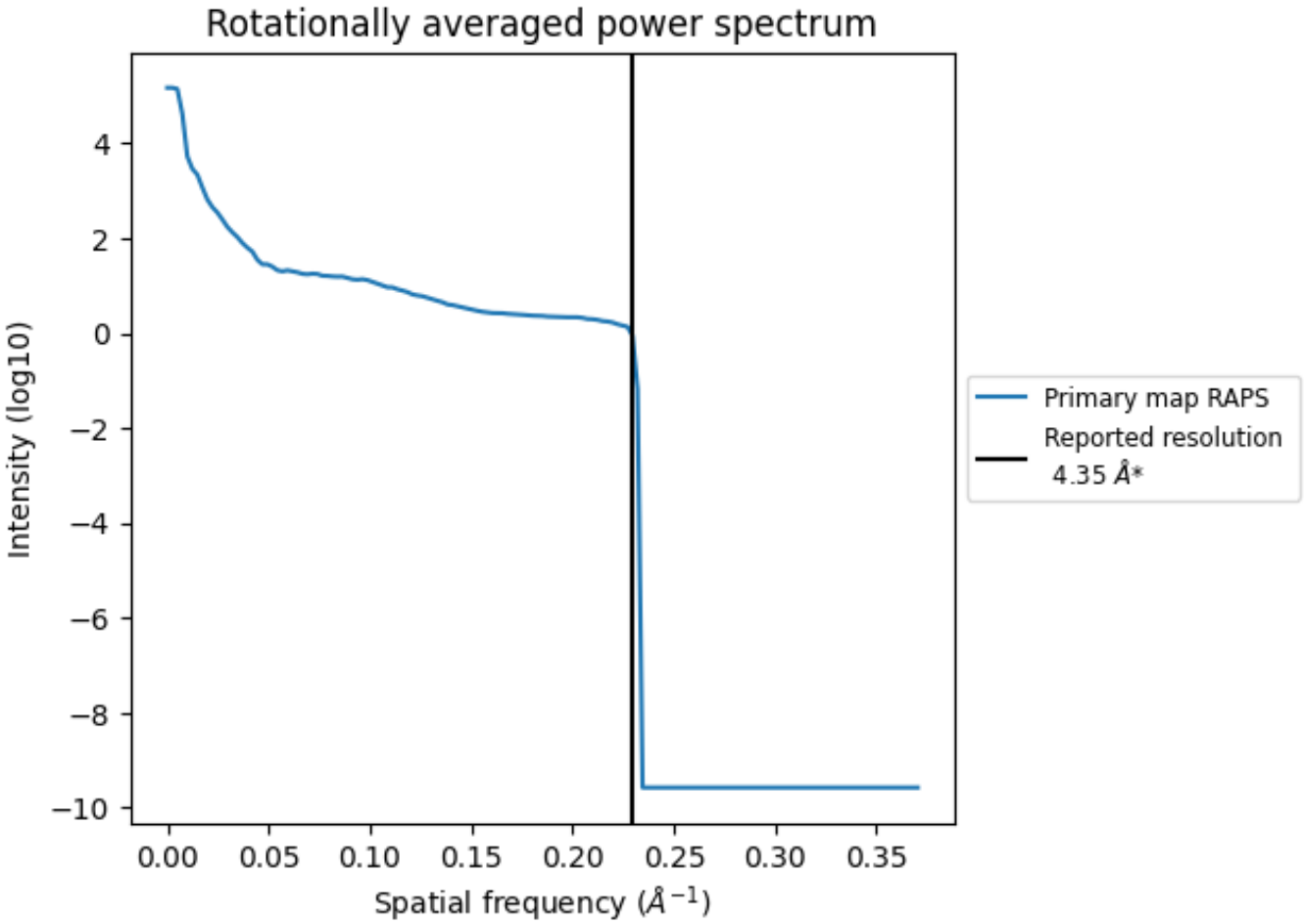
7.2 Volume estimate



The volume at the recommended contour level is 250 nm^3; this corresponds to an approximate mass of 226 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 0.230 Å^{-1}

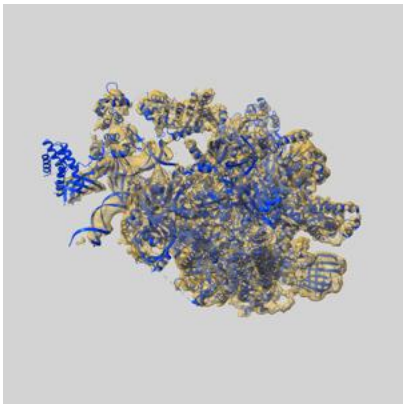
8 Fourier-Shell correlation (i)

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

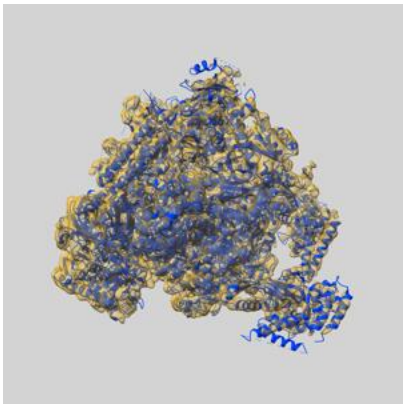
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3378 and PDB model 5FYW. Per-residue inclusion information can be found in section 3 on page 8.

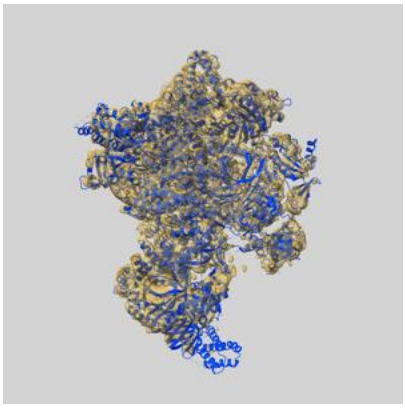
9.1 Map-model overlay



X



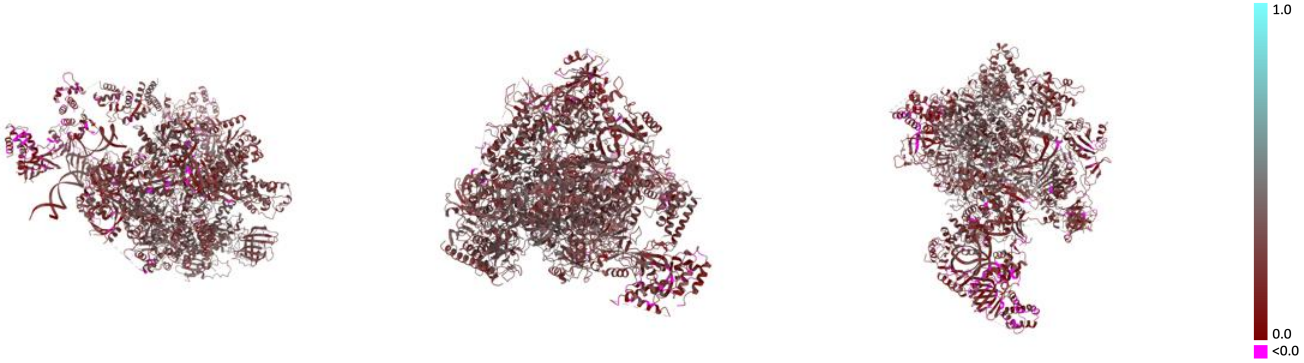
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0325 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

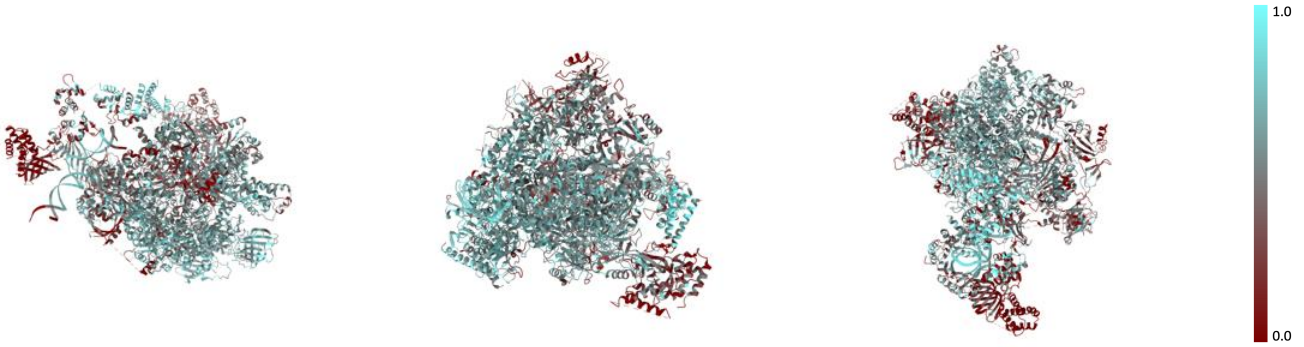
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

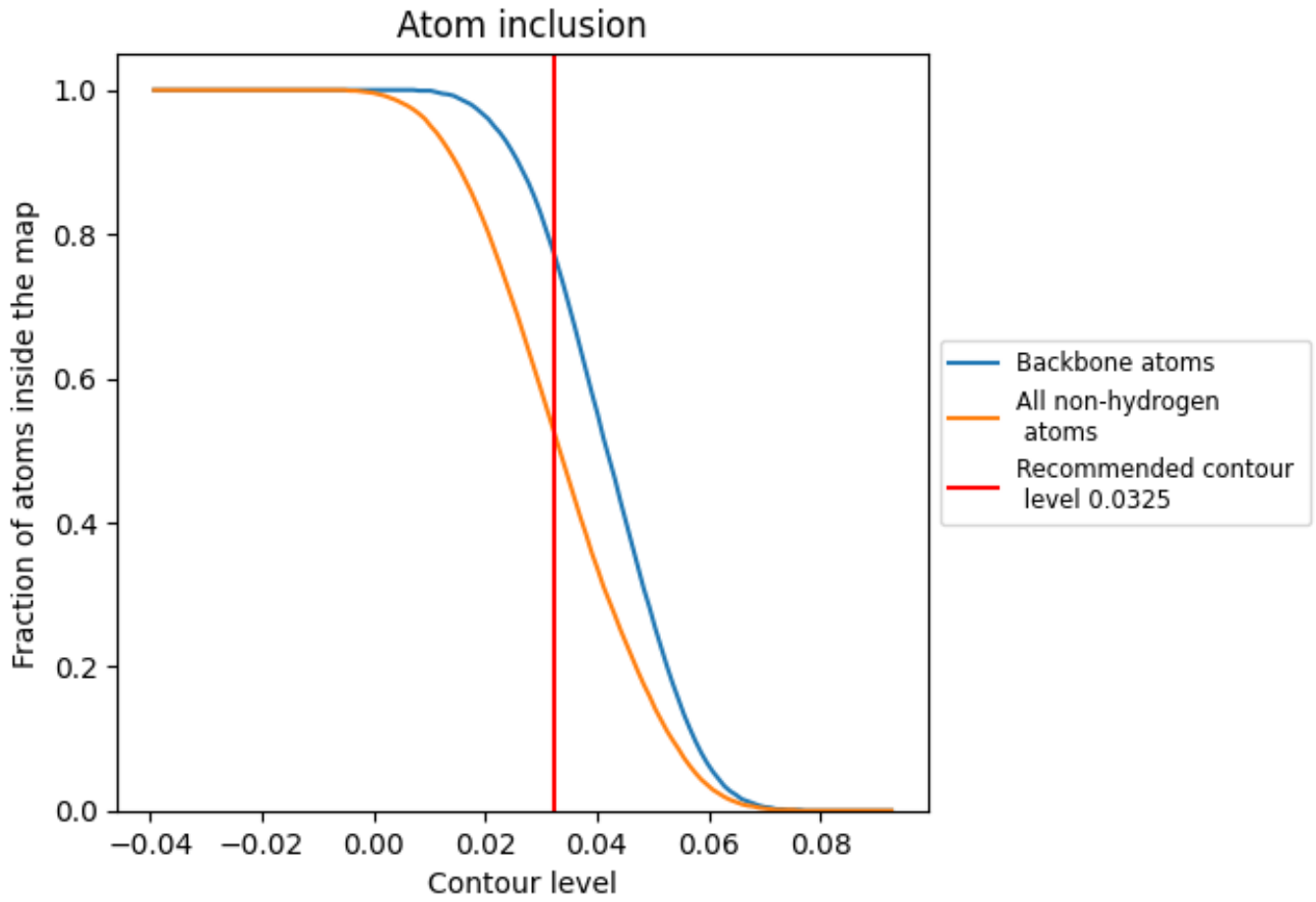
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0325).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 52% 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 (0.0325) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5210	0.2600
A	0.5660	0.2900
B	0.5770	0.3040
C	0.6790	0.3190
D	0.1920	0.1420
E	0.5400	0.2590
F	0.6170	0.2990
G	0.3910	0.2230
H	0.6470	0.2980
I	0.3760	0.2100
J	0.6690	0.3070
K	0.5470	0.2990
L	0.6160	0.3150
M	0.5350	0.2430
N	0.5680	0.2020
O	0.4430	0.1560
Q	0.3080	0.1880
R	0.3630	0.2010
T	0.5970	0.1930
U	0.0890	0.0950
V	0.0930	0.1140
W	0.6520	0.2270
X	0.5030	0.1730