Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 09:58 pm GMT

PDB ID	:	6TBM
EMDB ID	:	EMD-10446
Title	:	Structure of SAGA bound to TBP, including Spt8 and DUB
Authors	:	Papai, G.; Frechard, A.; Kolesnikova, O.; Crucifix, C.; Schultz, P.; Ben-Shem, A.
Deposited on	:	2019-11-01
Resolution	:	20.00 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:

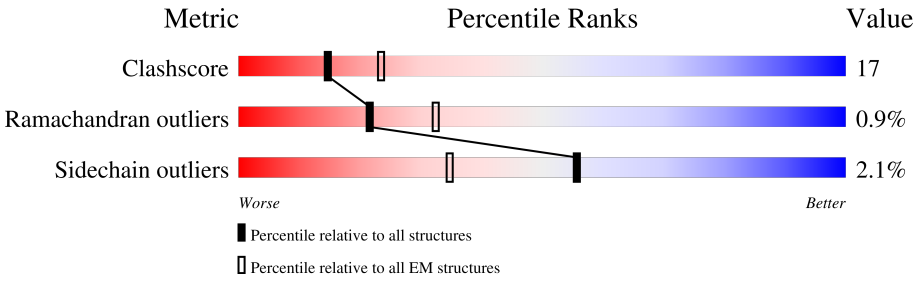
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 20.00 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	M	240	10% 37% 32% 6% 25%
2	A	448	9% 31% 7% 61%
3	C	698	5% 9% · 86%
4	F	517	· 33% 7% 59%
5	D	341	7% 37% 21% · 39%
6	E	1191	10% · · 87%
7	J	217	· 36% 7% 56%
8	K	609	· 17% 7% · 75%

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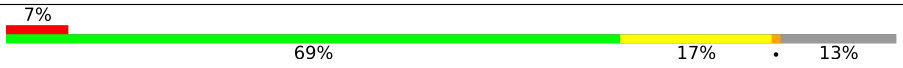
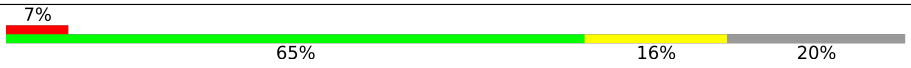
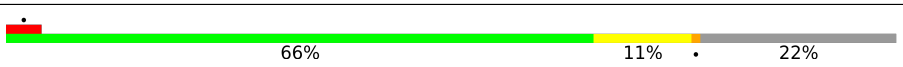
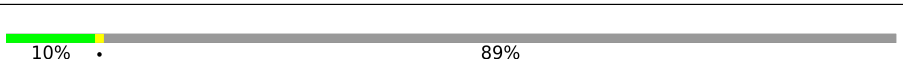
Mol	Chain	Length	Quality of chain
9	G	722	
10	H	485	
11	I	153	
12	L	3825	
13	B	722	
14	N	400	
15	R	76	
16	Q	502	
17	O	123	
18	P	96	

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 48800 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 TATA-box Binding Protein (TBP).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	180	Total	C	N	O	S	0	0
			1415	921	242	246	6		

- Molecule 2 is a protein called Transcriptional coactivator HFI1/ADA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	173	Total	C	N	O	S	0	0
			1300	816	228	250	6		

- Molecule 3 is a protein called Subunit of SAGA histone acetyltransferase complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	95	Total	C	N	O	S	0	0
			761	480	142	133	6		

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	645	LEU	-	expression tag	UNP C4QZ39
C	646	GLU	-	expression tag	UNP C4QZ39
C	647	GLY	-	expression tag	UNP C4QZ39
C	648	GLY	-	expression tag	UNP C4QZ39
C	649	GLY	-	expression tag	UNP C4QZ39
C	650	GLY	-	expression tag	UNP C4QZ39
C	651	SER	-	expression tag	UNP C4QZ39
C	652	MET	-	expression tag	UNP C4QZ39
C	653	ASP	-	expression tag	UNP C4QZ39
C	654	GLU	-	expression tag	UNP C4QZ39
C	655	LYS	-	expression tag	UNP C4QZ39
C	656	THR	-	expression tag	UNP C4QZ39
C	657	THR	-	expression tag	UNP C4QZ39
C	658	GLY	-	expression tag	UNP C4QZ39
C	659	TRP	-	expression tag	UNP C4QZ39

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Chain	Residue	Modelled	Actual	Comment	Reference
C	660	ARG	-	expression tag	UNP C4QZ39
C	661	GLY	-	expression tag	UNP C4QZ39
C	662	GLY	-	expression tag	UNP C4QZ39
C	663	HIS	-	expression tag	UNP C4QZ39
C	664	VAL	-	expression tag	UNP C4QZ39
C	665	VAL	-	expression tag	UNP C4QZ39
C	666	GLU	-	expression tag	UNP C4QZ39
C	667	GLY	-	expression tag	UNP C4QZ39
C	668	LEU	-	expression tag	UNP C4QZ39
C	669	ALA	-	expression tag	UNP C4QZ39
C	670	GLY	-	expression tag	UNP C4QZ39
C	671	GLU	-	expression tag	UNP C4QZ39
C	672	LEU	-	expression tag	UNP C4QZ39
C	673	GLU	-	expression tag	UNP C4QZ39
C	674	GLN	-	expression tag	UNP C4QZ39
C	675	LEU	-	expression tag	UNP C4QZ39
C	676	ARG	-	expression tag	UNP C4QZ39
C	677	ALA	-	expression tag	UNP C4QZ39
C	678	ARG	-	expression tag	UNP C4QZ39
C	679	LEU	-	expression tag	UNP C4QZ39
C	680	GLU	-	expression tag	UNP C4QZ39
C	681	HIS	-	expression tag	UNP C4QZ39
C	682	HIS	-	expression tag	UNP C4QZ39
C	683	PRO	-	expression tag	UNP C4QZ39
C	684	GLN	-	expression tag	UNP C4QZ39
C	685	GLY	-	expression tag	UNP C4QZ39
C	686	GLN	-	expression tag	UNP C4QZ39
C	687	ARG	-	expression tag	UNP C4QZ39
C	688	GLU	-	expression tag	UNP C4QZ39
C	689	PRO	-	expression tag	UNP C4QZ39
C	690	GLY	-	expression tag	UNP C4QZ39
C	691	GLY	-	expression tag	UNP C4QZ39
C	692	SER	-	expression tag	UNP C4QZ39
C	693	HIS	-	expression tag	UNP C4QZ39
C	694	HIS	-	expression tag	UNP C4QZ39
C	695	HIS	-	expression tag	UNP C4QZ39
C	696	HIS	-	expression tag	UNP C4QZ39
C	697	HIS	-	expression tag	UNP C4QZ39
C	698	HIS	-	expression tag	UNP C4QZ39

- Molecule 4 is a protein called Spt20.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	210	Total	C	N	O	S	0	0
			1682	1071	292	315	4		

- Molecule 5 is a protein called Subunit of the SAGA and SAGA-like transcriptional regulatory complexes, interacts with Spt15p to act.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	209	Total	C	N	O	S	0	0
			1616	1016	298	295	7		

- Molecule 6 is a protein called Subunit of the SAGA transcriptional regulatory complex, involved in proper assembly of the complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	154	Total	C	N	O	S	0	0
			1232	784	208	233	7		

- Molecule 7 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	96	Total	C	N	O	S	0	0
			768	489	120	156	3		

- Molecule 8 is a protein called Subunit (61/68 kDa) of TFIID and SAGA complexes.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	154	Total	C	N	O	S	0	0
			1192	747	216	226	3		

- Molecule 9 is a protein called Subunit (90 kDa) of TFIID and SAGA complexes.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	522	Total	C	N	O	S	0	0
			4075	2581	719	756	19		

- Molecule 10 is a protein called Subunit (60 kDa) of TFIID and SAGA complexes.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	421	Total	C	N	O	S	0	0
			3263	2084	556	617	6		

- Molecule 11 is a protein called Subunit (17 kDa) of TFIID and SAGA complexes, involved

in RNA polymerase II transcription initiation.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	123	Total	C	N	O	S	0	0
			981	632	169	178	2		

- Molecule 12 is a protein called Transcription-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	2968	Total	C	N	O	S	0	0
			22318	14296	3864	4071	87		

- Molecule 13 is a protein called Transcriptional regulator involved in glucose repression of Gal4p-regulated genes.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	B	76	Total	C	N	O	0	0
			373	221	76	76		

- Molecule 14 is a protein called Spt8.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	335	Total	C	N	O	0	0
			1648	978	335	335		

- Molecule 15 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	76	Total	C	N	O	S	2	0
			611	384	105	121	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	76	GLZ	-	expression tag	UNP J3QS39

- Molecule 16 is a protein called Ubiquitin carboxyl-terminal hydrolase.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	482	Total	C	N	O	S	0	0
			3817	2410	657	719	31		

- Molecule 17 is a protein called SAGA-associated factor 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	117	Total	C	N	O	S	0	0
			922	563	169	184	6		

- Molecule 18 is a protein called Transcription and mRNA export factor SUS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	90	Total	C	N	O	S	0	0
			735	470	122	142	1		

- Molecule 19 is water.

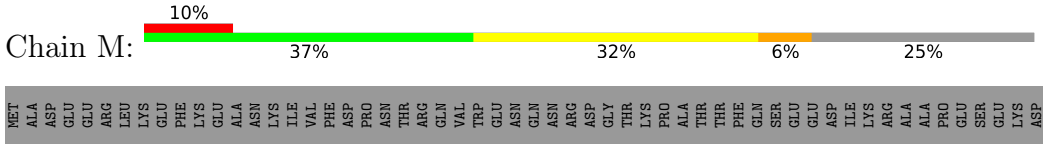
Mol	Chain	Residues	Atoms		AltConf
19	R	83	Total	O	0
			83	83	
19	Q	8	Total	O	0
			8	8	

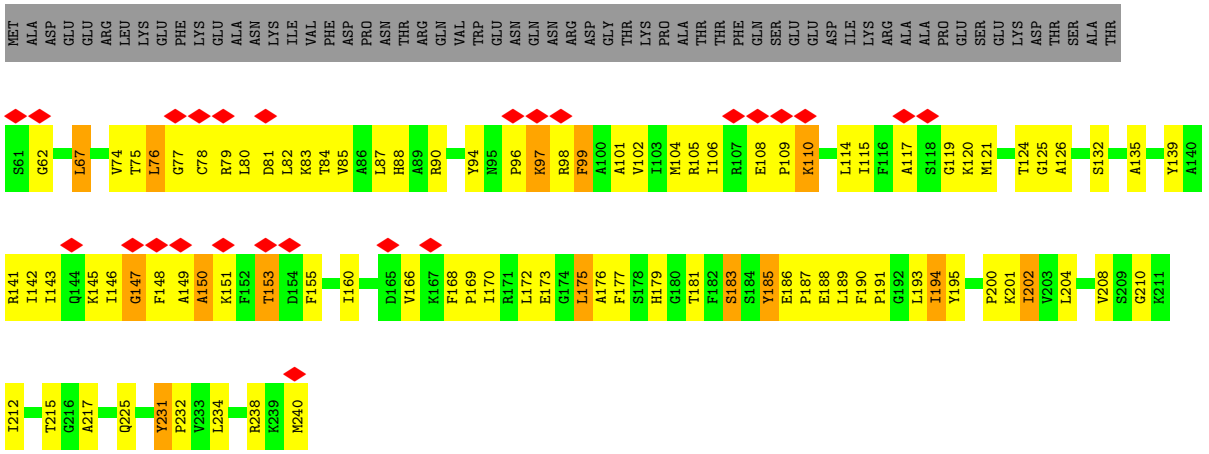
3 Residue-property plots (i)

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: TATA-box Binding Protein (TBP)

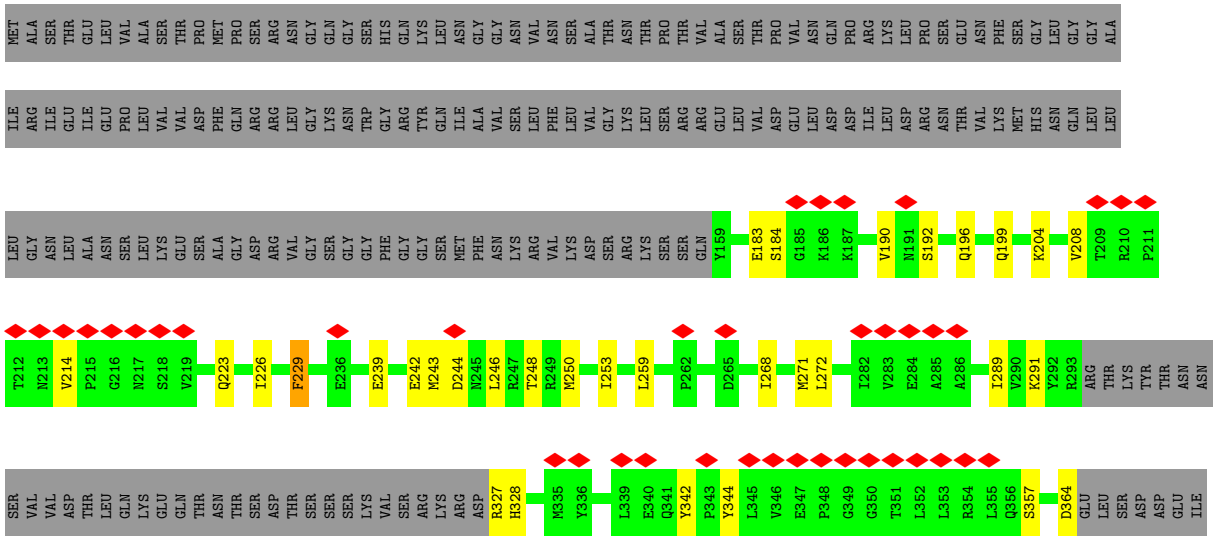
Chain M:





• Molecule 2: Transcriptional coactivator HFI1/ADA1

Chain A:



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

THR LYS GLU GLU LEU ASN TRP PHE ILE TYR ASP ILE LEU SER ASN ASN GLU

- Molecule 3: Subunit of SAGA histone acetyltransferase complex

Chain C: 5% 9% • 86%

MET GLN ASN PRO GLU ARG PRO VAL VAL TRP LYS GLU LEU GLY GLN TYR LEU ASP THR LEU GLN PRO ILE HIS GLN GLU LYS PRO SER SER LEU PRO ASP LEU PRO SER PRO SER TYR K31 D32 S33 L34 S35 N36 P37 L38 R39 Y40 R41 I42 C43 N44 N45 C46 D47 R48 P49 I50 L51

Q52 S53 C54 L55 S56 K57 H58 I59 K60 ILE CYS ASN GLN ILE VAL LYS VAL GLU LYS LEU GLU GLU ASP ASP LYS PRO MET ASN MET VAL ARG LYS ARG LYS ASN GLN VAL LEU GLU GLU SER LYS GLU SER THR PRO VAL THR ASN THR ASN SER THR ASN SER SER ASN ALA ILE ASN

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

GLY ALA LYS ARG ALA VAL PRO GLY ARG SER ALA PRO TYR ASP GLN LEU LEU VAL ALA TYR GLN ARG LYS ASN GLN ALA LYS PHE ALA ALA ASN ALA ALA ALA ALA HIS ALA ALA ARG ASP ASP LEU ILE HIS GLY SER GLN ILE PRO ILE ASP GLU ASP ASP GLU ALA H237 R253 K254

V255 I256 M257 P258 A259 R260 S261 E270 L277 PRO ARG VAL PRO THR ASN PRO PHE GLY ASN L288 Y289 S290 R291 T292 A293 R299 F305 S306 V307 P311 ARG MET PRO ASN GLN GLN GLN ASN LYS THR GLN LYS ASN PRO GLN PRO PRO ARG PRO GLN VAL GLN GLN GLN GLN

GLN ALA GLN LYS SER GLN GLN SER PRO PRO GLN ALA GLN GLN ILE SER GLN SER ALA GLY GLN GLN THR SER GLN THR VAL GLN ARG LEU VAL GLN GLN GLN GLN ARG LEU GLN GLN GLN ARG GLN GLN THR GLN ILE GLN GLN GLN GLN HIS GLN GLN GLN GLN GLN GLN

GLN HIS GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN THR HIS MET LEU GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN MET LEU LEU LEU GLN GLN GLN GLN GLN GLN ALA GLN GLN GLN SER PRO PRO ILE THR HIS GLN SER PRO ILE PRO ASP ASN

ARG PRO SER ASN GLN LEU PRO GLN GLN TYR SER GLN MET THR PRO GLN GLN LEU GLN LEU GLN GLN GLN LEU GLN LEU GLN GLN LYS GLN LYS GLU GLN PHE ARG LEU GLN GLN GLN GLN HIS LEU ARG ASN LEU UNK MET ARG UNK THR PRO GLN GLN GLN GLN GLN PHE ALA ASN LEU

THR PRO GLU LYS ARG ALA GLN PHE GLN ARG MET GLN LEU VAL GLN LEU GLN GLN GLN ILE LYS ASN GLN ALA ILE GLN ASN GLN MET GLN GLN GLN GLN GLN PRO SER HIS VAL GLN SER GLN ALA GLN THR GLN PHE GLN ALA GLN LEU LYS ALA GLN SER ARG ALA GLN VAL

LEU GLN ALA ALA GLN ARG GLN MET GLN ASN SER PRO THR SER PRO VAL THR SER MET SER SER PRO LEU ALA ILE PRO SER ASN LEU ALA ASN GLN GLY PRO ASN GLN THR SER GLN LEU PRO ASN GLU GLN LEU SER ASN PRO LEU MET GLY ASN GLN PHE GLN GLY GLN PHE ASN GLN

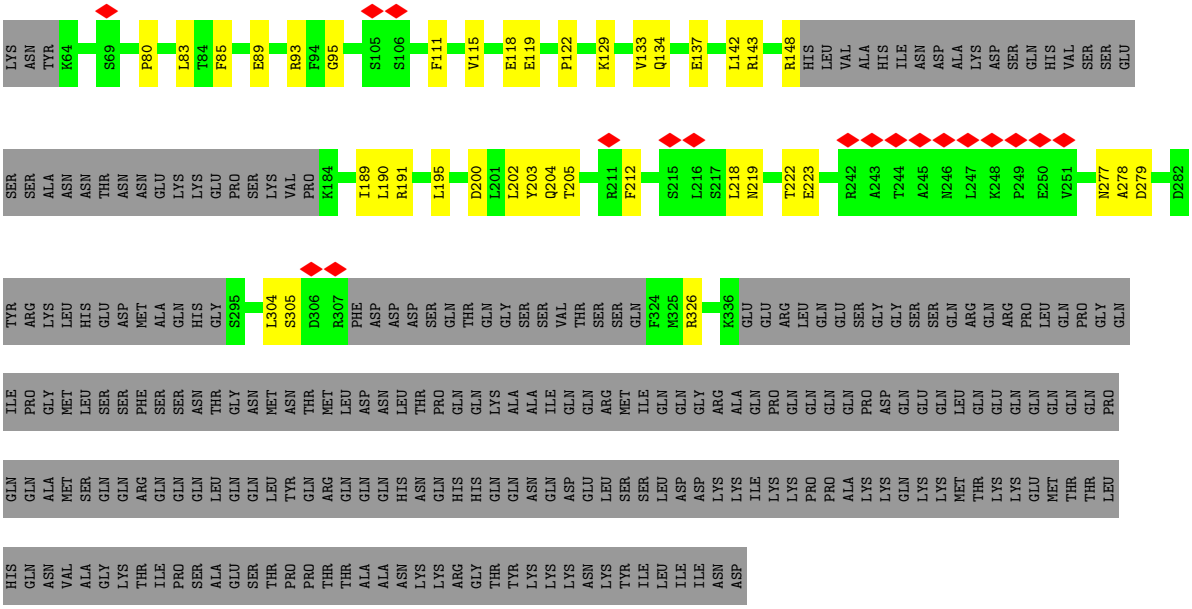
TYR GLN PRO ASN TYR ARG GLU ASN LEU GLU GLY GLY GLY GLY SER MET ASP GLU LYS THR THR GLY TRP ARG GLY GLY HIS VAL VAL GLU GLY LEU ALA GLY GLU LEU GLU GLN LEU ARG ALA ARG LEU GLU HIS HIS PRO GLN GLY GLN ARG GLU PRO GLY GLY SER HIS HIS HIS HIS

HIS HIS

- Molecule 4: Spt20

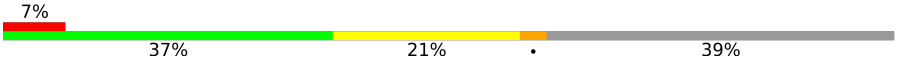
Chain F: • 33% 7% 59%

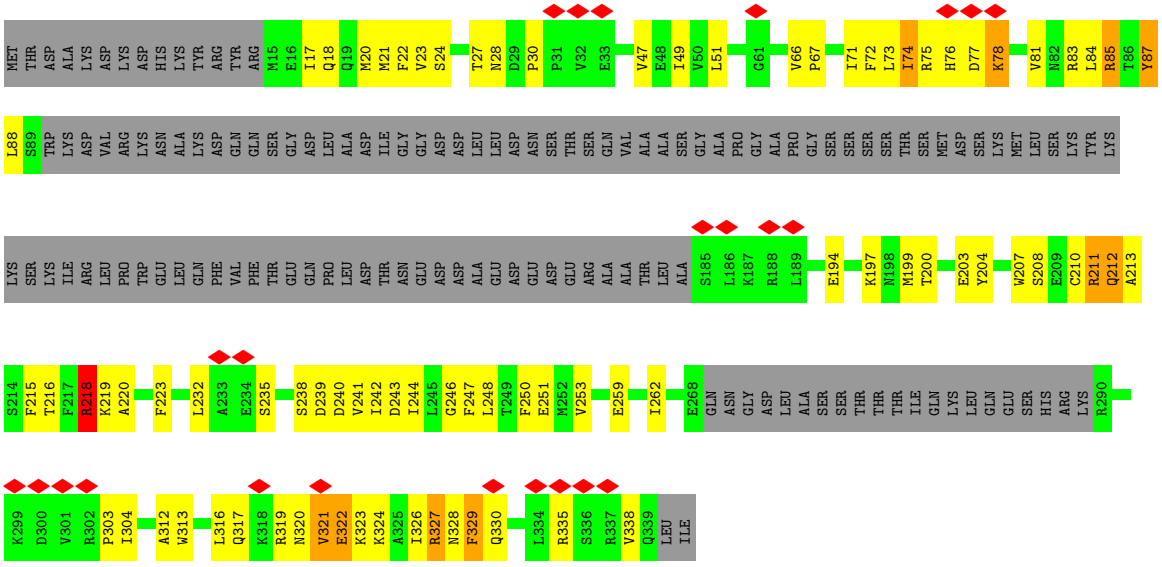
MET SER GLN ILE GLN SER SER GLN VAL GLY ALA LYS ASN MET GLN THR ALA GLN PRO GLN ALA GLN ARG PRO ILE ASN GLY SER VAL THR LEU SER ASN GLY GLN ARG ILE ASN PRO GLN ASN LEU THR PRO GLN GLN GLN ARG LEU LEU GLN GLN LYS VAL LEU HIS GLN LYS LEU



• Molecule 5: Subunit of the SAGA and SAGA-like transcriptional regulatory complexes, interacts with Spt15p to act

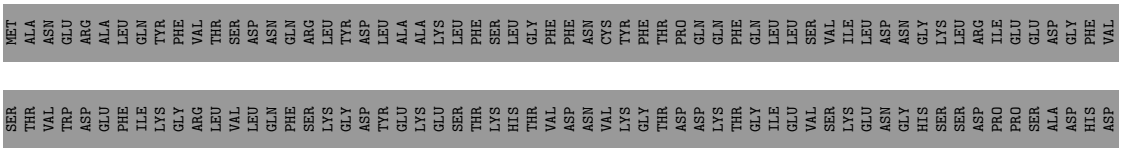
Chain D:

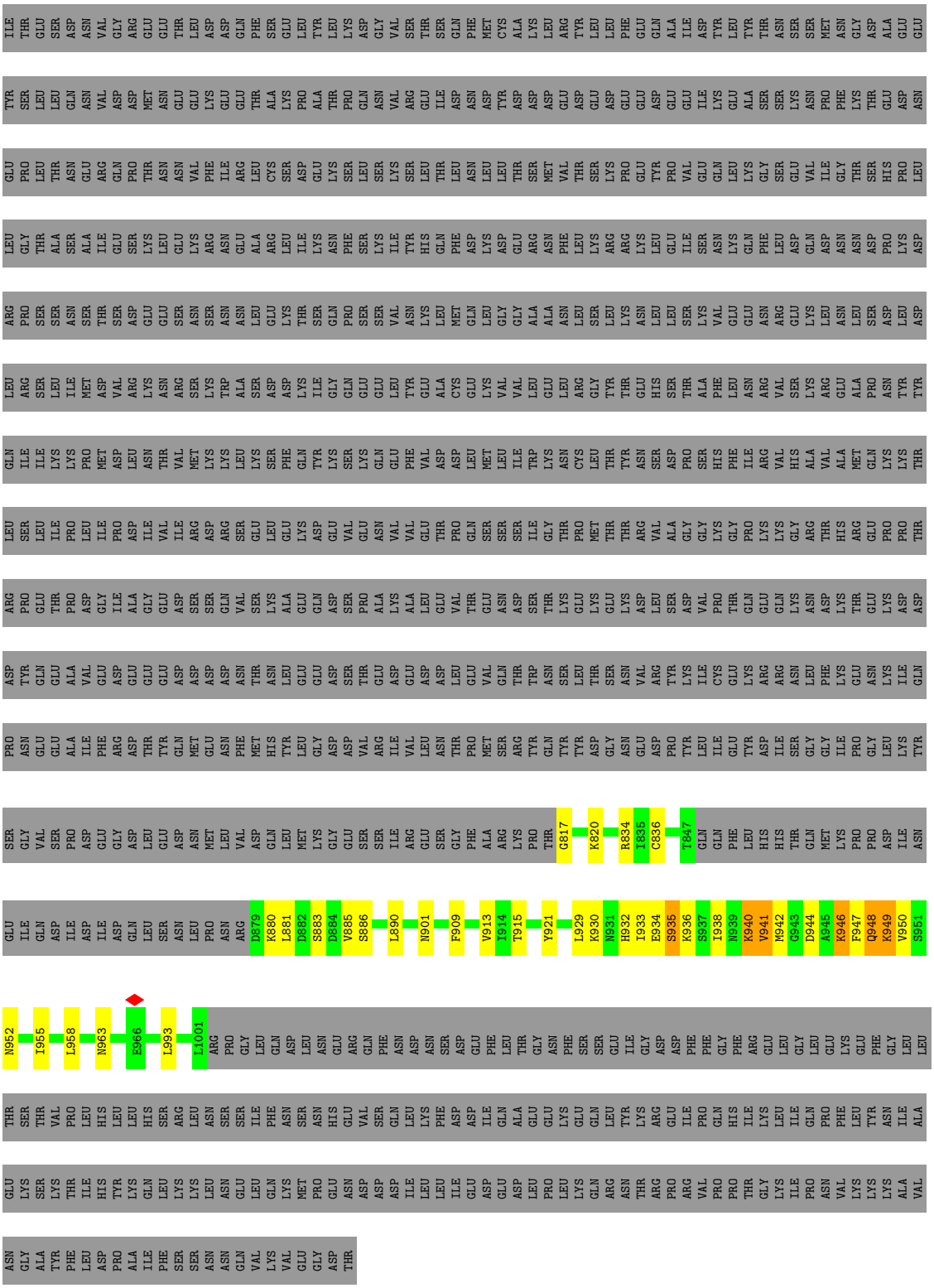




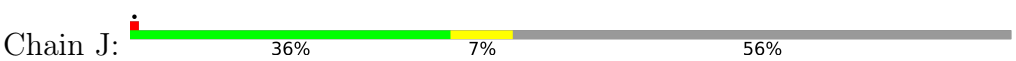
• Molecule 6: Subunit of the SAGA transcriptional regulatory complex, involved in proper assembly of the complex

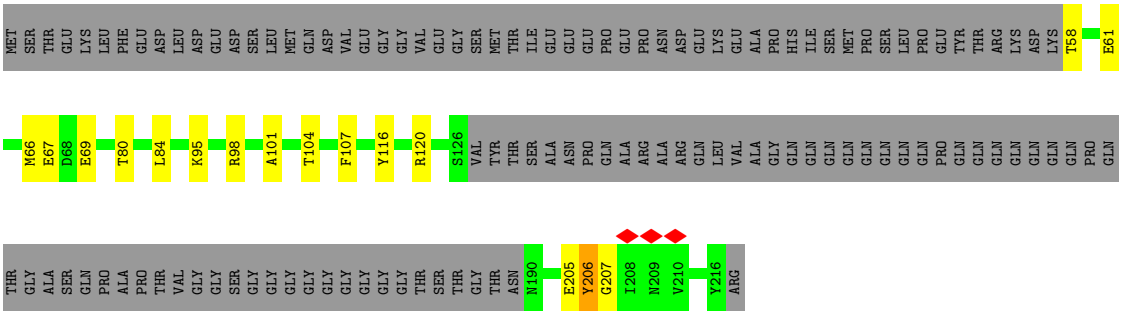
Chain E:





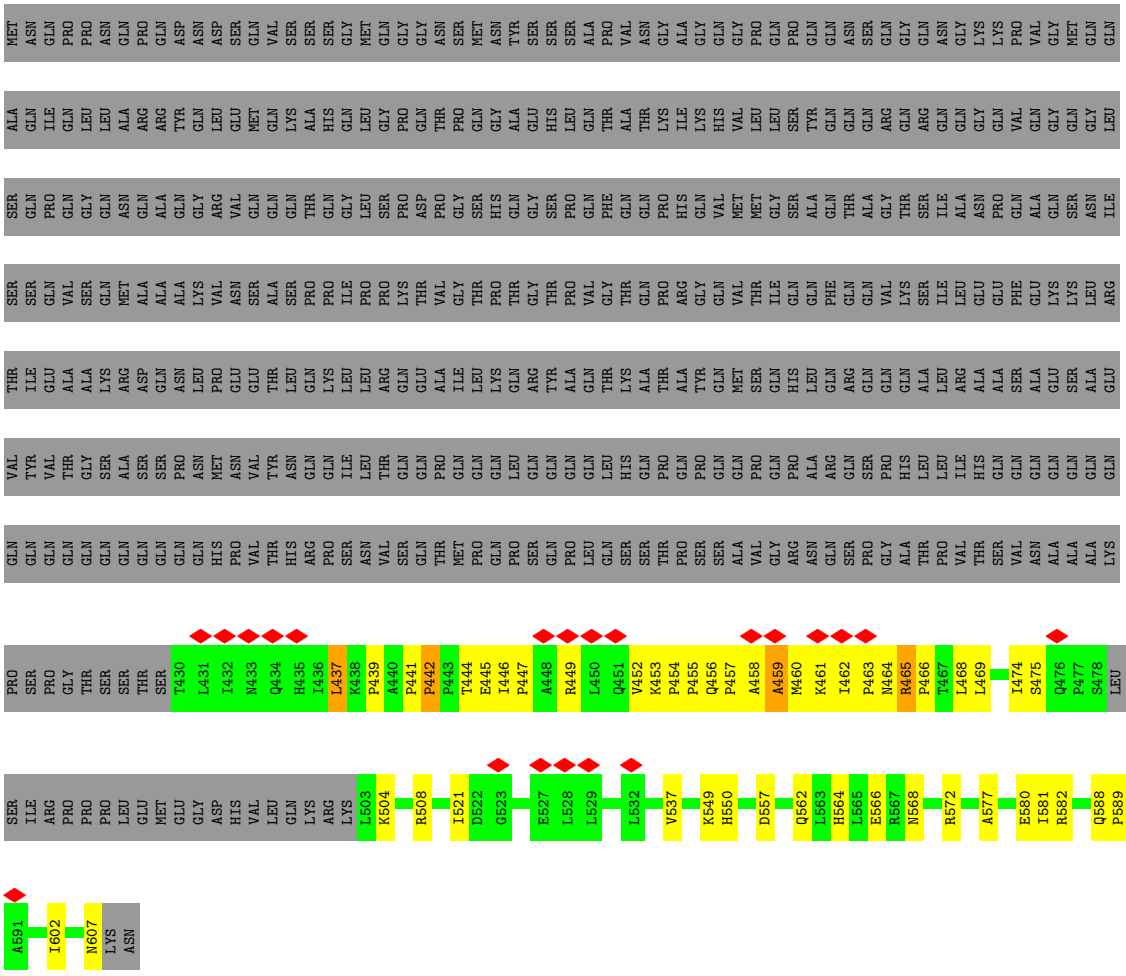
• Molecule 7: Transcription initiation factor TFIID subunit 10





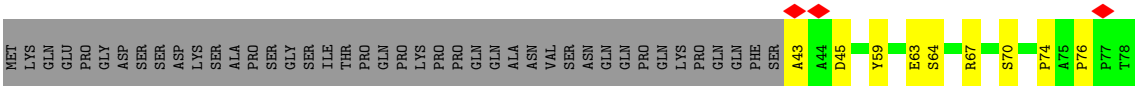
• Molecule 8: Subunit (61/68 kDa) of TFIID and SAGA complexes

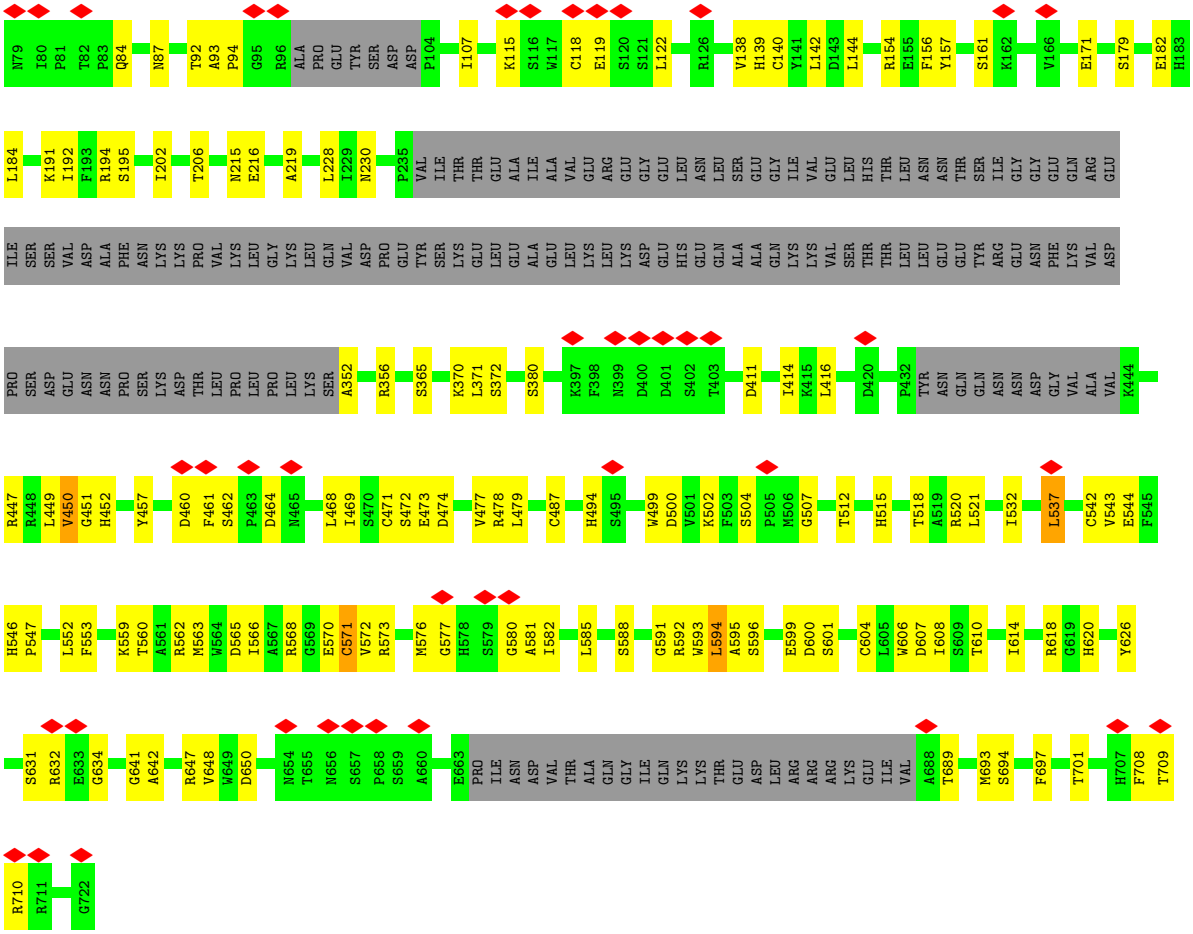
Chain K:



• Molecule 9: Subunit (90 kDa) of TFIID and SAGA complexes

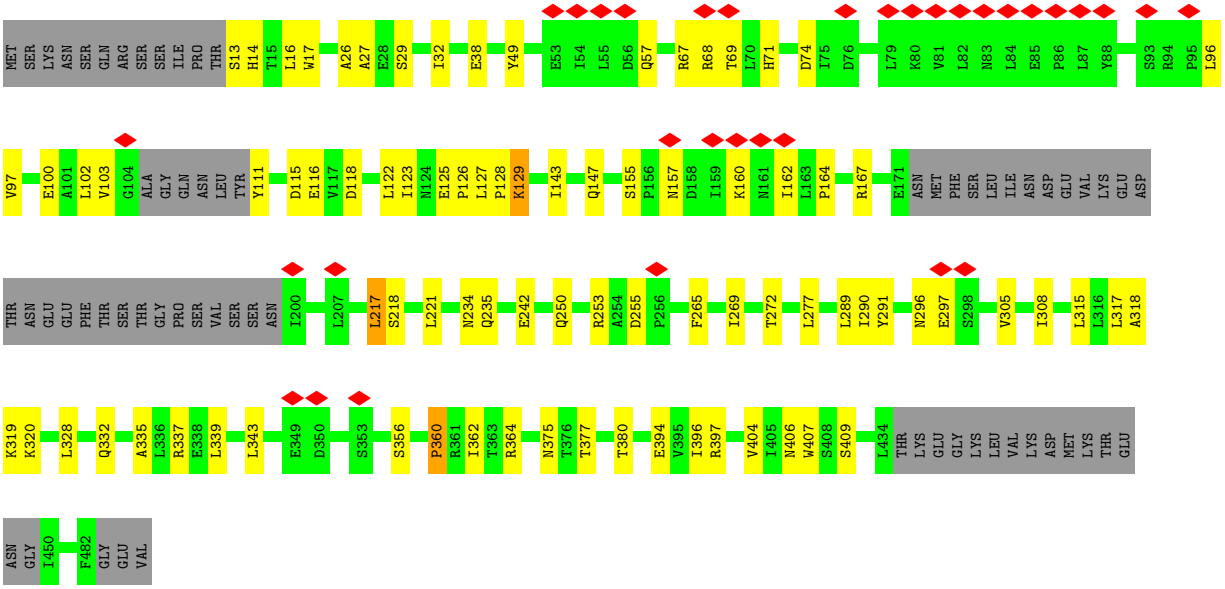
Chain G:





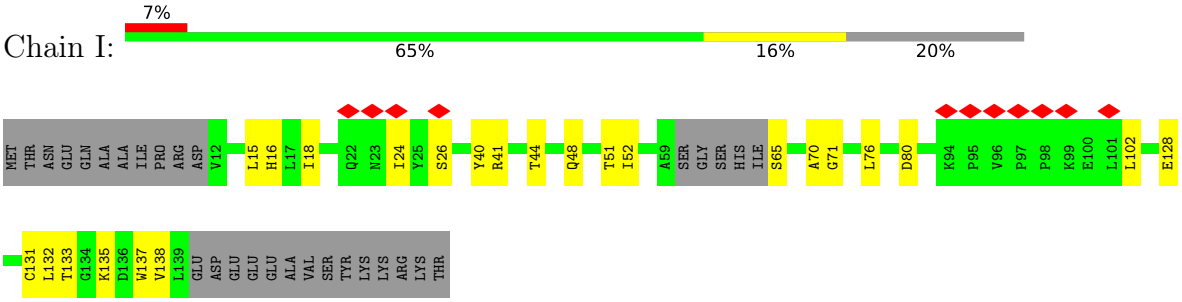
• Molecule 10: Subunit (60 kDa) of TFIID and SAGA complexes

Chain H:



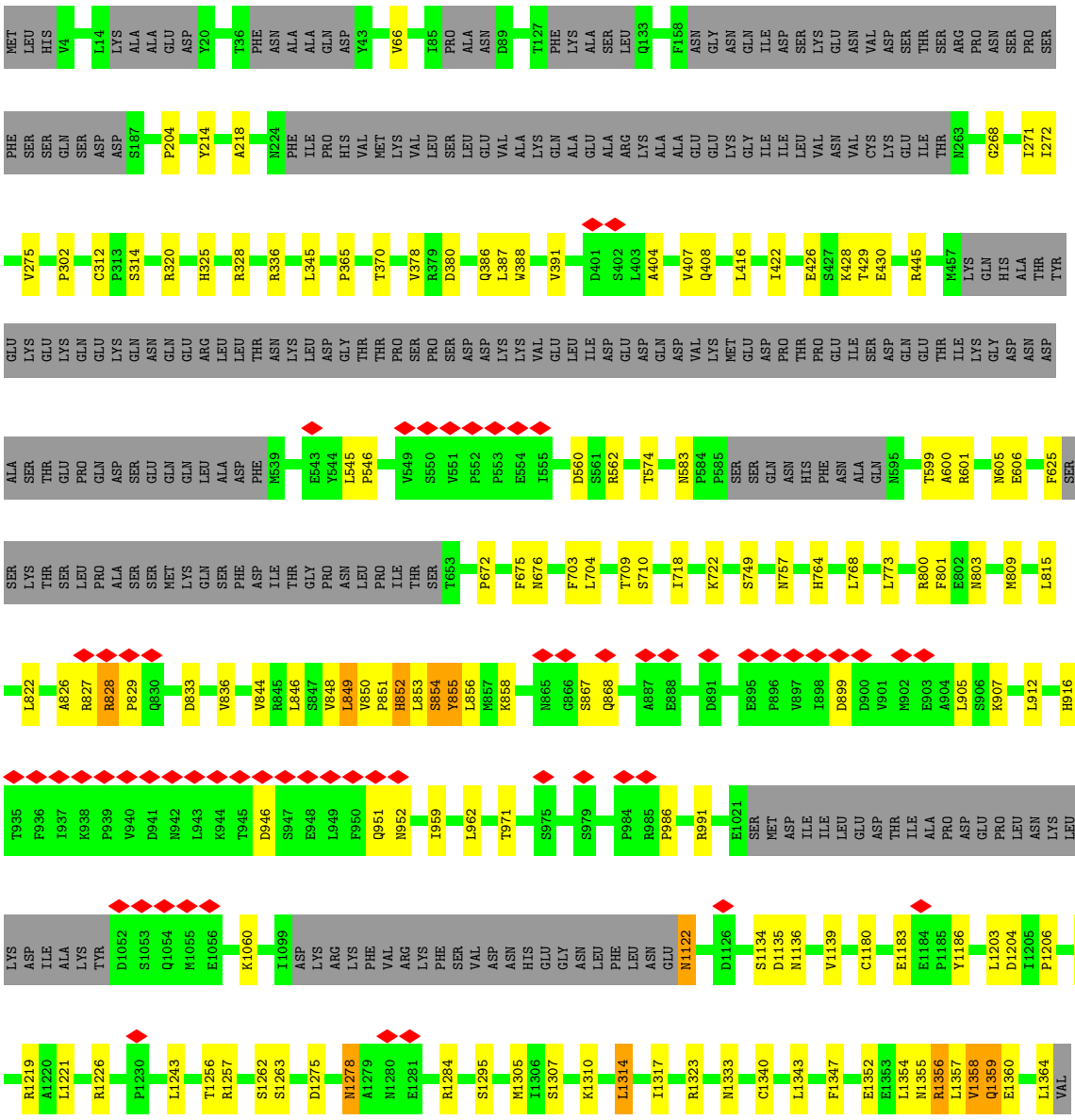
• Molecule 11: Subunit (17 kDa) of TFIID and SAGA complexes, involved in RNA polymerase II transcription initiation

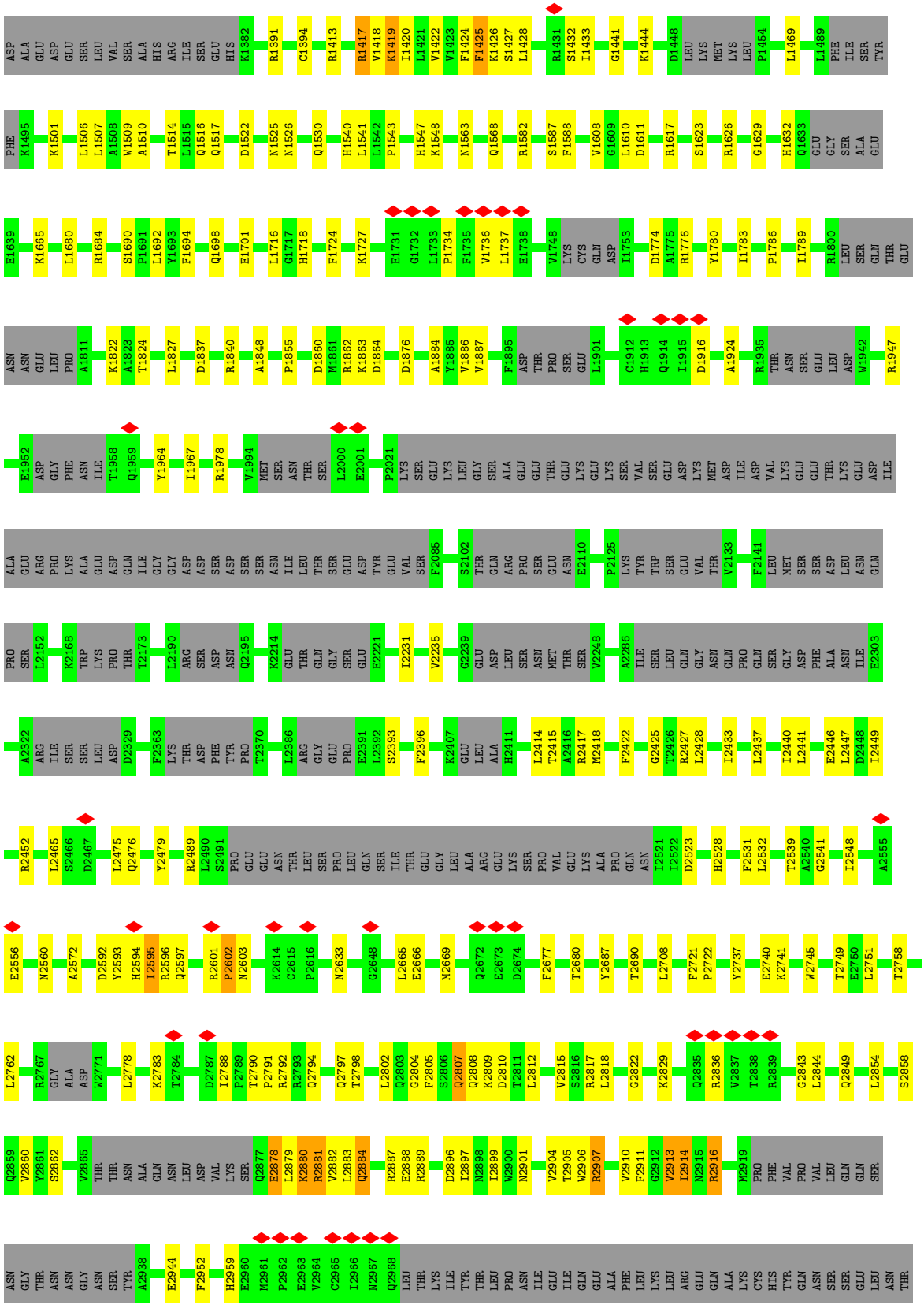
Chain I:

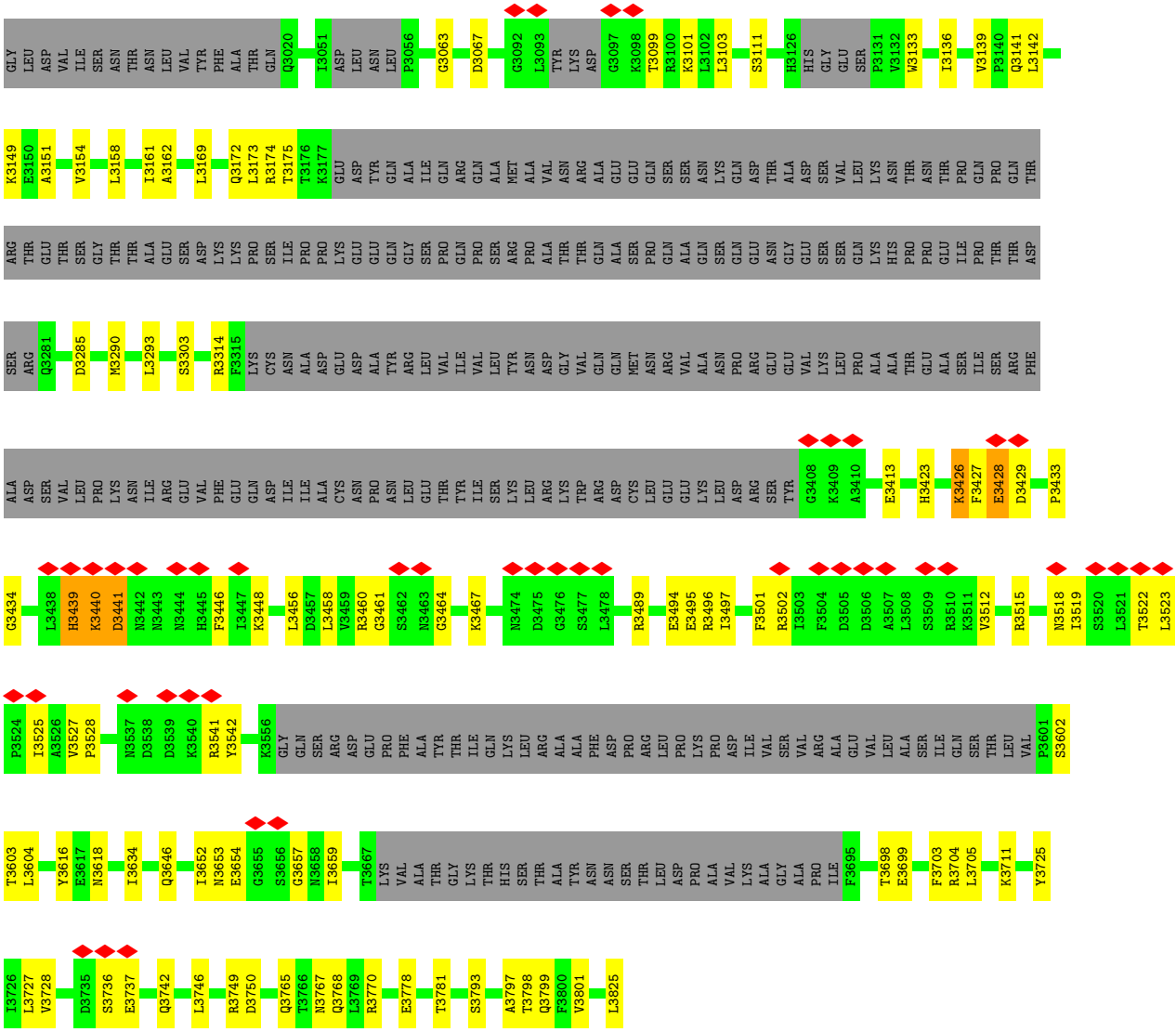


• Molecule 12: Transcription-associated protein

Chain L:

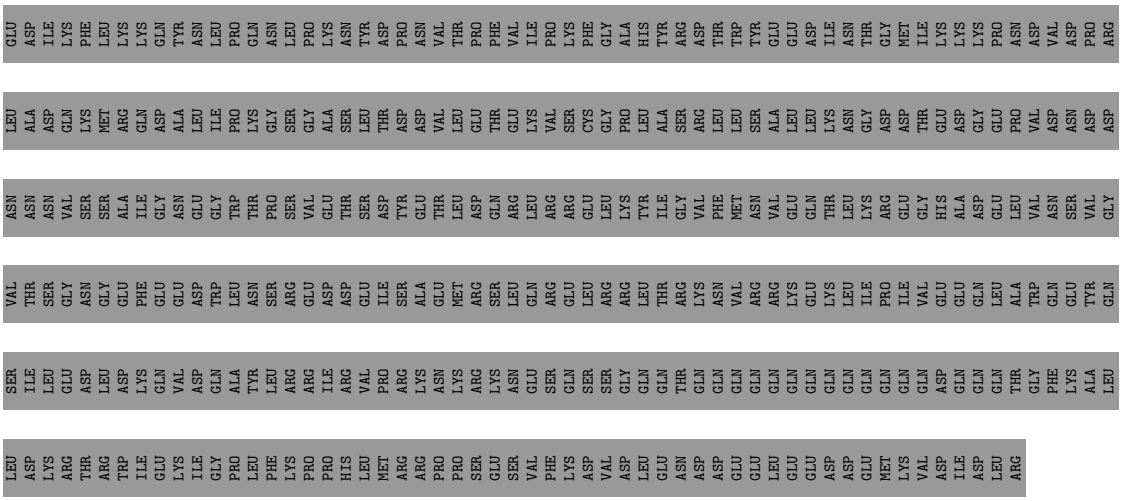






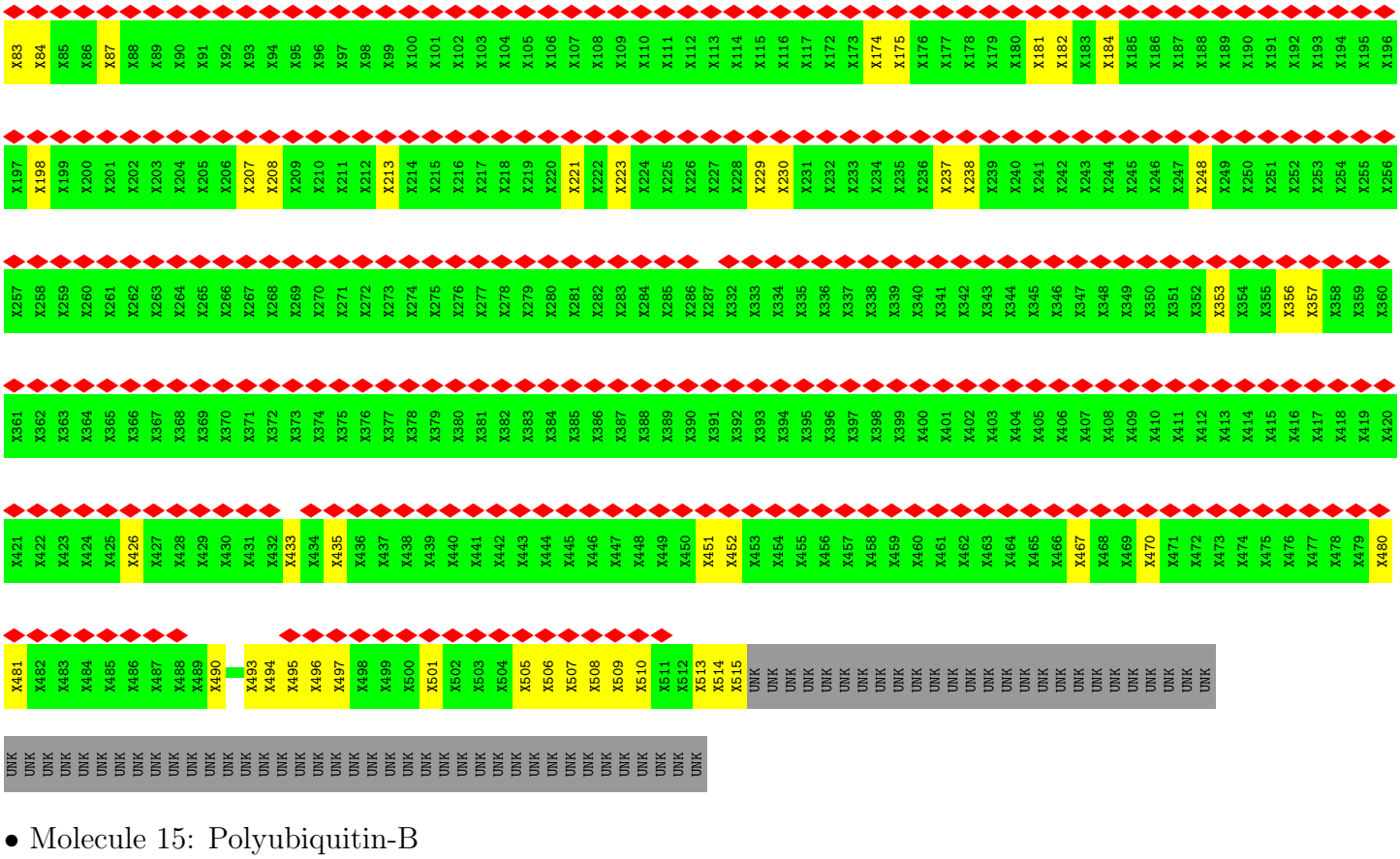
• Molecule 13: Transcriptional regulator involved in glucose repression of Gal4p-regulated genes

Chain B:



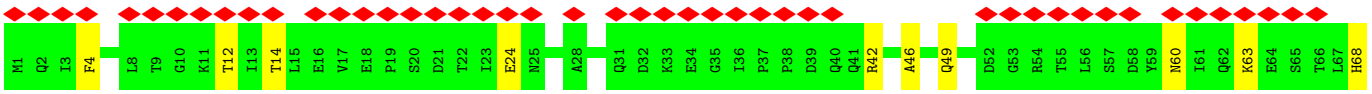
• Molecule 14: Spt8

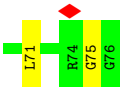
Chain N:



• Molecule 15: Polyubiquitin-B

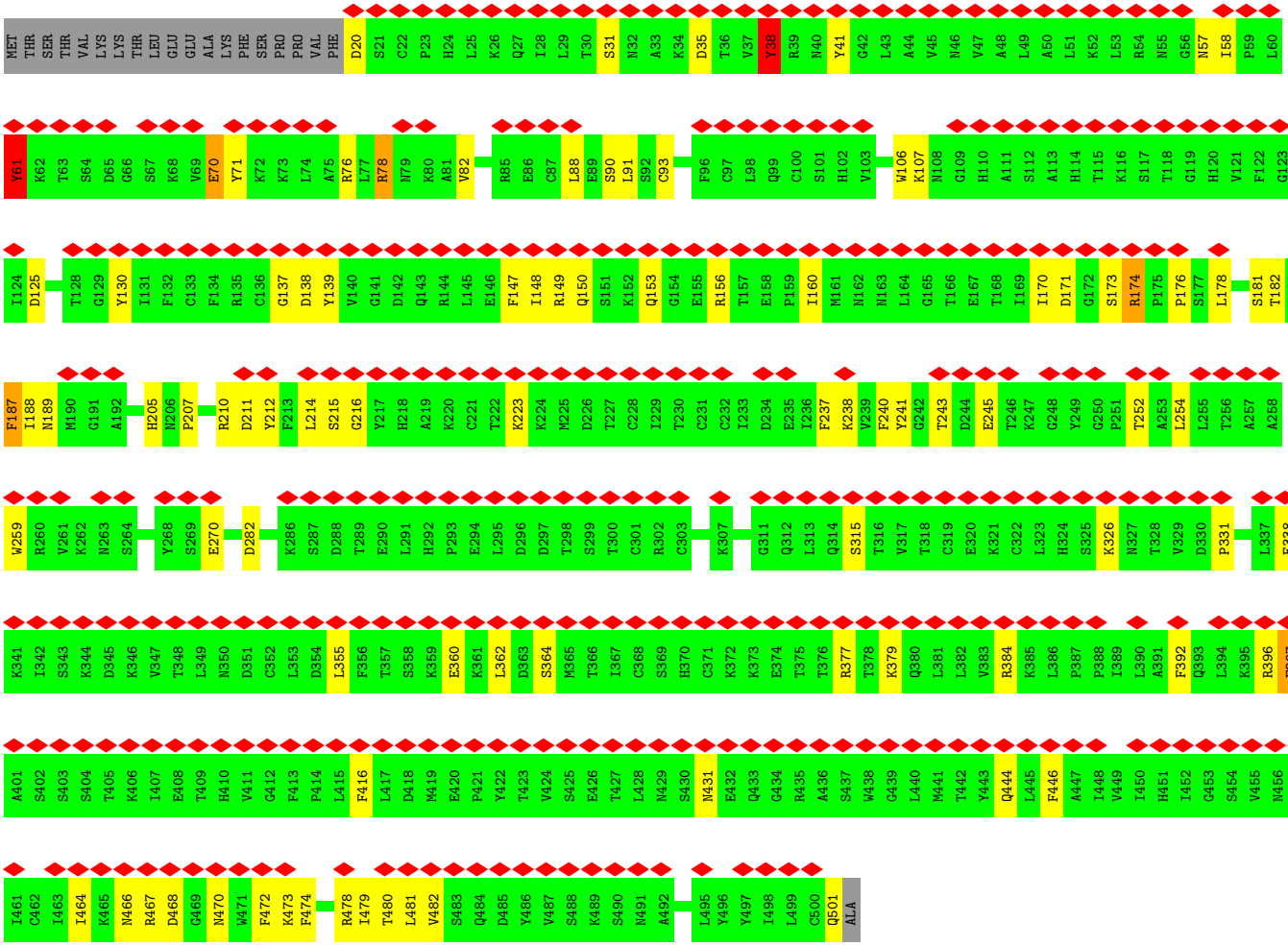
Chain R:





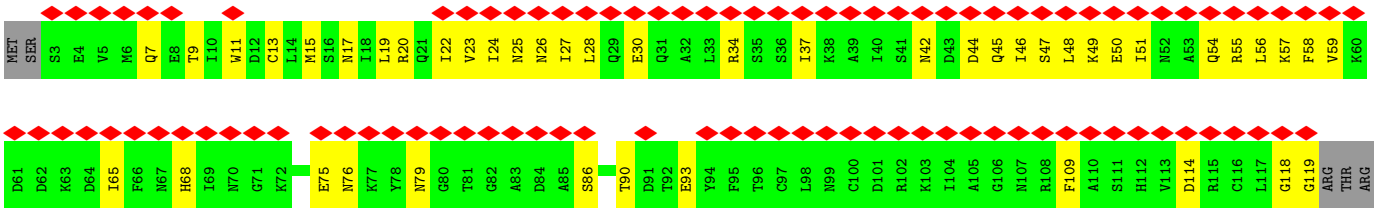
• Molecule 16: Ubiquitin carboxyl-terminal hydrolase

Chain Q:



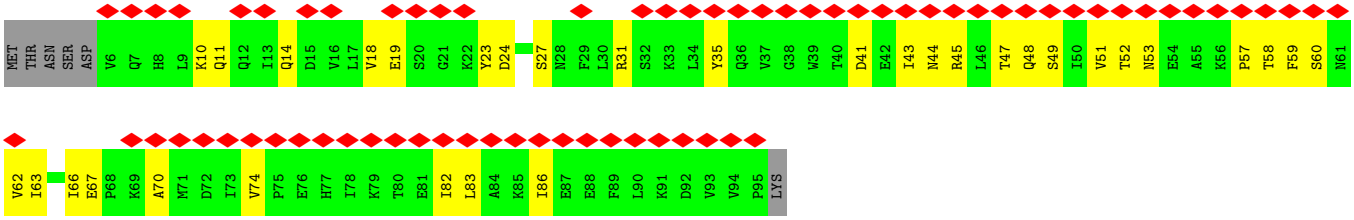
• Molecule 17: SAGA-associated factor 11

Chain O:



• Molecule 18: Transcription and mRNA export factor SUS1

Chain P:


MET
THR
ASN
SER
ASP
V6
Q7
H8
L9
K10
Q11
Q12
I13
Q14
D15
V16
L17
V18
E19
S20
G21
K22
Y23
D24
S27
N28
F29
L30
R31
S32
K33
L34
Y35
Q36
V37
G38
W39
T40
D41
E42
I43
N44
R45
L46
T47
Q48
S49
I50
V51
T52
N53
E54
A55
K56
P57
T58
F59
S60
N61
V62
I63
I66
E67
P68
K69
A70
M71
D72
I73
V74
P75
E76
H77
I78
K79
T80
E81
I82
L83
A84
K85
I86
E87
E88
F89
L90
K91
D92
V93
V94
P95
LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	354104	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	52.8	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.032	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	558.08, 558.08, 558.08	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.18, 2.18, 2.18	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	M	0.88	2/1442 (0.1%)	0.78	2/1942 (0.1%)
2	A	0.44	0/1319	0.60	0/1794
3	C	0.53	0/774	0.75	0/1039
4	F	0.34	0/1718	0.58	0/2335
5	D	0.51	0/1641	0.65	0/2213
6	E	0.45	0/1246	0.62	0/1667
7	J	0.47	0/779	0.60	0/1051
8	K	0.42	0/1213	0.66	0/1647
9	G	0.52	0/4177	0.60	0/5661
10	H	0.38	0/3315	0.60	0/4500
11	I	0.44	0/1006	0.63	0/1374
12	L	0.33	0/22712	0.54	0/30825
13	B	0.64	0/370	0.70	1/509 (0.2%)
15	R	0.83	1/619 (0.2%)	0.75	0/833
16	Q	0.71	0/3897	1.09	15/5265 (0.3%)
17	O	0.79	0/931	1.13	2/1250 (0.2%)
18	P	0.75	0/747	1.01	0/1011
All	All	0.47	3/47906 (0.0%)	0.67	20/64916 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	M	0	1
16	Q	2	5
All	All	2	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	194	ILE	C-N	27.38	1.97	1.34
1	M	183	SER	C-N	6.38	1.48	1.34
15	R	24	GLU	CB-CG	-5.25	1.42	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Q	61	TYR	CB-CG-CD1	9.83	126.90	121.00
16	Q	61	TYR	CB-CG-CD2	-9.38	115.37	121.00
1	M	62	GLY	N-CA-C	6.94	130.46	113.10
16	Q	78	ARG	NE-CZ-NH1	-6.80	116.90	120.30
13	B	527	PRO	N-CA-CB	6.57	111.18	103.30
17	O	119	GLY	N-CA-C	6.39	129.07	113.10
16	Q	240	PHE	CB-CG-CD1	6.28	125.20	120.80
1	M	194	ILE	CA-C-N	-6.13	103.71	117.20
16	Q	41	TYR	CB-CG-CD1	6.09	124.65	121.00
16	Q	396	ARG	NE-CZ-NH1	5.95	123.27	120.30
16	Q	384	ARG	NE-CZ-NH2	5.87	123.23	120.30
16	Q	78	ARG	NE-CZ-NH2	5.72	123.16	120.30
16	Q	187	PHE	CB-CG-CD1	5.58	124.71	120.80
16	Q	174	ARG	NE-CZ-NH2	5.57	123.09	120.30
16	Q	240	PHE	CB-CG-CD2	-5.31	117.08	120.80
16	Q	38	TYR	CA-CB-CG	5.28	123.44	113.40
16	Q	187	PHE	CB-CG-CD2	-5.18	117.18	120.80
16	Q	41	TYR	CB-CG-CD2	-5.13	117.92	121.00
17	O	118	GLY	C-N-CA	5.12	133.06	122.30
16	Q	392	PHE	CB-CG-CD2	-5.08	117.24	120.80

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	Q	31	SER	CA
16	Q	222	THR	CA

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	183	SER	Mainchain
16	Q	149	ARG	Sidechain
16	Q	212	TYR	Sidechain
16	Q	241	TYR	Sidechain
16	Q	38	TYR	Sidechain
16	Q	61	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	1415	0	1491	102	0
2	A	1300	0	1254	30	0
3	C	761	0	779	194	0
4	F	1682	0	1622	30	0
5	D	1616	0	1558	122	0
6	E	1232	0	1276	40	0
7	J	768	0	754	11	0
8	K	1192	0	1214	89	0
9	G	4075	0	3934	102	0
10	H	3263	0	3258	69	0
11	I	981	0	982	18	0
12	L	22318	0	20960	376	0
13	B	373	0	190	2	0
14	N	1648	0	382	61	0
15	R	611	0	636	20	0
16	Q	3817	0	3772	521	0
17	O	922	0	897	411	0
18	P	735	0	743	191	0
19	Q	8	0	0	10	0
19	R	83	0	0	7	0
All	All	48800	0	45702	1602	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 (1602) 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)
16:Q:472:PHE:CZ	17:O:45:GLN:HB3	1.29	1.65
17:O:11:TRP:CD1	18:P:83:LEU:HD23	1.14	1.61
16:Q:479:ILE:HG23	17:O:47:SER:CA	1.19	1.61
16:Q:479:ILE:CG2	17:O:47:SER:HA	1.14	1.60
17:O:34:ARG:HH11	18:P:57:PRO:CB	1.11	1.58
16:Q:464:ILE:CD1	17:O:46:ILE:CD1	1.74	1.57
17:O:9:THR:HG22	18:P:10:LYS:CE	1.29	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:22:ILE:CD1	18:P:43:ILE:HD11	1.14	1.55
3:C:38:LEU:HD22	16:Q:210:ARG:CD	1.33	1.55
16:Q:464:ILE:CG1	17:O:46:ILE:HD12	1.34	1.54
3:C:34:LEU:CD2	16:Q:446:PHE:HE1	0.95	1.54
3:C:38:LEU:HD13	16:Q:210:ARG:CZ	1.21	1.54
17:O:11:TRP:HD1	18:P:83:LEU:CD2	1.19	1.54
3:C:39:ARG:NH1	16:Q:148:ILE:CA	1.68	1.53
16:Q:178:LEU:HD13	17:O:37:ILE:CD1	1.34	1.53
17:O:22:ILE:HD13	18:P:43:ILE:CD1	1.13	1.53
3:C:34:LEU:HD22	16:Q:446:PHE:CE1	1.00	1.52
3:C:38:LEU:CD1	16:Q:210:ARG:NE	1.67	1.51
8:K:469:LEU:HD13	12:L:2788:ILE:CG2	1.31	1.51
16:Q:464:ILE:CD1	17:O:46:ILE:HD13	1.26	1.51
17:O:9:THR:CG2	18:P:10:LYS:HE3	1.08	1.50
14:N:207:UNK:C	14:N:208:UNK:H2	1.23	1.49
16:Q:472:PHE:CD2	17:O:46:ILE:HG12	1.45	1.49
3:C:49:PRO:HG2	16:Q:237:PHE:CE1	1.48	1.46
16:Q:178:LEU:CD1	17:O:37:ILE:HD13	1.42	1.45
17:O:11:TRP:NE1	18:P:83:LEU:HA	1.18	1.45
16:Q:182:THR:CG2	17:O:44:ASP:HB2	1.47	1.44
3:C:38:LEU:CD2	16:Q:210:ARG:HD2	1.46	1.44
17:O:56:LEU:CD1	18:P:52:THR:H	1.18	1.43
3:C:39:ARG:HH11	16:Q:148:ILE:CG2	1.29	1.41
17:O:9:THR:CG2	18:P:10:LYS:CE	1.86	1.41
14:N:207:UNK:C	14:N:208:UNK:N	1.79	1.40
17:O:11:TRP:CE2	18:P:86:ILE:HD12	1.55	1.40
16:Q:182:THR:N	17:O:44:ASP:CB	1.70	1.40
16:Q:482:VAL:HG12	17:O:49:LYS:N	1.30	1.39
17:O:11:TRP:CD1	18:P:83:LEU:CD2	1.93	1.39
16:Q:78:ARG:NH2	18:P:23:TYR:HE2	1.15	1.39
17:O:27:ILE:CD1	18:P:59:PHE:HA	1.53	1.38
16:Q:78:ARG:NH2	18:P:23:TYR:CE2	1.88	1.38
16:Q:479:ILE:HG23	17:O:47:SER:CB	1.53	1.38
16:Q:472:PHE:CD2	17:O:46:ILE:CG1	2.06	1.38
17:O:55:ARG:C	18:P:52:THR:HG21	1.01	1.37
1:M:88:HIS:O	14:N:515:UNK:C	1.71	1.36
15:R:4:PHE:CZ	16:Q:377:ARG:NH1	1.94	1.35
17:O:22:ILE:CD1	18:P:43:ILE:CD1	1.76	1.35
8:K:469:LEU:CD1	12:L:2788:ILE:HG21	1.57	1.34
17:O:55:ARG:C	18:P:52:THR:CG2	1.96	1.34
3:C:47:ASP:CB	16:Q:243:THR:O	1.75	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:19:LEU:HD23	18:P:67:GLU:CG	1.57	1.34
16:Q:464:ILE:HD12	17:O:46:ILE:CD1	1.44	1.33
14:N:451:UNK:C	14:N:452:UNK:H2	1.42	1.32
17:O:19:LEU:CD2	18:P:67:GLU:HG3	1.57	1.32
16:Q:106:TRP:HD1	17:O:20:ARG:CZ	1.41	1.31
16:Q:472:PHE:CB	17:O:46:ILE:HG13	1.60	1.31
16:Q:416:PHE:HE1	18:P:35:TYR:CE2	0.98	1.31
16:Q:479:ILE:HB	17:O:68:HIS:CE1	1.59	1.31
1:M:147:GLY:O	14:N:435:UNK:CB	1.78	1.30
3:C:34:LEU:CD2	16:Q:446:PHE:CE1	1.74	1.30
16:Q:416:PHE:CE1	18:P:35:TYR:CE2	1.87	1.30
16:Q:139:TYR:CB	17:O:28:LEU:HD21	1.62	1.29
3:C:38:LEU:CD1	16:Q:210:ARG:CZ	2.01	1.29
3:C:51:LEU:N	16:Q:214:LEU:HG	1.47	1.29
3:C:39:ARG:NH1	16:Q:148:ILE:N	1.74	1.28
3:C:54:CYS:SG	16:Q:215:SER:HA	1.72	1.28
17:O:30:GLU:OE1	18:P:51:VAL:HG11	1.28	1.28
17:O:27:ILE:HG23	18:P:57:PRO:O	1.20	1.27
17:O:19:LEU:HD21	18:P:67:GLU:CA	1.64	1.27
3:C:52:GLN:NE2	16:Q:153:GLN:HG3	1.47	1.27
16:Q:189:ASN:ND2	19:Q:602:HOH:O	1.59	1.27
16:Q:178:LEU:CD1	17:O:37:ILE:CD1	2.02	1.26
17:O:11:TRP:HE1	18:P:83:LEU:CA	1.46	1.26
16:Q:71:TYR:HD1	18:P:24:ASP:OD2	1.12	1.25
16:Q:93:CYS:SG	17:O:20:ARG:HD2	1.75	1.25
16:Q:472:PHE:HD2	17:O:46:ILE:CG1	1.45	1.25
17:O:34:ARG:NH1	18:P:57:PRO:HB3	0.93	1.24
16:Q:91:LEU:HD21	17:O:13:CYS:SG	1.76	1.24
3:C:54:CYS:SG	16:Q:215:SER:CA	2.26	1.23
17:O:56:LEU:HD11	18:P:52:THR:N	1.22	1.21
14:N:451:UNK:C	14:N:452:UNK:N	1.99	1.21
16:Q:139:TYR:CE1	17:O:24:ILE:HG12	1.37	1.21
16:Q:182:THR:CA	17:O:44:ASP:HB3	1.70	1.21
16:Q:71:TYR:CD1	18:P:24:ASP:OD2	1.92	1.21
3:C:50:ILE:N	16:Q:214:LEU:HD11	1.53	1.20
17:O:56:LEU:N	18:P:52:THR:HG21	1.55	1.20
12:L:828:ARG:H	12:L:829:PRO:HD3	1.06	1.20
16:Q:479:ILE:CG2	17:O:47:SER:CA	1.91	1.20
16:Q:416:PHE:CE1	18:P:35:TYR:CD2	2.29	1.20
16:Q:472:PHE:CZ	17:O:45:GLN:CB	2.23	1.20
17:O:27:ILE:HD13	18:P:59:PHE:CA	1.71	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:474:PHE:CG	17:O:47:SER:HB3	1.75	1.19
1:M:194:ILE:HG22	1:M:195:TYR:N	1.57	1.19
3:C:49:PRO:CG	16:Q:237:PHE:CE1	2.24	1.19
16:Q:182:THR:CB	17:O:44:ASP:CB	2.13	1.19
17:O:54:GLN:HE22	18:P:49:SER:N	1.37	1.18
17:O:55:ARG:O	18:P:52:THR:HG21	1.43	1.18
15:R:4:PHE:HZ	16:Q:377:ARG:CZ	1.57	1.18
16:Q:106:TRP:CD1	17:O:20:ARG:CZ	2.27	1.18
3:C:39:ARG:NH1	16:Q:148:ILE:HA	1.34	1.18
1:M:194:ILE:C	1:M:195:TYR:N	1.97	1.17
16:Q:259:TRP:CD1	17:O:114:ASP:OD1	1.97	1.17
17:O:11:TRP:NE1	18:P:83:LEU:CA	2.06	1.17
17:O:11:TRP:CD2	18:P:86:ILE:HD12	1.80	1.16
3:C:39:ARG:HD2	16:Q:147:PHE:CE1	1.80	1.16
16:Q:474:PHE:CD2	17:O:47:SER:HB3	1.79	1.16
17:O:19:LEU:CD2	18:P:67:GLU:HA	1.75	1.16
3:C:51:LEU:HD23	16:Q:214:LEU:HD23	1.27	1.16
16:Q:139:TYR:HB3	17:O:28:LEU:CD2	1.76	1.15
16:Q:479:ILE:HD12	17:O:47:SER:HB2	1.25	1.14
17:O:34:ARG:NH1	18:P:57:PRO:CB	1.82	1.14
3:C:40:TYR:CB	16:Q:214:LEU:HD21	1.78	1.13
19:R:153:HOH:O	16:Q:326:LYS:HB3	1.44	1.13
17:O:22:ILE:HD12	18:P:43:ILE:CD1	1.75	1.13
16:Q:184:LEU:HD12	17:O:44:ASP:O	1.49	1.13
3:C:47:ASP:HB2	16:Q:243:THR:O	1.29	1.13
16:Q:479:ILE:CB	17:O:68:HIS:CE1	2.26	1.12
3:C:51:LEU:HD11	16:Q:211:ASP:O	1.44	1.12
16:Q:182:THR:N	17:O:44:ASP:HB3	1.42	1.11
3:C:38:LEU:HD13	16:Q:210:ARG:NE	0.80	1.11
3:C:40:TYR:HB3	16:Q:214:LEU:HD21	1.33	1.11
16:Q:91:LEU:CD2	17:O:13:CYS:SG	2.37	1.11
16:Q:464:ILE:HD11	17:O:46:ILE:HD13	1.28	1.11
16:Q:474:PHE:CD2	17:O:47:SER:CB	2.33	1.11
17:O:11:TRP:CE2	18:P:86:ILE:CD1	2.32	1.11
3:C:39:ARG:NH1	16:Q:147:PHE:C	2.03	1.11
5:D:212:GLN:HE21	5:D:212:GLN:HA	1.12	1.11
16:Q:93:CYS:SG	17:O:20:ARG:HB2	1.89	1.11
16:Q:139:TYR:CE1	17:O:24:ILE:CG1	2.34	1.11
16:Q:464:ILE:HD11	17:O:46:ILE:HG21	1.18	1.10
3:C:49:PRO:C	16:Q:214:LEU:CD1	2.19	1.10
14:N:501:UNK:HA	14:N:505:UNK:HA	1.30	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:191:PRO:HA	5:D:211:ARG:HD2	1.25	1.09
16:Q:416:PHE:HE1	18:P:35:TYR:CD2	1.68	1.09
8:K:466:PRO:HA	12:L:2791:PRO:HG2	1.33	1.08
16:Q:130:TYR:CG	17:O:28:LEU:CD1	2.36	1.08
17:O:55:ARG:O	18:P:52:THR:CG2	1.95	1.08
17:O:27:ILE:CG2	18:P:57:PRO:O	2.00	1.08
3:C:39:ARG:NH1	16:Q:148:ILE:CG2	2.09	1.07
8:K:469:LEU:CD1	12:L:2788:ILE:CG2	2.22	1.07
8:K:468:LEU:HB3	12:L:2829:LYS:HZ1	1.05	1.07
8:K:469:LEU:HD13	12:L:2788:ILE:HG22	1.30	1.07
16:Q:482:VAL:CG2	17:O:49:LYS:HD2	1.61	1.07
3:C:34:LEU:CD2	16:Q:446:PHE:CD1	2.38	1.07
3:C:50:ILE:N	16:Q:214:LEU:CD1	2.17	1.07
17:O:11:TRP:CD2	18:P:86:ILE:CD1	2.38	1.06
16:Q:479:ILE:HG22	17:O:47:SER:HA	1.09	1.06
3:C:47:ASP:HB3	16:Q:243:THR:O	1.53	1.05
16:Q:182:THR:CA	17:O:44:ASP:CB	2.30	1.05
16:Q:464:ILE:HD11	17:O:46:ILE:CG2	1.86	1.05
16:Q:501:GLN:HB2	18:P:31:ARG:HH22	1.17	1.05
3:C:54:CYS:SG	16:Q:215:SER:O	2.13	1.05
5:D:78:LYS:HE3	5:D:78:LYS:HA	1.38	1.05
16:Q:482:VAL:HG23	17:O:49:LYS:HD2	1.29	1.05
17:O:11:TRP:NE1	18:P:83:LEU:HD23	1.71	1.05
8:K:468:LEU:HB3	12:L:2829:LYS:NZ	1.70	1.04
15:R:4:PHE:CE1	16:Q:377:ARG:NH1	2.25	1.04
16:Q:472:PHE:CG	17:O:46:ILE:HG13	1.90	1.04
16:Q:182:THR:HG23	17:O:44:ASP:CB	1.85	1.03
16:Q:472:PHE:CE2	17:O:50:GLU:HG2	1.93	1.03
16:Q:464:ILE:HG13	17:O:46:ILE:CD1	1.87	1.03
16:Q:472:PHE:HB3	17:O:47:SER:C	1.51	1.03
16:Q:482:VAL:CG1	17:O:49:LYS:H	1.70	1.03
3:C:34:LEU:CG	16:Q:446:PHE:HE1	1.70	1.03
17:O:34:ARG:HH12	18:P:57:PRO:HB3	1.23	1.02
16:Q:182:THR:CB	17:O:44:ASP:HB2	1.78	1.02
16:Q:472:PHE:HB2	17:O:46:ILE:CG1	1.88	1.02
3:C:39:ARG:HH11	16:Q:148:ILE:HG23	1.22	1.02
16:Q:472:PHE:CE1	17:O:45:GLN:HB3	1.94	1.02
16:Q:479:ILE:O	17:O:68:HIS:CE1	2.12	1.02
17:O:54:GLN:NE2	18:P:49:SER:N	2.07	1.01
3:C:38:LEU:CD2	16:Q:210:ARG:CD	2.18	1.01
3:C:52:GLN:HE21	16:Q:153:GLN:HG3	0.94	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:93:CYS:SG	17:O:20:ARG:CD	2.49	1.00
3:C:39:ARG:NH2	16:Q:147:PHE:O	1.94	1.00
16:Q:472:PHE:CE2	17:O:50:GLU:CG	2.44	1.00
16:Q:479:ILE:HB	17:O:68:HIS:HE1	0.83	1.00
16:Q:482:VAL:HG12	17:O:49:LYS:CA	1.73	1.00
16:Q:464:ILE:HD11	17:O:46:ILE:CD1	1.72	1.00
3:C:51:LEU:HG	16:Q:214:LEU:CB	1.92	1.00
3:C:34:LEU:CG	16:Q:446:PHE:CE1	2.42	0.99
16:Q:473:LYS:HA	17:O:48:LEU:HD23	1.40	0.99
3:C:51:LEU:HG	16:Q:214:LEU:HB3	1.43	0.99
3:C:51:LEU:CD1	16:Q:211:ASP:O	2.09	0.99
5:D:66:VAL:HG12	5:D:67:PRO:HD2	1.44	0.99
17:O:51:ILE:HG21	18:P:45:ARG:HG3	1.43	0.99
16:Q:472:PHE:HZ	17:O:45:GLN:HB3	1.21	0.98
17:O:9:THR:HG21	18:P:10:LYS:HE3	1.44	0.98
16:Q:259:TRP:HD1	17:O:114:ASP:OD1	1.39	0.98
17:O:55:ARG:HD2	18:P:53:ASN:OD1	1.63	0.98
16:Q:178:LEU:HD13	17:O:37:ILE:HD12	1.43	0.97
15:R:46:ALA:HA	16:Q:331:PRO:O	1.64	0.97
1:M:173:GLU:HG2	5:D:197:LYS:HA	1.44	0.97
16:Q:472:PHE:HB2	17:O:46:ILE:HG13	0.99	0.97
16:Q:474:PHE:CD1	17:O:47:SER:HB3	1.99	0.97
17:O:22:ILE:CD1	18:P:43:ILE:HD12	1.92	0.97
17:O:11:TRP:HD1	18:P:83:LEU:HD21	1.28	0.97
16:Q:479:ILE:HD12	17:O:47:SER:CB	1.94	0.96
3:C:50:ILE:CA	16:Q:214:LEU:HD11	1.95	0.96
3:C:34:LEU:HD22	16:Q:446:PHE:CD1	1.97	0.96
14:N:467:UNK:O	14:N:470:UNK:CB	2.14	0.96
3:C:39:ARG:HH11	16:Q:148:ILE:HG22	1.27	0.96
14:N:451:UNK:C	14:N:452:UNK:CA	2.43	0.96
8:K:465:ARG:HH21	12:L:2843:GLY:H	1.10	0.96
16:Q:93:CYS:SG	17:O:17:ASN:HA	2.06	0.96
16:Q:178:LEU:CD1	17:O:37:ILE:HD12	1.94	0.95
19:R:165:HOH:O	16:Q:355:LEU:HD11	1.63	0.95
16:Q:182:THR:CB	17:O:44:ASP:HB3	1.77	0.95
17:O:34:ARG:HH11	18:P:57:PRO:CG	1.78	0.95
16:Q:474:PHE:CE2	17:O:47:SER:CB	2.50	0.95
12:L:849:LEU:HD12	12:L:849:LEU:H	1.31	0.95
16:Q:479:ILE:CB	17:O:68:HIS:HE1	1.70	0.95
16:Q:481:LEU:HD12	17:O:50:GLU:H	1.28	0.95
16:Q:482:VAL:CG1	17:O:49:LYS:N	2.26	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:88:HIS:C	14:N:515:UNK:C	2.35	0.94
16:Q:444:GLN:NE2	18:P:35:TYR:HE2	1.65	0.94
3:C:51:LEU:N	16:Q:214:LEU:CG	2.31	0.94
16:Q:464:ILE:CD1	17:O:46:ILE:HD12	1.59	0.94
17:O:54:GLN:NE2	18:P:49:SER:HA	1.83	0.94
3:C:39:ARG:NH1	16:Q:148:ILE:CB	2.31	0.93
17:O:56:LEU:CD1	18:P:52:THR:N	1.91	0.93
16:Q:473:LYS:N	17:O:47:SER:O	2.00	0.93
16:Q:130:TYR:CD2	17:O:28:LEU:HD12	2.04	0.93
3:C:54:CYS:SG	16:Q:215:SER:C	2.47	0.93
5:D:66:VAL:CG1	5:D:67:PRO:HD2	1.99	0.93
14:N:182:UNK:HA	14:N:198:UNK:CB	1.97	0.93
17:O:54:GLN:NE2	18:P:49:SER:CA	2.31	0.93
3:C:34:LEU:CD1	16:Q:446:PHE:CE1	2.51	0.93
3:C:50:ILE:CA	16:Q:214:LEU:CD1	2.45	0.93
5:D:212:GLN:HA	5:D:212:GLN:NE2	1.81	0.93
16:Q:139:TYR:HE1	17:O:24:ILE:HG12	1.19	0.93
16:Q:474:PHE:CE2	17:O:47:SER:HB3	2.04	0.93
16:Q:88:LEU:CB	18:P:11:GLN:HG2	1.98	0.93
16:Q:106:TRP:HD1	17:O:20:ARG:NH2	1.66	0.93
16:Q:474:PHE:HA	17:O:47:SER:OG	1.69	0.93
3:C:51:LEU:HD12	16:Q:215:SER:OG	1.66	0.92
12:L:828:ARG:H	12:L:829:PRO:CD	1.82	0.92
8:K:441:PRO:HA	12:L:912:LEU:HD21	1.51	0.92
17:O:19:LEU:HD21	18:P:67:GLU:HA	0.93	0.92
16:Q:182:THR:CG2	17:O:44:ASP:CB	2.35	0.92
16:Q:472:PHE:HD2	17:O:46:ILE:HG12	0.79	0.92
3:C:34:LEU:HD21	16:Q:446:PHE:CD1	2.03	0.92
3:C:52:GLN:HE21	16:Q:153:GLN:CG	1.82	0.92
16:Q:78:ARG:CZ	18:P:23:TYR:CD2	2.53	0.92
1:M:99:PHE:CE2	1:M:101:ALA:HB3	2.05	0.91
1:M:172:LEU:HB3	1:M:193:LEU:HD13	1.50	0.91
12:L:828:ARG:N	12:L:829:PRO:HD3	1.83	0.91
16:Q:464:ILE:HG13	17:O:46:ILE:HD12	0.92	0.91
3:C:39:ARG:CD	16:Q:147:PHE:CE1	2.52	0.91
12:L:2916:ARG:NH2	12:L:2916:ARG:HB2	1.84	0.91
17:O:9:THR:HG23	18:P:10:LYS:HZ2	1.34	0.91
1:M:87:LEU:HD13	14:N:490:UNK:HA	1.52	0.91
16:Q:480:THR:O	17:O:47:SER:O	1.88	0.90
3:C:49:PRO:O	16:Q:214:LEU:HD12	1.71	0.90
9:G:546:HIS:CD2	9:G:547:PRO:HD2	2.06	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:38:LEU:CD1	16:Q:210:ARG:NH1	2.34	0.90
3:C:40:TYR:HB3	16:Q:214:LEU:CD2	2.01	0.90
16:Q:464:ILE:CG1	17:O:46:ILE:CD1	2.20	0.89
3:C:34:LEU:HD21	16:Q:446:PHE:CE1	2.03	0.89
16:Q:182:THR:HG23	17:O:44:ASP:HB2	0.91	0.89
3:C:51:LEU:H	16:Q:214:LEU:HG	1.26	0.89
3:C:39:ARG:NH1	16:Q:148:ILE:HG22	1.81	0.89
16:Q:181:SER:N	17:O:44:ASP:OD1	1.92	0.89
3:C:34:LEU:HD13	16:Q:446:PHE:CE1	2.08	0.89
3:C:40:TYR:HB2	16:Q:214:LEU:HD21	1.54	0.89
19:R:153:HOH:O	16:Q:326:LYS:CG	2.21	0.88
8:K:468:LEU:CB	12:L:2829:LYS:HZ1	1.87	0.88
9:G:543:VAL:HG22	9:G:552:LEU:HD11	1.55	0.88
3:C:39:ARG:HD2	16:Q:147:PHE:HE1	1.36	0.88
1:M:88:HIS:HB3	14:N:515:UNK:O	1.74	0.88
17:O:54:GLN:HE22	18:P:48:GLN:C	1.76	0.88
1:M:194:ILE:CG2	1:M:195:TYR:N	2.36	0.88
16:Q:93:CYS:SG	17:O:20:ARG:CB	2.62	0.88
16:Q:93:CYS:HG	17:O:20:ARG:HD2	1.37	0.88
17:O:27:ILE:HD11	18:P:62:VAL:HB	1.54	0.88
16:Q:444:GLN:NE2	18:P:35:TYR:CE2	2.38	0.88
16:Q:464:ILE:CD1	17:O:46:ILE:HG21	2.01	0.88
1:M:188:GLU:OE1	5:D:85:ARG:NH2	2.07	0.87
3:C:38:LEU:HD13	16:Q:210:ARG:NH1	1.88	0.87
6:E:938:ILE:HD12	6:E:938:ILE:H	1.38	0.87
16:Q:472:PHE:CG	17:O:46:ILE:CG1	2.54	0.87
17:O:9:THR:CG2	18:P:10:LYS:NZ	2.38	0.87
17:O:11:TRP:NE1	18:P:86:ILE:HD12	1.90	0.87
16:Q:178:LEU:CG	17:O:37:ILE:HD13	2.04	0.86
3:C:50:ILE:C	16:Q:214:LEU:HD11	1.95	0.86
16:Q:501:GLN:HB2	18:P:31:ARG:NH2	1.90	0.86
17:O:19:LEU:CD2	18:P:67:GLU:CB	2.53	0.86
5:D:216:THR:CG2	5:D:246:GLY:HA3	2.06	0.86
8:K:462:ILE:HB	12:L:2737:TYR:HE1	1.38	0.86
16:Q:178:LEU:HD12	17:O:37:ILE:CD1	2.04	0.86
17:O:30:GLU:OE1	18:P:51:VAL:CG1	2.20	0.86
16:Q:78:ARG:HH21	18:P:23:TYR:HE2	0.86	0.86
5:D:78:LYS:HE3	5:D:78:LYS:CA	2.06	0.86
17:O:56:LEU:N	18:P:52:THR:CG2	2.33	0.86
12:L:2854:LEU:HD13	12:L:2906:TRP:CH2	2.11	0.85
16:Q:78:ARG:NH2	18:P:23:TYR:CD2	2.42	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:125:ASP:OD1	17:O:24:ILE:HD13	1.75	0.85
16:Q:472:PHE:CB	17:O:46:ILE:C	2.43	0.85
16:Q:474:PHE:CD2	17:O:47:SER:HB2	2.11	0.85
16:Q:466:ASN:ND2	17:O:46:ILE:HG23	1.90	0.85
3:C:39:ARG:HH11	16:Q:148:ILE:CB	1.89	0.85
8:K:474:ILE:HD13	12:L:2592:ASP:HB3	1.59	0.85
8:K:469:LEU:HD13	12:L:2788:ILE:HG21	0.88	0.85
15:R:4:PHE:CZ	16:Q:377:ARG:CZ	2.44	0.85
16:Q:474:PHE:CE1	17:O:48:LEU:HG	2.11	0.85
17:O:19:LEU:CD2	18:P:67:GLU:CA	2.45	0.85
17:O:19:LEU:CD2	18:P:67:GLU:CG	2.31	0.85
8:K:442:PRO:HD2	12:L:912:LEU:HD22	1.58	0.85
16:Q:130:TYR:CD1	17:O:28:LEU:HD13	2.11	0.85
16:Q:139:TYR:CB	17:O:28:LEU:CD2	2.42	0.85
14:N:353:UNK:O	14:N:357:UNK:HA	1.76	0.85
17:O:19:LEU:HD21	18:P:67:GLU:CB	2.07	0.84
17:O:22:ILE:CD1	18:P:43:ILE:HD13	2.08	0.84
14:N:480:UNK:N	14:N:496:UNK:HA	1.93	0.84
16:Q:479:ILE:O	17:O:68:HIS:CD2	2.30	0.84
16:Q:78:ARG:CZ	18:P:23:TYR:HD2	1.91	0.83
3:C:38:LEU:CD1	16:Q:210:ARG:HE	1.52	0.83
16:Q:464:ILE:HD12	17:O:46:ILE:HD13	0.84	0.83
16:Q:472:PHE:CD2	17:O:46:ILE:HG13	1.92	0.83
3:C:38:LEU:HD22	16:Q:210:ARG:CG	2.08	0.83
12:L:1425:PHE:O	12:L:1428:LEU:N	2.10	0.83
17:O:9:THR:HG21	18:P:10:LYS:CE	1.97	0.83
16:Q:106:TRP:CD1	17:O:20:ARG:NH2	2.43	0.83
16:Q:464:ILE:O	17:O:46:ILE:HD11	1.77	0.83
16:Q:472:PHE:HB3	17:O:47:SER:CA	2.07	0.83
16:Q:481:LEU:HA	17:O:49:LYS:HA	1.58	0.83
3:C:38:LEU:HD11	16:Q:211:ASP:OD1	1.78	0.83
16:Q:479:ILE:HA	17:O:47:SER:OG	1.79	0.83
9:G:546:HIS:CD2	9:G:547:PRO:CD	2.62	0.82
16:Q:474:PHE:CG	17:O:47:SER:CB	2.56	0.82
10:H:27:ALA:HB1	10:H:32:ILE:HD11	1.62	0.82
3:C:49:PRO:O	16:Q:214:LEU:CD1	2.27	0.82
14:N:84:UNK:HA	14:N:506:UNK:O	1.80	0.82
16:Q:481:LEU:O	17:O:49:LYS:CE	2.23	0.82
16:Q:481:LEU:O	17:O:49:LYS:HE2	1.80	0.82
1:M:189:LEU:HA	5:D:85:ARG:HG2	1.61	0.81
14:N:353:UNK:HA	14:N:356:UNK:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:252:THR:HG23	17:O:109:PHE:CE1	2.15	0.81
8:K:454:PRO:N	8:K:455:PRO:HD2	1.95	0.81
1:M:82:LEU:HD13	1:M:101:ALA:HA	1.61	0.81
9:G:537:LEU:HD12	9:G:537:LEU:H	1.46	0.81
15:R:4:PHE:HZ	16:Q:377:ARG:NH1	1.47	0.81
2:A:246:LEU:HD11	8:K:537:VAL:HG21	1.62	0.81
3:C:51:LEU:CD2	16:Q:214:LEU:HD23	2.10	0.81
16:Q:474:PHE:CE1	17:O:47:SER:HB3	2.16	0.81
12:L:1203:LEU:O	12:L:1203:LEU:HD23	1.81	0.80
16:Q:178:LEU:HD13	17:O:37:ILE:HD13	0.82	0.80
16:Q:479:ILE:O	17:O:68:HIS:CG	2.34	0.80
3:C:45:ASN:HD21	16:Q:171:ASP:HA	1.44	0.80
16:Q:472:PHE:CD2	17:O:46:ILE:N	2.49	0.80
16:Q:479:ILE:HG23	17:O:47:SER:HB2	1.62	0.80
3:C:45:ASN:HD21	16:Q:171:ASP:CA	1.91	0.80
14:N:221:UNK:CA	14:N:230:UNK:HA	2.11	0.80
1:M:81:ASP:HB2	14:N:433:UNK:O	1.80	0.80
17:O:55:ARG:CA	18:P:52:THR:HG21	2.12	0.80
17:O:24:ILE:HG13	18:P:59:PHE:CE1	2.17	0.80
3:C:55:LEU:HD23	16:Q:160:ILE:HG12	1.63	0.80
9:G:478:ARG:NH1	9:G:487:CYS:SG	2.55	0.80
3:C:38:LEU:HD13	16:Q:210:ARG:HE	0.98	0.80
16:Q:91:LEU:HD23	17:O:13:CYS:HB3	1.62	0.80
16:Q:282:ASP:CG	19:Q:603:HOH:O	2.19	0.79
16:Q:470:ASN:HA	17:O:51:ILE:N	1.97	0.79
3:C:51:LEU:CD1	16:Q:215:SER:OG	2.31	0.79
16:Q:130:TYR:HB3	17:O:28:LEU:HD11	1.64	0.79
1:M:173:GLU:CG	5:D:197:LYS:HA	2.13	0.79
14:N:221:UNK:HA	14:N:230:UNK:HA	1.63	0.79
17:O:9:THR:HG23	18:P:10:LYS:NZ	1.97	0.79
16:Q:474:PHE:CZ	17:O:47:SER:N	2.49	0.79
17:O:51:ILE:CG2	18:P:45:ARG:HG3	2.12	0.79
3:C:51:LEU:CG	16:Q:214:LEU:HB3	2.13	0.79
16:Q:182:THR:HG21	17:O:45:GLN:H	1.47	0.79
16:Q:315:SER:CB	19:Q:605:HOH:O	2.31	0.79
16:Q:464:ILE:HD11	17:O:46:ILE:CB	2.13	0.79
17:O:9:THR:HG21	18:P:10:LYS:CD	2.13	0.79
16:Q:88:LEU:HB3	18:P:11:GLN:HG2	1.65	0.79
3:C:51:LEU:HD12	16:Q:215:SER:N	1.97	0.78
3:C:39:ARG:CZ	16:Q:148:ILE:HA	2.12	0.78
5:D:303:PRO:HB2	5:D:304:ILE:HG12	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:176:ALA:HB2	1:M:193:LEU:HD11	1.65	0.78
1:M:191:PRO:CA	5:D:211:ARG:HD2	2.09	0.78
8:K:465:ARG:HH21	12:L:2843:GLY:N	1.82	0.78
1:M:191:PRO:HA	5:D:211:ARG:CD	2.12	0.78
16:Q:472:PHE:CE2	17:O:46:ILE:N	2.51	0.78
6:E:938:ILE:HD12	6:E:938:ILE:N	1.99	0.78
16:Q:474:PHE:CD1	17:O:48:LEU:HG	2.18	0.78
3:C:39:ARG:CZ	16:Q:147:PHE:O	2.30	0.78
10:H:127:LEU:O	10:H:127:LEU:HD12	1.84	0.77
17:O:9:THR:HG23	18:P:10:LYS:CE	2.13	0.77
1:M:108:GLU:HA	1:M:110:LYS:N	1.99	0.77
17:O:27:ILE:HD12	18:P:59:PHE:CD1	2.18	0.77
16:Q:470:ASN:HA	17:O:51:ILE:H	1.50	0.77
16:Q:482:VAL:CG1	17:O:49:LYS:CA	2.48	0.77
3:C:38:LEU:CG	16:Q:210:ARG:NE	2.47	0.77
16:Q:107:LYS:CG	17:O:20:ARG:NH2	2.47	0.77
16:Q:178:LEU:HD22	17:O:37:ILE:HG21	1.64	0.77
16:Q:139:TYR:HB3	17:O:28:LEU:HD21	0.84	0.77
16:Q:474:PHE:CE1	17:O:48:LEU:N	2.52	0.77
17:O:27:ILE:HD13	18:P:59:PHE:HA	0.79	0.77
3:C:39:ARG:NH1	16:Q:147:PHE:O	2.16	0.77
3:C:45:ASN:ND2	16:Q:171:ASP:CA	2.48	0.77
12:L:2593:TYR:H	12:L:2596:ARG:HG2	1.48	0.77
16:Q:479:ILE:O	17:O:68:HIS:NE2	2.16	0.77
3:C:44:ASN:OD1	16:Q:174:ARG:HG3	1.85	0.76
12:L:1122:ASN:HD22	12:L:1122:ASN:N	1.82	0.76
16:Q:130:TYR:CG	17:O:28:LEU:HD13	2.20	0.76
16:Q:474:PHE:CE2	17:O:47:SER:HB2	2.18	0.76
17:O:11:TRP:CD1	18:P:83:LEU:CG	2.68	0.76
16:Q:479:ILE:CG2	17:O:47:SER:CB	2.49	0.76
12:L:1354:LEU:HA	12:L:1357:LEU:HD22	1.68	0.76
17:O:11:TRP:CZ2	18:P:86:ILE:HG13	2.20	0.76
16:Q:282:ASP:OD1	19:Q:603:HOH:O	2.02	0.76
1:M:101:ALA:HB1	1:M:115:ILE:O	1.85	0.76
12:L:2854:LEU:HD13	12:L:2906:TRP:HH2	1.49	0.76
2:A:239:GLU:N	2:A:239:GLU:OE1	2.18	0.76
3:C:37:PRO:O	16:Q:467:ARG:NH2	2.18	0.76
3:C:50:ILE:C	16:Q:214:LEU:CD1	2.54	0.76
5:D:323:LYS:HE2	7:J:107:PHE:HD1	1.51	0.76
12:L:2916:ARG:HB2	12:L:2916:ARG:CZ	2.16	0.76
16:Q:130:TYR:CB	17:O:28:LEU:HD11	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:44:ASN:HD21	16:Q:174:ARG:HG3	1.51	0.76
12:L:2907:ARG:HH11	12:L:2907:ARG:HG2	1.51	0.76
16:Q:130:TYR:CD2	17:O:28:LEU:CD1	2.67	0.76
12:L:2884:GLN:HA	12:L:2884:GLN:NE2	2.00	0.75
16:Q:107:LYS:NZ	17:O:13:CYS:HA	2.00	0.75
17:O:11:TRP:CD2	18:P:86:ILE:HD11	2.20	0.75
3:C:52:GLN:NE2	16:Q:153:GLN:CG	2.40	0.75
12:L:844:VAL:HB	12:L:849:LEU:HD22	1.68	0.75
3:C:45:ASN:ND2	16:Q:171:ASP:HA	2.01	0.75
3:C:49:PRO:C	16:Q:214:LEU:HD12	2.07	0.75
3:C:51:LEU:CA	16:Q:214:LEU:HG	2.16	0.75
12:L:2601:ARG:HB3	12:L:2602:PRO:HD2	1.68	0.75
16:Q:466:ASN:HD22	17:O:46:ILE:HG23	1.50	0.75
16:Q:478:ARG:HG3	17:O:68:HIS:HD2	1.51	0.75
17:O:34:ARG:HH22	18:P:51:VAL:HG11	1.52	0.75
16:Q:474:PHE:CZ	17:O:47:SER:HB3	2.20	0.75
8:K:462:ILE:HB	12:L:2737:TYR:CE1	2.20	0.75
16:Q:107:LYS:HZ3	17:O:13:CYS:HA	1.50	0.74
2:A:327:ARG:NH1	2:A:328:HIS:O	2.20	0.74
10:H:129:LYS:HZ2	10:H:129:LYS:HA	1.52	0.74
17:O:9:THR:HG21	18:P:10:LYS:HD2	1.69	0.74
5:D:322:GLU:OE2	5:D:322:GLU:HA	1.87	0.74
14:N:223:UNK:H	14:N:230:UNK:CB	2.00	0.74
16:Q:78:ARG:HH12	18:P:27:SER:CB	1.99	0.74
16:Q:474:PHE:HZ	17:O:46:ILE:HB	1.50	0.74
17:O:55:ARG:O	18:P:52:THR:HG23	1.84	0.74
12:L:428:LYS:HE2	12:L:430:GLU:HG3	1.68	0.74
16:Q:259:TRP:NE1	17:O:114:ASP:HA	2.02	0.74
3:C:38:LEU:CD1	16:Q:211:ASP:OD1	2.36	0.74
5:D:72:PHE:O	5:D:75:ARG:HB2	1.87	0.74
17:O:11:TRP:CE2	18:P:83:LEU:HA	2.20	0.74
3:C:55:LEU:HD11	16:Q:173:SER:OG	1.88	0.74
16:Q:478:ARG:HA	17:O:68:HIS:CD2	2.22	0.74
3:C:51:LEU:HD23	16:Q:214:LEU:CD2	2.15	0.74
8:K:441:PRO:HA	12:L:912:LEU:CD2	2.17	0.74
17:O:56:LEU:HD11	18:P:51:VAL:C	2.07	0.74
16:Q:130:TYR:HE2	17:O:25:ASN:OD1	1.70	0.73
3:C:49:PRO:CG	16:Q:237:PHE:HE1	1.85	0.73
9:G:414:ILE:HB	9:G:449:LEU:HB2	1.68	0.73
16:Q:78:ARG:NE	18:P:23:TYR:HD2	1.86	0.73
17:O:11:TRP:CG	18:P:86:ILE:HD12	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:19:LEU:HD23	18:P:67:GLU:HG3	0.78	0.73
16:Q:501:GLN:CB	18:P:31:ARG:HH22	2.00	0.73
16:Q:107:LYS:HG3	17:O:20:ARG:NH2	2.03	0.73
3:C:49:PRO:HG2	16:Q:237:PHE:HE1	0.98	0.73
12:L:1417:ARG:HA	12:L:1420:ILE:HD12	1.70	0.73
3:C:38:LEU:HB2	16:Q:210:ARG:NH2	2.03	0.73
8:K:453:LYS:C	8:K:455:PRO:HD2	2.08	0.73
14:N:207:UNK:C	14:N:208:UNK:CB	2.67	0.73
14:N:451:UNK:C	14:N:452:UNK:HA	2.19	0.73
9:G:537:LEU:HD12	9:G:537:LEU:N	2.04	0.73
9:G:568:ARG:HG2	9:G:570:GLU:HG2	1.69	0.73
9:G:546:HIS:HB2	9:G:553:PHE:HE1	1.54	0.72
14:N:221:UNK:C	14:N:230:UNK:HA	2.19	0.72
5:D:78:LYS:HA	5:D:78:LYS:CE	2.17	0.72
9:G:67:ARG:O	9:G:70:SER:OG	2.07	0.72
3:C:44:ASN:ND2	16:Q:174:ARG:HG3	2.05	0.72
3:C:54:CYS:SG	16:Q:215:SER:CB	2.77	0.72
4:F:115:VAL:HG22	4:F:190:LEU:HD21	1.71	0.72
12:L:849:LEU:HD12	12:L:849:LEU:N	2.03	0.72
17:O:54:GLN:NE2	18:P:48:GLN:C	2.40	0.72
17:O:54:GLN:HE21	18:P:49:SER:HA	1.53	0.72
16:Q:481:LEU:CD1	17:O:50:GLU:H	2.01	0.72
3:C:50:ILE:CA	16:Q:214:LEU:HD12	2.18	0.72
3:C:51:LEU:HD11	16:Q:211:ASP:C	2.09	0.72
8:K:453:LYS:HG2	8:K:455:PRO:HD2	1.71	0.72
17:O:19:LEU:HD13	18:P:70:ALA:CB	2.20	0.72
3:C:38:LEU:HD12	16:Q:210:ARG:NH1	2.03	0.72
5:D:73:LEU:HD23	5:D:73:LEU:O	1.89	0.72
5:D:317:GLN:C	5:D:319:ARG:H	1.93	0.72
15:R:12:THR:N	16:Q:360:GLU:OE1	2.22	0.72
1:M:188:GLU:CG	5:D:247:PHE:HA	2.20	0.72
16:Q:472:PHE:HB3	17:O:47:SER:N	2.05	0.72
5:D:216:THR:HB	5:D:243:ASP:HA	1.70	0.71
7:J:66:MET:O	7:J:98:ARG:NH1	2.24	0.71
16:Q:107:LYS:CG	17:O:20:ARG:HH22	2.03	0.71
17:O:7:GLN:HG3	18:P:86:ILE:HB	1.72	0.71
16:Q:91:LEU:HD21	17:O:13:CYS:HG	1.50	0.71
16:Q:130:TYR:CG	17:O:28:LEU:HD11	2.24	0.71
16:Q:482:VAL:O	17:O:50:GLU:O	2.09	0.71
14:N:451:UNK:O	14:N:452:UNK:N	2.21	0.71
1:M:87:LEU:CD1	14:N:490:UNK:CA	2.66	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:90:ARG:HH11	14:N:513:UNK:CB	2.04	0.70
3:C:49:PRO:C	16:Q:214:LEU:HD13	2.11	0.70
8:K:468:LEU:O	12:L:2829:LYS:NZ	2.18	0.70
9:G:457:TYR:HE2	9:G:473:GLU:HB3	1.57	0.70
17:O:7:GLN:HG2	18:P:83:LEU:CD2	2.21	0.70
3:C:39:ARG:CD	16:Q:147:PHE:HE1	1.96	0.70
16:Q:472:PHE:HE2	17:O:50:GLU:OE2	1.74	0.70
16:Q:76:ARG:HH22	18:P:19:GLU:N	1.89	0.70
1:M:188:GLU:HG2	5:D:247:PHE:HA	1.72	0.70
8:K:474:ILE:CD1	12:L:2592:ASP:HB3	2.21	0.70
14:N:207:UNK:C	14:N:208:UNK:CA	2.68	0.70
16:Q:482:VAL:HG12	17:O:49:LYS:H	0.87	0.70
3:C:55:LEU:CD2	16:Q:160:ILE:HG23	2.22	0.70
16:Q:464:ILE:HD11	17:O:46:ILE:CG1	2.20	0.70
12:L:846:LEU:HG	12:L:850:VAL:HG11	1.74	0.70
5:D:21:MET:CE	5:D:250:PHE:HA	2.21	0.70
16:Q:88:LEU:HB2	18:P:11:GLN:HG2	1.73	0.70
17:O:19:LEU:HD23	18:P:67:GLU:CB	2.19	0.70
16:Q:479:ILE:C	17:O:68:HIS:CE1	2.52	0.69
16:Q:125:ASP:OD1	17:O:24:ILE:CD1	2.40	0.69
16:Q:326:LYS:O	19:Q:604:HOH:O	2.08	0.69
3:C:39:ARG:HH22	16:Q:150:GLN:HE21	1.40	0.69
3:C:49:PRO:HG2	16:Q:237:PHE:CD1	2.21	0.69
8:K:466:PRO:CA	12:L:2791:PRO:HG2	2.19	0.69
8:K:550:HIS:NE2	11:I:80:ASP:OD1	2.25	0.69
16:Q:178:LEU:CB	17:O:37:ILE:HD13	2.22	0.69
8:K:580:GLU:O	11:I:65:SER:N	2.25	0.69
16:Q:472:PHE:HB3	17:O:46:ILE:C	2.10	0.69
3:C:47:ASP:HB3	16:Q:243:THR:HB	1.73	0.69
6:E:948:GLN:HA	6:E:948:GLN:OE1	1.93	0.69
16:Q:472:PHE:CE2	17:O:50:GLU:OE2	2.45	0.69
4:F:202:LEU:O	4:F:205:THR:OG1	2.08	0.69
17:O:11:TRP:CD2	18:P:82:ILE:HG23	2.28	0.69
17:O:11:TRP:CE3	18:P:86:ILE:HD11	2.27	0.69
17:O:11:TRP:CD1	18:P:86:ILE:HD12	2.27	0.69
3:C:39:ARG:CZ	16:Q:148:ILE:HG22	2.23	0.68
16:Q:473:LYS:O	17:O:47:SER:OG	2.11	0.68
5:D:20:MET:SD	5:D:213:ALA:HB3	2.34	0.68
3:C:39:ARG:NE	16:Q:147:PHE:CD1	2.62	0.68
8:K:456:GLN:HA	12:L:2669:MET:HG3	1.74	0.68
9:G:581:ALA:HB3	9:G:599:GLU:HG2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:20:MET:SD	5:D:210:CYS:HA	2.34	0.68
9:G:118:CYS:SG	9:G:119:GLU:N	2.67	0.68
16:Q:78:ARG:CZ	18:P:23:TYR:CE2	2.71	0.68
17:O:55:ARG:HB3	18:P:52:THR:HG22	1.74	0.68
16:Q:188:ILE:HD13	17:O:93:GLU:OE1	1.93	0.68
3:C:38:LEU:HD11	16:Q:210:ARG:HE	1.51	0.68
9:G:620:HIS:CE1	9:G:641:GLY:HA3	2.29	0.68
17:O:19:LEU:HD11	18:P:66:ILE:HG22	1.76	0.68
16:Q:464:ILE:O	17:O:48:LEU:HB2	1.93	0.67
16:Q:479:ILE:O	17:O:68:HIS:ND1	2.27	0.67
3:C:38:LEU:CD2	16:Q:210:ARG:CG	2.71	0.67
5:D:320:ASN:C	5:D:322:GLU:H	1.95	0.67
12:L:846:LEU:HA	12:L:850:VAL:HB	1.77	0.67
3:C:51:LEU:HG	16:Q:214:LEU:CG	2.24	0.67
6:E:817:GLY:N	7:J:69:GLU:OE2	2.26	0.67
12:L:849:LEU:H	12:L:849:LEU:CD1	2.06	0.67
14:N:175:UNK:HA	14:N:213:UNK:C	2.24	0.67
16:Q:416:PHE:CE1	18:P:35:TYR:CG	2.67	0.67
16:Q:479:ILE:CG2	17:O:47:SER:N	2.57	0.67
3:C:51:LEU:HD12	16:Q:215:SER:CB	2.25	0.67
9:G:594:LEU:HG	9:G:606:TRP:HB2	1.75	0.67
5:D:21:MET:HE2	5:D:253:VAL:HG21	1.77	0.67
5:D:66:VAL:HG12	5:D:67:PRO:CD	2.22	0.67
8:K:447:PRO:HG3	12:L:2788:ILE:HG23	1.77	0.67
11:I:48:GLN:O	11:I:51:THR:OG1	2.11	0.67
16:Q:91:LEU:HD23	17:O:13:CYS:CB	2.25	0.66
16:Q:338:GLU:OE2	19:Q:601:HOH:O	0.66	0.66
3:C:34:LEU:HD21	16:Q:446:PHE:HD1	1.60	0.66
8:K:453:LYS:HG2	8:K:455:PRO:CD	2.26	0.66
9:G:157:TYR:O	9:G:161:SER:N	2.28	0.66
5:D:241:VAL:HA	5:D:244:ILE:HD12	1.78	0.66
17:O:11:TRP:CE2	18:P:82:ILE:HG23	2.31	0.66
3:C:50:ILE:HA	16:Q:214:LEU:HD12	1.77	0.66
6:E:938:ILE:H	6:E:938:ILE:CD1	2.08	0.66
9:G:520:ARG:HG3	9:G:532:ILE:HG12	1.78	0.66
14:N:426:UNK:CB	14:N:481:UNK:HA	2.26	0.66
10:H:129:LYS:HA	10:H:129:LYS:NZ	2.11	0.66
10:H:404:VAL:HG12	10:H:407:TRP:CZ2	2.31	0.66
6:E:946:LYS:HE2	6:E:946:LYS:HA	1.78	0.66
14:N:83:UNK:N	14:N:506:UNK:HA	2.10	0.66
9:G:43:ALA:N	9:G:45:ASP:OD1	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:479:ILE:CD1	17:O:47:SER:HB2	2.16	0.65
12:L:2802:LEU:HD12	12:L:2815:VAL:HG11	1.77	0.65
12:L:2849:GLN:NE2	12:L:2889:ARG:O	2.29	0.65
16:Q:78:ARG:HD3	18:P:23:TYR:CD2	2.32	0.65
16:Q:182:THR:HG21	17:O:45:GLN:N	2.12	0.65
17:O:51:ILE:HD12	18:P:48:GLN:OE1	1.96	0.65
16:Q:107:LYS:HG2	17:O:20:ARG:NH2	2.11	0.65
14:N:84:UNK:HA	14:N:506:UNK:C	2.26	0.65
8:K:454:PRO:N	8:K:455:PRO:CD	2.59	0.65
16:Q:91:LEU:CD2	17:O:13:CYS:CB	2.75	0.65
4:F:278:ALA:HB3	8:K:521:ILE:HG12	1.79	0.65
16:Q:76:ARG:HH22	18:P:18:VAL:C	1.99	0.65
16:Q:472:PHE:CB	17:O:47:SER:C	2.36	0.65
11:I:128:GLU:N	11:I:128:GLU:OE1	2.28	0.64
16:Q:482:VAL:O	17:O:49:LYS:C	2.35	0.64
1:M:82:LEU:HB3	1:M:94:TYR:HE2	1.60	0.64
5:D:71:ILE:O	5:D:74:ILE:HG12	1.97	0.64
6:E:952:ASN:ND2	11:I:138:VAL:O	2.30	0.64
8:K:469:LEU:HD12	12:L:2788:ILE:HG21	1.72	0.64
16:Q:472:PHE:HZ	17:O:45:GLN:CB	1.89	0.64
17:O:34:ARG:HE	18:P:57:PRO:HG3	1.62	0.64
5:D:326:ILE:O	5:D:328:ASN:N	2.30	0.64
8:K:582:ARG:NH2	11:I:70:ALA:O	2.30	0.64
15:R:42:ARG:NH1	15:R:49:GLN:OE1	2.28	0.64
3:C:55:LEU:HD21	16:Q:160:ILE:HG23	1.80	0.64
9:G:154:ARG:NH2	9:G:179:SER:OG	2.31	0.64
12:L:1425:PHE:O	12:L:1427:SER:N	2.31	0.64
12:L:3303:SER:HB3	12:L:3427:PHE:HD2	1.61	0.64
3:C:34:LEU:HD13	16:Q:446:PHE:CZ	2.33	0.64
14:N:467:UNK:C	14:N:470:UNK:CB	2.76	0.64
16:Q:474:PHE:HE1	17:O:48:LEU:HG	1.61	0.64
16:Q:481:LEU:HD11	17:O:50:GLU:HB2	1.78	0.64
17:O:7:GLN:HG2	18:P:83:LEU:HD22	1.79	0.64
17:O:56:LEU:HD13	18:P:51:VAL:HB	1.80	0.64
3:C:51:LEU:HD12	16:Q:215:SER:CA	2.27	0.64
17:O:55:ARG:CB	18:P:52:THR:HG22	2.27	0.64
5:D:259:GLU:HG3	5:D:316:LEU:HD21	1.80	0.64
7:J:67:GLU:OE1	7:J:95:LYS:NZ	2.30	0.64
12:L:328:ARG:HD3	12:L:370:THR:HG22	1.79	0.64
1:M:169:PRO:HA	1:M:208:VAL:O	1.99	0.63
14:N:184:UNK:CB	14:N:237:UNK:HA	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:315:SER:HB2	19:Q:605:HOH:O	1.97	0.63
17:O:11:TRP:CZ2	18:P:86:ILE:CD1	2.81	0.63
5:D:248:LEU:O	5:D:251:GLU:HG2	1.98	0.63
9:G:494:HIS:NE2	9:G:520:ARG:HD3	2.14	0.63
10:H:375:ASN:ND2	10:H:377:THR:O	2.31	0.63
16:Q:478:ARG:CD	17:O:76:ASN:HD21	2.11	0.63
5:D:73:LEU:HD23	5:D:73:LEU:C	2.19	0.63
14:N:221:UNK:HA	14:N:229:UNK:O	1.97	0.63
17:O:55:ARG:CB	18:P:52:THR:CG2	2.77	0.63
8:K:468:LEU:C	12:L:2829:LYS:HZ3	2.01	0.63
12:L:2878:GLU:HA	12:L:2881:ARG:HD3	1.79	0.63
14:N:83:UNK:HA	14:N:505:UNK:O	1.99	0.63
16:Q:106:TRP:CD1	17:O:20:ARG:NE	2.67	0.63
3:C:38:LEU:CG	16:Q:210:ARG:CD	2.77	0.63
12:L:365:PRO:HB3	12:L:407:VAL:HG11	1.81	0.63
12:L:2854:LEU:HD13	12:L:2906:TRP:CZ2	2.33	0.62
17:O:15:MET:CE	18:P:74:VAL:HG21	2.28	0.62
9:G:647:ARG:NH2	10:H:167:ARG:O	2.32	0.62
1:M:177:PHE:HB2	5:D:194:GLU:HA	1.80	0.62
17:O:34:ARG:HH22	18:P:51:VAL:CG1	2.11	0.62
12:L:846:LEU:HA	12:L:850:VAL:CG2	2.29	0.62
16:Q:478:ARG:CA	17:O:68:HIS:CD2	2.81	0.62
16:Q:139:TYR:HB2	17:O:28:LEU:CD2	2.27	0.62
5:D:17:ILE:N	5:D:17:ILE:HD12	2.14	0.62
12:L:2880:LYS:H	12:L:2880:LYS:HD2	1.64	0.62
16:Q:464:ILE:O	17:O:46:ILE:CD1	2.46	0.62
9:G:462:SER:OG	9:G:464:ASP:OD1	2.04	0.62
8:K:439:PRO:HB3	12:L:916:HIS:CE1	2.34	0.62
10:H:217:LEU:HD12	10:H:218:SER:H	1.65	0.62
12:L:1122:ASN:N	12:L:1122:ASN:ND2	2.44	0.62
9:G:546:HIS:CD2	9:G:547:PRO:HD3	2.35	0.61
12:L:3501:PHE:HB2	12:L:3523:LEU:HD21	1.81	0.61
17:O:9:THR:CG2	18:P:10:LYS:CD	2.65	0.61
1:M:189:LEU:HB3	5:D:84:LEU:HD22	1.81	0.61
5:D:49:ILE:HG23	5:D:73:LEU:HD13	1.82	0.61
3:C:39:ARG:NH2	16:Q:150:GLN:HE21	1.97	0.61
3:C:51:LEU:HD11	16:Q:211:ASP:HA	1.82	0.61
16:Q:472:PHE:HZ	17:O:45:GLN:CG	2.13	0.61
3:C:38:LEU:CG	16:Q:210:ARG:HD2	2.26	0.61
10:H:317:LEU:O	10:H:380:THR:HG22	2.00	0.61
17:O:26:ASN:HD22	18:P:47:THR:CB	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:115:ILE:HD13	1:M:121:MET:SD	2.40	0.61
10:H:265:PHE:CE2	10:H:289:LEU:HD11	2.36	0.61
12:L:1611:ASP:HA	12:L:1617:ARG:HH12	1.65	0.61
9:G:87:ASN:ND2	9:G:219:ALA:O	2.33	0.61
9:G:450:VAL:HG22	9:G:451:GLY:H	1.65	0.61
12:L:2812:LEU:O	12:L:2815:VAL:HG22	1.99	0.61
16:Q:474:PHE:HE1	17:O:48:LEU:H	1.46	0.61
1:M:204:LEU:HD23	1:M:212:ILE:HD12	1.83	0.61
5:D:78:LYS:O	5:D:78:LYS:HD3	2.01	0.61
15:R:12:THR:HG21	16:Q:379:LYS:HE3	1.83	0.61
5:D:320:ASN:C	5:D:322:GLU:N	2.53	0.61
17:O:56:LEU:HD11	18:P:52:THR:H	0.45	0.60
2:A:289:ILE:O	6:E:958:LEU:HD21	2.01	0.60
5:D:21:MET:HE1	5:D:250:PHE:HA	1.82	0.60
5:D:320:ASN:CB	5:D:324:LYS:HB2	2.32	0.60
6:E:946:LYS:HA	6:E:946:LYS:CE	2.32	0.60
5:D:216:THR:HG23	5:D:246:GLY:HA3	1.83	0.60
12:L:428:LYS:HG3	12:L:430:GLU:HG2	1.84	0.60
3:C:39:ARG:CZ	16:Q:147:PHE:CD1	2.85	0.60
6:E:890:LEU:HD22	6:E:915:THR:HG23	1.83	0.60
3:C:44:ASN:OD1	16:Q:174:ARG:CG	2.49	0.60
12:L:2907:ARG:HG2	12:L:2907:ARG:NH1	2.10	0.60
16:Q:478:ARG:CG	17:O:68:HIS:HD2	2.14	0.60
5:D:76:HIS:C	5:D:78:LYS:N	2.53	0.60
9:G:620:HIS:HA	9:G:647:ARG:HE	1.67	0.60
12:L:704:LEU:HD13	12:L:749:SER:HB2	1.82	0.60
14:N:221:UNK:HA	14:N:230:UNK:CA	2.32	0.60
17:O:27:ILE:CD1	18:P:59:PHE:CA	2.49	0.60
5:D:76:HIS:C	5:D:78:LYS:H	2.04	0.60
9:G:518:THR:HG21	11:I:102:LEU:HD22	1.82	0.60
10:H:277:LEU:O	10:H:320:LYS:NZ	2.34	0.60
12:L:853:LEU:O	12:L:855:TYR:N	2.35	0.60
12:L:1837:ASP:OD1	12:L:1840:ARG:NH1	2.35	0.60
12:L:3652:ILE:HG22	12:L:3659:ILE:HG12	1.82	0.60
16:Q:184:LEU:CD1	17:O:44:ASP:O	2.39	0.60
16:Q:479:ILE:HA	17:O:47:SER:HG	1.65	0.60
1:M:188:GLU:HA	1:M:188:GLU:OE2	2.02	0.60
1:M:185:TYR:OH	5:D:211:ARG:HD3	2.02	0.59
5:D:21:MET:HE3	5:D:250:PHE:HA	1.84	0.59
10:H:269:ILE:O	10:H:272:THR:OG1	2.16	0.59
12:L:3736:SER:OG	12:L:3737:GLU:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:78:ARG:CD	18:P:23:TYR:CD2	2.85	0.59
16:Q:379:LYS:HE3	19:Q:607:HOH:O	2.02	0.59
1:M:202:ILE:HD11	1:M:217:ALA:HB2	1.84	0.59
3:C:38:LEU:CD1	16:Q:210:ARG:CD	2.75	0.59
3:C:38:LEU:HD12	16:Q:210:ARG:CZ	2.19	0.59
3:C:39:ARG:NE	16:Q:148:ILE:HG22	2.17	0.59
5:D:317:GLN:C	5:D:319:ARG:N	2.55	0.59
8:K:437:LEU:H	8:K:437:LEU:HD23	1.67	0.59
16:Q:91:LEU:HD23	17:O:13:CYS:SG	2.39	0.59
17:O:22:ILE:HD12	18:P:43:ILE:HD13	1.75	0.59
4:F:119:GLU:OE1	4:F:119:GLU:N	2.36	0.59
8:K:469:LEU:CD1	12:L:2788:ILE:HG22	2.14	0.59
12:L:848:VAL:C	12:L:851:PRO:HD2	2.23	0.59
16:Q:474:PHE:CZ	17:O:47:SER:CB	2.83	0.59
12:L:1352:GLU:HA	12:L:1355:ASN:HB2	1.83	0.59
2:A:226:ILE:HA	2:A:229:PHE:CE2	2.37	0.59
16:Q:468:ASP:O	17:O:51:ILE:HD11	2.03	0.59
12:L:3440:LYS:HG3	12:L:3446:PHE:CE1	2.38	0.59
12:L:3704:ARG:NH2	12:L:3825:LEU:O	2.36	0.59
12:L:3767:ASN:OD1	12:L:3770:ARG:NH2	2.35	0.59
3:C:59:ILE:CG2	16:Q:170:ILE:HD11	2.32	0.59
16:Q:139:TYR:CZ	17:O:24:ILE:CG2	2.86	0.59
1:M:90:ARG:NH1	14:N:513:UNK:CB	2.66	0.59
3:C:55:LEU:CD2	16:Q:160:ILE:HG12	2.30	0.59
17:O:56:LEU:N	18:P:52:THR:CB	2.64	0.59
3:C:44:ASN:CG	16:Q:174:ARG:HG3	2.23	0.59
6:E:952:ASN:OD1	11:I:137:TRP:NE1	2.35	0.59
12:L:3169:LEU:HG	12:L:3173:LEU:HD23	1.85	0.59
12:L:2805:PHE:CZ	12:L:2812:LEU:HG	2.38	0.58
16:Q:478:ARG:HD2	17:O:76:ASN:HD21	1.67	0.58
17:O:22:ILE:HG21	18:P:43:ILE:HG13	1.85	0.58
17:O:22:ILE:HG21	18:P:43:ILE:CD1	2.33	0.58
6:E:921:TYR:HD1	7:J:104:THR:HG22	1.68	0.58
8:K:446:ILE:HG13	12:L:2595:ILE:HG12	1.84	0.58
10:H:100:GLU:OE2	10:H:111:TYR:N	2.35	0.58
12:L:2913:VAL:HG12	12:L:2914:ILE:HD13	1.84	0.58
16:Q:93:CYS:N	17:O:17:ASN:OD1	2.26	0.58
5:D:84:LEU:HD23	5:D:84:LEU:O	2.02	0.58
12:L:2593:TYR:HB2	12:L:2596:ARG:HA	1.86	0.58
1:M:190:PHE:HB3	5:D:88:LEU:HG	1.84	0.58
3:C:52:GLN:CD	16:Q:153:GLN:HG3	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:38:GLU:N	10:H:38:GLU:OE1	2.36	0.58
10:H:162:ILE:HG22	10:H:164:PRO:HD2	1.86	0.58
4:F:223:GLU:HG2	9:G:576:MET:HB2	1.85	0.58
10:H:296:ASN:OD1	10:H:297:GLU:N	2.36	0.58
1:M:168:PHE:CD1	1:M:238:ARG:HG3	2.39	0.58
4:F:83:LEU:O	4:F:142:LEU:HD13	2.03	0.58
6:E:946:LYS:HD2	6:E:946:LYS:N	2.17	0.58
14:N:493:UNK:HA	14:N:510:UNK:O	2.03	0.58
12:L:2601:ARG:N	12:L:2601:ARG:HE	2.02	0.58
15:R:14:THR:OG1	16:Q:364:SER:HB3	2.04	0.58
16:Q:138:ASP:OD2	18:P:58:THR:HA	2.03	0.58
3:C:51:LEU:HD11	16:Q:211:ASP:CA	2.32	0.58
3:C:51:LEU:HG	16:Q:214:LEU:C	2.24	0.58
12:L:2428:LEU:HD11	12:L:2433:ILE:HD11	1.85	0.58
2:A:229:PHE:HZ	3:C:270:GLU:HG2	1.69	0.58
12:L:850:VAL:O	12:L:853:LEU:HB3	2.03	0.58
16:Q:472:PHE:CE2	17:O:50:GLU:HG3	2.37	0.58
1:M:82:LEU:CB	1:M:94:TYR:HE2	2.18	0.57
3:C:51:LEU:HG	16:Q:214:LEU:HG	1.84	0.57
5:D:87:TYR:CD1	5:D:87:TYR:C	2.77	0.57
15:R:4:PHE:HZ	16:Q:377:ARG:NH2	1.99	0.57
12:L:905:LEU:HD22	12:L:922:THR:HG23	1.85	0.57
12:L:1355:ASN:O	12:L:1358:VAL:HG13	2.04	0.57
12:L:2836:ARG:NH2	12:L:3618:ASN:OD1	2.37	0.57
10:H:125:GLU:N	10:H:126:PRO:HD3	2.18	0.57
6:E:921:TYR:CD1	7:J:104:THR:HG22	2.39	0.57
10:H:250:GLN:OE1	10:H:253:ARG:NE	2.33	0.57
11:I:41:ARG:O	11:I:44:THR:OG1	2.19	0.57
12:L:851:PRO:O	12:L:852:HIS:HB3	2.03	0.57
16:Q:472:PHE:CG	17:O:46:ILE:CA	2.82	0.57
10:H:129:LYS:HZ3	10:H:129:LYS:HB2	1.70	0.57
17:O:11:TRP:NE1	18:P:83:LEU:N	2.51	0.57
4:F:89:GLU:OE2	4:F:148:ARG:NH1	2.37	0.57
9:G:500:ASP:HB2	9:G:502:LYS:HE2	1.85	0.57
12:L:378:VAL:HG12	12:L:380:ASP:H	1.70	0.57
3:C:47:ASP:CB	16:Q:243:THR:HB	2.35	0.57
12:L:2860:VAL:HG13	12:L:2879:LEU:HD11	1.86	0.57
12:L:3458:LEU:H	12:L:3458:LEU:HD23	1.69	0.57
16:Q:473:LYS:O	17:O:47:SER:O	2.22	0.57
1:M:108:GLU:HA	1:M:110:LYS:H	1.70	0.57
9:G:620:HIS:NE2	9:G:641:GLY:HA3	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:3727:LEU:HD22	12:L:3798:THR:HG22	1.85	0.57
1:M:87:LEU:O	1:M:90:ARG:HG2	2.04	0.57
10:H:102:LEU:HD23	10:H:103:VAL:N	2.20	0.57
12:L:1355:ASN:HA	12:L:1358:VAL:CG1	2.35	0.57
16:Q:107:LYS:HG2	17:O:20:ARG:CZ	2.34	0.57
17:O:15:MET:HE1	18:P:74:VAL:HG21	1.87	0.57
17:O:19:LEU:HD13	18:P:70:ALA:HB1	1.86	0.57
1:M:191:PRO:HB3	5:D:212:GLN:CG	2.34	0.56
3:C:51:LEU:CD1	16:Q:215:SER:N	2.68	0.56
9:G:572:VAL:HG12	9:G:573:ARG:HG2	1.87	0.56
12:L:2880:LYS:N	12:L:2880:LYS:CD	2.67	0.56
16:Q:178:LEU:CD2	17:O:37:ILE:HG21	2.33	0.56
17:O:11:TRP:CZ2	18:P:86:ILE:CG1	2.86	0.56
3:C:288:LEU:HD21	3:C:292:THR:HG21	1.87	0.56
9:G:546:HIS:HB2	9:G:553:PHE:CE1	2.35	0.56
12:L:853:LEU:O	12:L:856:LEU:N	2.37	0.56
12:L:2880:LYS:HD2	12:L:2880:LYS:N	2.20	0.56
12:L:2880:LYS:CA	12:L:2880:LYS:HE3	2.35	0.56
4:F:111:PHE:CE1	4:F:115:VAL:HG21	2.41	0.56
6:E:885:VAL:HA	10:H:128:PRO:CG	2.35	0.56
12:L:3433:PRO:HB2	12:L:3527:VAL:HG11	1.86	0.56
1:M:74:VAL:HG23	1:M:155:PHE:HA	1.87	0.56
8:K:456:GLN:HG3	12:L:2677:PHE:CE2	2.41	0.56
6:E:932:HIS:O	6:E:935:SER:HB2	2.04	0.56
8:K:460:MET:SD	8:K:460:MET:N	2.76	0.56
12:L:302:PRO:HD3	12:L:336:ARG:HH22	1.71	0.56
12:L:3174:ARG:NH1	12:L:3290:MET:SD	2.79	0.56
15:R:12:THR:OG1	16:Q:360:GLU:OE2	2.22	0.56
12:L:2896:ASP:HB3	12:L:2899:ILE:HG12	1.86	0.56
16:Q:464:ILE:O	17:O:48:LEU:CB	2.53	0.56
1:M:87:LEU:CD1	14:N:490:UNK:HA	2.28	0.56
10:H:356:SER:O	10:H:360:PRO:HG2	2.05	0.56
12:L:827:ARG:O	12:L:828:ARG:HB2	2.05	0.56
5:D:320:ASN:HB3	5:D:324:LYS:HB2	1.89	0.55
12:L:946:ASP:O	12:L:951:GLN:NE2	2.39	0.55
12:L:3439:HIS:C	12:L:3440:LYS:HG2	2.27	0.55
12:L:583:ASN:ND2	12:L:600:ALA:O	2.39	0.55
3:C:42:ILE:HD12	16:Q:176:PRO:HA	1.87	0.55
3:C:54:CYS:SG	16:Q:215:SER:HB3	2.45	0.55
14:N:495:UNK:HA	14:N:508:UNK:O	2.07	0.55
16:Q:182:THR:CG2	17:O:45:GLN:N	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:188:ILE:HG23	17:O:90:THR:HG22	1.88	0.55
3:C:39:ARG:CZ	16:Q:147:PHE:C	2.70	0.55
3:C:40:TYR:CB	16:Q:214:LEU:CD2	2.64	0.55
8:K:455:PRO:HB2	8:K:457:PRO:HD2	1.88	0.55
12:L:2414:LEU:O	12:L:2417:ARG:NH1	2.40	0.55
16:Q:178:LEU:HD13	17:O:37:ILE:HG21	1.88	0.55
17:O:26:ASN:ND2	18:P:47:THR:HB	2.22	0.55
1:M:139:TYR:O	1:M:143:ILE:HG12	2.06	0.55
5:D:88:LEU:C	5:D:88:LEU:HD13	2.27	0.55
16:Q:501:GLN:OE1	18:P:31:ARG:NH2	2.28	0.55
5:D:326:ILE:HD12	5:D:327:ARG:N	2.21	0.55
10:H:265:PHE:HE2	10:H:289:LEU:HD11	1.70	0.55
9:G:546:HIS:CG	9:G:547:PRO:HD2	2.42	0.55
12:L:3698:THR:OG1	12:L:3699:GLU:N	2.39	0.55
1:M:143:ILE:O	1:M:150:ALA:HB2	2.06	0.55
1:M:189:LEU:HD21	5:D:81:VAL:HG12	1.87	0.55
5:D:212:GLN:HE21	5:D:212:GLN:CA	2.02	0.55
1:M:83:LYS:O	1:M:87:LEU:HG	2.07	0.54
1:M:187:PRO:CB	5:D:211:ARG:HB2	2.37	0.54
3:C:39:ARG:HE	16:Q:148:ILE:HG22	1.71	0.54
5:D:238:SER:OG	5:D:240:ASP:OD1	2.11	0.54
5:D:317:GLN:O	5:D:319:ARG:N	2.35	0.54
10:H:218:SER:OG	10:H:221:LEU:N	2.38	0.54
12:L:3429:ASP:HB2	12:L:3448:LYS:HD2	1.89	0.54
16:Q:182:THR:HB	17:O:45:GLN:O	2.07	0.54
16:Q:444:GLN:HE21	18:P:35:TYR:HE2	0.80	0.54
16:Q:252:THR:HG23	17:O:109:PHE:HE1	1.68	0.54
1:M:99:PHE:CZ	1:M:114:LEU:HD12	2.43	0.54
2:A:208:VAL:HG21	2:A:214:VAL:HG11	1.88	0.54
17:O:7:GLN:HG2	18:P:83:LEU:HD23	1.88	0.54
1:M:115:ILE:CD1	1:M:121:MET:SD	2.95	0.54
1:M:189:LEU:HD13	5:D:84:LEU:HD13	1.89	0.54
5:D:22:PHE:CE2	5:D:30:PRO:HD3	2.43	0.54
12:L:822:LEU:HD22	12:L:1186:TYR:H	1.72	0.54
12:L:3458:LEU:HD23	12:L:3458:LEU:N	2.22	0.54
16:Q:205:HIS:CE1	17:O:46:ILE:HG22	2.43	0.54
5:D:259:GLU:HB2	5:D:312:ALA:HB1	1.88	0.54
9:G:593:TRP:HE1	9:G:614:ILE:HD12	1.72	0.54
9:G:631:SER:OG	9:G:634:GLY:N	2.39	0.54
12:L:1822:LYS:NZ	12:L:1864:ASP:OD2	2.41	0.54
17:O:54:GLN:H	17:O:57:LYS:HB2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:173:GLU:HB2	5:D:204:TYR:CD1	2.43	0.54
4:F:212:PHE:HE2	4:F:218:LEU:HD21	1.72	0.54
5:D:199:MET:HA	5:D:203:GLU:CB	2.37	0.54
10:H:394:GLU:N	10:H:394:GLU:OE1	2.40	0.54
12:L:2916:ARG:HB2	12:L:2916:ARG:HH21	1.71	0.54
8:K:464:ASN:OD1	12:L:2669:MET:SD	2.65	0.54
10:H:115:ASP:OD1	10:H:116:GLU:N	2.41	0.54
11:I:40:TYR:O	11:I:44:THR:HG23	2.07	0.54
5:D:216:THR:CG2	5:D:243:ASP:HA	2.38	0.54
1:M:90:ARG:HD2	14:N:513:UNK:CB	2.38	0.54
3:C:51:LEU:CD2	16:Q:214:LEU:HB3	2.38	0.54
16:Q:93:CYS:SG	17:O:20:ARG:CG	2.95	0.54
16:Q:178:LEU:HB2	17:O:37:ILE:HD13	1.89	0.54
16:Q:468:ASP:O	17:O:51:ILE:CD1	2.56	0.54
5:D:17:ILE:HD12	5:D:17:ILE:H	1.72	0.54
12:L:3428:GLU:HG2	12:L:3429:ASP:H	1.73	0.54
16:Q:78:ARG:NH1	18:P:27:SER:CB	2.70	0.54
12:L:846:LEU:O	12:L:850:VAL:HB	2.08	0.53
17:O:11:TRP:CE3	18:P:82:ILE:CG2	2.91	0.53
17:O:27:ILE:HD12	18:P:59:PHE:HD1	1.70	0.53
5:D:216:THR:CB	5:D:243:ASP:HA	2.38	0.53
12:L:2911:PHE:CE2	12:L:2944:GLU:HG3	2.44	0.53
19:R:165:HOH:O	16:Q:355:LEU:CD1	2.39	0.53
17:O:23:VAL:HG21	18:P:63:ILE:HD12	1.90	0.53
12:L:1522:ASP:OD1	12:L:1522:ASP:N	2.41	0.53
16:Q:78:ARG:NE	18:P:23:TYR:CD2	2.70	0.53
5:D:66:VAL:HG13	5:D:67:PRO:HD2	1.87	0.53
5:D:317:GLN:HA	5:D:317:GLN:NE2	2.22	0.53
8:K:468:LEU:C	12:L:2829:LYS:NZ	2.61	0.53
4:F:93:ARG:NH2	4:F:95:GLY:O	2.41	0.53
10:H:332:GLN:N	10:H:332:GLN:OE1	2.42	0.53
12:L:1727:LYS:HG3	12:L:1776:ARG:HH21	1.73	0.53
12:L:3136:ILE:HG22	12:L:3161:ILE:HD13	1.89	0.53
17:O:56:LEU:CD1	18:P:51:VAL:HB	2.38	0.53
4:F:277:ASN:OD1	4:F:278:ALA:N	2.42	0.53
9:G:411:ASP:N	9:G:411:ASP:OD1	2.42	0.53
9:G:537:LEU:H	9:G:537:LEU:CD1	2.20	0.53
12:L:1219:ARG:NH1	12:L:3413:GLU:OE2	2.41	0.53
16:Q:188:ILE:HG23	17:O:90:THR:CG2	2.38	0.53
10:H:13:SER:OG	10:H:14:HIS:N	2.41	0.53
16:Q:106:TRP:HB3	17:O:20:ARG:HH21	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:340:ALA:HB3	19:Q:601:HOH:O	2.09	0.53
3:C:48:ARG:HH12	16:Q:216:GLY:HA2	1.74	0.53
9:G:521:LEU:HD23	9:G:521:LEU:O	2.08	0.53
12:L:959:ILE:HG21	12:L:2449:ILE:HD12	1.91	0.53
16:Q:474:PHE:CD2	16:Q:479:ILE:HD12	2.44	0.53
5:D:84:LEU:HD23	5:D:84:LEU:C	2.29	0.53
10:H:406:ASN:O	10:H:409:SER:OG	2.15	0.53
12:L:345:LEU:O	12:L:386:GLN:NE2	2.42	0.53
12:L:1278:ASN:O	12:L:1284:ARG:NH2	2.42	0.53
16:Q:106:TRP:HB3	17:O:20:ARG:NH2	2.23	0.53
16:Q:472:PHE:CD2	17:O:46:ILE:CA	2.92	0.53
17:O:22:ILE:HG23	18:P:44:ASN:OD1	2.08	0.53
1:M:173:GLU:HG2	5:D:197:LYS:CA	2.29	0.53
1:M:188:GLU:OE1	5:D:85:ARG:CZ	2.57	0.53
3:C:39:ARG:HH22	16:Q:150:GLN:NE2	2.05	0.53
3:C:47:ASP:HB3	16:Q:243:THR:C	2.25	0.53
5:D:313:TRP:O	5:D:317:GLN:HG2	2.08	0.53
5:D:323:LYS:HG3	5:D:323:LYS:O	2.08	0.53
10:H:217:LEU:HD12	10:H:218:SER:O	2.08	0.53
12:L:416:LEU:HD11	12:L:574:THR:HB	1.91	0.53
12:L:3101:LYS:O	12:L:3742:GLN:NE2	2.42	0.53
16:Q:474:PHE:CA	17:O:47:SER:OG	2.50	0.53
1:M:84:THR:HA	1:M:87:LEU:HD12	1.90	0.52
9:G:76:PRO:O	9:G:592:ARG:NH1	2.42	0.52
9:G:546:HIS:CG	9:G:547:PRO:CD	2.92	0.52
8:K:469:LEU:HD23	12:L:2790:THR:CG2	2.39	0.52
12:L:1526:ASN:O	12:L:1530:GLN:NE2	2.43	0.52
12:L:2528:HIS:O	12:L:2531:PHE:N	2.42	0.52
5:D:21:MET:HE2	5:D:253:VAL:CG2	2.38	0.52
7:J:80:THR:O	7:J:84:LEU:HD23	2.09	0.52
12:L:1886:VAL:HG22	12:L:1924:ALA:HB2	1.91	0.52
16:Q:259:TRP:HE1	17:O:114:ASP:HA	1.74	0.52
1:M:149:ALA:O	1:M:151:LYS:N	2.42	0.52
9:G:521:LEU:HD23	9:G:521:LEU:C	2.30	0.52
9:G:544:GLU:O	9:G:552:LEU:HD12	2.09	0.52
16:Q:130:TYR:CB	17:O:28:LEU:CD1	2.81	0.52
16:Q:472:PHE:CD2	17:O:50:GLU:HG2	2.44	0.52
3:C:39:ARG:NH2	16:Q:150:GLN:NE2	2.57	0.52
3:C:42:ILE:CD1	16:Q:176:PRO:HA	2.40	0.52
3:C:51:LEU:N	16:Q:214:LEU:CD1	2.72	0.52
9:G:562:ARG:HB3	9:G:571:CYS:SG	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:326:ILE:HD12	5:D:326:ILE:C	2.30	0.52
12:L:852:HIS:CG	12:L:852:HIS:O	2.62	0.52
12:L:1355:ASN:HA	12:L:1358:VAL:HG12	1.91	0.52
12:L:3515:ARG:NH1	12:L:3518:ASN:OD1	2.43	0.52
17:O:24:ILE:HG13	18:P:59:PHE:CZ	2.45	0.52
2:A:223:GLN:OE1	2:A:223:GLN:HA	2.09	0.52
2:A:226:ILE:HA	2:A:229:PHE:CD2	2.44	0.52
3:C:55:LEU:CD1	16:Q:173:SER:OG	2.57	0.52
8:K:442:PRO:CD	12:L:912:LEU:HD22	2.36	0.52
12:L:846:LEU:HA	12:L:850:VAL:CB	2.39	0.52
12:L:1307:SER:HA	12:L:1310:LYS:HD2	1.91	0.52
12:L:2884:GLN:NE2	12:L:2884:GLN:CA	2.72	0.52
5:D:218:ARG:C	5:D:220:ALA:H	2.12	0.52
8:K:468:LEU:CB	12:L:2829:LYS:NZ	2.58	0.52
8:K:602:ILE:O	8:K:607:ASN:N	2.43	0.52
15:R:12:THR:HG21	16:Q:379:LYS:CE	2.39	0.52
1:M:185:TYR:C	1:M:185:TYR:HD1	2.13	0.52
8:K:460:MET:HG3	12:L:2758:THR:HG22	1.92	0.52
12:L:710:SER:O	12:L:757:ASN:ND2	2.43	0.52
15:R:63:LYS:NZ	19:R:103:HOH:O	2.29	0.52
16:Q:106:TRP:HD1	17:O:20:ARG:NH1	1.97	0.52
1:M:102:VAL:HG12	1:M:115:ILE:HB	1.92	0.51
9:G:84:GLN:OE1	9:G:215:ASN:O	2.28	0.51
9:G:202:ILE:HD11	9:G:206:THR:HG21	1.92	0.51
10:H:27:ALA:HB1	10:H:32:ILE:CD1	2.35	0.51
16:Q:178:LEU:HD22	17:O:37:ILE:CG2	2.38	0.51
9:G:607:ASP:HB2	9:G:614:ILE:HG13	1.92	0.51
12:L:672:PRO:HA	12:L:675:PHE:HB3	1.93	0.51
12:L:1419:LYS:O	12:L:1422:VAL:HG22	2.11	0.51
12:L:1947:ARG:NH2	12:L:1964:TYR:OH	2.43	0.51
12:L:3141:GLN:NE2	12:L:3750:ASP:OD2	2.42	0.51
12:L:3495:GLU:HG3	12:L:3496:ARG:HD2	1.91	0.51
14:N:221:UNK:C	14:N:230:UNK:CA	2.88	0.51
15:R:68:HIS:HE1	19:R:113:HOH:O	1.92	0.51
6:E:940:LYS:O	6:E:941:VAL:HB	2.09	0.51
12:L:1221:LEU:HD21	12:L:1243:LEU:HB3	1.92	0.51
19:R:153:HOH:O	16:Q:326:LYS:CB	2.11	0.51
16:Q:182:THR:CG2	17:O:45:GLN:H	2.19	0.51
6:E:947:PHE:HD1	6:E:947:PHE:O	1.94	0.51
12:L:899:ASP:N	12:L:899:ASP:OD1	2.41	0.51
12:L:2805:PHE:CE1	12:L:2812:LEU:HG	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:232:LEU:HD22	5:D:235:SER:OG	2.11	0.51
10:H:255:ASP:OD1	10:H:255:ASP:N	2.43	0.51
12:L:986:PRO:O	12:L:991:ARG:NH2	2.44	0.51
12:L:2601:ARG:O	12:L:2603:ASN:N	2.43	0.51
2:A:364:ASP:N	2:A:364:ASP:OD1	2.42	0.51
3:C:49:PRO:HG3	16:Q:237:PHE:CE1	2.36	0.51
4:F:200:ASP:HA	4:F:203:TYR:HE2	1.75	0.51
6:E:935:SER:OG	6:E:940:LYS:HB2	2.11	0.51
10:H:362:ILE:N	10:H:362:ILE:HD13	2.24	0.51
12:L:3423:HIS:HA	12:L:3426:LYS:HB2	1.93	0.51
12:L:809:MET:HE1	12:L:844:VAL:HG21	1.92	0.51
12:L:1203:LEU:O	12:L:1206:PRO:HD2	2.10	0.51
12:L:1203:LEU:HD23	12:L:1206:PRO:HD2	1.93	0.51
16:Q:70:GLU:OE1	18:P:24:ASP:HA	2.11	0.51
17:O:15:MET:HE3	18:P:74:VAL:HG21	1.93	0.51
1:M:105:ARG:O	1:M:106:ILE:HG23	2.10	0.51
5:D:74:ILE:HG13	5:D:78:LYS:HB3	1.92	0.51
8:K:461:LYS:HZ1	12:L:2792:ARG:NH2	2.09	0.51
9:G:650:ASP:HB3	9:G:693:MET:HE2	1.93	0.51
12:L:3456:LEU:HD12	12:L:3467:LYS:HB3	1.93	0.51
4:F:212:PHE:CE2	4:F:218:LEU:HD21	2.46	0.51
9:G:471:CYS:SG	9:G:499:TRP:O	2.69	0.51
10:H:328:LEU:O	10:H:332:GLN:NE2	2.43	0.51
12:L:562:ARG:NH1	12:L:625:PHE:O	2.44	0.51
12:L:2802:LEU:HD11	12:L:2858:SER:HB2	1.93	0.51
2:A:246:LEU:O	2:A:250:MET:HG3	2.11	0.51
9:G:494:HIS:CE1	9:G:520:ARG:HD3	2.45	0.51
16:Q:472:PHE:CE2	17:O:50:GLU:CD	2.83	0.51
17:O:22:ILE:HD12	18:P:43:ILE:HD12	1.68	0.51
2:A:192:SER:O	2:A:196:GLN:NE2	2.44	0.50
12:L:1314:LEU:O	12:L:1317:ILE:HG22	2.10	0.50
16:Q:474:PHE:CZ	17:O:46:ILE:HB	2.39	0.50
16:Q:479:ILE:HD12	17:O:47:SER:OG	2.12	0.50
4:F:326:ARG:HG2	12:L:2751:LEU:HD11	1.92	0.50
6:E:836:CYS:SG	6:E:993:LEU:HD13	2.51	0.50
12:L:1698:GLN:HA	12:L:1701:GLU:HG2	1.93	0.50
12:L:2415:THR:HA	12:L:2418:MET:HE3	1.93	0.50
15:R:75:GLY:HA2	16:Q:270:GLU:OE2	2.11	0.50
1:M:170:ILE:HD13	1:M:234:LEU:HD22	1.93	0.50
9:G:565:ASP:HB3	9:G:568:ARG:HB3	1.93	0.50
12:L:703:PHE:O	12:L:709:THR:OG1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:1860:ASP:OD1	12:L:1860:ASP:N	2.45	0.50
12:L:2556:GLU:O	12:L:2560:ASN:ND2	2.44	0.50
12:L:2802:LEU:HD22	12:L:2854:LEU:HD12	1.92	0.50
1:M:185:TYR:C	1:M:185:TYR:CD1	2.84	0.50
9:G:380:SER:OG	10:H:143:ILE:O	2.20	0.50
12:L:1314:LEU:HG	12:L:1347:PHE:CZ	2.47	0.50
2:A:246:LEU:HG	2:A:250:MET:HE2	1.93	0.50
5:D:78:LYS:HE3	5:D:78:LYS:C	2.31	0.50
12:L:1507:LEU:HA	12:L:1510:ALA:HB3	1.92	0.50
16:Q:90:SER:H	18:P:14:GLN:NE2	2.10	0.50
16:Q:464:ILE:C	17:O:46:ILE:CD1	2.80	0.50
16:Q:472:PHE:CZ	17:O:50:GLU:HG2	2.44	0.50
12:L:2916:ARG:CZ	12:L:2916:ARG:CB	2.88	0.50
12:L:3746:LEU:HA	12:L:3749:ARG:HG2	1.93	0.50
1:M:67:LEU:HD13	1:M:160:ILE:HG23	1.94	0.50
3:C:38:LEU:HD22	16:Q:210:ARG:HD2	0.55	0.50
17:O:26:ASN:HB2	18:P:47:THR:HG21	1.94	0.50
1:M:142:ILE:HA	1:M:145:LYS:HE3	1.94	0.50
4:F:122:PRO:HG3	4:F:195:LEU:HD23	1.93	0.50
12:L:2880:LYS:HE3	12:L:2880:LYS:HA	1.94	0.50
12:L:3440:LYS:HG3	12:L:3446:PHE:HE1	1.75	0.50
10:H:290:ILE:HG22	10:H:343:LEU:HD11	1.93	0.50
12:L:1516:GLN:NE2	12:L:1563:ASN:O	2.45	0.50
14:N:174:UNK:O	14:N:213:UNK:O	2.30	0.50
6:E:948:GLN:HG3	6:E:950:VAL:O	2.11	0.49
9:G:122:LEU:HD21	10:H:291:TYR:CD1	2.46	0.49
9:G:469:ILE:HD11	9:G:479:LEU:HD12	1.93	0.49
12:L:1947:ARG:NH1	12:L:1978:ARG:O	2.45	0.49
17:O:56:LEU:HD11	18:P:51:VAL:CA	2.42	0.49
4:F:219:ASN:O	4:F:222:THR:OG1	2.31	0.49
12:L:2880:LYS:H	12:L:2880:LYS:CD	2.23	0.49
17:O:56:LEU:CA	18:P:52:THR:CG2	2.90	0.49
1:M:80:LEU:HD21	1:M:143:ILE:HD12	1.93	0.49
3:C:47:ASP:CG	16:Q:243:THR:HB	2.32	0.49
12:L:2797:GLN:HG2	12:L:2818:LEU:HD21	1.93	0.49
16:Q:107:LYS:CA	17:O:20:ARG:HH22	2.26	0.49
10:H:96:LEU:HD23	10:H:97:VAL:N	2.27	0.49
16:Q:107:LYS:HG2	17:O:20:ARG:NH1	2.27	0.49
17:O:34:ARG:NH1	18:P:57:PRO:CA	2.69	0.49
4:F:200:ASP:HA	4:F:203:TYR:CE2	2.48	0.49
5:D:67:PRO:O	5:D:71:ILE:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:428:LYS:HG3	12:L:430:GLU:CG	2.42	0.49
12:L:2465:LEU:HB3	12:L:2593:TYR:HB3	1.95	0.49
12:L:3653:ASN:HB3	12:L:3657:GLY:H	1.78	0.49
16:Q:479:ILE:CD1	17:O:47:SER:OG	2.61	0.49
2:A:208:VAL:CG2	2:A:214:VAL:HG11	2.42	0.49
3:C:56:SER:HB2	16:Q:156:ARG:HD3	1.94	0.49
12:L:1432:SER:OG	12:L:1433:ILE:N	2.45	0.49
12:L:2906:TRP:O	12:L:2910:VAL:HG23	2.12	0.49
4:F:279:ASP:O	8:K:521:ILE:HD11	2.12	0.49
5:D:329:PHE:N	5:D:329:PHE:CD1	2.80	0.49
1:M:82:LEU:CD1	1:M:101:ALA:HA	2.37	0.49
3:C:306:SER:OG	3:C:307:VAL:N	2.45	0.49
5:D:319:ARG:HG3	5:D:320:ASN:H	1.77	0.49
12:L:3175:THR:HG21	12:L:3528:PRO:HB2	1.94	0.49
13:B:556:VAL:O	13:B:557:VAL:C	2.50	0.49
1:M:108:GLU:HA	1:M:109:PRO:C	2.31	0.49
6:E:885:VAL:HA	10:H:128:PRO:HG3	1.95	0.49
12:L:1354:LEU:O	12:L:1358:VAL:HG12	2.13	0.49
12:L:1364:LEU:O	12:L:1391:ARG:NH1	2.45	0.49
16:Q:472:PHE:CB	17:O:46:ILE:CG1	2.55	0.49
1:M:175:LEU:O	1:M:179:HIS:HB2	2.13	0.49
2:A:190:VAL:HG22	2:A:192:SER:H	1.77	0.49
6:E:946:LYS:CE	6:E:946:LYS:CA	2.91	0.49
12:L:2475:LEU:O	12:L:2479:TYR:N	2.44	0.49
3:C:48:ARG:NH1	16:Q:216:GLY:HA2	2.27	0.48
4:F:223:GLU:OE1	4:F:223:GLU:N	2.46	0.48
5:D:78:LYS:O	5:D:78:LYS:CD	2.61	0.48
11:I:133:THR:O	11:I:135:LYS:N	2.44	0.48
12:L:2665:LEU:HD21	12:L:2680:THR:HB	1.95	0.48
3:C:34:LEU:C	16:Q:467:ARG:HG2	2.32	0.48
4:F:129:LYS:HG2	4:F:203:TYR:CE1	2.47	0.48
8:K:454:PRO:CD	8:K:455:PRO:CD	2.92	0.48
12:L:1256:THR:OG1	12:L:1257:ARG:N	2.47	0.48
12:L:1358:VAL:HG23	12:L:1394:CYS:HB3	1.95	0.48
16:Q:130:TYR:HD2	17:O:24:ILE:HG22	1.76	0.48
8:K:564:HIS:ND1	8:K:568:ASN:OD1	2.44	0.48
9:G:139:HIS:ND1	9:G:228:LEU:HD22	2.29	0.48
12:L:545:LEU:HD12	12:L:546:PRO:HD2	1.94	0.48
3:C:38:LEU:CG	16:Q:210:ARG:CZ	2.89	0.48
8:K:439:PRO:HB3	12:L:916:HIS:HE1	1.75	0.48
14:N:87:UNK:HA	14:N:497:UNK:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:93:CYS:H	17:O:17:ASN:CG	2.14	0.48
17:O:26:ASN:ND2	18:P:47:THR:CB	2.77	0.48
6:E:885:VAL:HG22	10:H:128:PRO:HB2	1.95	0.48
10:H:26:ALA:O	10:H:29:SER:OG	2.22	0.48
12:L:599:THR:O	12:L:601:ARG:NH1	2.46	0.48
17:O:11:TRP:CE3	18:P:82:ILE:HG23	2.48	0.48
12:L:426:GLU:HG3	12:L:428:LYS:HD3	1.94	0.48
16:Q:139:TYR:CZ	17:O:24:ILE:HG23	2.48	0.48
16:Q:481:LEU:HD12	17:O:50:GLU:N	2.11	0.48
10:H:118:ASP:OD1	10:H:118:ASP:N	2.46	0.48
12:L:605:ASN:OD1	12:L:1568:GLN:NE2	2.46	0.48
12:L:387:LEU:HD21	12:L:422:ILE:HG12	1.95	0.48
17:O:7:GLN:HG3	18:P:86:ILE:CB	2.41	0.48
17:O:19:LEU:CD1	18:P:70:ALA:CB	2.91	0.48
6:E:909:PHE:O	6:E:913:VAL:HG23	2.14	0.48
9:G:171:GLU:OE1	9:G:171:GLU:N	2.45	0.48
10:H:317:LEU:HD12	10:H:319:LYS:H	1.78	0.48
12:L:2807:GLN:CB	12:L:2809:LYS:HE3	2.44	0.48
18:P:47:THR:HA	18:P:66:ILE:HD11	1.96	0.48
1:M:96:PRO:O	1:M:98:ARG:N	2.47	0.48
5:D:23:VAL:HA	5:D:27:THR:O	2.14	0.48
6:E:834:ARG:NH2	6:E:901:ASN:O	2.47	0.48
12:L:1514:THR:O	12:L:1517:GLN:NE2	2.44	0.48
12:L:1724:PHE:HB3	12:L:1776:ARG:HD2	1.96	0.48
12:L:2528:HIS:CD2	12:L:2532:LEU:HD23	2.49	0.48
16:Q:259:TRP:NE1	17:O:114:ASP:OD1	2.42	0.48
1:M:194:ILE:CA	1:M:195:TYR:N	2.76	0.47
4:F:115:VAL:HG13	4:F:190:LEU:HD11	1.96	0.47
8:K:458:ALA:O	8:K:459:ALA:HB2	2.14	0.47
9:G:94:PRO:HB3	9:G:566:ILE:HD11	1.96	0.47
9:G:184:LEU:O	9:G:191:LYS:NZ	2.41	0.47
11:I:131:CYS:SG	11:I:132:LEU:N	2.87	0.47
12:L:1180:CYS:HA	12:L:1183:GLU:HG2	1.96	0.47
12:L:2878:GLU:O	12:L:2882:VAL:HG13	2.14	0.47
12:L:2879:LEU:O	12:L:2882:VAL:HG22	2.14	0.47
9:G:650:ASP:HB3	9:G:693:MET:CE	2.43	0.47
16:Q:315:SER:HB3	19:Q:605:HOH:O	2.04	0.47
17:O:55:ARG:HB3	18:P:52:THR:CG2	2.41	0.47
2:A:229:PHE:CZ	3:C:270:GLU:HG2	2.50	0.47
3:C:39:ARG:NE	16:Q:147:PHE:CE1	2.82	0.47
3:C:50:ILE:C	16:Q:214:LEU:CG	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:84:LEU:HA	5:D:87:TYR:HD2	1.79	0.47
8:K:468:LEU:O	12:L:2790:THR:HG22	2.14	0.47
12:L:853:LEU:HD23	12:L:853:LEU:N	2.28	0.47
12:L:1262:SER:OG	12:L:1263:SER:N	2.47	0.47
12:L:1855:PRO:HA	12:L:1862:ARG:HH22	1.79	0.47
5:D:319:ARG:HH12	5:D:335:ARG:HG2	1.79	0.47
8:K:469:LEU:HB3	12:L:2788:ILE:CG2	2.44	0.47
12:L:2904:VAL:HG21	12:L:2952:PHE:HB2	1.95	0.47
12:L:3519:ILE:O	12:L:3519:ILE:HG13	2.13	0.47
3:C:34:LEU:O	16:Q:467:ARG:HG2	2.15	0.47
3:C:54:CYS:HG	16:Q:215:SER:C	1.90	0.47
5:D:17:ILE:H	5:D:17:ILE:CD1	2.26	0.47
5:D:208:SER:HB3	5:D:211:ARG:CZ	2.44	0.47
9:G:559:LYS:HG2	9:G:580:GLY:O	2.14	0.47
1:M:191:PRO:HB3	5:D:212:GLN:HG2	1.96	0.47
5:D:47:VAL:O	5:D:51:LEU:HD23	2.14	0.47
5:D:73:LEU:C	5:D:73:LEU:CD2	2.82	0.47
5:D:328:ASN:ND2	6:E:963:ASN:OD1	2.48	0.47
10:H:305:VAL:HA	10:H:308:ILE:HG22	1.97	0.47
12:L:1469:LEU:O	12:L:1501:LYS:NZ	2.47	0.47
12:L:1824:THR:H	12:L:1827:LEU:HD21	1.79	0.47
12:L:2914:ILE:HD13	12:L:2914:ILE:N	2.28	0.47
12:L:3162:ALA:HB2	12:L:3169:LEU:HD23	1.95	0.47
2:A:246:LEU:HG	2:A:250:MET:CE	2.45	0.47
3:C:55:LEU:HD23	16:Q:160:ILE:CG1	2.41	0.47
4:F:118:GLU:O	4:F:191:ARG:N	2.45	0.47
4:F:189:ILE:C	4:F:190:LEU:HD12	2.35	0.47
4:F:304:LEU:CD2	8:K:475:SER:HB2	2.45	0.47
6:E:947:PHE:CD1	6:E:947:PHE:C	2.88	0.47
8:K:566:GLU:O	8:K:572:ARG:NH1	2.46	0.47
9:G:472:SER:OG	9:G:474:ASP:OD1	2.28	0.47
12:L:854:SER:C	12:L:856:LEU:H	2.18	0.47
12:L:867:SER:OG	12:L:868:GLN:N	2.48	0.47
12:L:1417:ARG:HG2	12:L:1418:VAL:N	2.29	0.47
12:L:1684:ARG:HH12	12:L:1692:LEU:HD13	1.80	0.47
14:N:238:UNK:HA	14:N:248:UNK:O	2.14	0.47
16:Q:474:PHE:HD1	17:O:48:LEU:HG	1.76	0.47
17:O:27:ILE:HD12	18:P:59:PHE:HA	1.77	0.47
1:M:82:LEU:HG	1:M:117:ALA:HB2	1.97	0.47
9:G:626:TYR:CE2	9:G:642:ALA:HB2	2.50	0.47
12:L:1716:LEU:HG	12:L:1718:HIS:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:3798:THR:OG1	12:L:3799:GLN:N	2.44	0.47
16:Q:478:ARG:HD3	17:O:76:ASN:HD21	1.79	0.47
9:G:546:HIS:NE2	9:G:547:PRO:HD2	2.29	0.47
10:H:157:ASN:HD22	10:H:160:LYS:HZ3	1.62	0.47
12:L:1134:SER:OG	12:L:1135:ASP:N	2.47	0.47
12:L:2808:GLN:HA	12:L:2808:GLN:OE1	2.14	0.47
16:Q:91:LEU:CD2	17:O:13:CYS:HB3	2.36	0.47
16:Q:479:ILE:CD1	17:O:47:SER:CB	2.79	0.47
2:A:244:ASP:O	2:A:248:THR:HG23	2.15	0.47
10:H:16:LEU:HD22	11:I:18:ILE:HG12	1.97	0.47
12:L:312:CYS:O	12:L:320:ARG:NH2	2.47	0.47
12:L:1203:LEU:HD22	12:L:1210:PHE:CE2	2.50	0.47
12:L:1848:ALA:HB2	12:L:1887:VAL:HG23	1.97	0.47
15:R:46:ALA:CA	16:Q:331:PRO:O	2.50	0.47
16:Q:464:ILE:C	17:O:46:ILE:HD11	2.36	0.47
1:M:151:LYS:O	1:M:153:THR:HG22	2.15	0.46
2:A:271:MET:SD	8:K:537:VAL:HG23	2.55	0.46
3:C:33:SER:HB2	16:Q:207:PRO:HG3	1.96	0.46
8:K:441:PRO:CA	12:L:912:LEU:HD21	2.33	0.46
8:K:504:LYS:O	8:K:508:ARG:NH1	2.48	0.46
12:L:853:LEU:O	12:L:854:SER:C	2.54	0.46
17:O:22:ILE:HG21	18:P:43:ILE:CG1	2.44	0.46
17:O:56:LEU:HD23	18:P:52:THR:HG23	1.76	0.46
3:C:38:LEU:HB2	16:Q:210:ARG:HH21	1.76	0.46
9:G:576:MET:SD	9:G:577:GLY:N	2.88	0.46
12:L:952:ASN:OD1	12:L:952:ASN:N	2.48	0.46
15:R:71:LEU:HD12	16:Q:397:PHE:HB2	1.97	0.46
16:Q:472:PHE:HZ	17:O:45:GLN:CD	2.18	0.46
16:Q:130:TYR:CE2	17:O:25:ASN:OD1	2.59	0.46
16:Q:416:PHE:CE2	18:P:35:TYR:O	2.69	0.46
17:O:34:ARG:NH1	18:P:57:PRO:CG	2.55	0.46
4:F:137:GLU:O	9:G:59:TYR:N	2.45	0.46
5:D:75:ARG:O	5:D:75:ARG:HG2	2.16	0.46
8:K:444:THR:OG1	8:K:445:GLU:N	2.48	0.46
12:L:1441:GLY:HA2	12:L:1444:LYS:HG2	1.98	0.46
12:L:2601:ARG:O	12:L:2602:PRO:C	2.53	0.46
12:L:2959:HIS:HA	12:L:3512:VAL:HG11	1.96	0.46
1:M:75:THR:HB	1:M:120:LYS:HG2	1.97	0.46
1:M:88:HIS:HA	14:N:514:UNK:O	2.16	0.46
2:A:357:SER:O	2:A:357:SER:OG	2.34	0.46
9:G:477:VAL:HG21	9:G:512:THR:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:1354:LEU:CA	12:L:1357:LEU:HD22	2.43	0.46
12:L:2425:GLY:HA2	12:L:2428:LEU:HD23	1.98	0.46
12:L:2812:LEU:HD11	12:L:2862:SER:HB2	1.97	0.46
16:Q:472:PHE:CB	17:O:47:SER:N	2.73	0.46
8:K:465:ARG:O	12:L:2829:LYS:HE2	2.16	0.46
8:K:588:GLN:NE2	8:K:589:PRO:O	2.45	0.46
12:L:853:LEU:HD23	12:L:853:LEU:H	1.80	0.46
12:L:934:ARG:H	12:L:934:ARG:HG2	1.55	0.46
17:O:55:ARG:CB	18:P:52:THR:HG21	2.43	0.46
12:L:606:GLU:HB2	12:L:1694:PHE:HB2	1.98	0.46
5:D:78:LYS:CE	5:D:78:LYS:O	2.64	0.46
10:H:234:ASN:OD1	10:H:235:GLN:NE2	2.49	0.46
12:L:3434:GLY:HA3	12:L:3525:ILE:HD12	1.97	0.46
12:L:3602:SER:OG	12:L:3603:THR:N	2.48	0.46
1:M:117:ALA:C	1:M:119:GLY:H	2.19	0.46
9:G:642:ALA:O	10:H:68:ARG:NH2	2.49	0.46
10:H:69:THR:O	10:H:71:HIS:ND1	2.47	0.46
12:L:2901:ASN:O	12:L:2905:THR:HG22	2.16	0.46
15:R:4:PHE:CE1	16:Q:362:LEU:HD13	2.51	0.46
17:O:7:GLN:HG3	18:P:86:ILE:CG2	2.45	0.46
3:C:39:ARG:CG	16:Q:147:PHE:HE1	2.28	0.46
3:C:51:LEU:CG	16:Q:214:LEU:HG	2.46	0.46
5:D:66:VAL:CG1	5:D:67:PRO:CD	2.84	0.46
8:K:469:LEU:HB3	12:L:2788:ILE:HG22	1.97	0.46
12:L:2807:GLN:HB3	12:L:2809:LYS:HE3	1.98	0.46
16:Q:472:PHE:CZ	17:O:50:GLU:CG	2.98	0.46
1:M:172:LEU:HB2	5:D:204:TYR:CE2	2.52	0.45
5:D:17:ILE:N	5:D:17:ILE:CD1	2.79	0.45
7:J:58:THR:N	7:J:61:GLU:OE2	2.49	0.45
9:G:709:THR:HG22	9:G:710:ARG:H	1.80	0.45
12:L:828:ARG:N	12:L:829:PRO:CD	2.57	0.45
12:L:1608:VAL:O	12:L:1617:ARG:NH2	2.49	0.45
16:Q:472:PHE:CG	17:O:46:ILE:N	2.80	0.45
17:O:11:TRP:CG	18:P:86:ILE:CD1	2.94	0.45
3:C:290:SER:OG	3:C:291:ARG:N	2.49	0.45
12:L:2807:GLN:HB3	12:L:2809:LYS:HG3	1.97	0.45
12:L:3458:LEU:H	12:L:3458:LEU:CD2	2.28	0.45
5:D:76:HIS:O	5:D:78:LYS:N	2.49	0.45
7:J:98:ARG:O	7:J:101:ALA:HB3	2.16	0.45
12:L:827:ARG:HH21	12:L:829:PRO:HB3	1.80	0.45
12:L:1136:ASN:HB3	12:L:1139:VAL:HG12	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:2807:GLN:OE1	12:L:2807:GLN:HA	2.16	0.45
16:Q:130:TYR:CD2	17:O:24:ILE:HG22	2.51	0.45
16:Q:182:THR:CA	17:O:44:ASP:HB2	2.18	0.45
5:D:239:ASP:HA	5:D:242:ILE:HD12	1.97	0.45
8:K:462:ILE:HG23	8:K:463:PRO:HD3	1.98	0.45
16:Q:91:LEU:CD2	17:O:13:CYS:HG	2.19	0.45
16:Q:106:TRP:CD1	17:O:20:ARG:NH1	2.79	0.45
16:Q:107:LYS:N	17:O:20:ARG:HH22	2.14	0.45
16:Q:416:PHE:HZ	18:P:41:ASP:OD2	1.99	0.45
17:O:24:ILE:CG1	18:P:59:PHE:CE1	2.94	0.45
1:M:166:VAL:HG22	1:M:210:GLY:O	2.17	0.45
8:K:562:GLN:CD	8:K:577:ALA:HB3	2.36	0.45
12:L:1916:ASP:OD1	12:L:1916:ASP:N	2.49	0.45
4:F:326:ARG:HD3	12:L:2751:LEU:HD21	1.97	0.45
10:H:17:TRP:HZ3	11:I:15:LEU:HD21	1.81	0.45
12:L:854:SER:C	12:L:856:LEU:N	2.69	0.45
12:L:1418:VAL:O	12:L:1422:VAL:HG13	2.17	0.45
3:C:49:PRO:HB2	16:Q:214:LEU:HD13	1.97	0.45
9:G:460:ASP:O	9:G:468:LEU:HD12	2.17	0.45
9:G:546:HIS:NE2	9:G:591:GLY:HA2	2.32	0.45
9:G:594:LEU:CG	9:G:606:TRP:HB2	2.45	0.45
12:L:3461:GLY:N	12:L:3464:GLY:O	2.50	0.45
14:N:221:UNK:HA	14:N:230:UNK:CB	2.47	0.45
1:M:124:THR:CG2	1:M:125:GLY:N	2.80	0.45
1:M:189:LEU:HD13	5:D:84:LEU:HD22	1.98	0.45
8:K:465:ARG:HG3	12:L:2844:LEU:CD1	2.47	0.45
9:G:697:PHE:O	10:H:147:GLN:NE2	2.50	0.45
12:L:962:LEU:HG	12:L:2572:ALA:HB2	1.98	0.45
12:L:1543:PRO:O	12:L:1547:HIS:NE2	2.49	0.45
12:L:3494:GLU:HA	12:L:3497:ILE:HG12	1.99	0.45
16:Q:35:ASP:HA	16:Q:38:TYR:CD2	2.52	0.45
1:M:135:ALA:O	1:M:139:TYR:CD2	2.70	0.45
5:D:27:THR:HG22	5:D:28:ASN:H	1.81	0.45
9:G:632:ARG:NH1	9:G:708:PHE:O	2.46	0.45
12:L:2708:LEU:HD21	12:L:3793:SER:HB2	1.98	0.45
12:L:2745:TRP:O	12:L:2749:THR:OG1	2.35	0.45
14:N:426:UNK:CB	14:N:481:UNK:CA	2.94	0.45
14:N:426:UNK:CB	14:N:481:UNK:CB	2.95	0.45
16:Q:130:TYR:CD1	17:O:28:LEU:CD1	2.77	0.45
16:Q:130:TYR:HB3	17:O:28:LEU:CD1	2.42	0.45
3:C:38:LEU:HB2	16:Q:210:ARG:CZ	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:437:LEU:H	8:K:437:LEU:CD2	2.28	0.45
9:G:107:ILE:HD11	9:G:140:CYS:HB2	1.99	0.45
14:N:83:UNK:C	14:N:506:UNK:C	2.95	0.45
2:A:342:TYR:HD1	2:A:344:TYR:HH	1.64	0.44
3:C:39:ARG:NH1	16:Q:148:ILE:HG23	2.06	0.44
4:F:305:SER:O	8:K:452:VAL:HG21	2.16	0.44
6:E:946:LYS:N	6:E:946:LYS:CD	2.79	0.44
9:G:450:VAL:HG22	9:G:451:GLY:N	2.29	0.44
8:K:465:ARG:HD3	8:K:465:ARG:H	1.83	0.44
12:L:271:ILE:O	12:L:275:VAL:N	2.48	0.44
12:L:854:SER:O	12:L:856:LEU:N	2.50	0.44
12:L:1425:PHE:C	12:L:1427:SER:N	2.70	0.44
12:L:1780:TYR:HA	12:L:1783:ILE:HG22	1.99	0.44
12:L:1876:ASP:OD1	12:L:1876:ASP:N	2.51	0.44
12:L:2539:THR:HG23	12:L:2541:GLY:H	1.83	0.44
9:G:371:LEU:HD12	9:G:372:SER:H	1.83	0.44
9:G:544:GLU:HG2	9:G:553:PHE:HB2	1.98	0.44
12:L:214:TYR:O	12:L:218:ALA:N	2.49	0.44
12:L:1340:CYS:HA	12:L:1343:LEU:HD13	1.98	0.44
12:L:2804:GLY:O	12:L:2809:LYS:N	2.50	0.44
12:L:3725:TYR:HA	12:L:3728:VAL:HG12	1.98	0.44
3:C:38:LEU:HD21	16:Q:210:ARG:HG2	1.99	0.44
9:G:192:ILE:O	9:G:195:SER:OG	2.31	0.44
12:L:3172:GLN:O	12:L:3175:THR:OG1	2.34	0.44
8:K:465:ARG:O	12:L:2791:PRO:HG3	2.18	0.44
9:G:63:GLU:OE1	9:G:64:SER:OG	2.31	0.44
9:G:215:ASN:OD1	9:G:216:GLU:N	2.50	0.44
9:G:352:ALA:O	9:G:356:ARG:N	2.46	0.44
9:G:504:SER:OG	9:G:507:GLY:N	2.44	0.44
12:L:1610:LEU:O	12:L:1617:ARG:NH2	2.51	0.44
6:E:946:LYS:HD2	6:E:946:LYS:H	1.82	0.44
9:G:618:ARG:HD3	9:G:689:THR:HG21	2.00	0.44
12:L:1623:SER:OG	12:L:1626:ARG:NE	2.51	0.44
12:L:2393:SER:HA	12:L:2396:PHE:HB3	1.99	0.44
12:L:2446:GLU:O	12:L:2452:ARG:NE	2.46	0.44
1:M:78:CYS:SG	1:M:80:LEU:HD11	2.57	0.44
3:C:38:LEU:CB	16:Q:210:ARG:CZ	2.95	0.44
5:D:24:SER:HB3	5:D:210:CYS:CB	2.48	0.44
12:L:1356:ARG:N	12:L:1356:ARG:NE	2.65	0.44
12:L:1358:VAL:O	12:L:1359:GLN:C	2.56	0.44
12:L:1727:LYS:HD2	12:L:1734:PRO:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:138:VAL:O	9:G:142:LEU:HD23	2.18	0.44
9:G:596:SER:OG	9:G:604:CYS:HB2	2.18	0.44
12:L:404:ALA:HB3	12:L:407:VAL:HG22	1.99	0.44
12:L:1358:VAL:O	12:L:1360:GLU:N	2.51	0.44
12:L:3522:THR:O	12:L:3522:THR:OG1	2.33	0.44
16:Q:137:GLY:O	18:P:60:SER:OG	2.27	0.44
17:O:26:ASN:CB	18:P:47:THR:HG21	2.48	0.44
8:K:461:LYS:HZ2	12:L:2792:ARG:NE	2.16	0.44
9:G:74:PRO:HB3	9:G:610:THR:CG2	2.47	0.44
12:L:722:LYS:HG2	12:L:768:LEU:HD21	2.00	0.44
12:L:2437:LEU:HA	12:L:2440:ILE:HD12	2.00	0.44
12:L:2897:ILE:HD12	12:L:2897:ILE:HA	1.86	0.44
14:N:507:UNK:C	14:N:509:UNK:N	2.78	0.44
15:R:4:PHE:CE1	16:Q:362:LEU:CD1	3.01	0.44
1:M:76:LEU:O	1:M:78:CYS:N	2.51	0.43
6:E:880:LYS:C	6:E:881:LEU:HD12	2.38	0.43
8:K:461:LYS:HD2	12:L:2762:LEU:HD11	1.99	0.43
8:K:557:ASP:OD1	8:K:557:ASP:N	2.46	0.43
3:C:59:ILE:HG22	16:Q:170:ILE:HD11	1.99	0.43
13:B:413:ASP:O	13:B:414:ASP:C	2.56	0.43
1:M:126:ALA:HB3	1:M:132:SER:OG	2.19	0.43
5:D:259:GLU:HA	5:D:262:ILE:HD12	2.00	0.43
12:L:408:GLN:OE1	12:L:445:ARG:NH1	2.39	0.43
12:L:850:VAL:N	12:L:851:PRO:CD	2.82	0.43
12:L:2860:VAL:HG13	12:L:2879:LEU:CD1	2.49	0.43
12:L:3151:ALA:HA	12:L:3154:VAL:HG12	2.01	0.43
1:M:79:ARG:O	1:M:80:LEU:HD12	2.17	0.43
3:C:48:ARG:HG3	16:Q:238:LYS:HG2	2.00	0.43
5:D:215:PHE:HB3	5:D:223:PHE:HB2	2.01	0.43
8:K:452:VAL:O	12:L:2666:GLU:OE2	2.36	0.43
8:K:469:LEU:CD2	12:L:2790:THR:CG2	2.96	0.43
16:Q:130:TYR:CE2	17:O:28:LEU:HD12	2.51	0.43
10:H:318:ALA:HB3	10:H:337:ARG:NH1	2.32	0.43
12:L:801:PHE:HD1	12:L:803:ASN:H	1.66	0.43
12:L:850:VAL:HG13	12:L:853:LEU:HD13	1.99	0.43
12:L:3765:GLN:HB3	12:L:3768:GLN:HB3	2.00	0.43
14:N:207:UNK:CA	14:N:208:UNK:CB	2.96	0.43
1:M:200:PRO:HD3	1:M:225:GLN:OE1	2.18	0.43
5:D:321:VAL:HG12	5:D:321:VAL:O	2.17	0.43
8:K:469:LEU:HD23	8:K:469:LEU:N	2.33	0.43
12:L:773:LEU:HD13	12:L:815:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:3541:ARG:HB2	12:L:3654:GLU:HB2	2.01	0.43
17:O:11:TRP:CD1	18:P:83:LEU:HG	2.51	0.43
1:M:88:HIS:CB	14:N:515:UNK:O	2.56	0.43
3:C:51:LEU:HG	16:Q:214:LEU:CA	2.48	0.43
5:D:71:ILE:HD12	5:D:74:ILE:HD11	2.01	0.43
12:L:2741:LYS:NZ	12:L:2896:ASP:OD1	2.52	0.43
12:L:3099:THR:HG22	12:L:3103:LEU:HD13	2.00	0.43
12:L:3285:ASP:OD1	12:L:3285:ASP:N	2.48	0.43
12:L:2523:ASP:OD1	12:L:2523:ASP:N	2.42	0.43
3:C:36:ASN:CB	16:Q:467:ARG:NH2	2.81	0.43
3:C:51:LEU:HD12	16:Q:215:SER:H	1.81	0.43
4:F:204:GLN:OE1	4:F:204:GLN:HA	2.19	0.43
5:D:17:ILE:HG22	5:D:21:MET:SD	2.59	0.43
5:D:207:TRP:CD1	5:D:207:TRP:C	2.91	0.43
7:J:206:TYR:HB3	7:J:207:GLY:H	1.71	0.43
9:G:92:THR:OG1	9:G:93:ALA:N	2.51	0.43
12:L:560:ASP:N	12:L:560:ASP:OD1	2.51	0.43
12:L:1204:ASP:OD1	12:L:1204:ASP:N	2.52	0.43
12:L:1690:SER:O	12:L:1690:SER:OG	2.32	0.43
12:L:2447:LEU:HD23	12:L:2447:LEU:HA	1.89	0.43
1:M:177:PHE:CB	5:D:194:GLU:HA	2.49	0.43
2:A:243:MET:CB	2:A:268:ILE:HD12	2.49	0.43
6:E:883:SER:O	6:E:886:SER:OG	2.28	0.43
12:L:1884:ALA:HA	12:L:1887:VAL:HG12	2.00	0.43
12:L:1967:ILE:HD12	12:L:1967:ILE:HA	1.91	0.43
14:N:181:UNK:O	14:N:198:UNK:CB	2.67	0.43
5:D:319:ARG:HD2	5:D:319:ARG:HA	1.65	0.42
6:E:885:VAL:HG13	10:H:128:PRO:HG2	2.01	0.42
6:E:929:LEU:CD1	6:E:955:ILE:HG22	2.49	0.42
6:E:950:VAL:O	6:E:950:VAL:HG23	2.19	0.42
12:L:1317:ILE:HD11	12:L:1333:ASN:HA	2.01	0.42
12:L:1357:LEU:N	12:L:1357:LEU:CD1	2.81	0.42
12:L:1736:VAL:HG13	12:L:1737:LEU:HD23	2.01	0.42
16:Q:78:ARG:HA	16:Q:82:VAL:HB	2.01	0.42
3:C:51:LEU:HD12	16:Q:211:ASP:O	2.08	0.42
12:L:1060:LYS:HD2	12:L:1060:LYS:HA	1.72	0.42
12:L:1786:PRO:HA	12:L:1789:ILE:HG12	2.01	0.42
12:L:2805:PHE:HA	12:L:2810:ASP:O	2.19	0.42
5:D:240:ASP:OD1	5:D:241:VAL:N	2.52	0.42
9:G:581:ALA:O	9:G:582:ILE:HD13	2.19	0.42
10:H:122:LEU:HD12	10:H:123:ILE:HB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:129:LYS:NZ	10:H:129:LYS:CB	2.82	0.42
10:H:129:LYS:HZ3	10:H:129:LYS:CB	2.31	0.42
12:L:1226:ARG:NH2	12:L:1275:ASP:OD2	2.52	0.42
12:L:1354:LEU:O	12:L:1357:LEU:HB2	2.19	0.42
12:L:2601:ARG:NE	12:L:2601:ARG:CA	2.81	0.42
2:A:183:GLU:O	2:A:184:SER:OG	2.26	0.42
8:K:581:ILE:HD12	11:I:52:ILE:HD11	2.01	0.42
10:H:317:LEU:HD12	10:H:318:ALA:N	2.34	0.42
12:L:848:VAL:O	12:L:851:PRO:HD2	2.19	0.42
12:L:1541:LEU:HD12	12:L:1541:LEU:HA	1.93	0.42
12:L:3173:LEU:HD21	12:L:3293:LEU:HD22	2.02	0.42
5:D:22:PHE:HE2	5:D:30:PRO:HD3	1.85	0.42
6:E:817:GLY:O	6:E:820:LYS:N	2.52	0.42
8:K:437:LEU:HD23	8:K:437:LEU:N	2.32	0.42
12:L:846:LEU:CA	12:L:850:VAL:HB	2.45	0.42
12:L:907:LYS:HE3	12:L:907:LYS:HB3	1.83	0.42
12:L:3111:SER:O	12:L:3111:SER:OG	2.33	0.42
17:O:34:ARG:NH2	18:P:51:VAL:CG1	2.79	0.42
3:C:47:ASP:HB3	16:Q:243:THR:CA	2.48	0.42
9:G:416:LEU:N	9:G:447:ARG:O	2.52	0.42
10:H:242:GLU:OE1	10:H:242:GLU:N	2.52	0.42
12:L:1356:ARG:NE	12:L:1356:ARG:CA	2.82	0.42
12:L:1417:ARG:HH21	12:L:1417:ARG:HG3	1.85	0.42
12:L:2422:PHE:HE2	12:L:2441:LEU:HD22	1.85	0.42
12:L:2889:ARG:O	12:L:2889:ARG:HG2	2.20	0.42
16:Q:139:TYR:HE1	18:P:59:PHE:CD1	2.36	0.42
3:C:288:LEU:CD2	3:C:292:THR:HG21	2.48	0.42
5:D:72:PHE:HD1	5:D:72:PHE:HA	1.70	0.42
12:L:1727:LYS:O	12:L:1776:ARG:NH2	2.53	0.42
14:N:83:UNK:C	14:N:507:UNK:N	2.82	0.42
1:M:186:GLU:HB3	1:M:189:LEU:HB2	2.01	0.42
5:D:244:ILE:O	5:D:248:LEU:HG	2.20	0.42
6:E:947:PHE:HE1	6:E:949:LYS:HA	1.85	0.42
7:J:116:TYR:OH	7:J:120:ARG:NH2	2.53	0.42
8:K:582:ARG:NH1	11:I:71:GLY:O	2.52	0.42
10:H:315:LEU:O	10:H:318:ALA:HB2	2.20	0.42
12:L:2476:GLN:HG2	12:L:2548:ILE:HD12	2.02	0.42
12:L:2592:ASP:OD1	12:L:2592:ASP:N	2.53	0.42
12:L:2740:GLU:HB2	12:L:2745:TRP:CH2	2.55	0.42
16:Q:416:PHE:CZ	18:P:41:ASP:OD2	2.73	0.42
16:Q:478:ARG:HG3	17:O:68:HIS:CD2	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:187:PRO:HB3	5:D:211:ARG:HB2	2.02	0.42
2:A:204:LYS:HA	3:C:293:ALA:HB3	2.02	0.42
2:A:250:MET:O	2:A:253:ILE:N	2.52	0.42
3:C:253:ARG:NH2	10:H:49:TYR:OH	2.51	0.42
10:H:67:ARG:NH2	10:H:74:ASP:OD1	2.53	0.42
12:L:1863:LYS:HA	12:L:1863:LYS:HD2	1.78	0.42
14:N:494:UNK:O	14:N:509:UNK:HA	2.20	0.42
17:O:26:ASN:HD22	18:P:47:THR:HG21	1.85	0.42
2:A:259:LEU:HD21	8:K:549:LYS:HB2	2.02	0.41
3:C:38:LEU:CD1	16:Q:210:ARG:HH11	2.27	0.41
9:G:600:ASP:OD1	9:G:601:SER:N	2.53	0.41
11:I:24:ILE:O	11:I:26:SER:N	2.51	0.41
12:L:328:ARG:HH11	12:L:370:THR:HG22	1.84	0.41
12:L:3149:LYS:HD3	12:L:3149:LYS:HA	1.89	0.41
6:E:930:LYS:O	6:E:934:GLU:HG2	2.21	0.41
9:G:144:LEU:HD22	9:G:156:PHE:CE2	2.56	0.41
9:G:450:VAL:HG13	9:G:451:GLY:N	2.35	0.41
10:H:155:SER:OG	10:H:157:ASN:OD1	2.36	0.41
12:L:718:ILE:HD12	12:L:718:ILE:HA	1.95	0.41
12:L:3634:ILE:HD12	12:L:3703:PHE:HB2	2.02	0.41
14:N:184:UNK:CB	14:N:238:UNK:N	2.82	0.41
14:N:496:UNK:N	14:N:508:UNK:CB	2.83	0.41
16:Q:178:LEU:HD12	17:O:37:ILE:HD12	1.81	0.41
1:M:74:VAL:HG23	1:M:155:PHE:CA	2.49	0.41
3:C:41:ARG:HB3	16:Q:173:SER:HB3	2.02	0.41
8:K:442:PRO:HB3	12:L:2817:ARG:NH1	2.35	0.41
8:K:469:LEU:CD2	12:L:2790:THR:HG23	2.50	0.41
9:G:515:HIS:NE2	10:H:57:GLN:OE1	2.53	0.41
9:G:585:LEU:HA	9:G:595:ALA:O	2.21	0.41
10:H:69:THR:HG23	10:H:71:HIS:HE1	1.84	0.41
12:L:764:HIS:NE2	12:L:1525:ASN:OD1	2.37	0.41
12:L:3603:THR:HG22	12:L:3711:LYS:HG2	2.01	0.41
16:Q:472:PHE:HE2	17:O:50:GLU:CG	2.18	0.41
2:A:223:GLN:OE1	2:A:223:GLN:CA	2.68	0.41
12:L:1444:LYS:HE3	12:L:1444:LYS:HB2	1.80	0.41
12:L:2798:THR:HA	12:L:2818:LEU:HD23	2.02	0.41
12:L:3705:LEU:HD12	12:L:3705:LEU:HA	1.95	0.41
1:M:146:ILE:O	1:M:147:GLY:C	2.58	0.41
3:C:52:GLN:CG	16:Q:153:GLN:HG3	2.50	0.41
8:K:466:PRO:HA	12:L:2791:PRO:CG	2.23	0.41
9:G:709:THR:HG22	9:G:710:ARG:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:185:TYR:HD2	5:D:204:TYR:HH	1.64	0.41
1:M:189:LEU:CD1	5:D:84:LEU:HD13	2.49	0.41
3:C:44:ASN:OD1	16:Q:174:ARG:CD	2.69	0.41
6:E:934:GLU:O	6:E:936:LYS:N	2.45	0.41
8:K:454:PRO:CD	8:K:455:PRO:HD2	2.50	0.41
9:G:460:ASP:OD1	9:G:461:PHE:N	2.54	0.41
12:L:388:TRP:HA	12:L:391:VAL:HG12	2.03	0.41
12:L:1587:SER:OG	12:L:1588:PHE:N	2.53	0.41
12:L:3133:TRP:CZ3	12:L:3441:ASP:HB3	2.56	0.41
17:O:11:TRP:CE2	18:P:86:ILE:CG1	2.97	0.41
1:M:84:THR:O	1:M:87:LEU:HB2	2.20	0.41
2:A:268:ILE:O	2:A:272:LEU:HD23	2.20	0.41
9:G:365:SER:O	9:G:370:LYS:N	2.49	0.41
9:G:563:MET:HE3	9:G:608:ILE:HD13	2.03	0.41
10:H:129:LYS:NZ	10:H:129:LYS:CA	2.82	0.41
12:L:268:GLY:O	12:L:272:ILE:N	2.53	0.41
12:L:672:PRO:O	12:L:676:ASN:ND2	2.54	0.41
12:L:1629:GLY:HA2	12:L:1632:HIS:HD2	1.86	0.41
12:L:2794:GLN:HG2	12:L:2822:GLY:HA3	2.02	0.41
1:M:231:TYR:HB3	1:M:232:PRO:HD3	2.03	0.41
8:K:469:LEU:HD22	12:L:2790:THR:HG23	2.03	0.41
12:L:1295:SER:OG	12:L:1305:MET:SD	2.68	0.41
12:L:3136:ILE:HA	12:L:3139:VAL:HG23	2.03	0.41
2:A:242:GLU:O	2:A:243:MET:C	2.58	0.41
3:C:51:LEU:CG	16:Q:214:LEU:CG	2.97	0.41
4:F:133:VAL:HG23	4:F:134:GLN:CD	2.41	0.41
9:G:648:VAL:HG13	9:G:694:SER:H	1.86	0.41
9:G:701:THR:O	9:G:701:THR:OG1	2.39	0.41
10:H:396:ILE:HG23	10:H:397:ARG:N	2.36	0.41
11:I:51:THR:HG22	11:I:76:LEU:HD21	2.03	0.41
12:L:314:SER:O	12:L:314:SER:OG	2.33	0.41
12:L:853:LEU:H	12:L:853:LEU:CD2	2.34	0.41
12:L:858:LYS:HB2	12:L:858:LYS:HE3	1.87	0.41
12:L:1540:HIS:O	12:L:1582:ARG:NH2	2.54	0.41
12:L:2465:LEU:H	12:L:2465:LEU:HG	1.71	0.41
12:L:2778:LEU:HD23	12:L:2778:LEU:HA	1.96	0.41
12:L:3142:LEU:HB3	12:L:3158:LEU:HD11	2.03	0.41
14:N:175:UNK:HA	14:N:213:UNK:O	2.21	0.41
10:H:335:ALA:O	10:H:339:LEU:HD23	2.20	0.41
16:Q:107:LYS:HZ2	17:O:13:CYS:HA	1.83	0.41
1:M:105:ARG:O	1:M:106:ILE:CG2	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:115:ILE:HD13	1:M:121:MET:CG	2.51	0.40
2:A:199:GLN:NE2	3:C:305:PHE:O	2.54	0.40
8:K:460:MET:HG3	12:L:2758:THR:CG2	2.51	0.40
12:L:325:HIS:HA	12:L:328:ARG:HB3	2.03	0.40
12:L:1358:VAL:HG22	12:L:1359:GLN:N	2.36	0.40
12:L:1506:LEU:HA	12:L:1509:TRP:HD1	1.86	0.40
12:L:2231:ILE:O	12:L:2235:VAL:N	2.53	0.40
12:L:2721:PHE:HA	12:L:2722:PRO:HD3	1.90	0.40
12:L:3604:LEU:HD12	12:L:3604:LEU:HA	1.93	0.40
12:L:2687:TYR:HB2	12:L:2690:THR:HG22	2.02	0.40
12:L:2817:ARG:HA	12:L:2817:ARG:HD2	1.91	0.40
12:L:2907:ARG:HH11	12:L:2907:ARG:CG	2.25	0.40
12:L:3798:THR:HB	12:L:3801:VAL:HG22	2.04	0.40
17:O:9:THR:HG22	18:P:10:LYS:HE3	0.41	0.40
1:M:78:CYS:SG	1:M:80:LEU:CD1	3.10	0.40
3:C:49:PRO:CD	16:Q:238:LYS:HA	2.52	0.40
4:F:85:PHE:N	4:F:143:ARG:O	2.46	0.40
6:E:944:ASP:OD1	6:E:944:ASP:N	2.54	0.40
9:G:588:SER:HB3	9:G:593:TRP:HB2	2.04	0.40
10:H:127:LEU:HD12	10:H:127:LEU:C	2.39	0.40
10:H:217:LEU:HB2	10:H:221:LEU:HD22	2.02	0.40
12:L:833:ASP:HA	12:L:836:VAL:HG12	2.03	0.40
12:L:1611:ASP:OD1	12:L:1611:ASP:N	2.53	0.40
16:Q:20:ASP:N	16:Q:20:ASP:OD1	2.55	0.40
5:D:84:LEU:HA	5:D:87:TYR:CD2	2.56	0.40
8:K:461:LYS:HE2	8:K:463:PRO:HD2	2.03	0.40
9:G:45:ASP:OD1	9:G:45:ASP:N	2.55	0.40
12:L:2783:LYS:HA	12:L:2783:LYS:HD3	1.74	0.40
12:L:3063:GLY:O	12:L:3067:ASP:N	2.47	0.40
16:Q:182:THR:CB	17:O:45:GLN:O	2.69	0.40
17:O:22:ILE:CB	18:P:43:ILE:HD12	2.52	0.40
1:M:85:VAL:HG11	1:M:143:ILE:HG22	2.04	0.40
1:M:88:HIS:CA	14:N:515:UNK:C	2.98	0.40
9:G:182:GLU:OE1	9:G:182:GLU:N	2.49	0.40
12:L:3778:GLU:HA	12:L:3781:THR:HG22	2.04	0.40
17:O:11:TRP:CZ2	18:P:82:ILE:HG23	2.55	0.40
17:O:22:ILE:CG2	18:P:44:ASN:OD1	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	M	178/240 (74%)	147 (83%)	24 (14%)	7 (4%)	3 23
2	A	169/448 (38%)	151 (89%)	18 (11%)	0	100 100
3	C	89/698 (13%)	83 (93%)	6 (7%)	0	100 100
4	F	202/517 (39%)	177 (88%)	24 (12%)	1 (0%)	29 69
5	D	203/341 (60%)	177 (87%)	19 (9%)	7 (3%)	3 26
6	E	150/1191 (13%)	135 (90%)	13 (9%)	2 (1%)	12 48
7	J	92/217 (42%)	82 (89%)	9 (10%)	1 (1%)	14 52
8	K	150/609 (25%)	125 (83%)	23 (15%)	2 (1%)	12 48
9	G	512/722 (71%)	448 (88%)	63 (12%)	1 (0%)	47 81
10	H	413/485 (85%)	365 (88%)	48 (12%)	0	100 100
11	I	119/153 (78%)	98 (82%)	21 (18%)	0	100 100
12	L	2874/3825 (75%)	2623 (91%)	233 (8%)	18 (1%)	25 66
13	B	70/722 (10%)	63 (90%)	7 (10%)	0	100 100
15	R	76/76 (100%)	75 (99%)	1 (1%)	0	100 100
16	Q	480/502 (96%)	444 (92%)	30 (6%)	6 (1%)	12 48
17	O	115/123 (94%)	103 (90%)	6 (5%)	6 (5%)	2 19
18	P	88/96 (92%)	85 (97%)	3 (3%)	0	100 100
All	All	5980/10965 (54%)	5381 (90%)	548 (9%)	51 (1%)	21 57

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	77	GLY
1	M	99	PHE
1	M	110	LYS
5	D	200	THR
5	D	327	ARG

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Mol	Chain	Res	Type
6	E	935	SER
8	K	459	ALA
12	L	66	VAL
12	L	204	PRO
12	L	828	ARG
12	L	854	SER
12	L	855	TYR
12	L	1425	PHE
12	L	1426	LYS
12	L	2602	PRO
12	L	3428	GLU
12	L	3797	ALA
16	Q	31	SER
16	Q	58	ILE
16	Q	223	LYS
17	O	59	VAL
17	O	75	GLU
17	O	79	ASN
1	M	97	LYS
1	M	147	GLY
1	M	150	ALA
5	D	219	LYS
5	D	330	GLN
7	J	206	TYR
9	G	450	VAL
12	L	826	ALA
12	L	2597	GLN
16	Q	70	GLU
17	O	65	ILE
1	M	201	LYS
5	D	77	ASP
6	E	941	VAL
12	L	1774	ASP
12	L	3460	ARG
16	Q	431	ASN
17	O	58	PHE
8	K	442	PRO
12	L	2594	HIS
12	L	3439	HIS
17	O	86	SER
4	F	80	PRO
5	D	218	ARG

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Mol	Chain	Res	Type
12	L	3616	TYR
16	Q	245	GLU
12	L	1359	GLN
5	D	321	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	M	152/205 (74%)	138 (91%)	14 (9%)	9 29
2	A	134/394 (34%)	132 (98%)	2 (2%)	65 80
3	C	85/627 (14%)	85 (100%)	0	100 100
4	F	179/471 (38%)	179 (100%)	0	100 100
5	D	166/306 (54%)	154 (93%)	12 (7%)	14 39
6	E	142/1101 (13%)	136 (96%)	6 (4%)	30 54
7	J	85/183 (46%)	84 (99%)	1 (1%)	71 83
8	K	133/524 (25%)	130 (98%)	3 (2%)	50 70
9	G	439/635 (69%)	430 (98%)	9 (2%)	53 72
10	H	352/438 (80%)	348 (99%)	4 (1%)	73 84
11	I	104/130 (80%)	103 (99%)	1 (1%)	76 86
12	L	2156/3450 (62%)	2114 (98%)	42 (2%)	57 75
15	R	70/68 (103%)	69 (99%)	1 (1%)	67 80
16	Q	431/449 (96%)	425 (99%)	6 (1%)	67 80
17	O	103/109 (94%)	102 (99%)	1 (1%)	76 86
18	P	85/91 (93%)	85 (100%)	0	100 100
All	All	4816/9181 (52%)	4714 (98%)	102 (2%)	56 72

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	67	LEU
1	M	76	LEU
1	M	97	LYS
1	M	104	MET
1	M	141	ARG
1	M	148	PHE
1	M	153	THR
1	M	175	LEU
1	M	181	THR
1	M	185	TYR
1	M	202	ILE
1	M	215	THR
1	M	231	TYR
1	M	240	MET
2	A	229	PHE
2	A	291	LYS
5	D	18	GLN
5	D	74	ILE
5	D	78	LYS
5	D	83	ARG
5	D	85	ARG
5	D	87	TYR
5	D	211	ARG
5	D	212	GLN
5	D	218	ARG
5	D	322	GLU
5	D	329	PHE
5	D	338	VAL
6	E	933	ILE
6	E	940	LYS
6	E	942	MET
6	E	946	LYS
6	E	948	GLN
6	E	949	LYS
7	J	205	GLU
8	K	437	LEU
8	K	449	ARG
8	K	465	ARG
9	G	115	LYS
9	G	194	ARG
9	G	230	ASN
9	G	452	HIS
9	G	537	LEU

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Mol	Chain	Res	Type
9	G	542	CYS
9	G	560	THR
9	G	571	CYS
9	G	594	LEU
10	H	129	LYS
10	H	217	LEU
10	H	360	PRO
10	H	364	ARG
11	I	16	HIS
12	L	429	THR
12	L	800	ARG
12	L	849	LEU
12	L	852	HIS
12	L	971	THR
12	L	1122	ASN
12	L	1278	ASN
12	L	1314	LEU
12	L	1323	ARG
12	L	1356	ARG
12	L	1358	VAL
12	L	1413	ARG
12	L	1417	ARG
12	L	1419	LYS
12	L	1424	PHE
12	L	1548	LYS
12	L	1665	LYS
12	L	1680	LEU
12	L	2427	ARG
12	L	2489	ARG
12	L	2595	ILE
12	L	2633	ASN
12	L	2807	GLN
12	L	2878	GLU
12	L	2880	LYS
12	L	2881	ARG
12	L	2883	LEU
12	L	2884	GLN
12	L	2887	ARG
12	L	2888	GLU
12	L	2907	ARG
12	L	2913	VAL
12	L	2914	ILE

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Mol	Chain	Res	Type
12	L	2916	ARG
12	L	3314	ARG
12	L	3426	LYS
12	L	3440	LYS
12	L	3441	ASP
12	L	3489	ARG
12	L	3502	ARG
12	L	3542	TYR
12	L	3646	GLN
15	R	60	ASN
16	Q	38	TYR
16	Q	57	ASN
16	Q	61	TYR
16	Q	187	PHE
16	Q	254	LEU
16	Q	397	PHE
17	O	42	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	91	ASN
1	M	95	ASN
1	M	179	HIS
2	A	227	HIS
3	C	52	GLN
5	D	212	GLN
5	D	317	GLN
9	G	391	ASN
10	H	64	HIS
10	H	157	ASN
10	H	306	HIS
12	L	1632	HIS
12	L	2633	ASN
12	L	2698	GLN
12	L	2884	GLN
15	R	2	GLN
15	R	25	ASN
15	R	60	ASN
15	R	62	GLN
15	R	68	HIS
16	Q	110	HIS

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Mol	Chain	Res	Type
16	Q	150	GLN
16	Q	205	HIS
16	Q	466	ASN
17	O	26	ASN
17	O	52	ASN
17	O	54	GLN
17	O	76	ASN
18	P	14	GLN
18	P	36	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	GLZ	R	76	16,15	3,3,3	0.70	0	0,2,2	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	GLZ	R	76	16,15	-	0/0/1/1	-

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.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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
14	N	6
13	B	2
1	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	414:ASP	C	462:ALA	N	28.86
1	B	471:ASP	C	509:ASP	N	23.98
1	N	117:UNK	C	172:UNK	N	15.59
1	N	287:UNK	C	332:UNK	N	5.97
1	N	213:UNK	C	214:UNK	N	4.21
1	N	467:UNK	C	468:UNK	N	2.43
1	N	451:UNK	C	452:UNK	N	1.99
1	M	194:ILE	C	195:TYR	N	1.97
1	N	207:UNK	C	208:UNK	N	1.79

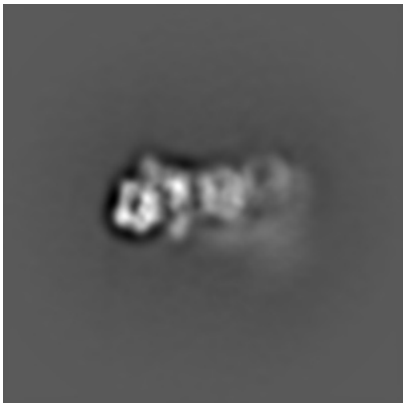
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10446. These allow visual inspection of the internal detail of the map and identification of artifacts.

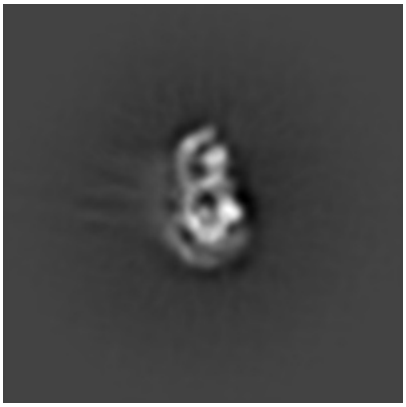
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map



X



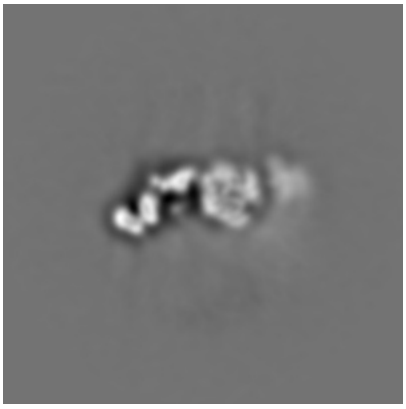
Y

Z

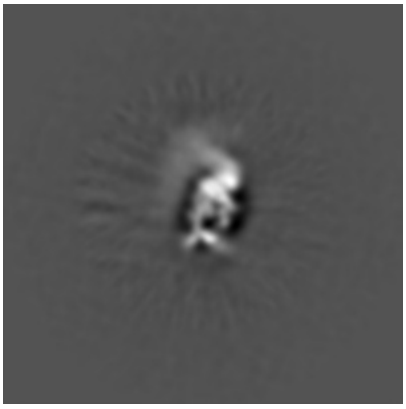
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 128



Y Index: 128

Z Index: 128

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: 121

Y Index: 93

Z Index: 133

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

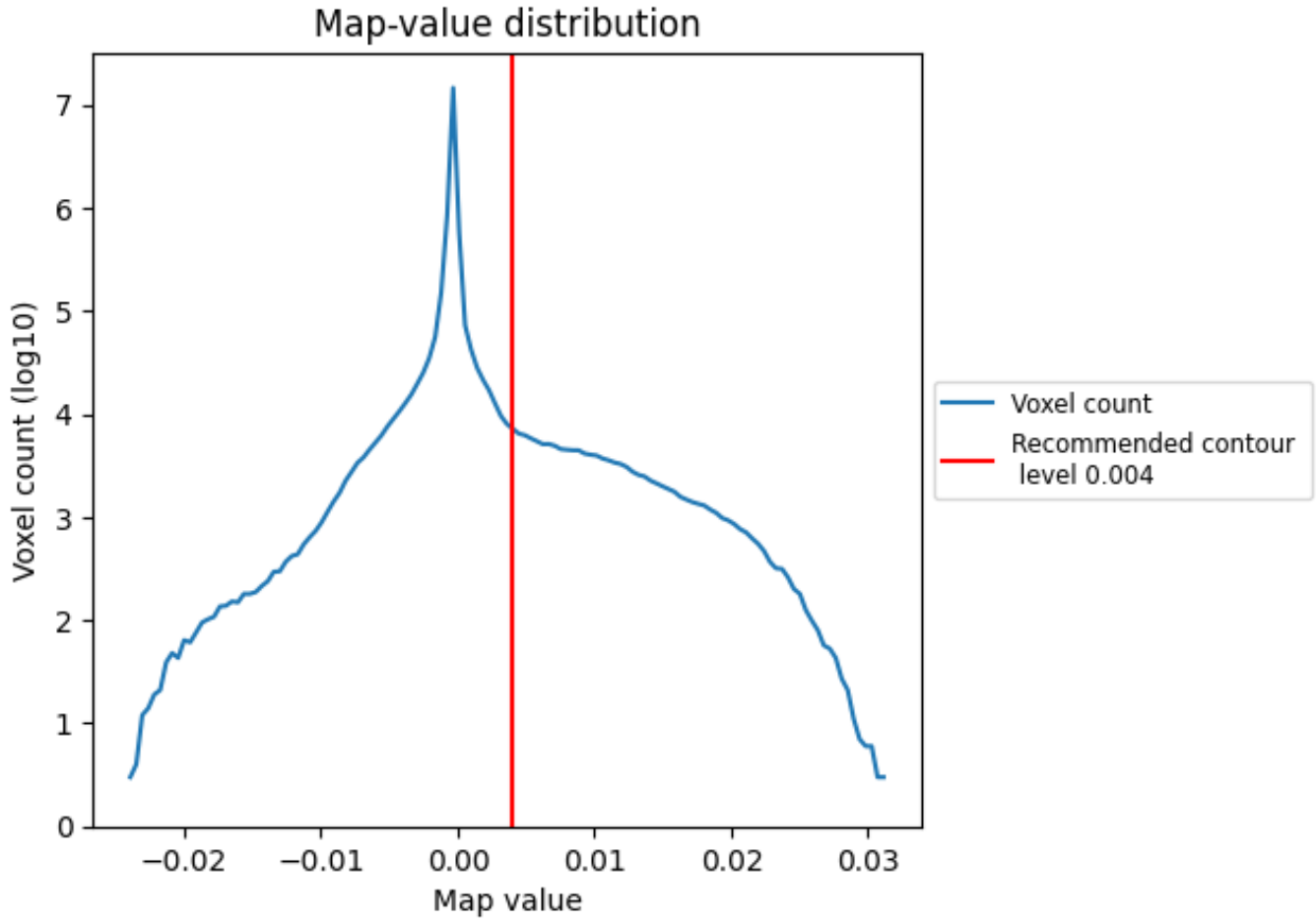
6.5 Mask visualisation (i)

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

7 Map analysis

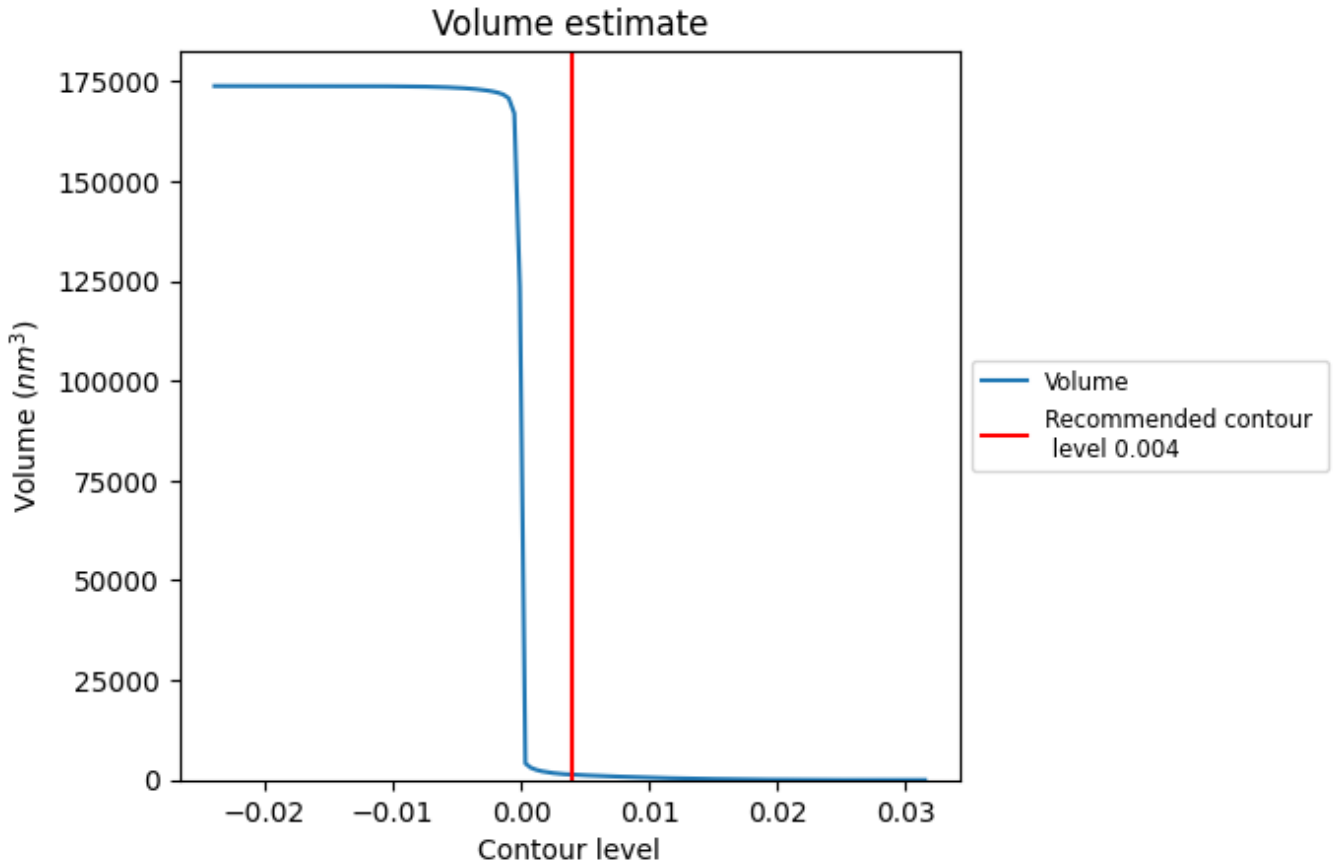
This section contains the results of statistical analysis of the map.

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.

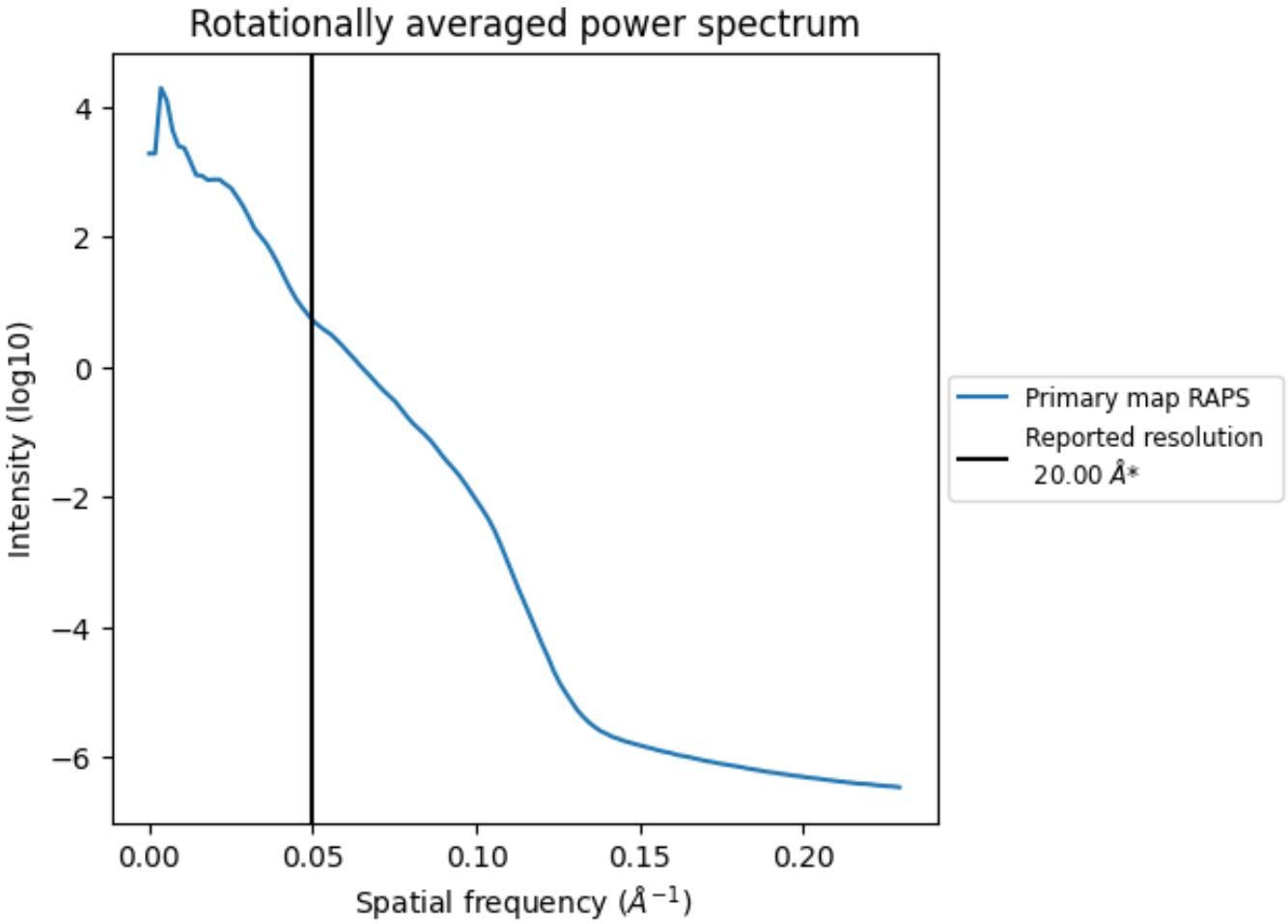
7.2 Volume estimate



The volume at the recommended contour level is 1341 nm^3; this corresponds to an approximate mass of 1211 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 0.050 Å^{-1}

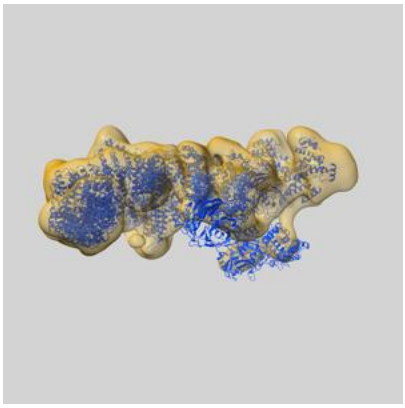
8 Fourier-Shell correlation

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

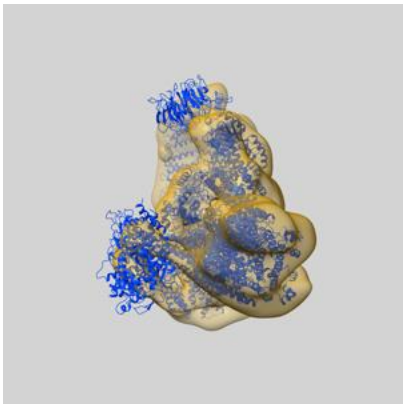
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10446 and PDB model 6TBM. Per-residue inclusion information can be found in section 3 on page 9.

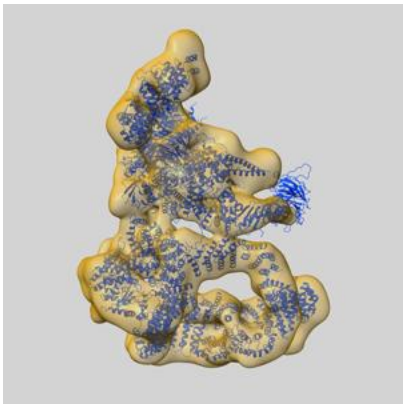
9.1 Map-model overlay



X



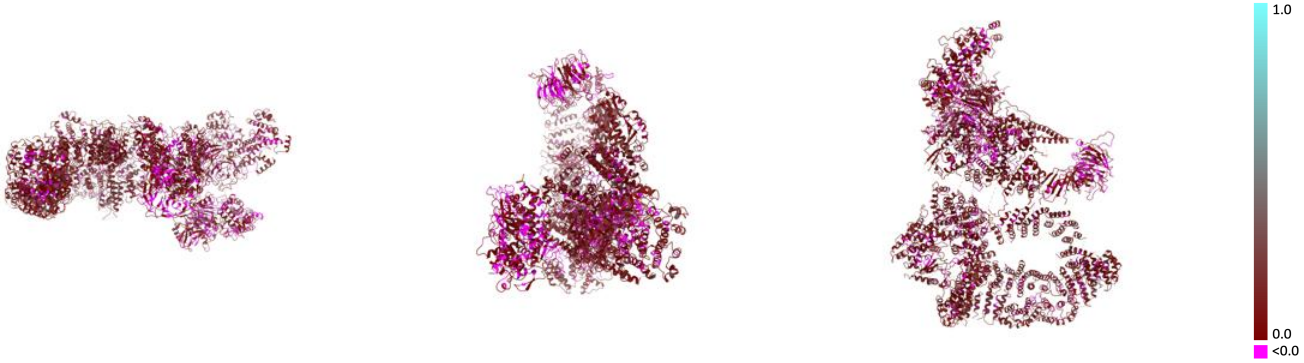
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.004 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.

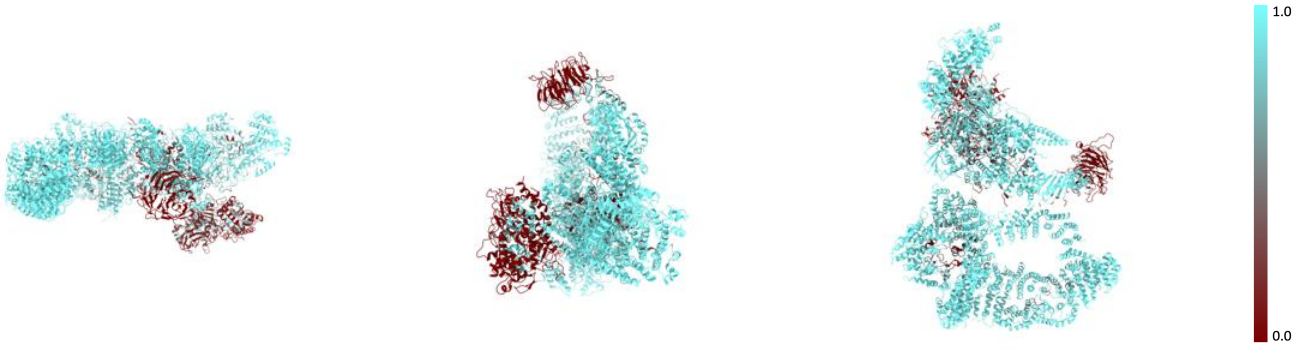
9.2 Q-score mapped to coordinate model (i)



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.

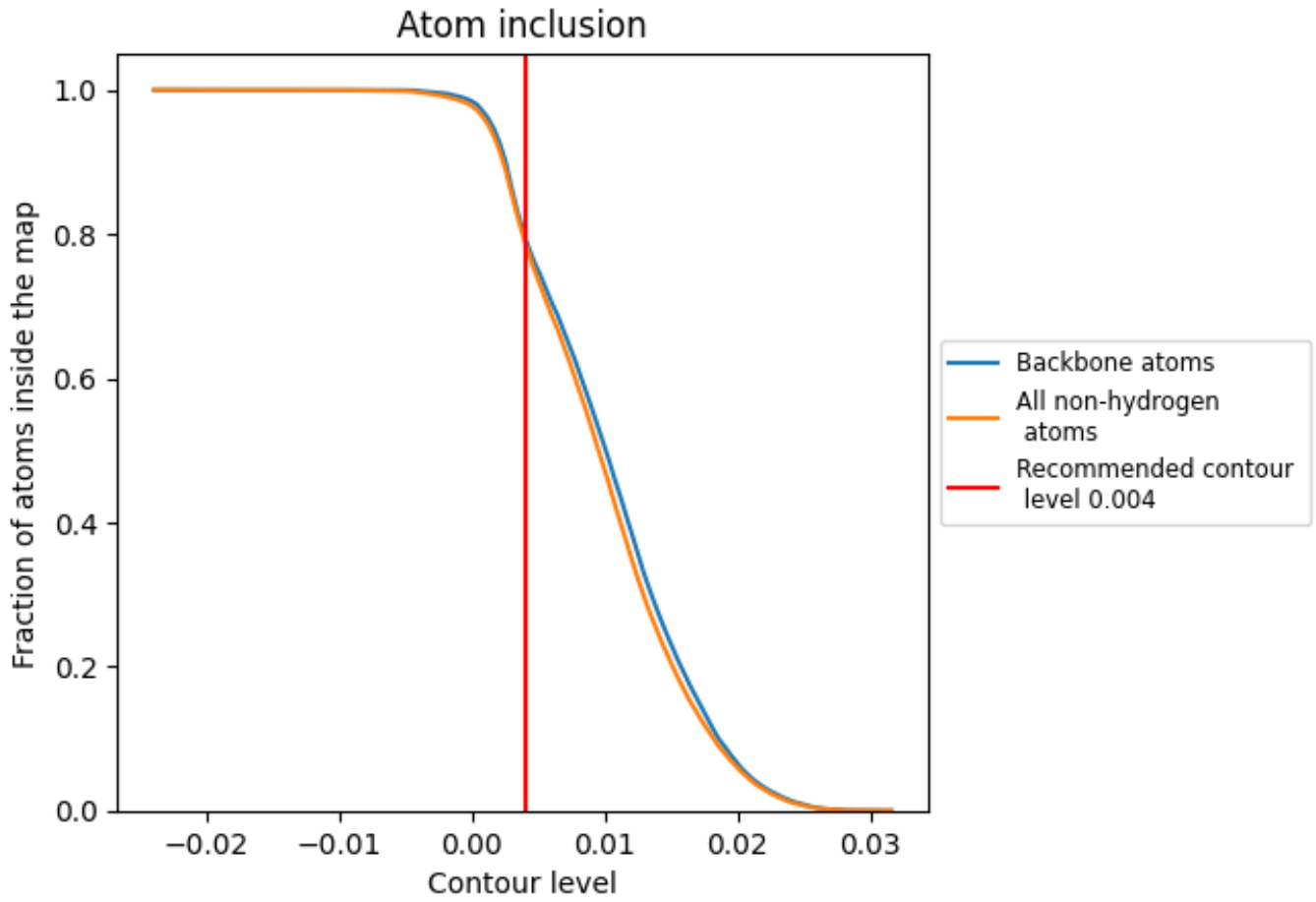
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.004).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 79% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7876	0.0800
A	0.7335	0.0550
B	1.0000	0.1030
C	0.5899	0.0520
D	0.8776	0.0850
E	0.9844	0.1110
F	0.8987	0.0920
G	0.8956	0.0740
H	0.9007	0.0800
I	0.8677	0.0710
J	0.9483	0.0730
K	0.8178	0.0500
L	0.9283	0.1010
M	0.8061	0.0760
N	0.0382	0.0210
O	0.1702	0.0130
P	0.2190	0.0410
Q	0.2215	0.0270
R	0.3801	0.0620