Full wwPDB EM Validation Report ⓘ

Dec 12, 2022 – 02:34 am GMT

PDB ID	:	6TNT
EMDB ID	:	EMD-10536
Title	:	SUMOylated apoAPC/C with repositioned APC2 WHB domain
Authors	:	Barford, D.; Yatskevich, S.
Deposited on	:	2019-12-10
Resolution	:	3.78 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:

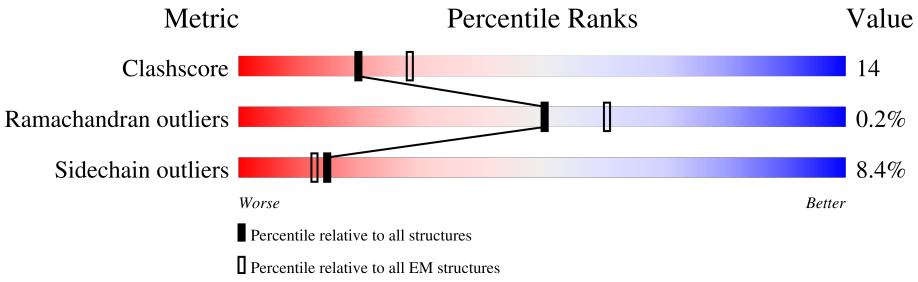
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.78 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1944	52% 26% 19%
2	B	84	81% 67% 29%
3	C	597	63% 22% 12%
3	P	597	5% 61% 20% 18%
4	D	121	33% 12% 55%
5	E	110	35% 15% 49%
6	F	824	37% 17% 44%
6	H	824	41% 16% 41%

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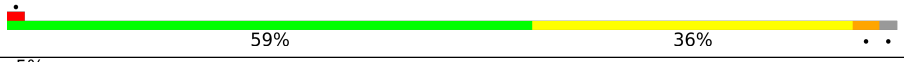
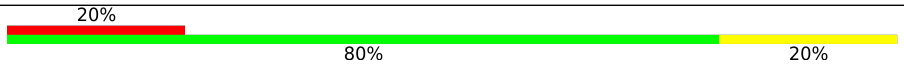
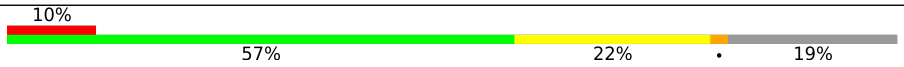
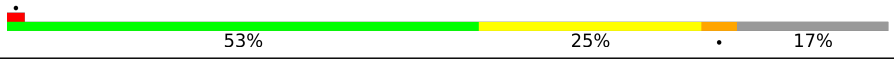
Mol	Chain	Length	Quality of chain
7	G	85	
7	W	85	
8	I	808	
9	J	620	
9	K	620	
10	L	185	
11	M	74	
12	N	822	
13	O	755	
14	T	15	
15	X	599	
15	Y	599	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 63827 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 Anaphase-promoting complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1583	11990	7717	2035	2158	80	0	0

- Molecule 2 is a protein called Anaphase-promoting complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	84	649	416	117	99	17	1	0

- Molecule 3 is a protein called Cell division cycle protein 23 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	524	4306	2774	727	781	24	0	0
3	P	492	Total	C	N	O	S	0	0
			4046	2613	679	730	24		

- Molecule 4 is a protein called Anaphase-promoting complex subunit 15.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	55	436	277	73	86	0	0

- Molecule 5 is a protein called Anaphase-promoting complex subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	56	450	290	74	85	1	0	0

- Molecule 6 is a protein called Cell division cycle protein 27 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	460	Total	C	N	O	S	0	0
			3618	2320	608	666	24		
6	H	488	Total	C	N	O	S	0	0
			3879	2489	655	709	26		

- Molecule 7 is a protein called Anaphase-promoting complex subunit CDC26.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	25	Total	C	N	O	S	0	0
			220	137	41	41	1		
7	W	26	Total	C	N	O	S	0	0
			218	136	41	40	1		

- Molecule 8 is a protein called Anaphase-promoting complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	723	Total	C	N	O	S	0	0
			5634	3619	940	1041	34		

- Molecule 9 is a protein called Cell division cycle protein 16 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	504	Total	C	N	O	S	0	0
			4053	2604	687	737	25		
9	K	493	Total	C	N	O	S	0	0
			3988	2564	672	728	24		

- Molecule 10 is a protein called Anaphase-promoting complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	182	Total	C	N	O	S	0	0
			1435	898	263	268	6		

- Molecule 11 is a protein called Anaphase-promoting complex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	59	Total	C	N	O	S	0	0
			481	304	79	96	2		

- Molecule 12 is a protein called Anaphase-promoting complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	672	Total	C	N	O	S	0	0
			5313	3409	941	938	25		

- Molecule 13 is a protein called Anaphase-promoting complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	688	Total	C	N	O	S	0	0
			5400	3443	940	989	28		

- Molecule 14 is a protein called UNIDENTIFIED PEPTIDE.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	T	15	Total	C	N	O	0	0
			79	47	16	16		

- Molecule 15 is a protein called Anaphase-promoting complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	484	Total	C	N	O	S	0	0
			3767	2390	649	704	24		
15	Y	496	Total	C	N	O	S	0	0
			3862	2446	666	724	26		

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

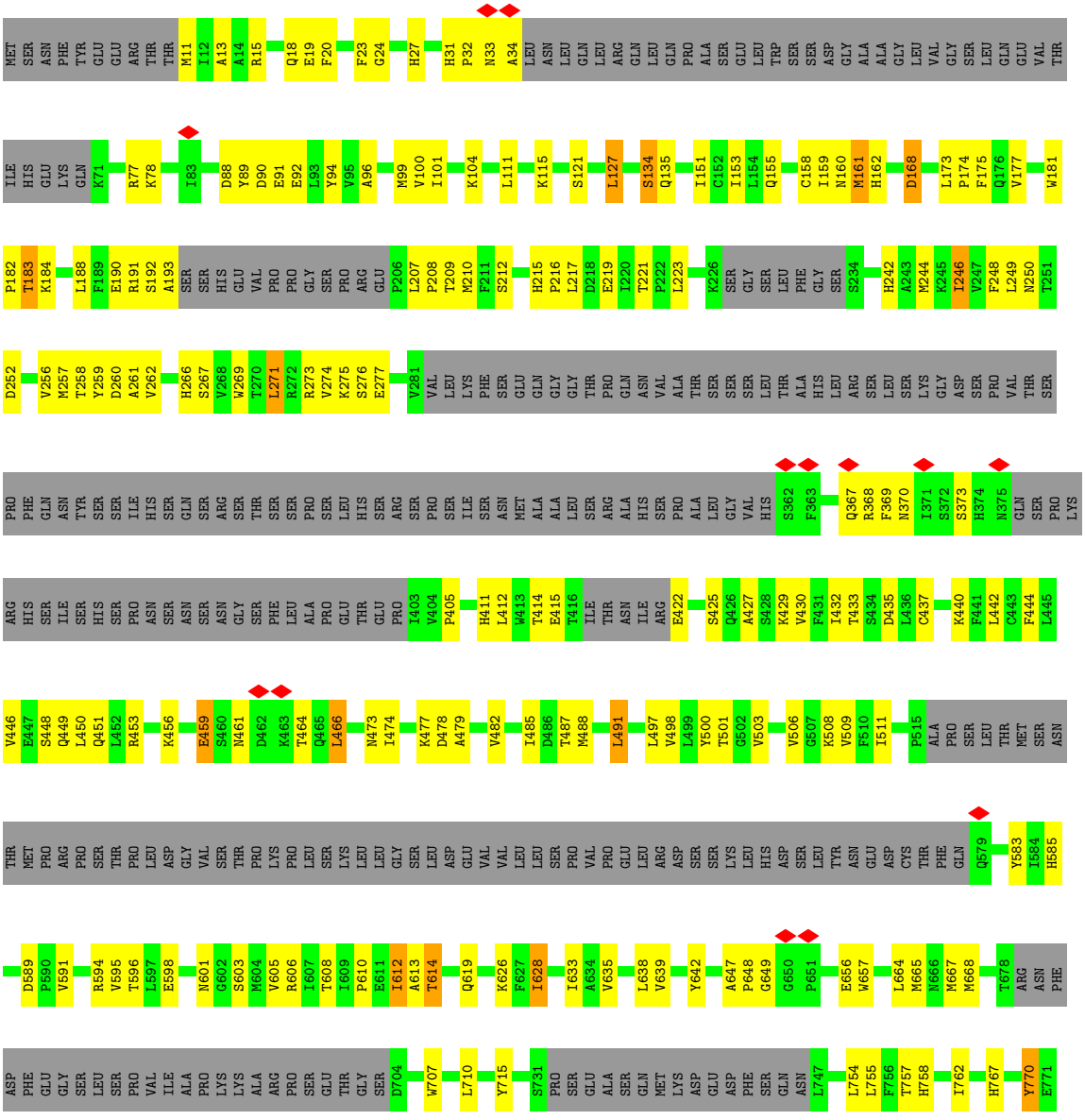
Mol	Chain	Residues	Atoms		AltConf
16	B	3	Total	Zn	0
			3	3	

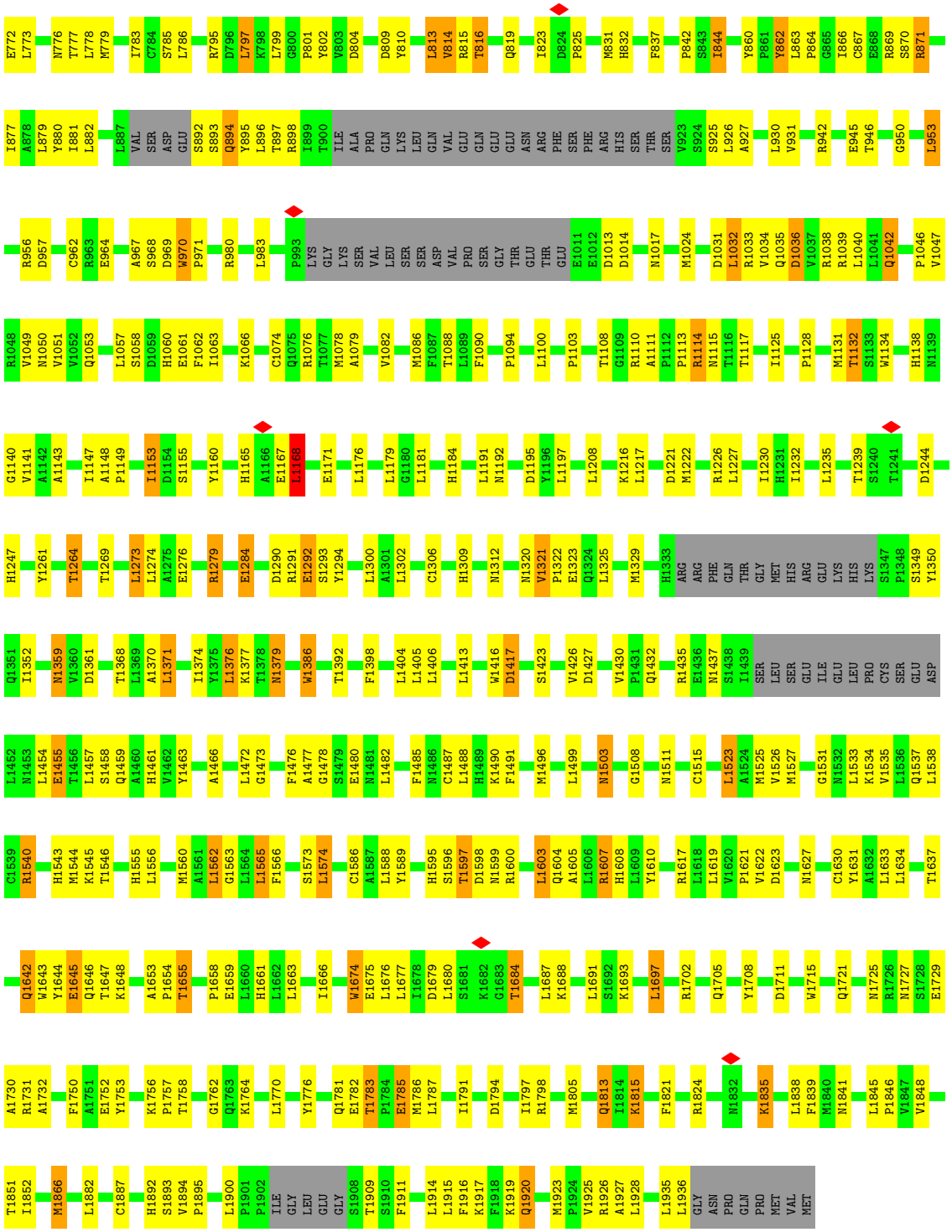
3 Residue-property plots (i)

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: Anaphase-promoting complex subunit 1

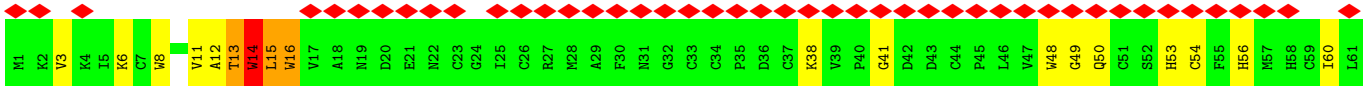
Chain A:





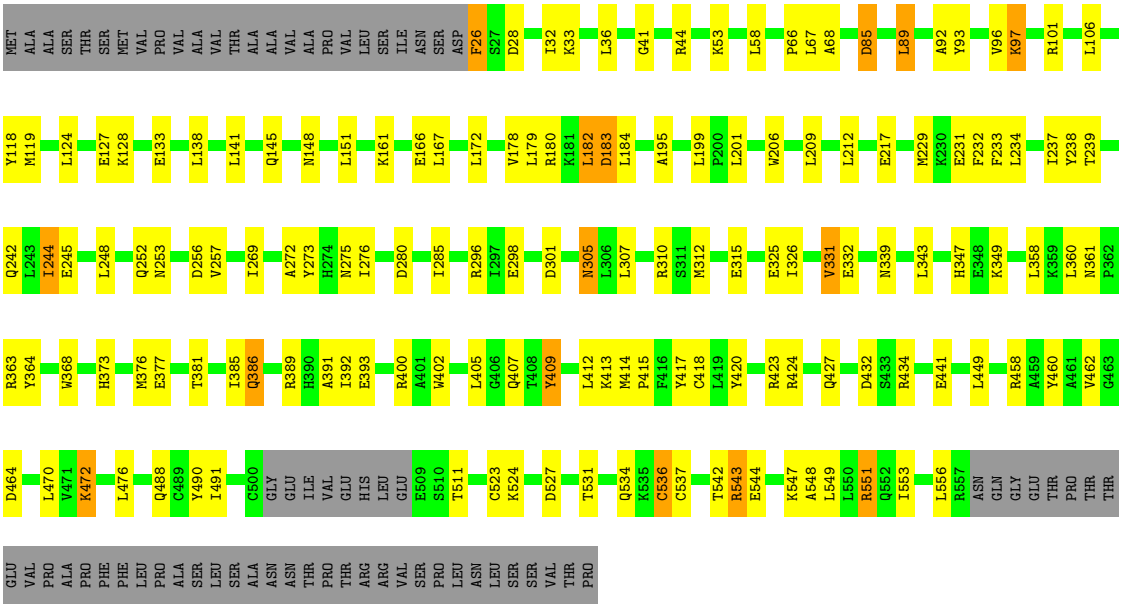
• Molecule 2: Anaphase-promoting complex subunit 11

Chain B:



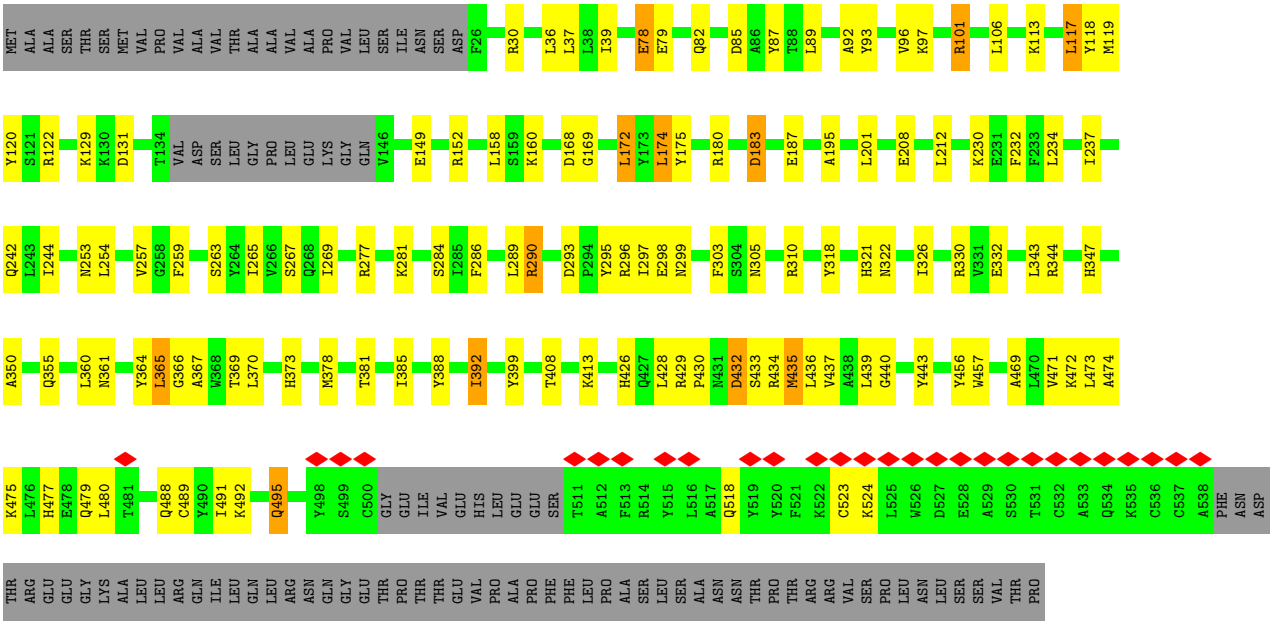
• Molecule 3: Cell division cycle protein 23 homolog

Chain C:



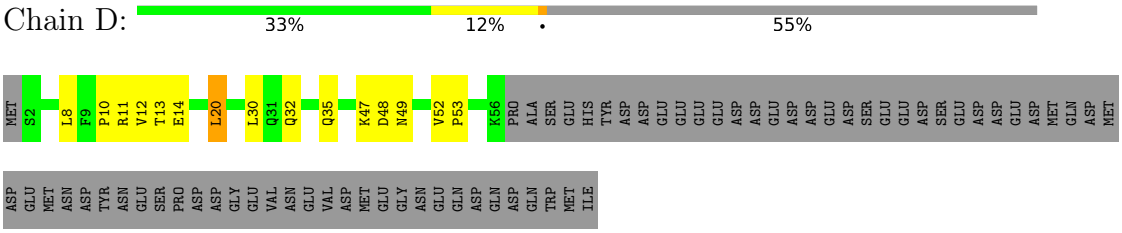
• Molecule 3: Cell division cycle protein 23 homolog

Chain P:



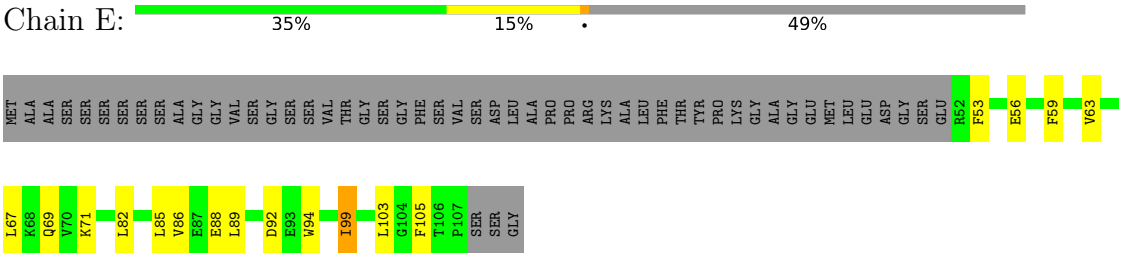
• Molecule 4: Anaphase-promoting complex subunit 15

Chain D:



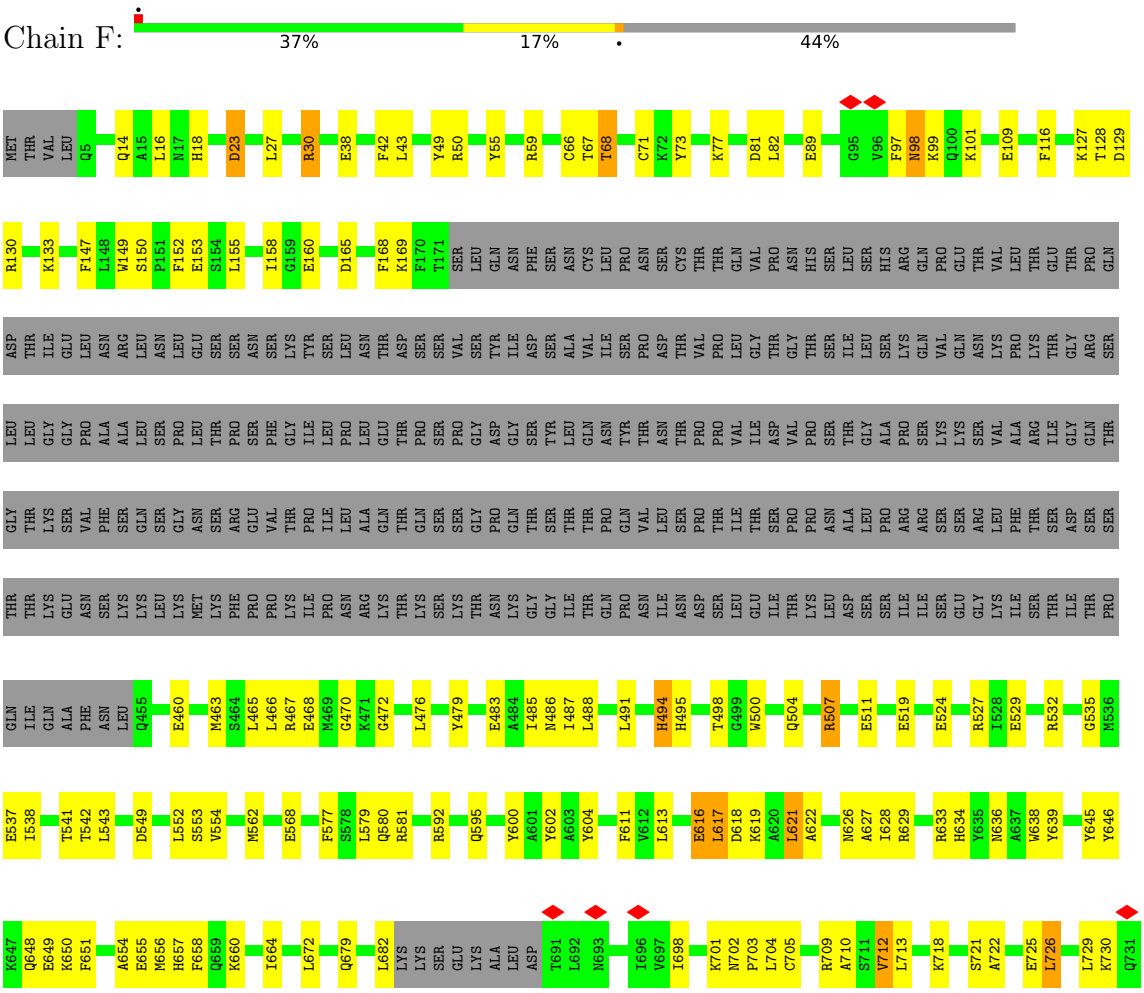
• Molecule 5: Anaphase-promoting complex subunit 16

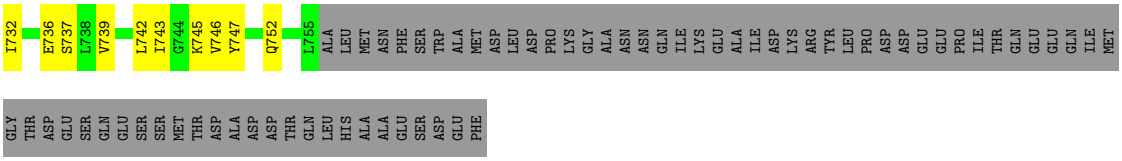
Chain E:



• Molecule 6: Cell division cycle protein 27 homolog

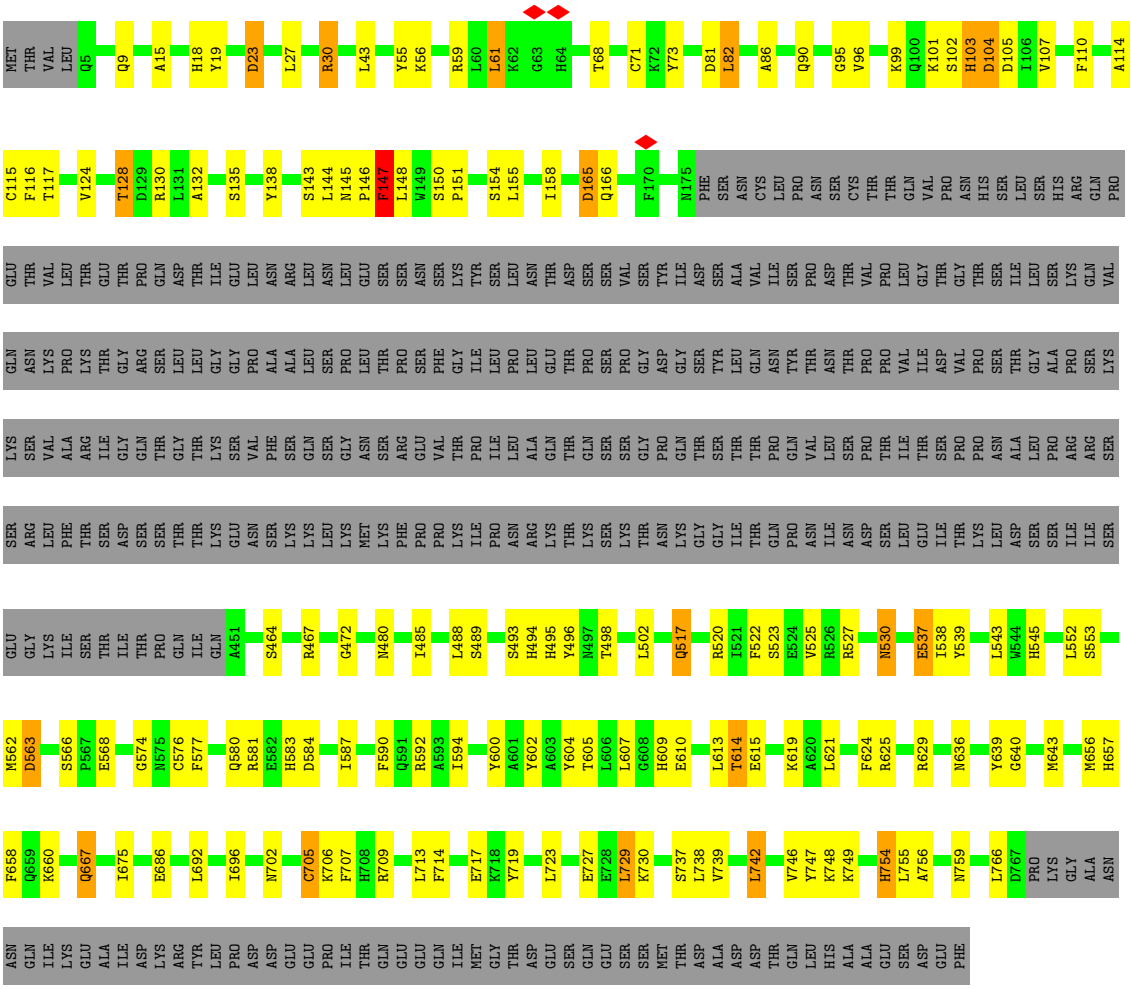
Chain F:





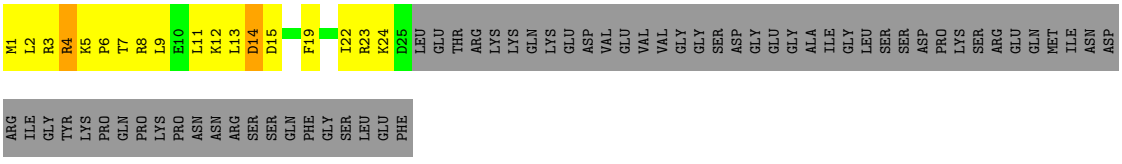
• Molecule 6: Cell division cycle protein 27 homolog

Chain H: 41% 16% 41%



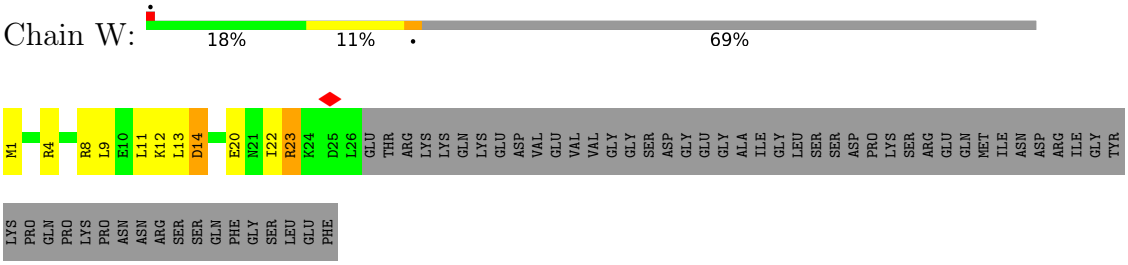
• Molecule 7: Anaphase-promoting complex subunit CDC26

Chain G: 8% 19% 71%



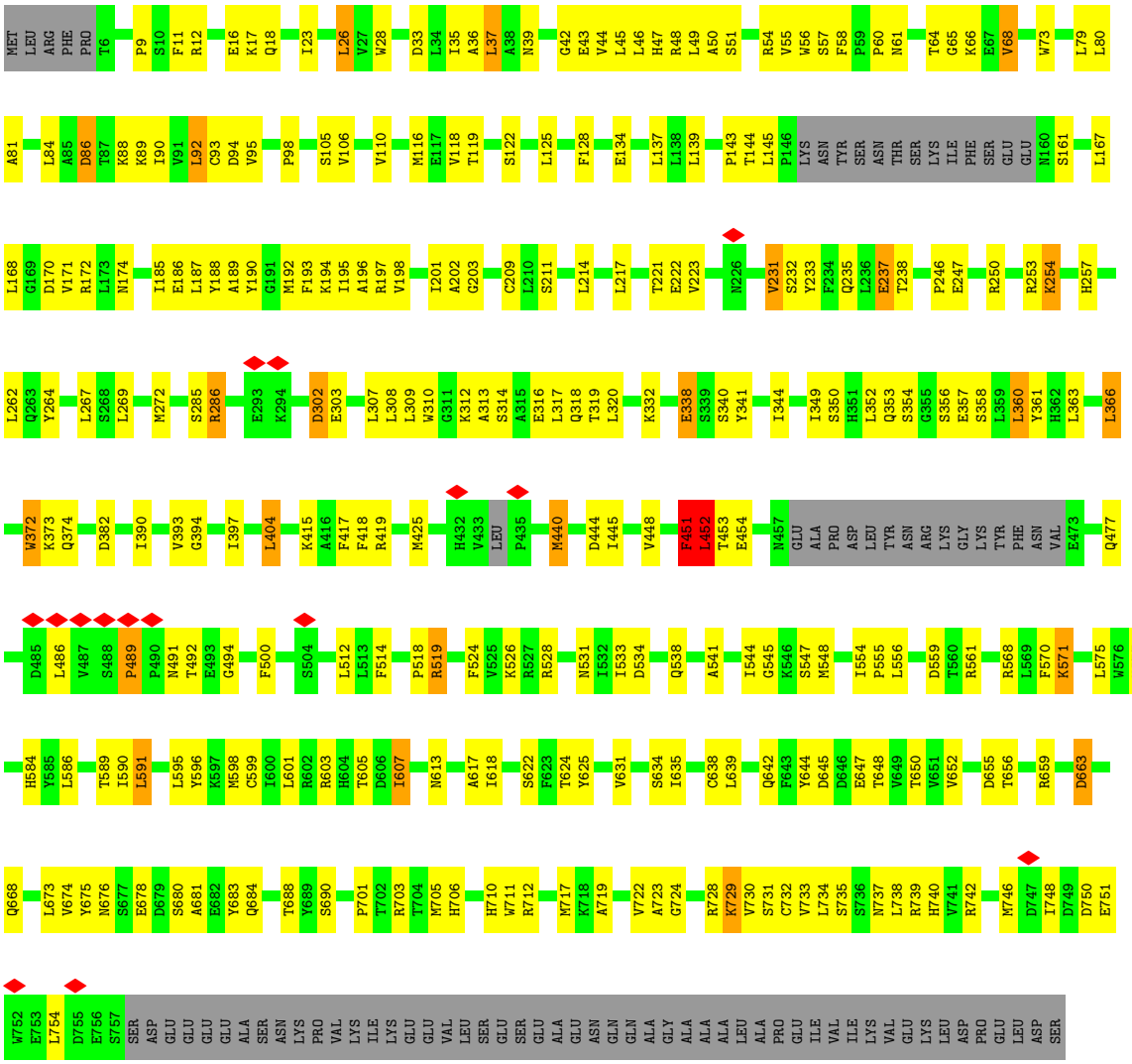
• Molecule 7: Anaphase-promoting complex subunit CDC26

Chain W:



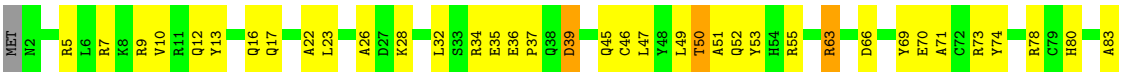
• Molecule 8: Anaphase-promoting complex subunit 4

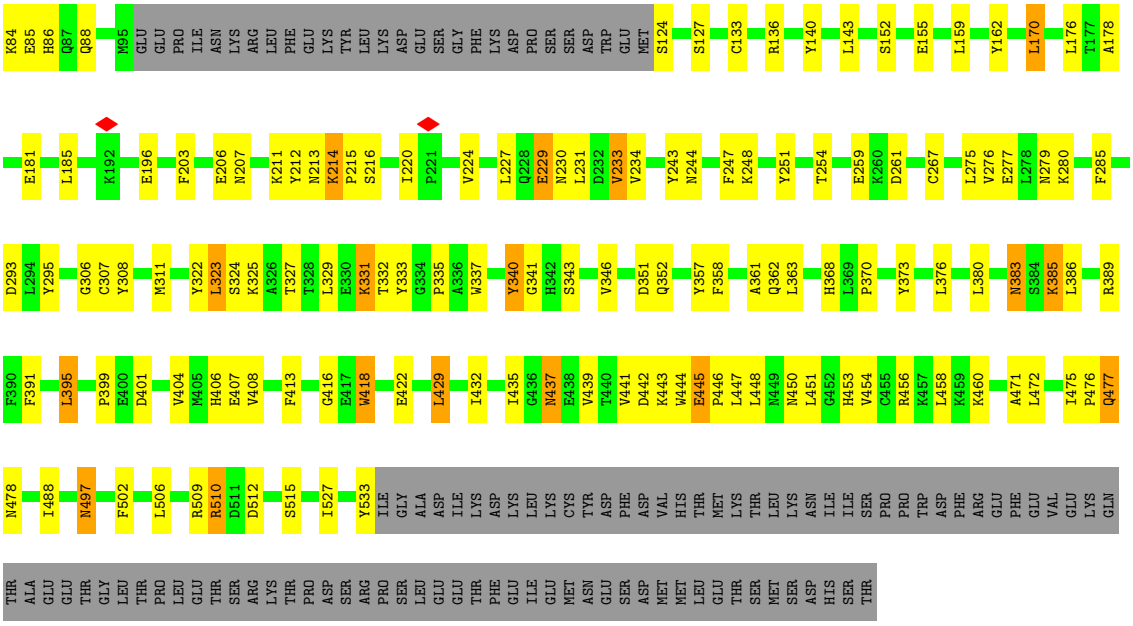
Chain I:



• Molecule 9: Cell division cycle protein 16 homolog

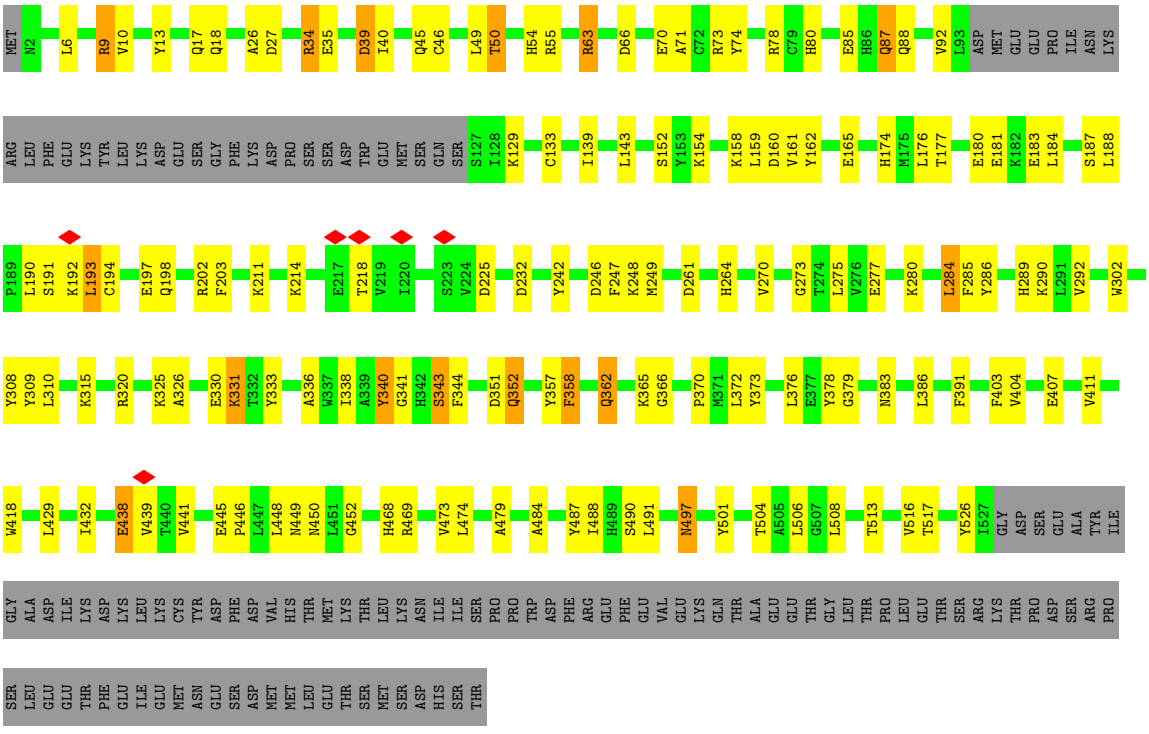
Chain J:





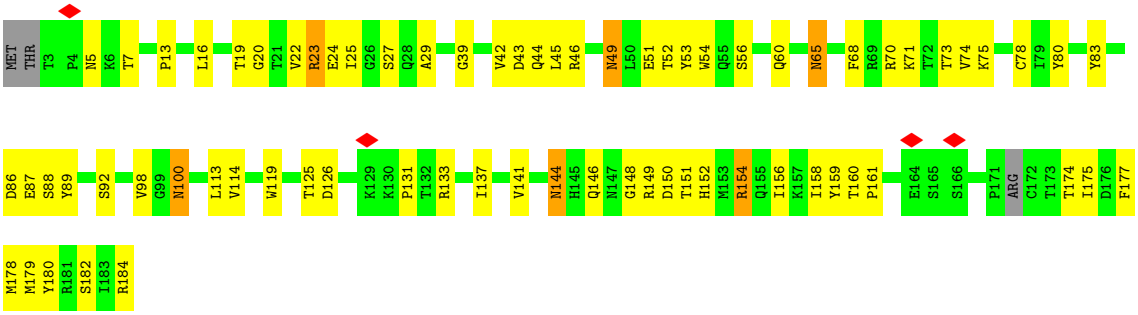
• Molecule 9: Cell division cycle protein 16 homolog

Chain K:



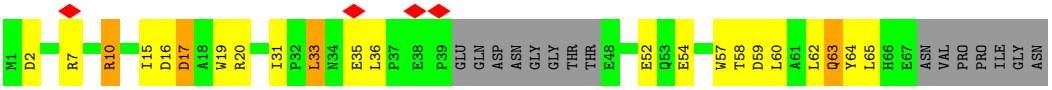
• Molecule 10: Anaphase-promoting complex subunit 10

Chain L:



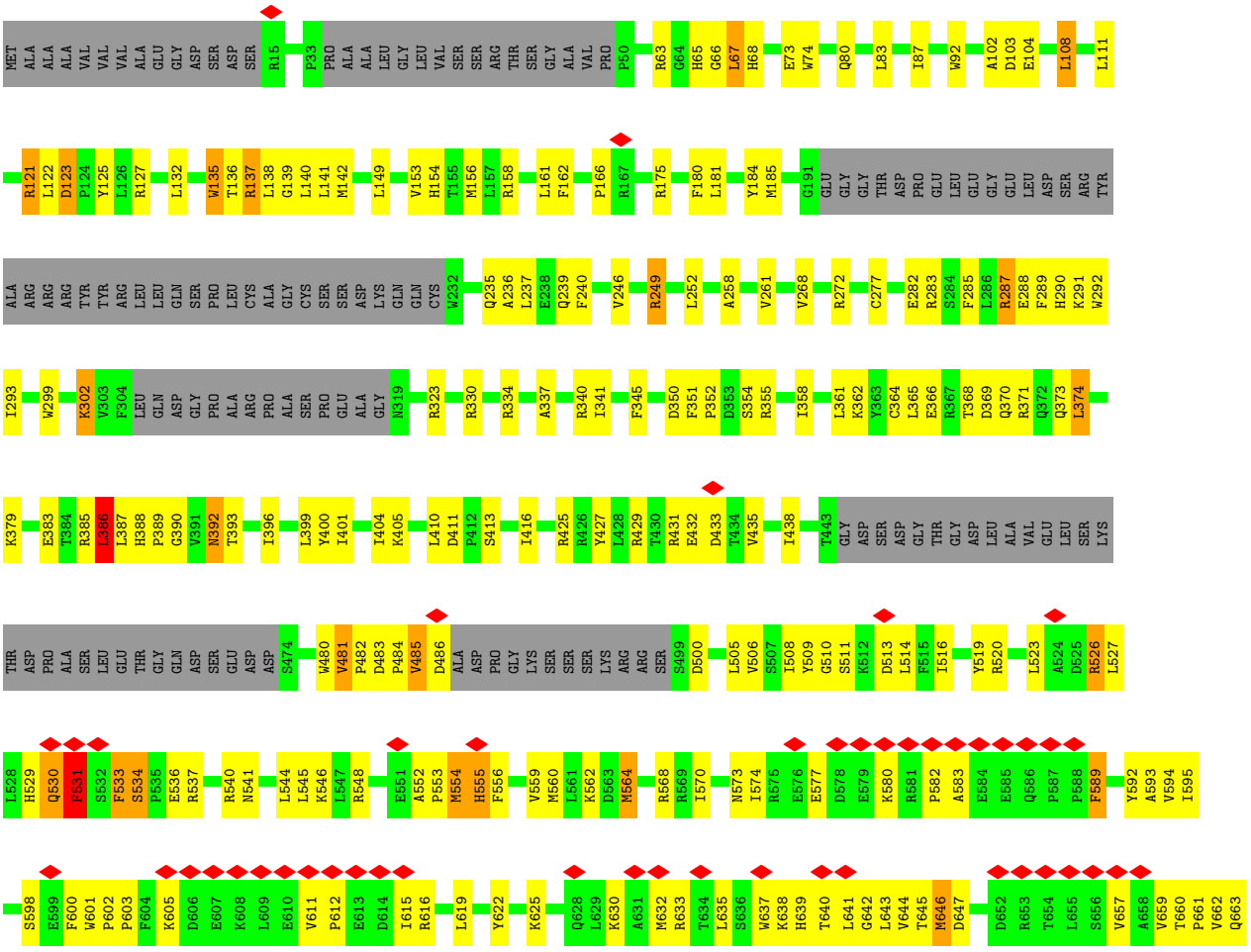
• Molecule 11: Anaphase-promoting complex subunit 13

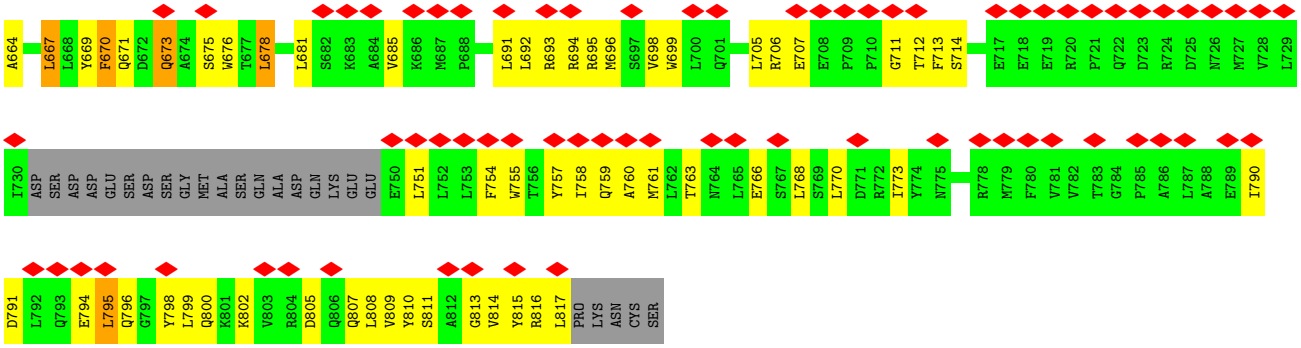
Chain M:



• Molecule 12: Anaphase-promoting complex subunit 2

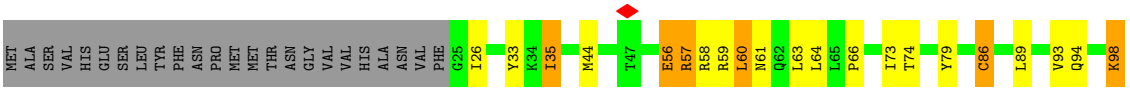
Chain N:

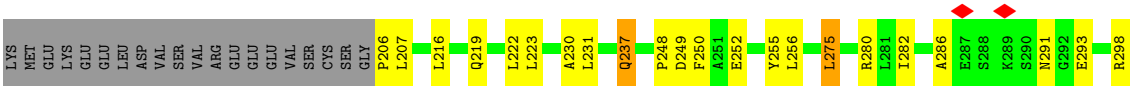


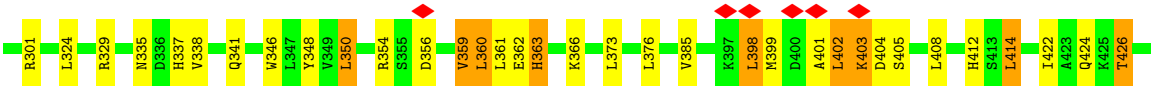


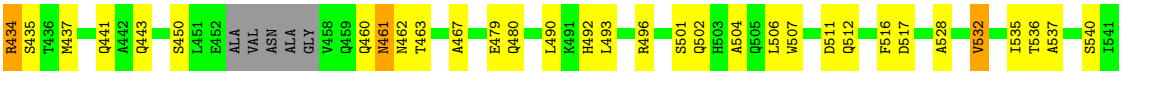
• Molecule 13: Anaphase-promoting complex subunit 5

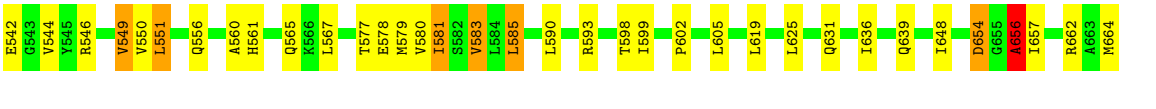
Chain O:

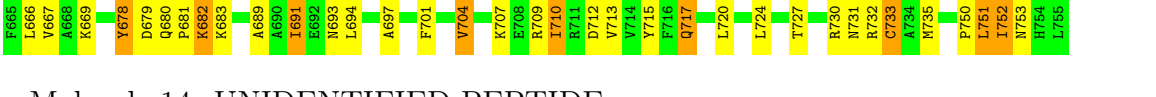










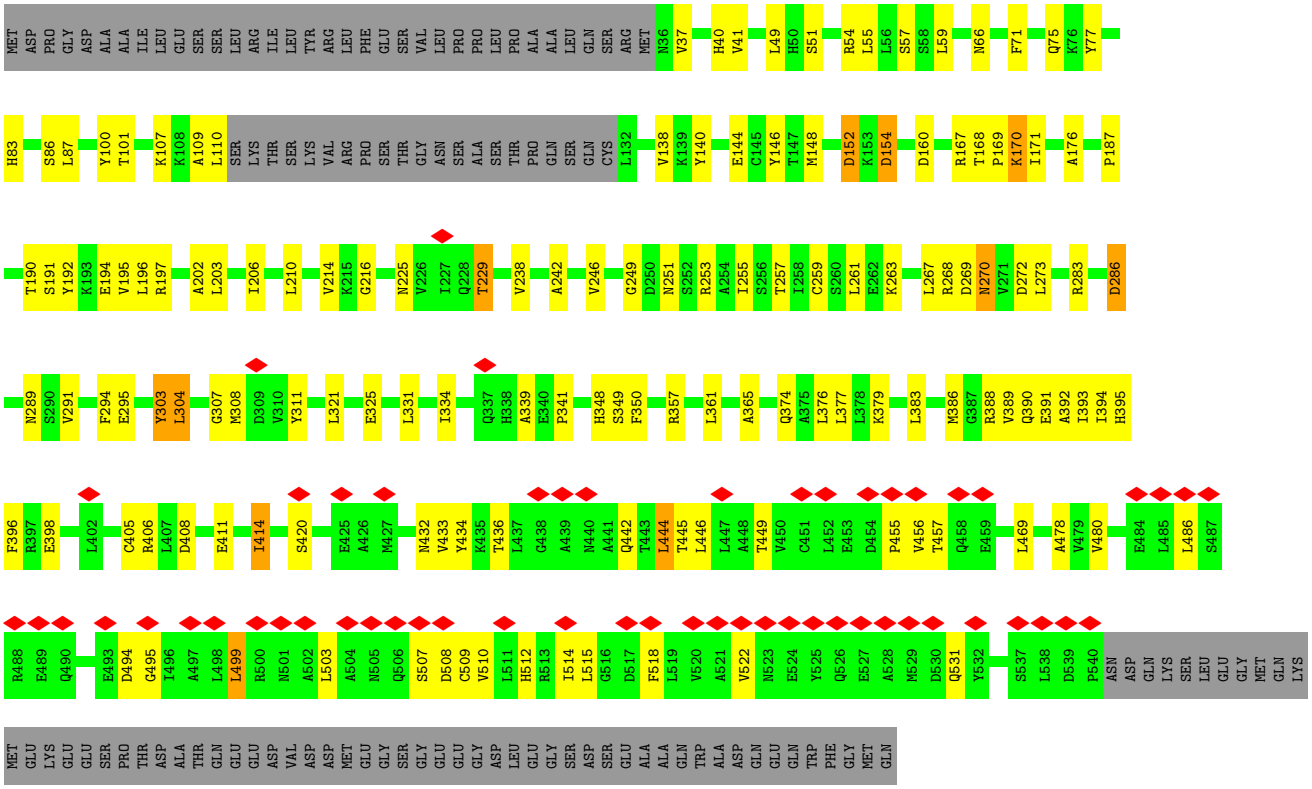


• Molecule 14: UNIDENTIFIED PEPTIDE

Chain T:

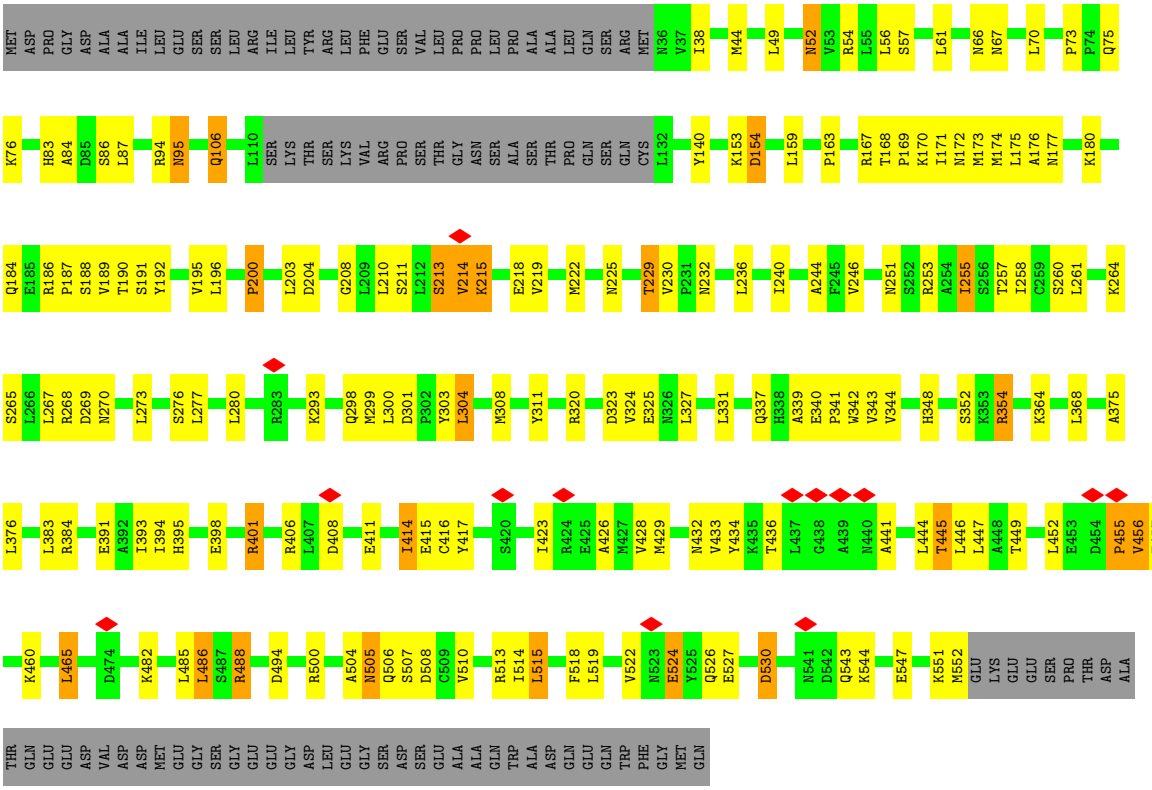
• Molecule 15: Anaphase-promoting complex subunit 7

Chain X:



• Molecule 15: Anaphase-promoting complex subunit 7

Chain Y:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	137954	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 ($e^-/Å^2$)	0.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.060	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0117	Depositor
Map size (Å)	366.73, 366.73, 366.73	wwPDB
Map dimensions	338, 338, 338	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.085, 1.085, 1.085	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.33	0/12269	0.47	2/16722 (0.0%)
2	B	0.25	0/674	0.41	0/913
3	C	0.36	0/4404	0.43	0/5945
3	P	0.31	0/4141	0.41	0/5593
4	D	0.32	0/446	0.44	0/610
5	E	0.30	0/459	0.38	0/619
6	F	0.30	0/3704	0.38	0/5019
6	H	0.33	0/3969	0.42	0/5366
7	G	0.29	0/221	0.49	0/292
7	W	0.26	0/219	0.47	0/291
8	I	0.30	0/5754	0.45	1/7806 (0.0%)
9	J	0.31	0/4152	0.43	0/5623
9	K	0.31	0/4086	0.39	0/5533
10	L	0.31	0/1468	0.46	0/1993
11	M	0.30	0/490	0.47	0/665
12	N	0.27	0/5417	0.45	2/7341 (0.0%)
13	O	0.33	0/5499	0.45	0/7432
14	T	0.31	0/78	0.63	0/107
15	X	0.26	0/3827	0.40	0/5180
15	Y	0.26	0/3922	0.40	0/5304
All	All	0.31	0/65199	0.43	5/88354 (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	A	0	1
2	B	0	1
8	I	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
9	K	0	1
13	O	0	3
15	Y	0	1
All	All	0	8

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	N	121	ARG	C-N-CA	6.95	139.07	121.70
1	A	1168	LEU	CA-CB-CG	5.33	127.56	115.30
1	A	1032	LEU	CA-CB-CG	5.26	127.41	115.30
8	I	489	PRO	C-N-CD	-5.12	109.34	120.60
12	N	386	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1455	GLU	Peptide
2	B	14	TRP	Peptide
8	I	451	PHE	Peptide
9	K	87	GLN	Peptide
13	O	129	THR	Peptide
13	O	130	SER	Peptide
13	O	656	ALA	Peptide
15	Y	455	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11990	0	11648	365	0
2	B	649	0	598	29	0
3	C	4306	0	4275	105	0
3	P	4046	0	3998	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	436	0	396	14	0
5	E	450	0	435	11	0
6	F	3618	0	3452	109	0
6	H	3879	0	3805	112	0
7	G	220	0	233	14	0
7	W	218	0	222	15	0
8	I	5634	0	5527	181	0
9	J	4053	0	3960	124	0
9	K	3988	0	3913	103	0
10	L	1435	0	1382	57	0
11	M	481	0	457	18	0
12	N	5313	0	5240	205	0
13	O	5400	0	5418	143	0
14	T	79	0	77	3	0
15	X	3767	0	3820	102	0
15	Y	3862	0	3915	124	0
16	B	3	0	0	0	0
All	All	63827	0	62771	1755	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 14.

All (1755) 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)
10:L:89:TYR:HE2	10:L:150:ASP:CG	1.30	1.35
10:L:89:TYR:HE2	10:L:150:ASP:OD2	1.09	1.31
10:L:89:TYR:CE2	10:L:150:ASP:CG	2.12	1.22
10:L:89:TYR:CE2	10:L:150:ASP:OD2	1.95	1.20
10:L:89:TYR:CE2	10:L:150:ASP:OD1	2.02	1.12
12:N:121:ARG:HB3	12:N:122:LEU:HB2	1.32	1.05
6:H:101:LYS:O	6:H:105:ASP:HB3	1.61	0.99
1:A:1914:LEU:HD11	1:A:1936:LEU:HD21	1.59	0.82
6:H:102:SER:O	6:H:105:ASP:N	2.13	0.81
13:O:581:ILE:HD11	13:O:619:LEU:HB3	1.61	0.81
12:N:509:TYR:HB2	12:N:510:GLY:HA2	1.62	0.80
8:I:303:GLU:HB3	8:I:317:LEU:HD22	1.63	0.80
12:N:766:GLU:HA	12:N:768:LEU:H	1.43	0.79
10:L:89:TYR:CD2	10:L:150:ASP:OD1	2.35	0.79
6:H:90:GLN:HA	6:H:95:GLY:H	1.48	0.78
8:I:719:ALA:HA	8:I:735:SER:HA	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:406:HIS:HE1	9:J:450:ASN:HD22	1.27	0.78
1:A:1909:THR:H	1:A:1936:LEU:HD22	1.47	0.78
6:H:696:ILE:HG12	6:H:705:CYS:HB3	1.67	0.77
13:O:291:ASN:O	13:O:298:ARG:NH2	2.19	0.76
6:F:23:ASP:N	6:F:23:ASP:OD1	2.14	0.76
2:B:12:ALA:H	12:N:594:VAL:HG12	1.51	0.75
12:N:574:ILE:HG13	12:N:625:LYS:HZ2	1.50	0.75
4:D:52:VAL:O	9:J:510:ARG:NH2	2.17	0.75
12:N:640:THR:HG23	12:N:641:LEU:HG	1.67	0.75
3:C:361:ASN:HD22	3:C:363:ARG:H	1.35	0.74
1:A:657:TRP:NE1	1:A:785:SER:OG	2.20	0.74
8:I:26:LEU:HB3	8:I:37:LEU:HB3	1.70	0.74
8:I:723:ALA:HB3	8:I:732:CYS:HB3	1.70	0.73
9:K:479:ALA:HB2	9:K:508:LEU:HB2	1.70	0.73
4:D:47:LYS:HE3	3:P:355:GLN:HE22	1.53	0.73
9:K:232:ASP:OD1	9:K:264:HIS:NE2	2.22	0.73
9:K:309:TYR:OH	11:M:59:ASP:OD2	2.06	0.73
1:A:1643:TRP:HB3	14:T:3:ALA:H	1.53	0.72
2:B:63:TRP:NE1	2:B:72:HIS:O	2.22	0.72
1:A:1329:MET:HE2	1:A:1368:THR:HA	1.71	0.72
12:N:523:LEU:HA	12:N:526:ARG:HD3	1.71	0.72
1:A:950:GLY:H	1:A:1813:GLN:HG3	1.55	0.72
6:F:128:THR:HG21	6:F:130:ARG:HH21	1.54	0.72
3:C:381:THR:HG21	3:C:412:LEU:HD21	1.72	0.71
9:J:497:ASN:OD1	9:J:497:ASN:N	2.20	0.71
13:O:435:SER:HB3	13:O:654:ASP:HB3	1.72	0.71
6:F:698:ILE:O	6:F:702:ASN:N	2.20	0.71
10:L:60:GLN:NE2	10:L:149:ARG:O	2.23	0.71
13:O:216:LEU:HD22	13:O:256:LEU:HD12	1.71	0.71
3:C:85:ASP:OD1	3:C:85:ASP:N	2.20	0.71
6:F:710:ALA:HB2	6:F:725:GLU:HG2	1.71	0.71
13:O:130:SER:HB2	13:O:133:GLY:H	1.55	0.71
2:B:15:LEU:HD21	12:N:635:LEU:HA	1.72	0.71
1:A:1866:MET:SD	1:A:1866:MET:N	2.60	0.70
12:N:707:GLU:HB3	12:N:712:THR:HB	1.74	0.70
10:L:174:THR:O	10:L:177:PHE:N	2.23	0.70
1:A:810:TYR:HB3	1:A:813:LEU:HD11	1.74	0.70
3:C:301:ASP:OD2	3:C:364:TYR:OH	2.10	0.70
6:H:527:ARG:NH1	15:Y:303:TYR:OH	2.25	0.70
12:N:121:ARG:CB	12:N:122:LEU:HB2	2.18	0.70
8:I:680:SER:O	8:I:684:GLN:NE2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:461:ASN:HD22	13:O:462:ASN:H	1.39	0.69
1:A:1128:PRO:HG2	1:A:1131:MET:HB2	1.75	0.69
1:A:1455:GLU:H	1:A:1458:SER:H	1.39	0.69
9:K:158:LYS:HG2	9:K:188:LEU:HA	1.75	0.69
15:X:303:TYR:HB3	15:X:334:ILE:HD12	1.75	0.69
9:J:23:LEU:HD11	9:J:47:LEU:HD23	1.75	0.69
9:K:46:CYS:O	9:K:50:THR:OG1	2.09	0.69
15:Y:225:ASN:O	15:Y:229:THR:OG1	2.09	0.69
13:O:679:ASP:HA	13:O:683:LYS:HD2	1.74	0.68
1:A:1599:ASN:HB2	1:A:1603:LEU:HA	1.76	0.68
8:I:12:ARG:NH1	8:I:751:GLU:OE1	2.27	0.68
13:O:61:ASN:HA	13:O:64:LEU:HD23	1.76	0.68
1:A:869:ARG:NH2	1:A:946:THR:OG1	2.27	0.68
1:A:1276:GLU:HG2	1:A:1294:TYR:HE1	1.58	0.68
6:F:97:PHE:HD2	6:F:99:LYS:HG3	1.59	0.68
13:O:701:PHE:HB3	13:O:710:ILE:HG22	1.74	0.68
1:A:1036:ASP:N	1:A:1036:ASP:OD1	2.24	0.68
6:F:155:LEU:HG	6:F:160:GLU:HB2	1.74	0.68
13:O:654:ASP:N	13:O:654:ASP:OD1	2.26	0.68
12:N:560:MET:SD	12:N:601:TRP:NE1	2.66	0.68
12:N:706:ARG:HB3	12:N:714:SER:HB2	1.74	0.68
1:A:956:ARG:NH1	1:A:1785:GLU:OE2	2.27	0.68
9:J:406:HIS:CE1	9:J:450:ASN:HD22	2.11	0.68
6:F:14:GLN:O	6:F:18:HIS:ND1	2.21	0.67
15:X:225:ASN:O	15:X:229:THR:OG1	2.11	0.67
15:Y:176:ALA:HB2	15:Y:191:SER:HB2	1.76	0.67
1:A:258:THR:OG1	1:A:269:TRP:NE1	2.27	0.67
15:Y:434:TYR:HA	15:Y:444:LEU:HD13	1.76	0.67
6:H:128:THR:HG21	9:K:473:VAL:HG22	1.76	0.67
9:J:456:ARG:HD3	9:J:488:ILE:HG22	1.77	0.67
8:I:93:CYS:SG	8:I:94:ASP:N	2.68	0.67
12:N:411:ASP:O	12:N:413:SER:N	2.24	0.67
7:G:6:PRO:HB3	9:J:406:HIS:CD2	2.30	0.67
10:L:39:GLY:O	10:L:44:GLN:NE2	2.27	0.67
10:L:88:SER:HB2	10:L:148:GLY:HA3	1.75	0.67
6:F:73:TYR:OH	6:H:18:HIS:O	2.09	0.67
1:A:1039:ARG:O	1:A:1042:GLN:NE2	2.27	0.67
15:Y:376:LEU:HD21	15:Y:398:GLU:HG3	1.74	0.67
9:K:176:LEU:HB3	9:K:180:GLU:HB2	1.76	0.66
6:H:563:ASP:OD1	6:H:566:SER:OG	2.13	0.66
15:X:214:VAL:HG12	15:X:216:GLY:H	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:491:ASN:HD21	8:I:494:GLY:HA3	1.60	0.66
2:B:14:TRP:HE3	2:B:15:LEU:HB2	1.59	0.66
3:C:373:HIS:NE2	3:C:377:GLU:OE2	2.28	0.66
8:I:451:PHE:O	8:I:453:THR:N	2.28	0.66
9:J:46:CYS:O	9:J:50:THR:OG1	2.13	0.66
6:H:520:ARG:NH2	15:X:101:THR:OG1	2.29	0.66
9:J:215:PRO:HB2	9:J:435:ILE:HD11	1.77	0.66
15:X:331:LEU:HB3	15:X:341:PRO:HG3	1.77	0.66
3:C:385:ILE:HG23	3:C:405:LEU:HD11	1.78	0.66
15:Y:433:VAL:HA	15:Y:436:THR:HG22	1.76	0.66
15:Y:513:ARG:NH1	15:Y:547:GLU:OE1	2.27	0.66
1:A:1032:LEU:HD23	12:N:485:VAL:HG22	1.78	0.66
9:K:194:CYS:HB3	9:K:197:GLU:HG2	1.77	0.66
10:L:24:GLU:OE2	10:L:46:ARG:NH2	2.28	0.66
12:N:287:ARG:O	12:N:291:LYS:NZ	2.27	0.66
13:O:460:GLN:HE21	13:O:496:ARG:HH22	1.41	0.66
1:A:89:TYR:HB3	13:O:536:THR:HG23	1.77	0.66
3:P:432:ASP:OD1	3:P:432:ASP:N	2.28	0.66
8:I:625:TYR:OH	8:I:711:TRP:O	2.11	0.66
6:H:130:ARG:NH1	9:K:469:ARG:O	2.29	0.65
3:P:267:SER:OG	3:P:299:ASN:ND2	2.28	0.65
15:Y:210:LEU:HD22	15:Y:244:ALA:HB2	1.77	0.65
12:N:136:THR:HA	12:N:140:LEU:HB3	1.77	0.65
1:A:244:MET:N	1:A:244:MET:SD	2.69	0.65
10:L:16:LEU:O	10:L:19:THR:OG1	2.15	0.65
1:A:1149:PRO:O	1:A:1153:ILE:HB	1.96	0.65
1:A:1531:GLY:HA2	1:A:1565:LEU:HD22	1.77	0.65
1:A:77:ARG:NH2	1:A:91:GLU:OE2	2.28	0.65
1:A:1057:LEU:HD12	1:A:1061:GLU:HB3	1.79	0.65
1:A:1134:TRP:HD1	1:A:1597:THR:HA	1.62	0.65
3:P:373:HIS:ND1	3:P:388:TYR:OH	2.27	0.65
8:I:349:ILE:O	8:I:353:GLN:HB2	1.97	0.65
8:I:622:SER:H	8:I:706:HIS:HA	1.62	0.65
12:N:760:ALA:O	12:N:763:THR:OG1	2.13	0.65
13:O:461:ASN:O	13:O:462:ASN:ND2	2.30	0.65
1:A:191:ARG:NH1	1:A:208:PRO:O	2.30	0.64
1:A:1100:LEU:HG	1:A:1147:ILE:HD11	1.79	0.64
8:I:222:GLU:HB2	8:I:231:VAL:HG13	1.77	0.64
1:A:757:THR:OG1	1:A:758:HIS:N	2.29	0.64
1:A:1653:ALA:O	1:A:1655:THR:N	2.31	0.64
10:L:144:ASN:N	10:L:144:ASN:OD1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:X:455:PRO:O	15:X:457:THR:N	2.31	0.64
1:A:1417:ASP:OD1	1:A:1417:ASP:N	2.28	0.64
12:N:334:ARG:NH1	12:N:369:ASP:OD1	2.31	0.64
12:N:370:GLN:NE2	12:N:373:GLN:OE1	2.24	0.64
12:N:795:LEU:HA	12:N:798:TYR:HB3	1.79	0.64
3:P:435:MET:SD	3:P:435:MET:N	2.70	0.64
3:C:347:HIS:NE2	3:C:377:GLU:OE1	2.31	0.64
3:C:413:LYS:O	13:O:329:ARG:NH2	2.30	0.64
8:I:9:PRO:HG2	8:I:750:ASP:HB3	1.80	0.64
12:N:554:MET:N	12:N:554:MET:SD	2.69	0.64
6:H:495:HIS:O	6:H:498:THR:OG1	2.16	0.64
6:H:667:GLN:NE2	6:H:667:GLN:O	2.31	0.64
6:H:696:ILE:HD13	6:H:706:LYS:HG3	1.80	0.63
12:N:802:LYS:HD3	12:N:805:ASP:HB3	1.80	0.63
12:N:379:LYS:NZ	12:N:383:GLU:OE2	2.27	0.63
12:N:580:LYS:HB3	12:N:582:PRO:HD2	1.79	0.63
9:J:39:ASP:N	9:J:39:ASP:OD1	2.31	0.63
1:A:1279:ARG:O	1:A:1291:ARG:NH2	2.32	0.63
12:N:334:ARG:NH1	12:N:368:THR:OG1	2.32	0.63
13:O:293:GLU:O	13:O:301:ARG:NH2	2.31	0.63
15:Y:510:VAL:HG23	15:Y:544:LYS:HZ3	1.62	0.63
4:D:20:LEU:HD11	13:O:252:GLU:HG2	1.80	0.63
3:P:399:TYR:HB3	3:P:428:LEU:HD22	1.79	0.63
15:Y:258:ILE:HD12	15:Y:273:LEU:HD11	1.81	0.63
8:I:361:TYR:OH	13:O:434:ARG:NH2	2.32	0.63
12:N:87:ILE:HD12	12:N:121:ARG:HG2	1.79	0.63
15:X:376:LEU:HD21	15:X:398:GLU:HG3	1.81	0.63
1:A:1473:GLY:HA2	1:A:1526:VAL:HG13	1.81	0.62
6:H:594:ILE:HD11	6:H:604:TYR:HA	1.80	0.62
12:N:673:GLN:NE2	12:N:675:SER:O	2.32	0.62
1:A:596:THR:HB	1:A:606:ARG:HG2	1.80	0.62
2:B:14:TRP:HA	2:B:15:LEU:HD23	1.80	0.62
3:C:161:LYS:NZ	3:C:166:GLU:OE1	2.32	0.62
6:H:615:GLU:OE2	10:L:23:ARG:NH1	2.32	0.62
11:M:7:ARG:NH1	3:P:360:LEU:O	2.30	0.62
3:C:310:ARG:HB3	3:C:312:MET:HG3	1.82	0.62
12:N:392:ASN:OD1	12:N:392:ASN:N	2.28	0.62
6:F:562:MET:SD	6:H:59:ARG:NH1	2.72	0.62
3:P:469:ALA:O	3:P:473:LEU:N	2.29	0.62
6:H:493:SER:HA	6:H:496:TYR:HB3	1.81	0.62
8:I:663:ASP:OD1	8:I:663:ASP:N	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:89:TYR:CD2	10:L:150:ASP:CG	2.71	0.62
1:A:797:LEU:HB3	1:A:799:LEU:HD13	1.82	0.62
8:I:349:ILE:HG12	8:I:404:LEU:HD11	1.80	0.62
9:J:383:ASN:HB3	9:J:386:LEU:HD13	1.82	0.62
6:H:636:ASN:ND2	10:L:184:ARG:O	2.31	0.62
15:Y:38:ILE:HG13	15:Y:75:GLN:HB3	1.81	0.62
7:G:9:LEU:O	9:J:453:HIS:NE2	2.33	0.61
3:P:456:TYR:HB2	3:P:473:LEU:HD13	1.81	0.61
1:A:1589:TYR:O	1:A:1607:ARG:NH2	2.32	0.61
6:H:124:VAL:O	6:H:128:THR:OG1	2.17	0.61
9:K:190:LEU:HD13	9:K:202:ARG:HE	1.64	0.61
12:N:527:LEU:HD22	12:N:530:GLN:HB2	1.81	0.61
6:F:155:LEU:HD12	6:F:158:ILE:HD11	1.82	0.61
1:A:258:THR:OG1	1:A:267:SER:OG	2.14	0.61
1:A:451:GLN:NE2	1:A:473:ASN:OD1	2.32	0.61
12:N:766:GLU:HA	12:N:768:LEU:N	2.15	0.61
1:A:1915:LEU:HD22	12:N:67:LEU:HD22	1.82	0.61
3:C:101:ARG:HG2	3:P:295:TYR:HB2	1.82	0.61
9:J:229:GLU:OE2	9:K:34:ARG:NH2	2.34	0.61
9:K:351:ASP:OD1	9:K:352:GLN:NE2	2.33	0.61
12:N:429:ARG:NH2	12:N:508:ILE:O	2.33	0.61
9:J:74:TYR:OH	9:J:78:ARG:NH1	2.33	0.61
1:A:153:ILE:N	1:A:160:ASN:O	2.31	0.61
6:F:730:LYS:HD3	6:F:743:ILE:HD11	1.81	0.61
8:I:233:TYR:HB3	8:I:554:ILE:HB	1.83	0.61
8:I:586:LEU:HB3	8:I:601:LEU:HB3	1.83	0.61
9:J:261:ASP:OD2	9:K:55:ARG:NH1	2.33	0.61
15:Y:352:SER:O	15:Y:354:ARG:NH1	2.30	0.61
1:A:1197:LEU:HD21	1:A:1208:LEU:HD22	1.82	0.61
8:I:48:ARG:NH1	12:N:390:GLY:O	2.34	0.61
9:K:325:LYS:NZ	11:M:54:GLU:O	2.34	0.61
9:K:358:PHE:O	9:K:362:GLN:NE2	2.34	0.61
10:L:98:VAL:HG12	10:L:137:ILE:HG12	1.83	0.61
11:M:15:ILE:HG22	11:M:17:ASP:H	1.65	0.61
15:X:267:LEU:HG	15:X:270:ASN:HD21	1.66	0.61
15:X:445:THR:O	15:X:449:THR:HG23	2.00	0.61
3:C:432:ASP:OD2	3:C:434:ARG:NH1	2.34	0.60
1:A:425:SER:HB2	1:A:448:SER:HB3	1.83	0.60
1:A:1839:PHE:O	1:A:1841:ASN:N	2.35	0.60
15:X:270:ASN:HB2	15:X:273:LEU:HB2	1.82	0.60
13:O:73:ILE:O	13:O:161:TYR:OH	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Y:414:ILE:HG21	15:Y:447:LEU:HD22	1.82	0.60
1:A:478:ASP:HB3	1:A:491:LEU:HD21	1.82	0.60
10:L:46:ARG:NH1	10:L:156:ILE:O	2.34	0.60
7:G:7:THR:O	9:J:450:ASN:ND2	2.35	0.60
1:A:1247:HIS:CE1	1:A:1294:TYR:HB2	2.37	0.60
3:C:66:PRO:HG2	3:C:68:ALA:HB3	1.82	0.60
1:A:1480:GLU:HA	1:A:1527:MET:HG2	1.82	0.60
6:H:30:ARG:HA	6:H:30:ARG:HH11	1.67	0.60
1:A:1306:CYS:HB2	1:A:1374:ILE:HG12	1.84	0.59
3:C:386:GLN:HE22	13:O:282:ILE:HD11	1.65	0.59
8:I:185:ILE:HG13	8:I:201:ILE:HG13	1.84	0.59
3:P:242:GLN:HE22	3:P:429:ARG:HG3	1.67	0.59
15:X:169:PRO:HB2	15:Y:49:LEU:HD21	1.83	0.59
6:H:609:HIS:HD2	10:L:184:ARG:HG3	1.66	0.59
8:I:48:ARG:HD2	8:I:50:ALA:HB3	1.83	0.59
6:H:581:ARG:NH1	10:L:19:THR:O	2.36	0.59
9:K:445:GLU:OE2	7:W:8:ARG:NH2	2.34	0.59
15:X:383:LEU:HD11	15:X:388:ARG:HB2	1.84	0.59
1:A:1051:VAL:HG21	1:A:1066:LYS:HA	1.84	0.59
6:H:605:THR:HG21	6:H:636:ASN:HB3	1.84	0.59
3:P:180:ARG:NH1	3:P:208:GLU:OE1	2.36	0.59
1:A:168:ASP:OD1	1:A:168:ASP:N	2.33	0.59
9:J:70:GLU:HA	9:J:73:ARG:HB3	1.84	0.59
13:O:681:PRO:HB2	13:O:682:LYS:HE2	1.85	0.59
10:L:87:GLU:HG3	10:L:146:GLN:HE22	1.66	0.59
1:A:191:ARG:HH22	1:A:207:LEU:HB3	1.68	0.59
3:C:242:GLN:OE1	3:C:275:ASN:ND2	2.36	0.59
3:C:536:CYS:O	3:C:542:THR:OG1	2.21	0.59
13:O:426:THR:HB	13:O:441:GLN:HB3	1.84	0.59
3:P:437:VAL:HG22	3:P:469:ALA:HB2	1.85	0.59
15:Y:391:GLU:O	15:Y:395:HIS:ND1	2.34	0.59
6:F:549:ASP:O	6:F:553:SER:N	2.33	0.59
8:I:571:LYS:NZ	8:I:722:VAL:O	2.36	0.59
8:I:624:THR:O	8:I:711:TRP:NE1	2.31	0.59
9:K:441:VAL:HG11	9:K:474:LEU:HD22	1.84	0.59
12:N:340:ARG:HB2	12:N:361:LEU:HD13	1.84	0.59
12:N:527:LEU:HA	12:N:530:GLN:HA	1.84	0.59
13:O:504:ALA:HA	13:O:507:TRP:CD1	2.38	0.59
3:C:460:TYR:HA	3:C:464:ASP:HB2	1.84	0.59
6:F:507:ARG:NH1	6:F:511:GLU:OE2	2.35	0.59
9:K:40:ILE:HD13	9:K:63:ARG:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:17:ASP:HA	11:M:20:ARG:HB3	1.85	0.59
12:N:299:TRP:HA	12:N:302:LYS:HD2	1.84	0.59
15:X:308:MET:HG3	15:X:331:LEU:HD21	1.85	0.59
6:F:618:ASP:O	6:F:622:ALA:N	2.34	0.58
8:I:586:LEU:N	8:I:601:LEU:O	2.33	0.58
9:K:180:GLU:HA	9:K:183:GLU:HB3	1.85	0.58
12:N:108:LEU:HD22	12:N:239:GLN:HB3	1.85	0.58
1:A:369:PHE:HB3	3:C:400:ARG:HD2	1.85	0.58
6:F:604:TYR:HB2	6:F:627:ALA:HB2	1.84	0.58
15:X:283:ARG:NH1	15:X:405:CYS:SG	2.76	0.58
3:C:280:ASP:OD1	3:C:310:ARG:NH2	2.36	0.58
9:J:327:THR:OG1	9:J:337:TRP:NE1	2.36	0.58
9:J:437:ASN:N	9:J:437:ASN:OD1	2.35	0.58
6:F:18:HIS:O	6:H:73:TYR:OH	2.13	0.58
12:N:664:ALA:HA	12:N:699:TRP:HZ2	1.68	0.58
2:B:50:GLN:N	2:B:81:LYS:O	2.33	0.58
3:C:441:GLU:OE2	3:C:472:LYS:NZ	2.36	0.58
8:I:171:VAL:HA	8:I:253:ARG:HH21	1.68	0.58
12:N:63:ARG:NH2	12:N:139:GLY:O	2.36	0.58
15:Y:343:VAL:HG22	15:Y:375:ALA:HB2	1.84	0.58
1:A:155:GLN:NE2	1:A:158:CYS:SG	2.72	0.58
1:A:459:GLU:HA	1:A:466:LEU:HA	1.86	0.58
6:F:524:GLU:OE2	6:F:527:ARG:NH2	2.35	0.58
9:K:66:ASP:N	9:K:66:ASP:OD1	2.36	0.58
12:N:386:LEU:HD22	12:N:396:ILE:HG13	1.84	0.58
3:P:281:LYS:O	3:P:284:SER:OG	2.21	0.58
15:Y:192:TYR:HA	15:Y:195:VAL:HG22	1.86	0.58
15:Y:428:VAL:O	15:Y:432:ASN:ND2	2.31	0.58
1:A:1033:ARG:NH1	1:A:1531:GLY:O	2.37	0.58
1:A:1432:GLN:HA	1:A:1435:ARG:HD2	1.84	0.58
8:I:11:PHE:O	8:I:712:ARG:NH1	2.36	0.58
3:P:263:SER:OG	3:P:296:ARG:NH2	2.34	0.58
15:X:154:ASP:OD1	15:X:154:ASP:N	2.36	0.58
1:A:20:PHE:HB2	1:A:606:ARG:HG3	1.84	0.58
1:A:1094:PRO:HB3	1:A:1100:LEU:HD11	1.85	0.58
2:B:49:GLY:N	2:B:53:HIS:O	2.35	0.58
9:K:70:GLU:OE1	9:K:129:LYS:NZ	2.37	0.58
1:A:1376:LEU:HD22	1:A:1377:LYS:HG3	1.85	0.58
9:K:45:GLN:O	9:K:49:LEU:HG	2.04	0.58
9:K:248:LYS:N	9:K:438:GLU:OE2	2.31	0.58
12:N:530:GLN:O	12:N:531:PHE:HB2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Y:260:SER:O	15:Y:264:LYS:NZ	2.34	0.58
15:Y:455:PRO:O	15:Y:457:THR:N	2.36	0.58
1:A:34:ALA:HB3	13:O:237:GLN:HE22	1.69	0.57
1:A:256:VAL:HB	1:A:269:TRP:HB2	1.85	0.57
3:C:151:LEU:HD22	3:C:178:VAL:HG13	1.85	0.57
15:X:203:LEU:HD11	15:Y:56:LEU:HD13	1.85	0.57
1:A:260:ASP:OD1	1:A:261:ALA:N	2.36	0.57
1:A:707:TRP:CD1	13:O:730:ARG:HD2	2.38	0.57
6:F:101:LYS:NZ	6:F:109:GLU:OE1	2.31	0.57
9:K:391:PHE:HE2	9:K:411:VAL:HG21	1.68	0.57
3:C:106:LEU:HB3	3:C:118:TYR:HB2	1.87	0.57
8:I:512:LEU:HD21	13:O:480:GLN:HG3	1.86	0.57
9:J:448:LEU:HB3	9:J:471:ALA:HB2	1.87	0.57
9:K:338:ILE:HD11	9:K:370:PRO:HD3	1.87	0.57
10:L:144:ASN:ND2	10:L:150:ASP:O	2.37	0.57
3:P:296:ARG:HH11	3:P:298:GLU:HB3	1.69	0.57
15:Y:159:LEU:HD11	15:Y:174:MET:HE3	1.86	0.57
15:Y:230:VAL:HG12	15:Y:232:ASN:H	1.68	0.57
6:F:656:MET:HB3	15:Y:526:GLN:HB2	1.87	0.57
3:P:93:TYR:OH	3:P:101:ARG:NH2	2.38	0.57
15:X:263:LYS:O	15:X:268:ARG:NH2	2.37	0.57
6:F:554:VAL:HG21	9:K:286:TYR:HB2	1.86	0.57
8:I:440:MET:HB3	8:I:444:ASP:HB3	1.87	0.57
8:I:518:PRO:HB2	8:I:519:ARG:HD3	1.86	0.57
8:I:740:HIS:HE1	8:I:742:ARG:HH21	1.53	0.57
9:J:78:ARG:NH2	9:K:17:GLN:O	2.38	0.57
15:X:59:LEU:HD22	15:Y:270:ASN:HD22	1.68	0.57
15:X:269:ASP:H	15:Y:66:ASN:HD21	1.53	0.57
8:I:356:SER:HB3	8:I:397:ILE:HG12	1.86	0.57
12:N:236:ALA:HA	12:N:239:GLN:HE21	1.70	0.57
13:O:501:SER:OG	13:O:502:GLN:N	2.37	0.57
3:P:187:GLU:N	3:P:187:GLU:OE1	2.37	0.57
1:A:613:ALA:HB1	1:A:619:GLN:HB2	1.85	0.57
1:A:1782:GLU:OE1	1:A:1782:GLU:N	2.38	0.57
6:H:104:ASP:OD1	6:H:104:ASP:N	2.24	0.57
8:I:491:ASN:OD1	8:I:492:THR:N	2.37	0.57
12:N:691:LEU:HA	12:N:694:ARG:HD2	1.87	0.57
12:N:770:LEU:HA	12:N:813:GLY:HA3	1.87	0.57
13:O:467:ALA:HB1	13:O:506:LEU:HD11	1.87	0.57
15:Y:95:ASN:N	15:Y:95:ASN:OD1	2.36	0.57
15:Y:452:LEU:HD13	15:Y:460:LYS:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:970:TRP:CD1	1:A:971:PRO:HD2	2.40	0.57
9:J:368:HIS:NE2	9:J:401:ASP:OD2	2.38	0.57
13:O:398:LEU:HD13	13:O:399:MET:H	1.69	0.57
1:A:594:ARG:HG2	1:A:608:THR:HG22	1.86	0.56
8:I:302:ASP:OD1	13:O:58:ARG:NH1	2.38	0.56
8:I:440:MET:SD	8:I:440:MET:N	2.78	0.56
12:N:657:VAL:HG22	12:N:659:VAL:HB	1.87	0.56
13:O:577:THR:O	13:O:581:ILE:HG23	2.05	0.56
1:A:1508:GLY:HA3	1:A:1511:ASN:HD22	1.70	0.56
3:C:206:TRP:HB3	3:C:233:PHE:HB2	1.86	0.56
9:J:85:GLU:OE1	9:J:88:GLN:NE2	2.38	0.56
12:N:137:ARG:HH11	12:N:137:ARG:HB2	1.69	0.56
8:I:89:LYS:HA	8:I:105:SER:HA	1.87	0.56
9:J:86:HIS:HB3	9:J:143:LEU:HD13	1.87	0.56
9:K:35:GLU:OE1	9:K:63:ARG:NH1	2.36	0.56
8:I:307:LEU:HA	8:I:313:ALA:HB3	1.86	0.56
9:K:446:PRO:HB3	7:W:8:ARG:HB2	1.87	0.56
12:N:277:CYS:HA	12:N:285:PHE:HE2	1.70	0.56
6:F:618:ASP:HB2	6:F:621:LEU:HD22	1.87	0.56
8:I:740:HIS:CE1	8:I:742:ARG:HH21	2.24	0.56
9:J:439:VAL:HG21	9:J:448:LEU:HD21	1.87	0.56
9:K:302:TRP:HB2	9:K:326:ALA:HB2	1.87	0.56
12:N:678:LEU:HD23	12:N:678:LEU:H	1.70	0.56
13:O:109:GLU:HB3	3:P:344:ARG:HH21	1.70	0.56
1:A:1758:THR:OG1	13:O:639:GLN:OE1	2.19	0.56
9:J:53:TYR:HB2	9:J:83:ALA:HB2	1.87	0.56
9:J:361:ALA:HB2	9:J:370:PRO:HB2	1.88	0.56
1:A:161:MET:SD	1:A:161:MET:N	2.79	0.56
12:N:646:MET:N	12:N:646:MET:SD	2.79	0.56
12:N:759:GLN:HG2	12:N:817:LEU:HD21	1.88	0.56
3:P:293:ASP:HB3	3:P:296:ARG:HB2	1.88	0.56
1:A:31:HIS:ND1	1:A:99:MET:SD	2.79	0.56
8:I:624:THR:HB	8:I:631:VAL:HA	1.87	0.56
8:I:717:MET:HG3	8:I:719:ALA:HB2	1.88	0.56
1:A:100:VAL:HG21	1:A:153:ILE:HD12	1.88	0.56
3:C:33:LYS:NZ	3:P:85:ASP:OD2	2.31	0.56
12:N:104:GLU:HG2	12:N:175:ARG:HH21	1.70	0.56
12:N:388:HIS:ND1	12:N:389:PRO:O	2.38	0.56
1:A:209:THR:OG1	1:A:210:MET:SD	2.62	0.56
3:C:145:GLN:NE2	13:O:206:PRO:O	2.39	0.56
8:I:33:ASP:OD1	8:I:33:ASP:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:706:ARG:O	12:N:714:SER:N	2.39	0.56
1:A:1679:ASP:N	1:A:1679:ASP:OD1	2.36	0.55
1:A:1752:GLU:HA	1:A:1756:LYS:HD3	1.88	0.55
7:G:14:ASP:N	7:G:14:ASP:OD1	2.39	0.55
7:W:13:LEU:H	7:W:13:LEU:HD12	1.72	0.55
15:Y:507:SER:OG	15:Y:508:ASP:N	2.40	0.55
1:A:1013:ASP:OD1	1:A:1017:ASN:ND2	2.40	0.55
15:X:57:SER:HG	15:X:83:HIS:HD1	1.55	0.55
1:A:1477:ALA:HB1	1:A:1574:LEU:HD13	1.87	0.55
1:A:1753:TYR:O	13:O:631:GLN:NE2	2.39	0.55
3:C:360:LEU:HD12	11:M:19:TRP:HH2	1.70	0.55
3:C:548:ALA:HA	3:C:551:ARG:HH11	1.71	0.55
4:D:12:VAL:HG23	4:D:13:THR:HG23	1.88	0.55
6:H:537:GLU:OE2	6:H:600:TYR:OH	2.25	0.55
8:I:36:ALA:HB2	8:I:46:LEU:HD13	1.87	0.55
12:N:258:ALA:HA	12:N:261:VAL:HG22	1.87	0.55
12:N:794:GLU:O	12:N:798:TYR:N	2.35	0.55
6:H:574:GLY:HA3	6:H:590:PHE:CE1	2.41	0.55
15:X:349:SER:OG	15:X:357:ARG:NH1	2.39	0.55
1:A:1086:MET:HG2	1:A:1610:TYR:CZ	2.42	0.55
1:A:1676:LEU:HD22	1:A:1677:LEU:H	1.72	0.55
8:I:46:LEU:O	8:I:55:VAL:N	2.40	0.55
8:I:534:ASP:O	8:I:538:GLN:HG2	2.07	0.55
10:L:141:VAL:HG11	10:L:151:THR:HG21	1.89	0.55
12:N:809:VAL:HG22	12:N:816:ARG:H	1.70	0.55
15:X:66:ASN:ND2	15:Y:265:SER:O	2.36	0.55
15:Y:184:GLN:O	15:Y:188:SER:OG	2.15	0.55
1:A:461:ASN:H	1:A:464:THR:HB	1.71	0.55
1:A:770:TYR:OH	1:A:809:ASP:OD2	2.23	0.55
1:A:1926:ARG:NH1	12:N:73:GLU:OE1	2.40	0.55
3:C:252:GLN:NE2	3:C:256:ASP:OD1	2.40	0.55
15:X:253:ARG:O	15:X:257:THR:HG22	2.06	0.55
15:X:291:VAL:HG13	15:X:311:TYR:HE1	1.71	0.55
1:A:1797:ILE:HG22	1:A:1852:ILE:HD11	1.89	0.55
8:I:90:ILE:HD11	8:I:110:VAL:HG21	1.88	0.55
1:A:246:ILE:HA	1:A:258:THR:HA	1.89	0.55
9:K:85:GLU:HB3	9:K:88:GLN:HB2	1.89	0.55
10:L:56:SER:OG	10:L:151:THR:N	2.40	0.55
13:O:248:PRO:O	13:O:280:ARG:NH2	2.40	0.55
1:A:1141:VAL:HG11	1:A:1608:HIS:CG	2.41	0.55
3:P:364:TYR:HD2	3:P:367:ALA:H	1.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:X:51:SER:OG	15:Y:204:ASP:OD2	2.22	0.55
1:A:491:LEU:HB3	1:A:497:LEU:HD23	1.89	0.54
1:A:601:ASN:ND2	1:A:603:SER:OG	2.40	0.54
6:H:530:ASN:N	6:H:530:ASN:OD1	2.40	0.54
8:I:56:TRP:CE3	8:I:98:PRO:HB3	2.42	0.54
15:Y:518:PHE:O	15:Y:522:VAL:HG23	2.07	0.54
1:A:799:LEU:O	1:A:801:PRO:HD2	2.08	0.54
1:A:1916:PHE:HE1	12:N:65:HIS:HB3	1.73	0.54
10:L:44:GLN:HB3	10:L:52:THR:HB	1.88	0.54
15:X:238:VAL:HB	15:X:261:LEU:HD21	1.88	0.54
1:A:1622:VAL:N	1:A:1697:LEU:O	2.34	0.54
1:A:1675:GLU:HG2	1:A:1676:LEU:H	1.73	0.54
7:W:14:ASP:N	7:W:14:ASP:OD1	2.38	0.54
15:Y:384:ARG:HH12	15:Y:415:GLU:HB3	1.72	0.54
1:A:94:TYR:HE1	1:A:96:ALA:HB2	1.72	0.54
1:A:1232:ILE:HD11	1:A:1235:LEU:HD22	1.90	0.54
1:A:1730:ALA:HB2	1:A:1776:TYR:CD2	2.42	0.54
8:I:81:ALA:HA	8:I:92:LEU:HA	1.90	0.54
12:N:383:GLU:HA	12:N:387:LEU:HB2	1.90	0.54
3:P:477:HIS:HA	3:P:480:LEU:HB2	1.90	0.54
1:A:776:ASN:HD21	1:A:778:LEU:HB2	1.72	0.54
8:I:170:ASP:O	8:I:253:ARG:NH2	2.40	0.54
9:K:73:ARG:HG3	9:K:92:VAL:HG12	1.88	0.54
9:K:246:ASP:HB3	9:K:249:MET:HB2	1.90	0.54
9:K:315:LYS:NZ	11:M:63:GLN:HE22	2.06	0.54
10:L:75:LYS:HB2	10:L:161:PRO:HG3	1.89	0.54
10:L:86:ASP:HB3	10:L:89:TYR:HB2	1.90	0.54
3:P:96:VAL:N	3:P:97:LYS:HA	2.22	0.54
5:E:105:PHE:HZ	6:H:619:LYS:HG3	1.72	0.54
8:I:86:ASP:OD1	8:I:86:ASP:N	2.31	0.54
12:N:509:TYR:CB	12:N:510:GLY:HA2	2.34	0.54
15:Y:383:LEU:HD13	15:Y:391:GLU:HB3	1.88	0.54
1:A:27:HIS:HB3	1:A:101:ILE:HD13	1.90	0.54
1:A:506:VAL:HG13	1:A:639:VAL:HG23	1.88	0.54
1:A:1455:GLU:OE2	1:A:1459:GLN:NE2	2.41	0.54
1:A:1674:TRP:N	1:A:1674:TRP:CD1	2.74	0.54
6:F:529:GLU:HG2	6:F:532:ARG:HB2	1.90	0.54
8:I:214:LEU:O	8:I:238:THR:OG1	2.25	0.54
9:J:418:TRP:HB2	9:J:458:LEU:HD21	1.90	0.54
13:O:689:ALA:O	13:O:693:ASN:ND2	2.40	0.54
1:A:1040:LEU:HD23	1:A:1562:LEU:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1115:ASN:O	1:A:1115:ASN:ND2	2.41	0.54
6:F:150:SER:OG	6:H:23:ASP:OD2	2.19	0.54
9:J:325:LYS:NZ	11:M:35:GLU:O	2.34	0.54
9:K:162:TYR:OH	9:K:197:GLU:OE1	2.26	0.54
10:L:125:THR:HA	10:L:126:ASP:HB3	1.90	0.54
12:N:393:THR:HA	12:N:396:ILE:HG22	1.89	0.54
1:A:1060:HIS:HA	1:A:1063:ILE:HG22	1.89	0.54
1:A:1141:VAL:HG11	1:A:1608:HIS:CD2	2.43	0.54
8:I:634:SER:OG	8:I:635:ILE:N	2.40	0.54
12:N:508:ILE:HG23	12:N:509:TYR:CD2	2.42	0.54
1:A:89:TYR:HE2	1:A:104:LYS:HD2	1.73	0.54
1:A:275:LYS:O	1:A:277:GLU:N	2.41	0.54
9:J:413:PHE:CD1	9:J:454:VAL:HG12	2.43	0.54
10:L:80:TYR:HB2	10:L:119:TRP:CD2	2.43	0.54
1:A:772:GLU:HG3	1:A:867:CYS:HA	1.90	0.53
1:A:1835:LYS:HB2	1:A:1838:LEU:HB2	1.90	0.53
1:A:1925:VAL:HG21	12:N:74:TRP:HB2	1.89	0.53
6:F:718:LYS:HB3	6:F:721:SER:HB3	1.89	0.53
6:H:624:PHE:CE1	6:H:640:GLY:HA3	2.43	0.53
8:I:514:PHE:H	13:O:443:GLN:HE21	1.55	0.53
9:J:13:TYR:HB3	9:J:22:ALA:HB2	1.90	0.53
9:K:180:GLU:O	9:K:184:LEU:N	2.30	0.53
9:K:487:TYR:O	9:K:490:SER:OG	2.18	0.53
12:N:570:ILE:HA	12:N:573:ASN:ND2	2.23	0.53
6:H:502:LEU:HB3	6:H:525:VAL:HG22	1.89	0.53
6:H:754:HIS:CD2	6:H:755:LEU:H	2.26	0.53
13:O:338:VAL:HG13	13:O:373:LEU:HD21	1.90	0.53
6:F:494:HIS:HD2	6:F:495:HIS:H	1.56	0.53
9:J:133:CYS:O	9:J:152:SER:OG	2.26	0.53
9:K:74:TYR:CZ	9:K:78:ARG:HD2	2.44	0.53
12:N:546:LYS:HG3	12:N:554:MET:HE2	1.90	0.53
15:Y:519:LEU:HD22	15:Y:524:GLU:HG3	1.90	0.53
1:A:488:MET:N	1:A:500:TYR:O	2.33	0.53
15:X:286:ASP:HB3	15:X:289:ASN:HD22	1.73	0.53
15:Y:44:MET:HG3	15:Y:49:LEU:HD12	1.89	0.53
3:P:277:ARG:HH22	3:P:434:ARG:HH11	1.57	0.53
1:A:212:SER:OG	1:A:221:THR:OG1	2.27	0.53
1:A:585:HIS:N	1:A:598:GLU:O	2.34	0.53
15:Y:154:ASP:N	15:Y:154:ASP:OD1	2.41	0.53
15:Y:398:GLU:HA	15:Y:401:ARG:HG2	1.90	0.53
4:D:11:ARG:NH1	4:D:14:GLU:OE2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:650:LYS:O	6:F:654:ALA:N	2.38	0.53
6:H:132:ALA:O	6:H:135:SER:OG	2.24	0.53
8:I:360:LEU:HD21	8:I:390:ILE:HG23	1.90	0.53
10:L:71:LYS:HG2	10:L:133:ARG:HG2	1.89	0.53
3:P:78:GLU:OE1	3:P:79:GLU:N	2.39	0.53
8:I:731:SER:OG	8:I:746:MET:SD	2.58	0.53
9:K:497:ASN:OD1	9:K:497:ASN:N	2.41	0.53
13:O:402:LEU:HB3	13:O:403:LYS:HE2	1.91	0.53
3:C:96:VAL:N	3:C:97:LYS:HA	2.23	0.53
6:H:520:ARG:NH1	15:X:146:TYR:OH	2.41	0.53
13:O:219:GLN:NE2	13:O:231:LEU:H	2.07	0.53
1:A:1797:ILE:HG21	1:A:1848:VAL:HG13	1.91	0.52
3:C:392:ILE:HD13	3:C:402:TRP:CE2	2.43	0.52
6:F:752:GLN:N	6:F:752:GLN:OE1	2.40	0.52
3:P:168:ASP:OD1	3:P:169:GLY:N	2.43	0.52
2:B:16:TRP:HA	2:B:16:TRP:CE3	2.44	0.52
8:I:269:LEU:HA	8:I:272:MET:HE2	1.92	0.52
9:K:39:ASP:OD1	9:K:39:ASP:N	2.40	0.52
9:K:174:HIS:CE1	9:K:211:LYS:HD2	2.44	0.52
10:L:65:ASN:N	10:L:65:ASN:OD1	2.41	0.52
15:X:160:ASP:OD1	15:X:167:ARG:NH2	2.42	0.52
15:X:259:CYS:O	15:X:263:LYS:HG2	2.10	0.52
15:X:390:GLN:O	15:X:393:ILE:HG12	2.09	0.52
7:G:12:LYS:N	7:G:15:ASP:OD2	2.42	0.52
8:I:43:GLU:HB3	8:I:60:PRO:HD3	1.91	0.52
8:I:302:ASP:OD1	8:I:302:ASP:N	2.42	0.52
9:K:275:LEU:HD22	9:K:280:LYS:HB2	1.92	0.52
1:A:134:SER:H	1:A:135:GLN:HA	1.74	0.52
1:A:1503:ASN:N	1:A:1503:ASN:OD1	2.43	0.52
6:F:577:PHE:HE1	11:M:65:LEU:HD23	1.74	0.52
8:I:65:GLY:H	8:I:84:LEU:HG	1.74	0.52
8:I:642:GLN:O	8:I:650:THR:N	2.40	0.52
9:J:401:ASP:HB3	9:J:404:VAL:HG12	1.89	0.52
10:L:22:VAL:HB	10:L:159:TYR:HB3	1.90	0.52
11:M:7:ARG:NH1	3:P:361:ASN:O	2.41	0.52
12:N:341:ILE:HG12	12:N:374:LEU:HD12	1.92	0.52
12:N:401:ILE:HG22	12:N:405:LYS:HE2	1.91	0.52
3:P:318:TYR:HA	3:P:321:HIS:CE1	2.45	0.52
15:Y:364:LYS:HE2	15:Y:368:LEU:HG	1.92	0.52
15:Y:485:LEU:O	15:Y:488:ARG:HG3	2.10	0.52
13:O:593:ARG:HG2	13:O:753:ASN:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:332:GLU:OE1	3:P:332:GLU:N	2.40	0.52
15:X:286:ASP:OD1	15:X:286:ASP:N	2.42	0.52
15:X:383:LEU:HD11	15:X:391:GLU:HB2	1.92	0.52
15:Y:213:SER:OG	15:Y:214:VAL:N	2.39	0.52
6:F:616:GLU:OE1	6:F:617:LEU:N	2.43	0.52
12:N:181:LEU:HD12	12:N:268:VAL:HG21	1.90	0.52
1:A:612:ILE:HG23	1:A:642:TYR:HD2	1.75	0.52
8:I:189:ALA:N	8:I:193:PHE:O	2.42	0.52
15:Y:163:PRO:O	15:Y:167:ARG:N	2.42	0.52
1:A:24:GLY:HA3	1:A:94:TYR:CG	2.44	0.52
1:A:249:LEU:HD13	1:A:256:VAL:HG22	1.92	0.52
3:C:326:ILE:O	3:P:129:LYS:NZ	2.43	0.52
8:I:655:ASP:N	8:I:663:ASP:O	2.43	0.52
15:X:54:ARG:HD2	15:X:87:LEU:HD23	1.90	0.52
6:F:89:GLU:OE2	6:F:130:ARG:NH1	2.42	0.52
6:F:709:ARG:O	6:F:713:LEU:N	2.43	0.52
12:N:65:HIS:HB2	12:N:66:GLY:HA2	1.91	0.52
15:X:196:LEU:HD23	15:X:202:ALA:HB3	1.92	0.52
1:A:422:GLU:HA	1:A:449:GLN:HE21	1.74	0.51
6:H:517:GLN:HA	6:H:517:GLN:HE21	1.75	0.51
9:J:13:TYR:OH	9:K:160:ASP:OD2	2.26	0.51
9:J:391:PHE:HB3	9:J:408:VAL:HG22	1.91	0.51
12:N:602:PRO:N	12:N:603:PRO:HD2	2.25	0.51
13:O:123:GLU:N	13:O:124:PRO:HA	2.25	0.51
15:X:194:GLU:HA	15:X:197:ARG:HG2	1.91	0.51
15:Y:331:LEU:HB3	15:Y:341:PRO:HG3	1.91	0.51
1:A:1711:ASP:OD1	1:A:1715:TRP:N	2.43	0.51
2:B:63:TRP:CG	2:B:74:PRO:HG3	2.46	0.51
6:H:755:LEU:O	6:H:759:ASN:ND2	2.35	0.51
12:N:536:GLU:O	12:N:540:ARG:HG2	2.10	0.51
12:N:706:ARG:N	12:N:714:SER:O	2.33	0.51
12:N:795:LEU:O	12:N:799:LEU:N	2.39	0.51
3:C:488:GLN:O	3:C:491:ILE:HG13	2.09	0.51
6:H:146:PRO:O	6:H:148:LEU:N	2.43	0.51
12:N:481:VAL:HG12	12:N:482:PRO:HD2	1.92	0.51
15:Y:308:MET:HA	15:Y:311:TYR:HB3	1.93	0.51
1:A:435:ASP:HB2	1:A:501:THR:HG22	1.92	0.51
9:J:37:PRO:HB3	9:J:69:TYR:CE2	2.46	0.51
9:J:450:ASN:O	9:J:454:VAL:HG13	2.11	0.51
15:Y:170:LYS:HG3	15:Y:171:ILE:HD12	1.92	0.51
1:A:11:MET:N	1:A:508:LYS:HZ2	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1643:TRP:HB3	14:T:3:ALA:N	2.24	0.51
15:Y:52:ASN:OD1	15:Y:52:ASN:N	2.43	0.51
1:A:1659:GLU:OE1	1:A:1661:HIS:NE2	2.42	0.51
3:C:239:THR:O	3:C:242:GLN:NE2	2.43	0.51
6:F:645:TYR:HA	6:F:648:GLN:HB2	1.93	0.51
8:I:681:ALA:HA	8:I:684:GLN:HE21	1.75	0.51
11:M:33:LEU:HA	11:M:36:LEU:HD13	1.93	0.51
15:X:518:PHE:O	15:X:522:VAL:HG23	2.11	0.51
1:A:1619:LEU:HD21	1:A:1697:LEU:HD12	1.92	0.51
2:B:16:TRP:HA	2:B:16:TRP:HE3	1.76	0.51
3:C:101:ARG:NH2	3:P:293:ASP:OD2	2.41	0.51
8:I:372:TRP:HZ3	8:I:374:GLN:HB3	1.74	0.51
8:I:382:ASP:OD1	8:I:382:ASP:N	2.34	0.51
8:I:559:ASP:OD2	8:I:561:ARG:NE	2.43	0.51
12:N:400:TYR:CZ	12:N:404:ILE:HD11	2.45	0.51
12:N:505:LEU:O	12:N:510:GLY:HA3	2.11	0.51
7:W:20:GLU:O	7:W:23:ARG:HG3	2.11	0.51
1:A:215:HIS:CG	1:A:216:PRO:HD2	2.46	0.51
9:J:84:LYS:HD3	9:J:86:HIS:CE1	2.46	0.51
9:K:506:LEU:HD21	9:K:516:VAL:HG22	1.93	0.51
12:N:757:TYR:O	12:N:761:MET:HG2	2.11	0.51
3:P:183:ASP:N	3:P:183:ASP:OD1	2.43	0.51
1:A:23:PHE:HB2	1:A:111:LEU:HD22	1.93	0.51
1:A:968:SER:OG	1:A:969:ASP:N	2.43	0.51
6:H:737:SER:HB2	6:H:766:LEU:HB2	1.93	0.51
9:J:7:ARG:HA	9:J:10:VAL:HG12	1.91	0.51
13:O:493:LEU:HD13	13:O:507:TRP:HB2	1.93	0.51
3:C:368:TRP:HB3	3:C:391:ALA:HB2	1.93	0.51
7:G:19:PHE:HA	7:G:22:ILE:HG22	1.93	0.51
8:I:668:GLN:HB2	8:I:710:HIS:HB3	1.93	0.51
9:J:51:ALA:HA	9:J:53:TYR:CE1	2.46	0.51
9:K:284:LEU:HD12	9:K:308:TYR:HB2	1.93	0.51
13:O:404:ASP:OD1	13:O:405:SER:N	2.44	0.51
15:X:507:SER:OG	15:X:508:ASP:N	2.44	0.51
15:Y:187:PRO:HA	15:Y:190:THR:HG22	1.92	0.51
1:A:478:ASP:OD1	1:A:479:ALA:N	2.43	0.50
1:A:980:ARG:NH1	1:A:1674:TRP:O	2.44	0.50
3:C:66:PRO:O	3:C:67:LEU:HB3	2.11	0.50
9:J:285:PHE:HB2	9:J:308:TYR:CE1	2.46	0.50
10:L:53:TYR:HB3	10:L:154:ARG:HH21	1.77	0.50
6:F:466:LEU:O	6:F:470:GLY:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:393:VAL:O	8:I:397:ILE:HG13	2.10	0.50
15:Y:215:LYS:O	15:Y:219:VAL:HG23	2.11	0.50
15:Y:339:ALA:O	15:Y:343:VAL:HG23	2.11	0.50
1:A:1463:TYR:HE2	1:A:1511:ASN:HB3	1.76	0.50
8:I:187:LEU:HD13	8:I:196:ALA:HB3	1.94	0.50
10:L:175:ILE:HA	10:L:178:MET:HB2	1.92	0.50
12:N:678:LEU:HB2	12:N:692:LEU:HD21	1.92	0.50
3:P:472:LYS:HA	3:P:475:LYS:HB3	1.94	0.50
1:A:863:LEU:HD12	1:A:864:PRO:HD2	1.92	0.50
1:A:931:VAL:HG21	1:A:962:CYS:SG	2.51	0.50
9:K:10:VAL:HG21	9:K:26:ALA:HB2	1.94	0.50
10:L:49:ASN:HB2	10:L:52:THR:HG23	1.93	0.50
12:N:796:GLN:OE1	12:N:800:GLN:NE2	2.44	0.50
15:X:499:LEU:HB3	15:X:515:LEU:HG	1.94	0.50
1:A:248:PHE:HB3	1:A:257:MET:HB3	1.93	0.50
2:B:14:TRP:CE3	2:B:15:LEU:HB2	2.42	0.50
8:I:144:THR:HG23	8:I:161:SER:HA	1.93	0.50
9:J:5:ARG:O	9:J:9:ARG:HG2	2.12	0.50
9:J:230:ASN:O	9:J:234:VAL:HG13	2.11	0.50
10:L:7:THR:HG1	10:L:114:VAL:H	1.60	0.50
12:N:755:TRP:CH2	12:N:807:GLN:HB3	2.46	0.50
8:I:734:LEU:HD11	8:I:738:LEU:HA	1.92	0.50
12:N:83:LEU:HD12	12:N:87:ILE:HB	1.94	0.50
13:O:105:LEU:HD11	13:O:151:VAL:HG12	1.94	0.50
1:A:181:TRP:HB3	1:A:249:LEU:HD23	1.93	0.50
1:A:880:TYR:HB2	1:A:930:LEU:HD22	1.94	0.50
6:F:66:CYS:HB2	6:F:71:CYS:HB3	1.93	0.50
6:H:494:HIS:O	6:H:498:THR:HG23	2.12	0.50
8:I:9:PRO:HD3	8:I:754:LEU:HB2	1.92	0.50
1:A:90:ASP:HB3	1:A:594:ARG:HH21	1.76	0.50
1:A:127:LEU:HD23	1:A:182:PRO:HB3	1.94	0.50
1:A:266:HIS:HE1	1:A:427:ALA:H	1.59	0.50
6:F:49:TYR:OH	6:F:81:ASP:OD2	2.21	0.50
15:Y:186:ARG:HA	15:Y:189:VAL:HG12	1.94	0.50
1:A:121:SER:OG	1:A:155:GLN:OE1	2.28	0.50
1:A:1031:ASP:OD1	12:N:482:PRO:HG2	2.12	0.50
3:C:180:ARG:HG3	3:C:212:LEU:HD21	1.93	0.50
8:I:12:ARG:HH21	8:I:748:ILE:HB	1.77	0.50
8:I:202:ALA:O	8:I:221:THR:OG1	2.21	0.50
12:N:644:VAL:HG13	12:N:661:PRO:HG3	1.92	0.50
1:A:715:TYR:HE1	13:O:750:PRO:HD2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1321:VAL:HG23	1:A:1322:PRO:HD3	1.94	0.49
12:N:663:GLN:O	12:N:699:TRP:NE1	2.35	0.49
3:P:265:ILE:O	3:P:269:ILE:N	2.34	0.49
1:A:256:VAL:HG21	1:A:271:LEU:HD13	1.94	0.49
1:A:449:GLN:OE1	1:A:449:GLN:N	2.44	0.49
1:A:1244:ASP:OD1	1:A:1244:ASP:N	2.44	0.49
6:H:86:ALA:HA	9:K:473:VAL:HG12	1.95	0.49
8:I:203:GLY:HA3	8:I:223:VAL:HG11	1.94	0.49
9:J:203:PHE:CD2	9:J:227:LEU:HD22	2.47	0.49
9:K:484:ALA:HA	7:W:11:LEU:HD11	1.94	0.49
3:P:426:HIS:CD2	3:P:430:PRO:HA	2.46	0.49
15:Y:325:GLU:OE2	15:Y:348:HIS:NE2	2.45	0.49
1:A:258:THR:O	1:A:267:SER:OG	2.29	0.49
1:A:1226:ARG:HH21	3:C:511:THR:HG21	1.77	0.49
6:F:494:HIS:CD2	6:F:495:HIS:H	2.30	0.49
6:H:86:ALA:HB2	9:K:474:LEU:HA	1.93	0.49
6:H:102:SER:O	6:H:104:ASP:N	2.44	0.49
6:H:702:ASN:OD1	6:H:705:CYS:N	2.38	0.49
9:K:133:CYS:O	9:K:152:SER:OG	2.30	0.49
3:P:149:GLU:HB3	3:P:152:ARG:HH21	1.75	0.49
1:A:369:PHE:CZ	1:A:373:SER:HB3	2.47	0.49
6:F:16:LEU:HD11	6:F:50:ARG:HD2	1.93	0.49
7:G:8:ARG:NH2	9:J:445:GLU:OE2	2.45	0.49
13:O:149:SER:O	13:O:153:LYS:HG2	2.12	0.49
13:O:730:ARG:NH2	13:O:731:ASN:OD1	2.33	0.49
1:A:1168:LEU:O	1:A:1171:GLU:HG3	2.12	0.49
3:C:415:PRO:HA	3:C:418:CYS:SG	2.52	0.49
8:I:561:ARG:HH22	8:I:590:ILE:HA	1.78	0.49
9:J:66:ASP:OD1	9:J:66:ASP:N	2.40	0.49
12:N:63:ARG:HG3	12:N:68:HIS:CE1	2.47	0.49
3:P:253:ASN:O	3:P:257:VAL:N	2.43	0.49
1:A:248:PHE:CZ	1:A:250:ASN:HB2	2.46	0.49
6:F:59:ARG:NH1	6:H:562:MET:SD	2.85	0.49
6:F:68:THR:HG23	6:F:71:CYS:HB2	1.95	0.49
6:H:154:SER:O	6:H:158:ILE:HG13	2.12	0.49
8:I:559:ASP:OD1	8:I:559:ASP:N	2.46	0.49
9:J:17:GLN:NE2	9:K:45:GLN:OE1	2.46	0.49
9:K:273:GLY:O	9:K:277:GLU:HG2	2.12	0.49
3:P:381:THR:OG1	3:P:408:THR:OG1	2.30	0.49
1:A:246:ILE:HB	1:A:258:THR:HG22	1.95	0.49
1:A:367:GLN:HB3	1:A:368:ARG:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1427:ASP:O	1:A:1435:ARG:NH2	2.45	0.49
3:C:234:LEU:HG	3:C:238:TYR:CE2	2.47	0.49
3:C:420:TYR:HA	3:C:423:ARG:NH1	2.27	0.49
6:H:537:GLU:OE1	6:H:538:ILE:N	2.37	0.49
8:I:524:PHE:HZ	8:I:528:ARG:HH21	1.59	0.49
9:J:476:PRO:O	9:J:477:GLN:NE2	2.45	0.49
13:O:348:TYR:HA	13:O:359:VAL:HG21	1.94	0.49
13:O:360:LEU:HD22	13:O:360:LEU:H	1.78	0.49
14:T:5:ALA:O	14:T:6:GLN:NE2	2.46	0.49
15:Y:54:ARG:HB2	15:Y:86:SER:HB2	1.94	0.49
15:Y:340:GLU:OE1	15:Y:340:GLU:N	2.32	0.49
1:A:1103:PRO:HD2	1:A:1143:ALA:HB2	1.95	0.49
2:B:48:TRP:CH2	12:N:632:MET:HG2	2.48	0.49
3:C:537:CYS:O	3:C:543:ARG:NH1	2.46	0.49
7:G:13:LEU:HD22	7:G:13:LEU:H	1.78	0.49
6:H:581:ARG:HD2	10:L:20:GLY:HA3	1.95	0.49
6:H:692:LEU:O	6:H:696:ILE:HG13	2.12	0.49
8:I:188:TYR:HA	8:I:194:LYS:HA	1.95	0.49
8:I:639:LEU:HB2	8:I:652:VAL:HG13	1.94	0.49
9:J:12:GLN:HE22	9:J:16:GLN:NE2	2.11	0.49
9:K:333:TYR:HD2	9:K:336:ALA:H	1.61	0.49
12:N:577:GLU:HG2	12:N:583:ALA:HB2	1.94	0.49
13:O:335:ASN:ND2	13:O:335:ASN:O	2.45	0.49
1:A:964:GLU:OE1	1:A:1702:ARG:NH2	2.46	0.49
6:F:729:LEU:HD23	6:F:739:VAL:HB	1.94	0.49
12:N:810:TYR:O	12:N:811:SER:OG	2.30	0.49
1:A:13:ALA:HB2	1:A:648:PRO:HB3	1.95	0.49
1:A:892:SER:OG	1:A:893:SER:N	2.44	0.49
3:C:244:ILE:HD12	3:C:245:GLU:H	1.76	0.49
4:D:48:ASP:N	4:D:48:ASP:OD1	2.45	0.49
6:F:42:PHE:HB2	6:F:71:CYS:SG	2.52	0.49
8:I:88:LYS:O	8:I:106:VAL:HG22	2.12	0.49
12:N:350:ASP:O	12:N:354:SER:OG	2.27	0.49
4:D:13:THR:HG22	13:O:255:TYR:HE2	1.77	0.48
4:D:13:THR:HG22	13:O:255:TYR:CE2	2.48	0.48
9:J:37:PRO:HB3	9:J:69:TYR:CZ	2.48	0.48
15:X:249:GLY:HA2	15:X:405:CYS:SG	2.53	0.48
1:A:370:ASN:HB2	3:C:400:ARG:HB3	1.95	0.48
1:A:1063:ILE:HA	1:A:1066:LYS:HG2	1.94	0.48
1:A:1113:PRO:HD2	1:A:1114:ARG:HD2	1.96	0.48
3:C:409:TYR:HB3	3:C:418:CYS:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:802:LYS:HG2	12:N:808:LEU:HD12	1.95	0.48
13:O:662:ARG:HD3	13:O:709:ARG:HH11	1.78	0.48
15:X:434:TYR:HE2	15:X:445:THR:HG22	1.78	0.48
1:A:596:THR:HA	1:A:606:ARG:HA	1.95	0.48
2:B:11:VAL:HG11	12:N:642:GLY:HA2	1.95	0.48
3:C:127:GLU:OE1	3:C:148:ASN:ND2	2.46	0.48
6:F:656:MET:HE1	15:Y:526:GLN:H	1.78	0.48
8:I:514:PHE:H	13:O:443:GLN:NE2	2.11	0.48
9:K:320:ARG:NH2	9:K:343:SER:O	2.41	0.48
12:N:83:LEU:HA	12:N:87:ILE:HG12	1.95	0.48
12:N:438:ILE:HG21	12:N:505:LEU:HD21	1.95	0.48
12:N:663:GLN:HG2	12:N:699:TRP:NE1	2.28	0.48
15:X:192:TYR:HA	15:X:195:VAL:HG22	1.96	0.48
15:Y:253:ARG:O	15:Y:257:THR:HG22	2.12	0.48
15:Y:267:LEU:HG	15:Y:270:ASN:HD21	1.79	0.48
3:C:172:LEU:HB3	3:C:195:ALA:HB2	1.94	0.48
6:H:485:ILE:O	6:H:489:SER:OG	2.17	0.48
8:I:676:ASN:HD21	8:I:678:GLU:HB2	1.78	0.48
15:X:331:LEU:HD23	15:X:334:ILE:HD11	1.96	0.48
1:A:1284:GLU:CD	1:A:1284:GLU:H	2.17	0.48
1:A:1781:GLN:O	1:A:1783:THR:N	2.42	0.48
6:F:476:LEU:HD21	6:F:507:ARG:HB3	1.96	0.48
6:H:55:TYR:HA	6:H:82:LEU:HD21	1.96	0.48
12:N:80:GLN:HB2	12:N:156:MET:SD	2.54	0.48
12:N:556:PHE:O	12:N:559:VAL:HG12	2.13	0.48
13:O:337:HIS:O	13:O:341:GLN:HG2	2.13	0.48
15:Y:408:ASP:O	15:Y:411:GLU:HG2	2.13	0.48
1:A:1148:ALA:HB3	1:A:1153:ILE:HG12	1.96	0.48
1:A:1284:GLU:HB2	1:A:1350:TYR:CE2	2.48	0.48
1:A:1426:VAL:HG11	1:A:1491:PHE:HE2	1.78	0.48
1:A:1770:LEU:HD21	1:A:1794:ASP:HB3	1.96	0.48
2:B:72:HIS:HA	2:B:80:TRP:H	1.79	0.48
8:I:44:VAL:O	8:I:58:PHE:N	2.41	0.48
9:J:533:TYR:CD2	3:P:426:HIS:HE1	2.32	0.48
12:N:639:HIS:NE2	12:N:661:PRO:HB2	2.29	0.48
13:O:581:ILE:HD12	13:O:585:LEU:HD23	1.94	0.48
15:X:100:TYR:CD1	15:X:138:VAL:HG13	2.49	0.48
1:A:192:SER:HA	1:A:193:ALA:HA	1.59	0.48
1:A:881:ILE:HG22	1:A:882:LEU:HD12	1.95	0.48
1:A:1312:ASN:ND2	1:A:1312:ASN:O	2.46	0.48
1:A:1371:LEU:HD23	1:A:1371:LEU:HA	1.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:251:TYR:HA	9:J:254:THR:HG22	1.96	0.48
9:K:331:LYS:H	9:K:331:LYS:HD2	1.78	0.48
3:P:457:TRP:HE3	3:P:473:LEU:HD21	1.79	0.48
15:X:176:ALA:HB2	15:X:191:SER:HB2	1.96	0.48
15:Y:543:GLN:HE21	15:Y:547:GLU:HG3	1.79	0.48
1:A:1535:VAL:HB	1:A:1565:LEU:HD11	1.96	0.48
6:F:655:GLU:HG3	6:F:702:ASN:HD22	1.78	0.48
9:J:351:ASP:OD1	9:J:352:GLN:N	2.45	0.48
9:J:429:LEU:HA	9:J:432:ILE:HG22	1.95	0.48
1:A:369:PHE:HD2	3:C:400:ARG:HB2	1.79	0.48
1:A:799:LEU:HD23	1:A:802:TYR:CG	2.49	0.48
1:A:1197:LEU:HD13	1:A:1227:LEU:HD11	1.96	0.48
1:A:1617:ARG:HA	1:A:1691:LEU:HD13	1.96	0.48
1:A:1621:PRO:HG2	1:A:1630:CYS:O	2.14	0.48
5:E:82:LEU:O	5:E:86:VAL:HG23	2.14	0.48
6:H:729:LEU:HD13	6:H:739:VAL:HG22	1.96	0.48
8:I:642:GLN:OE1	8:I:724:GLY:N	2.43	0.48
13:O:490:LEU:HD13	13:O:511:ASP:HB2	1.96	0.48
3:P:347:HIS:HA	3:P:350:ALA:HB3	1.94	0.48
1:A:773:LEU:HD22	1:A:779:MET:HG3	1.96	0.48
8:I:316:GLU:O	8:I:319:THR:OG1	2.28	0.48
9:K:80:HIS:HB3	9:K:85:GLU:HB2	1.95	0.48
10:L:51:GLU:O	10:L:154:ARG:NH2	2.47	0.48
2:B:60:ILE:O	2:B:64:LEU:HG	2.14	0.47
3:C:449:LEU:HD22	3:C:476:LEU:HD11	1.96	0.47
6:F:168:PHE:CE2	6:F:466:LEU:HB3	2.49	0.47
12:N:132:LEU:HA	12:N:135:TRP:HB2	1.96	0.47
13:O:35:ILE:HD11	13:O:112:PHE:HZ	1.79	0.47
3:P:120:TYR:HD1	3:P:174:LEU:HD21	1.78	0.47
15:X:304:LEU:O	15:X:308:MET:HG2	2.14	0.47
15:Y:441:ALA:HB3	15:Y:444:LEU:HD12	1.96	0.47
1:A:153:ILE:HB	1:A:160:ASN:HB2	1.95	0.47
1:A:612:ILE:HG23	1:A:642:TYR:CD2	2.49	0.47
1:A:767:HIS:NE2	1:A:842:PRO:HD2	2.29	0.47
1:A:772:GLU:OE2	1:A:870:SER:N	2.40	0.47
1:A:1114:ARG:HD2	1:A:1114:ARG:N	2.29	0.47
6:F:38:GLU:OE2	6:F:67:THR:N	2.43	0.47
8:I:247:GLU:OE1	8:I:247:GLU:N	2.36	0.47
8:I:313:ALA:HA	8:I:314:SER:HA	1.58	0.47
8:I:366:LEU:HD12	8:I:366:LEU:HA	1.73	0.47
8:I:683:TYR:HD1	8:I:701:PRO:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:449:ASN:ND2	7:W:8:ARG:HG3	2.29	0.47
12:N:798:TYR:O	12:N:802:LYS:N	2.43	0.47
15:Y:452:LEU:HA	15:Y:455:PRO:HG2	1.96	0.47
3:C:93:TYR:OH	3:C:101:ARG:NH2	2.47	0.47
8:I:122:SER:HB2	8:I:125:LEU:HG	1.97	0.47
9:K:372:LEU:HD13	9:K:404:VAL:HG13	1.97	0.47
10:L:73:THR:O	10:L:160:THR:OG1	2.24	0.47
12:N:802:LYS:NZ	12:N:805:ASP:OD2	2.43	0.47
13:O:362:GLU:OE1	13:O:362:GLU:N	2.38	0.47
13:O:648:ILE:HD12	13:O:667:VAL:HG21	1.96	0.47
1:A:799:LEU:C	1:A:801:PRO:HD2	2.35	0.47
1:A:1261:TYR:O	1:A:1264:THR:OG1	2.30	0.47
1:A:1573:SER:OG	1:A:1617:ARG:NH1	2.47	0.47
3:C:201:LEU:HA	3:C:229:MET:HG3	1.96	0.47
3:C:325:GLU:O	3:P:129:LYS:NZ	2.28	0.47
6:H:165:ASP:OD1	6:H:165:ASP:N	2.46	0.47
12:N:282:GLU:HA	12:N:354:SER:HA	1.96	0.47
12:N:559:VAL:HA	12:N:562:LYS:HG2	1.96	0.47
12:N:758:ILE:HD13	12:N:808:LEU:HD11	1.96	0.47
13:O:35:ILE:HD11	13:O:112:PHE:CZ	2.50	0.47
1:A:433:THR:HG21	1:A:488:MET:HE2	1.95	0.47
3:C:183:ASP:N	3:C:183:ASP:OD1	2.47	0.47
4:D:10:PRO:HG2	13:O:346:TRP:CE2	2.49	0.47
8:I:231:VAL:HB	8:I:556:LEU:HB2	1.96	0.47
9:K:320:ARG:HH21	9:K:344:PHE:HA	1.80	0.47
10:L:74:VAL:HG11	10:L:158:ILE:HD11	1.95	0.47
12:N:389:PRO:HA	12:N:431:ARG:HH22	1.78	0.47
12:N:511:SER:HB3	12:N:514:LEU:HG	1.95	0.47
15:X:446:LEU:O	15:X:449:THR:OG1	2.22	0.47
1:A:446:VAL:HG21	1:A:453:ARG:NH1	2.30	0.47
1:A:862:TYR:HB3	1:A:896:LEU:HD22	1.96	0.47
6:F:476:LEU:HD21	6:F:507:ARG:HD2	1.97	0.47
6:H:101:LYS:O	6:H:105:ASP:CB	2.49	0.47
9:J:324:SER:HA	9:J:327:THR:HG22	1.97	0.47
12:N:593:ALA:HB1	12:N:595:ILE:HG12	1.97	0.47
13:O:678:TYR:HB2	13:O:680:GLN:HG2	1.96	0.47
3:P:289:LEU:HD11	3:P:296:ARG:HG2	1.96	0.47
15:Y:269:ASP:HB3	15:Y:300:LEU:HD21	1.96	0.47
1:A:115:LYS:HE2	1:A:162:HIS:HE1	1.79	0.47
1:A:487:THR:HG22	1:A:501:THR:HA	1.97	0.47
1:A:862:TYR:OH	1:A:871:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:580:GLN:NE2	11:M:62:LEU:HD11	2.30	0.47
8:I:56:TRP:HZ3	8:I:58:PHE:HB2	1.80	0.47
8:I:584:HIS:N	8:I:603:ARG:O	2.44	0.47
8:I:688:THR:HG22	8:I:690:SER:H	1.79	0.47
9:J:475:ILE:HG13	9:J:475:ILE:O	2.15	0.47
9:K:379:GLY:HA3	9:K:411:VAL:HG22	1.97	0.47
10:L:92:SER:HA	10:L:113:LEU:HB2	1.97	0.47
15:X:283:ARG:HE	15:X:406:ARG:HE	1.61	0.47
15:X:433:VAL:HA	15:X:436:THR:HG22	1.96	0.47
15:Y:140:TYR:HB2	15:Y:171:ILE:HD11	1.95	0.47
1:A:1791:ILE:HB	13:O:598:THR:HG21	1.96	0.47
2:B:60:ILE:HG12	2:B:80:TRP:CE2	2.50	0.47
3:C:145:GLN:HE22	13:O:207:LEU:HB3	1.80	0.47
3:C:182:LEU:HD12	3:C:182:LEU:HA	1.74	0.47
6:H:102:SER:O	6:H:103:HIS:C	2.53	0.47
6:H:714:PHE:HD2	6:H:746:VAL:HG22	1.80	0.47
9:J:45:GLN:O	9:J:49:LEU:HG	2.15	0.47
3:P:305:ASN:HD21	3:P:370:LEU:HD11	1.80	0.47
15:Y:277:LEU:HD23	15:Y:293:LYS:HD2	1.97	0.47
15:Y:411:GLU:O	15:Y:414:ILE:HG22	2.14	0.47
15:Y:465:LEU:HD12	15:Y:482:LYS:HD2	1.97	0.47
1:A:1631:TYR:HB2	1:A:1708:TYR:HB2	1.95	0.47
6:F:23:ASP:OD2	6:H:148:LEU:HD22	2.14	0.47
6:F:129:ASP:HB2	15:Y:506:GLN:HE22	1.80	0.47
6:F:129:ASP:HB2	15:Y:506:GLN:NE2	2.30	0.47
12:N:545:LEU:HD21	12:N:553:PRO:HB3	1.96	0.47
12:N:574:ILE:HA	12:N:625:LYS:HZ3	1.80	0.47
13:O:580:VAL:O	13:O:583:VAL:HG12	2.15	0.47
3:P:297:ILE:HD13	3:P:330:ARG:HD3	1.96	0.47
1:A:710:LEU:HD11	13:O:715:TYR:HD1	1.79	0.47
1:A:1110:ARG:HH12	1:A:1117:THR:HG22	1.80	0.47
1:A:1134:TRP:CZ3	1:A:1605:ALA:HB2	2.50	0.47
1:A:1487:CYS:SG	1:A:1488:LEU:N	2.88	0.47
1:A:1752:GLU:HG3	1:A:1753:TYR:HD2	1.80	0.47
1:A:1892:HIS:HB3	1:A:1927:ALA:HB2	1.96	0.47
3:C:148:ASN:HB3	3:C:151:LEU:HG	1.97	0.47
3:C:305:ASN:HD22	3:C:305:ASN:HA	1.58	0.47
8:I:254:LYS:HD3	8:I:254:LYS:HA	1.68	0.47
9:J:214:LYS:HG2	9:J:216:SER:H	1.80	0.47
9:J:502:PHE:HE1	9:J:515:SER:HA	1.79	0.47
12:N:431:ARG:HG3	12:N:432:GLU:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:479:GLU:HB3	13:O:656:ALA:HA	1.95	0.47
15:Y:414:ILE:HG12	15:Y:426:ALA:HB1	1.97	0.47
1:A:1882:LEU:HD23	1:A:1882:LEU:H	1.80	0.46
3:C:26:PHE:N	3:C:26:PHE:CD1	2.84	0.46
6:F:656:MET:O	6:F:660:LYS:HG2	2.15	0.46
8:I:61:ASN:OD1	8:I:64:THR:N	2.48	0.46
8:I:168:LEU:HD13	8:I:257:HIS:CE1	2.50	0.46
12:N:611:VAL:HG23	12:N:616:ARG:HG2	1.97	0.46
12:N:612:PRO:O	12:N:616:ARG:HG3	2.15	0.46
15:X:321:LEU:HB3	15:X:348:HIS:NE2	2.30	0.46
15:Y:87:LEU:HD22	15:Y:95:ASN:HB2	1.96	0.46
1:A:610:PRO:O	1:A:642:TYR:OH	2.19	0.46
1:A:1642:GLN:HG3	1:A:1643:TRP:CE2	2.50	0.46
1:A:1919:LYS:NZ	12:N:67:LEU:HA	2.30	0.46
6:H:102:SER:O	6:H:102:SER:OG	2.33	0.46
8:I:185:ILE:O	8:I:198:VAL:N	2.48	0.46
8:I:394:GLY:HA3	8:I:514:PHE:CE1	2.50	0.46
9:J:224:VAL:HG23	9:J:227:LEU:HD21	1.97	0.46
9:J:231:LEU:HA	9:J:234:VAL:HG22	1.96	0.46
9:J:295:TYR:CE1	9:K:54:HIS:HD2	2.32	0.46
3:P:39:ILE:HG12	3:P:201:LEU:O	2.15	0.46
15:X:434:TYR:CD2	15:X:444:LEU:HB2	2.50	0.46
1:A:369:PHE:CE1	1:A:373:SER:HB3	2.51	0.46
1:A:1379:ASN:OD1	1:A:1379:ASN:N	2.47	0.46
2:B:3:VAL:HB	12:N:671:GLN:OE1	2.15	0.46
6:F:465:LEU:HD11	6:F:495:HIS:CG	2.50	0.46
8:I:673:LEU:HA	8:I:676:ASN:HB2	1.96	0.46
9:J:447:LEU:O	9:J:451:LEU:HG	2.16	0.46
9:K:192:LYS:HG2	9:K:198:GLN:HG3	1.96	0.46
1:A:477:LYS:HD2	1:A:491:LEU:HD11	1.96	0.46
1:A:1058:SER:H	1:A:1061:GLU:HB2	1.81	0.46
1:A:1463:TYR:CE2	1:A:1511:ASN:HB3	2.51	0.46
1:A:1815:LYS:HZ1	1:A:1893:SER:HB3	1.80	0.46
5:E:89:LEU:O	6:H:592:ARG:NH2	2.49	0.46
6:F:726:LEU:HD11	6:F:742:LEU:HB3	1.97	0.46
8:I:589:THR:HB	8:I:596:TYR:HB3	1.97	0.46
15:Y:168:THR:HB	15:Y:169:PRO:HD2	1.97	0.46
15:Y:304:LEU:HB3	15:Y:308:MET:HE2	1.97	0.46
1:A:950:GLY:N	1:A:1813:GLN:HG3	2.28	0.46
2:B:48:TRP:HA	2:B:54:CYS:HA	1.97	0.46
3:C:393:GLU:OE2	13:O:280:ARG:NE	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:616:GLU:OE1	6:F:619:LYS:HB2	2.14	0.46
9:J:279:ASN:HA	9:J:311:MET:HE1	1.98	0.46
12:N:92:TRP:CZ3	12:N:166:PRO:HG3	2.50	0.46
12:N:246:VAL:HG23	12:N:249:ARG:HH21	1.81	0.46
3:P:172:LEU:HB3	3:P:195:ALA:HB2	1.96	0.46
7:W:12:LYS:HD3	7:W:12:LYS:HA	1.75	0.46
1:A:1485:PHE:HD1	1:A:1523:LEU:HD21	1.80	0.46
1:A:1731:ARG:HA	1:A:1732:ALA:HA	1.69	0.46
6:H:115:CYS:SG	6:H:116:PHE:N	2.88	0.46
15:X:515:LEU:HB3	15:X:531:GLN:HG3	1.98	0.46
1:A:89:TYR:HB2	13:O:537:ALA:HB2	1.98	0.46
1:A:626:LYS:HD3	1:A:638:LEU:HD21	1.98	0.46
5:E:85:LEU:O	5:E:88:GLU:HG3	2.16	0.46
6:H:609:HIS:CD2	10:L:184:ARG:HG3	2.46	0.46
9:J:35:GLU:OE2	9:J:63:ARG:NH1	2.48	0.46
9:J:52:GLN:OE1	9:J:55:ARG:NH2	2.38	0.46
12:N:341:ILE:HG12	12:N:374:LEU:HB2	1.97	0.46
12:N:611:VAL:HG21	12:N:637:TRP:CZ2	2.50	0.46
15:X:509:CYS:HA	15:X:512:HIS:HD2	1.81	0.46
15:Y:406:ARG:HD3	15:Y:406:ARG:HA	1.74	0.46
1:A:1160:TYR:CE1	1:A:1191:LEU:HD13	2.51	0.46
8:I:194:LYS:HG2	8:I:541:ALA:HB1	1.97	0.46
9:J:441:VAL:HG23	9:J:443:LYS:H	1.80	0.46
9:K:403:PHE:O	9:K:407:GLU:HG2	2.14	0.46
13:O:249:ASP:HA	13:O:280:ARG:HH22	1.80	0.46
13:O:691:ILE:HD13	13:O:720:LEU:HD23	1.98	0.46
3:P:149:GLU:HA	3:P:152:ARG:HE	1.79	0.46
3:P:436:LEU:HD23	3:P:439:LEU:HD12	1.98	0.46
15:X:251:ASN:HD21	15:X:283:ARG:HB3	1.80	0.46
15:X:379:LYS:HD2	15:X:395:HIS:CD2	2.51	0.46
15:X:394:ILE:O	15:X:398:GLU:HG2	2.16	0.46
15:X:509:CYS:HA	15:X:512:HIS:CD2	2.50	0.46
9:K:203:PHE:HE1	9:K:218:THR:HB	1.80	0.46
13:O:127:HIS:ND1	13:O:127:HIS:O	2.49	0.46
15:X:357:ARG:O	15:X:361:LEU:HG	2.16	0.46
1:A:1676:LEU:HD13	1:A:1677:LEU:N	2.31	0.46
3:C:305:ASN:ND2	3:C:339:ASN:HD21	2.13	0.46
6:H:55:TYR:OH	6:H:56:LYS:NZ	2.49	0.46
6:H:96:VAL:HG11	9:K:448:LEU:HD11	1.98	0.46
6:H:610:GLU:O	6:H:614:THR:OG1	2.34	0.46
8:I:451:PHE:CG	8:I:452:LEU:N	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:500:PHE:CZ	13:O:492:HIS:HB2	2.52	0.46
8:I:676:ASN:ND2	8:I:678:GLU:OE1	2.41	0.46
15:Y:515:LEU:O	15:Y:519:LEU:HG	2.15	0.46
1:A:1426:VAL:HG11	1:A:1491:PHE:CE2	2.51	0.45
1:A:1478:GLY:N	1:A:1525:MET:O	2.43	0.45
8:I:143:PRO:O	8:I:264:TYR:OH	2.26	0.45
8:I:209:CYS:HB2	8:I:575:LEU:HB3	1.98	0.45
8:I:352:LEU:HD12	8:I:352:LEU:HA	1.80	0.45
15:Y:393:ILE:HG12	15:Y:416:CYS:SG	2.57	0.45
15:Y:446:LEU:O	15:Y:449:THR:OG1	2.28	0.45
6:F:626:ASN:OD1	6:F:629:ARG:NH2	2.50	0.45
6:F:639:TYR:CD1	6:F:672:LEU:HD22	2.52	0.45
6:H:552:LEU:HG	6:H:576:CYS:SG	2.57	0.45
8:I:235:GLN:OE1	8:I:603:ARG:NH1	2.50	0.45
10:L:24:GLU:OE2	10:L:27:SER:N	2.49	0.45
12:N:531:PHE:HB3	12:N:534:SER:N	2.32	0.45
12:N:544:LEU:O	12:N:548:ARG:HG2	2.15	0.45
12:N:670:PHE:CZ	12:N:713:PHE:HB3	2.51	0.45
13:O:691:ILE:HD12	13:O:691:ILE:HA	1.81	0.45
3:P:296:ARG:HD2	3:P:298:GLU:HB2	1.99	0.45
15:Y:505:ASN:OD1	15:Y:505:ASN:N	2.48	0.45
1:A:1017:ASN:HA	1:A:1038:ARG:HH21	1.81	0.45
2:B:13:THR:HG21	12:N:605:LYS:HD3	1.97	0.45
3:C:36:LEU:HD21	3:C:58:LEU:HB2	1.97	0.45
3:C:424:ARG:HB3	3:C:424:ARG:HH11	1.80	0.45
6:F:549:ASP:HB3	6:F:579:LEU:HD12	1.97	0.45
6:H:656:MET:HG3	6:H:657:HIS:HD2	1.81	0.45
10:L:100:ASN:N	10:L:100:ASN:OD1	2.50	0.45
12:N:484:PRO:O	12:N:486:ASP:N	2.50	0.45
12:N:570:ILE:HA	12:N:573:ASN:HD21	1.81	0.45
13:O:360:LEU:HD23	13:O:363:HIS:HB2	1.99	0.45
13:O:376:LEU:HD12	13:O:376:LEU:HA	1.74	0.45
3:P:475:LYS:O	3:P:479:GLN:NE2	2.50	0.45
3:C:36:LEU:HD12	3:C:36:LEU:HA	1.74	0.45
9:J:422:GLU:OE2	9:J:460:LYS:NZ	2.40	0.45
9:K:285:PHE:HB2	9:K:308:TYR:CE1	2.51	0.45
9:K:341:GLY:HA3	9:K:357:TYR:CE1	2.50	0.45
12:N:180:PHE:HB2	12:N:240:PHE:CZ	2.52	0.45
13:O:585:LEU:HD13	13:O:585:LEU:HA	1.81	0.45
15:X:383:LEU:HD12	15:X:392:ALA:N	2.32	0.45
15:X:389:VAL:HG21	15:X:420:SER:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Y:73:PRO:HB3	15:Y:106:GLN:HE22	1.81	0.45
15:Y:180:LYS:HG3	15:Y:188:SER:HB3	1.99	0.45
1:A:181:TRP:NE1	1:A:190:GLU:OE2	2.45	0.45
1:A:269:TRP:CZ3	1:A:411:HIS:HB2	2.51	0.45
2:B:13:THR:HG23	12:N:638:LYS:HD2	1.99	0.45
8:I:28:TRP:CZ3	8:I:35:ILE:HB	2.51	0.45
9:J:322:TYR:CE1	11:M:31:ILE:HG12	2.52	0.45
9:K:176:LEU:HD12	9:K:181:GLU:HG2	1.99	0.45
9:K:383:ASN:HB3	9:K:386:LEU:HD13	1.98	0.45
12:N:640:THR:HA	12:N:662:VAL:HG21	1.99	0.45
1:A:1221:ASP:OD1	1:A:1222:MET:N	2.49	0.45
1:A:1423:SER:OG	1:A:1490:LYS:NZ	2.40	0.45
6:F:745:LYS:HD2	6:F:745:LYS:HA	1.73	0.45
6:H:727:GLU:HA	6:H:730:LYS:HE2	1.99	0.45
8:I:197:ARG:O	8:I:545:GLY:HA2	2.16	0.45
12:N:290:HIS:HA	12:N:293:ILE:HB	1.98	0.45
13:O:450:SER:HB2	13:O:461:ASN:HB2	1.98	0.45
13:O:546:ARG:O	13:O:549:VAL:HG12	2.16	0.45
13:O:750:PRO:C	13:O:752:ILE:H	2.19	0.45
15:Y:276:SER:O	15:Y:280:LEU:HG	2.16	0.45
1:A:1138:HIS:HD2	1:A:1608:HIS:NE2	2.15	0.45
1:A:1604:GLN:O	1:A:1607:ARG:HB2	2.16	0.45
6:F:543:LEU:HB2	6:F:552:LEU:HD13	1.99	0.45
6:F:703:PRO:HG2	6:F:704:LEU:HD22	1.98	0.45
6:H:138:TYR:HB2	6:H:155:LEU:HD13	1.99	0.45
9:J:214:LYS:HD3	9:J:216:SER:HB2	1.98	0.45
9:J:276:VAL:HA	9:J:311:MET:SD	2.57	0.45
9:J:512:ASP:OD2	9:J:515:SER:OG	2.30	0.45
9:K:439:VAL:O	9:K:441:VAL:HG23	2.17	0.45
10:L:87:GLU:HG3	10:L:146:GLN:NE2	2.32	0.45
13:O:717:GLN:HB3	13:O:733:CYS:SG	2.57	0.45
15:X:325:GLU:HG3	15:X:348:HIS:NE2	2.32	0.45
15:X:480:VAL:HG13	15:X:514:ILE:HG13	1.98	0.45
1:A:970:TRP:HD1	1:A:971:PRO:HD2	1.82	0.45
3:C:26:PHE:CE1	3:C:257:VAL:HG21	2.52	0.45
3:C:269:ILE:HG22	3:C:285:ILE:HD13	1.99	0.45
3:C:307:LEU:HD21	3:C:315:GLU:HB2	1.99	0.45
6:F:645:TYR:O	6:F:649:GLU:N	2.50	0.45
6:H:600:TYR:CE2	6:H:602:TYR:HB3	2.52	0.45
8:I:188:TYR:CZ	8:I:194:LYS:HB2	2.52	0.45
8:I:445:ILE:HD13	13:O:131:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:131:PRO:HG2	10:L:161:PRO:HG2	1.99	0.45
12:N:516:ILE:HG12	12:N:553:PRO:HB3	1.99	0.45
15:Y:434:TYR:CD2	15:Y:444:LEU:HB3	2.52	0.45
1:A:215:HIS:CD2	1:A:217:LEU:H	2.35	0.45
1:A:258:THR:HG1	1:A:267:SER:HG	1.60	0.45
1:A:435:ASP:OD1	1:A:437:CYS:N	2.50	0.45
1:A:980:ARG:HG3	1:A:983:LEU:H	1.81	0.45
6:F:77:LYS:NZ	6:H:19:TYR:O	2.49	0.45
8:I:417:PHE:HA	8:I:448:VAL:HG22	1.99	0.45
1:A:127:LEU:H	1:A:127:LEU:HD13	1.82	0.45
1:A:219:GLU:HA	3:C:458:ARG:NH2	2.32	0.45
1:A:258:THR:HG1	1:A:269:TRP:HE1	1.63	0.45
6:H:545:HIS:HE1	10:L:182:SER:O	2.00	0.45
6:H:621:LEU:HD13	6:H:625:ARG:HH21	1.82	0.45
8:I:139:LEU:HD23	8:I:139:LEU:HA	1.81	0.45
9:K:450:ASN:OD1	7:W:9:LEU:N	2.42	0.45
10:L:13:PRO:HG3	10:L:78:CYS:SG	2.57	0.45
12:N:345:PHE:CD2	12:N:385:ARG:HD2	2.52	0.45
12:N:808:LEU:HD22	12:N:815:TYR:HB3	1.98	0.45
3:P:474:ALA:HB2	3:P:489:CYS:HB2	1.98	0.45
15:X:283:ARG:HE	15:X:406:ARG:NE	2.15	0.45
15:X:374:GLN:HA	15:X:377:LEU:HG	1.99	0.45
15:Y:298:GLN:HE22	15:Y:327:LEU:HD13	1.82	0.45
3:C:180:ARG:HG3	3:C:212:LEU:HD11	2.00	0.44
6:F:651:PHE:HA	6:F:654:ALA:HB3	1.98	0.44
6:H:110:PHE:CD1	6:H:117:THR:HG21	2.53	0.44
6:H:583:HIS:CE1	6:H:613:LEU:HG	2.52	0.44
8:I:735:SER:HB2	8:I:737:ASN:OD1	2.17	0.44
9:K:452:GLY:HA3	9:K:468:HIS:CE1	2.52	0.44
12:N:506:VAL:HA	12:N:510:GLY:HA3	1.98	0.44
12:N:523:LEU:O	12:N:527:LEU:HG	2.16	0.44
12:N:531:PHE:HB3	12:N:533:PHE:HA	1.97	0.44
12:N:564:MET:O	12:N:568:ARG:HG3	2.17	0.44
1:A:1114:ARG:N	1:A:1114:ARG:HH11	2.15	0.44
1:A:1349:SER:OG	1:A:1352:ILE:O	2.26	0.44
1:A:1674:TRP:N	1:A:1674:TRP:HD1	2.15	0.44
6:F:98:ASN:OD1	6:F:98:ASN:N	2.49	0.44
6:H:742:LEU:O	6:H:746:VAL:HG23	2.17	0.44
9:K:484:ALA:O	9:K:488:ILE:HG12	2.17	0.44
12:N:351:PHE:CG	12:N:352:PRO:HA	2.52	0.44
13:O:707:LYS:HA	13:O:710:ILE:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:290:ARG:HD3	3:P:290:ARG:HA	1.84	0.44
15:X:469:LEU:HG	15:X:478:ALA:HB1	2.00	0.44
15:Y:208:GLY:O	15:Y:211:SER:OG	2.27	0.44
15:Y:267:LEU:HG	15:Y:270:ASN:ND2	2.31	0.44
1:A:31:HIS:CD2	1:A:32:PRO:HD2	2.53	0.44
1:A:864:PRO:HG3	1:A:898:ARG:HD2	2.00	0.44
5:E:99:ILE:HG12	5:E:103:LEU:HD13	1.98	0.44
6:F:168:PHE:HB3	6:F:463:MET:SD	2.58	0.44
6:F:472:GLY:HA3	6:F:488:LEU:HD21	2.00	0.44
6:F:580:GLN:HE21	11:M:60:LEU:HD13	1.82	0.44
6:F:726:LEU:HD13	6:F:726:LEU:HA	1.76	0.44
12:N:513:ASP:OD1	12:N:513:ASP:N	2.50	0.44
12:N:530:GLN:HE21	12:N:530:GLN:HB3	1.52	0.44
13:O:63:LEU:O	13:O:66:PRO:HD2	2.18	0.44
1:A:174:PRO:HG2	1:A:175:PHE:HD2	1.81	0.44
1:A:1757:PRO:O	1:A:1758:THR:OG1	2.36	0.44
1:A:1894:VAL:HA	1:A:1923:MET:HE2	1.98	0.44
1:A:1909:THR:HA	1:A:1936:LEU:HD13	1.99	0.44
3:C:361:ASN:HD22	3:C:363:ARG:N	2.09	0.44
3:C:527:ASP:OD1	3:C:527:ASP:N	2.45	0.44
6:F:127:LYS:HA	6:F:127:LYS:HD3	1.83	0.44
6:F:655:GLU:HG3	6:F:702:ASN:ND2	2.32	0.44
6:H:581:ARG:HH11	10:L:20:GLY:HA3	1.83	0.44
6:H:629:ARG:HB2	9:K:504:THR:HB	2.00	0.44
8:I:338:GLU:HG3	8:I:415:LYS:NZ	2.32	0.44
8:I:350:SER:O	8:I:354:SER:OG	2.20	0.44
8:I:676:ASN:ND2	8:I:678:GLU:HB2	2.32	0.44
8:I:737:ASN:ND2	8:I:739:ARG:HB2	2.33	0.44
12:N:519:TYR:HE2	12:N:541:ASN:HD21	1.65	0.44
13:O:385:VAL:HG21	13:O:401:ALA:HB3	1.99	0.44
15:X:495:GLY:HA3	15:X:518:PHE:CE2	2.52	0.44
1:A:628:ILE:HD11	1:A:762:ILE:HD13	2.00	0.44
1:A:1595:HIS:CE1	1:A:1598:ASP:HB2	2.52	0.44
1:A:1684:THR:O	1:A:1688:LYS:HB2	2.17	0.44
6:H:658:PHE:HB3	6:H:675:ILE:HG12	1.98	0.44
9:K:177:THR:HG22	9:K:365:LYS:HB3	1.98	0.44
12:N:570:ILE:HD12	12:N:573:ASN:OD1	2.17	0.44
15:Y:246:VAL:HG13	15:Y:280:LEU:HD21	2.00	0.44
1:A:1086:MET:HB2	1:A:1563:GLY:HA3	1.99	0.44
1:A:1545:LYS:HB3	1:A:1545:LYS:HE2	1.76	0.44
9:K:373:TYR:CE2	7:W:4:ARG:HG2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:413:LYS:HE2	3:P:413:LYS:HB3	1.86	0.44
15:X:55:LEU:HB3	15:Y:203:LEU:HD12	2.00	0.44
1:A:158:CYS:SG	3:C:427:GLN:NE2	2.90	0.44
1:A:174:PRO:HG2	1:A:175:PHE:CD2	2.53	0.44
1:A:647:ALA:O	1:A:649:GLY:N	2.48	0.44
1:A:831:MET:HA	1:A:832:HIS:HA	1.58	0.44
1:A:1386:TRP:C	1:A:1386:TRP:CD1	2.91	0.44
1:A:1454:LEU:HD22	1:A:1454:LEU:H	1.83	0.44
2:B:16:TRP:NE1	2:B:41:GLY:O	2.45	0.44
6:F:483:GLU:HA	6:F:486:ASN:HD22	1.81	0.44
6:F:549:ASP:OD1	6:F:549:ASP:N	2.48	0.44
7:G:4:ARG:HB2	9:J:373:TYR:CE1	2.53	0.44
8:I:237:GLU:H	8:I:237:GLU:CD	2.19	0.44
12:N:283:ARG:NH2	12:N:288:GLU:OE2	2.49	0.44
13:O:542:GLU:OE2	13:O:546:ARG:NH2	2.50	0.44
1:A:188:LEU:HD11	1:A:223:LEU:HD22	1.99	0.44
1:A:1398:PHE:CZ	10:L:70:ARG:HD3	2.53	0.44
1:A:1928:LEU:HD13	1:A:1928:LEU:HA	1.84	0.44
2:B:73:CYS:N	2:B:78:GLN:O	2.33	0.44
6:F:460:GLU:HG3	6:F:467:ARG:HH22	1.82	0.44
6:F:581:ARG:HG2	6:F:682:LEU:HB3	1.98	0.44
6:F:698:ILE:O	6:F:701:LYS:N	2.51	0.44
6:H:464:SER:HA	6:H:467:ARG:NH1	2.32	0.44
8:I:186:GLU:OE2	8:I:197:ARG:NH1	2.51	0.44
12:N:132:LEU:HB3	12:N:149:LEU:HD13	1.99	0.44
12:N:500:ASP:OD1	12:N:500:ASP:N	2.44	0.44
13:O:129:THR:C	13:O:133:GLY:HA3	2.38	0.44
15:X:66:ASN:ND2	15:Y:268:ARG:HB3	2.33	0.44
15:X:77:TYR:CE1	15:X:107:LYS:HD3	2.53	0.44
15:Y:173:MET:O	15:Y:177:ASN:ND2	2.51	0.44
1:A:894:GLN:CD	1:A:895:TYR:H	2.21	0.44
1:A:1086:MET:SD	1:A:1560:MET:HG3	2.58	0.44
1:A:1675:GLU:HG2	1:A:1676:LEU:N	2.32	0.44
3:C:556:LEU:HD13	3:C:556:LEU:HA	1.90	0.44
6:F:519:GLU:HB3	6:F:542:THR:HG21	1.99	0.44
9:J:332:THR:H	9:J:363:LEU:HD21	1.82	0.44
9:J:386:LEU:HD12	9:J:386:LEU:H	1.82	0.44
12:N:355:ARG:HA	12:N:358:ILE:HG22	1.99	0.44
13:O:350:LEU:HD22	13:O:350:LEU:HA	1.75	0.44
3:P:365:LEU:HD12	3:P:366:GLY:H	1.83	0.44
3:P:429:ARG:HB3	3:P:432:ASP:OD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:X:140:TYR:HB2	15:X:171:ILE:HD11	1.98	0.44
15:X:325:GLU:HG3	15:X:348:HIS:CD2	2.53	0.44
1:A:430:VAL:HG13	1:A:444:PHE:HB3	1.99	0.43
1:A:877:ILE:HG23	1:A:881:ILE:HD13	1.98	0.43
6:H:723:LEU:HG	6:H:746:VAL:HG11	2.00	0.43
8:I:125:LEU:HD21	8:I:246:PRO:HA	2.00	0.43
8:I:674:VAL:HG22	8:I:705:MET:HE1	2.00	0.43
9:K:70:GLU:HG3	9:K:71:ALA:N	2.33	0.43
13:O:712:ASP:OD2	13:O:751:LEU:HB3	2.18	0.43
3:P:523:CYS:O	3:P:524:LYS:HG2	2.18	0.43
7:W:11:LEU:O	7:W:12:LYS:NZ	2.28	0.43
15:X:389:VAL:O	15:X:393:ILE:HG23	2.19	0.43
15:Y:364:LYS:HA	15:Y:364:LYS:HD2	1.87	0.43
15:Y:500:ARG:HE	15:Y:515:LEU:HD11	1.82	0.43
15:Y:527:GLU:HA	15:Y:530:ASP:HB3	1.99	0.43
1:A:953:LEU:HD22	1:A:953:LEU:HA	1.84	0.43
6:H:738:LEU:HD12	6:H:738:LEU:HA	1.88	0.43
8:I:360:LEU:HB3	13:O:437:MET:SD	2.57	0.43
8:I:644:TYR:OH	8:I:729:LYS:HA	2.18	0.43
12:N:289:PHE:C	12:N:291:LYS:H	2.22	0.43
13:O:286:ALA:HB2	13:O:298:ARG:HD2	2.00	0.43
13:O:532:VAL:O	13:O:536:THR:HG22	2.18	0.43
3:P:474:ALA:HA	3:P:477:HIS:ND1	2.32	0.43
15:X:408:ASP:O	15:X:411:GLU:HG2	2.18	0.43
1:A:432:ILE:HG12	1:A:442:LEU:HD13	2.00	0.43
1:A:1476:PHE:O	1:A:1526:VAL:HA	2.18	0.43
8:I:419:ARG:HH21	8:I:440:MET:HG3	1.83	0.43
8:I:598:MET:HB2	8:I:638:CYS:SG	2.58	0.43
9:J:376:LEU:HD23	9:J:376:LEU:HA	1.82	0.43
12:N:123:ASP:HB3	12:N:127:ARG:CZ	2.49	0.43
12:N:691:LEU:HB3	12:N:695:ARG:NH1	2.33	0.43
13:O:128:LYS:O	13:O:137:ARG:NH2	2.52	0.43
3:P:277:ARG:NH2	3:P:434:ARG:HH11	2.16	0.43
15:X:170:LYS:HG2	15:X:171:ILE:N	2.33	0.43
2:B:56:HIS:O	2:B:60:ILE:HG22	2.18	0.43
7:G:1:MET:O	7:G:3:ARG:HG3	2.17	0.43
9:J:9:ARG:HD3	9:K:162:TYR:CD1	2.53	0.43
9:K:191:SER:O	9:K:193:LEU:HG	2.18	0.43
12:N:108:LEU:HD13	12:N:239:GLN:NE2	2.34	0.43
12:N:122:LEU:HA	12:N:125:TYR:HD2	1.83	0.43
12:N:692:LEU:HD11	12:N:713:PHE:HZ	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:433:SER:HA	3:P:436:LEU:HD12	2.00	0.43
15:X:37:VAL:O	15:X:41:VAL:HG23	2.17	0.43
15:X:202:ALA:HA	15:Y:52:ASN:HD22	1.83	0.43
1:A:667:MET:O	1:A:755:LEU:HB3	2.19	0.43
1:A:1053:GLN:HB3	1:A:1062:PHE:CE1	2.53	0.43
3:C:128:LYS:HE3	11:M:10:ARG:HH22	1.83	0.43
6:H:714:PHE:CD2	6:H:746:VAL:HG22	2.53	0.43
8:I:186:GLU:HG2	8:I:197:ARG:HG3	1.99	0.43
9:J:55:ARG:NH1	9:K:261:ASP:OD2	2.42	0.43
10:L:5:ASN:OD1	10:L:5:ASN:N	2.52	0.43
12:N:345:PHE:HZ	12:N:386:LEU:HG	1.83	0.43
12:N:386:LEU:HG	12:N:399:LEU:HD23	2.00	0.43
13:O:502:GLN:C	13:O:504:ALA:H	2.22	0.43
3:P:87:TYR:CE2	3:P:117:LEU:HD12	2.53	0.43
3:P:92:ALA:O	3:P:96:VAL:HG23	2.19	0.43
15:X:377:LEU:HA	15:X:396:PHE:HE1	1.83	0.43
15:Y:57:SER:O	15:Y:61:LEU:HB2	2.18	0.43
15:Y:196:LEU:O	15:Y:200:PRO:HB3	2.18	0.43
15:Y:261:LEU:HA	15:Y:264:LYS:HG2	2.00	0.43
15:Y:320:ARG:O	15:Y:324:VAL:HG23	2.18	0.43
1:A:78:LYS:HZ2	1:A:88:ASP:HA	1.82	0.43
1:A:1078:MET:SD	1:A:1132:THR:HG23	2.59	0.43
1:A:1534:LYS:O	1:A:1537:GLN:HG2	2.19	0.43
1:A:1917:LYS:O	1:A:1920:GLN:HG2	2.18	0.43
6:F:152:PHE:HE1	6:F:470:GLY:HA2	1.84	0.43
8:I:363:LEU:HB3	8:I:390:ILE:HG12	2.00	0.43
12:N:154:HIS:HB3	12:N:158:ARG:NH2	2.34	0.43
12:N:350:ASP:N	12:N:350:ASP:OD1	2.50	0.43
12:N:362:LYS:HB2	12:N:410:LEU:HD23	2.00	0.43
1:A:31:HIS:CG	1:A:32:PRO:HD2	2.53	0.43
1:A:1437:ASN:OD1	1:A:1437:ASN:N	2.52	0.43
1:A:1627:ASN:O	1:A:1627:ASN:ND2	2.51	0.43
1:A:1895:PRO:HB2	1:A:1900:LEU:HB2	2.01	0.43
6:F:655:GLU:HA	6:F:658:PHE:HB2	2.01	0.43
8:I:238:THR:HG22	8:I:548:MET:SD	2.59	0.43
9:J:343:SER:O	9:J:346:VAL:HG12	2.19	0.43
9:K:190:LEU:O	9:K:198:GLN:NE2	2.44	0.43
9:K:270:VAL:HG22	7:W:1:MET:SD	2.59	0.43
12:N:289:PHE:O	12:N:290:HIS:HB2	2.18	0.43
12:N:691:LEU:HD23	12:N:694:ARG:HD2	2.00	0.43
3:P:440:GLY:HA2	3:P:443:TYR:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:23:ARG:NH1	7:W:23:ARG:HB2	2.33	0.43
15:X:71:PHE:HB3	15:X:75:GLN:HB2	2.00	0.43
1:A:815:ARG:HA	1:A:816:THR:HA	1.68	0.43
4:D:30:LEU:HD21	13:O:137:ARG:HG2	2.00	0.43
6:F:537:GLU:O	6:F:541:THR:N	2.45	0.43
8:I:79:LEU:HD23	8:I:79:LEU:HA	1.89	0.43
9:J:341:GLY:HA3	9:J:357:TYR:CE1	2.54	0.43
9:J:395:LEU:HD22	9:J:395:LEU:HA	1.87	0.43
12:N:659:VAL:HG13	12:N:660:THR:O	2.18	0.43
13:O:724:LEU:HD23	13:O:724:LEU:HA	1.83	0.43
15:Y:494:ASP:OD1	15:Y:494:ASP:N	2.51	0.43
1:A:1644:TYR:O	1:A:1646:GLN:N	2.52	0.43
3:C:41:GLY:HA2	3:C:44:ARG:NH1	2.34	0.43
4:D:8:LEU:HD11	13:O:424:GLN:HE22	1.84	0.43
4:D:20:LEU:HA	4:D:20:LEU:HD12	1.72	0.43
6:F:500:TRP:CH2	6:F:504:GLN:HG3	2.53	0.43
8:I:49:LEU:HD13	8:I:730:VAL:HG21	2.01	0.43
8:I:394:GLY:HA3	8:I:514:PHE:CZ	2.54	0.43
9:K:139:ILE:O	9:K:143:LEU:N	2.51	0.43
10:L:149:ARG:HA	10:L:149:ARG:HD3	1.76	0.43
13:O:79:TYR:OH	13:O:94:GLN:HG2	2.18	0.43
13:O:540:SER:O	13:O:544:VAL:HG22	2.18	0.43
13:O:599:ILE:O	13:O:602:PRO:HD2	2.19	0.43
3:P:254:LEU:O	3:P:257:VAL:HG12	2.19	0.43
15:X:510:VAL:O	15:X:514:ILE:HG12	2.19	0.43
15:Y:513:ARG:HG3	15:Y:544:LYS:HB3	2.01	0.43
1:A:626:LYS:HE2	1:A:626:LYS:HB3	1.78	0.43
1:A:1300:LEU:HD21	1:A:1586:CYS:HA	1.99	0.43
9:J:136:ARG:HG2	9:J:140:TYR:CE2	2.54	0.43
9:J:445:GLU:HG3	9:J:475:ILE:HG12	2.01	0.43
9:K:174:HIS:O	9:K:366:GLY:N	2.40	0.43
10:L:80:TYR:HA	10:L:119:TRP:HA	2.00	0.43
12:N:102:ALA:HA	12:N:103:ASP:HA	1.82	0.43
12:N:751:LEU:HA	12:N:754:PHE:HB2	2.01	0.43
12:N:759:GLN:HE21	12:N:759:GLN:HB3	1.62	0.43
13:O:26:ILE:HD11	13:O:145:LYS:HD2	2.00	0.43
13:O:108:MET:HE3	13:O:155:TYR:HD1	1.84	0.43
13:O:348:TYR:CE1	13:O:361:LEU:HD21	2.54	0.43
13:O:727:THR:HB	13:O:730:ARG:HH22	1.84	0.43
15:X:144:GLU:O	15:X:148:MET:HG2	2.19	0.43
1:A:776:ASN:ND2	1:A:778:LEU:H	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1063:ILE:HG13	1:A:1066:LYS:HE2	2.01	0.42
1:A:1165:HIS:C	1:A:1167:GLU:H	2.22	0.42
1:A:1320:ASN:HB3	1:A:1323:GLU:HB3	2.00	0.42
3:C:124:LEU:HD23	3:C:124:LEU:HA	1.73	0.42
3:C:209:LEU:HD23	3:C:209:LEU:HA	1.87	0.42
3:C:409:TYR:HD1	3:C:409:TYR:HA	1.77	0.42
8:I:722:VAL:HG12	8:I:733:VAL:HG13	2.01	0.42
9:J:331:LYS:H	9:J:331:LYS:HD2	1.84	0.42
9:K:88:GLN:O	9:K:92:VAL:HG23	2.19	0.42
11:M:10:ARG:H	11:M:10:ARG:HD2	1.84	0.42
12:N:137:ARG:O	12:N:138:LEU:HD13	2.19	0.42
13:O:362:GLU:O	13:O:366:LYS:HD3	2.18	0.42
13:O:542:GLU:HG3	13:O:546:ARG:HE	1.83	0.42
13:O:551:LEU:HB3	13:O:560:ALA:HB2	2.00	0.42
1:A:767:HIS:CD2	1:A:842:PRO:HD2	2.54	0.42
5:E:63:VAL:HG21	15:Y:364:LYS:HB2	2.01	0.42
6:F:613:LEU:HD12	6:F:679:GLN:HG2	2.00	0.42
6:H:502:LEU:HD23	6:H:502:LEU:HA	1.79	0.42
6:H:520:ARG:O	6:H:523:SER:OG	2.31	0.42
8:I:134:GLU:O	8:I:137:LEU:HB3	2.19	0.42
8:I:676:ASN:HD22	8:I:703:ARG:NH2	2.17	0.42
9:J:63:ARG:N	9:J:63:ARG:HD3	2.34	0.42
9:J:275:LEU:HD22	9:J:280:LYS:HB2	2.00	0.42
9:J:306:GLY:HA3	9:J:323:LEU:HD13	2.01	0.42
9:J:357:TYR:CE2	9:J:373:TYR:HB3	2.53	0.42
15:Y:395:HIS:HA	15:Y:398:GLU:OE2	2.18	0.42
1:A:414:THR:HA	1:A:415:GLU:HA	1.76	0.42
1:A:614:THR:HB	1:A:656:GLU:OE1	2.19	0.42
1:A:823:ILE:C	1:A:825:PRO:HD3	2.40	0.42
1:A:844:ILE:HG12	1:A:860:TYR:CZ	2.54	0.42
1:A:1269:THR:HG22	1:A:1273:LEU:HD22	2.00	0.42
2:B:13:THR:HG22	12:N:598:SER:HB2	2.01	0.42
3:C:217:GLU:H	3:C:217:GLU:CD	2.23	0.42
6:F:468:GLU:HB3	6:F:491:LEU:HD11	2.00	0.42
8:I:47:HIS:NE2	8:I:54:ARG:HG2	2.34	0.42
8:I:544:ILE:O	8:I:547:SER:HB3	2.20	0.42
8:I:613:ASN:HB2	8:I:675:TYR:CE1	2.54	0.42
8:I:645:ASP:OD2	8:I:648:THR:OG1	2.22	0.42
9:J:247:PHE:CE2	9:J:277:GLU:HG3	2.54	0.42
9:J:445:GLU:N	9:J:446:PRO:HD2	2.33	0.42
9:K:184:LEU:HD12	9:K:187:SER:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:337:ALA:HB2	12:N:364:CYS:HB3	2.01	0.42
13:O:324:LEU:HA	13:O:324:LEU:HD12	1.69	0.42
1:A:183:THR:OG1	1:A:184:LYS:N	2.52	0.42
1:A:619:GLN:OE1	13:O:556:GLN:NE2	2.46	0.42
1:A:1413:LEU:HD23	1:A:1413:LEU:HA	1.83	0.42
1:A:1596:SER:O	1:A:1597:THR:HG22	2.19	0.42
3:C:28:ASP:OD1	3:C:28:ASP:N	2.52	0.42
3:C:248:LEU:HD21	3:C:273:TYR:CE2	2.55	0.42
6:F:600:TYR:CE2	6:F:602:TYR:HB3	2.54	0.42
6:F:722:ALA:HB3	6:F:746:VAL:HG21	2.01	0.42
6:H:115:CYS:SG	6:H:145:ASN:ND2	2.92	0.42
8:I:17:LYS:NZ	8:I:51:SER:O	2.34	0.42
8:I:262:LEU:HD11	8:I:533:ILE:HG21	2.02	0.42
8:I:599:CYS:HA	8:I:617:ALA:HA	2.02	0.42
10:L:179:MET:HE2	10:L:180:TYR:CE2	2.54	0.42
12:N:431:ARG:O	12:N:433:ASP:N	2.45	0.42
12:N:659:VAL:HG22	12:N:660:THR:H	1.84	0.42
13:O:57:ARG:HB3	13:O:57:ARG:HH11	1.85	0.42
3:P:296:ARG:HD2	3:P:298:GLU:CB	2.49	0.42
3:P:435:MET:O	3:P:439:LEU:N	2.44	0.42
3:P:492:LYS:HA	3:P:495:GLN:NE2	2.35	0.42
15:X:152:ASP:OD1	15:X:152:ASP:N	2.52	0.42
1:A:250:ASN:OD1	1:A:252:ASP:N	2.51	0.42
1:A:589:ASP:N	1:A:589:ASP:OD1	2.53	0.42
1:A:967:ALA:O	1:A:1676:LEU:HD12	2.19	0.42
3:C:179:LEU:HD22	3:C:184:LEU:HD12	2.01	0.42
3:C:272:ALA:O	3:C:276:ILE:HG13	2.20	0.42
3:C:296:ARG:HD2	3:C:298:GLU:H	1.84	0.42
3:C:432:ASP:OD1	3:C:434:ARG:HG2	2.19	0.42
6:F:633:ARG:HE	6:F:664:ILE:HG23	1.83	0.42
7:G:23:ARG:HA	7:G:24:LYS:HA	1.73	0.42
6:H:143:SER:OG	6:H:166:GLN:NE2	2.53	0.42
6:H:660:LYS:HE3	6:H:660:LYS:HB2	1.88	0.42
9:J:28:LYS:HA	9:J:28:LYS:HD3	1.84	0.42
9:J:124:SER:O	9:J:127:SER:OG	2.28	0.42
9:K:497:ASN:O	9:K:501:TYR:N	2.47	0.42
12:N:383:GLU:HA	12:N:387:LEU:HD12	2.00	0.42
12:N:796:GLN:O	12:N:799:LEU:HB3	2.20	0.42
12:N:808:LEU:HD13	12:N:815:TYR:HB3	2.02	0.42
3:P:434:ARG:H	3:P:434:ARG:HG3	1.64	0.42
15:X:206:ILE:O	15:X:210:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Y:391:GLU:HA	15:Y:394:ILE:HG12	2.01	0.42
3:C:26:PHE:HB2	3:C:32:ILE:HD11	2.02	0.42
3:C:66:PRO:C	3:C:68:ALA:H	2.21	0.42
6:F:633:ARG:HH21	6:F:664:ILE:HG23	1.84	0.42
12:N:552:ALA:HA	12:N:555:HIS:HB2	2.02	0.42
3:P:180:ARG:HG3	3:P:212:LEU:HD11	2.02	0.42
1:A:1179:LEU:HD12	1:A:1179:LEU:HA	1.85	0.42
6:H:90:GLN:HE21	6:H:90:GLN:HB2	1.66	0.42
8:I:659:ARG:HA	8:I:663:ASP:HB3	2.02	0.42
8:I:723:ALA:N	8:I:732:CYS:O	2.34	0.42
9:J:476:PRO:HD3	3:P:152:ARG:HD3	2.02	0.42
9:K:292:VAL:HG21	11:M:57:TRP:HB3	2.02	0.42
13:O:94:GLN:OE1	13:O:98:LYS:NZ	2.52	0.42
13:O:666:LEU:HD12	13:O:669:LYS:HD3	2.02	0.42
1:A:1076:ARG:HB2	1:A:1555:HIS:CE1	2.55	0.42
1:A:1079:ALA:HB1	1:A:1556:LEU:HA	2.01	0.42
1:A:1276:GLU:OE2	1:A:1294:TYR:OH	2.25	0.42
1:A:1658:PRO:HG2	1:A:1663:LEU:HD13	2.01	0.42
1:A:1727:ASN:C	1:A:1729:GLU:H	2.22	0.42
3:C:548:ALA:HA	3:C:551:ARG:NH1	2.35	0.42
6:F:655:GLU:OE1	6:F:704:LEU:HB2	2.20	0.42
6:F:726:LEU:HG	6:F:743:ILE:HA	2.02	0.42
6:H:472:GLY:HA3	6:H:488:LEU:HD21	2.01	0.42
6:H:656:MET:HE3	9:K:526:TYR:CD2	2.55	0.42
9:J:211:LYS:C	9:J:213:ASN:H	2.23	0.42
9:J:231:LEU:O	9:J:234:VAL:HG22	2.20	0.42
9:J:333:TYR:CE2	9:J:335:PRO:HG2	2.55	0.42
9:K:247:PHE:CE1	9:K:277:GLU:HG3	2.54	0.42
12:N:630:LYS:O	12:N:633:ARG:HD2	2.20	0.42
13:O:127:HIS:C	13:O:129:THR:H	2.23	0.42
13:O:422:ILE:O	13:O:426:THR:HG22	2.20	0.42
1:A:1292:GLU:H	1:A:1292:GLU:HG2	1.46	0.42
1:A:1560:MET:HE1	1:A:1607:ARG:HG3	2.01	0.42
4:D:53:PRO:HB3	3:P:385:ILE:HG21	2.01	0.42
6:F:709:ARG:O	6:F:712:VAL:HG12	2.20	0.42
7:G:6:PRO:HG2	9:J:444:TRP:CZ3	2.55	0.42
6:H:61:LEU:HA	6:H:61:LEU:HD12	1.78	0.42
6:H:101:LYS:O	6:H:102:SER:O	2.37	0.42
8:I:340:SER:O	8:I:344:ILE:HG13	2.20	0.42
8:I:363:LEU:HD23	8:I:363:LEU:HA	1.79	0.42
8:I:486:LEU:O	8:I:519:ARG:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:591:LEU:HB3	8:I:596:TYR:CE1	2.55	0.42
9:J:170:LEU:HD11	9:J:176:LEU:HD11	2.01	0.42
9:K:242:TYR:OH	7:W:1:MET:O	2.30	0.42
12:N:365:LEU:HD23	12:N:365:LEU:HA	1.84	0.42
3:P:230:LYS:HE2	3:P:234:LEU:HD11	2.01	0.42
15:X:83:HIS:O	15:X:86:SER:OG	2.31	0.42
15:X:339:ALA:HB1	15:X:365:ALA:HB1	2.02	0.42
1:A:24:GLY:HA3	1:A:94:TYR:CD1	2.55	0.42
1:A:459:GLU:HB3	1:A:466:LEU:HD23	2.02	0.42
1:A:594:ARG:HB3	1:A:606:ARG:HH21	1.85	0.42
1:A:1050:ASN:OD1	1:A:1050:ASN:N	2.53	0.42
1:A:1293:SER:HB3	1:A:1600:ARG:O	2.20	0.42
1:A:1359:ASN:HD22	1:A:1359:ASN:H	1.68	0.42
1:A:1633:LEU:HA	1:A:1633:LEU:HD12	1.82	0.42
1:A:1815:LYS:NZ	1:A:1893:SER:HB3	2.34	0.42
1:A:1838:LEU:HD23	1:A:1838:LEU:HA	1.91	0.42
3:C:89:LEU:HD23	3:C:89:LEU:HA	1.82	0.42
8:I:190:TYR:CZ	8:I:253:ARG:HD3	2.55	0.42
9:J:55:ARG:NH1	9:K:264:HIS:HA	2.34	0.42
9:J:383:ASN:OD1	9:J:383:ASN:N	2.52	0.42
9:K:161:VAL:HG13	9:K:188:LEU:HD12	2.02	0.42
9:K:176:LEU:HB2	9:K:181:GLU:HG3	2.01	0.42
12:N:427:TYR:OH	12:N:431:ARG:NH2	2.53	0.42
12:N:630:LYS:HB3	12:N:630:LYS:HE2	1.92	0.42
13:O:147:SER:N	13:O:150:GLN:OE1	2.46	0.42
15:Y:236:LEU:O	15:Y:240:ILE:HG13	2.20	0.42
15:Y:445:THR:O	15:Y:449:THR:HG23	2.20	0.42
15:Y:510:VAL:O	15:Y:514:ILE:HG12	2.19	0.42
1:A:664:LEU:O	1:A:668:MET:HG2	2.20	0.41
3:C:544:GLU:HA	3:C:547:LYS:HB2	2.01	0.41
7:G:12:LYS:HB2	7:G:12:LYS:HE3	1.78	0.41
6:H:522:PHE:CD1	6:H:539:TYR:HB2	2.54	0.41
6:H:543:LEU:HB2	6:H:552:LEU:HD13	2.02	0.41
6:H:587:ILE:HG23	6:H:607:LEU:HD11	2.02	0.41
8:I:94:ASP:OD1	8:I:95:VAL:N	2.53	0.41
8:I:187:LEU:O	8:I:195:ILE:N	2.50	0.41
8:I:607:ILE:HD12	8:I:607:ILE:H	1.84	0.41
9:J:230:ASN:HB3	9:J:233:VAL:HG13	2.02	0.41
9:J:333:TYR:O	9:J:337:TRP:HD1	2.02	0.41
9:J:395:LEU:HD22	9:J:399:PRO:HA	2.02	0.41
12:N:302:LYS:HE3	12:N:302:LYS:HB3	1.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:667:LEU:HD23	12:N:670:PHE:HB3	2.01	0.41
12:N:669:TYR:HB3	12:N:676:TRP:CZ2	2.54	0.41
13:O:44:MET:HE2	13:O:60:LEU:HD11	2.02	0.41
13:O:106:LYS:HD2	13:O:107:ASP:N	2.35	0.41
15:X:187:PRO:HA	15:X:190:THR:HG22	2.02	0.41
15:X:383:LEU:CD1	15:X:388:ARG:HB2	2.50	0.41
15:X:411:GLU:HA	15:X:414:ILE:HG22	2.02	0.41
1:A:1082:VAL:O	1:A:1086:MET:HG3	2.20	0.41
1:A:1111:ALA:O	1:A:1115:ASN:N	2.51	0.41
1:A:1227:LEU:O	1:A:1230:ILE:HG22	2.20	0.41
6:F:116:PHE:CZ	6:H:15:ALA:HA	2.55	0.41
7:G:2:LEU:HD13	7:G:2:LEU:HA	1.85	0.41
6:H:707:PHE:HB2	6:H:729:LEU:HD11	2.02	0.41
8:I:128:PHE:HB2	8:I:250:ARG:HH21	1.85	0.41
8:I:613:ASN:HB2	8:I:675:TYR:HE1	1.85	0.41
9:J:34:ARG:HD3	9:J:34:ARG:HA	1.84	0.41
9:K:13:TYR:HD1	9:K:18:GLN:HB2	1.85	0.41
12:N:162:PHE:CE1	12:N:252:LEU:HD23	2.55	0.41
12:N:330:ARG:O	12:N:334:ARG:HG3	2.20	0.41
12:N:511:SER:OG	12:N:513:ASP:OD1	2.24	0.41
3:P:37:LEU:HD23	3:P:37:LEU:HA	1.89	0.41
3:P:388:TYR:O	3:P:392:ILE:HG22	2.19	0.41
15:X:37:VAL:HA	15:X:40:HIS:CD2	2.55	0.41
1:A:1074:CYS:O	1:A:1078:MET:HG2	2.19	0.41
2:B:14:TRP:HB3	12:N:595:ILE:HG23	2.02	0.41
4:D:8:LEU:HD23	4:D:8:LEU:HA	1.82	0.41
8:I:167:LEU:HD22	8:I:192:MET:SD	2.59	0.41
9:J:244:ASN:HB3	9:J:435:ILE:HD13	2.02	0.41
12:N:755:TRP:CZ2	12:N:817:LEU:HD22	2.55	0.41
13:O:89:LEU:HD12	13:O:89:LEU:HA	1.95	0.41
3:P:87:TYR:CZ	3:P:113:LYS:HD2	2.55	0.41
3:P:119:MET:HG2	3:P:158:LEU:HD21	2.02	0.41
15:X:406:ARG:HD3	15:X:406:ARG:HA	1.84	0.41
15:Y:167:ARG:HB3	15:Y:172:ASN:OD1	2.20	0.41
1:A:1140:GLY:HA3	1:A:1171:GLU:O	2.21	0.41
1:A:1192:ASN:HD22	1:A:1195:ASP:N	2.18	0.41
3:C:349:LYS:HE2	3:C:349:LYS:HB3	1.87	0.41
3:C:405:LEU:HD12	3:C:405:LEU:HA	1.86	0.41
8:I:16:GLU:HG3	8:I:742:ARG:HG3	2.01	0.41
8:I:42:GLY:HA3	8:I:66:LYS:O	2.20	0.41
8:I:45:LEU:HA	8:I:57:SER:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:568:ARG:HD2	8:I:570:PHE:CD1	2.55	0.41
9:J:155:GLU:O	9:J:159:LEU:HG	2.20	0.41
9:K:6:LEU:HD23	9:K:9:ARG:HG3	2.01	0.41
12:N:520:ARG:NH2	12:N:602:PRO:HD3	2.35	0.41
12:N:711:GLY:O	12:N:713:PHE:N	2.53	0.41
13:O:33:TYR:CE2	13:O:73:ILE:HG12	2.54	0.41
13:O:57:ARG:NH2	13:O:58:ARG:HA	2.35	0.41
13:O:681:PRO:O	13:O:682:LYS:HB2	2.19	0.41
13:O:701:PHE:O	13:O:704:VAL:HG12	2.21	0.41
3:P:158:LEU:HD23	3:P:158:LEU:HA	1.86	0.41
15:Y:57:SER:OG	15:Y:83:HIS:ND1	2.32	0.41
15:Y:177:ASN:HA	15:Y:180:LYS:HE2	2.03	0.41
15:Y:255:ILE:HG12	15:Y:277:LEU:HD11	2.01	0.41
1:A:259:TYR:HA	1:A:266:HIS:HA	2.02	0.41
1:A:274:VAL:HG21	1:A:405:PRO:HG2	2.03	0.41
1:A:863:LEU:HD23	1:A:866:ILE:HG22	2.03	0.41
1:A:1235:LEU:HA	1:A:1235:LEU:HD12	1.78	0.41
3:C:53:LYS:HD3	3:P:96:VAL:HG21	2.01	0.41
6:F:645:TYR:HE2	6:F:657:HIS:CE1	2.39	0.41
8:I:309:LEU:HD23	13:O:64:LEU:HD21	2.03	0.41
9:J:69:TYR:C	9:J:71:ALA:H	2.24	0.41
9:J:80:HIS:CD2	9:J:85:GLU:HG3	2.56	0.41
9:J:212:TYR:HB3	9:J:243:TYR:CD2	2.56	0.41
9:K:320:ARG:HG2	9:K:340:TYR:HE1	1.85	0.41
9:K:445:GLU:N	9:K:446:PRO:HD2	2.35	0.41
11:M:2:ASP:HB3	3:P:120:TYR:OH	2.21	0.41
12:N:791:ASP:HA	12:N:795:LEU:HB2	2.03	0.41
13:O:222:LEU:HB3	13:O:230:ALA:HB2	2.01	0.41
13:O:512:GLN:HB3	13:O:535:ILE:HG12	2.02	0.41
3:P:471:VAL:O	3:P:475:LYS:N	2.50	0.41
15:X:499:LEU:HD23	15:X:515:LEU:HA	2.02	0.41
3:C:231:GLU:OE2	3:C:253:ASN:ND2	2.54	0.41
8:I:42:GLY:HA2	8:I:68:VAL:HG12	2.03	0.41
8:I:312:LYS:N	13:O:127:HIS:HB2	2.35	0.41
9:J:36:GLU:HB2	9:J:39:ASP:CG	2.41	0.41
9:K:154:LYS:HE2	9:K:184:LEU:HD13	2.03	0.41
9:K:513:THR:O	9:K:517:THR:HG22	2.21	0.41
12:N:184:TYR:CZ	12:N:302:LYS:HD3	2.56	0.41
13:O:412:HIS:HB2	13:O:414:LEU:HD11	2.03	0.41
13:O:516:PHE:CE2	13:O:528:ALA:HB1	2.55	0.41
3:P:366:GLY:HA2	3:P:369:THR:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:X:57:SER:HB2	15:X:83:HIS:HB2	2.02	0.41
15:X:100:TYR:HD1	15:X:138:VAL:HG13	1.85	0.41
15:Y:167:ARG:HG2	15:Y:171:ILE:HG21	2.03	0.41
15:Y:411:GLU:HA	15:Y:414:ILE:HG22	2.02	0.41
15:Y:460:LYS:HD2	15:Y:460:LYS:N	2.35	0.41
15:Y:482:LYS:O	15:Y:486:LEU:HD22	2.21	0.41
1:A:925:SER:C	1:A:927:ALA:H	2.24	0.41
1:A:1623:ASP:O	1:A:1627:ASN:N	2.49	0.41
3:C:167:LEU:HD12	3:C:167:LEU:HA	1.91	0.41
3:C:549:LEU:O	3:C:553:ILE:HG13	2.21	0.41
5:E:53:PHE:O	5:E:56:GLU:HG3	2.21	0.41
6:F:628:ILE:HD12	6:F:638:TRP:CE2	2.56	0.41
6:H:150:SER:N	6:H:151:PRO:HD2	2.36	0.41
6:H:747:TYR:CD2	6:H:755:LEU:HB3	2.56	0.41
8:I:18:GLN:HG2	8:I:740:HIS:CD2	2.56	0.41
8:I:211:SER:HA	8:I:577:ASN:ND2	2.35	0.41
9:J:327:THR:HG1	9:J:337:TRP:HE1	1.55	0.41
9:J:376:LEU:O	9:J:380:LEU:HG	2.20	0.41
9:J:506:LEU:HD12	9:J:509:ARG:O	2.21	0.41
12:N:287:ARG:HD3	12:N:287:ARG:HA	1.84	0.41
12:N:556:PHE:HD1	12:N:600:PHE:HB3	1.86	0.41
12:N:639:HIS:HD2	12:N:662:VAL:HG22	1.85	0.41
15:X:109:ALA:O	15:X:110:LEU:HG	2.20	0.41
1:A:1485:PHE:CD1	1:A:1523:LEU:HD21	2.56	0.41
1:A:1531:GLY:HA3	1:A:1566:PHE:CZ	2.55	0.41
1:A:1637:THR:HG22	1:A:1648:LYS:HG2	2.02	0.41
1:A:1653:ALA:HB3	1:A:1654:PRO:HD3	2.02	0.41
1:A:1677:LEU:HD21	1:A:1687:LEU:HD23	2.03	0.41
1:A:1750:PHE:HB2	13:O:605:LEU:HD13	2.02	0.41
3:C:92:ALA:O	3:C:96:VAL:HG23	2.21	0.41
3:C:212:LEU:HA	3:C:212:LEU:HD23	1.83	0.41
3:C:386:GLN:HE21	3:C:386:GLN:HB2	1.48	0.41
6:H:709:ARG:HH21	6:H:713:LEU:HD11	1.86	0.41
6:H:749:LYS:HA	6:H:749:LYS:HD3	1.82	0.41
8:I:33:ASP:HB3	8:I:728:ARG:NH1	2.36	0.41
8:I:310:TRP:CE3	13:O:126:VAL:HG22	2.56	0.41
9:J:85:GLU:HB3	9:J:88:GLN:HB2	2.03	0.41
9:J:178:ALA:HA	9:J:181:GLU:OE1	2.20	0.41
12:N:605:LYS:O	12:N:638:LYS:HA	2.21	0.41
12:N:693:ARG:HA	12:N:696:MET:HE2	2.02	0.41
13:O:252:GLU:OE1	13:O:252:GLU:N	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:398:LEU:HD22	13:O:398:LEU:HA	1.86	0.41
13:O:680:GLN:HB2	13:O:681:PRO:HD2	2.03	0.41
3:P:322:ASN:O	3:P:326:ILE:HG13	2.21	0.41
15:X:170:LYS:HG2	15:X:171:ILE:HD12	2.02	0.41
15:X:494:ASP:OD1	15:X:494:ASP:N	2.54	0.41
1:A:1370:ALA:O	1:A:1374:ILE:HG13	2.21	0.41
1:A:1472:LEU:HD12	1:A:1472:LEU:HA	1.89	0.41
1:A:1540:ARG:NH1	1:A:1544:MET:SD	2.94	0.41
1:A:1560:MET:HE1	1:A:1607:ARG:CG	2.51	0.41
1:A:1824:ARG:NE	12:N:142:MET:HA	2.35	0.41
1:A:1845:LEU:N	1:A:1846:PRO:HD2	2.36	0.41
2:B:13:THR:OG1	12:N:638:LYS:HB2	2.20	0.41
5:E:82:LEU:HB3	6:H:577:PHE:HE2	1.86	0.41
5:E:94:TRP:CE2	6:F:592:ARG:HD3	2.56	0.41
6:F:155:LEU:HD12	6:F:155:LEU:HA	1.85	0.41
6:F:648:GLN:HB3	6:F:650:LYS:HG2	2.03	0.41
6:H:144:LEU:HD23	6:H:144:LEU:HA	1.90	0.41
6:H:553:SER:HA	6:H:576:CYS:SG	2.60	0.41
8:I:209:CYS:O	8:I:217:LEU:HD12	2.21	0.41
8:I:232:SER:HA	8:I:555:PRO:HA	2.03	0.41
8:I:285:SER:OG	8:I:286:ARG:N	2.54	0.41
8:I:645:ASP:OD1	8:I:647:GLU:N	2.40	0.41
9:J:340:TYR:O	9:J:343:SER:OG	2.27	0.41
9:J:385:LYS:O	9:J:389:ARG:HG2	2.21	0.41
9:J:416:GLY:HA2	9:J:418:TRP:CZ3	2.56	0.41
9:J:527:ILE:HD13	9:J:527:ILE:HA	1.83	0.41
12:N:161:LEU:HD23	12:N:161:LEU:HA	1.90	0.41
12:N:663:GLN:HE22	12:N:698:VAL:HG11	1.86	0.41
13:O:223:LEU:HD23	13:O:223:LEU:HA	1.88	0.41
13:O:732:ARG:HD3	13:O:732:ARG:HA	1.80	0.41
3:P:488:GLN:OE1	3:P:518:GLN:NE2	2.54	0.41
15:X:77:TYR:CZ	15:X:107:LYS:HD3	2.56	0.41
15:X:294:PHE:HE2	15:X:307:GLY:HA3	1.85	0.41
15:Y:251:ASN:O	15:Y:255:ILE:HG22	2.21	0.41
15:Y:417:TYR:HB3	15:Y:426:ALA:HB2	2.03	0.41
1:A:159:ILE:HB	1:A:173:LEU:HD21	2.03	0.41
1:A:271:LEU:HD12	1:A:271:LEU:HA	1.85	0.41
1:A:1040:LEU:HG	1:A:1543:HIS:ND1	2.36	0.41
1:A:1155:SER:HB3	1:A:1184:HIS:ND1	2.36	0.41
1:A:1821:PHE:HZ	1:A:1839:PHE:HD2	1.69	0.41
3:C:460:TYR:CE1	3:C:470:LEU:HD11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:523:CYS:O	3:C:524:LYS:HG2	2.21	0.41
5:E:67:LEU:HD22	15:Y:342:TRP:HH2	1.86	0.41
6:F:16:LEU:HD21	6:F:50:ARG:HD2	2.02	0.41
8:I:23:ILE:HA	8:I:39:ASN:HA	2.03	0.41
8:I:491:ASN:ND2	8:I:494:GLY:HA3	2.30	0.41
9:J:143:LEU:HD12	9:J:143:LEU:HA	1.95	0.41
9:K:491:LEU:HD22	7:W:22:ILE:HG21	2.03	0.41
10:L:29:ALA:HB2	10:L:68:PHE:HD2	1.86	0.41
12:N:362:LYS:HD2	12:N:410:LEU:H	1.86	0.41
12:N:433:ASP:O	12:N:435:VAL:HG23	2.21	0.41
13:O:152:PHE:CD1	3:P:321:HIS:HB2	2.56	0.41
13:O:561:HIS:CE1	13:O:565:GLN:HE21	2.38	0.41
13:O:664:MET:HB2	13:O:697:ALA:HB2	2.03	0.41
3:P:106:LEU:HB3	3:P:118:TYR:HB2	2.02	0.41
15:X:499:LEU:HD21	15:X:514:ILE:HG22	2.03	0.41
15:X:515:LEU:HA	15:X:515:LEU:HD23	1.92	0.41
1:A:635:VAL:O	1:A:639:VAL:HG12	2.20	0.40
1:A:1377:LYS:HG2	1:A:1416:TRP:CG	2.56	0.40
1:A:1762:GLY:C	1:A:1764:LYS:H	2.24	0.40
6:F:30:ARG:HH21	6:H:498:THR:HG21	1.86	0.40
6:F:147:PHE:O	6:H:27:LEU:HD11	2.21	0.40
6:F:655:GLU:OE2	6:F:705:CYS:N	2.42	0.40
6:H:639:TYR:OH	6:H:643:MET:SD	2.68	0.40
9:J:10:VAL:HG21	9:J:26:ALA:HB2	2.03	0.40
9:K:330:GLU:HG3	9:K:333:TYR:HB2	2.03	0.40
15:Y:173:MET:HG2	15:Y:177:ASN:HD21	1.86	0.40
15:Y:426:ALA:HA	15:Y:429:MET:HE2	2.03	0.40
1:A:15:ARG:NH1	1:A:610:PRO:HA	2.37	0.40
1:A:370:ASN:HB2	3:C:400:ARG:CB	2.51	0.40
1:A:1090:PHE:CE2	1:A:1149:PRO:HG3	2.56	0.40
1:A:1457:LEU:HD12	1:A:1457:LEU:HA	1.80	0.40
1:A:1466:ALA:HB2	1:A:1515:CYS:HB2	2.03	0.40
2:B:6:LYS:HB2	12:N:647:ASP:HB2	2.03	0.40
2:B:38:LYS:O	12:N:600:PHE:HZ	2.04	0.40
6:F:55:TYR:HA	6:F:82:LEU:HD21	2.03	0.40
6:F:535:GLY:O	6:F:538:ILE:HG12	2.21	0.40
8:I:188:TYR:CE2	8:I:194:LYS:HB2	2.56	0.40
8:I:246:PRO:O	8:I:250:ARG:HG2	2.21	0.40
12:N:181:LEU:O	12:N:185:MET:HG2	2.20	0.40
12:N:272:ARG:HD3	12:N:292:TRP:CE2	2.56	0.40
12:N:612:PRO:HG2	12:N:615:ILE:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:79:TYR:OH	13:O:94:GLN:HA	2.21	0.40
13:O:275:LEU:HD12	13:O:275:LEU:HA	1.79	0.40
3:P:232:PHE:HZ	3:P:259:PHE:CE1	2.40	0.40
3:P:491:ILE:HD12	3:P:518:GLN:HB3	2.03	0.40
15:Y:73:PRO:HA	15:Y:76:LYS:HD2	2.03	0.40
1:A:18:GLN:HE21	1:A:18:GLN:HB2	1.67	0.40
1:A:94:TYR:CE1	1:A:96:ALA:HB2	2.56	0.40
1:A:795:ARG:HH21	1:A:814:VAL:HG22	1.85	0.40
1:A:879:LEU:O	1:A:926:LEU:HD11	2.21	0.40
1:A:1032:LEU:HG	12:N:483:ASP:CB	2.52	0.40
1:A:1290:ASP:OD1	1:A:1290:ASP:N	2.54	0.40
1:A:1300:LEU:HD12	1:A:1300:LEU:HA	1.71	0.40
1:A:1476:PHE:HB2	1:A:1526:VAL:HG12	2.02	0.40
1:A:1783:THR:O	1:A:1783:THR:OG1	2.23	0.40
2:B:8:TRP:HB3	12:N:589:PHE:CD2	2.56	0.40
3:C:331:VAL:HG13	3:C:332:GLU:OE1	2.22	0.40
3:C:414:MET:HE3	3:C:417:TYR:CG	2.56	0.40
3:C:531:THR:HA	3:C:534:GLN:HG2	2.04	0.40
6:H:107:VAL:HG22	6:H:114:ALA:HB1	2.03	0.40
6:H:717:GLU:HA	6:H:719:TYR:CE1	2.56	0.40
9:J:276:VAL:HG21	9:J:307:CYS:HB3	2.03	0.40
12:N:433:ASP:O	12:N:435:VAL:N	2.54	0.40
15:X:295:GLU:OE2	15:X:311:TYR:OH	2.29	0.40
15:Y:159:LEU:HB2	15:Y:175:LEU:HD13	2.02	0.40
15:Y:218:GLU:O	15:Y:222:MET:HG2	2.21	0.40
1:A:1642:GLN:HG3	1:A:1643:TRP:CD2	2.57	0.40
1:A:1725:ASN:C	1:A:1727:ASN:H	2.24	0.40
3:C:234:LEU:HD12	3:C:234:LEU:HA	1.89	0.40
6:F:27:LEU:HD11	6:H:147:PHE:O	2.20	0.40
6:F:149:TRP:NE1	6:F:153:GLU:OE2	2.54	0.40
6:F:479:TYR:CE2	6:F:664:ILE:HG22	2.56	0.40
6:F:622:ALA:O	6:F:626:ASN:N	2.49	0.40
6:H:580:GLN:HE21	6:H:580:GLN:HB3	1.67	0.40
6:H:748:LYS:HG3	6:H:756:ALA:HB1	2.03	0.40
8:I:119:THR:O	8:I:172:ARG:NE	2.47	0.40
9:J:211:LYS:O	9:J:213:ASN:N	2.55	0.40
10:L:25:ILE:HG13	10:L:160:THR:HB	2.03	0.40
10:L:54:TRP:O	10:L:152:HIS:HA	2.22	0.40
13:O:56:GLU:HG3	13:O:86:CYS:SG	2.62	0.40
15:X:383:LEU:CD1	15:X:391:GLU:HB2	2.50	0.40
15:Y:84:ALA:HA	15:Y:87:LEU:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Y:246:VAL:HG22	15:Y:280:LEU:HD21	2.04	0.40
1:A:19:GLU:HA	1:A:605:VAL:HG12	2.03	0.40
1:A:1032:LEU:HD12	1:A:1032:LEU:O	2.22	0.40
1:A:1046:PRO:HG2	1:A:1110:ARG:HD3	2.04	0.40
1:A:1406:LEU:HD23	1:A:1406:LEU:HA	1.96	0.40
5:E:92:ASP:HA	6:F:595:GLN:HE22	1.87	0.40
6:F:133:LYS:HD2	15:Y:504:ALA:O	2.21	0.40
6:F:736:GLU:OE1	6:F:737:SER:N	2.54	0.40
8:I:66:LYS:N	8:I:86:ASP:OD2	2.35	0.40
8:I:73:TRP:CD2	8:I:80:LEU:HD13	2.57	0.40
8:I:618:ILE:HD13	8:I:618:ILE:HA	1.94	0.40
8:I:624:THR:OG1	8:I:625:TYR:N	2.55	0.40
9:J:475:ILE:HD12	9:J:478:ASN:HB2	2.03	0.40
9:K:87:GLN:HB2	9:K:143:LEU:HD11	2.04	0.40
12:N:527:LEU:HD12	12:N:601:TRP:CZ2	2.57	0.40
15:X:242:ALA:O	15:X:246:VAL:HG23	2.21	0.40
15:Y:331:LEU:HD12	15:Y:344:VAL:HG11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1551/1944 (80%)	1377 (89%)	171 (11%)	3 (0%)	47	78
2	B	83/84 (99%)	78 (94%)	5 (6%)	0	100	100
3	C	520/597 (87%)	494 (95%)	26 (5%)	0	100	100
3	P	486/597 (81%)	459 (94%)	27 (6%)	0	100	100
4	D	53/121 (44%)	46 (87%)	7 (13%)	0	100	100
5	E	54/110 (49%)	54 (100%)	0	0	100	100
6	F	454/824 (55%)	428 (94%)	26 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	H	484/824 (59%)	451 (93%)	31 (6%)	2 (0%)	34 69
7	G	23/85 (27%)	23 (100%)	0	0	100 100
7	W	24/85 (28%)	23 (96%)	1 (4%)	0	100 100
8	I	717/808 (89%)	664 (93%)	50 (7%)	3 (0%)	34 69
9	J	500/620 (81%)	469 (94%)	31 (6%)	0	100 100
9	K	489/620 (79%)	462 (94%)	27 (6%)	0	100 100
10	L	180/185 (97%)	163 (91%)	17 (9%)	0	100 100
11	M	55/74 (74%)	50 (91%)	5 (9%)	0	100 100
12	N	658/822 (80%)	587 (89%)	69 (10%)	2 (0%)	41 74
13	O	682/755 (90%)	644 (94%)	36 (5%)	2 (0%)	41 74
14	T	13/15 (87%)	10 (77%)	3 (23%)	0	100 100
15	X	480/599 (80%)	458 (95%)	21 (4%)	1 (0%)	47 78
15	Y	492/599 (82%)	471 (96%)	17 (4%)	4 (1%)	19 56
All	All	7998/10368 (77%)	7411 (93%)	570 (7%)	17 (0%)	50 78

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	I	452	LEU
1	A	276	SER
6	H	103	HIS
6	H	147	PHE
13	O	130	SER
15	X	456	VAL
1	A	1645	GLU
8	I	451	PHE
8	I	489	PRO
12	N	531	PHE
13	O	656	ALA
1	A	1721	GLN
12	N	485	VAL
15	Y	214	VAL
15	Y	215	LYS
15	Y	456	VAL
15	Y	200	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1252/1720 (73%)	1108 (88%)	144 (12%)	5 28
2	B	65/75 (87%)	59 (91%)	6 (9%)	9 36
3	C	452/520 (87%)	423 (94%)	29 (6%)	17 49
3	P	422/520 (81%)	395 (94%)	27 (6%)	17 49
4	D	46/115 (40%)	42 (91%)	4 (9%)	10 39
5	E	47/89 (53%)	43 (92%)	4 (8%)	10 40
6	F	371/727 (51%)	347 (94%)	24 (6%)	17 48
6	H	408/727 (56%)	380 (93%)	28 (7%)	15 47
7	G	25/77 (32%)	21 (84%)	4 (16%)	2 16
7	W	23/77 (30%)	21 (91%)	2 (9%)	10 39
8	I	607/730 (83%)	562 (93%)	45 (7%)	13 44
9	J	425/548 (78%)	388 (91%)	37 (9%)	10 39
9	K	423/548 (77%)	395 (93%)	28 (7%)	16 48
10	L	155/170 (91%)	145 (94%)	10 (6%)	17 48
11	M	52/67 (78%)	44 (85%)	8 (15%)	2 17
12	N	547/724 (76%)	496 (91%)	51 (9%)	9 36
13	O	573/650 (88%)	514 (90%)	59 (10%)	7 31
14	T	1/2 (50%)	1 (100%)	0	100 100
15	X	406/513 (79%)	385 (95%)	21 (5%)	23 55
15	Y	417/513 (81%)	386 (93%)	31 (7%)	13 44
All	All	6717/9112 (74%)	6155 (92%)	562 (8%)	14 40

All (562) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	92	GLU
1	A	127	LEU

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Mol	Chain	Res	Type
1	A	134	SER
1	A	151	ILE
1	A	161	MET
1	A	168	ASP
1	A	177	VAL
1	A	183	THR
1	A	242	HIS
1	A	246	ILE
1	A	262	VAL
1	A	271	LEU
1	A	273	ARG
1	A	412	LEU
1	A	429	LYS
1	A	440	LYS
1	A	450	LEU
1	A	456	LYS
1	A	459	GLU
1	A	466	LEU
1	A	474	ILE
1	A	482	VAL
1	A	485	ILE
1	A	491	LEU
1	A	498	VAL
1	A	503	VAL
1	A	509	VAL
1	A	511	ILE
1	A	583	TYR
1	A	591	VAL
1	A	595	VAL
1	A	612	ILE
1	A	614	THR
1	A	628	ILE
1	A	633	ILE
1	A	665	MET
1	A	754	LEU
1	A	770	TYR
1	A	777	THR
1	A	783	ILE
1	A	786	LEU
1	A	797	LEU
1	A	804	ASP
1	A	813	LEU

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Mol	Chain	Res	Type
1	A	814	VAL
1	A	816	THR
1	A	819	GLN
1	A	837	PHE
1	A	844	ILE
1	A	862	TYR
1	A	871	ARG
1	A	894	GLN
1	A	897	THR
1	A	942	ARG
1	A	945	GLU
1	A	953	LEU
1	A	957	ASP
1	A	970	TRP
1	A	1014	ASP
1	A	1024	MET
1	A	1034	VAL
1	A	1035	GLN
1	A	1036	ASP
1	A	1042	GLN
1	A	1047	VAL
1	A	1049	VAL
1	A	1088	THR
1	A	1108	THR
1	A	1114	ARG
1	A	1125	ILE
1	A	1132	THR
1	A	1153	ILE
1	A	1168	LEU
1	A	1176	LEU
1	A	1181	LEU
1	A	1216	LYS
1	A	1217	LEU
1	A	1239	THR
1	A	1264	THR
1	A	1273	LEU
1	A	1274	LEU
1	A	1279	ARG
1	A	1284	GLU
1	A	1292	GLU
1	A	1302	LEU
1	A	1309	HIS

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Mol	Chain	Res	Type
1	A	1321	VAL
1	A	1325	LEU
1	A	1359	ASN
1	A	1361	ASP
1	A	1371	LEU
1	A	1376	LEU
1	A	1379	ASN
1	A	1386	TRP
1	A	1392	THR
1	A	1404	LEU
1	A	1405	LEU
1	A	1417	ASP
1	A	1430	VAL
1	A	1461	HIS
1	A	1482	LEU
1	A	1496	MET
1	A	1499	LEU
1	A	1503	ASN
1	A	1523	LEU
1	A	1533	LEU
1	A	1538	LEU
1	A	1540	ARG
1	A	1546	THR
1	A	1562	LEU
1	A	1565	LEU
1	A	1574	LEU
1	A	1588	LEU
1	A	1597	THR
1	A	1603	LEU
1	A	1607	ARG
1	A	1634	LEU
1	A	1642	GLN
1	A	1645	GLU
1	A	1647	THR
1	A	1655	THR
1	A	1666	ILE
1	A	1674	TRP
1	A	1680	LEU
1	A	1684	THR
1	A	1693	LYS
1	A	1697	LEU
1	A	1705	GLN

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Mol	Chain	Res	Type
1	A	1783	THR
1	A	1785	GLU
1	A	1786	MET
1	A	1787	LEU
1	A	1798	ARG
1	A	1805	MET
1	A	1813	GLN
1	A	1815	LYS
1	A	1835	LYS
1	A	1851	THR
1	A	1866	MET
1	A	1887	CYS
1	A	1911	PHE
1	A	1920	GLN
1	A	1935	LEU
2	B	13	THR
2	B	14	TRP
2	B	15	LEU
2	B	16	TRP
2	B	65	HIS
2	B	75	MET
3	C	26	PHE
3	C	85	ASP
3	C	89	LEU
3	C	97	LYS
3	C	119	MET
3	C	133	GLU
3	C	138	LEU
3	C	141	LEU
3	C	182	LEU
3	C	183	ASP
3	C	199	LEU
3	C	232	PHE
3	C	237	ILE
3	C	244	ILE
3	C	305	ASN
3	C	331	VAL
3	C	343	LEU
3	C	358	LEU
3	C	376	MET
3	C	386	GLN
3	C	389	ARG

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Mol	Chain	Res	Type
3	C	407	GLN
3	C	409	TYR
3	C	462	VAL
3	C	472	LYS
3	C	490	TYR
3	C	536	CYS
3	C	543	ARG
3	C	551	ARG
4	D	20	LEU
4	D	32	GLN
4	D	35	GLN
4	D	49	ASN
5	E	59	PHE
5	E	69	GLN
5	E	71	LYS
5	E	99	ILE
6	F	23	ASP
6	F	30	ARG
6	F	43	LEU
6	F	68	THR
6	F	98	ASN
6	F	165	ASP
6	F	169	LYS
6	F	485	ILE
6	F	487	ILE
6	F	494	HIS
6	F	498	THR
6	F	507	ARG
6	F	568	GLU
6	F	611	PHE
6	F	616	GLU
6	F	617	LEU
6	F	621	LEU
6	F	634	HIS
6	F	636	ASN
6	F	646	TYR
6	F	712	VAL
6	F	726	LEU
6	F	732	ILE
6	F	747	TYR
7	G	4	ARG
7	G	5	LYS

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Mol	Chain	Res	Type
7	G	11	LEU
7	G	14	ASP
6	H	9	GLN
6	H	23	ASP
6	H	30	ARG
6	H	43	LEU
6	H	61	LEU
6	H	68	THR
6	H	71	CYS
6	H	81	ASP
6	H	82	LEU
6	H	99	LYS
6	H	104	ASP
6	H	128	THR
6	H	147	PHE
6	H	165	ASP
6	H	480	ASN
6	H	517	GLN
6	H	530	ASN
6	H	537	GLU
6	H	563	ASP
6	H	568	GLU
6	H	584	ASP
6	H	614	THR
6	H	667	GLN
6	H	686	GLU
6	H	705	CYS
6	H	729	LEU
6	H	742	LEU
6	H	754	HIS
8	I	26	LEU
8	I	37	LEU
8	I	68	VAL
8	I	86	ASP
8	I	92	LEU
8	I	116	MET
8	I	118	VAL
8	I	145	LEU
8	I	174	ASN
8	I	231	VAL
8	I	237	GLU
8	I	254	LYS

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Mol	Chain	Res	Type
8	I	267	LEU
8	I	286	ARG
8	I	302	ASP
8	I	308	LEU
8	I	318	GLN
8	I	320	LEU
8	I	332	LYS
8	I	338	GLU
8	I	341	TYR
8	I	357	GLU
8	I	358	SER
8	I	360	LEU
8	I	366	LEU
8	I	372	TRP
8	I	373	LYS
8	I	404	LEU
8	I	418	PHE
8	I	425	MET
8	I	440	MET
8	I	452	LEU
8	I	454	GLU
8	I	477	GLN
8	I	519	ARG
8	I	526	LYS
8	I	531	ASN
8	I	571	LYS
8	I	591	LEU
8	I	595	LEU
8	I	605	THR
8	I	607	ILE
8	I	656	THR
8	I	663	ASP
8	I	729	LYS
9	J	32	LEU
9	J	39	ASP
9	J	50	THR
9	J	63	ARG
9	J	162	TYR
9	J	170	LEU
9	J	185	LEU
9	J	196	GLU
9	J	206	GLU

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Mol	Chain	Res	Type
9	J	207	ASN
9	J	214	LYS
9	J	220	ILE
9	J	229	GLU
9	J	233	VAL
9	J	248	LYS
9	J	259	GLU
9	J	267	CYS
9	J	293	ASP
9	J	323	LEU
9	J	329	LEU
9	J	331	LYS
9	J	340	TYR
9	J	358	PHE
9	J	362	GLN
9	J	383	ASN
9	J	385	LYS
9	J	395	LEU
9	J	407	GLU
9	J	418	TRP
9	J	429	LEU
9	J	437	ASN
9	J	442	ASP
9	J	445	GLU
9	J	472	LEU
9	J	477	GLN
9	J	497	ASN
9	J	510	ARG
9	K	9	ARG
9	K	27	ASP
9	K	34	ARG
9	K	39	ASP
9	K	50	THR
9	K	63	ARG
9	K	159	LEU
9	K	165	GLU
9	K	193	LEU
9	K	214	LYS
9	K	225	ASP
9	K	284	LEU
9	K	289	HIS
9	K	290	LYS

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Mol	Chain	Res	Type
9	K	310	LEU
9	K	331	LYS
9	K	340	TYR
9	K	343	SER
9	K	352	GLN
9	K	358	PHE
9	K	362	GLN
9	K	376	LEU
9	K	378	TYR
9	K	418	TRP
9	K	429	LEU
9	K	432	ILE
9	K	438	GLU
9	K	497	ASN
10	L	23	ARG
10	L	42	VAL
10	L	43	ASP
10	L	45	LEU
10	L	49	ASN
10	L	65	ASN
10	L	83	TYR
10	L	100	ASN
10	L	144	ASN
10	L	154	ARG
11	M	10	ARG
11	M	16	ASP
11	M	17	ASP
11	M	33	LEU
11	M	52	GLU
11	M	58	THR
11	M	63	GLN
11	M	64	TYR
12	N	67	LEU
12	N	108	LEU
12	N	111	LEU
12	N	123	ASP
12	N	135	TRP
12	N	137	ARG
12	N	141	LEU
12	N	153	VAL
12	N	235	GLN
12	N	237	LEU

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Mol	Chain	Res	Type
12	N	249	ARG
12	N	287	ARG
12	N	302	LYS
12	N	323	ARG
12	N	366	GLU
12	N	371	ARG
12	N	374	LEU
12	N	386	LEU
12	N	392	ASN
12	N	416	ILE
12	N	425	ARG
12	N	480	TRP
12	N	481	VAL
12	N	526	ARG
12	N	529	HIS
12	N	530	GLN
12	N	531	PHE
12	N	533	PHE
12	N	534	SER
12	N	537	ARG
12	N	554	MET
12	N	555	HIS
12	N	564	MET
12	N	589	PHE
12	N	592	TYR
12	N	619	LEU
12	N	622	TYR
12	N	643	LEU
12	N	645	THR
12	N	646	MET
12	N	667	LEU
12	N	670	PHE
12	N	673	GLN
12	N	678	LEU
12	N	681	LEU
12	N	685	VAL
12	N	705	LEU
12	N	773	ILE
12	N	790	ILE
12	N	795	LEU
12	N	814	VAL
13	O	35	ILE

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Mol	Chain	Res	Type
13	O	56	GLU
13	O	57	ARG
13	O	59	ARG
13	O	60	LEU
13	O	74	THR
13	O	86	CYS
13	O	93	VAL
13	O	98	LYS
13	O	106	LYS
13	O	110	GLN
13	O	117	ASP
13	O	138	HIS
13	O	237	GLN
13	O	250	PHE
13	O	275	LEU
13	O	350	LEU
13	O	354	ARG
13	O	356	ASP
13	O	359	VAL
13	O	360	LEU
13	O	363	HIS
13	O	398	LEU
13	O	402	LEU
13	O	403	LYS
13	O	408	LEU
13	O	414	LEU
13	O	426	THR
13	O	434	ARG
13	O	461	ASN
13	O	463	THR
13	O	517	ASP
13	O	532	VAL
13	O	549	VAL
13	O	550	VAL
13	O	551	LEU
13	O	567	LEU
13	O	578	GLU
13	O	579	MET
13	O	581	ILE
13	O	583	VAL
13	O	585	LEU
13	O	590	LEU

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Mol	Chain	Res	Type
13	O	625	LEU
13	O	636	ILE
13	O	654	ASP
13	O	657	ILE
13	O	678	TYR
13	O	682	LYS
13	O	691	ILE
13	O	694	LEU
13	O	704	VAL
13	O	710	ILE
13	O	713	VAL
13	O	717	GLN
13	O	733	CYS
13	O	735	MET
13	O	751	LEU
13	O	752	ILE
3	P	30	ARG
3	P	36	LEU
3	P	78	GLU
3	P	82	GLN
3	P	89	LEU
3	P	101	ARG
3	P	117	LEU
3	P	122	ARG
3	P	131	ASP
3	P	160	LYS
3	P	172	LEU
3	P	174	LEU
3	P	175	TYR
3	P	183	ASP
3	P	237	ILE
3	P	244	ILE
3	P	286	PHE
3	P	290	ARG
3	P	303	PHE
3	P	310	ARG
3	P	343	LEU
3	P	365	LEU
3	P	378	MET
3	P	392	ILE
3	P	432	ASP
3	P	435	MET

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Mol	Chain	Res	Type
3	P	495	GLN
7	W	14	ASP
7	W	23	ARG
15	X	49	LEU
15	X	152	ASP
15	X	154	ASP
15	X	168	THR
15	X	170	LYS
15	X	229	THR
15	X	255	ILE
15	X	270	ASN
15	X	272	ASP
15	X	286	ASP
15	X	303	TYR
15	X	304	LEU
15	X	350	PHE
15	X	386	MET
15	X	414	ILE
15	X	432	ASN
15	X	442	GLN
15	X	444	LEU
15	X	486	LEU
15	X	499	LEU
15	X	503	LEU
15	Y	52	ASN
15	Y	67	ASN
15	Y	70	LEU
15	Y	94	ARG
15	Y	95	ASN
15	Y	106	GLN
15	Y	153	LYS
15	Y	154	ASP
15	Y	213	SER
15	Y	229	THR
15	Y	255	ILE
15	Y	299	MET
15	Y	301	ASP
15	Y	304	LEU
15	Y	323	ASP
15	Y	337	GLN
15	Y	354	ARG
15	Y	401	ARG

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Mol	Chain	Res	Type
15	Y	414	ILE
15	Y	423	ILE
15	Y	445	THR
15	Y	456	VAL
15	Y	465	LEU
15	Y	486	LEU
15	Y	488	ARG
15	Y	505	ASN
15	Y	515	LEU
15	Y	524	GLU
15	Y	530	ASP
15	Y	551	LYS
15	Y	552	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (184) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	125	GLN
1	A	162	HIS
1	A	215	HIS
1	A	367	GLN
1	A	374	HIS
1	A	411	HIS
1	A	451	GLN
1	A	473	ASN
1	A	601	ASN
1	A	623	GLN
1	A	636	GLN
1	A	654	HIS
1	A	776	ASN
1	A	819	GLN
1	A	981	GLN
1	A	1106	ASN
1	A	1124	ASN
1	A	1138	HIS
1	A	1192	ASN
1	A	1231	HIS
1	A	1247	HIS
1	A	1481	ASN
1	A	1511	ASN
1	A	1591	HIS

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Mol	Chain	Res	Type
1	A	1602	HIS
1	A	1604	GLN
1	A	1642	GLN
1	A	1705	GLN
1	A	1795	GLN
1	A	1920	GLN
2	B	31	ASN
2	B	50	GLN
2	B	71	GLN
3	C	71	GLN
3	C	82	GLN
3	C	163	GLN
3	C	197	HIS
3	C	202	HIS
3	C	249	GLN
3	C	252	GLN
3	C	274	HIS
3	C	305	ASN
3	C	321	HIS
3	C	361	ASN
3	C	386	GLN
3	C	407	GLN
3	C	427	GLN
3	C	431	ASN
3	C	479	GLN
3	C	488	GLN
3	C	518	GLN
3	C	552	GLN
4	D	31	GLN
4	D	38	GLN
4	D	49	ASN
6	F	486	ASN
6	F	494	HIS
6	F	495	HIS
6	F	547	GLN
6	F	595	GLN
6	F	667	GLN
6	F	702	ASN
6	H	14	GLN
6	H	90	GLN
6	H	145	ASN
6	H	166	GLN

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Mol	Chain	Res	Type
6	H	480	ASN
6	H	497	ASN
6	H	517	GLN
6	H	545	HIS
6	H	580	GLN
6	H	583	HIS
6	H	595	GLN
6	H	609	HIS
6	H	636	ASN
6	H	648	GLN
6	H	657	HIS
6	H	667	GLN
6	H	754	HIS
8	I	21	GLN
8	I	114	HIS
8	I	323	ASN
8	I	401	ASN
8	I	477	GLN
8	I	684	GLN
8	I	740	HIS
9	J	16	GLN
9	J	18	GLN
9	J	38	GLN
9	J	80	HIS
9	J	88	GLN
9	J	271	HIS
9	J	352	GLN
9	J	362	GLN
9	J	406	HIS
9	J	477	GLN
9	J	503	HIS
9	K	18	GLN
9	K	38	GLN
9	K	54	HIS
9	K	271	HIS
9	K	352	GLN
9	K	362	GLN
10	L	28	GLN
10	L	103	HIS
10	L	104	ASN
10	L	146	GLN
10	L	155	GLN

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Mol	Chain	Res	Type
11	M	53	GLN
11	M	63	GLN
12	N	80	GLN
12	N	97	GLN
12	N	170	GLN
12	N	174	GLN
12	N	239	GLN
12	N	329	GLN
12	N	372	GLN
12	N	530	GLN
12	N	541	ASN
12	N	722	GLN
12	N	759	GLN
13	O	62	GLN
13	O	69	GLN
13	O	88	GLN
13	O	219	GLN
13	O	237	GLN
13	O	242	ASN
13	O	318	GLN
13	O	319	GLN
13	O	342	HIS
13	O	370	HIS
13	O	382	GLN
13	O	409	HIS
13	O	424	GLN
13	O	440	GLN
13	O	441	GLN
13	O	443	GLN
13	O	460	GLN
13	O	461	ASN
13	O	472	HIS
13	O	565	GLN
13	O	617	GLN
13	O	680	GLN
13	O	717	GLN
13	O	741	HIS
3	P	71	GLN
3	P	163	GLN
3	P	197	HIS
3	P	268	GLN
3	P	299	ASN

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Mol	Chain	Res	Type
3	P	305	ASN
3	P	355	GLN
3	P	361	ASN
3	P	386	GLN
3	P	390	HIS
3	P	426	HIS
3	P	427	GLN
3	P	479	GLN
3	P	485	GLN
3	P	488	GLN
3	P	495	GLN
3	P	518	GLN
15	X	78	GLN
15	X	151	GLN
15	X	184	GLN
15	X	289	ASN
15	X	298	GLN
15	X	337	GLN
15	X	338	HIS
15	X	371	ASN
15	X	432	ASN
15	X	506	GLN
15	X	512	HIS
15	Y	50	HIS
15	Y	66	ASN
15	Y	298	GLN
15	Y	337	GLN
15	Y	367	GLN
15	Y	385	ASN
15	Y	506	GLN
15	Y	512	HIS
15	Y	531	GLN
15	Y	543	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

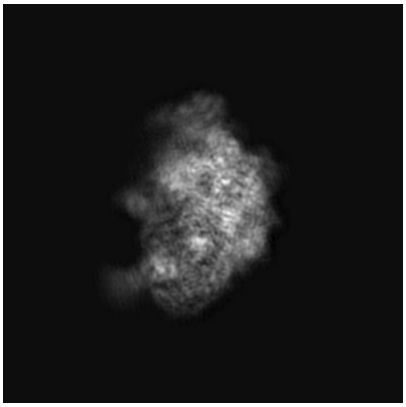
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10536. These allow visual inspection of the internal detail of the map and identification of artifacts.

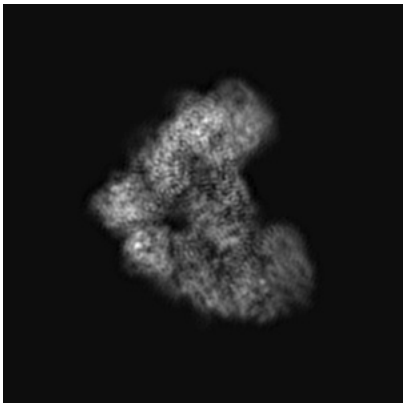
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

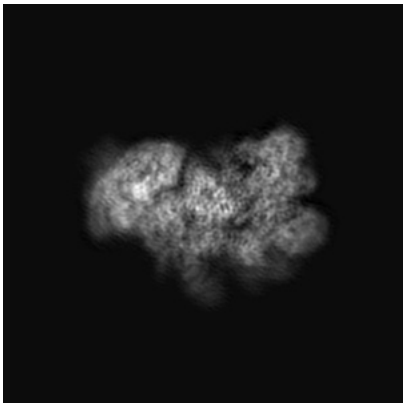
6.1.1 Primary map



X



Y

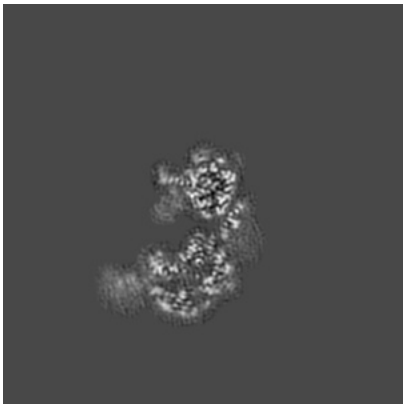


Z

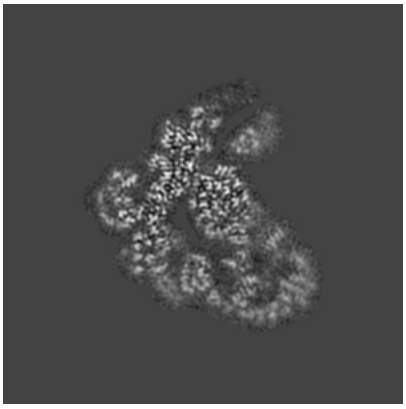
The images above show the map projected in three orthogonal directions.

6.2 Central slices

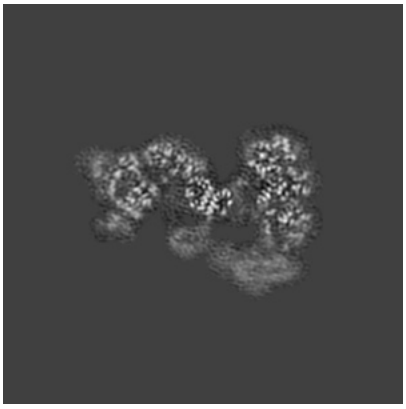
6.2.1 Primary map



X Index: 169



Y Index: 169

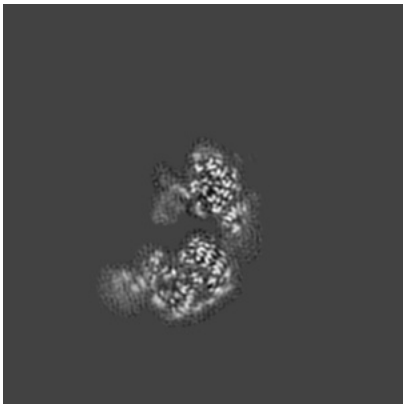


Z Index: 169

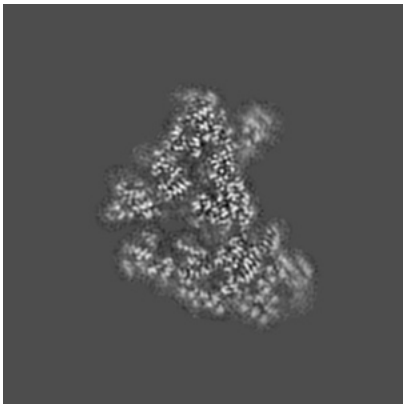
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

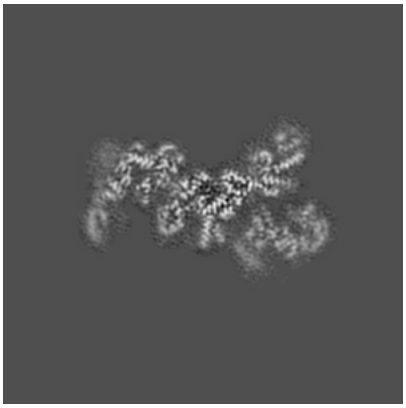
6.3.1 Primary map



X Index: 165



Y Index: 182



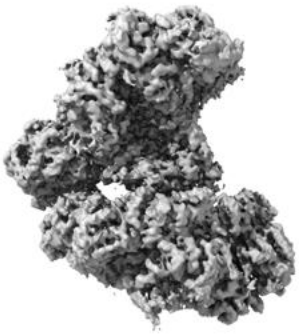
Z Index: 188

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 0.0117. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

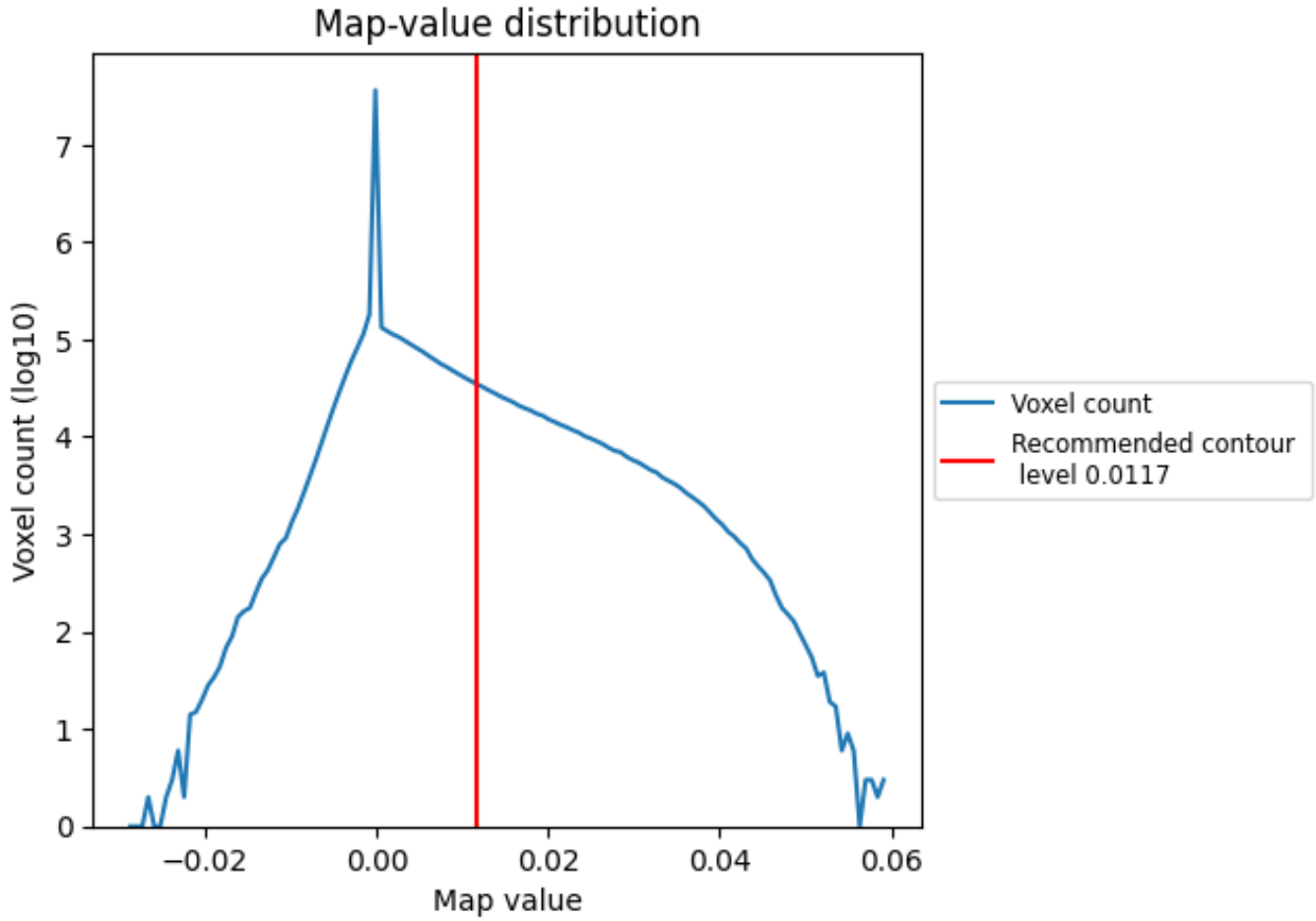
6.5 Mask visualisation (i)

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

7 Map analysis

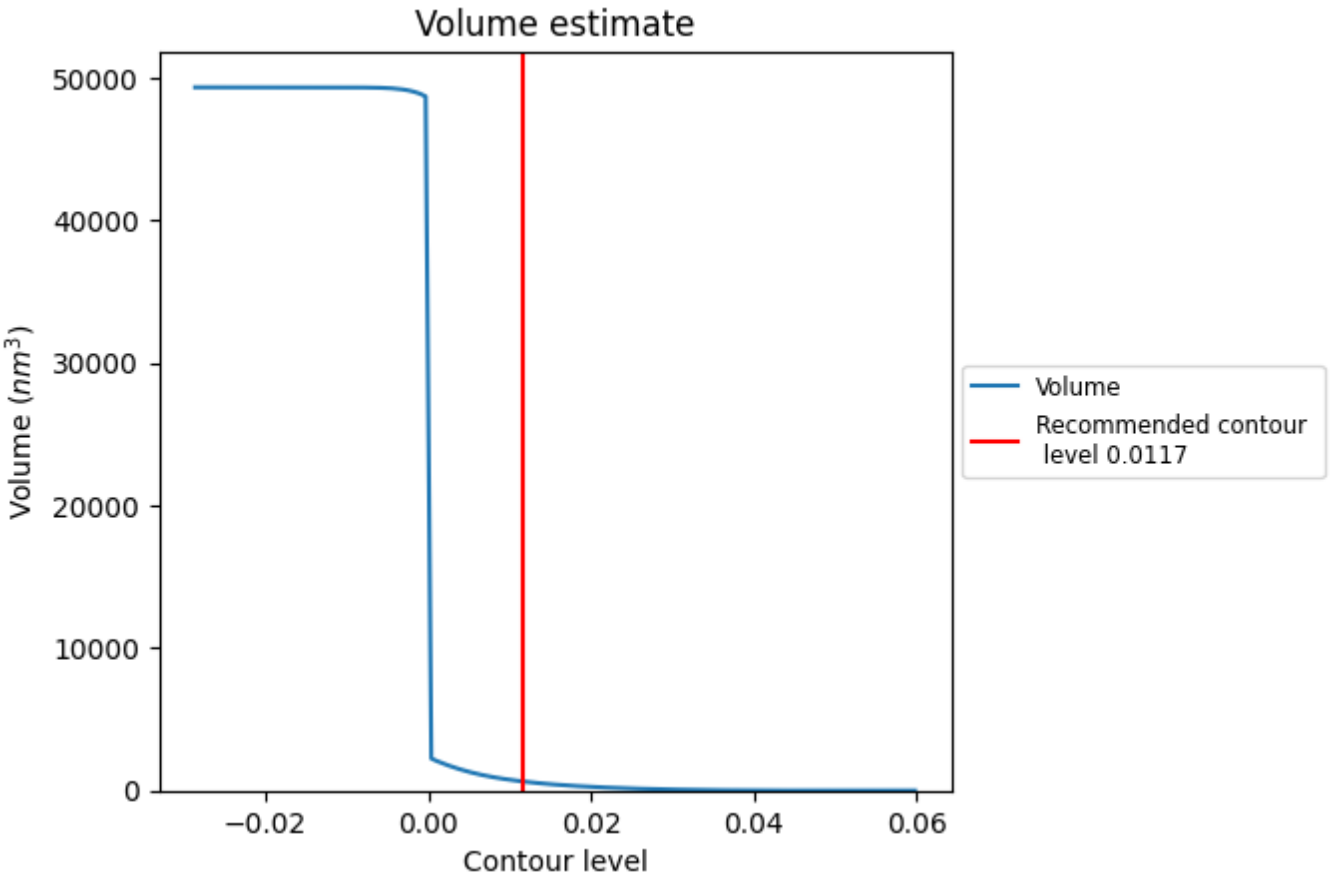
This section contains the results of statistical analysis of the map.

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.

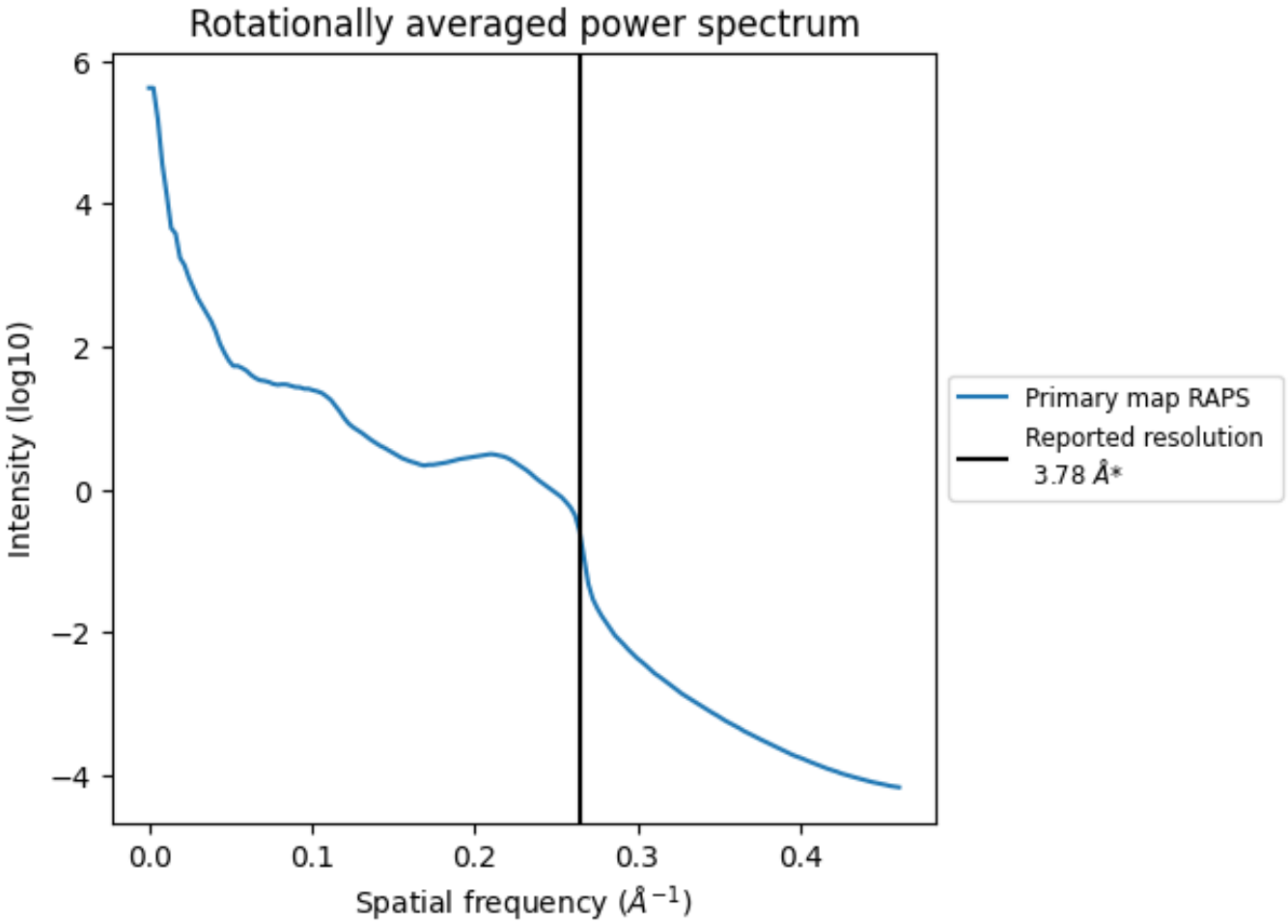
7.2 Volume estimate



The volume at the recommended contour level is 632 nm^3; this corresponds to an approximate mass of 571 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 0.265 Å^{-1}

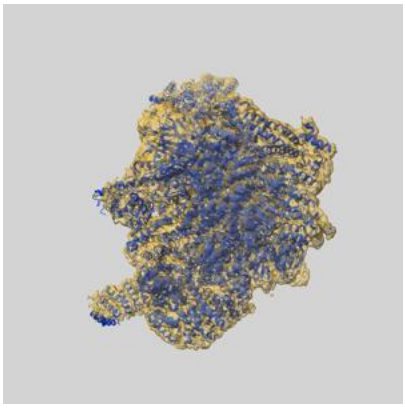
8 Fourier-Shell correlation

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

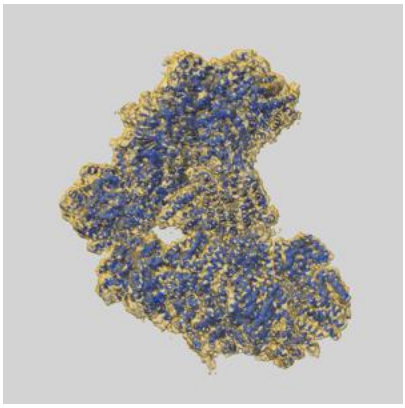
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10536 and PDB model 6TNT. Per-residue inclusion information can be found in section 3 on page 7.

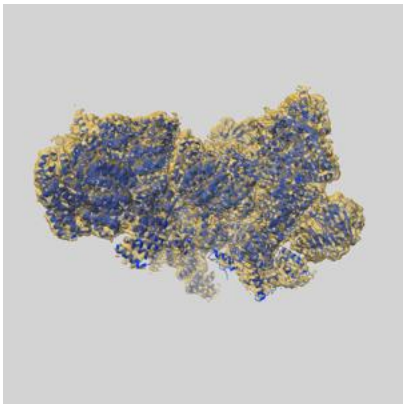
9.1 Map-model overlay



X



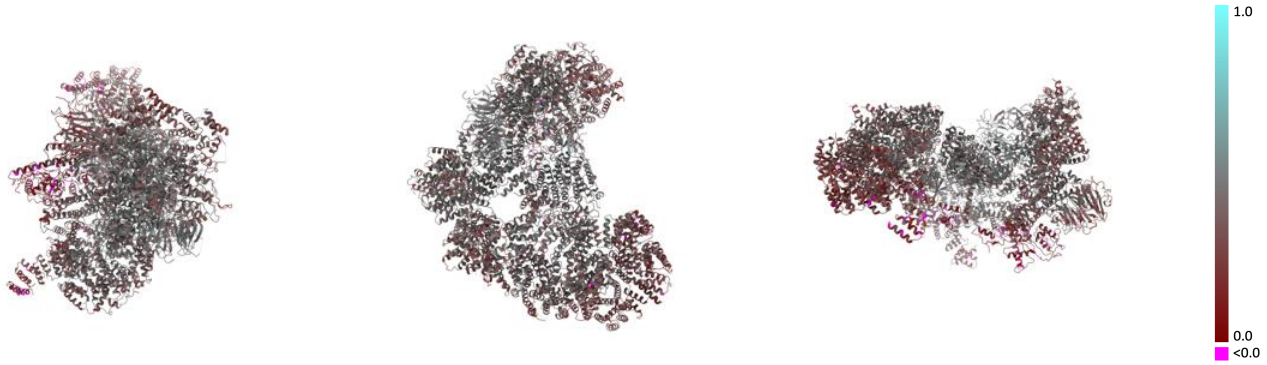
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0117 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.

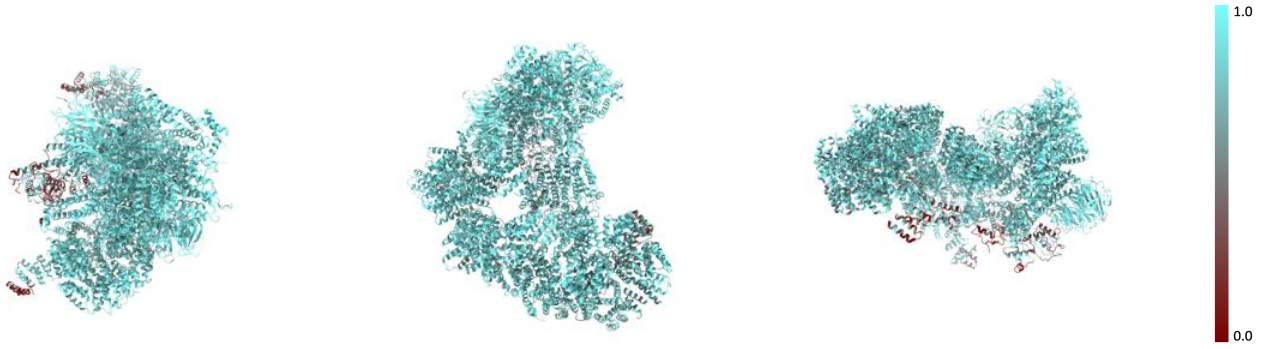
9.2 Q-score mapped to coordinate model (i)



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.

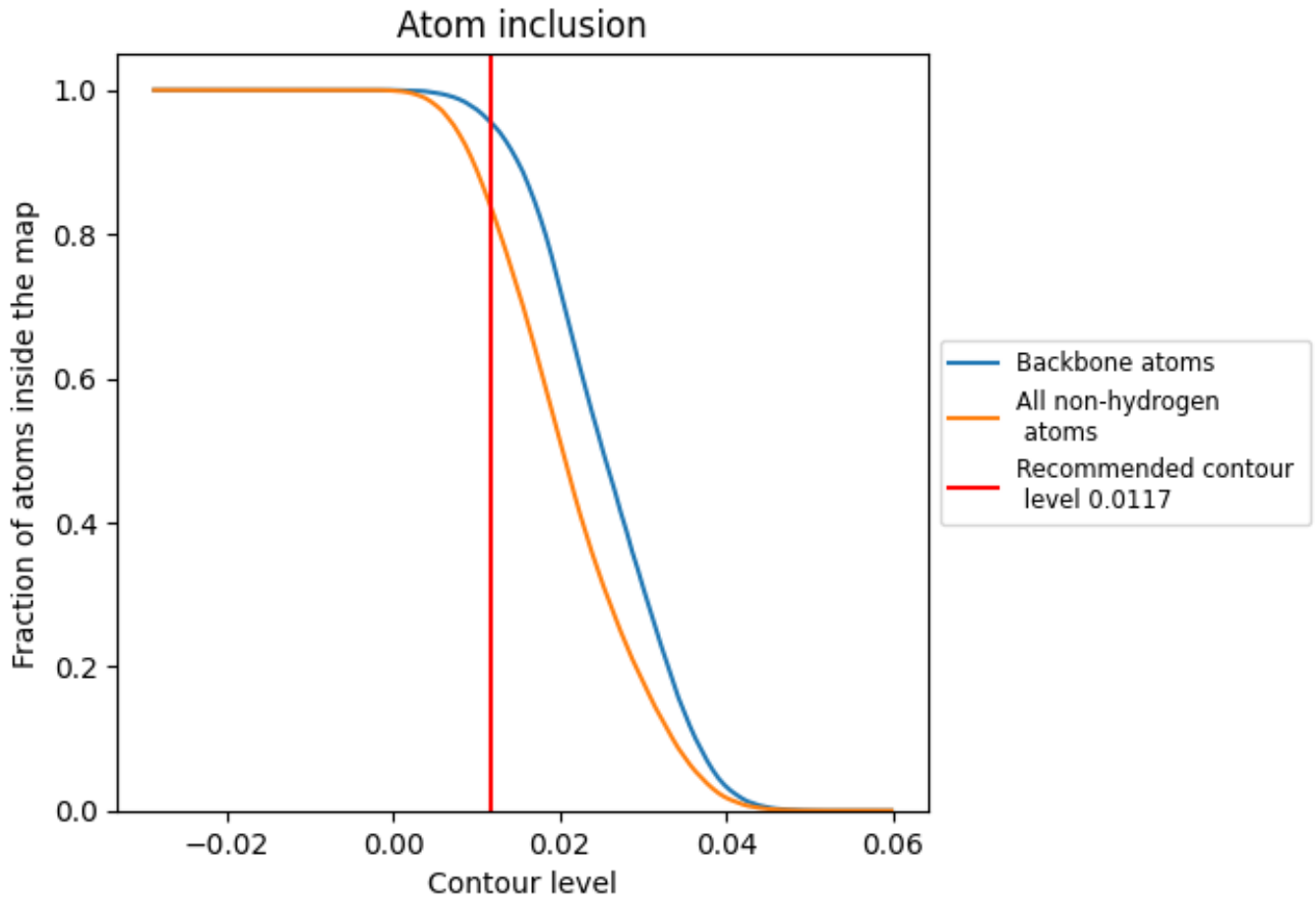
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0117).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 84% 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 (0.0117) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8376	0.3900
A	0.8929	0.4460
B	0.1962	0.1300
C	0.8860	0.4400
D	0.8426	0.4380
E	0.8333	0.4090
F	0.8626	0.3950
G	0.7972	0.3690
H	0.8670	0.4210
I	0.8747	0.3850
J	0.8753	0.3910
K	0.8839	0.4240
L	0.8466	0.4170
M	0.7643	0.4260
N	0.7058	0.2840
O	0.8820	0.4430
P	0.8399	0.3860
T	0.8354	0.4670
W	0.7810	0.3990
X	0.7172	0.2860
Y	0.7691	0.2920