Full wwPDB EM Validation Report

Mar 28, 2026 – 05:54 AM UTC

PDB ID	:	6TNT / pdb_00006tnt
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:

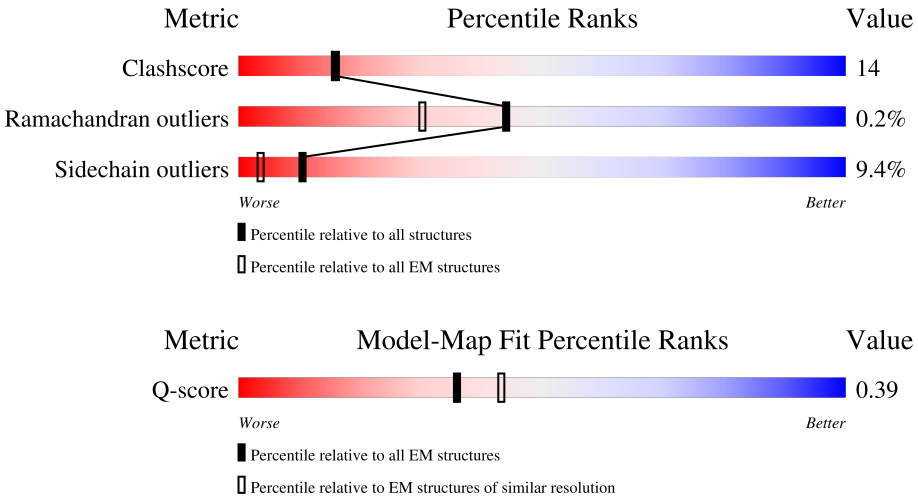
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.78 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10074 (3.28 - 4.27)

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	62% 24% 12%
3	P	597	5% 59% 21% 18%

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Mol	Chain	Length	Quality of chain
4	D	121	31% 14% 55%
5	E	110	37% 11% 49%
6	F	824	37% 18% 44%
6	H	824	41% 16% 41%
7	G	85	8% 18% 71%
7	W	85	18% 9% 69%
8	I	808	54% 31% 11%
9	J	620	52% 26% 19%
9	K	620	54% 23% 20%
10	L	185	58% 37%
11	M	74	5% 47% 27% 5% 20%
12	N	822	15% 47% 31% 18%
13	O	755	63% 22% 6% 9%
14	T	15	20% 80% 20%
15	X	599	10% 56% 23% 19%
15	Y	599	53% 26% 17%

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
			Total	C	N	O	S		
3	P	492	4046	2613	679	730	24	0	0

- 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 (CCD ID: ZN) (formula: Zn).

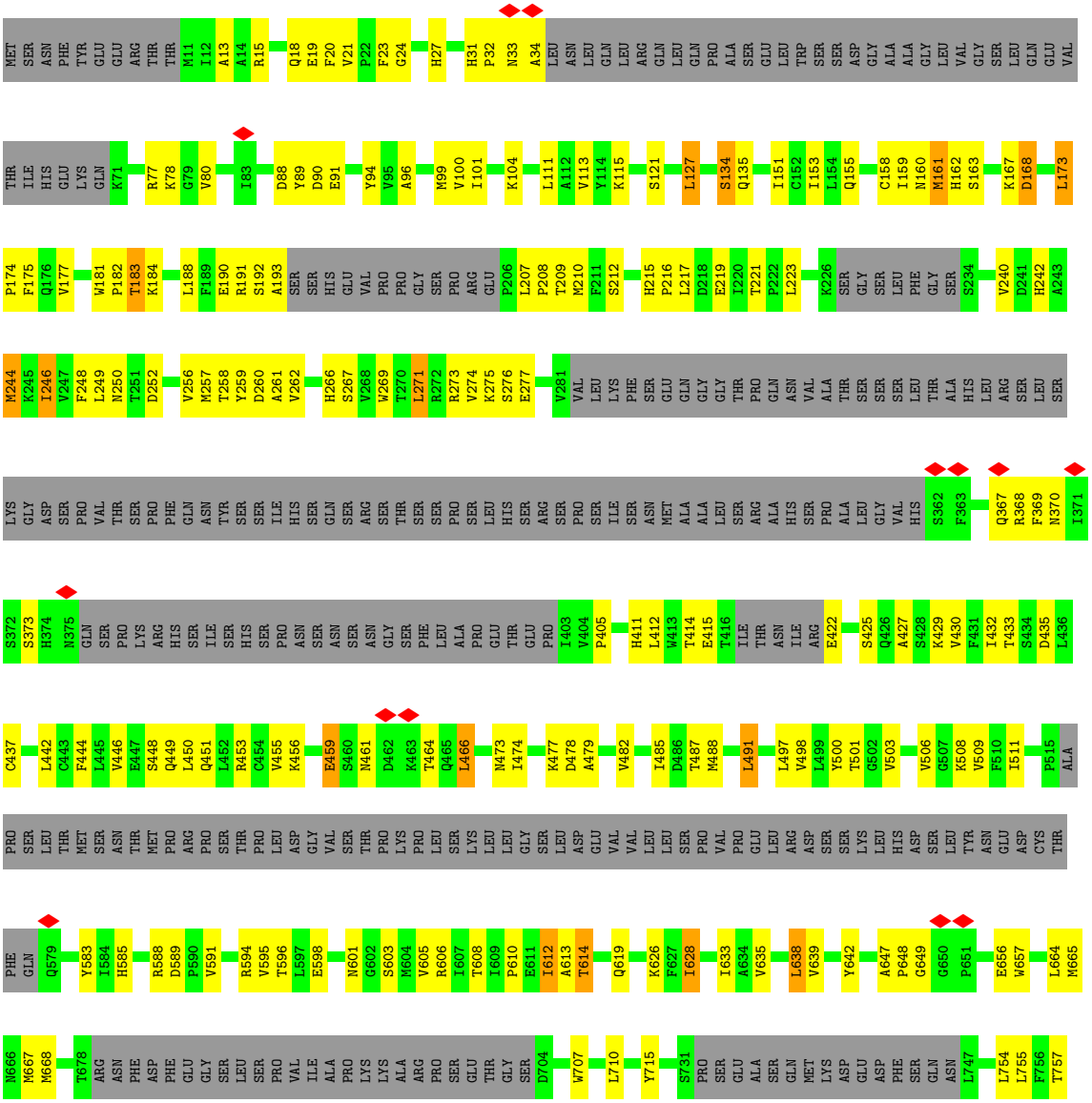
Mol	Chain	Residues	Atoms		AltConf
16	B	3	Total	Zn	0
			3	3	

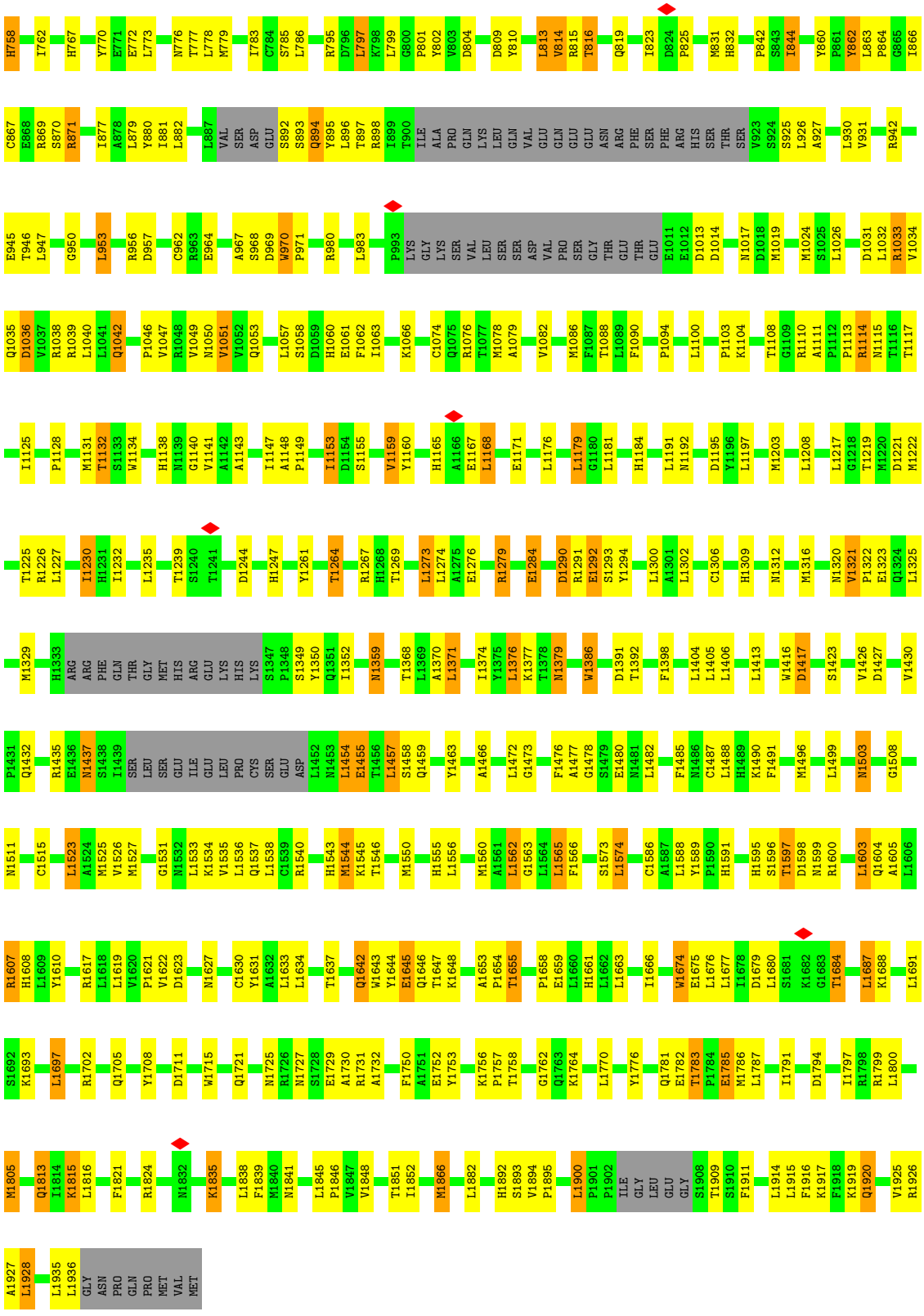
3 Residue-property plots (i)

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:



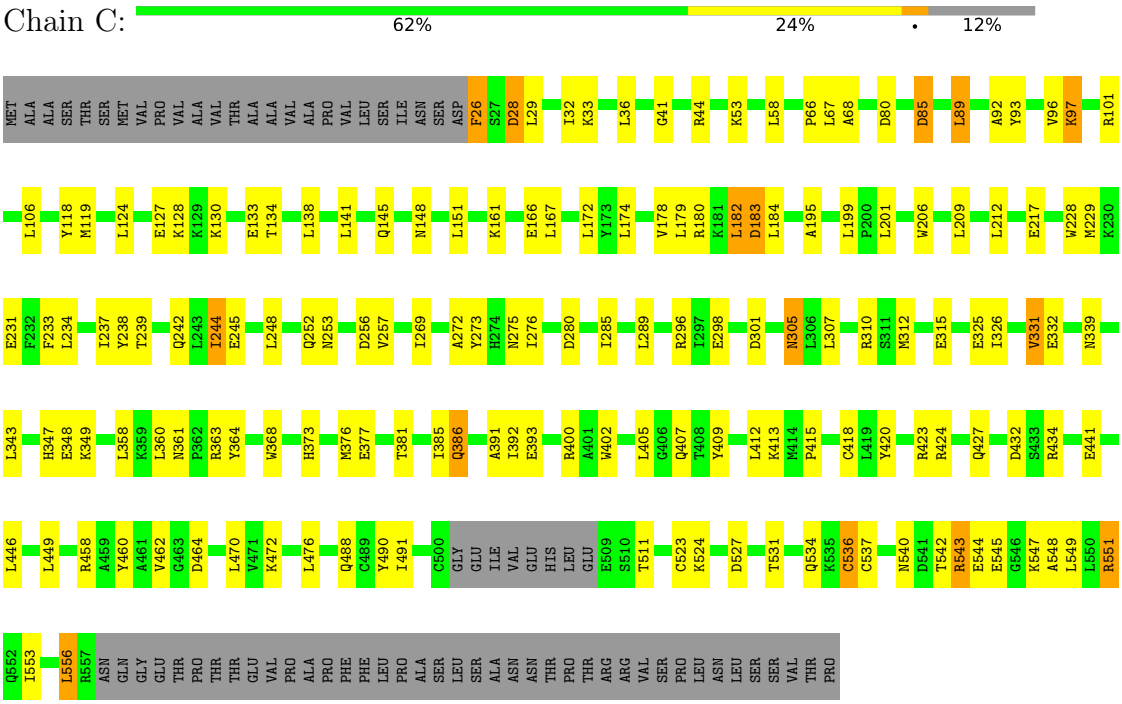


• Molecule 2: Anaphase-promoting complex subunit 11

Chain B:

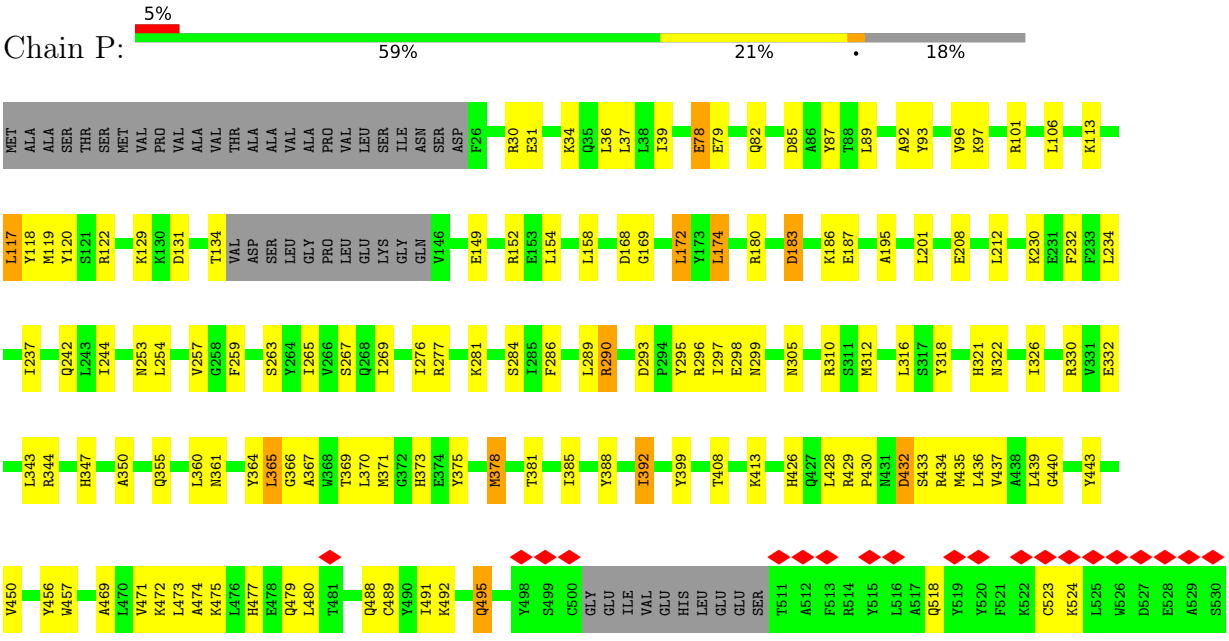
• Molecule 3: Cell division cycle protein 23 homolog

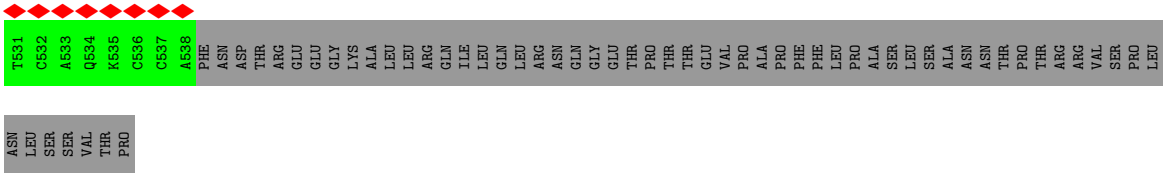
Chain C:



• Molecule 3: Cell division cycle protein 23 homolog

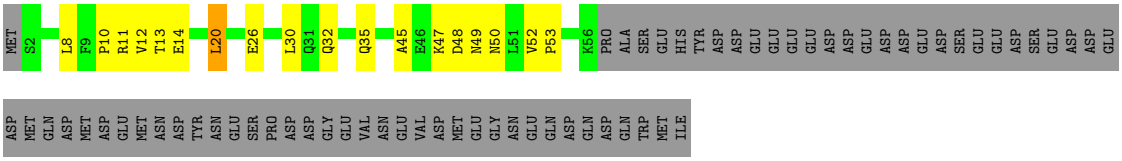
Chain P:





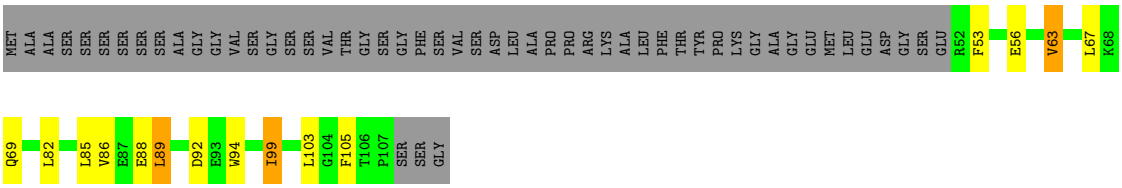
• Molecule 4: Anaphase-promoting complex subunit 15

Chain D:



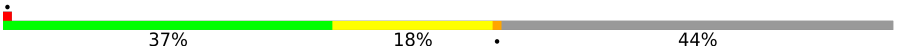
• Molecule 5: Anaphase-promoting complex subunit 16

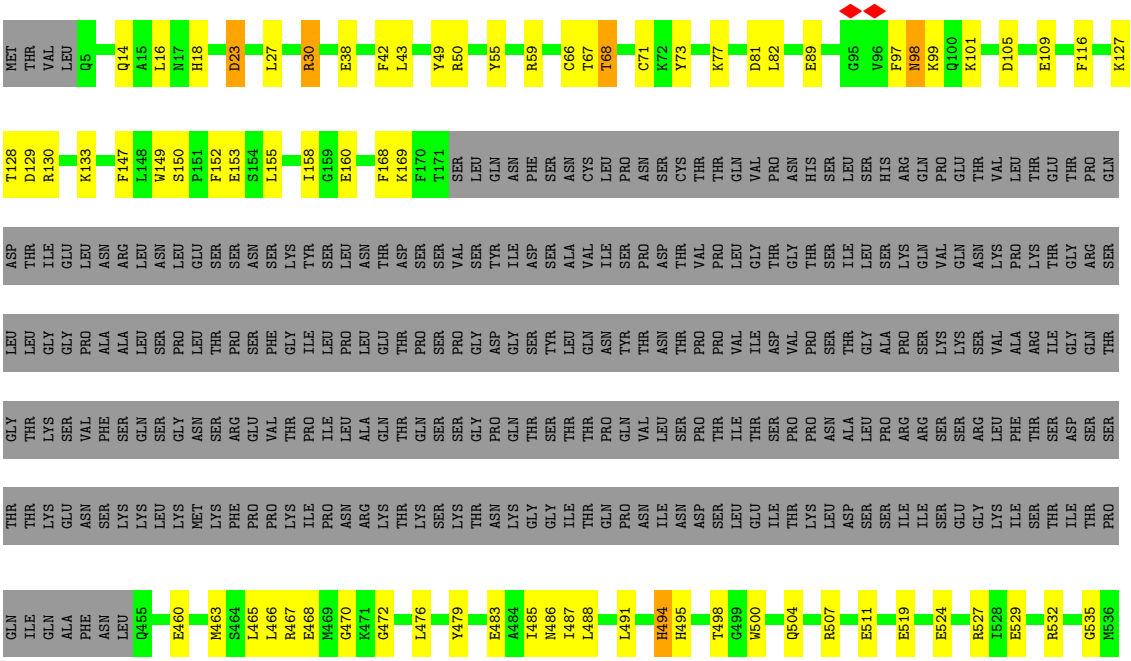
Chain E:

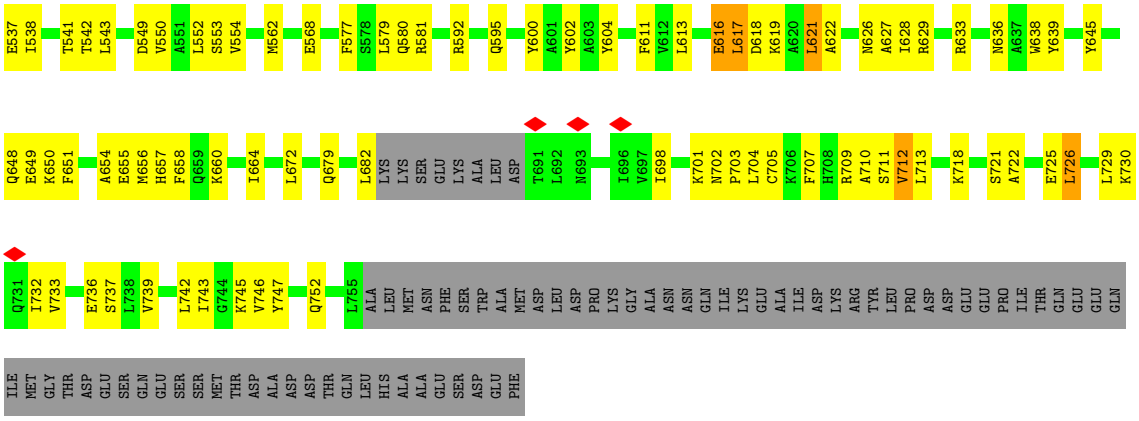


• Molecule 6: Cell division cycle protein 27 homolog

Chain F:

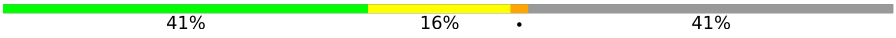


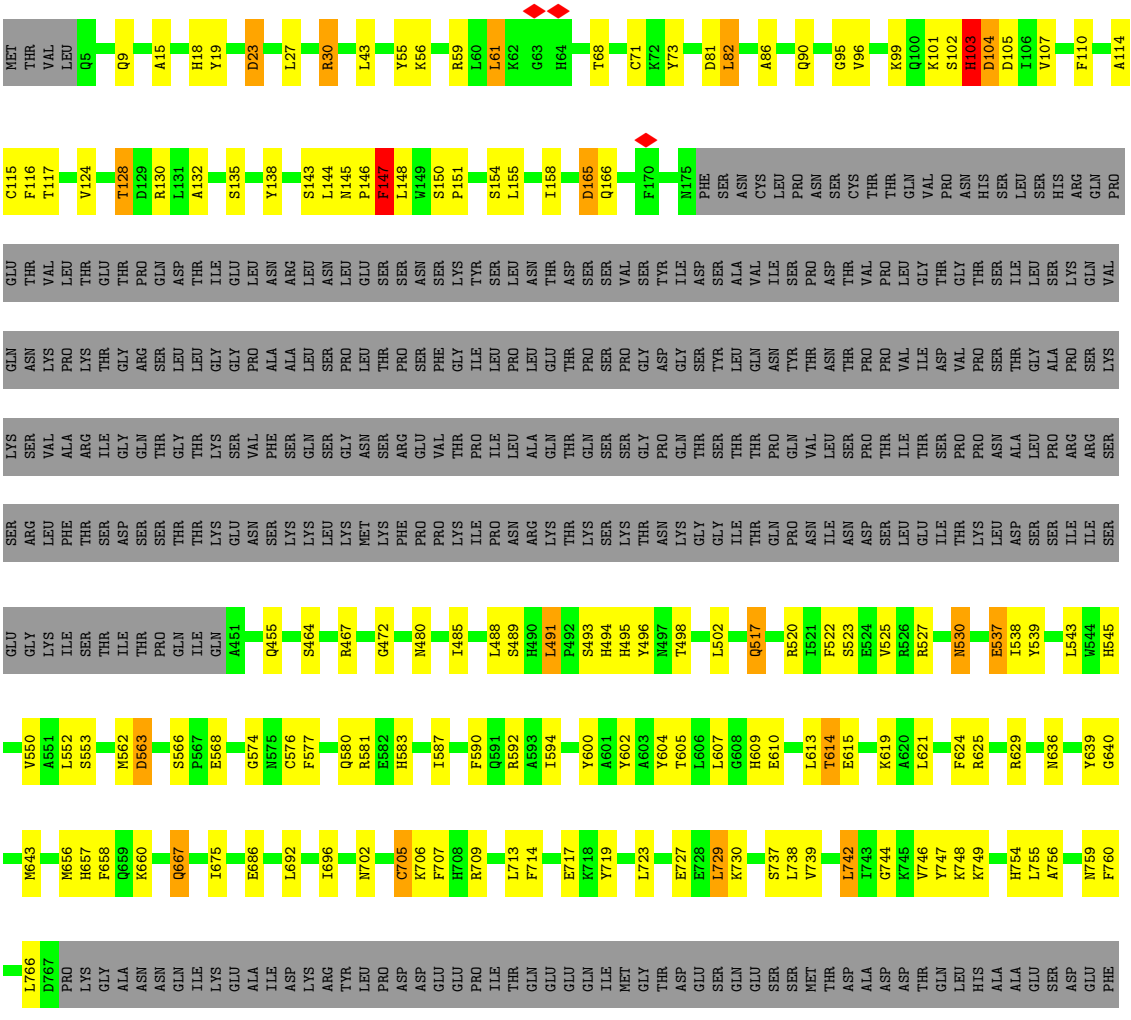




• Molecule 6: Cell division cycle protein 27 homolog

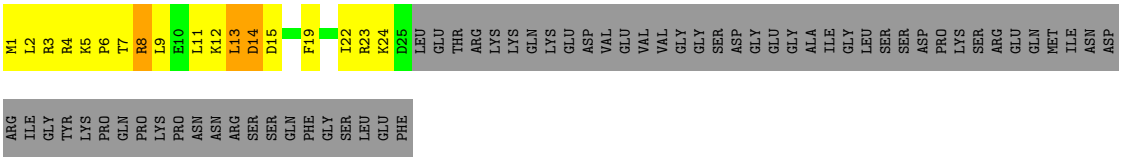
Chain H:





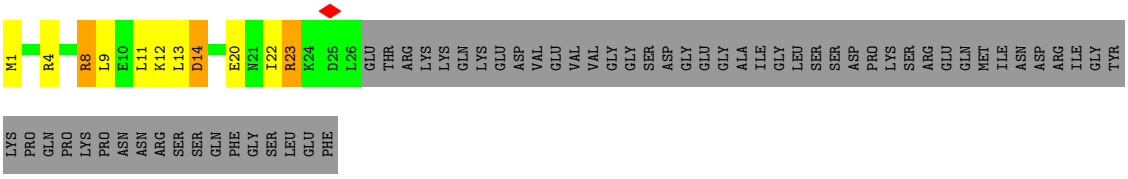
• Molecule 7: Anaphase-promoting complex subunit CDC26

Chain G:



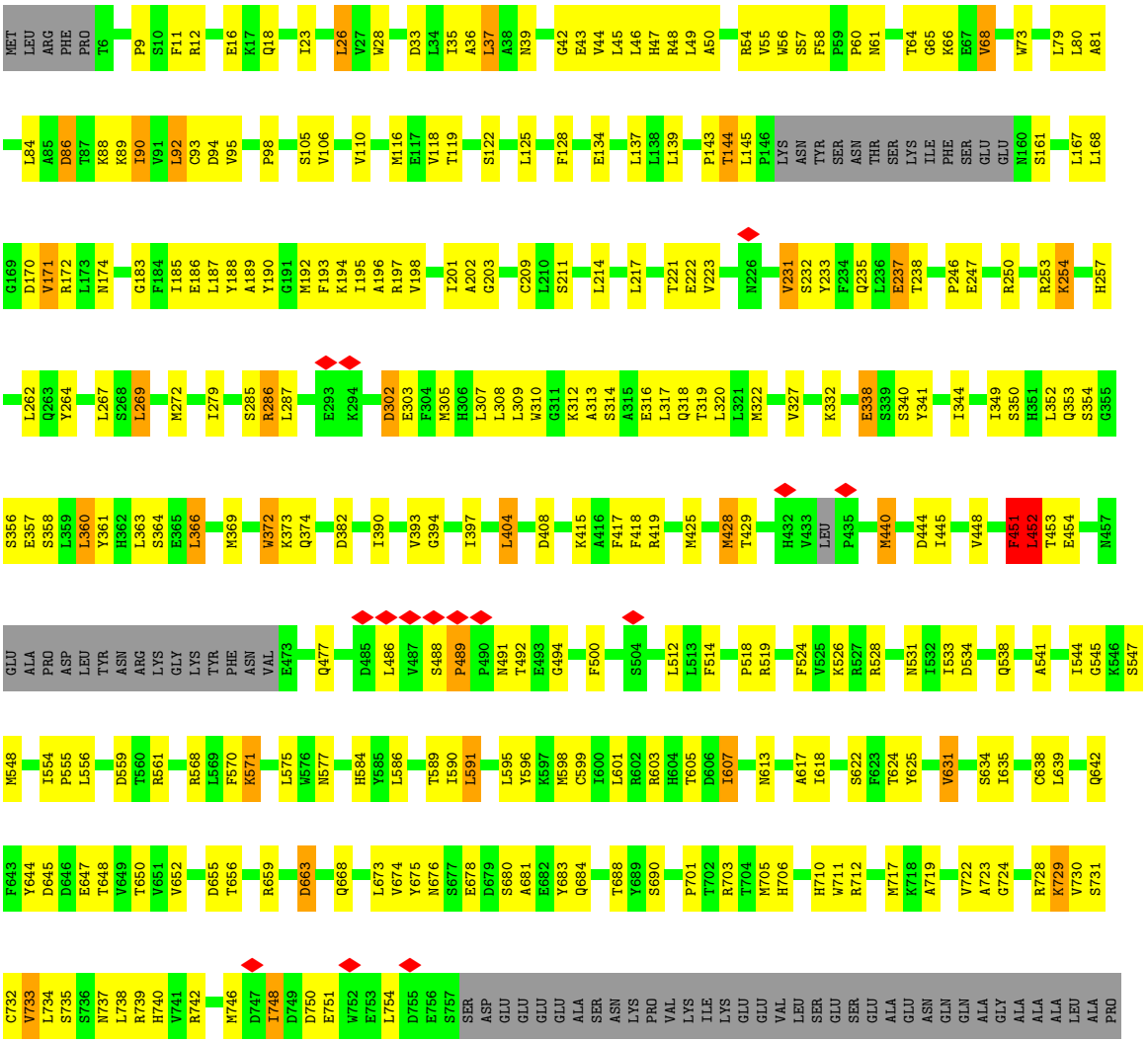
• Molecule 7: Anaphase-promoting complex subunit CDC26

Chain W:



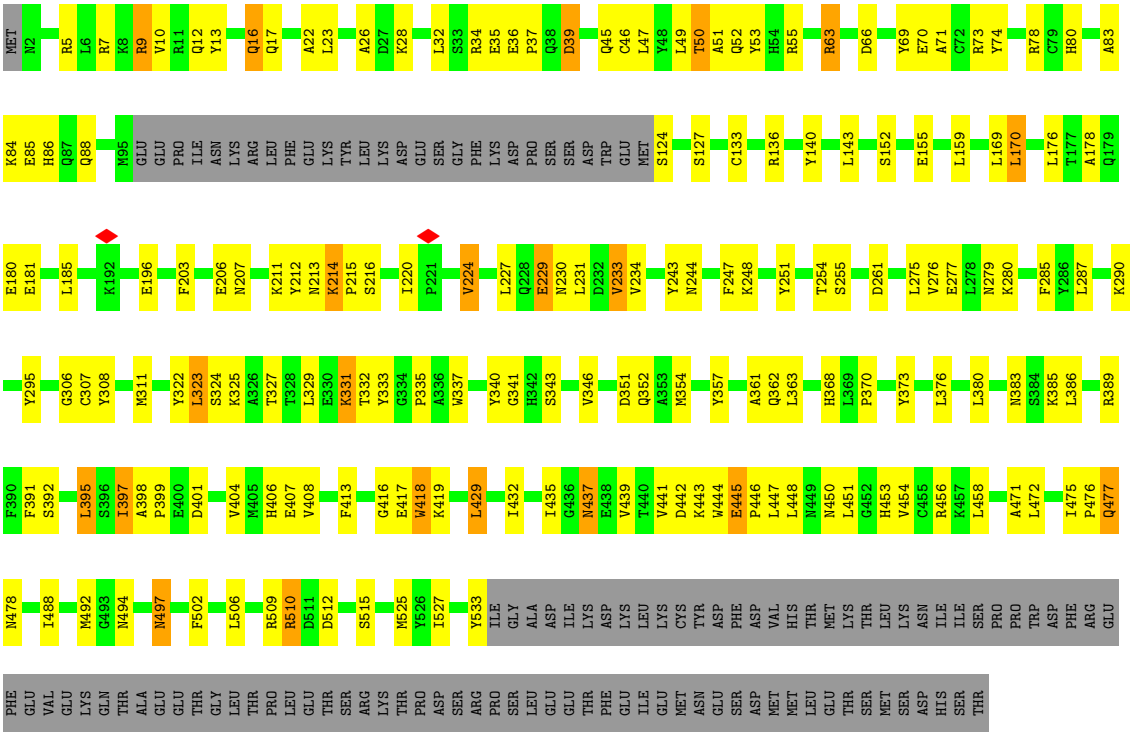
• Molecule 8: Anaphase-promoting complex subunit 4

Chain I:



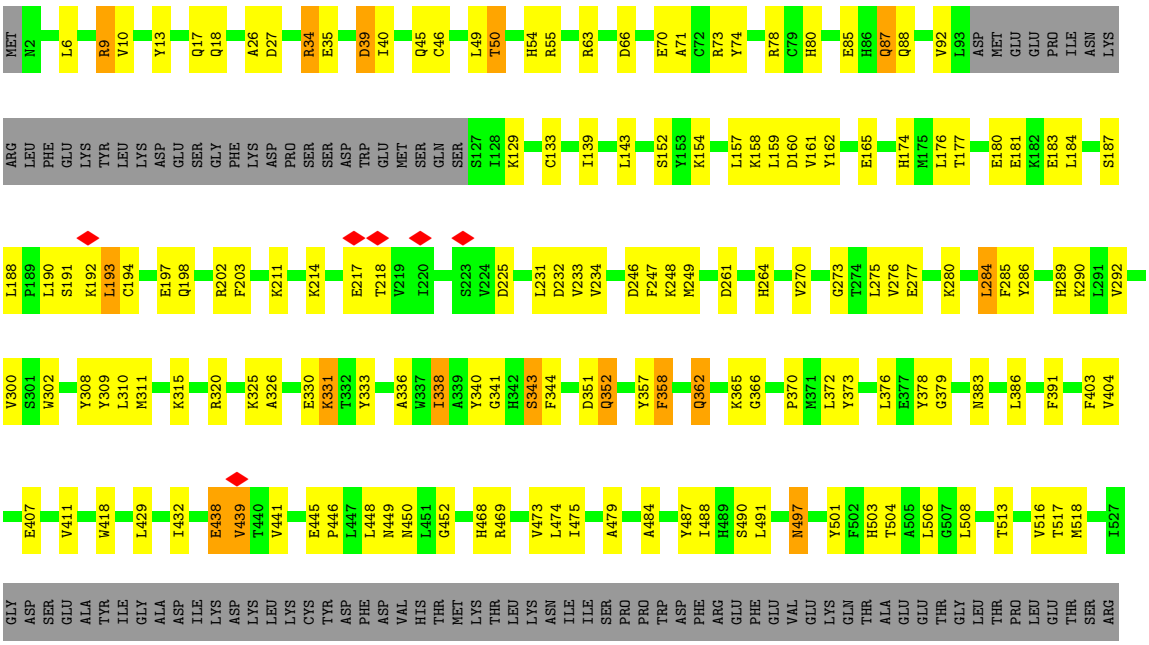
• Molecule 9: Cell division cycle protein 16 homolog

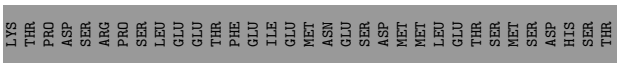
Chain J:



• Molecule 9: Cell division cycle protein 16 homolog

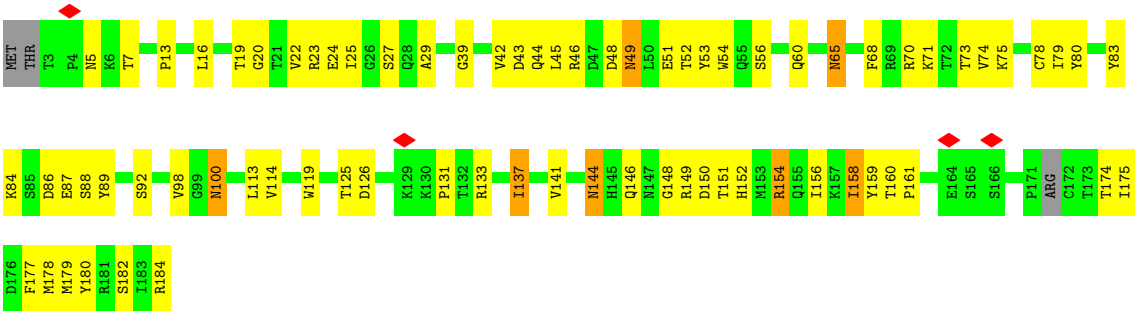
Chain K:





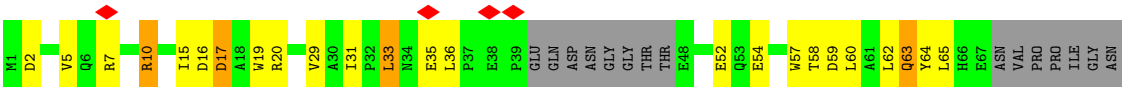
• Molecule 10: Anaphase-promoting complex subunit 10

Chain L:



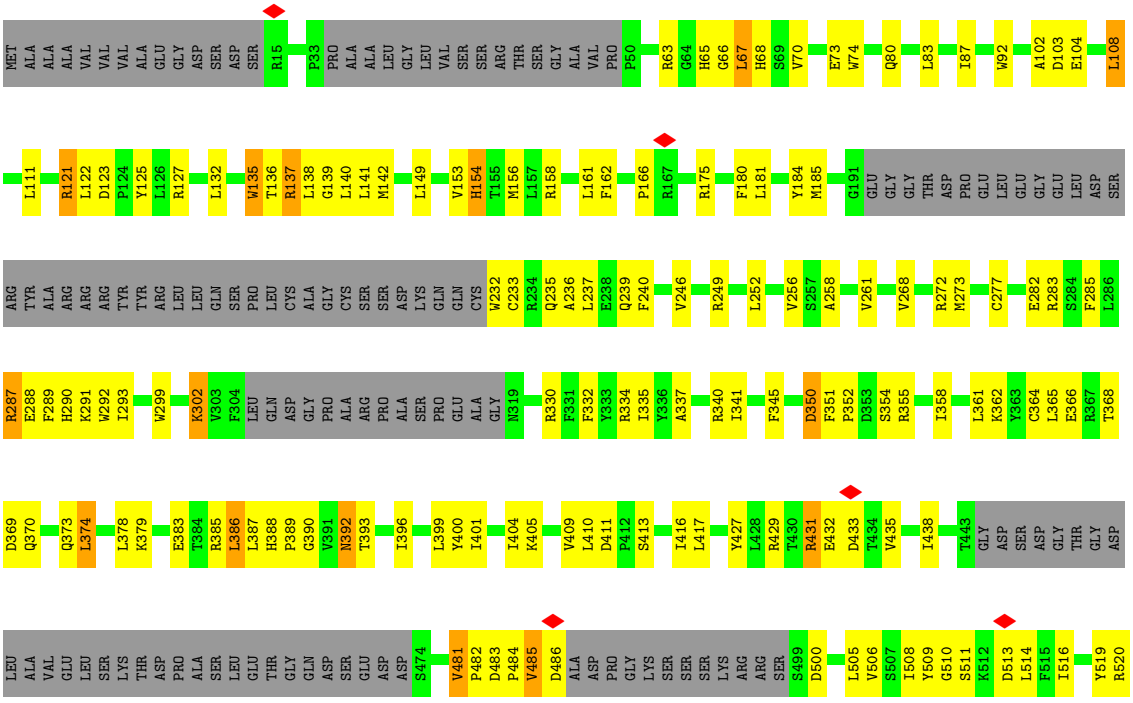
• Molecule 11: Anaphase-promoting complex subunit 13

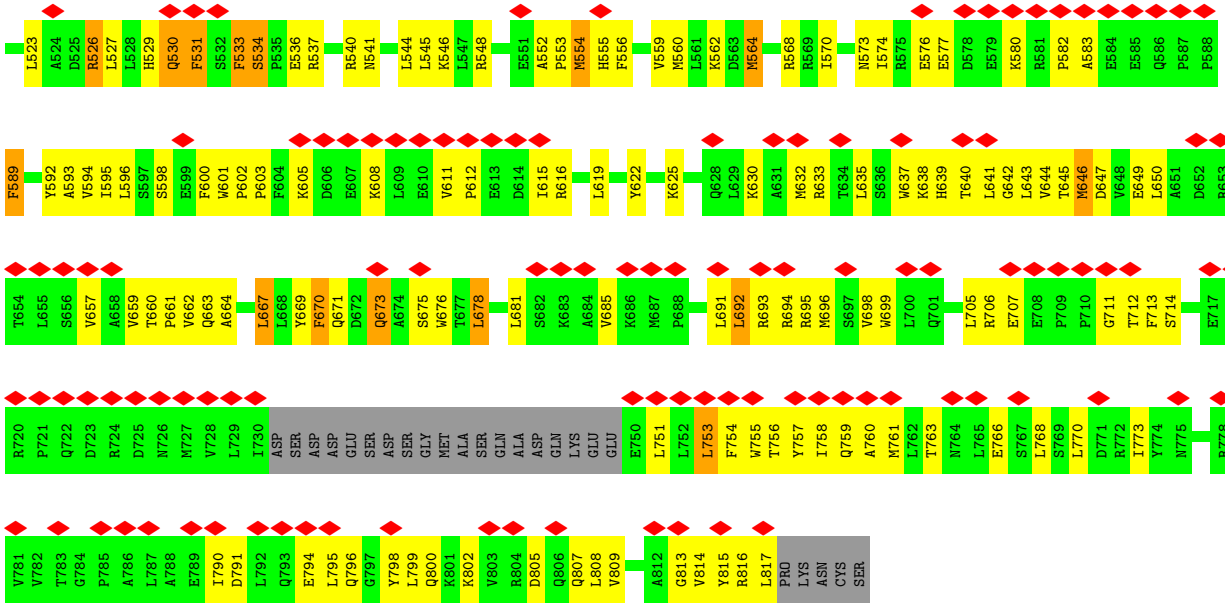
Chain M:



• Molecule 12: Anaphase-promoting complex subunit 2

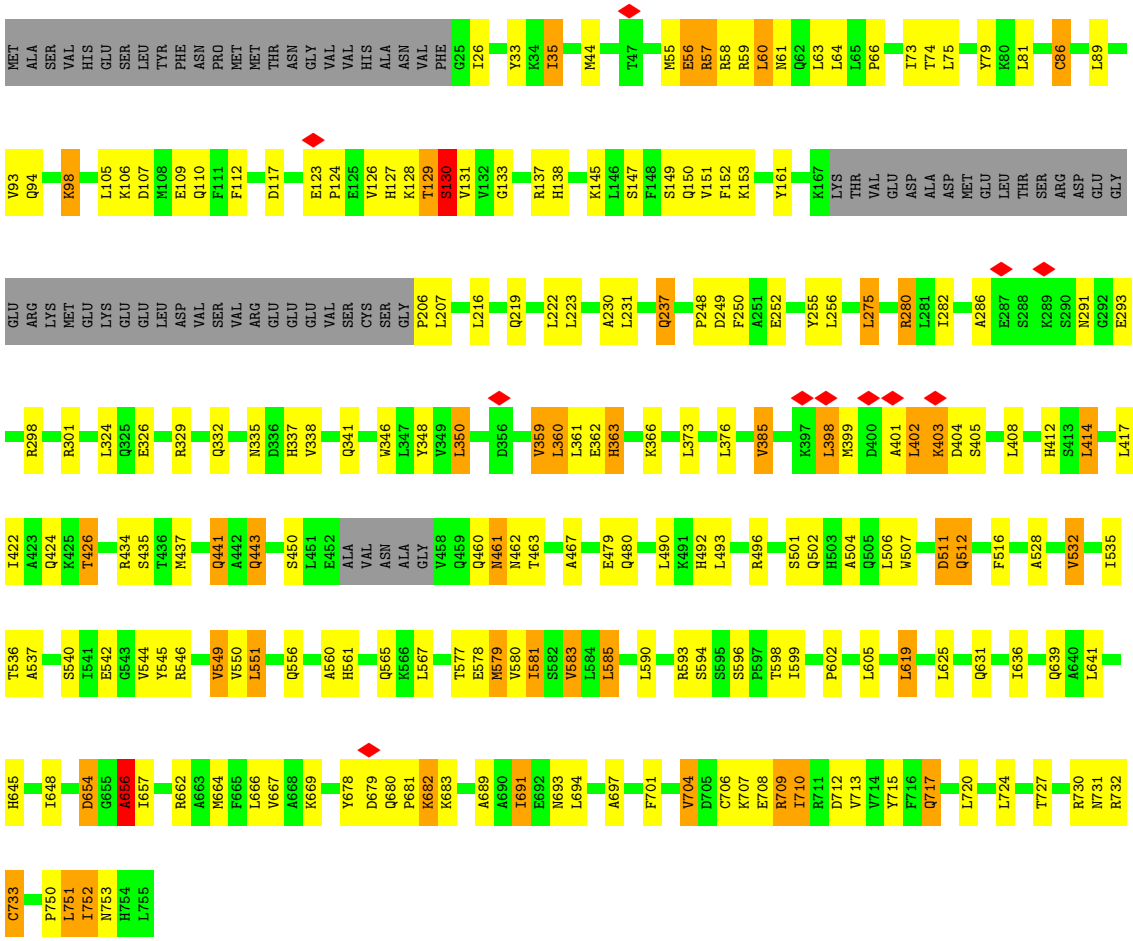
Chain N:





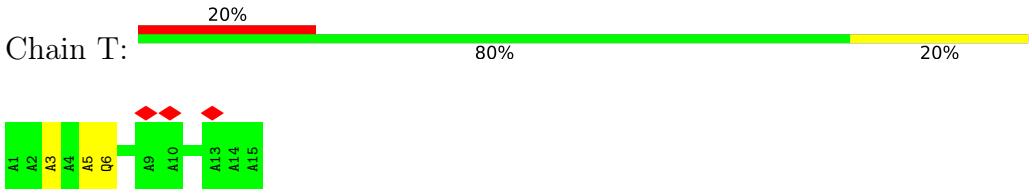
• Molecule 13: Anaphase-promoting complex subunit 5

Chain O:



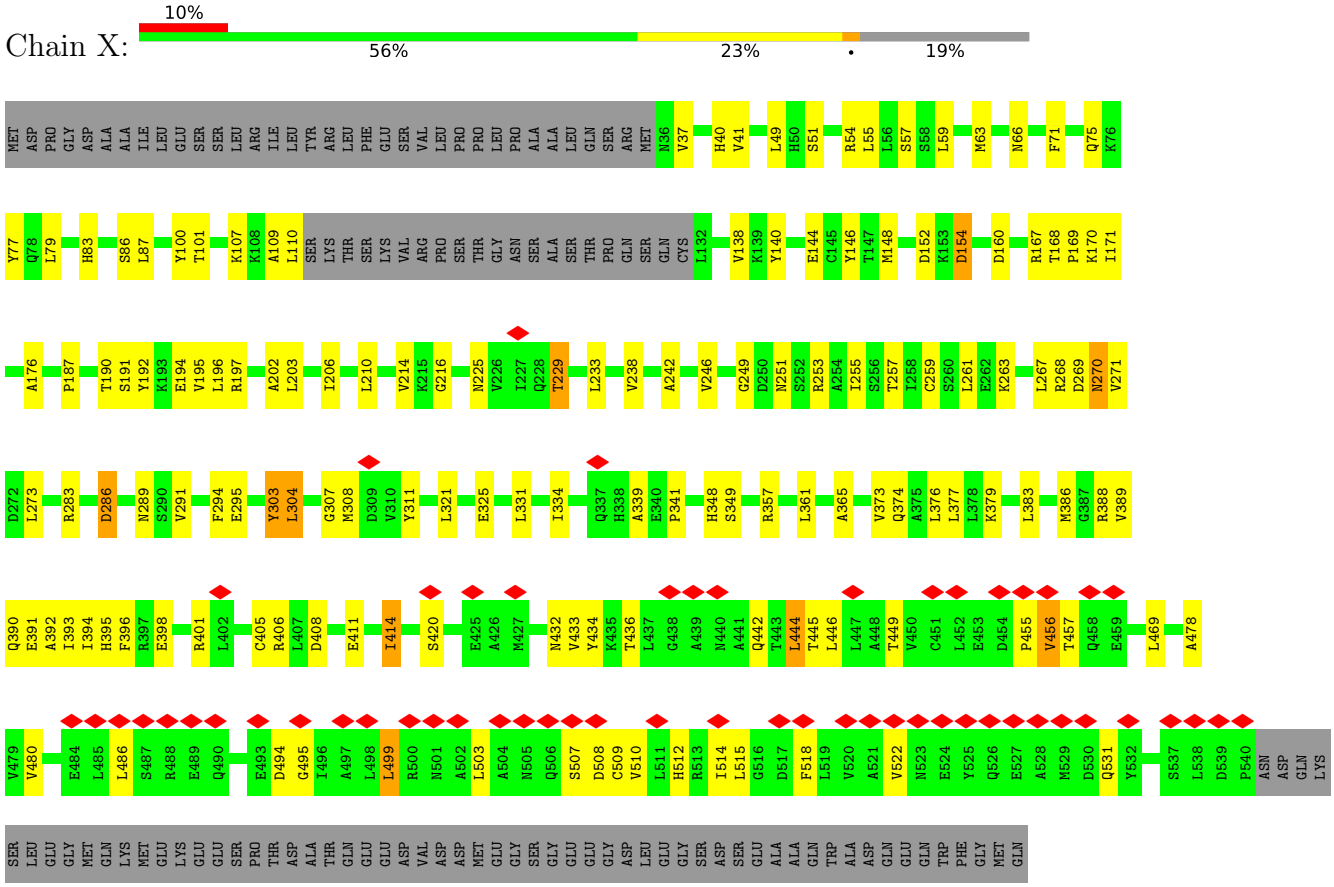
• Molecule 14: UNIDENTIFIED PEPTIDE

Chain T:



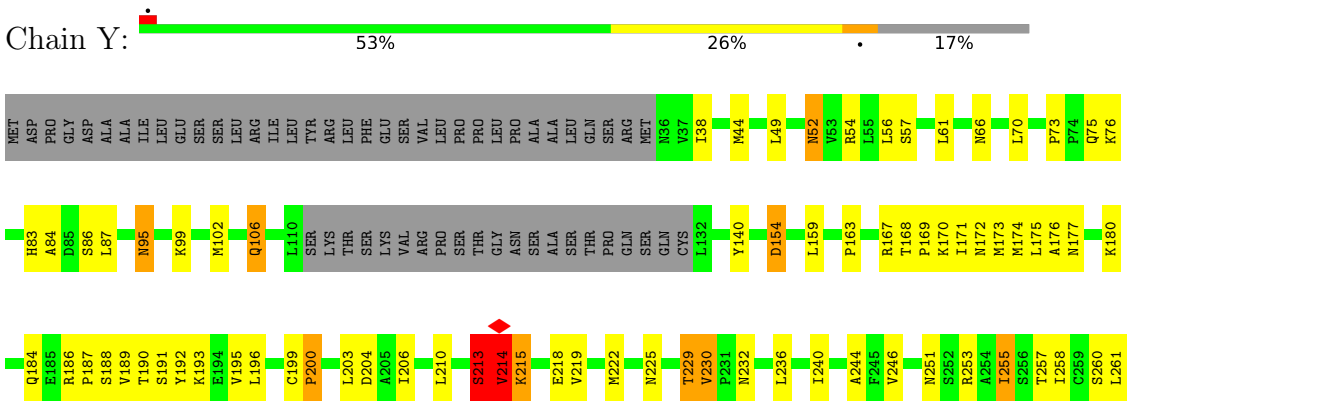
• Molecule 15: Anaphase-promoting complex subunit 7

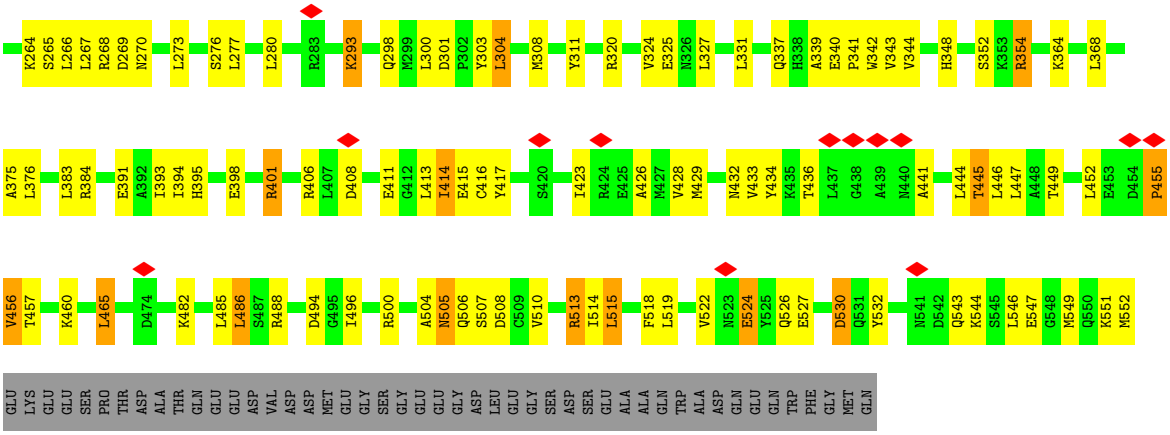
Chain X:



• Molecule 15: Anaphase-promoting complex subunit 7

Chain Y:




K264 S265 L266 L267 R268 D269 N270 L273 S276 L277 L280 R283 K293 Q298 M299 L300 D301 P302 Y303 L304 M308 Y311 R320 V324 E325 N326 L327 L331 Q337 H338 A339 E340 P341 W342 V343 V344 H348 S352 K353 R354 K364 L368
A375 L376 L383 R384 E391 A392 I393 I394 H395 E398 R401 R406 L407 D408 E411 G412 L413 I414 E415 C416 Y417 S420 I423 R424 E425 A426 M427 V428 M429 N432 V433 Y434 K435 T436 L437 G438 A439 N440 A441 L444 T445 L446 L447 A448 T449 L452 E453 D454 P455
V456 T457 K460 L465 D474 K482 L485 L486 S487 R488 D494 G495 I496 R500 A504 N505 Q506 S507 D508 Q509 V510 R513 I514 L515 F518 L519 V522 N523 E524 Y525 Q526 E527 D530 Q531 Y532 N541 D542 Q543 K544 S545 L546 E547 Q548 M549 Q550 K551 M552
GLU LYS GLU GLU SER PRO THR ASP ALA THR GLN GLU GLU ASP VAL ASP ASP MET GLU GLY SER GLY GLU GLU GLY ASP LEU GLU GLY SER ASP SER GLU ALA ALA GLN TRP ALA ASP GLN GLU GLN TRP PHE GLY MET GLN

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	0.26	0/12269	0.45	2/16722 (0.0%)
2	B	0.14	0/674	0.38	0/913
3	C	0.26	0/4404	0.39	0/5945
3	P	0.21	0/4141	0.36	0/5593
4	D	0.26	0/446	0.39	0/610
5	E	0.19	0/459	0.30	0/619
6	F	0.19	0/3704	0.31	0/5019
6	H	0.23	0/3969	0.36	0/5366
7	G	0.24	0/221	0.45	0/292
7	W	0.23	0/219	0.52	0/291
8	I	0.20	0/5754	0.39	3/7806 (0.0%)
9	J	0.21	0/4152	0.38	0/5623
9	K	0.21	0/4086	0.34	0/5533
10	L	0.22	0/1468	0.41	0/1993
11	M	0.22	0/490	0.45	0/665
12	N	0.18	0/5417	0.47	3/7341 (0.0%)
13	O	0.27	0/5499	0.43	0/7432
14	T	0.25	0/78	0.86	0/107
15	X	0.16	0/3827	0.35	0/5180
15	Y	0.16	0/3922	0.37	1/5304 (0.0%)
All	All	0.22	0/65199	0.40	9/88354 (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 (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	N	121	ARG	CA-C-N	9.65	139.07	121.70
12	N	121	ARG	C-N-CA	9.65	139.07	121.70
1	A	758	HIS	CA-C-N	6.47	124.31	120.24
1	A	758	HIS	C-N-CA	6.47	124.31	120.24
15	Y	213	SER	N-CA-C	6.42	116.47	108.19
12	N	121	ARG	N-CA-C	5.60	117.07	110.97
8	I	489	PRO	CA-C-N	5.22	139.54	127.00
8	I	489	PRO	C-N-CA	5.22	139.54	127.00
8	I	489	PRO	C-N-CD	-5.12	109.34	120.60

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	375	0
2	B	649	0	598	32	0
3	C	4306	0	4275	109	0
3	P	4046	0	3998	95	0
4	D	436	0	396	15	0
5	E	450	0	435	11	0
6	F	3618	0	3452	111	0
6	H	3879	0	3805	116	0
7	G	220	0	233	15	0
7	W	218	0	222	14	0
8	I	5634	0	5527	190	0
9	J	4053	0	3960	129	0
9	K	3988	0	3913	104	0
10	L	1435	0	1382	57	0
11	M	481	0	457	20	0
12	N	5313	0	5240	217	0
13	O	5400	0	5418	148	0
14	T	79	0	77	3	0
15	X	3767	0	3820	105	0
15	Y	3862	0	3915	134	0
16	B	3	0	0	0	0
All	All	63827	0	62771	1823	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 (1823) 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	1.39
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	1.25
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	1.10
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:657:TRP:NE1	1:A:785:SER:OG	2.20	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:276:VAL:HA	9:K:311:MET:HE2	1.74	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
12:N:560:MET:HE3	12:N:600:PHE:HB2	1.74	0.70
8:I:680:SER:O	8:I:684:GLN:NE2	2.25	0.69
13:O:461:ASN:HD22	13:O:462:ASN:H	1.39	0.69
7:G:23:ARG:HG3	9:J:525:MET:HE1	1.74	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
10:L:89:TYR:CD2	10:L:150:ASP:CG	2.71	0.68
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
8:I:625:TYR:OH	8:I:711:TRP:O	2.11	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
8:I:674:VAL:HG22	8:I:705:MET:HE1	1.75	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
8:I:93:CYS:SG	8:I:94:ASP:N	2.68	0.66
3:P:432:ASP:OD1	3:P:432:ASP:N	2.28	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
6:F:18:HIS:O	6:H:73:TYR:OH	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:546:LYS:HG3	12:N:554:MET:HE2	1.78	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
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
15:Y:510:VAL:HG23	15:Y:544:LYS:HZ3	1.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:P:119:MET:HE3	3:P:154:LEU:HG	1.80	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
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
15:Y:184:GLN:O	15:Y:188:SER:OG	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
12:N:232:TRP:CD1	12:N:233:CYS:HG	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:159:LEU:HD11	15:Y:174:MET:HE3	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:269:LEU:HA	8:I:272:MET:HE2	1.86	0.57
8:I:356:SER:HB3	8:I:397:ILE:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
13:O:44:MET:HE2	13:O:60:LEU:HD11	1.88	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
12:N:706:ARG:O	12:N:714:SER:N	2.39	0.56
1:A:770:TYR:OH	1:A:809:ASP:OD2	2.23	0.55
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
1:A:1013:ASP:OD1	1:A:1017:ASN:ND2	2.40	0.55
13:O:55:MET:HE1	13:O:58:ARG:HH21	1.70	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
1:A:461:ASN:H	1:A:464:THR:HB	1.71	0.55
1:A:1926:ARG:NH1	12:N:73:GLU:OE1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
12:N:511:SER:OG	12:N:513:ASP:OD1	2.24	0.55
3:P:31:GLU:OE2	3:P:34:LYS:NZ	2.38	0.55
3:P:364:TYR:HD2	3:P:367:ALA:H	1.53	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:OD1	6:H:530:ASN:N	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:1267:ARG:HA	1:A:1316:MET:HE2	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
1:A:1799:ARG:HD2	1:A:1805:MET:HE3	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1783:THR:O	1:A:1783:THR:OG1	2.23	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
8:I:250:ARG:HB2	8:I:369:MET:HE1	1.89	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:C:33:LYS:NZ	3:P:85:ASP:OD2	2.31	0.53
9:K:487:TYR:HE1	9:K:518:MET:HE3	1.72	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
1:A:1284:GLU:CD	1:A:1284:GLU:H	2.17	0.53
4:D:11:ARG:NH1	4:D:14:GLU:OE2	2.38	0.53
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:325:LYS:NZ	11:M:35:GLU:O	2.34	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
3:P:332:GLU:OE1	3:P:332:GLU:N	2.40	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
15:Y:507:SER:OG	15:Y:508:ASP:N	2.40	0.52
1:A:80:VAL:O	1:A:89:TYR:OH	2.24	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
15:Y:298:GLN:HB2	15:Y:308:MET:HE1	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:325:GLU:O	3:P:129:LYS:NZ	2.28	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
1:A:799:LEU:C	1:A:801:PRO:HD2	2.35	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:X:286:ASP:OD1	15:X:286:ASP:N	2.42	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:1643:TRP:HB3	14:T:3:ALA:N	2.24	0.51
8:I:202:ALA:O	8:I:221:THR:OG1	2.21	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
2:B:42:ASP:HA	12:N:630:LYS:HZ1	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:102:SER:O	6:H:103:HIS:C	2.53	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
15:Y:426:ALA:HA	15:Y:429:MET:HE2	1.91	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
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
3:C:228:TRP:CD1	3:C:228:TRP:H	2.29	0.50
4:D:45:ALA:HA	3:P:378:MET:HE2	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:W:11:LEU:O	7:W:12:LYS:NZ	2.28	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
9:J:327:THR:HG1	9:J:337:TRP:NE1	2.10	0.50
15:Y:186:ARG:HA	15:Y:189:VAL:HG12	1.94	0.50
15:Y:206:ILE:HD11	15:Y:222:MET:HE2	1.93	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
10:L:73:THR:O	10:L:160:THR:OG1	2.24	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
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
13:O:750:PRO:C	13:O:752:ILE:H	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
12:N:753:LEU:O	12:N:756:THR:OG1	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:492:MET:HE3	9:J:494:ASN:HD22	1.77	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
6:H:656:MET:HE2	6:H:660:LYS:HZ3	1.77	0.49
12:N:545:LEU:HB3	12:N:554:MET:HE1	1.94	0.49
1:A:13:ALA:HB2	1:A:648:PRO:HB3	1.95	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
8:I:237:GLU:H	8:I:237:GLU:CD	2.19	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:894:GLN:CD	1:A:895:TYR:H	2.21	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
1:A:1386:TRP:C	1:A:1386:TRP:CD1	2.91	0.48
3:C:409:TYR:HB3	3:C:418:CYS:HB3	1.95	0.48
12:N:802:LYS:HG2	12:N:808:LEU:HD12	1.95	0.48
13:O:129:THR:C	13:O:133:GLY:HA3	2.38	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
15:Y:304:LEU:HD13	15:Y:308:MET:HE2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:289:PHE:C	12:N:291:LYS:H	2.22	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
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
12:N:693:ARG:HA	12:N:696:MET:HE2	1.94	0.48
3:P:457:TRP:HE3	3:P:473:LEU:HD21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
13:O:502:GLN:C	13:O:504:ALA:H	2.22	0.48
3:P:310:ARG:HG2	3:P:312:MET:HE3	1.96	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
6:H:639:TYR:OH	6:H:643:MET:SD	2.68	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
1:A:892:SER:OG	1:A:893:SER:N	2.44	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
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:1165:HIS:C	1:A:1167:GLU:H	2.22	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
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:1082:VAL:HG11	1:A:1560:MET:HE2	1.95	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:823:ILE:C	1:A:825:PRO:HD3	2.40	0.47
1:A:862:TYR:HB3	1:A:896:LEU:HD22	1.96	0.47
3:C:66:PRO:C	3:C:68:ALA:H	2.21	0.47
3:C:217:GLU:H	3:C:217:GLU:CD	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:862:TYR:OH	1:A:871:ARG:NH2	2.47	0.47
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: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:1727:ASN:C	1:A:1729:GLU:H	2.22	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: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:NE2	2.30	0.47
6:F:129:ASP:HB2	15:Y:506:GLN:HE22	1.80	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:211:LYS:C	9:J:213:ASN:H	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:431:ARG:HG3	12:N:432:GLU:H	1.80	0.47
13:O:127:HIS:C	13:O:129:THR:H	2.23	0.47
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
8:I:361:TYR:O	8:I:364:SER:OG	2.31	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
8:I:645:ASP:OD2	8:I:648:THR:OG1	2.22	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
9:J:311:MET:HE2	9:J:311:MET:HB3	1.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Y:168:THR:HB	15:Y:169:PRO:HD2	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
6:F:616:GLU:OE1	6:F:619:LYS:HB2	2.14	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
15:X:63:MET:HE3	15:Y:266:LEU:HB3	1.96	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
9:J:69:TYR:C	9:J:71:ALA:H	2.24	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
3:C:183:ASP:N	3:C:183:ASP:OD1	2.47	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
8:I:322:MET:HE3	8:I:429:THR:OG1	2.16	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
9:J:475:ILE:HG13	9:J:475:ILE:O	2.15	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:36:GLU:HB2	9:J:39:ASP:CG	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:203:PHE:HE1	9:K:218:THR:HB	1.80	0.46
12:N:560:MET:HE2	12:N:560:MET:HA	1.98	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
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:925:SER:C	1:A:927:ALA:H	2.24	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:371:MET:HE2	3:P:375:TYR:CE2	2.52	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: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
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:78:LYS:HZ2	1:A:88:ASP:HA	1.81	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1725:ASN:C	1:A:1727:ASN:H	2.24	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
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
8:I:192:MET:HE2	8:I:192:MET:HB3	1.90	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
3:C:312:MET:HE3	3:C:315:GLU:HG3	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
1:A:1762:GLY:C	1:A:1764:LYS:H	2.24	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:1909:THR:HA	1:A:1936:LEU:HD13	1.99	0.44
2:B:3:VAL:HG13	12:N:649:GLU:CD	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
15:X:83:HIS:O	15:X:86:SER:OG	2.31	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: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
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:656:MET:HE1	15:Y:524:GLU:HA	2.00	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
15:X:66:ASN:ND2	15:Y:268:ARG:HB3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1086:MET:SD	1:A:1560:MET:HG3	2.58	0.44
1:A:1134:TRP:CE2	1:A:1203:MET:HE1	2.52	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
9:K:217:GLU:CD	9:K:218:THR:H	2.26	0.44
11:M:57:TRP:HE1	11:M:59:ASP:CG	2.26	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
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
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
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
1:A:1019:MET:HE2	1:A:1019:MET:HB3	1.70	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
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:163:SER:OG	1:A:167:LYS:O	2.30	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
1:A:1919:LYS:HZ3	12:N:67:LEU:HA	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:I:66:LYS:H	8:I:86:ASP:CG	2.23	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
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
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:51:SER:OG	15:Y:204:ASP:OD2	2.22	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:199:CYS:HB3	15:Y:200:PRO:C	2.44	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:545:TYR:CD2	13:O:579:MET:HE1	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1596:SER:C	1:A:1598:ASP:H	2.27	0.43
3:C:543:ARG:C	3:C:545:GLU:H	2.27	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: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
1:A:1063:ILE:HG13	1:A:1066:LYS:HE2	2.01	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
2:B:14:TRP:HD1	12:N:596:LEU:C	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:1379:ASN:HD21	1:A:1417:ASP:CG	2.27	0.42
2:B:13:THR:HG22	12:N:598:SER:HB2	2.01	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
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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:540:ASN:C	3:C:542:THR:H	2.28	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
15:Y:391:GLU:HA	15:Y:394:ILE:HG12	2.01	0.42
1:A:433:THR:HG21	1:A:488:MET:HE2	2.00	0.42
1:A:1550:MET:HE2	1:A:1550:MET:HB2	1.85	0.42
3:C:26:PHE:HB2	3:C:32:ILE:HD11	2.02	0.42
6:F:633:ARG:HH21	6:F:664:ILE:HG23	1.84	0.42
8:I:183:GLY:C	8:I:201:ILE:HB	2.43	0.42
10:L:179:MET:HE2	10:L:180:TYR:CE2	2.54	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
6:H:102:SER:C	6:H:104:ASP:N	2.77	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:1658:PRO:HG2	1:A:1663:LEU:HD13	2.01	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:707:PHE:O	6:F:711:SER:OG	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:744:GLY:C	6:H:760:PHE:HE1	2.28	0.42
8:I:222:GLU:CD	8:I:231:VAL:HG22	2.45	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:422:ILE:O	13:O:426:THR:HG22	2.20	0.42
15:Y:429:MET:HE3	15:Y:429:MET:HB2	1.68	0.42
1:A:1292:GLU:H	1:A:1292:GLU:HG2	1.46	0.42
4:D:53:PRO:HB3	3:P:385:ILE:HG21	2.01	0.42
6:F:537:GLU:H	6:F:537:GLU:CD	2.28	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
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
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: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:588:ARG:HG3	1:A:589:ASP:CG	2.45	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
3:C:307:LEU:HG	3:C:312:MET:HE2	2.01	0.42
8:I:190:TYR:CZ	8:I:253:ARG:HD3	2.55	0.42
8:I:486:LEU:C	8:I:488:SER:H	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:273:MET:HE2	12:N:332:PHE:HD1	1.85	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
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: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
13:O:326:GLU:CD	13:O:329:ARG:HH12	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:X:37:VAL:HA	15:X:40:HIS:CD2	2.55	0.41
1:A:1053:GLN:CD	1:A:1053:GLN:H	2.29	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
12:N:779:MET:HE3	12:N:779:MET:HB3	1.85	0.41
13:O:89:LEU:HD12	13:O:89:LEU:HA	1.95	0.41
13:O:706:CYS:C	13:O:708:GLU:H	2.28	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
15:Y:455:PRO:C	15:Y:457:THR:H	2.28	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
8:I:286:ARG:HG3	12:N:608:LYS:HZ3	1.84	0.41
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:X:455:PRO:C	15:X:457:THR:H	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
11:M:20:ARG:HD3	3:P:134:THR:C	2.46	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
15:Y:87:LEU:HD13	15:Y:95:ASN:C	2.46	0.41
15:Y:532:TYR:HB2	15:Y:549:MET:HE2	2.03	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:376:LEU:O	9:J:380:LEU:HG	2.20	0.41
9:J:389:ARG:O	9:J:392:SER:OG	2.30	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
13:O:252:GLU:OE1	13:O:252:GLU:N	2.39	0.41
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:354:MET:HE3	9:J:354:MET:HB2	1.86	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:594:SER:C	13:O:596:SER:H	2.29	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:X:408:ASP:HA	15:X:411:GLU:CD	2.46	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
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:273:MET:HE1	12:N:335:ILE:HB	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
15:Y:413:LEU:HG	15:Y:429:MET:HE1	2.03	0.41
1:A:635:VAL:O	1:A:639:VAL:HG12	2.20	0.40
1:A:1159:VAL:HG11	13:O:332:GLN:CD	2.46	0.40
1:A:1276:GLU:OE2	1:A:1294:TYR:OH	2.25	0.40
1:A:1377:LYS:HG2	1:A:1416:TRP:CG	2.56	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
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
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
6:H:491:LEU:C	6:H:493:SER:H	2.28	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:527:ARG:NH1	15:Y:303:TYR:HH	2.16	0.40
6:H:717:GLU:HA	6:H:719:TYR:CE1	2.56	0.40
8:I:428:MET:HE2	8:I:428:MET:HA	2.03	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
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
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:397:ILE:O	9:J:398:ALA:C	2.64	0.40
9:J:417:GLU:C	9:J:419:LYS:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:99:LYS:HD3	15:Y:102:MET:HE2	2.03	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%)	43 72
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
6	H	484/824 (59%)	451 (93%)	31 (6%)	2 (0%)	30 61
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%)	30 61
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
12	N	658/822 (80%)	587 (89%)	69 (10%)	2 (0%)	36 67
13	O	682/755 (90%)	644 (94%)	36 (5%)	2 (0%)	36 67
14	T	13/15 (87%)	10 (77%)	3 (23%)	0	100 100
15	X	480/599 (80%)	458 (95%)	21 (4%)	1 (0%)	43 72
15	Y	492/599 (82%)	471 (96%)	17 (4%)	4 (1%)	16 47
All	All	7998/10368 (77%)	7411 (93%)	570 (7%)	17 (0%)	44 72

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%)	1086 (87%)	166 (13%)	4 19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	65/75 (87%)	60 (92%)	5 (8%)	12 36
3	C	452/520 (87%)	417 (92%)	35 (8%)	12 36
3	P	422/520 (81%)	397 (94%)	25 (6%)	18 43
4	D	46/115 (40%)	40 (87%)	6 (13%)	4 19
5	E	47/89 (53%)	43 (92%)	4 (8%)	10 33
6	F	371/727 (51%)	348 (94%)	23 (6%)	16 42
6	H	408/727 (56%)	378 (93%)	30 (7%)	13 38
7	G	25/77 (32%)	20 (80%)	5 (20%)	1 8
7	W	23/77 (30%)	20 (87%)	3 (13%)	4 19
8	I	607/730 (83%)	550 (91%)	57 (9%)	8 30
9	J	425/548 (78%)	386 (91%)	39 (9%)	8 31
9	K	423/548 (77%)	388 (92%)	35 (8%)	10 34
10	L	155/170 (91%)	141 (91%)	14 (9%)	9 32
11	M	52/67 (78%)	42 (81%)	10 (19%)	1 9
12	N	547/724 (76%)	493 (90%)	54 (10%)	7 29
13	O	573/650 (88%)	508 (89%)	65 (11%)	5 23
14	T	1/2 (50%)	1 (100%)	0	100 100
15	X	406/513 (79%)	383 (94%)	23 (6%)	18 44
15	Y	417/513 (81%)	385 (92%)	32 (8%)	12 36
All	All	6717/9112 (74%)	6086 (91%)	631 (9%)	10 30

All (631) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	33	ASN
1	A	113	VAL
1	A	127	LEU
1	A	134	SER
1	A	151	ILE
1	A	161	MET
1	A	168	ASP
1	A	173	LEU
1	A	177	VAL
1	A	183	THR

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Mol	Chain	Res	Type
1	A	240	VAL
1	A	242	HIS
1	A	244	MET
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	450	LEU
1	A	455	VAL
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	508	LYS
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	638	LEU
1	A	665	MET
1	A	754	LEU
1	A	777	THR
1	A	783	ILE
1	A	786	LEU
1	A	797	LEU
1	A	804	ASP
1	A	813	LEU
1	A	814	VAL
1	A	816	THR
1	A	819	GLN

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Mol	Chain	Res	Type
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	947	LEU
1	A	953	LEU
1	A	957	ASP
1	A	970	TRP
1	A	1014	ASP
1	A	1024	MET
1	A	1026	LEU
1	A	1033	ARG
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	1051	VAL
1	A	1088	THR
1	A	1104	LYS
1	A	1108	THR
1	A	1114	ARG
1	A	1125	ILE
1	A	1132	THR
1	A	1153	ILE
1	A	1159	VAL
1	A	1168	LEU
1	A	1176	LEU
1	A	1179	LEU
1	A	1181	LEU
1	A	1217	LEU
1	A	1219	THR
1	A	1225	THR
1	A	1230	ILE
1	A	1239	THR
1	A	1264	THR
1	A	1273	LEU
1	A	1274	LEU

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Mol	Chain	Res	Type
1	A	1279	ARG
1	A	1284	GLU
1	A	1290	ASP
1	A	1292	GLU
1	A	1302	LEU
1	A	1309	HIS
1	A	1321	VAL
1	A	1325	LEU
1	A	1359	ASN
1	A	1371	LEU
1	A	1376	LEU
1	A	1379	ASN
1	A	1386	TRP
1	A	1391	ASP
1	A	1392	THR
1	A	1404	LEU
1	A	1405	LEU
1	A	1417	ASP
1	A	1430	VAL
1	A	1437	ASN
1	A	1454	LEU
1	A	1457	LEU
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	1536	LEU
1	A	1538	LEU
1	A	1544	MET
1	A	1546	THR
1	A	1562	LEU
1	A	1565	LEU
1	A	1574	LEU
1	A	1588	LEU
1	A	1591	HIS
1	A	1597	THR
1	A	1603	LEU
1	A	1607	ARG
1	A	1634	LEU
1	A	1642	GLN

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Mol	Chain	Res	Type
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	1687	LEU
1	A	1693	LYS
1	A	1697	LEU
1	A	1705	GLN
1	A	1783	THR
1	A	1785	GLU
1	A	1786	MET
1	A	1787	LEU
1	A	1800	LEU
1	A	1805	MET
1	A	1813	GLN
1	A	1815	LYS
1	A	1816	LEU
1	A	1835	LYS
1	A	1851	THR
1	A	1866	MET
1	A	1894	VAL
1	A	1900	LEU
1	A	1911	PHE
1	A	1920	GLN
1	A	1928	LEU
1	A	1935	LEU
2	B	13	THR
2	B	14	TRP
2	B	15	LEU
2	B	16	TRP
2	B	65	HIS
3	C	26	PHE
3	C	28	ASP
3	C	29	LEU
3	C	80	ASP
3	C	85	ASP
3	C	89	LEU
3	C	97	LYS
3	C	119	MET

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Mol	Chain	Res	Type
3	C	130	LYS
3	C	133	GLU
3	C	134	THR
3	C	138	LEU
3	C	141	LEU
3	C	174	LEU
3	C	182	LEU
3	C	183	ASP
3	C	199	LEU
3	C	237	ILE
3	C	244	ILE
3	C	289	LEU
3	C	305	ASN
3	C	331	VAL
3	C	343	LEU
3	C	348	GLU
3	C	358	LEU
3	C	376	MET
3	C	386	GLN
3	C	407	GLN
3	C	446	LEU
3	C	462	VAL
3	C	490	TYR
3	C	536	CYS
3	C	543	ARG
3	C	551	ARG
3	C	556	LEU
4	D	20	LEU
4	D	26	GLU
4	D	32	GLN
4	D	35	GLN
4	D	49	ASN
4	D	50	ASN
5	E	63	VAL
5	E	69	GLN
5	E	89	LEU
5	E	99	ILE
6	F	23	ASP
6	F	30	ARG
6	F	43	LEU
6	F	68	THR
6	F	98	ASN

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Mol	Chain	Res	Type
6	F	105	ASP
6	F	169	LYS
6	F	485	ILE
6	F	487	ILE
6	F	494	HIS
6	F	498	THR
6	F	550	VAL
6	F	568	GLU
6	F	611	PHE
6	F	616	GLU
6	F	617	LEU
6	F	621	LEU
6	F	636	ASN
6	F	712	VAL
6	F	726	LEU
6	F	732	ILE
6	F	733	VAL
6	F	747	TYR
7	G	5	LYS
7	G	8	ARG
7	G	11	LEU
7	G	13	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	103	HIS
6	H	104	ASP
6	H	128	THR
6	H	147	PHE
6	H	165	ASP
6	H	455	GLN
6	H	480	ASN
6	H	491	LEU
6	H	517	GLN

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Mol	Chain	Res	Type
6	H	530	ASN
6	H	537	GLU
6	H	550	VAL
6	H	563	ASP
6	H	568	GLU
6	H	614	THR
6	H	667	GLN
6	H	686	GLU
6	H	705	CYS
6	H	729	LEU
6	H	742	LEU
8	I	26	LEU
8	I	37	LEU
8	I	68	VAL
8	I	86	ASP
8	I	90	ILE
8	I	92	LEU
8	I	116	MET
8	I	118	VAL
8	I	144	THR
8	I	145	LEU
8	I	171	VAL
8	I	174	ASN
8	I	231	VAL
8	I	237	GLU
8	I	254	LYS
8	I	267	LEU
8	I	269	LEU
8	I	279	ILE
8	I	286	ARG
8	I	287	LEU
8	I	302	ASP
8	I	305	MET
8	I	308	LEU
8	I	318	GLN
8	I	320	LEU
8	I	327	VAL
8	I	332	LYS
8	I	338	GLU
8	I	341	TYR
8	I	357	GLU
8	I	358	SER

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Mol	Chain	Res	Type
8	I	360	LEU
8	I	366	LEU
8	I	372	TRP
8	I	373	LYS
8	I	404	LEU
8	I	408	ASP
8	I	418	PHE
8	I	425	MET
8	I	428	MET
8	I	440	MET
8	I	452	LEU
8	I	454	GLU
8	I	477	GLN
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	631	VAL
8	I	656	THR
8	I	663	ASP
8	I	729	LYS
8	I	733	VAL
8	I	748	ILE
9	J	9	ARG
9	J	16	GLN
9	J	32	LEU
9	J	39	ASP
9	J	50	THR
9	J	63	ARG
9	J	169	LEU
9	J	170	LEU
9	J	180	GLU
9	J	185	LEU
9	J	196	GLU
9	J	206	GLU
9	J	207	ASN
9	J	214	LYS
9	J	220	ILE
9	J	224	VAL

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Mol	Chain	Res	Type
9	J	229	GLU
9	J	233	VAL
9	J	248	LYS
9	J	255	SER
9	J	279	ASN
9	J	287	LEU
9	J	290	LYS
9	J	323	LEU
9	J	329	LEU
9	J	331	LYS
9	J	362	GLN
9	J	395	LEU
9	J	397	ILE
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	157	LEU
9	K	159	LEU
9	K	165	GLU
9	K	193	LEU
9	K	214	LYS
9	K	225	ASP
9	K	231	LEU
9	K	233	VAL
9	K	234	VAL
9	K	284	LEU
9	K	289	HIS
9	K	290	LYS
9	K	300	VAL
9	K	310	LEU

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Mol	Chain	Res	Type
9	K	331	LYS
9	K	338	ILE
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	439	VAL
9	K	475	ILE
9	K	497	ASN
9	K	503	HIS
10	L	42	VAL
10	L	43	ASP
10	L	45	LEU
10	L	48	ASP
10	L	49	ASN
10	L	65	ASN
10	L	79	ILE
10	L	83	TYR
10	L	84	LYS
10	L	100	ASN
10	L	137	ILE
10	L	144	ASN
10	L	154	ARG
10	L	158	ILE
11	M	5	VAL
11	M	10	ARG
11	M	16	ASP
11	M	17	ASP
11	M	29	VAL
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	70	VAL

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Mol	Chain	Res	Type
12	N	108	LEU
12	N	111	LEU
12	N	135	TRP
12	N	137	ARG
12	N	141	LEU
12	N	153	VAL
12	N	154	HIS
12	N	235	GLN
12	N	237	LEU
12	N	256	VAL
12	N	287	ARG
12	N	302	LYS
12	N	350	ASP
12	N	366	GLU
12	N	374	LEU
12	N	378	LEU
12	N	386	LEU
12	N	392	ASN
12	N	409	VAL
12	N	416	ILE
12	N	417	LEU
12	N	431	ARG
12	N	481	VAL
12	N	526	ARG
12	N	529	HIS
12	N	530	GLN
12	N	533	PHE
12	N	534	SER
12	N	537	ARG
12	N	554	MET
12	N	564	MET
12	N	576	GLU
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	650	LEU
12	N	667	LEU
12	N	670	PHE

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Mol	Chain	Res	Type
12	N	673	GLN
12	N	678	LEU
12	N	681	LEU
12	N	685	VAL
12	N	692	LEU
12	N	705	LEU
12	N	753	LEU
12	N	773	ILE
12	N	790	ILE
12	N	814	VAL
13	O	35	ILE
13	O	56	GLU
13	O	57	ARG
13	O	59	ARG
13	O	60	LEU
13	O	74	THR
13	O	75	LEU
13	O	81	LEU
13	O	86	CYS
13	O	93	VAL
13	O	98	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	280	ARG
13	O	350	LEU
13	O	359	VAL
13	O	360	LEU
13	O	363	HIS
13	O	385	VAL
13	O	398	LEU
13	O	402	LEU
13	O	403	LYS
13	O	408	LEU
13	O	414	LEU
13	O	417	LEU
13	O	426	THR
13	O	441	GLN
13	O	443	GLN

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Mol	Chain	Res	Type
13	O	461	ASN
13	O	463	THR
13	O	511	ASP
13	O	512	GLN
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
13	O	619	LEU
13	O	625	LEU
13	O	636	ILE
13	O	641	LEU
13	O	645	HIS
13	O	654	ASP
13	O	657	ILE
13	O	682	LYS
13	O	691	ILE
13	O	694	LEU
13	O	704	VAL
13	O	709	ARG
13	O	710	ILE
13	O	713	VAL
13	O	717	GLN
13	O	733	CYS
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	117	LEU
3	P	122	ARG
3	P	131	ASP
3	P	172	LEU

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Mol	Chain	Res	Type
3	P	174	LEU
3	P	183	ASP
3	P	186	LYS
3	P	237	ILE
3	P	244	ILE
3	P	276	ILE
3	P	286	PHE
3	P	290	ARG
3	P	316	LEU
3	P	343	LEU
3	P	365	LEU
3	P	378	MET
3	P	392	ILE
3	P	432	ASP
3	P	450	VAL
3	P	495	GLN
7	W	8	ARG
7	W	14	ASP
7	W	23	ARG
15	X	49	LEU
15	X	79	LEU
15	X	154	ASP
15	X	168	THR
15	X	229	THR
15	X	233	LEU
15	X	255	ILE
15	X	270	ASN
15	X	271	VAL
15	X	286	ASP
15	X	303	TYR
15	X	304	LEU
15	X	373	VAL
15	X	386	MET
15	X	401	ARG
15	X	414	ILE
15	X	432	ASN
15	X	442	GLN
15	X	444	LEU
15	X	456	VAL
15	X	486	LEU
15	X	499	LEU
15	X	503	LEU

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Mol	Chain	Res	Type
15	Y	52	ASN
15	Y	70	LEU
15	Y	95	ASN
15	Y	106	GLN
15	Y	154	ASP
15	Y	193	LYS
15	Y	213	SER
15	Y	214	VAL
15	Y	229	THR
15	Y	230	VAL
15	Y	255	ILE
15	Y	293	LYS
15	Y	301	ASP
15	Y	304	LEU
15	Y	337	GLN
15	Y	354	ARG
15	Y	401	ARG
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	496	ILE
15	Y	505	ASN
15	Y	513	ARG
15	Y	515	LEU
15	Y	524	GLU
15	Y	530	ASP
15	Y	546	LEU
15	Y	551	LYS
15	Y	552	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (211) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	27	HIS
1	A	124	GLN
1	A	125	GLN
1	A	162	HIS
1	A	176	GLN

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Mol	Chain	Res	Type
1	A	263	GLN
1	A	367	GLN
1	A	451	GLN
1	A	473	ASN
1	A	601	ASN
1	A	623	GLN
1	A	636	GLN
1	A	776	ASN
1	A	819	GLN
1	A	833	HIS
1	A	981	GLN
1	A	1106	ASN
1	A	1138	HIS
1	A	1192	ASN
1	A	1231	HIS
1	A	1247	HIS
1	A	1266	HIS
1	A	1309	HIS
1	A	1359	ASN
1	A	1481	ASN
1	A	1486	ASN
1	A	1510	HIS
1	A	1591	HIS
1	A	1602	HIS
1	A	1604	GLN
1	A	1642	GLN
1	A	1705	GLN
1	A	1765	GLN
1	A	1795	GLN
1	A	1920	GLN
2	B	9	ASN
2	B	31	ASN
2	B	50	GLN
2	B	71	GLN
3	C	71	GLN
3	C	82	GLN
3	C	145	GLN
3	C	163	GLN
3	C	197	HIS
3	C	249	GLN
3	C	252	GLN
3	C	274	HIS

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Mol	Chain	Res	Type
3	C	287	ASN
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	477	HIS
3	C	479	GLN
3	C	488	GLN
3	C	552	GLN
4	D	31	GLN
4	D	32	GLN
4	D	36	GLN
4	D	37	HIS
4	D	38	GLN
4	D	49	ASN
5	E	75	GLN
6	F	486	ASN
6	F	494	HIS
6	F	495	HIS
6	F	517	GLN
6	F	547	GLN
6	F	595	GLN
6	F	636	ASN
6	F	667	GLN
6	F	702	ASN
6	H	14	GLN
6	H	90	GLN
6	H	145	ASN
6	H	166	GLN
6	H	480	ASN
6	H	490	HIS
6	H	494	HIS
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	599	ASN

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Mol	Chain	Res	Type
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	53	HIS
8	I	114	HIS
8	I	257	HIS
8	I	266	ASN
8	I	323	ASN
8	I	345	GLN
8	I	353	GLN
8	I	374	GLN
8	I	401	ASN
8	I	477	GLN
8	I	531	ASN
8	I	577	ASN
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	241	HIS
9	J	271	HIS
9	J	352	GLN
9	J	362	GLN
9	J	406	HIS
9	J	477	GLN
9	J	494	ASN
9	J	503	HIS
9	K	18	GLN
9	K	20	GLN
9	K	38	GLN
9	K	271	HIS
9	K	352	GLN
9	K	362	GLN
10	L	28	GLN
10	L	44	GLN

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Mol	Chain	Res	Type
10	L	103	HIS
10	L	128	HIS
10	L	146	GLN
10	L	155	GLN
11	M	53	GLN
11	M	63	GLN
12	N	65	HIS
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
12	N	764	ASN
13	O	62	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	441	GLN
13	O	443	GLN
13	O	449	ASN
13	O	460	GLN
13	O	461	ASN
13	O	472	HIS
13	O	512	GLN
13	O	617	GLN
13	O	671	GLN
13	O	680	GLN
13	O	728	GLN

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Mol	Chain	Res	Type
13	O	741	HIS
3	P	35	GLN
3	P	71	GLN
3	P	163	GLN
3	P	197	HIS
3	P	249	GLN
3	P	268	GLN
3	P	299	ASN
3	P	305	ASN
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	251	ASN
15	X	289	ASN
15	X	298	GLN
15	X	337	GLN
15	X	338	HIS
15	X	369	ASN
15	X	371	ASN
15	X	385	ASN
15	Y	50	HIS
15	Y	66	ASN
15	Y	184	GLN
15	Y	298	GLN
15	Y	337	GLN
15	Y	367	GLN
15	Y	374	GLN
15	Y	506	GLN
15	Y	512	HIS
15	Y	526	GLN
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 (i)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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.

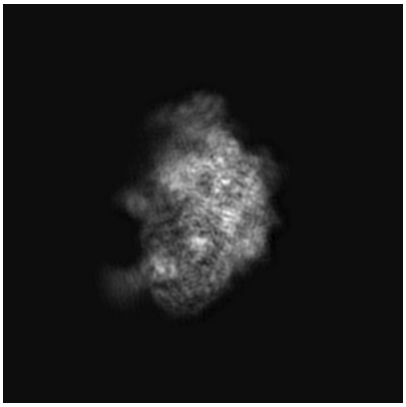
6 Map visualisation

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.

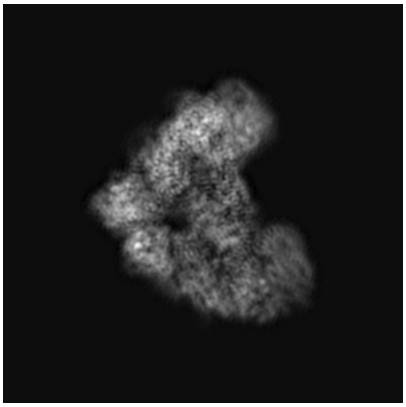
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

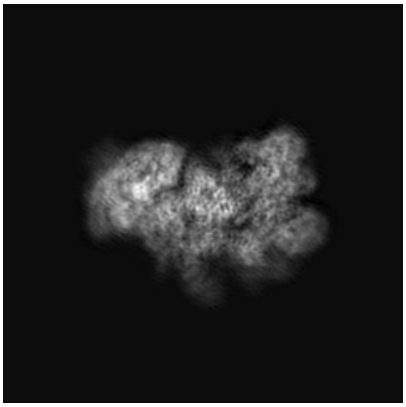
6.1.1 Primary map



X



Y

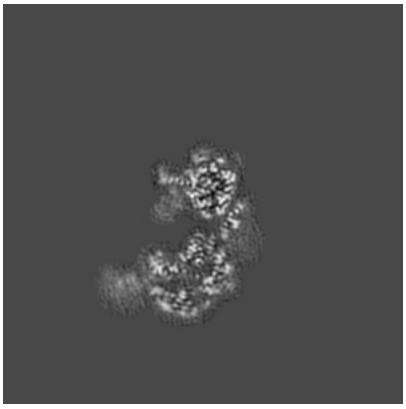


Z

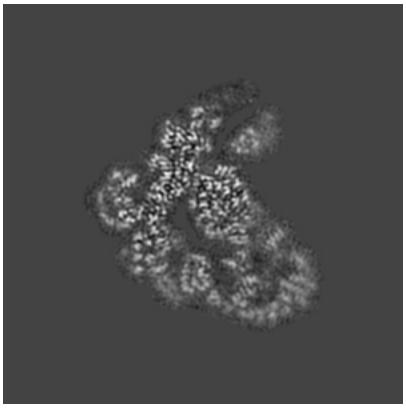
The images above show the map projected in three orthogonal directions.

6.2 Central slices

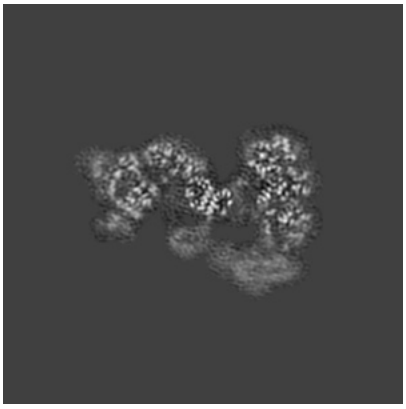
6.2.1 Primary map



X Index: 169



Y Index: 169

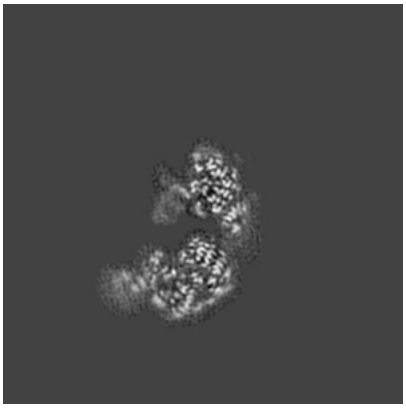


Z Index: 169

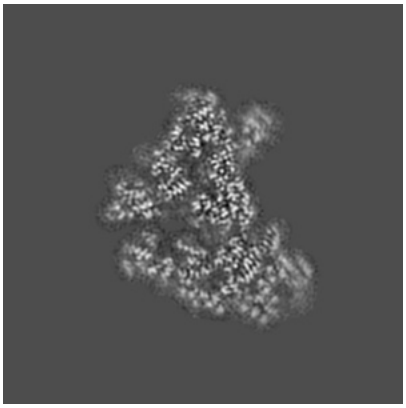
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

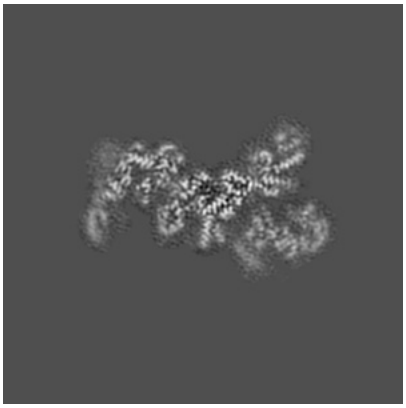
6.3.1 Primary map



X Index: 165



Y Index: 182

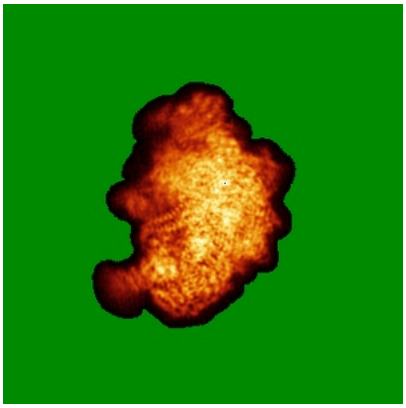


Z Index: 188

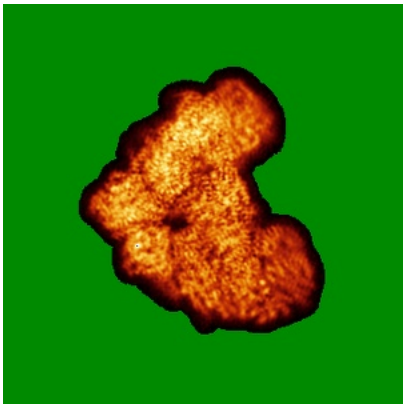
The images above show the largest variance slices of the map in three orthogonal directions.

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

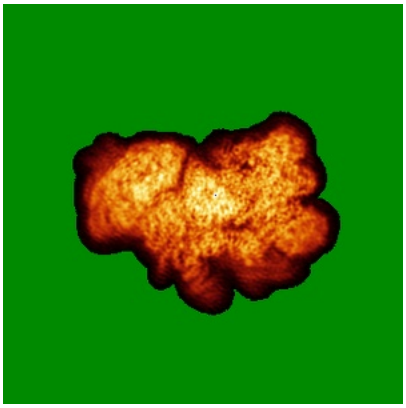
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0117. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

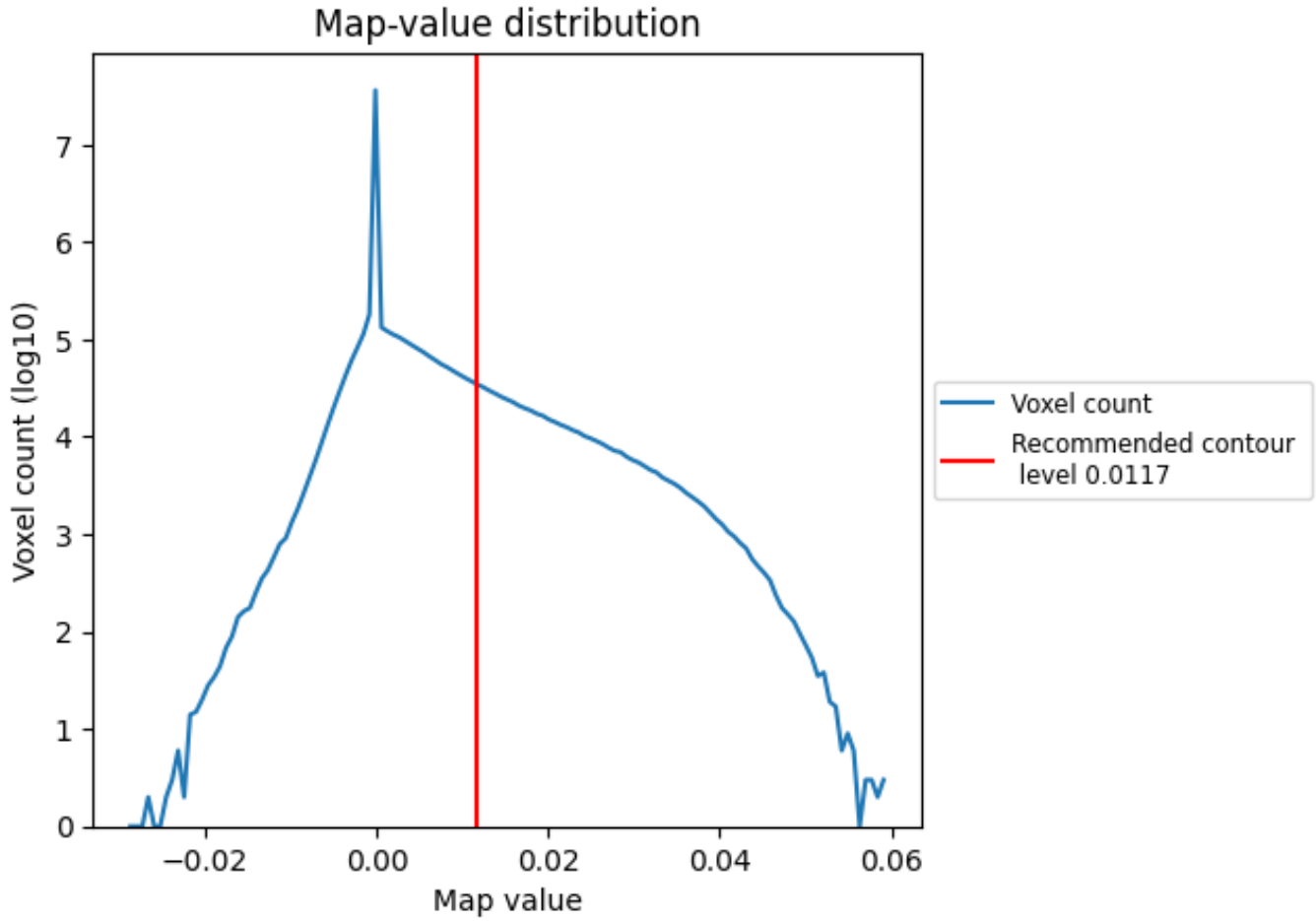
6.6 Mask visualisation (i)

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

7 Map analysis

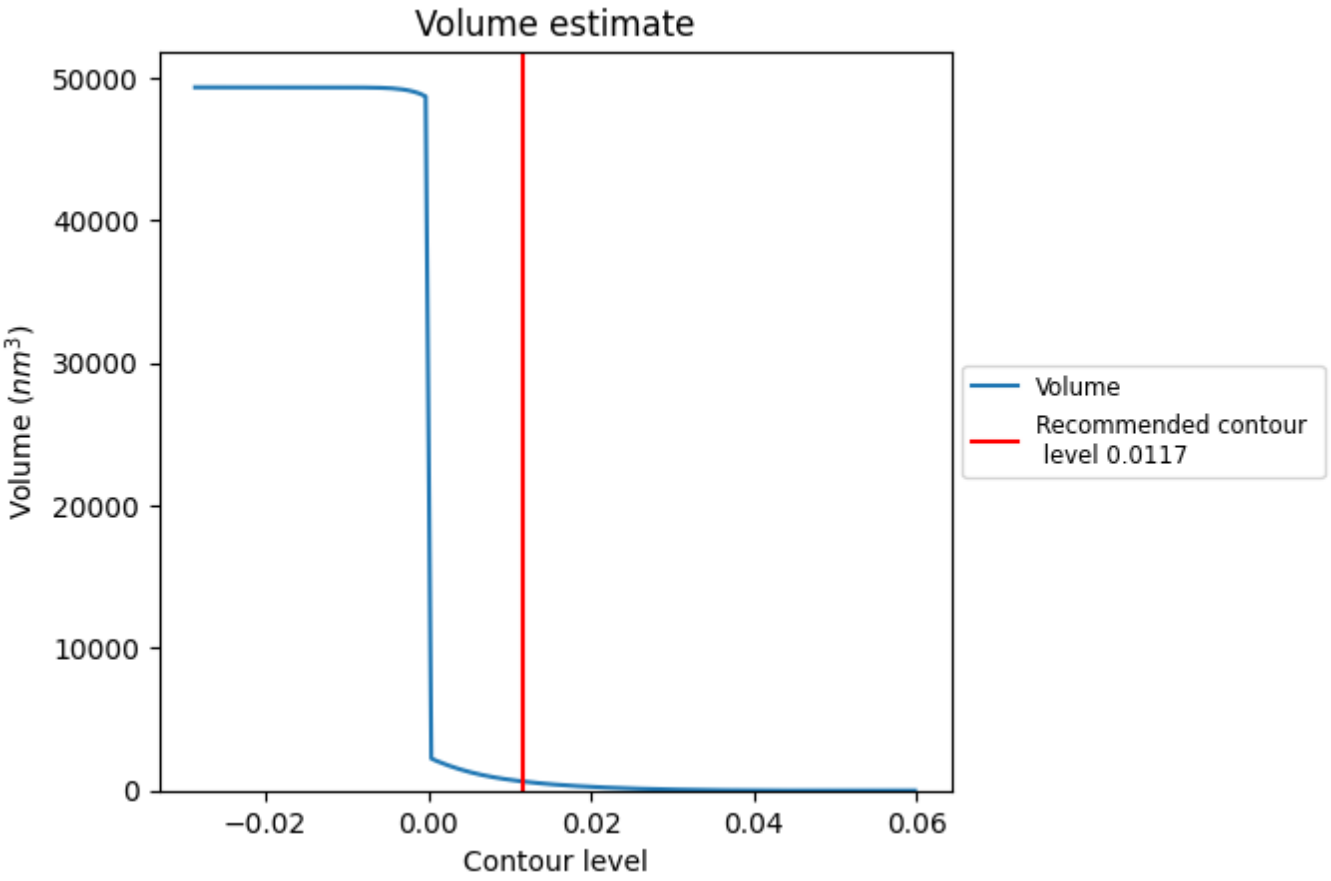
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

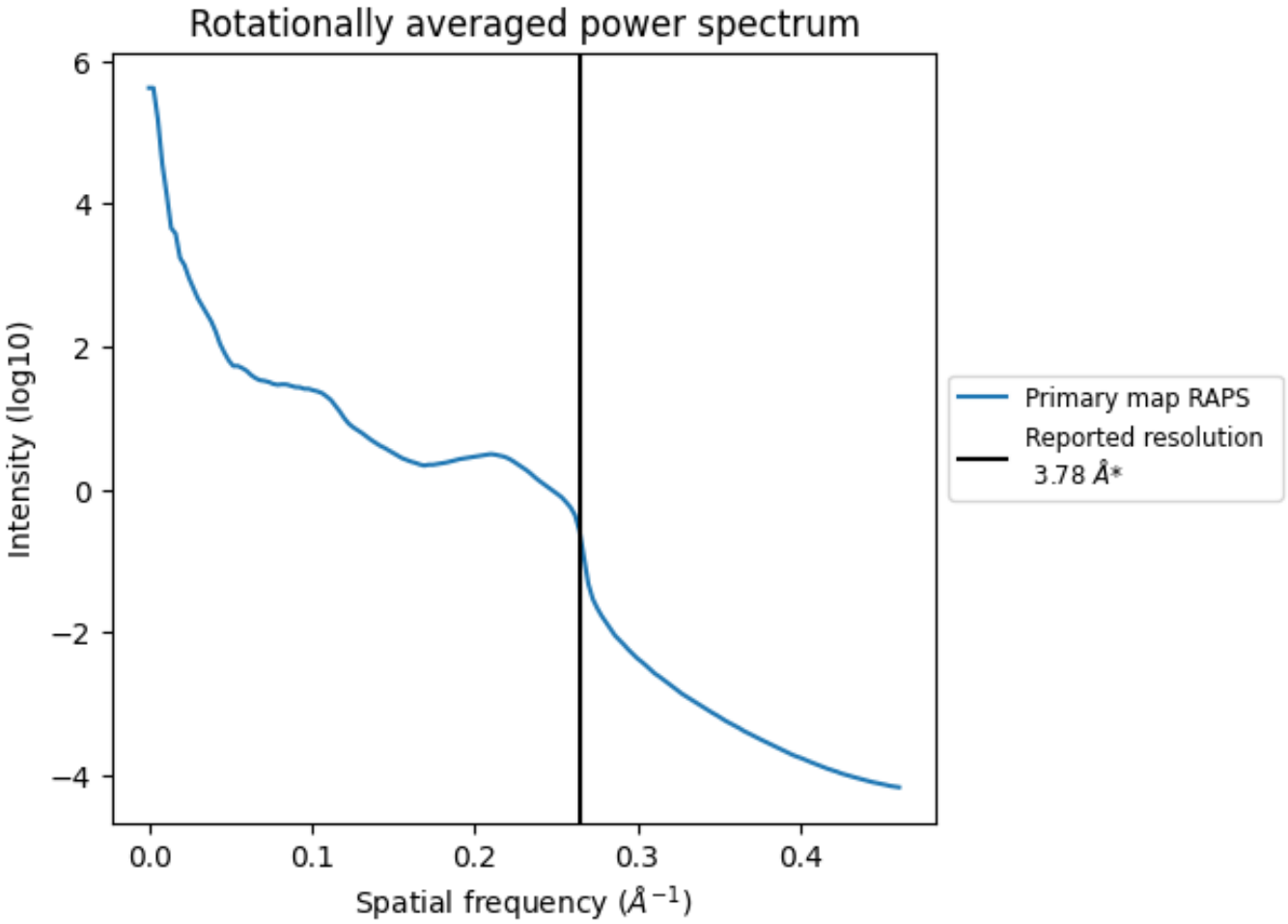
7.2 Volume estimate



The volume at the recommended contour level is 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}

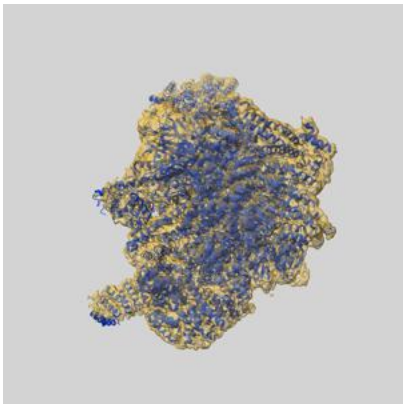
8 Fourier-Shell correlation

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

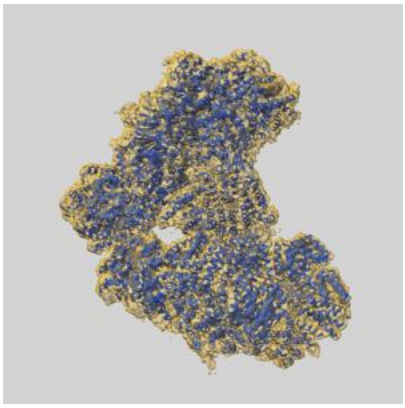
9 Map-model fit

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.

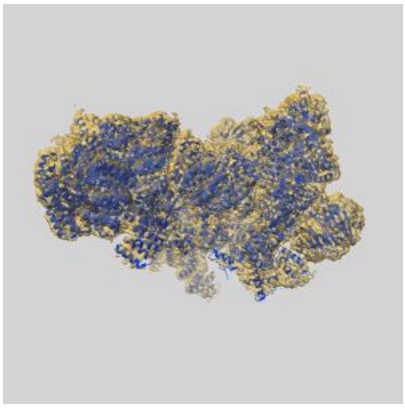
9.1 Map-model overlay



X



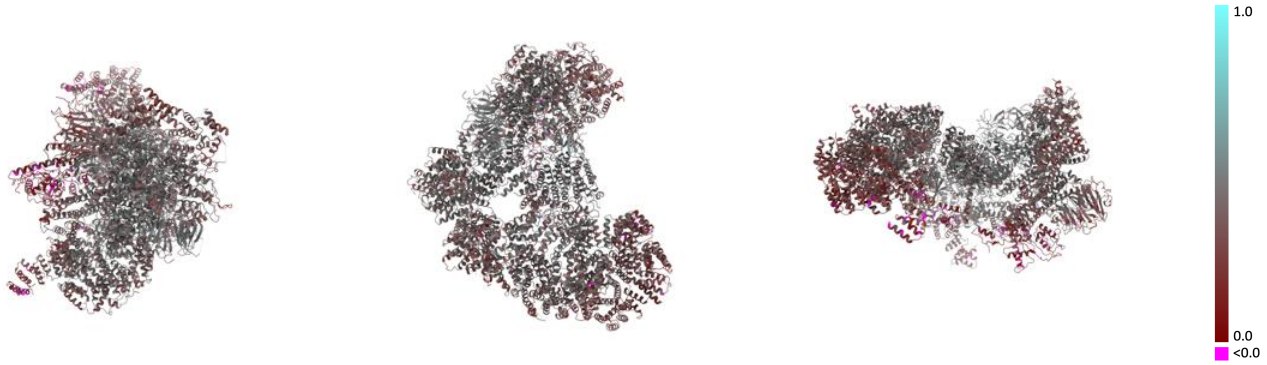
Y



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.

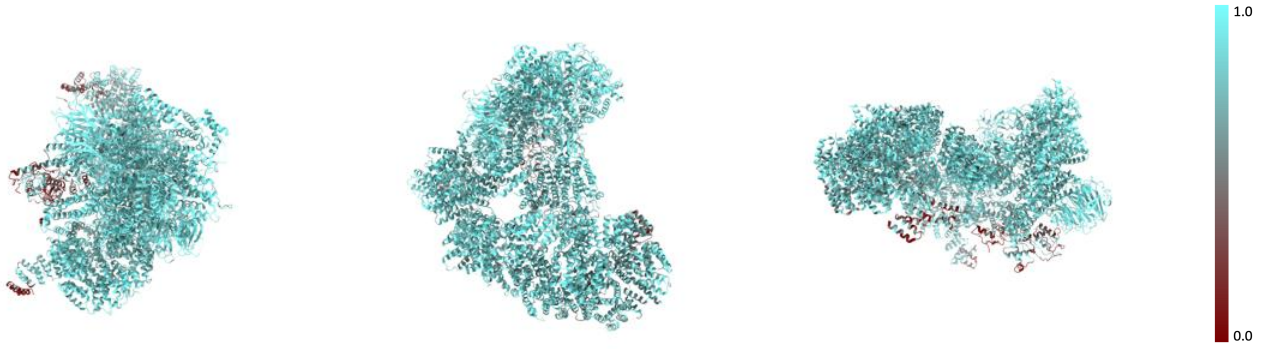
9.2 Q-score mapped to coordinate model (i)



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.

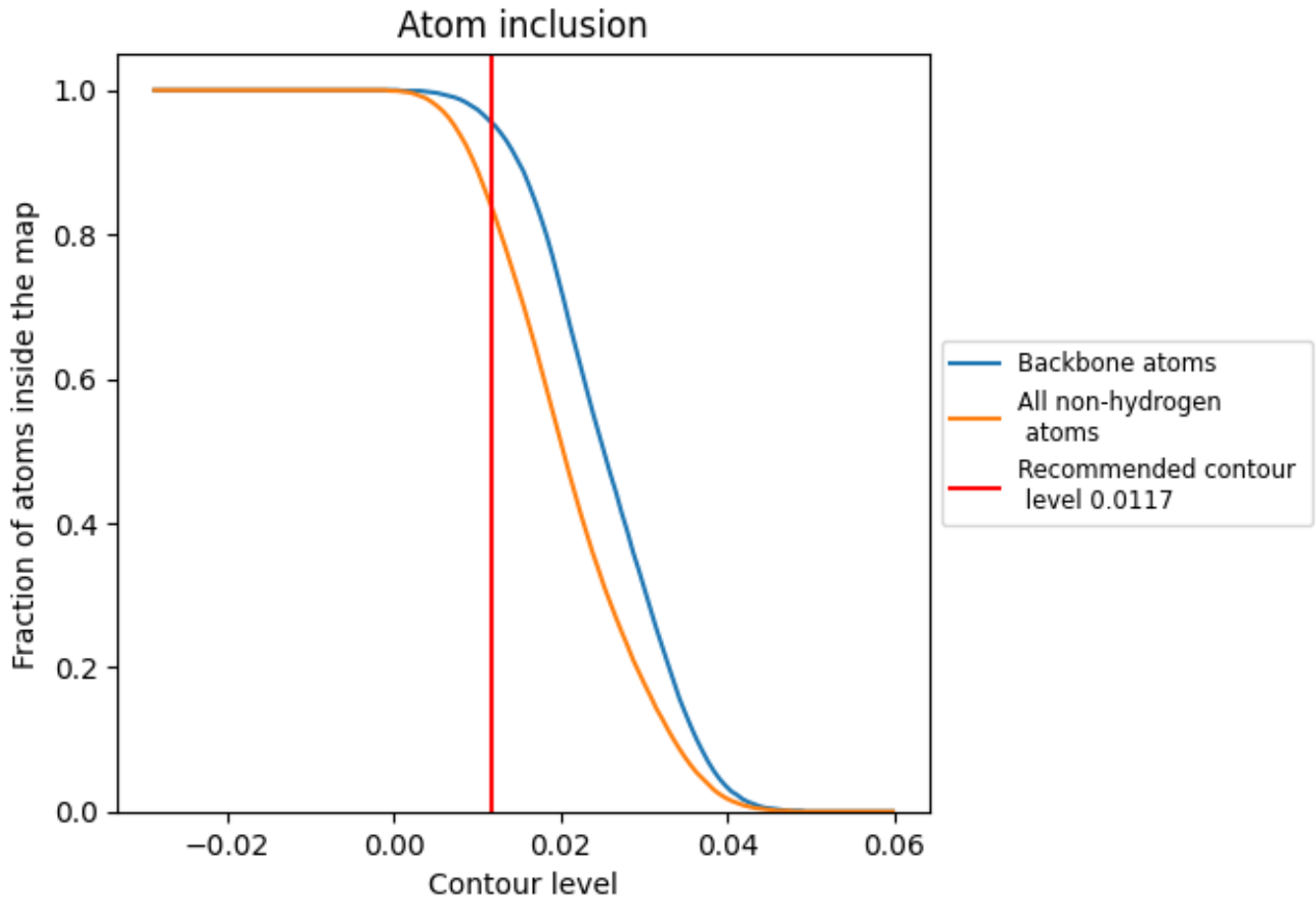
9.3 Atom inclusion mapped to coordinate model (i)



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	0.8380	0.3900
A	0.8930	0.4460
B	0.1960	0.1300
C	0.8860	0.4400
D	0.8430	0.4380
E	0.8330	0.4090
F	0.8630	0.3950
G	0.7970	0.3690
H	0.8670	0.4210
I	0.8750	0.3850
J	0.8750	0.3910
K	0.8840	0.4240
L	0.8470	0.4170
M	0.7640	0.4260
N	0.7060	0.2840
O	0.8820	0.4430
P	0.8400	0.3860
T	0.8350	0.4670
W	0.7810	0.3990
X	0.7170	0.2860
Y	0.7690	0.2920