Full wwPDB EM Validation Report (i)

Dec 17, 2022 – 01:56 pm GMT

PDB ID	:	6Z9M
EMDB ID	:	EMD-11123
Title	:	Pseudoatomic model of the pre-fusion conformation of glycoprotein B of Herpes simplex virus 1
Authors	:	Vollmer, B.; Prazak, V.; Vasishtan, D.; Jefferys, E.E.; Hernandez-Duran, A.; Vallbracht, M.; Klupp, B.; Mettenleiter, T.C.; Backovic, M.; Rey, F.A.; Topf, M.; Gruenewald, K.
Deposited on	:	2020-06-04
Resolution	:	9.10 Å(reported)
Based on initial model	:	5V2S

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 (i) 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 (i)) were used in the production of this report:

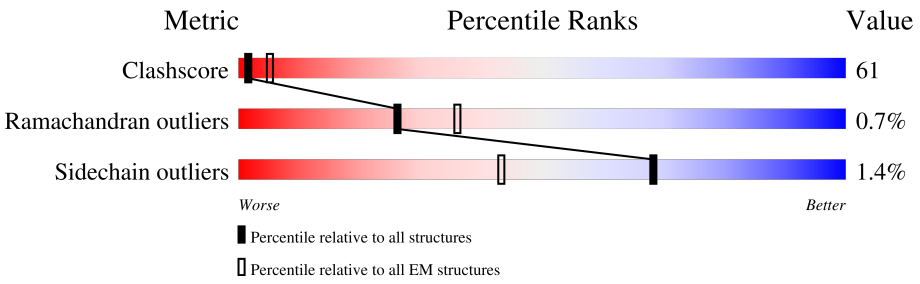
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 9.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	904	20% 15% 50% • 33%
1	B	904	20% 15% 50% • 33%
1	C	904	22% 16% 50% • 33%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 14694 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 Envelope glycoprotein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	606	4898	3089	863	924	22	0	0
1	B	606	4898	3089	863	924	22	0	0
1	C	606	4898	3089	863	924	22	0	0

There are 3 discrepancies between the modelled and reference sequences:

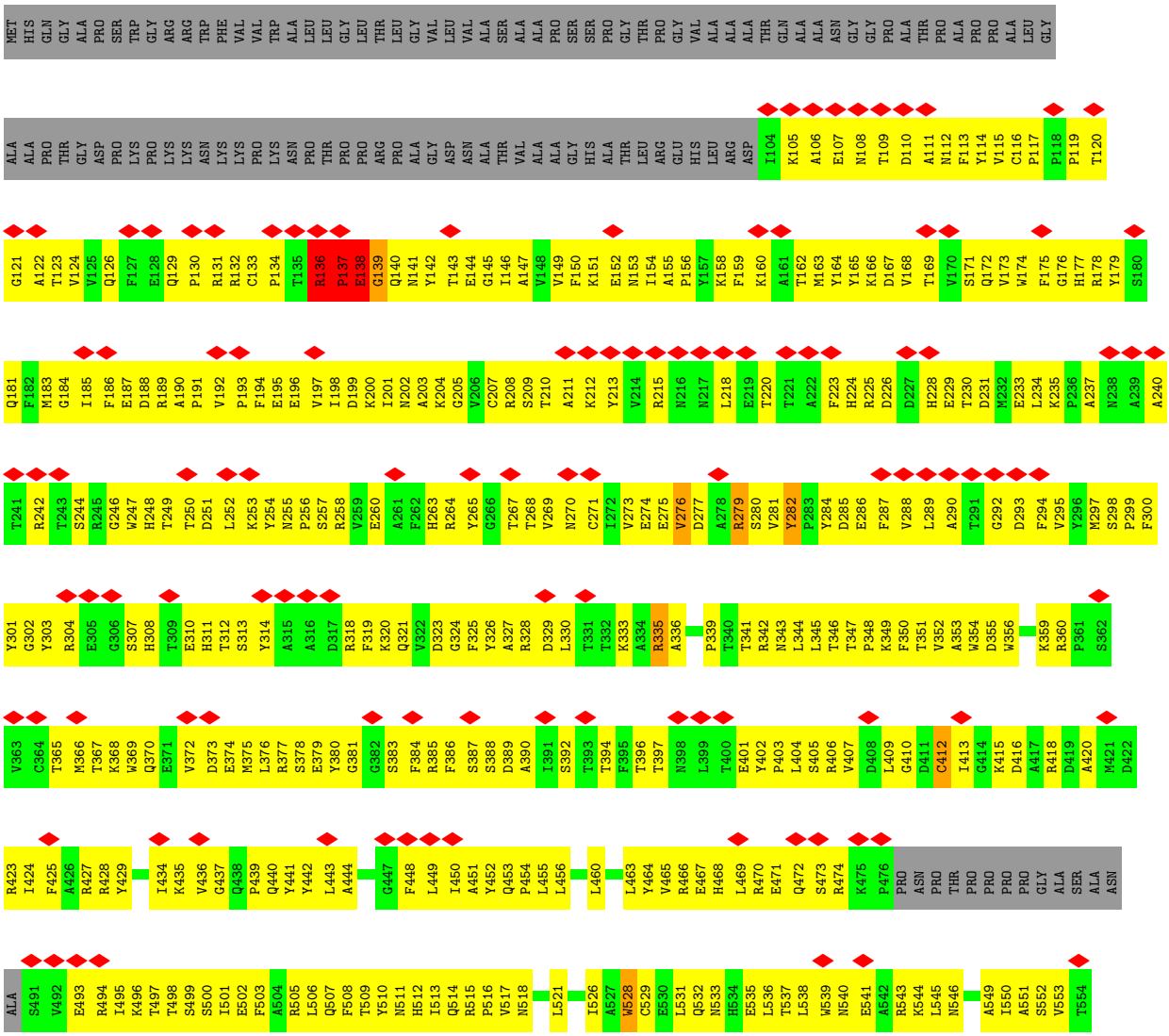
Chain	Residue	Modelled	Actual	Comment	Reference
A	516	PRO	HIS	engineered mutation	UNP A1Z0P7
B	516	PRO	HIS	engineered mutation	UNP A1Z0P7
C	516	PRO	HIS	engineered mutation	UNP A1Z0P7

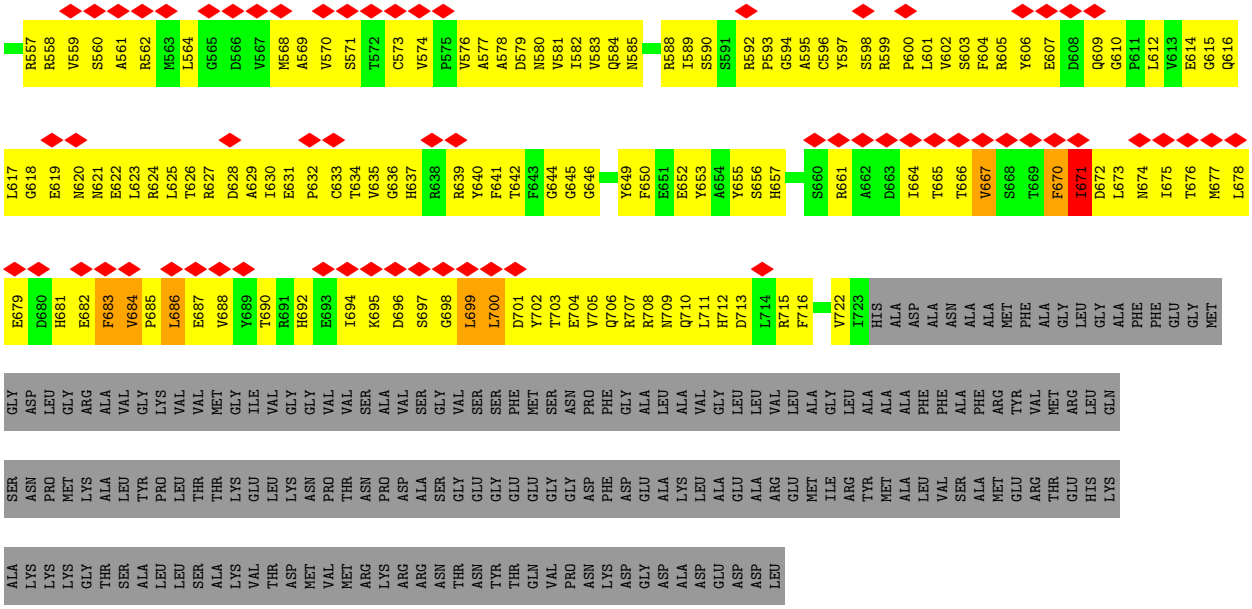
3 Residue-property plots (i)

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: Envelope glycoprotein B

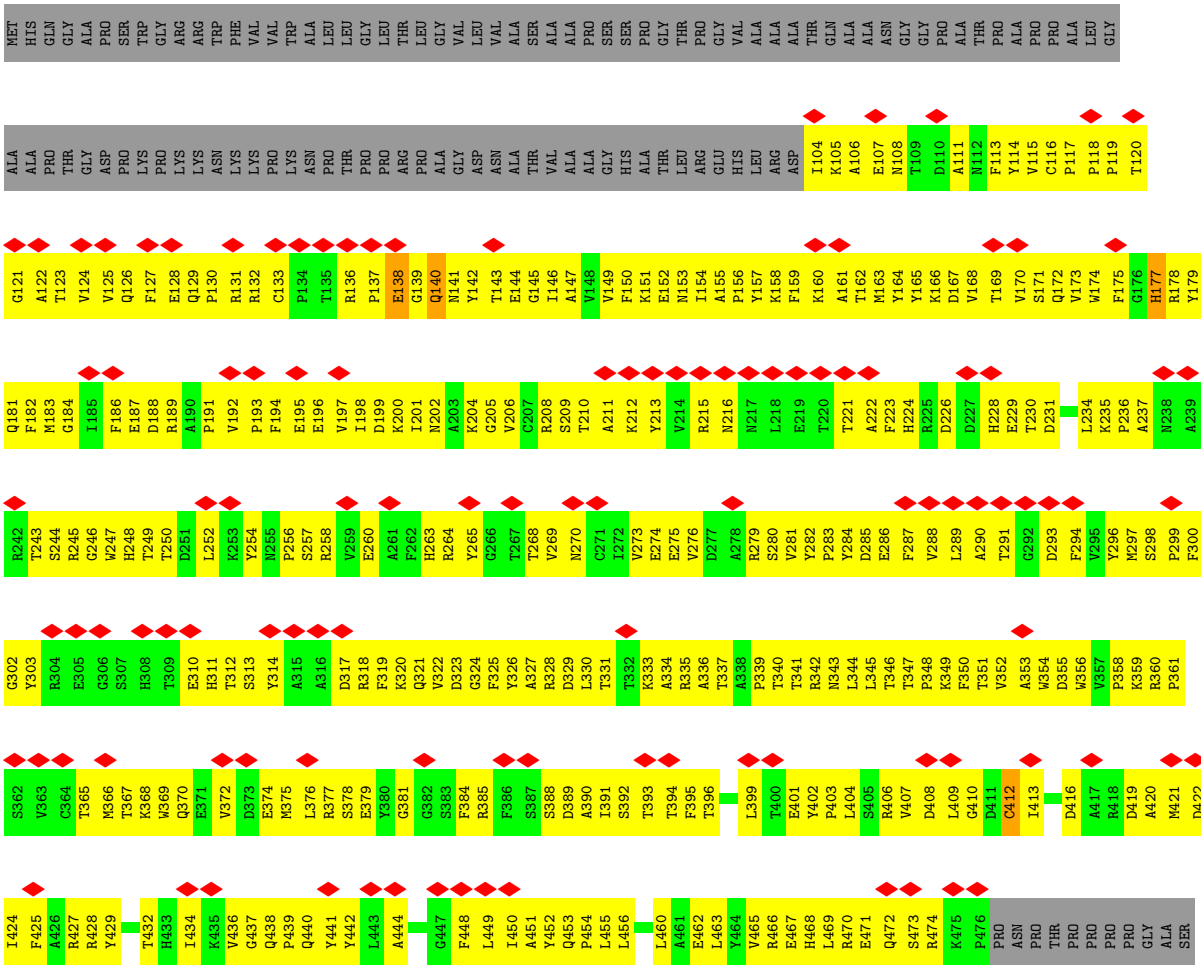
Chain A: 20% 15% 50% • 33%

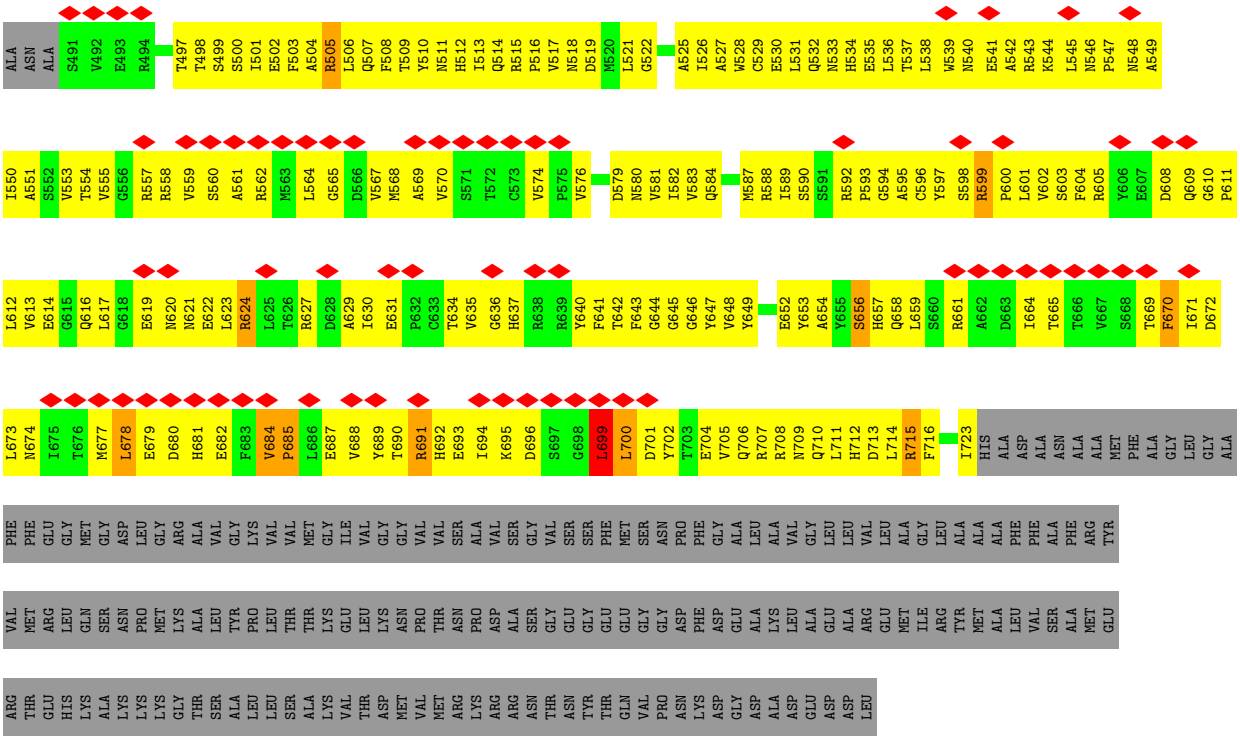




- Molecule 1: Envelope glycoprotein B

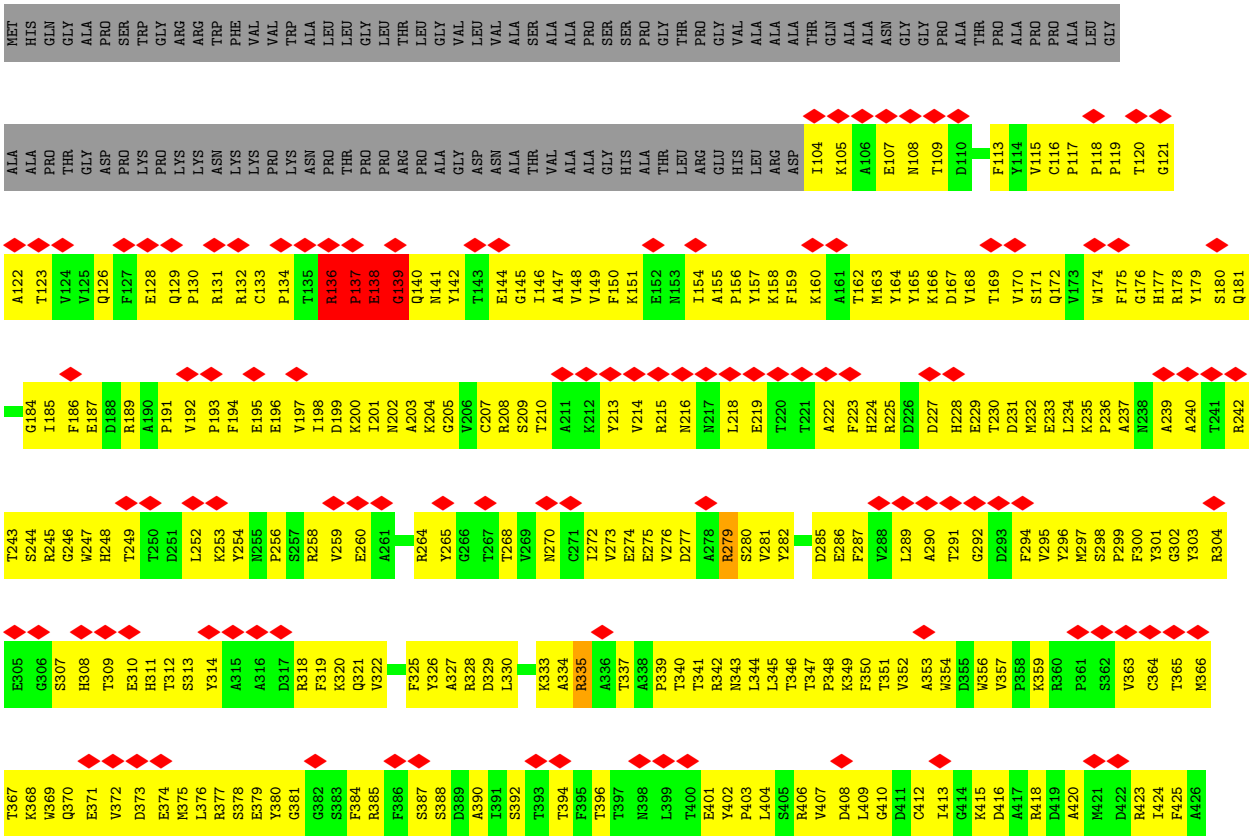
Chain B: 20% 15% 50% • 33%

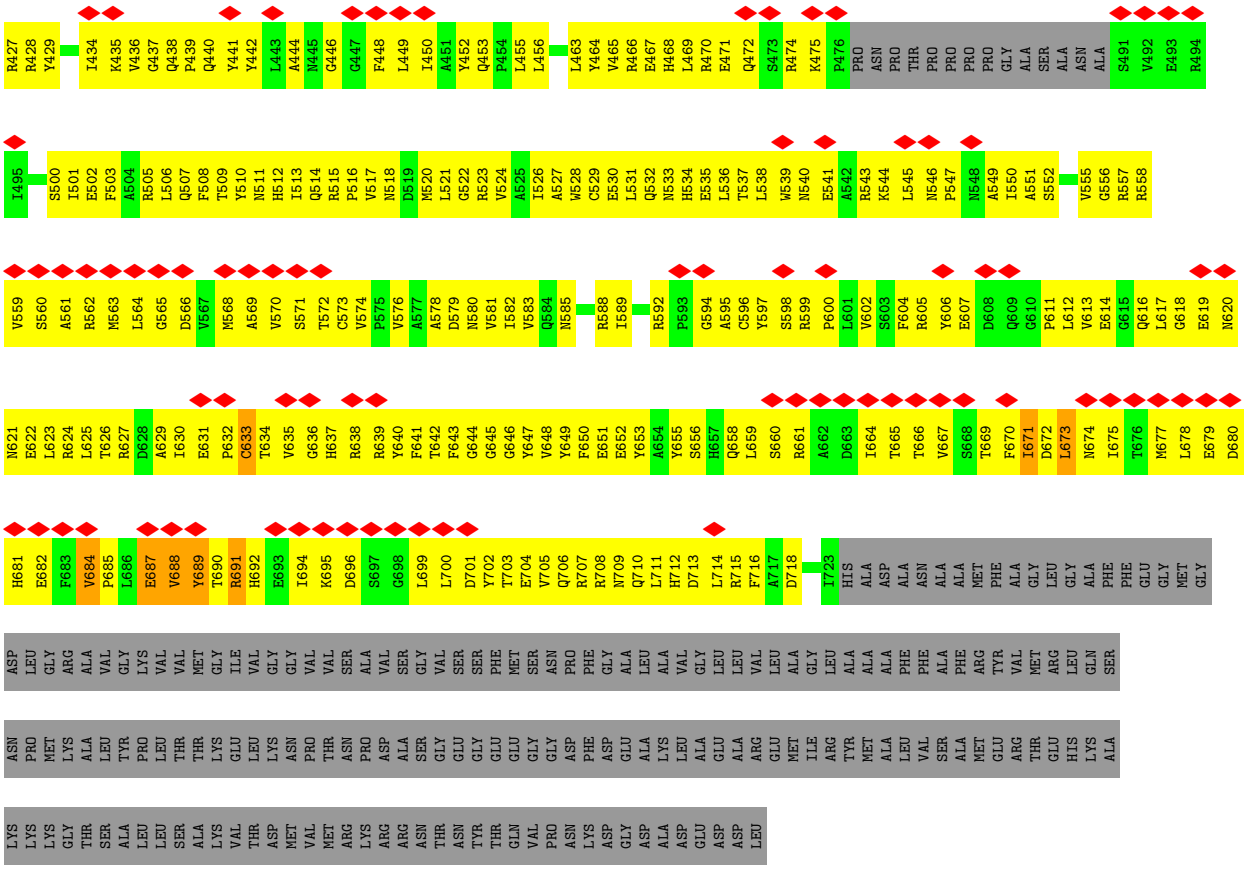




• Molecule 1: Envelope glycoprotein B

Chain C:




R427 R428 Y429 I434 K435 V436 G437 Q438 P439 Q440 Y441 Y442 L443 A444 W445 G446 G447 F448 L449 I450 A451 Y452 Q453 P454 L455 L456 L463 Y464 V465 R466 E467 H468 L469 R470 E471 Q472 S473 R474 K475 P476 PRO ASN PRO THR PRO PRO PRO PRO GLY ALA SER ALA ASN ALA S491 V492 E493 R494
I495 S500 I501 E502 F503 A504 R505 L506 Q507 F508 T509 Y510 N511 H512 I513 Q514 R515 P516 V517 N518 D519 M520 L521 G522 R523 V524 A525 T526 A527 W528 C529 E530 L531 Q532 N533 H534 E535 L536 T537 L538 W539 N540 E541 A542 R543 K544 L545 N546 P547 N548 A549 I550 A551 S552 V555 G556 R557 R558
V559 S560 A561 R562 M563 L564 G565 D566 V567 M568 A569 V570 S571 T572 C573 V574 P575 V576 A577 A578 D579 N580 V581 I582 V583 Q584 N585 R588 I589 R592 P593 G594 A595 C596 Y597 S598 R599 P600 L601 V602 S603 F604 R605 Y606 E607 D608 Q609 G610 P611 L612 V613 E614 G615 Q616 L617 G618 E619 N620
N621 E622 L623 R624 L625 T626 R627 D628 A629 I630 E631 P632 C633 T634 V635 G636 H637 R638 R639 Y640 F641 T642 F643 G644 G645 G646 Y647 V648 Y649 F650 E651 E652 Y653 A654 Y655 S656 H657 Q658 L659 S660 R661 A662 D663 I664 T665 T666 V667 S668 T669 F670 I671 D672 L673 N674 I675 T676 M677 L678 E679 D680
H681 E682 F683 V684 P685 L686 E687 V688 Y689 T690 R691 H692 E693 I694 K695 D696 S697 G698 L699 L700 D701 Y702 T703 E704 V705 Q706 R707 R708 N709 Q710 L711 H712 D713 L714 R715 F716 A717 D718 I723 HIS ALA ASP ALA ASN ALA ALA MET PHE ALA GLY LEU GLY ALA PHE MET GLY
ASP LEU GLY ARG ALA VAL GLY LYS VAL VAL MET GLY ILE VAL GLY GLY VAL VAL SER ALA VAL SER GLY VAL SER SER PHE MET SER ASN PRO PHE GLY ALA LEU ALA VAL GLY LEU LEU VAL LEU ALA GLY LEU ALA ALA PHE PHE ALA PHE ARG TYR VAL MET ARG LEU GLN SER
ASN PRO MET LYS ALA LEU TYR PRO LEU THR THR LYS GLU LEU LYS ASN PRO THR ASN PRO ASP ALA SER GLY GLU GLY GLU GLU GLY GLY ASP PHE ASP GLU ALA LYS LEU ALA GLU ALA ARG GLU MET ILE ARG TYR MET ALA LEU VAL SER ALA MET GLU ARG THR GLU HIS LYS ALA
LYS LYS LYS GLY THR SER ALA LEU LEU SER ALA LYS VAL THR ASP MET VAL MET ARG LYS ARG ARG ASN THR ASN TYR THR GLN VAL PRO ASN LYS ASP GLY ASP ALA ASP GLU ASP ASP LEU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of subtomograms used	46067	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	2.3	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.311	Depositor
Minimum map value	-0.336	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.056	Depositor
Map size (Å)	160.0, 160.0, 160.0	wwPDB
Map dimensions	100, 100, 100	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.6, 1.6, 1.6	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.36	0/5018	0.58	1/6817 (0.0%)
1	B	0.35	0/5018	0.57	2/6817 (0.0%)
1	C	0.36	0/5018	0.58	2/6817 (0.0%)
All	All	0.36	0/15054	0.58	5/20451 (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	10
1	B	0	6
1	C	0	8
All	All	0	24

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	699	LEU	CA-CB-CG	6.85	131.06	115.30
1	C	137	PRO	C-N-CA	5.86	136.36	121.70
1	C	139	GLY	N-CA-C	5.35	126.47	113.10
1	B	678	LEU	CA-CB-CG	5.18	127.21	115.30
1	B	699	LEU	C-N-CA	5.11	134.48	121.70

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	136	ARG	Peptide
1	A	137	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	A	138	GLU	Peptide
1	A	139	GLY	Peptide
1	A	670	PHE	Peptide
1	A	671	ILE	Peptide
1	A	683	PHE	Peptide
1	A	684	VAL	Peptide
1	A	686	LEU	Peptide
1	A	700	LEU	Peptide
1	B	138	GLU	Peptide
1	B	140	GLN	Peptide
1	B	670	PHE	Peptide
1	B	684	VAL	Peptide
1	B	699	LEU	Peptide
1	B	716	PHE	Peptide
1	C	136	ARG	Peptide
1	C	138	GLU	Peptide
1	C	363	VAL	Peptide
1	C	671	ILE	Peptide
1	C	673	LEU	Peptide
1	C	684	VAL	Peptide
1	C	687	GLU	Peptide
1	C	688	VAL	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	4898	0	4726	645	0
1	B	4898	0	4726	639	0
1	C	4898	0	4726	571	0
All	All	14694	0	14178	1757	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 61.

All (1757) 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)
1:B:439:PRO:HA	1:B:452:TYR:O	1.36	1.20
1:B:604:PHE:O	1:B:612:LEU:HA	1.42	1.15
1:C:604:PHE:O	1:C:612:LEU:HA	1.48	1.13
1:C:149:VAL:HA	1:C:449:LEU:O	1.56	1.06
1:B:174:TRP:HB2	1:B:183:MET:HG2	1.40	1.02
1:A:142:TYR:HA	1:A:377:ARG:O	1.61	0.99
1:A:145:GLY:O	1:A:375:MET:HB2	1.63	0.98
1:A:441:TYR:HA	1:A:450:ILE:O	1.64	0.97
1:A:343:ASN:O	1:A:353:ALA:HA	1.64	0.96
1:A:156:PRO:HA	1:A:280:SER:O	1.66	0.96
1:A:604:PHE:O	1:A:612:LEU:HA	1.66	0.95
1:B:672:ASP:HA	1:B:673:LEU:HB3	1.48	0.95
1:C:145:GLY:O	1:C:375:MET:HB3	1.67	0.94
1:C:692:HIS:HA	1:C:695:LYS:HE2	1.50	0.92
1:B:169:THR:HA	1:B:186:PHE:O	1.69	0.92
1:A:381:GLY:HA3	1:A:385:ARG:HH21	1.34	0.92
1:B:106:ALA:HB2	1:B:581:VAL:HB	1.52	0.89
1:A:617:LEU:O	1:A:624:ARG:NH1	2.06	0.89
1:A:149:VAL:HG13	1:A:369:TRP:HB2	1.53	0.88
1:B:589:ILE:HG22	1:B:595:ALA:HB3	1.53	0.88
1:B:699:LEU:H	1:B:700:LEU:HB2	1.38	0.88
1:A:386:PHE:O	1:A:394:THR:HA	1.72	0.88
1:C:589:ILE:HG22	1:C:595:ALA:HB3	1.55	0.88
1:B:154:ILE:HB	1:B:282:TYR:HB3	1.54	0.88
1:A:115:VAL:HG12	1:A:117:PRO:HD3	1.55	0.87
1:C:440:GLN:HB3	1:C:442:TYR:HE1	1.38	0.86
1:A:588:ARG:HA	1:A:596:CYS:HA	1.58	0.86
1:B:502:GLU:HA	1:B:505:ARG:HB2	1.59	0.85
1:C:682:GLU:HA	1:C:689:TYR:HD1	1.42	0.85
1:A:242:ARG:NH1	1:A:623:LEU:O	2.08	0.85
1:B:600:PRO:HB2	1:B:617:LEU:HB3	1.57	0.85
1:A:707:ARG:O	1:A:710:GLN:NE2	2.10	0.84
1:A:388:SER:O	1:A:392:SER:HA	1.77	0.84
1:B:136:ARG:HB2	1:B:526:ILE:HD11	1.58	0.83
1:B:149:VAL:HA	1:B:449:LEU:O	1.79	0.83
1:C:423:ARG:HB3	1:C:427:ARG:HH21	1.42	0.83
1:C:529:CYS:SG	1:C:533:ASN:ND2	2.50	0.83
1:B:640:TYR:HA	1:B:648:VAL:O	1.78	0.83
1:B:344:LEU:HA	1:B:352:VAL:O	1.78	0.82
1:A:558:ARG:HH22	1:A:576:VAL:HG12	1.44	0.82
1:B:113:PHE:HA	1:B:621:ASN:HB3	1.60	0.82
1:A:149:VAL:HA	1:A:449:LEU:O	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:ARG:NH2	1:B:507:GLN:OE1	2.12	0.82
1:B:637:HIS:HB3	1:B:652:GLU:HA	1.61	0.81
1:B:710:GLN:HE22	1:B:713:ASP:HB3	1.45	0.81
1:C:597:TYR:HA	1:C:630:ILE:HA	1.60	0.81
1:B:561:ALA:HA	1:B:569:ALA:O	1.81	0.81
1:B:470:ARG:NH1	1:B:471:GLU:OE2	2.12	0.81
1:C:638:ARG:HH11	1:C:651:GLU:HB2	1.44	0.81
1:A:163:MET:O	1:A:273:VAL:HA	1.82	0.80
1:A:712:HIS:HB3	1:A:715:ARG:HH21	1.46	0.80
1:C:599:ARG:NE	1:C:617:LEU:O	2.13	0.80
1:B:423:ARG:HB3	1:B:427:ARG:HH21	1.46	0.80
1:B:164:TYR:HB3	1:B:192:VAL:HB	1.63	0.80
1:A:701:ASP:HB3	1:A:704:GLU:HB2	1.64	0.80
1:A:470:ARG:O	1:A:474:ARG:NH1	2.15	0.80
1:A:616:GLN:OE1	1:A:624:ARG:NH2	2.14	0.80
1:B:300:PHE:HB2	1:B:310:GLU:HG2	1.64	0.80
1:C:318:ARG:HH21	1:C:347:THR:HA	1.47	0.80
1:C:470:ARG:HH22	1:C:474:ARG:HH21	1.24	0.80
1:A:464:TYR:O	1:A:468:HIS:HB2	1.81	0.79
1:B:597:TYR:HA	1:B:630:ILE:HA	1.61	0.79
1:A:440:GLN:H	1:A:452:TYR:H	1.29	0.79
1:C:707:ARG:O	1:C:710:GLN:NE2	2.16	0.78
1:A:171:SER:HA	1:A:184:GLY:O	1.83	0.78
1:A:545:LEU:HD22	1:C:541:GLU:HB2	1.63	0.78
1:A:558:ARG:NH2	1:A:574:VAL:O	2.16	0.78
1:C:514:GLN:HG2	1:C:518:ASN:HD21	1.47	0.78
1:C:147:ALA:HB2	1:C:375:MET:HG2	1.66	0.78
1:C:444:ALA:HB3	1:C:448:PHE:HB2	1.66	0.77
1:B:466:ARG:NH2	1:B:467:GLU:OE2	2.16	0.77
1:B:699:LEU:HB3	1:B:700:LEU:HG	1.66	0.77
1:C:708:ARG:O	1:C:715:ARG:NH2	2.17	0.77
1:A:425:PHE:HA	1:A:429:TYR:HD1	1.49	0.77
1:C:541:GLU:HA	1:C:544:LYS:HD2	1.67	0.77
1:C:588:ARG:HA	1:C:596:CYS:HA	1.65	0.77
1:C:233:GLU:O	1:C:235:LYS:NZ	2.17	0.77
1:C:160:LYS:NZ	1:C:277:ASP:OD1	2.17	0.76
1:A:113:PHE:O	1:A:558:ARG:NH1	2.19	0.76
1:A:444:ALA:HB3	1:A:448:PHE:HB2	1.67	0.76
1:B:285:ASP:HA	1:B:298:SER:HB2	1.67	0.76
1:B:210:THR:HG22	1:B:223:PHE:HA	1.68	0.76
1:B:329:ASP:N	1:B:334:ALA:O	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:581:VAL:HG13	1:B:602:VAL:HG11	1.66	0.76
1:A:470:ARG:NH1	1:A:471:GLU:OE1	2.19	0.76
1:A:631:GLU:OE2	1:B:707:ARG:NH1	2.19	0.76
1:A:150:PHE:HA	1:A:368:LYS:HA	1.67	0.76
1:A:466:ARG:NH2	1:A:507:GLN:OE1	2.19	0.76
1:C:121:GLY:HA3	1:C:292:GLY:HA2	1.68	0.75
1:C:133:CYS:SG	1:C:533:ASN:ND2	2.60	0.75
1:B:142:TYR:HB3	1:B:376:LEU:HD22	1.68	0.75
1:B:279:ARG:HH21	1:C:678:LEU:HD13	1.50	0.75
1:C:466:ARG:NH2	1:C:467:GLU:OE2	2.20	0.75
1:B:444:ALA:HB3	1:B:448:PHE:HB2	1.69	0.75
1:A:378:SER:HB3	1:A:385:ARG:HB2	1.69	0.74
1:C:439:PRO:HA	1:C:452:TYR:O	1.86	0.74
1:B:712:HIS:O	1:B:715:ARG:NH1	2.20	0.74
1:A:686:LEU:HD12	1:C:187:GLU:HG2	1.68	0.74
1:C:296:TYR:O	1:C:313:SER:OG	2.05	0.74
1:C:169:THR:HA	1:C:186:PHE:O	1.85	0.74
1:B:582:ILE:O	1:B:602:VAL:HA	1.87	0.74
1:A:105:LYS:HA	1:A:582:ILE:HG13	1.69	0.74
1:A:377:ARG:NH1	1:A:379:GLU:OE1	2.21	0.74
1:C:379:GLU:HG3	1:C:384:PHE:HE1	1.51	0.74
1:C:377:ARG:NH2	1:C:471:GLU:OE1	2.21	0.73
1:C:131:ARG:NH2	1:C:394:THR:O	2.20	0.73
1:C:376:LEU:HG	1:C:387:SER:HB2	1.71	0.73
1:A:598:SER:OG	1:A:624:ARG:NH2	2.21	0.73
1:B:551:ALA:O	1:B:555:VAL:HB	1.87	0.73
1:C:207:CYS:O	1:C:232:MET:N	2.21	0.73
1:C:328:ARG:HA	1:C:335:ARG:HA	1.69	0.73
1:C:644:GLY:O	1:C:661:ARG:NH2	2.21	0.73
1:C:163:MET:HA	1:C:351:THR:O	1.88	0.73
1:A:436:VAL:O	1:A:453:GLN:NE2	2.21	0.73
1:B:530:GLU:O	1:B:534:HIS:N	2.21	0.73
1:B:644:GLY:O	1:B:661:ARG:NH1	2.16	0.73
1:C:142:TYR:N	1:C:377:ARG:O	2.22	0.73
1:C:156:PRO:HA	1:C:281:VAL:HA	1.68	0.73
1:A:235:LYS:O	1:A:248:HIS:N	2.19	0.72
1:A:605:ARG:HE	1:A:612:LEU:HD13	1.51	0.72
1:A:502:GLU:HA	1:A:505:ARG:HB2	1.70	0.72
1:B:210:THR:OG1	1:B:229:GLU:OE2	2.06	0.72
1:A:169:THR:HA	1:A:186:PHE:O	1.89	0.72
1:B:226:ASP:OD2	1:B:264:ARG:NH2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:439:PRO:HG3	1:C:453:GLN:HB2	1.70	0.72
1:B:236:PRO:HA	1:B:247:TRP:HA	1.70	0.72
1:B:588:ARG:HA	1:B:596:CYS:HA	1.71	0.72
1:C:132:ARG:NH1	1:C:133:CYS:O	2.23	0.72
1:A:151:LYS:HG3	1:A:369:TRP:NE1	2.04	0.72
1:A:318:ARG:O	1:A:320:LYS:NZ	2.23	0.72
1:A:117:PRO:O	1:A:560:SER:OG	2.06	0.72
1:A:149:VAL:O	1:A:369:TRP:N	2.22	0.72
1:A:178:ARG:HA	1:A:258:ARG:HH22	1.53	0.72
1:A:275:GLU:HG3	1:A:330:LEU:HD12	1.72	0.72
1:C:142:TYR:CA	1:C:377:ARG:O	2.38	0.72
1:C:404:LEU:HB2	1:C:410:GLY:HA3	1.71	0.72
1:C:344:LEU:HA	1:C:352:VAL:O	1.90	0.72
1:A:210:THR:OG1	1:A:229:GLU:OE2	2.08	0.71
1:A:703:THR:O	1:C:702:TYR:OH	2.07	0.71
1:C:225:ARG:HD3	1:C:254:TYR:HB2	1.72	0.71
1:A:703:THR:OG1	1:A:707:ARG:NH2	2.23	0.71
1:B:602:VAL:HB	1:B:623:LEU:HD11	1.73	0.71
1:B:167:ASP:HA	1:B:188:ASP:O	1.91	0.71
1:A:209:SER:N	1:A:230:THR:O	2.23	0.71
1:A:463:LEU:HD22	1:A:466:ARG:HE	1.56	0.71
1:B:463:LEU:HD13	1:B:466:ARG:HH11	1.54	0.71
1:C:210:THR:OG1	1:C:229:GLU:OE1	2.08	0.71
1:A:402:TYR:HE2	1:A:407:VAL:HG13	1.56	0.71
1:C:235:LYS:N	1:C:248:HIS:O	2.23	0.71
1:B:535:GLU:HA	1:B:538:LEU:HD13	1.72	0.71
1:B:162:THR:HA	1:B:275:GLU:HA	1.73	0.71
1:A:624:ARG:NH1	1:B:701:ASP:OD1	2.23	0.71
1:B:132:ARG:NH1	1:B:133:CYS:O	2.24	0.71
1:C:704:GLU:OE1	1:C:707:ARG:NE	2.23	0.71
1:B:200:LYS:O	1:B:206:VAL:N	2.22	0.70
1:B:408:ASP:HB2	1:B:409:LEU:HD12	1.72	0.70
1:B:649:TYR:HB3	1:B:657:HIS:O	1.91	0.70
1:C:378:SER:OG	1:C:385:ARG:HB2	1.91	0.70
1:A:120:THR:OG1	1:B:680:ASP:OD1	2.06	0.70
1:A:123:THR:O	1:A:126:GLN:NE2	2.23	0.70
1:A:713:ASP:OD1	1:A:713:ASP:N	2.22	0.70
1:B:634:THR:OG1	1:B:692:HIS:O	2.09	0.70
1:C:159:PHE:CE2	1:C:354:TRP:HB2	2.26	0.70
1:C:322:VAL:HG22	1:C:325:PHE:HB2	1.73	0.70
1:A:388:SER:O	1:A:392:SER:CA	2.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:LYS:HZ2	1:B:369:TRP:HA	1.54	0.70
1:B:156:PRO:HB2	1:B:158:LYS:HZ3	1.55	0.70
1:B:596:CYS:O	1:B:631:GLU:N	2.25	0.70
1:B:164:TYR:HD1	1:B:273:VAL:HG22	1.57	0.70
1:C:647:TYR:O	1:C:658:GLN:HA	1.91	0.70
1:A:142:TYR:HB3	1:A:376:LEU:HD11	1.73	0.70
1:A:234:LEU:HB2	1:A:333:LYS:HE2	1.74	0.69
1:A:601:LEU:HD12	1:A:616:GLN:HG2	1.73	0.69
1:B:501:ILE:HD12	1:B:504:ALA:HB3	1.74	0.69
1:C:466:ARG:O	1:C:469:LEU:HB3	1.91	0.69
1:B:501:ILE:HG13	1:B:505:ARG:HD2	1.74	0.69
1:A:175:PHE:HB3	1:A:260:GLU:HG2	1.73	0.69
1:C:471:GLU:OE2	1:C:510:TYR:OH	2.10	0.69
1:C:598:SER:N	1:C:629:ALA:O	2.18	0.69
1:A:692:HIS:HA	1:A:695:LYS:HD2	1.74	0.69
1:C:620:ASN:HA	1:C:642:THR:HB	1.74	0.69
1:A:644:GLY:O	1:A:661:ARG:NH2	2.25	0.69
1:A:160:LYS:NZ	1:A:277:ASP:OD1	2.20	0.69
1:B:620:ASN:H	1:B:642:THR:HB	1.58	0.69
1:B:138:GLU:O	1:B:140:GLN:NE2	2.26	0.69
1:B:498:THR:HG21	1:B:504:ALA:H	1.56	0.69
1:B:723:ILE:HA	1:C:181:GLN:HE21	1.57	0.69
1:C:142:TYR:HA	1:C:377:ARG:O	1.93	0.69
1:C:209:SER:H	1:C:230:THR:H	1.39	0.69
1:A:672:ASP:HB2	1:A:674:ASN:HD21	1.58	0.69
1:A:187:GLU:OE2	1:A:188:ASP:N	2.25	0.68
1:A:665:THR:OG1	1:C:126:GLN:NE2	2.26	0.68
1:B:209:SER:N	1:B:230:THR:O	2.23	0.68
1:B:637:HIS:N	1:B:652:GLU:OE1	2.24	0.68
1:C:298:SER:HB2	1:C:311:HIS:HB3	1.74	0.68
1:C:465:VAL:HA	1:C:468:HIS:HE1	1.58	0.68
1:A:303:TYR:N	1:A:321:GLN:OE1	2.26	0.68
1:B:114:TYR:HA	1:B:576:VAL:HG21	1.75	0.68
1:A:576:VAL:HG11	1:A:623:LEU:HD22	1.75	0.68
1:C:151:LYS:O	1:C:367:THR:N	2.25	0.68
1:C:196:GLU:HG3	1:C:200:LYS:HB2	1.75	0.68
1:A:247:TRP:HZ3	1:A:275:GLU:H	1.40	0.68
1:A:301:TYR:O	1:A:308:HIS:ND1	2.26	0.68
1:B:235:LYS:O	1:B:248:HIS:ND1	2.27	0.68
1:C:298:SER:HB3	1:C:301:TYR:HB2	1.75	0.68
1:C:637:HIS:O	1:C:652:GLU:N	2.17	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:ALA:H	1:C:247:TRP:HA	1.59	0.68
1:A:122:ALA:HB3	1:A:123:THR:HA	1.74	0.68
1:A:712:HIS:HA	1:A:715:ARG:HE	1.59	0.68
1:C:372:VAL:HG22	1:C:390:ALA:HB3	1.75	0.68
1:A:708:ARG:NH2	1:C:631:GLU:OE1	2.26	0.68
1:B:143:THR:O	1:B:452:TYR:OH	2.12	0.68
1:B:208:ARG:HA	1:B:231:ASP:HA	1.76	0.68
1:B:106:ALA:H	1:B:581:VAL:H	1.42	0.68
1:A:558:ARG:HH12	1:A:576:VAL:H	1.40	0.67
1:B:526:ILE:O	1:B:529:CYS:HB3	1.93	0.67
1:A:700:LEU:HD11	1:A:708:ARG:HG3	1.74	0.67
1:B:634:THR:N	1:B:653:TYR:OH	2.28	0.67
1:A:142:TYR:HD1	1:A:376:LEU:HD21	1.59	0.67
1:B:130:PRO:HG3	1:B:536:LEU:HB2	1.76	0.67
1:A:147:ALA:HB3	1:A:375:MET:HG3	1.77	0.67
1:A:551:ALA:HB3	1:A:559:VAL:HG11	1.76	0.67
1:A:466:ARG:NH1	1:A:467:GLU:HG2	2.09	0.67
1:A:303:TYR:HA	1:A:308:HIS:HB2	1.76	0.67
1:B:178:ARG:O	1:B:258:ARG:NH2	2.27	0.67
1:B:297:MET:H	1:B:311:HIS:CE1	2.13	0.67
1:A:703:THR:HG21	1:C:545:LEU:HD13	1.75	0.67
1:B:463:LEU:HD21	1:B:506:LEU:HB2	1.76	0.67
1:B:159:PHE:HE2	1:B:354:TRP:HB2	1.59	0.67
1:C:208:ARG:HB3	1:C:229:GLU:HG3	1.77	0.67
1:B:303:TYR:N	1:B:321:GLN:OE1	2.25	0.66
1:C:682:GLU:HA	1:C:689:TYR:CD1	2.27	0.66
1:A:369:TRP:O	1:B:669:THR:OG1	2.09	0.66
1:A:405:SER:OG	1:A:406:ARG:NH1	2.28	0.66
1:B:637:HIS:O	1:B:652:GLU:N	2.15	0.66
1:A:276:VAL:HB	1:A:290:ALA:HB3	1.75	0.66
1:A:328:ARG:HA	1:A:335:ARG:HA	1.76	0.66
1:B:509:THR:O	1:B:513:ILE:N	2.27	0.66
1:C:234:LEU:HB3	1:C:247:TRP:HB2	1.77	0.66
1:C:296:TYR:O	1:C:311:HIS:HE1	1.79	0.66
1:A:571:SER:HA	1:B:677:MET:H	1.59	0.66
1:B:117:PRO:HD2	1:B:560:SER:HB2	1.77	0.66
1:B:118:PRO:HB2	1:C:680:ASP:HB3	1.77	0.66
1:B:152:GLU:HA	1:B:366:MET:HA	1.78	0.66
1:C:240:ALA:H	1:C:245:ARG:HD3	1.61	0.66
1:C:343:ASN:O	1:C:353:ALA:HA	1.95	0.66
1:A:435:LYS:NZ	1:A:437:GLY:O	2.20	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:THR:HG22	1:A:223:PHE:HA	1.78	0.66
1:A:466:ARG:NH2	1:A:467:GLU:OE2	2.27	0.66
1:A:618:GLY:N	1:A:622:GLU:O	2.20	0.66
1:B:240:ALA:HA	1:B:246:GLY:H	1.60	0.66
1:C:242:ARG:NH1	1:C:572:THR:O	2.29	0.66
1:A:558:ARG:NH1	1:A:576:VAL:H	1.94	0.66
1:B:196:GLU:HG3	1:B:200:LYS:HB2	1.76	0.66
1:B:547:PRO:HB2	1:B:561:ALA:H	1.59	0.66
1:C:444:ALA:HB2	1:C:450:ILE:HD11	1.77	0.66
1:A:121:GLY:HA3	1:A:569:ALA:HA	1.77	0.66
1:B:320:LYS:HZ1	1:B:346:THR:HG23	1.60	0.66
1:B:590:SER:HA	1:B:594:GLY:H	1.61	0.66
1:A:196:GLU:HA	1:A:200:LYS:HG2	1.78	0.66
1:A:281:VAL:N	1:A:286:GLU:OE2	2.23	0.66
1:B:122:ALA:H	1:B:123:THR:HA	1.59	0.66
1:B:194:PHE:HB2	1:B:320:LYS:HE3	1.78	0.66
1:C:463:LEU:HD13	1:C:467:GLU:HG2	1.78	0.66
1:C:144:GLU:O	1:C:455:LEU:N	2.26	0.65
1:C:158:LYS:HD2	1:C:279:ARG:HG3	1.76	0.65
1:A:369:TRP:HA	1:B:670:PHE:HD1	1.62	0.65
1:C:245:ARG:NH1	1:C:246:GLY:O	2.28	0.65
1:C:435:LYS:NZ	1:C:437:GLY:O	2.24	0.65
1:A:597:TYR:HA	1:A:630:ILE:HA	1.76	0.65
1:C:194:PHE:HD1	1:C:344:LEU:HD22	1.61	0.65
1:C:605:ARG:HE	1:C:612:LEU:HG	1.60	0.65
1:C:589:ILE:HB	1:C:630:ILE:HG21	1.77	0.65
1:C:672:ASP:N	1:C:673:LEU:O	2.29	0.65
1:A:215:ARG:HE	1:A:218:LEU:HD23	1.61	0.65
1:B:152:GLU:HG3	1:B:365:THR:HB	1.79	0.65
1:C:602:VAL:N	1:C:627:ARG:HH21	1.95	0.65
1:B:140:GLN:HG3	1:B:518:ASN:HB3	1.79	0.65
1:B:171:SER:HA	1:B:184:GLY:O	1.97	0.65
1:A:208:ARG:HH22	1:A:212:LYS:H	1.45	0.65
1:B:582:ILE:H	1:B:602:VAL:HG13	1.61	0.65
1:A:156:PRO:CA	1:A:280:SER:O	2.42	0.65
1:B:150:PHE:HA	1:B:368:LYS:HA	1.79	0.65
1:B:288:VAL:HG12	1:B:294:PHE:HD1	1.62	0.65
1:C:530:GLU:OE1	1:C:534:HIS:NE2	2.29	0.65
1:C:508:PHE:O	1:C:512:HIS:ND1	2.30	0.64
1:C:166:LYS:NZ	1:C:210:THR:O	2.29	0.64
1:C:402:TYR:N	1:C:441:TYR:O	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ARG:HB2	1:B:557:ARG:HH22	1.61	0.64
1:A:174:TRP:HB3	1:A:181:GLN:HB2	1.78	0.64
1:A:223:PHE:CD1	1:A:228:HIS:HA	2.33	0.64
1:A:386:PHE:HE1	1:A:397:THR:HG1	1.45	0.64
1:B:392:SER:HA	1:B:528:TRP:HE1	1.62	0.64
1:B:531:LEU:O	1:B:534:HIS:HB3	1.98	0.64
1:C:109:THR:HA	1:C:645:GLY:H	1.61	0.64
1:B:462:GLU:HG3	1:B:506:LEU:HD13	1.78	0.64
1:A:605:ARG:NH1	1:A:610:GLY:O	2.29	0.64
1:B:462:GLU:HG2	1:B:463:LEU:HG	1.79	0.64
1:C:224:HIS:CE1	1:C:268:THR:HG23	2.32	0.64
1:A:234:LEU:HB3	1:A:247:TRP:HB3	1.79	0.64
1:B:320:LYS:HZ1	1:B:346:THR:H	1.46	0.64
1:B:463:LEU:HD22	1:B:466:ARG:HE	1.62	0.64
1:A:197:VAL:O	1:A:202:ASN:N	2.20	0.64
1:A:540:ASN:HB3	1:A:543:ARG:HH21	1.61	0.64
1:A:557:ARG:NH1	1:A:558:ARG:O	2.29	0.64
1:B:149:VAL:O	1:B:369:TRP:N	2.30	0.64
1:B:374:GLU:OE1	1:B:390:ALA:N	2.31	0.64
1:A:700:LEU:HG	1:A:705:VAL:HA	1.79	0.64
1:B:378:SER:OG	1:B:385:ARG:HB2	1.97	0.64
1:B:257:SER:H	1:B:264:ARG:HH21	1.45	0.63
1:B:616:GLN:HE22	1:B:629:ALA:HB3	1.63	0.63
1:B:589:ILE:O	1:B:595:ALA:N	2.21	0.63
1:B:709:ASN:HA	1:B:712:HIS:HE1	1.64	0.63
1:C:148:VAL:HG22	1:C:371:GLU:HG2	1.80	0.63
1:C:197:VAL:HA	1:C:201:ILE:HB	1.78	0.63
1:C:522:GLY:O	1:C:526:ILE:HG13	1.97	0.63
1:A:113:PHE:HA	1:A:621:ASN:HB3	1.79	0.63
1:A:599:ARG:HE	1:A:617:LEU:HG	1.62	0.63
1:B:584:GLN:OE1	1:B:603:SER:N	2.32	0.63
1:B:505:ARG:O	1:B:508:PHE:HB3	1.98	0.63
1:C:403:PRO:HG2	1:C:406:ARG:HG3	1.80	0.63
1:B:153:ASN:N	1:B:365:THR:O	2.32	0.63
1:B:193:PRO:HB2	1:B:195:GLU:HG3	1.79	0.63
1:B:282:TYR:HA	1:B:284:TYR:N	2.13	0.63
1:B:438:GLN:O	1:B:440:GLN:NE2	2.31	0.63
1:A:639:ARG:NH1	1:C:563:MET:SD	2.72	0.63
1:C:166:LYS:HZ1	1:C:208:ARG:HB2	1.64	0.63
1:A:224:HIS:CE1	1:A:268:THR:HG23	2.33	0.63
1:B:140:GLN:HE22	1:B:378:SER:HB2	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:PHE:HD1	1:B:344:LEU:HD22	1.63	0.63
1:B:324:GLY:HA2	1:B:339:PRO:HB2	1.80	0.63
1:C:279:ARG:NH2	1:C:289:LEU:O	2.31	0.63
1:A:178:ARG:HE	1:A:258:ARG:HH22	1.47	0.63
1:A:210:THR:HG23	1:A:229:GLU:HA	1.81	0.63
1:C:258:ARG:NE	1:C:260:GLU:OE1	2.25	0.63
1:B:123:THR:N	1:B:126:GLN:OE1	2.29	0.62
1:B:164:TYR:HB2	1:B:351:THR:HB	1.80	0.62
1:A:114:TYR:O	1:A:623:LEU:N	2.32	0.62
1:A:201:ILE:O	1:A:328:ARG:NH1	2.24	0.62
1:A:436:VAL:HG22	1:A:456:LEU:HD23	1.81	0.62
1:C:691:ARG:HG2	1:C:695:LYS:HZ3	1.64	0.62
1:B:198:ILE:HD13	1:B:325:PHE:CZ	2.34	0.62
1:A:330:LEU:HA	1:A:333:LYS:HD3	1.81	0.62
1:A:605:ARG:HH21	1:A:612:LEU:HB2	1.64	0.62
1:A:664:ILE:HB	1:C:126:GLN:HG3	1.81	0.62
1:C:239:ALA:HB1	1:C:611:PRO:HG2	1.81	0.62
1:C:369:TRP:CD2	1:C:370:GLN:HG2	2.35	0.62
1:A:424:ILE:HD12	1:A:427:ARG:HH22	1.65	0.62
1:A:599:ARG:NH1	1:A:619:GLU:OE2	2.32	0.62
1:C:585:ASN:OD1	1:C:655:TYR:N	2.31	0.62
1:C:704:GLU:O	1:C:708:ARG:HG2	1.98	0.62
1:C:280:SER:HA	1:C:287:PHE:HB3	1.82	0.62
1:A:670:PHE:HB3	1:C:369:TRP:NE1	2.14	0.62
1:C:640:TYR:HA	1:C:648:VAL:O	1.99	0.62
1:B:256:PRO:HB2	1:B:264:ARG:HG3	1.82	0.62
1:C:151:LYS:HG3	1:C:367:THR:HB	1.81	0.62
1:C:517:VAL:O	1:C:521:LEU:HG	2.00	0.62
1:C:381:GLY:HA3	1:C:385:ARG:NH2	2.14	0.62
1:C:470:ARG:HH21	1:C:471:GLU:CD	2.02	0.62
1:A:151:LYS:O	1:A:367:THR:N	2.22	0.61
1:A:463:LEU:HD13	1:A:466:ARG:HH11	1.65	0.61
1:A:709:ASN:HA	1:A:712:HIS:CE1	2.35	0.61
1:A:110:ASP:HB2	1:A:645:GLY:HA3	1.82	0.61
1:B:164:TYR:HD2	1:B:351:THR:HB	1.65	0.61
1:B:174:TRP:HE3	1:B:181:GLN:HB2	1.64	0.61
1:A:343:ASN:HD21	1:A:356:TRP:HB2	1.65	0.61
1:A:558:ARG:NH2	1:A:576:VAL:HG12	2.16	0.61
1:B:235:LYS:N	1:B:248:HIS:O	2.33	0.61
1:C:164:TYR:HB2	1:C:351:THR:HB	1.82	0.61
1:C:303:TYR:N	1:C:321:GLN:OE1	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:THR:HA	1:A:274:GLU:O	2.01	0.61
1:C:150:PHE:HZ	1:C:416:ASP:HB2	1.64	0.61
1:C:168:VAL:O	1:C:187:GLU:HA	2.01	0.61
1:C:440:GLN:HB3	1:C:442:TYR:CE1	2.30	0.61
1:B:463:LEU:HD11	1:B:506:LEU:HB3	1.83	0.61
1:B:687:GLU:HG2	1:B:688:VAL:H	1.65	0.61
1:C:174:TRP:HE3	1:C:181:GLN:HB2	1.64	0.61
1:B:515:ARG:O	1:B:519:ASP:N	2.28	0.61
1:C:240:ALA:HB3	1:C:245:ARG:HB3	1.82	0.61
1:C:640:TYR:HB3	1:C:647:TYR:CD2	2.36	0.61
1:A:678:LEU:HD13	1:C:276:VAL:HG12	1.83	0.61
1:B:105:LYS:HD2	1:B:582:ILE:HD11	1.82	0.61
1:B:142:TYR:HA	1:B:377:ARG:O	2.01	0.61
1:C:470:ARG:NH2	1:C:474:ARG:HH21	1.96	0.61
1:C:600:PRO:HG2	1:C:617:LEU:HD23	1.83	0.61
1:A:420:ALA:HA	1:A:423:ARG:HE	1.66	0.61
1:C:164:TYR:HB3	1:C:192:VAL:HB	1.83	0.60
1:C:225:ARG:NH1	1:C:268:THR:OG1	2.34	0.60
1:C:259:VAL:HB	1:C:264:ARG:HD2	1.82	0.60
1:A:154:ILE:HA	1:A:282:TYR:HD2	1.66	0.60
1:B:555:VAL:HG12	1:C:674:ASN:HD21	1.65	0.60
1:A:149:VAL:HG22	1:A:369:TRP:CD1	2.35	0.60
1:B:562:ARG:HG2	1:B:569:ALA:HB3	1.83	0.60
1:C:616:GLN:HB2	1:C:624:ARG:HG3	1.83	0.60
1:A:173:VAL:HG21	1:A:255:ASN:HD22	1.66	0.60
1:A:637:HIS:HB3	1:A:652:GLU:HA	1.83	0.60
1:B:199:ASP:OD2	1:B:200:LYS:N	2.34	0.60
1:B:366:MET:HB3	1:B:413:ILE:HD11	1.81	0.60
1:B:439:PRO:CA	1:B:452:TYR:O	2.31	0.60
1:C:177:HIS:CD2	1:C:178:ARG:H	2.19	0.60
1:A:153:ASN:N	1:A:365:THR:O	2.35	0.60
1:A:191:PRO:HA	1:A:350:PHE:HA	1.84	0.60
1:A:639:ARG:HH11	1:C:565:GLY:N	1.99	0.60
1:A:681:HIS:CE1	1:C:291:THR:HB	2.37	0.60
1:B:170:VAL:HG22	1:B:186:PHE:HB3	1.83	0.60
1:B:379:GLU:OE2	1:B:474:ARG:NH1	2.35	0.60
1:C:379:GLU:OE2	1:C:474:ARG:NH1	2.35	0.60
1:A:196:GLU:O	1:A:201:ILE:N	2.35	0.60
1:A:329:ASP:O	1:A:333:LYS:N	2.34	0.60
1:A:389:ASP:HB3	1:A:528:TRP:CE2	2.35	0.60
1:C:425:PHE:HA	1:C:429:TYR:HD1	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ASN:HB3	1:A:577:ALA:HA	1.83	0.60
1:B:159:PHE:CE2	1:B:354:TRP:HB2	2.36	0.60
1:B:428:ARG:HB3	1:B:429:TYR:CE1	2.37	0.60
1:B:465:VAL:HA	1:B:468:HIS:CD2	2.36	0.60
1:C:634:THR:O	1:C:637:HIS:N	2.34	0.60
1:A:535:GLU:HB3	1:A:539:TRP:CZ2	2.37	0.60
1:B:111:ALA:O	1:B:621:ASN:ND2	2.34	0.60
1:A:156:PRO:HB3	1:A:281:VAL:HG12	1.83	0.60
1:A:158:LYS:HD2	1:A:279:ARG:HG3	1.84	0.60
1:A:297:MET:HB2	1:A:314:TYR:HE2	1.66	0.60
1:A:355:ASP:N	1:A:355:ASP:OD1	2.33	0.60
1:A:607:GLU:HG2	1:A:609:GLN:H	1.67	0.60
1:B:440:GLN:H	1:B:452:TYR:H	1.50	0.60
1:A:701:ASP:OD2	1:A:704:GLU:N	2.32	0.60
1:B:177:HIS:HB3	1:B:179:TYR:CE1	2.37	0.60
1:B:602:VAL:HG12	1:B:604:PHE:HD1	1.66	0.60
1:C:373:ASP:OD1	1:C:428:ARG:NH1	2.35	0.60
1:B:126:GLN:HE22	1:B:567:VAL:HG23	1.67	0.59
1:B:202:ASN:O	1:B:328:ARG:NE	2.23	0.59
1:B:210:THR:HA	1:B:222:ALA:O	2.02	0.59
1:B:327:ALA:H	1:B:337:THR:HG1	1.50	0.59
1:C:150:PHE:HB2	1:C:449:LEU:HB3	1.83	0.59
1:C:155:ALA:H	1:C:282:TYR:HB3	1.66	0.59
1:C:210:THR:HA	1:C:222:ALA:O	2.01	0.59
1:A:113:PHE:HB2	1:A:576:VAL:HG13	1.83	0.59
1:A:376:LEU:HB3	1:A:387:SER:OG	2.02	0.59
1:A:452:TYR:O	1:A:454:PRO:HD3	2.02	0.59
1:B:150:PHE:HZ	1:B:416:ASP:HB2	1.66	0.59
1:B:235:LYS:HE3	1:B:248:HIS:CE1	2.37	0.59
1:B:374:GLU:HB3	1:B:390:ALA:HB2	1.83	0.59
1:A:318:ARG:HE	1:A:345:LEU:HD11	1.66	0.59
1:A:428:ARG:HB3	1:A:429:TYR:CE1	2.38	0.59
1:A:558:ARG:NE	1:A:573:CYS:SG	2.64	0.59
1:B:127:PHE:HZ	1:B:567:VAL:HA	1.66	0.59
1:B:377:ARG:NH2	1:B:474:ARG:HD2	2.17	0.59
1:B:600:PRO:O	1:B:617:LEU:N	2.22	0.59
1:C:343:ASN:HB2	1:C:354:TRP:CE2	2.36	0.59
1:C:561:ALA:HA	1:C:569:ALA:O	2.03	0.59
1:A:108:ASN:O	1:A:645:GLY:N	2.26	0.59
1:A:141:ASN:OD1	1:A:474:ARG:NH2	2.36	0.59
1:A:518:ASN:HA	1:A:521:LEU:HD12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:PRO:HB2	1:B:158:LYS:NZ	2.17	0.59
1:C:175:PHE:HB3	1:C:260:GLU:HG2	1.83	0.59
1:C:640:TYR:HB3	1:C:647:TYR:HD2	1.67	0.59
1:A:640:TYR:CD1	1:A:649:TYR:HB2	2.37	0.59
1:B:125:VAL:HG13	1:C:667:VAL:HA	1.84	0.59
1:C:159:PHE:HE2	1:C:354:TRP:HB2	1.64	0.59
1:C:650:PHE:CZ	1:C:655:TYR:HB2	2.37	0.59
1:B:157:TYR:O	1:B:158:LYS:NZ	2.30	0.59
1:A:303:TYR:HB2	1:A:304:ARG:CZ	2.32	0.59
1:A:141:ASN:HB3	1:A:377:ARG:NH2	2.17	0.59
1:B:329:ASP:O	1:B:333:LYS:N	2.36	0.59
1:B:510:TYR:O	1:B:514:GLN:HG3	2.03	0.59
1:A:620:ASN:HA	1:A:642:THR:HG21	1.84	0.59
1:A:667:VAL:HG23	1:A:670:PHE:CE1	2.38	0.59
1:B:375:MET:O	1:B:452:TYR:OH	2.21	0.59
1:A:176:GLY:HA3	1:A:179:TYR:CE2	2.38	0.58
1:A:599:ARG:HG2	1:A:600:PRO:HD2	1.85	0.58
1:B:516:PRO:O	1:B:519:ASP:HB2	2.03	0.58
1:B:646:GLY:HA2	1:B:661:ARG:HG3	1.85	0.58
1:A:124:VAL:HG22	1:B:665:THR:H	1.68	0.58
1:A:473:SER:OG	1:A:474:ARG:NH1	2.36	0.58
1:A:108:ASN:HB3	1:A:645:GLY:N	2.17	0.58
1:A:537:THR:HA	1:A:540:ASN:ND2	2.17	0.58
1:B:276:VAL:HB	1:B:290:ALA:HB3	1.85	0.58
1:C:465:VAL:HA	1:C:468:HIS:CE1	2.36	0.58
1:C:598:SER:OG	1:C:631:GLU:HG2	2.03	0.58
1:C:713:ASP:OD1	1:C:713:ASP:N	2.34	0.58
1:A:682:GLU:HA	1:A:684:VAL:HG13	1.84	0.58
1:C:194:PHE:O	1:C:198:ILE:HG12	2.02	0.58
1:A:143:THR:HB	1:A:377:ARG:HB3	1.84	0.58
1:B:129:GLN:H	1:B:131:ARG:NH2	2.00	0.58
1:B:200:LYS:HA	1:B:204:LYS:HD2	1.86	0.58
1:A:129:GLN:OE1	1:B:661:ARG:NH1	2.36	0.58
1:A:168:VAL:HG12	1:A:269:VAL:HG22	1.86	0.58
1:A:634:THR:O	1:A:653:TYR:OH	2.21	0.58
1:C:116:CYS:HB2	1:C:623:LEU:O	2.03	0.58
1:C:649:TYR:CD1	1:C:656:SER:HB3	2.39	0.58
1:A:178:ARG:HA	1:A:258:ARG:NH2	2.18	0.58
1:B:711:LEU:HD12	1:B:714:LEU:HB2	1.84	0.58
1:C:502:GLU:HA	1:C:505:ARG:HD2	1.85	0.58
1:C:661:ARG:HA	1:C:664:ILE:HG12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:THR:N	1:A:350:PHE:O	2.37	0.58
1:B:589:ILE:N	1:B:595:ALA:O	2.31	0.58
1:B:681:HIS:CG	1:B:682:GLU:H	2.21	0.58
1:C:200:LYS:HA	1:C:204:LYS:HB2	1.85	0.58
1:C:209:SER:N	1:C:230:THR:O	2.36	0.58
1:C:298:SER:OG	1:C:310:GLU:OE1	2.14	0.58
1:C:377:ARG:NH2	1:C:474:ARG:HG3	2.19	0.58
1:C:600:PRO:HB2	1:C:617:LEU:HB3	1.86	0.58
1:A:369:TRP:CD2	1:B:670:PHE:HE1	2.22	0.58
1:B:542:ALA:O	1:B:546:ASN:ND2	2.37	0.58
1:B:605:ARG:NE	1:B:610:GLY:O	2.37	0.58
1:B:705:VAL:HA	1:B:708:ARG:NE	2.19	0.58
1:C:116:CYS:SG	1:C:622:GLU:HB3	2.44	0.58
1:C:138:GLU:OE2	1:C:518:ASN:HB2	2.04	0.58
1:C:439:PRO:HB2	1:C:441:TYR:CE2	2.38	0.58
1:A:156:PRO:HA	1:A:281:VAL:HA	1.86	0.57
1:A:257:SER:O	1:A:264:ARG:NH1	2.37	0.57
1:A:642:THR:HG23	1:A:661:ARG:NH2	2.19	0.57
1:B:151:LYS:HD3	1:B:369:TRP:CG	2.39	0.57
1:B:320:LYS:NZ	1:B:346:THR:H	2.01	0.57
1:B:555:VAL:O	1:C:674:ASN:ND2	2.37	0.57
1:C:141:ASN:H	1:C:379:GLU:HB3	1.68	0.57
1:A:436:VAL:HB	1:A:454:PRO:HB2	1.85	0.57
1:A:585:ASN:OD1	1:A:655:TYR:N	2.36	0.57
1:A:605:ARG:NH2	1:A:612:LEU:HB2	2.19	0.57
1:B:402:TYR:HA	1:B:406:ARG:HH21	1.69	0.57
1:B:599:ARG:HB3	1:B:616:GLN:HG2	1.86	0.57
1:C:319:PHE:CE1	1:C:343:ASN:HB3	2.40	0.57
1:C:326:TYR:HB3	1:C:335:ARG:HG2	1.86	0.57
1:A:154:ILE:O	1:A:282:TYR:N	2.37	0.57
1:A:307:SER:HB2	1:A:356:TRP:HZ2	1.69	0.57
1:B:441:TYR:HD1	1:B:449:LEU:HD11	1.69	0.57
1:B:507:GLN:HE21	1:B:511:ASN:HD21	1.52	0.57
1:C:156:PRO:HA	1:C:280:SER:O	2.05	0.57
1:C:289:LEU:HD13	1:C:294:PHE:HA	1.87	0.57
1:A:174:TRP:HB2	1:A:183:MET:HG2	1.87	0.57
1:A:634:THR:N	1:A:653:TYR:OH	2.37	0.57
1:B:161:ALA:HA	1:B:353:ALA:O	2.04	0.57
1:B:532:GLN:NE2	1:B:533:ASN:OD1	2.37	0.57
1:C:632:PRO:HB3	1:C:695:LYS:HG3	1.87	0.57
1:A:116:CYS:SG	1:A:622:GLU:HB3	2.45	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:GLU:HB3	1:C:189:ARG:HD2	1.86	0.57
1:C:614:GLU:HB2	1:C:627:ARG:HD2	1.86	0.57
1:C:700:LEU:HD22	1:C:705:VAL:HA	1.85	0.57
1:A:557:ARG:NE	1:B:674:ASN:O	2.31	0.57
1:A:701:ASP:OD2	1:A:703:THR:OG1	2.19	0.57
1:B:343:ASN:HB2	1:B:354:TRP:CE2	2.40	0.57
1:B:401:GLU:HA	1:B:441:TYR:O	2.04	0.57
1:C:428:ARG:HB3	1:C:429:TYR:CE1	2.39	0.57
1:A:388:SER:O	1:A:392:SER:N	2.38	0.57
1:B:213:TYR:OH	1:B:348:PRO:O	2.17	0.57
1:B:329:ASP:HB2	1:B:336:ALA:HB2	1.87	0.57
1:A:434:ILE:HB	1:A:456:LEU:HG	1.86	0.57
1:B:155:ALA:O	1:B:284:TYR:OH	2.17	0.57
1:B:343:ASN:ND2	1:B:356:TRP:HB2	2.20	0.57
1:C:191:PRO:HD2	1:C:213:TYR:CZ	2.39	0.57
1:C:598:SER:HB2	1:C:629:ALA:HB1	1.85	0.57
1:A:290:ALA:HB1	1:B:679:GLU:CD	2.24	0.57
1:B:508:PHE:O	1:B:512:HIS:ND1	2.33	0.57
1:C:242:ARG:NH2	1:C:574:VAL:HG12	2.19	0.57
1:C:633:CYS:HA	1:C:653:TYR:CE2	2.40	0.57
1:C:640:TYR:CE1	1:C:649:TYR:HB2	2.39	0.57
1:C:666:THR:HG22	1:C:667:VAL:H	1.68	0.57
1:A:424:ILE:HD13	1:A:427:ARG:HH12	1.70	0.57
1:A:671:ILE:O	1:C:557:ARG:NH2	2.38	0.57
1:B:147:ALA:HB3	1:B:375:MET:HG3	1.87	0.57
1:C:199:ASP:OD2	1:C:204:LYS:NZ	2.32	0.57
1:C:436:VAL:O	1:C:453:GLN:NE2	2.38	0.57
1:A:165:TYR:HA	1:A:192:VAL:H	1.69	0.56
1:A:297:MET:HG2	1:A:313:SER:H	1.69	0.56
1:A:372:VAL:O	1:A:375:MET:HG2	2.05	0.56
1:A:675:ILE:H	1:A:675:ILE:HD12	1.70	0.56
1:B:502:GLU:HA	1:B:505:ARG:HD3	1.86	0.56
1:C:171:SER:HA	1:C:184:GLY:O	2.05	0.56
1:C:618:GLY:N	1:C:622:GLU:O	2.38	0.56
1:A:590:SER:HA	1:A:594:GLY:H	1.69	0.56
1:B:286:GLU:HB2	1:B:294:PHE:CE1	2.40	0.56
1:C:385:ARG:HG3	1:C:396:THR:HA	1.85	0.56
1:B:437:GLY:O	1:B:453:GLN:NE2	2.30	0.56
1:C:164:TYR:HD1	1:C:273:VAL:HG22	1.70	0.56
1:C:185:ILE:HG23	1:C:253:LYS:HE3	1.87	0.56
1:C:639:ARG:NH2	1:C:696:ASP:OD2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:646:GLY:O	1:C:661:ARG:NH1	2.39	0.56
1:B:149:VAL:HG13	1:B:370:GLN:H	1.70	0.56
1:B:635:VAL:N	1:B:693:GLU:OE1	2.39	0.56
1:B:328:ARG:NH1	1:B:333:LYS:O	2.28	0.56
1:B:144:GLU:OE1	1:B:144:GLU:N	2.36	0.56
1:C:223:PHE:HD1	1:C:228:HIS:HA	1.69	0.56
1:A:151:LYS:HG3	1:A:369:TRP:HE1	1.69	0.56
1:A:297:MET:HB2	1:A:314:TYR:CE2	2.41	0.56
1:A:319:PHE:CE1	1:A:343:ASN:HB3	2.41	0.56
1:B:279:ARG:O	1:B:288:VAL:HG22	2.06	0.56
1:B:296:TYR:HB2	1:B:313:SER:OG	2.06	0.56
1:B:329:ASP:OD1	1:B:331:THR:OG1	2.20	0.56
1:B:711:LEU:HA	1:B:714:LEU:HD12	1.88	0.56
1:C:680:ASP:OD1	1:C:681:HIS:N	2.38	0.56
1:A:140:GLN:O	1:A:379:GLU:HG2	2.05	0.56
1:B:256:PRO:HB2	1:B:264:ARG:NE	2.21	0.56
1:B:410:GLY:HA2	1:B:413:ILE:HD13	1.88	0.56
1:C:119:PRO:O	1:C:562:ARG:NE	2.37	0.56
1:C:564:LEU:HD21	1:C:569:ALA:HB2	1.87	0.56
1:A:117:PRO:HD2	1:A:560:SER:HB2	1.88	0.56
1:A:145:GLY:HA3	1:A:454:PRO:HA	1.88	0.56
1:A:174:TRP:N	1:A:181:GLN:O	2.33	0.56
1:A:540:ASN:O	1:A:544:LYS:HG3	2.06	0.56
1:A:639:ARG:HH11	1:C:565:GLY:H	1.54	0.56
1:B:498:THR:HG21	1:B:504:ALA:N	2.21	0.56
1:B:677:MET:HG3	1:B:678:LEU:H	1.70	0.56
1:C:703:THR:O	1:C:706:GLN:NE2	2.38	0.56
1:A:223:PHE:HD1	1:A:228:HIS:HA	1.70	0.56
1:A:713:ASP:HA	1:A:716:PHE:CE1	2.41	0.56
1:B:442:TYR:HB2	1:B:450:ILE:HB	1.88	0.56
1:B:592:ARG:HD3	1:B:593:PRO:HD2	1.88	0.56
1:B:598:SER:N	1:B:629:ALA:O	2.33	0.56
1:B:705:VAL:O	1:B:708:ARG:HG2	2.05	0.56
1:B:245:ARG:NH1	1:B:329:ASP:OD1	2.40	0.55
1:B:424:ILE:O	1:B:427:ARG:HG2	2.06	0.55
1:B:502:GLU:O	1:B:506:LEU:N	2.29	0.55
1:B:549:ALA:O	1:B:553:VAL:HG12	2.05	0.55
1:C:150:PHE:HB3	1:C:366:MET:HB3	1.87	0.55
1:A:136:ARG:CZ	1:A:526:ILE:HD12	2.36	0.55
1:A:237:ALA:HA	1:A:248:HIS:ND1	2.21	0.55
1:A:535:GLU:HA	1:A:538:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:THR:O	1:A:667:VAL:HG22	2.06	0.55
1:B:149:VAL:HG13	1:B:369:TRP:HB3	1.88	0.55
1:B:202:ASN:C	1:B:328:ARG:HE	2.07	0.55
1:B:466:ARG:HD2	1:B:507:GLN:HB2	1.88	0.55
1:B:470:ARG:CZ	1:B:514:GLN:HE22	2.18	0.55
1:A:235:LYS:N	1:A:248:HIS:O	2.39	0.55
1:A:704:GLU:HA	1:A:707:ARG:HE	1.70	0.55
1:B:106:ALA:N	1:B:579:ASP:O	2.39	0.55
1:B:106:ALA:HA	1:B:643:PHE:HZ	1.72	0.55
1:B:452:TYR:HE2	1:B:454:PRO:HA	1.70	0.55
1:C:140:GLN:OE1	1:C:378:SER:HB2	2.06	0.55
1:C:563:MET:HA	1:C:568:MET:HE2	1.89	0.55
1:A:404:LEU:HB3	1:A:410:GLY:HA3	1.89	0.55
1:A:631:GLU:HG3	1:A:632:PRO:HD2	1.89	0.55
1:B:146:ILE:HD13	1:B:421:MET:HG2	1.88	0.55
1:C:325:PHE:O	1:C:340:THR:OG1	2.20	0.55
1:A:258:ARG:NH2	1:A:260:GLU:OE2	2.31	0.55
1:A:284:TYR:CG	1:A:300:PHE:HE2	2.25	0.55
1:A:375:MET:SD	1:A:388:SER:HB2	2.46	0.55
1:A:702:TYR:O	1:A:706:GLN:NE2	2.40	0.55
1:B:302:GLY:HA3	1:B:356:TRP:CE2	2.41	0.55
1:B:209:SER:O	1:B:269:VAL:HB	2.07	0.55
1:B:558:ARG:HD3	1:B:559:VAL:H	1.72	0.55
1:C:297:MET:SD	1:C:312:THR:HA	2.46	0.55
1:C:578:ALA:HB1	1:C:643:PHE:HE2	1.72	0.55
1:A:517:VAL:O	1:A:521:LEU:HG	2.06	0.55
1:A:676:THR:O	1:C:279:ARG:NH2	2.39	0.55
1:C:424:ILE:HG22	1:C:429:TYR:HE1	1.70	0.55
1:C:439:PRO:HB2	1:C:441:TYR:HE2	1.71	0.55
1:A:152:GLU:OE1	1:A:282:TYR:OH	2.16	0.55
1:B:538:LEU:H	1:B:538:LEU:HD12	1.72	0.55
1:B:702:TYR:O	1:B:705:VAL:HB	2.06	0.55
1:C:154:ILE:H	1:C:154:ILE:HD12	1.70	0.55
1:C:685:PRO:HG2	1:C:690:THR:HG21	1.89	0.55
1:A:242:ARG:N	1:A:606:TYR:OH	2.39	0.55
1:A:502:GLU:HB3	1:A:506:LEU:HD12	1.87	0.55
1:A:541:GLU:HA	1:A:544:LYS:HD3	1.88	0.55
1:C:116:CYS:O	1:C:118:PRO:HD3	2.06	0.55
1:B:154:ILE:HG13	1:B:156:PRO:HD3	1.89	0.55
1:A:300:PHE:CG	1:A:359:LYS:HA	2.42	0.54
1:A:301:TYR:CZ	1:A:312:THR:HB	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:PRO:HA	1:A:452:TYR:C	2.27	0.54
1:A:672:ASP:OD1	1:A:672:ASP:N	2.35	0.54
1:B:256:PRO:HB3	1:B:265:TYR:C	2.28	0.54
1:B:537:THR:HA	1:B:540:ASN:OD1	2.06	0.54
1:A:704:GLU:HG3	1:A:707:ARG:CZ	2.38	0.54
1:B:142:TYR:CD1	1:B:376:LEU:HB3	2.43	0.54
1:A:147:ALA:HA	1:A:451:ALA:O	2.07	0.54
1:A:256:PRO:HB2	1:A:264:ARG:NE	2.21	0.54
1:A:701:ASP:O	1:A:704:GLU:N	2.40	0.54
1:B:150:PHE:HB3	1:B:366:MET:SD	2.48	0.54
1:B:587:MET:O	1:B:588:ARG:HG3	2.08	0.54
1:B:712:HIS:O	1:B:715:ARG:HD3	2.06	0.54
1:C:213:TYR:OH	1:C:348:PRO:O	2.25	0.54
1:C:583:VAL:HG22	1:C:602:VAL:HG12	1.90	0.54
1:C:711:LEU:HB2	1:C:715:ARG:NH2	2.22	0.54
1:B:318:ARG:O	1:B:320:LYS:NZ	2.34	0.54
1:B:562:ARG:HB3	1:C:699:LEU:HD23	1.88	0.54
1:B:710:GLN:NE2	1:B:713:ASP:HB3	2.20	0.54
1:A:320:LYS:NZ	1:A:344:LEU:O	2.29	0.54
1:C:146:ILE:O	1:C:452:TYR:HA	2.08	0.54
1:C:701:ASP:O	1:C:704:GLU:N	2.41	0.54
1:A:187:GLU:HG3	1:B:684:VAL:HG12	1.90	0.54
1:A:199:ASP:O	1:A:204:LYS:N	2.40	0.54
1:B:372:VAL:HG13	1:B:391:ILE:HG23	1.89	0.54
1:C:107:GLU:OE1	1:C:660:SER:OG	2.22	0.54
1:C:150:PHE:CE2	1:C:413:ILE:HG23	2.43	0.54
1:A:330:LEU:O	1:A:333:LYS:NZ	2.30	0.54
1:A:540:ASN:HA	1:A:543:ARG:HE	1.72	0.54
1:A:650:PHE:CZ	1:A:655:TYR:HB2	2.43	0.54
1:B:108:ASN:O	1:B:645:GLY:N	2.28	0.54
1:B:115:VAL:HG23	1:B:576:VAL:HG22	1.90	0.54
1:B:723:ILE:HA	1:C:181:GLN:NE2	2.22	0.54
1:C:559:VAL:HG12	1:C:572:THR:HA	1.89	0.54
1:C:589:ILE:N	1:C:595:ALA:O	2.30	0.54
1:A:133:CYS:HB3	1:A:526:ILE:HG23	1.90	0.54
1:A:151:LYS:HE2	1:A:369:TRP:CZ2	2.42	0.54
1:B:144:GLU:O	1:B:455:LEU:N	2.30	0.54
1:B:163:MET:HA	1:B:351:THR:O	2.07	0.54
1:B:235:LYS:HE2	1:B:250:THR:N	2.22	0.54
1:A:132:ARG:HD3	1:B:557:ARG:HH21	1.73	0.54
1:A:570:VAL:HG13	1:B:677:MET:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:616:GLN:HG3	1:A:626:THR:O	2.08	0.54
1:B:302:GLY:HA2	1:B:319:PHE:HZ	1.72	0.54
1:C:223:PHE:CD1	1:C:228:HIS:HA	2.43	0.54
1:C:560:SER:OG	1:C:571:SER:OG	2.25	0.54
1:A:199:ASP:HA	1:A:203:ALA:HB3	1.90	0.54
1:A:208:ARG:HH12	1:A:212:LYS:HE2	1.73	0.54
1:A:615:GLY:O	1:A:627:ARG:NE	2.40	0.54
1:C:420:ALA:O	1:C:424:ILE:HG12	2.08	0.54
1:C:424:ILE:O	1:C:427:ARG:HG2	2.08	0.54
1:A:344:LEU:HA	1:A:352:VAL:O	2.08	0.53
1:A:369:TRP:HB3	1:A:370:GLN:OE1	2.08	0.53
1:A:500:SER:HB3	1:A:503:PHE:CE2	2.42	0.53
1:A:637:HIS:N	1:A:652:GLU:OE2	2.41	0.53
1:A:401:GLU:HA	1:A:441:TYR:O	2.07	0.53
1:B:114:TYR:O	1:B:622:GLU:HA	2.08	0.53
1:B:244:SER:HB2	1:B:275:GLU:C	2.28	0.53
1:C:215:ARG:O	1:C:218:LEU:HG	2.08	0.53
1:C:300:PHE:CG	1:C:359:LYS:HA	2.44	0.53
1:C:329:ASP:N	1:C:334:ALA:O	2.40	0.53
1:A:634:THR:OG1	1:A:692:HIS:O	2.19	0.53
1:B:499:SER:HB3	1:B:503:PHE:HE1	1.73	0.53
1:B:536:LEU:HA	1:B:539:TRP:HD1	1.74	0.53
1:C:256:PRO:HB2	1:C:264:ARG:NE	2.22	0.53
1:C:616:GLN:O	1:C:624:ARG:N	2.41	0.53
1:A:546:ASN:O	1:A:550:ILE:HG12	2.08	0.53
1:A:670:PHE:CD2	1:A:671:ILE:HB	2.43	0.53
1:B:202:ASN:O	1:B:326:TYR:OH	2.16	0.53
1:C:523:ARG:HA	1:C:526:ILE:HD12	1.89	0.53
1:A:701:ASP:CB	1:A:704:GLU:HB2	2.37	0.53
1:A:709:ASN:HB2	1:B:710:GLN:OE1	2.08	0.53
1:B:245:ARG:O	1:B:275:GLU:HG2	2.08	0.53
1:B:402:TYR:N	1:B:441:TYR:HB2	2.24	0.53
1:A:150:PHE:CE1	1:A:368:LYS:HB3	2.43	0.53
1:A:541:GLU:HG3	1:B:545:LEU:HD22	1.91	0.53
1:A:683:PHE:O	1:A:690:THR:HG21	2.09	0.53
1:B:119:PRO:HB3	1:B:560:SER:O	2.09	0.53
1:B:245:ARG:HH22	1:B:329:ASP:HA	1.74	0.53
1:B:634:THR:OG1	1:B:695:LYS:HE3	2.07	0.53
1:C:364:CYS:HA	1:C:409:LEU:HD13	1.91	0.53
1:A:287:PHE:CE1	1:A:295:VAL:HB	2.44	0.53
1:B:147:ALA:HA	1:B:451:ALA:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:LYS:HE3	1:B:248:HIS:NE2	2.23	0.53
1:B:243:THR:HG23	1:B:244:SER:O	2.08	0.53
1:B:467:GLU:OE1	1:B:471:GLU:HG2	2.08	0.53
1:A:136:ARG:HB3	1:A:137:PRO:CD	2.39	0.53
1:B:460:LEU:HD22	1:B:506:LEU:HD22	1.91	0.53
1:C:150:PHE:CZ	1:C:368:LYS:HB2	2.43	0.53
1:A:114:TYR:CE2	1:A:558:ARG:HA	2.44	0.53
1:A:143:THR:O	1:A:452:TYR:OH	2.27	0.53
1:B:146:ILE:HG22	1:B:453:GLN:HB3	1.91	0.53
1:B:527:ALA:O	1:B:531:LEU:HG	2.09	0.53
1:B:694:ILE:HG22	1:B:708:ARG:HH22	1.74	0.53
1:C:559:VAL:HA	1:C:572:THR:HA	1.91	0.53
1:C:704:GLU:HA	1:C:707:ARG:HG3	1.91	0.53
1:A:113:PHE:CE2	1:A:578:ALA:HA	2.44	0.53
1:A:702:TYR:OH	1:B:706:GLN:HB2	2.09	0.53
1:B:164:TYR:CD2	1:B:351:THR:HB	2.44	0.53
1:B:375:MET:SD	1:B:388:SER:HB2	2.49	0.53
1:C:144:GLU:HG2	1:C:455:LEU:HB2	1.91	0.53
1:A:344:LEU:HG	1:A:353:ALA:HB2	1.90	0.52
1:B:548:ASN:ND2	1:B:620:ASN:HB2	2.24	0.52
1:C:463:LEU:HG	1:C:506:LEU:HB3	1.90	0.52
1:A:297:MET:HA	1:A:311:HIS:HE1	1.74	0.52
1:A:301:TYR:CE1	1:A:312:THR:HB	2.44	0.52
1:A:345:LEU:O	1:A:351:THR:HA	2.09	0.52
1:A:682:GLU:HG2	1:C:165:TYR:HE1	1.74	0.52
1:C:130:PRO:HG3	1:C:536:LEU:HD22	1.91	0.52
1:A:151:LYS:HE2	1:A:369:TRP:HZ2	1.74	0.52
1:A:343:ASN:HB2	1:A:354:TRP:CE2	2.45	0.52
1:A:505:ARG:O	1:A:509:THR:HG23	2.09	0.52
1:A:677:MET:HG3	1:C:290:ALA:O	2.10	0.52
1:B:209:SER:HB2	1:B:224:HIS:HB2	1.91	0.52
1:B:297:MET:H	1:B:311:HIS:HE1	1.54	0.52
1:C:235:LYS:O	1:C:248:HIS:ND1	2.42	0.52
1:A:149:VAL:HG22	1:A:369:TRP:HD1	1.75	0.52
1:A:178:ARG:HE	1:A:258:ARG:HH12	1.56	0.52
1:A:589:ILE:O	1:A:595:ALA:N	2.29	0.52
1:B:559:VAL:HG11	1:B:622:GLU:OE2	2.09	0.52
1:C:113:PHE:HA	1:C:621:ASN:HB3	1.91	0.52
1:C:242:ARG:HH21	1:C:574:VAL:HG12	1.73	0.52
1:A:646:GLY:O	1:A:661:ARG:NH2	2.37	0.52
1:A:698:GLY:C	1:A:700:LEU:HB2	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ASN:HA	1:C:670:PHE:CZ	2.44	0.52
1:B:198:ILE:HD11	1:B:322:VAL:HG21	1.90	0.52
1:A:324:GLY:HA2	1:A:339:PRO:HB2	1.92	0.52
1:A:706:GLN:HA	1:A:709:ASN:HD21	1.75	0.52
1:B:215:ARG:HH11	1:B:216:ASN:ND2	2.08	0.52
1:B:279:ARG:NH2	1:C:678:LEU:HA	2.25	0.52
1:A:598:SER:N	1:A:629:ALA:O	2.36	0.52
1:B:151:LYS:HE3	1:C:669:THR:H	1.74	0.52
1:B:288:VAL:HB	1:C:678:LEU:HD11	1.92	0.52
1:C:547:PRO:HB2	1:C:561:ALA:HB3	1.91	0.52
1:A:194:PHE:HD1	1:A:344:LEU:HD22	1.75	0.52
1:A:196:GLU:HA	1:A:200:LYS:CG	2.40	0.52
1:B:123:THR:H	1:B:126:GLN:CD	2.13	0.52
1:B:201:ILE:O	1:B:328:ARG:HD2	2.08	0.52
1:C:595:ALA:HB1	1:C:630:ILE:HD12	1.92	0.52
1:A:115:VAL:HA	1:A:623:LEU:HB2	1.92	0.52
1:A:132:ARG:NH1	1:A:133:CYS:O	2.43	0.52
1:A:583:VAL:HG23	1:A:600:PRO:HB3	1.91	0.52
1:A:602:VAL:HG23	1:A:604:PHE:HE1	1.75	0.52
1:A:646:GLY:HA2	1:A:661:ARG:HG2	1.91	0.52
1:B:224:HIS:CE1	1:B:268:THR:HG23	2.44	0.52
1:C:505:ARG:O	1:C:509:THR:HG23	2.10	0.52
1:C:598:SER:OG	1:C:630:ILE:O	2.28	0.52
1:A:132:ARG:HB2	1:B:557:ARG:NH2	2.25	0.52
1:A:369:TRP:HA	1:B:670:PHE:CD1	2.43	0.52
1:B:463:LEU:HD13	1:B:466:ARG:NH1	2.24	0.52
1:C:142:TYR:CD2	1:C:518:ASN:HB3	2.44	0.52
1:C:468:HIS:HD2	1:C:472:GLN:HE22	1.56	0.52
1:A:200:LYS:HA	1:A:204:LYS:HD3	1.92	0.51
1:A:208:ARG:HD2	1:A:229:GLU:CD	2.30	0.51
1:A:709:ASN:HA	1:A:712:HIS:NE2	2.25	0.51
1:B:548:ASN:HD21	1:B:620:ASN:HB2	1.74	0.51
1:B:657:HIS:ND1	1:B:658:GLN:O	2.31	0.51
1:B:677:MET:HG3	1:B:678:LEU:HD12	1.92	0.51
1:C:235:LYS:O	1:C:248:HIS:N	2.26	0.51
1:C:691:ARG:HA	1:C:694:ILE:HD12	1.91	0.51
1:A:343:ASN:ND2	1:A:356:TRP:HB2	2.26	0.51
1:A:466:ARG:HH12	1:A:467:GLU:HG2	1.74	0.51
1:A:618:GLY:HA3	1:A:622:GLU:HB2	1.91	0.51
1:B:122:ALA:N	1:B:123:THR:HA	2.25	0.51
1:C:150:PHE:CD2	1:C:413:ILE:HG23	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:VAL:HG22	1:C:186:PHE:HB3	1.90	0.51
1:C:244:SER:HB2	1:C:275:GLU:HB2	1.92	0.51
1:A:467:GLU:OE1	1:A:471:GLU:HG2	2.10	0.51
1:A:583:VAL:HA	1:A:602:VAL:HG12	1.93	0.51
1:A:589:ILE:N	1:A:595:ALA:O	2.39	0.51
1:A:673:LEU:HB3	1:C:557:ARG:HH21	1.75	0.51
1:B:114:TYR:HB2	1:B:622:GLU:OE2	2.10	0.51
1:B:608:ASP:OD1	1:B:609:GLN:NE2	2.43	0.51
1:B:700:LEU:HB3	1:B:701:ASP:O	2.10	0.51
1:C:157:TYR:HB3	1:C:280:SER:HB3	1.92	0.51
1:C:326:TYR:HA	1:C:339:PRO:HA	1.91	0.51
1:C:649:TYR:HD1	1:C:656:SER:HB3	1.74	0.51
1:A:439:PRO:HA	1:A:452:TYR:O	2.09	0.51
1:A:681:HIS:CG	1:A:682:GLU:N	2.79	0.51
1:B:359:LYS:NZ	1:B:361:PRO:HA	2.25	0.51
1:B:403:PRO:HD2	1:B:406:ARG:HE	1.75	0.51
1:B:587:MET:HB3	1:B:653:TYR:HB3	1.92	0.51
1:B:605:ARG:NH2	1:B:612:LEU:HG	2.25	0.51
1:B:710:GLN:O	1:B:714:LEU:HG	2.11	0.51
1:C:276:VAL:HB	1:C:290:ALA:HB3	1.92	0.51
1:A:341:THR:HG23	1:A:356:TRP:H	1.76	0.51
1:A:420:ALA:O	1:A:424:ILE:HG12	2.11	0.51
1:A:502:GLU:OE1	1:A:502:GLU:N	2.37	0.51
1:A:666:THR:O	1:A:667:VAL:HG13	2.10	0.51
1:B:105:LYS:HZ2	1:B:612:LEU:HD11	1.76	0.51
1:B:212:LYS:NZ	1:B:229:GLU:OE2	2.38	0.51
1:A:147:ALA:HB2	1:A:452:TYR:HD1	1.76	0.51
1:A:175:PHE:HB2	1:A:260:GLU:HA	1.92	0.51
1:A:502:GLU:O	1:A:506:LEU:HB2	2.10	0.51
1:A:564:LEU:HD11	1:A:569:ALA:HB2	1.91	0.51
1:A:614:GLU:HB2	1:A:627:ARG:HG3	1.92	0.51
1:B:151:LYS:N	1:B:367:THR:O	2.31	0.51
1:B:183:MET:HG3	1:B:263:HIS:CE1	2.45	0.51
1:A:208:ARG:NH1	1:A:229:GLU:OE2	2.42	0.51
1:B:640:TYR:CE1	1:B:649:TYR:HB2	2.45	0.51
1:C:104:ILE:N	1:C:582:ILE:HG13	2.26	0.51
1:C:162:THR:HB	1:C:164:TYR:OH	2.09	0.51
1:C:537:THR:HA	1:C:540:ASN:ND2	2.25	0.51
1:C:605:ARG:NE	1:C:612:LEU:HG	2.25	0.51
1:A:234:LEU:HD13	1:A:273:VAL:HB	1.93	0.51
1:B:343:ASN:O	1:B:353:ALA:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:ASP:HA	1:B:528:TRP:CE2	2.45	0.51
1:C:198:ILE:HG23	1:C:325:PHE:CE1	2.46	0.51
1:C:470:ARG:HH22	1:C:474:ARG:NH2	2.03	0.51
1:C:536:LEU:HA	1:C:539:TRP:CE3	2.45	0.51
1:A:167:ASP:HB2	1:A:270:ASN:OD1	2.11	0.51
1:B:636:GLY:N	1:B:652:GLU:OE1	2.43	0.51
1:C:302:GLY:HA2	1:C:319:PHE:CZ	2.46	0.51
1:C:680:ASP:O	1:C:681:HIS:ND1	2.44	0.51
1:C:240:ALA:N	1:C:245:ARG:HD3	2.25	0.51
1:A:425:PHE:HA	1:A:429:TYR:CD1	2.38	0.50
1:B:151:LYS:NZ	1:B:369:TRP:HA	2.25	0.50
1:B:158:LYS:HZ1	1:B:279:ARG:HB3	1.76	0.50
1:B:342:ARG:HH21	1:B:354:TRP:HA	1.77	0.50
1:B:358:PRO:HD2	1:B:360:ARG:NH2	2.27	0.50
1:B:699:LEU:CB	1:B:700:LEU:HG	2.40	0.50
1:A:134:PRO:HD2	1:A:526:ILE:HG12	1.93	0.50
1:A:208:ARG:NH1	1:A:212:LYS:HE2	2.26	0.50
1:A:701:ASP:O	1:A:705:VAL:N	2.36	0.50
1:B:115:VAL:O	1:B:117:PRO:HD3	2.11	0.50
1:C:105:LYS:HG3	1:C:579:ASP:H	1.76	0.50
1:C:208:ARG:HA	1:C:231:ASP:HA	1.93	0.50
1:C:285:ASP:O	1:C:311:HIS:ND1	2.44	0.50
1:C:716:PHE:CE2	1:C:718:ASP:HB3	2.46	0.50
1:A:348:PRO:HD2	1:A:349:LYS:NZ	2.26	0.50
1:A:442:TYR:HB2	1:A:450:ILE:HD12	1.93	0.50
1:B:150:PHE:HA	1:B:369:TRP:H	1.76	0.50
1:B:165:TYR:HA	1:B:192:VAL:H	1.76	0.50
1:B:318:ARG:NE	1:B:346:THR:OG1	2.26	0.50
1:B:555:VAL:HG11	1:B:558:ARG:HB3	1.94	0.50
1:B:616:GLN:NE2	1:B:629:ALA:HB3	2.25	0.50
1:B:657:HIS:CE1	1:B:659:LEU:HG	2.46	0.50
1:A:599:ARG:NH1	1:A:641:PHE:HD2	2.09	0.50
1:B:240:ALA:HA	1:B:246:GLY:N	2.25	0.50
1:B:434:ILE:HB	1:B:456:LEU:HB2	1.93	0.50
1:C:279:ARG:HH12	1:C:290:ALA:HB2	1.75	0.50
1:C:534:HIS:O	1:C:538:LEU:HG	2.11	0.50
1:A:237:ALA:HA	1:A:248:HIS:HB3	1.93	0.50
1:A:386:PHE:HE1	1:A:397:THR:OG1	1.93	0.50
1:A:678:LEU:HD12	1:C:243:THR:HB	1.93	0.50
1:B:121:GLY:N	1:B:569:ALA:HA	2.26	0.50
1:C:690:THR:HG21	1:C:692:HIS:ND1	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ASN:HD21	1:A:470:ARG:HH12	1.59	0.50
1:A:704:GLU:O	1:A:708:ARG:HG2	2.12	0.50
1:B:141:ASN:HB3	1:B:377:ARG:HH12	1.76	0.50
1:B:291:THR:HG23	1:C:681:HIS:HB2	1.94	0.50
1:B:525:ALA:O	1:B:528:TRP:HB3	2.11	0.50
1:B:705:VAL:HA	1:B:708:ARG:HE	1.75	0.50
1:A:172:GLN:HE21	1:A:183:MET:HB3	1.77	0.50
1:C:287:PHE:CE1	1:C:295:VAL:HB	2.46	0.50
1:C:326:TYR:CZ	1:C:339:PRO:HD3	2.47	0.50
1:C:588:ARG:HH21	1:C:594:GLY:H	1.60	0.50
1:A:589:ILE:HG22	1:A:630:ILE:HG21	1.93	0.50
1:A:636:GLY:N	1:A:652:GLU:OE2	2.41	0.50
1:B:143:THR:H	1:B:377:ARG:H	1.59	0.50
1:B:286:GLU:O	1:B:299:PRO:HD3	2.11	0.50
1:C:707:ARG:NH1	1:C:708:ARG:HB3	2.27	0.50
1:A:185:ILE:HG21	1:A:253:LYS:NZ	2.26	0.50
1:A:701:ASP:OD2	1:A:707:ARG:NH2	2.43	0.50
1:B:348:PRO:HB2	1:B:349:LYS:HD3	1.94	0.50
1:B:614:GLU:HB3	1:B:627:ARG:HD2	1.93	0.50
1:C:374:GLU:OE1	1:C:390:ALA:HB2	2.12	0.50
1:A:142:TYR:CD2	1:A:518:ASN:HB3	2.47	0.49
1:A:153:ASN:N	1:A:365:THR:OG1	2.45	0.49
1:A:202:ASN:HA	1:A:328:ARG:HD2	1.94	0.49
1:B:546:ASN:O	1:B:550:ILE:HG12	2.12	0.49
1:B:194:PHE:CD2	1:B:320:LYS:HG2	2.46	0.49
1:B:347:THR:N	1:B:350:PHE:O	2.45	0.49
1:B:709:ASN:HA	1:B:712:HIS:CE1	2.46	0.49
1:C:196:GLU:O	1:C:201:ILE:N	2.45	0.49
1:C:464:TYR:O	1:C:468:HIS:ND1	2.43	0.49
1:C:501:ILE:O	1:C:505:ARG:HG3	2.12	0.49
1:A:302:GLY:HA2	1:A:319:PHE:CZ	2.47	0.49
1:A:465:VAL:O	1:A:469:LEU:HG	2.12	0.49
1:A:562:ARG:NH2	1:B:680:ASP:OD2	2.45	0.49
1:B:402:TYR:CE2	1:B:407:VAL:HB	2.47	0.49
1:C:149:VAL:O	1:C:369:TRP:N	2.41	0.49
1:C:466:ARG:HH12	1:C:470:ARG:HG3	1.77	0.49
1:A:528:TRP:HA	1:A:531:LEU:HD12	1.94	0.49
1:A:683:PHE:O	1:A:685:PRO:HD2	2.12	0.49
1:B:285:ASP:O	1:B:311:HIS:ND1	2.46	0.49
1:C:500:SER:HB3	1:C:503:PHE:CZ	2.47	0.49
1:C:555:VAL:HG23	1:C:557:ARG:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:588:ARG:CA	1:C:596:CYS:HA	2.39	0.49
1:A:109:THR:HA	1:A:578:ALA:HB3	1.94	0.49
1:A:225:ARG:HA	1:A:254:TYR:CD2	2.48	0.49
1:B:151:LYS:HE2	1:C:670:PHE:CD1	2.48	0.49
1:B:246:GLY:HA3	1:B:274:GLU:OE1	2.12	0.49
1:B:592:ARG:NH1	1:C:714:LEU:O	2.45	0.49
1:A:469:LEU:HA	1:A:472:GLN:HG2	1.95	0.49
1:A:512:HIS:O	1:A:516:PRO:HD3	2.12	0.49
1:A:544:LYS:HE2	1:B:545:LEU:HD13	1.95	0.49
1:A:584:GLN:OE1	1:A:603:SER:N	2.45	0.49
1:A:598:SER:OG	1:A:616:GLN:OE1	2.27	0.49
1:B:200:LYS:O	1:B:205:GLY:N	2.45	0.49
1:B:243:THR:HG21	1:B:276:VAL:HG12	1.93	0.49
1:B:468:HIS:CE1	1:B:469:LEU:HG	2.48	0.49
1:B:602:VAL:C	1:B:627:ARG:HH21	2.16	0.49
1:B:624:ARG:H	1:B:624:ARG:HD3	1.78	0.49
1:C:195:GLU:OE1	1:C:208:ARG:NH2	2.34	0.49
1:C:616:GLN:OE1	1:C:629:ALA:HB3	2.12	0.49
1:B:234:LEU:HB3	1:B:247:TRP:HB3	1.95	0.49
1:C:466:ARG:O	1:C:470:ARG:N	2.36	0.49
1:A:119:PRO:HG2	1:A:569:ALA:CB	2.42	0.49
1:A:160:LYS:HG2	1:A:277:ASP:HA	1.94	0.49
1:A:225:ARG:HG2	1:A:254:TYR:HB2	1.94	0.49
1:A:465:VAL:O	1:A:468:HIS:HB3	2.13	0.49
1:A:549:ALA:O	1:A:553:VAL:HG12	2.12	0.49
1:B:199:ASP:O	1:B:204:LYS:N	2.46	0.49
1:B:208:ARG:HD2	1:B:229:GLU:OE2	2.12	0.49
1:C:140:GLN:HG2	1:C:380:TYR:HB2	1.94	0.49
1:C:520:MET:SD	1:C:521:LEU:HD23	2.52	0.49
1:C:618:GLY:H	1:C:623:LEU:HA	1.78	0.49
1:B:166:LYS:HB2	1:B:211:ALA:HB2	1.94	0.49
1:C:388:SER:O	1:C:392:SER:HA	2.13	0.49
1:C:636:GLY:HA2	1:C:638:ARG:HH21	1.77	0.49
1:A:172:GLN:HG3	1:A:263:HIS:HB3	1.95	0.49
1:A:183:MET:HG3	1:A:263:HIS:HE1	1.77	0.49
1:A:470:ARG:HD3	1:A:510:TYR:CE2	2.48	0.49
1:B:146:ILE:HG21	1:B:421:MET:HG2	1.94	0.49
1:B:518:ASN:HA	1:B:521:LEU:HD12	1.94	0.49
1:B:649:TYR:CD2	1:B:656:SER:HB2	2.48	0.49
1:C:580:ASN:O	1:C:604:PHE:HA	2.13	0.49
1:C:711:LEU:O	1:C:714:LEU:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ARG:HB3	1:A:137:PRO:HD3	1.94	0.48
1:A:237:ALA:HA	1:A:248:HIS:HD1	1.76	0.48
1:A:670:PHE:CG	1:A:670:PHE:O	2.66	0.48
1:A:682:GLU:N	1:A:682:GLU:OE2	2.46	0.48
1:B:280:SER:HA	1:B:287:PHE:HA	1.94	0.48
1:B:282:TYR:HA	1:B:284:TYR:H	1.77	0.48
1:B:469:LEU:HD23	1:B:472:GLN:NE2	2.28	0.48
1:C:252:LEU:HD12	1:C:253:LYS:H	1.77	0.48
1:C:463:LEU:O	1:C:467:GLU:HB2	2.12	0.48
1:A:498:THR:HG21	1:A:503:PHE:HB2	1.95	0.48
1:A:607:GLU:HG2	1:A:609:GLN:N	2.27	0.48
1:B:279:ARG:NH2	1:B:289:LEU:O	2.46	0.48
1:C:274:GLU:HG2	1:C:274:GLU:O	2.13	0.48
1:A:708:ARG:HE	1:A:711:LEU:HD11	1.78	0.48
1:B:191:PRO:HD2	1:B:213:TYR:CZ	2.49	0.48
1:B:210:THR:OG1	1:B:212:LYS:NZ	2.46	0.48
1:B:282:TYR:CG	1:B:283:PRO:HA	2.48	0.48
1:B:565:GLY:H	1:C:639:ARG:NH1	2.10	0.48
1:C:122:ALA:HB1	1:C:123:THR:HG22	1.94	0.48
1:C:134:PRO:HG2	1:C:526:ILE:HA	1.95	0.48
1:C:166:LYS:HZ1	1:C:208:ARG:HD2	1.77	0.48
1:C:201:ILE:O	1:C:205:GLY:N	2.44	0.48
1:A:162:THR:HG23	1:A:274:GLU:C	2.34	0.48
1:A:215:ARG:NE	1:A:220:THR:OG1	2.47	0.48
1:A:304:ARG:HB2	1:A:356:TRP:CH2	2.49	0.48
1:A:602:VAL:HG23	1:A:604:PHE:CE1	2.48	0.48
1:B:264:ARG:HD2	1:B:265:TYR:H	1.78	0.48
1:C:169:THR:HG23	1:C:268:THR:HB	1.94	0.48
1:C:343:ASN:OD1	1:C:356:TRP:HB2	2.13	0.48
1:A:119:PRO:HG3	1:A:561:ALA:HA	1.94	0.48
1:A:286:GLU:HB2	1:A:294:PHE:CZ	2.48	0.48
1:B:120:THR:OG1	1:C:678:LEU:HB3	2.13	0.48
1:B:162:THR:HG23	1:B:275:GLU:N	2.27	0.48
1:B:201:ILE:HG21	1:B:273:VAL:HG21	1.94	0.48
1:C:301:TYR:CE1	1:C:312:THR:HB	2.48	0.48
1:A:463:LEU:HD21	1:A:506:LEU:CB	2.43	0.48
1:A:681:HIS:CG	1:A:682:GLU:H	2.31	0.48
1:B:247:TRP:N	1:B:274:GLU:OE2	2.45	0.48
1:B:634:THR:HG23	1:B:693:GLU:HA	1.94	0.48
1:C:233:GLU:OE1	1:C:234:LEU:N	2.46	0.48
1:C:711:LEU:HA	1:C:714:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LYS:HZ3	1:A:207:CYS:HB3	1.79	0.48
1:A:327:ALA:O	1:A:336:ALA:N	2.46	0.48
1:B:301:TYR:CE1	1:B:312:THR:HB	2.48	0.48
1:B:470:ARG:HD2	1:B:507:GLN:OE1	2.13	0.48
1:B:528:TRP:HA	1:B:531:LEU:HD12	1.96	0.48
1:B:599:ARG:HH22	1:B:619:GLU:HA	1.79	0.48
1:B:599:ARG:HG3	1:B:617:LEU:O	2.14	0.48
1:B:673:LEU:O	1:B:674:ASN:ND2	2.46	0.48
1:B:700:LEU:HD22	1:B:701:ASP:HB2	1.95	0.48
1:C:685:PRO:HG2	1:C:690:THR:CG2	2.44	0.48
1:A:164:TYR:HB2	1:A:351:THR:HB	1.95	0.48
1:A:402:TYR:HE1	1:A:443:LEU:HD22	1.78	0.48
1:A:415:LYS:HA	1:A:418:ARG:NH1	2.29	0.48
1:A:529:CYS:SG	1:A:533:ASN:ND2	2.87	0.48
1:B:157:TYR:H	1:B:284:TYR:HE2	1.61	0.48
1:B:589:ILE:HD13	1:B:597:TYR:HE1	1.79	0.48
1:C:177:HIS:CD2	1:C:178:ARG:N	2.82	0.48
1:C:198:ILE:HG23	1:C:325:PHE:HE1	1.79	0.48
1:C:237:ALA:HB2	1:C:248:HIS:HB3	1.95	0.48
1:C:303:TYR:CD2	1:C:321:GLN:HB3	2.49	0.48
1:A:285:ASP:HA	1:A:298:SER:HA	1.95	0.48
1:A:541:GLU:OE2	1:B:546:ASN:ND2	2.47	0.48
1:A:677:MET:HG2	1:C:120:THR:H	1.78	0.48
1:B:130:PRO:HG3	1:B:536:LEU:HD13	1.95	0.48
1:B:234:LEU:HD13	1:B:273:VAL:HB	1.96	0.48
1:B:297:MET:HG3	1:B:312:THR:HA	1.95	0.48
1:B:326:TYR:HB2	1:B:336:ALA:O	2.13	0.48
1:B:565:GLY:N	1:C:639:ARG:HH11	2.11	0.48
1:C:176:GLY:HA3	1:C:179:TYR:CE2	2.49	0.48
1:C:704:GLU:HA	1:C:707:ARG:CG	2.44	0.48
1:A:119:PRO:HB3	1:A:571:SER:OG	2.13	0.48
1:A:162:THR:HG21	1:A:330:LEU:HD11	1.96	0.48
1:A:164:TYR:HD1	1:A:273:VAL:HG22	1.78	0.48
1:A:392:SER:OG	1:A:532:GLN:HG2	2.13	0.48
1:A:570:VAL:HG13	1:B:677:MET:CB	2.44	0.48
1:A:599:ARG:CG	1:A:600:PRO:HD2	2.43	0.48
1:A:678:LEU:HG	1:A:679:GLU:H	1.78	0.48
1:B:319:PHE:CE2	1:B:321:GLN:HB2	2.49	0.48
1:B:401:GLU:OE1	1:B:440:GLN:HB3	2.14	0.48
1:C:223:PHE:HB3	1:C:227:ASP:O	2.13	0.48
1:C:564:LEU:HD11	1:C:569:ALA:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:641:PHE:O	1:C:648:VAL:HG12	2.13	0.48
1:C:651:GLU:OE2	1:C:651:GLU:N	2.44	0.48
1:A:138:GLU:HG3	1:A:515:ARG:HA	1.94	0.47
1:A:242:ARG:HE	1:A:625:LEU:HD23	1.78	0.47
1:A:297:MET:HA	1:A:311:HIS:CE1	2.48	0.47
1:A:436:VAL:O	1:A:454:PRO:HD2	2.13	0.47
1:A:502:GLU:OE2	1:A:505:ARG:NH1	2.48	0.47
1:A:592:ARG:HD2	1:A:593:PRO:HD2	1.96	0.47
1:B:208:ARG:HG3	1:B:210:THR:O	2.13	0.47
1:B:282:TYR:CD1	1:B:283:PRO:HA	2.49	0.47
1:B:582:ILE:N	1:B:602:VAL:HG13	2.28	0.47
1:C:700:LEU:HD21	1:C:708:ARG:NE	2.29	0.47
1:A:403:PRO:HG2	1:A:406:ARG:HG2	1.96	0.47
1:B:168:VAL:O	1:B:187:GLU:HA	2.14	0.47
1:B:197:VAL:HA	1:B:201:ILE:HB	1.95	0.47
1:B:642:THR:HA	1:B:647:TYR:CD1	2.49	0.47
1:B:706:GLN:HA	1:B:709:ASN:OD1	2.14	0.47
1:C:209:SER:HB2	1:C:224:HIS:HB2	1.96	0.47
1:C:529:CYS:HA	1:C:532:GLN:HG2	1.95	0.47
1:C:541:GLU:OE2	1:C:544:LYS:HB2	2.14	0.47
1:A:576:VAL:HG23	1:A:580:ASN:HB2	1.96	0.47
1:B:125:VAL:HG21	1:C:672:ASP:HB3	1.96	0.47
1:C:165:TYR:CA	1:C:192:VAL:HG23	2.44	0.47
1:C:605:ARG:HG3	1:C:612:LEU:HD23	1.96	0.47
1:A:167:ASP:HA	1:A:188:ASP:O	2.14	0.47
1:B:199:ASP:O	1:B:204:LYS:HG3	2.15	0.47
1:B:420:ALA:HA	1:B:423:ARG:CZ	2.45	0.47
1:C:198:ILE:O	1:C:202:ASN:HB3	2.15	0.47
1:A:380:TYR:C	1:A:385:ARG:HE	2.18	0.47
1:A:409:LEU:HG	1:A:412:CYS:HB3	1.96	0.47
1:A:560:SER:O	1:A:571:SER:OG	2.29	0.47
1:A:580:ASN:OD1	1:A:605:ARG:HG3	2.14	0.47
1:B:564:LEU:HB3	1:C:639:ARG:HG2	1.96	0.47
1:B:699:LEU:N	1:B:700:LEU:HB2	2.18	0.47
1:C:467:GLU:OE2	1:C:470:ARG:HD3	2.14	0.47
1:A:420:ALA:HA	1:A:423:ARG:HH21	1.79	0.47
1:B:196:GLU:HG3	1:B:200:LYS:HD2	1.96	0.47
1:B:517:VAL:O	1:B:521:LEU:HG	2.13	0.47
1:A:164:TYR:OH	1:A:353:ALA:HB3	2.15	0.47
1:A:192:VAL:HG13	1:A:196:GLU:HB2	1.97	0.47
1:A:208:ARG:NH2	1:A:212:LYS:HG2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:GLY:HA3	1:A:385:ARG:NH2	2.14	0.47
1:A:540:ASN:O	1:A:543:ARG:NE	2.48	0.47
1:B:108:ASN:HB2	1:B:643:PHE:HD2	1.80	0.47
1:B:117:PRO:HD2	1:B:560:SER:CB	2.45	0.47
1:B:156:PRO:HB3	1:B:281:VAL:HA	1.95	0.47
1:B:172:GLN:O	1:B:183:MET:N	2.47	0.47
1:B:705:VAL:HG13	1:B:708:ARG:HH21	1.80	0.47
1:C:175:PHE:CG	1:C:258:ARG:HG3	2.49	0.47
1:C:328:ARG:HE	1:C:334:ALA:HA	1.80	0.47
1:C:402:TYR:CE2	1:C:407:VAL:HG13	2.49	0.47
1:C:438:GLN:HB2	1:C:475:LYS:NZ	2.29	0.47
1:C:555:VAL:HG23	1:C:557:ARG:N	2.30	0.47
1:C:706:GLN:O	1:C:710:GLN:HG3	2.15	0.47
1:A:105:LYS:HD2	1:A:579:ASP:O	2.14	0.47
1:A:154:ILE:HD12	1:A:282:TYR:CD2	2.50	0.47
1:A:171:SER:O	1:A:265:TYR:HA	2.15	0.47
1:A:273:VAL:HG12	1:A:330:LEU:CD1	2.44	0.47
1:A:706:GLN:HA	1:A:709:ASN:ND2	2.30	0.47
1:B:142:TYR:CE1	1:B:378:SER:HB3	2.50	0.47
1:B:700:LEU:HB3	1:B:701:ASP:C	2.35	0.47
1:C:166:LYS:NZ	1:C:208:ARG:HB2	2.29	0.47
1:C:242:ARG:HH21	1:C:606:TYR:HE1	1.63	0.47
1:C:514:GLN:HG2	1:C:518:ASN:ND2	2.22	0.47
1:C:540:ASN:O	1:C:543:ARG:HG3	2.15	0.47
1:C:588:ARG:NH2	1:C:589:ILE:O	2.48	0.47
1:C:659:LEU:HD23	1:C:659:LEU:HA	1.80	0.47
1:A:124:VAL:HG23	1:B:664:ILE:HD12	1.97	0.47
1:A:507:GLN:NE2	1:A:511:ASN:OD1	2.48	0.47
1:A:637:HIS:HE1	1:A:650:PHE:HB3	1.80	0.47
1:B:425:PHE:HA	1:B:429:TYR:HD1	1.80	0.47
1:B:522:GLY:O	1:B:526:ILE:HG13	2.15	0.47
1:C:243:THR:HG22	1:C:276:VAL:HA	1.97	0.47
1:C:531:LEU:O	1:C:535:GLU:HG2	2.15	0.47
1:C:546:ASN:O	1:C:550:ILE:HG12	2.14	0.47
1:C:617:LEU:HG	1:C:618:GLY:O	2.15	0.47
1:A:189:ARG:HG3	1:B:684:VAL:HG13	1.96	0.47
1:A:300:PHE:HB2	1:A:310:GLU:OE1	2.14	0.47
1:A:318:ARG:NH1	1:A:348:PRO:HD3	2.30	0.47
1:A:494:ARG:HB3	1:A:496:LYS:NZ	2.30	0.47
1:A:508:PHE:HA	1:A:511:ASN:ND2	2.30	0.47
1:B:141:ASN:O	1:B:377:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:SER:HB3	1:B:528:TRP:HZ2	1.80	0.47
1:B:532:GLN:HE21	1:B:536:LEU:HD11	1.79	0.47
1:C:166:LYS:NZ	1:C:208:ARG:HD2	2.30	0.47
1:C:552:SER:OG	1:C:558:ARG:HA	2.14	0.47
1:A:120:THR:O	1:B:678:LEU:HB2	2.15	0.46
1:A:130:PRO:HG3	1:A:536:LEU:HD13	1.97	0.46
1:A:368:LYS:O	1:B:670:PHE:HB3	2.14	0.46
1:A:582:ILE:HD13	1:A:612:LEU:HD11	1.97	0.46
1:C:109:THR:HA	1:C:644:GLY:HA3	1.97	0.46
1:C:165:TYR:O	1:C:272:ILE:HB	2.14	0.46
1:C:189:ARG:NH2	1:C:350:PHE:HB3	2.30	0.46
1:A:138:GLU:OE2	1:A:518:ASN:HB2	2.15	0.46
1:A:463:LEU:HD22	1:A:466:ARG:HH11	1.80	0.46
1:B:126:GLN:HB3	1:C:666:THR:HA	1.96	0.46
1:B:223:PHE:CD1	1:B:228:HIS:HA	2.51	0.46
1:B:318:ARG:HH21	1:B:346:THR:HG21	1.80	0.46
1:C:599:ARG:HD3	1:C:624:ARG:HD2	1.96	0.46
1:A:144:GLU:OE1	1:A:455:LEU:HB2	2.15	0.46
1:A:163:MET:SD	1:A:352:VAL:HG22	2.54	0.46
1:A:164:TYR:CE1	1:A:273:VAL:HG13	2.50	0.46
1:A:342:ARG:NH2	1:A:354:TRP:HA	2.30	0.46
1:A:373:ASP:HB2	1:A:424:ILE:HG21	1.96	0.46
1:A:466:ARG:CZ	1:A:507:GLN:HB2	2.45	0.46
1:B:120:THR:HA	1:B:569:ALA:HB1	1.97	0.46
1:B:395:PHE:CD1	1:B:444:ALA:HB1	2.50	0.46
1:C:632:PRO:CB	1:C:695:LYS:HG3	2.44	0.46
1:A:131:ARG:NH2	1:A:532:GLN:OE1	2.48	0.46
1:A:175:PHE:CE1	1:A:264:ARG:HB3	2.50	0.46
1:B:136:ARG:HB3	1:B:137:PRO:HD3	1.96	0.46
1:B:163:MET:HE1	1:B:352:VAL:HG13	1.98	0.46
1:C:108:ASN:O	1:C:646:GLY:N	2.48	0.46
1:C:150:PHE:CD1	1:C:449:LEU:HD22	2.51	0.46
1:A:113:PHE:HB3	1:A:623:LEU:HD13	1.98	0.46
1:A:198:ILE:HD13	1:A:325:PHE:HE1	1.81	0.46
1:A:244:SER:HB2	1:A:276:VAL:HA	1.98	0.46
1:A:318:ARG:NH2	1:A:347:THR:HA	2.30	0.46
1:A:596:CYS:N	1:A:633:CYS:SG	2.88	0.46
1:B:164:TYR:O	1:B:350:PHE:HA	2.14	0.46
1:C:318:ARG:NH2	1:C:347:THR:HA	2.23	0.46
1:C:352:VAL:HB	1:C:354:TRP:CZ3	2.50	0.46
1:A:121:GLY:HA2	1:A:570:VAL:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:PHE:CZ	1:A:368:LYS:HB3	2.49	0.46
1:A:389:ASP:O	1:A:528:TRP:NE1	2.48	0.46
1:A:466:ARG:HD2	1:A:507:GLN:HB2	1.96	0.46
1:A:500:SER:O	1:A:503:PHE:N	2.22	0.46
1:B:105:LYS:HE3	1:B:580:ASN:HA	1.98	0.46
1:B:168:VAL:HG12	1:B:269:VAL:HG13	1.98	0.46
1:B:589:ILE:HB	1:B:597:TYR:CE1	2.51	0.46
1:B:699:LEU:HB3	1:B:700:LEU:CG	2.42	0.46
1:B:704:GLU:HB3	1:B:707:ARG:HE	1.81	0.46
1:C:341:THR:OG1	1:C:356:TRP:HB3	2.16	0.46
1:A:177:HIS:CD2	1:A:179:TYR:HE1	2.34	0.46
1:A:559:VAL:HG23	1:A:571:SER:O	2.16	0.46
1:A:640:TYR:HD1	1:A:649:TYR:HB2	1.81	0.46
1:B:345:LEU:HG	1:B:347:THR:HG22	1.98	0.46
1:B:616:GLN:CG	1:B:624:ARG:HH21	2.28	0.46
1:C:415:LYS:NZ	1:C:418:ARG:HD2	2.31	0.46
1:C:468:HIS:HD2	1:C:472:GLN:NE2	2.13	0.46
1:C:520:MET:O	1:C:524:VAL:HG13	2.16	0.46
1:A:240:ALA:HB1	1:A:246:GLY:H	1.80	0.46
1:A:672:ASP:HA	1:A:673:LEU:HB2	1.98	0.46
1:A:692:HIS:HA	1:A:695:LYS:CD	2.45	0.46
1:A:704:GLU:HG3	1:A:707:ARG:NE	2.31	0.46
1:B:234:LEU:HB3	1:B:247:TRP:CB	2.45	0.46
1:C:296:TYR:C	1:C:314:TYR:HE2	2.19	0.46
1:C:384:PHE:HZ	1:C:474:ARG:HB3	1.80	0.46
1:C:556:GLY:O	1:C:558:ARG:NH2	2.44	0.46
1:A:195:GLU:OE1	1:A:196:GLU:HG3	2.15	0.46
1:A:667:VAL:HG12	1:C:369:TRP:CZ3	2.50	0.46
1:C:156:PRO:CA	1:C:280:SER:O	2.63	0.46
1:C:156:PRO:HB3	1:C:281:VAL:HG22	1.97	0.46
1:C:215:ARG:HD2	1:C:216:ASN:ND2	2.31	0.46
1:C:233:GLU:O	1:C:249:THR:HG22	2.15	0.46
1:C:319:PHE:HE1	1:C:343:ASN:HB3	1.80	0.46
1:C:651:GLU:OE1	1:C:656:SER:HB2	2.16	0.46
1:A:273:VAL:HG12	1:A:330:LEU:HD11	1.98	0.46
1:A:511:ASN:O	1:A:514:GLN:HB2	2.15	0.46
1:A:631:GLU:HA	1:B:711:LEU:HD13	1.98	0.46
1:B:245:ARG:HD2	1:B:331:THR:HG21	1.96	0.46
1:B:247:TRP:HE1	1:B:331:THR:CG2	2.28	0.46
1:B:302:GLY:HA2	1:B:319:PHE:CZ	2.50	0.46
1:C:699:LEU:N	1:C:700:LEU:HB2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:GLU:CD	1:A:389:ASP:HB2	2.36	0.45
1:B:300:PHE:O	1:B:310:GLU:HB3	2.17	0.45
1:B:470:ARG:O	1:B:473:SER:OG	2.26	0.45
1:C:142:TYR:CD1	1:C:376:LEU:HD13	2.51	0.45
1:C:164:TYR:CB	1:C:192:VAL:HB	2.46	0.45
1:C:194:PHE:CD1	1:C:344:LEU:HD22	2.47	0.45
1:C:500:SER:HB3	1:C:503:PHE:CE2	2.51	0.45
1:C:605:ARG:HB3	1:C:607:GLU:O	2.16	0.45
1:C:709:ASN:O	1:C:715:ARG:NH1	2.47	0.45
1:C:711:LEU:O	1:C:715:ARG:HG3	2.16	0.45
1:B:157:TYR:N	1:B:284:TYR:OH	2.49	0.45
1:B:175:PHE:HB3	1:B:260:GLU:HG2	1.97	0.45
1:B:191:PRO:HD2	1:B:213:TYR:CE1	2.50	0.45
1:C:175:PHE:CE2	1:C:258:ARG:HA	2.52	0.45
1:C:380:TYR:O	1:C:385:ARG:NE	2.49	0.45
1:C:566:ASP:OD1	1:C:566:ASP:N	2.47	0.45
1:C:664:ILE:O	1:C:665:THR:OG1	2.35	0.45
1:A:208:ARG:HA	1:A:231:ASP:HA	1.99	0.45
1:B:498:THR:HG23	1:B:500:SER:O	2.16	0.45
1:B:507:GLN:HE21	1:B:511:ASN:ND2	2.14	0.45
1:C:243:THR:CG2	1:C:277:ASP:H	2.29	0.45
1:C:300:PHE:CD2	1:C:359:LYS:HA	2.52	0.45
1:A:119:PRO:HG2	1:A:569:ALA:HB3	1.99	0.45
1:A:120:THR:HG21	1:A:292:GLY:HA2	1.98	0.45
1:A:250:THR:OG1	1:A:251:ASP:N	2.50	0.45
1:A:326:TYR:CE1	1:A:339:PRO:HB3	2.52	0.45
1:A:589:ILE:CG2	1:A:595:ALA:HB3	2.46	0.45
1:B:145:GLY:HA2	1:B:455:LEU:HG	1.97	0.45
1:B:168:VAL:HG22	1:B:188:ASP:HB2	1.99	0.45
1:B:235:LYS:O	1:B:248:HIS:N	2.37	0.45
1:B:558:ARG:NH1	1:B:574:VAL:HB	2.32	0.45
1:B:623:LEU:HD13	1:B:623:LEU:HA	1.80	0.45
1:C:581:VAL:HA	1:C:604:PHE:HA	1.97	0.45
1:A:141:ASN:HB2	1:A:379:GLU:OE1	2.16	0.45
1:A:165:TYR:HA	1:A:192:VAL:N	2.31	0.45
1:A:297:MET:SD	1:A:298:SER:N	2.89	0.45
1:A:365:THR:O	1:A:367:THR:HG23	2.17	0.45
1:B:105:LYS:HB2	1:B:107:GLU:OE1	2.15	0.45
1:B:106:ALA:HA	1:B:643:PHE:CZ	2.52	0.45
1:B:167:ASP:OD1	1:B:189:ARG:HG2	2.16	0.45
1:B:318:ARG:O	1:B:345:LEU:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:LYS:HB2	1:B:344:LEU:HB2	1.98	0.45
1:C:105:LYS:HG3	1:C:579:ASP:N	2.31	0.45
1:C:113:PHE:HB2	1:C:576:VAL:HG22	1.98	0.45
1:C:113:PHE:HD2	1:C:576:VAL:O	2.00	0.45
1:C:151:LYS:HG2	1:C:369:TRP:HB2	1.99	0.45
1:C:319:PHE:CZ	1:C:321:GLN:HB2	2.51	0.45
1:C:322:VAL:O	1:C:325:PHE:HB3	2.16	0.45
1:C:348:PRO:HG2	1:C:349:LYS:NZ	2.31	0.45
1:C:639:ARG:HH21	1:C:696:ASP:CG	2.19	0.45
1:A:189:ARG:HG3	1:B:684:VAL:CG1	2.47	0.45
1:A:286:GLU:O	1:A:299:PRO:HD3	2.17	0.45
1:A:348:PRO:HD2	1:A:349:LYS:HZ3	1.82	0.45
1:A:377:ARG:NH2	1:A:471:GLU:OE2	2.50	0.45
1:A:667:VAL:HG23	1:A:670:PHE:CZ	2.52	0.45
1:A:670:PHE:HB3	1:C:369:TRP:HE1	1.79	0.45
1:B:147:ALA:HB1	1:B:450:ILE:HG23	1.98	0.45
1:B:294:PHE:HE2	1:B:296:TYR:CZ	2.35	0.45
1:B:348:PRO:C	1:B:349:LYS:HD3	2.37	0.45
1:C:117:PRO:O	1:C:560:SER:OG	2.15	0.45
1:C:611:PRO:O	1:C:613:VAL:HG23	2.17	0.45
1:A:108:ASN:HB3	1:A:645:GLY:H	1.81	0.45
1:A:138:GLU:HG3	1:A:515:ARG:HG3	1.99	0.45
1:A:151:LYS:CG	1:A:369:TRP:HE1	2.28	0.45
1:B:237:ALA:HA	1:B:248:HIS:CE1	2.52	0.45
1:B:388:SER:HB3	1:B:393:THR:HG22	1.98	0.45
1:B:707:ARG:NH2	1:B:708:ARG:HB3	2.32	0.45
1:C:163:MET:HG3	1:C:291:THR:HG21	1.99	0.45
1:C:165:TYR:HA	1:C:192:VAL:H	1.81	0.45
1:C:379:GLU:HG3	1:C:384:PHE:CE1	2.41	0.45
1:C:700:LEU:HD22	1:C:705:VAL:CA	2.47	0.45
1:A:196:GLU:OE2	1:A:208:ARG:NH2	2.46	0.45
1:A:279:ARG:O	1:A:288:VAL:HG22	2.15	0.45
1:A:379:GLU:OE1	1:A:474:ARG:HG2	2.17	0.45
1:B:108:ASN:HB2	1:B:643:PHE:CD2	2.52	0.45
1:B:471:GLU:OE1	1:B:474:ARG:NE	2.43	0.45
1:C:196:GLU:HG3	1:C:200:LYS:CB	2.45	0.45
1:A:513:ILE:O	1:A:517:VAL:HG12	2.16	0.45
1:A:634:THR:OG1	1:A:696:ASP:HB2	2.17	0.45
1:A:637:HIS:O	1:A:652:GLU:N	2.28	0.45
1:B:249:THR:OG1	1:B:270:ASN:HB3	2.16	0.45
1:B:541:GLU:HA	1:B:544:LYS:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:ILE:HG12	1:C:582:ILE:HG13	1.99	0.45
1:C:434:ILE:HB	1:C:456:LEU:HB3	1.99	0.45
1:C:649:TYR:CZ	1:C:651:GLU:HB3	2.51	0.45
1:A:194:PHE:CD1	1:A:344:LEU:HD22	2.51	0.45
1:A:428:ARG:NH1	1:A:429:TYR:OH	2.50	0.45
1:A:597:TYR:HB3	1:A:616:GLN:NE2	2.32	0.45
1:B:384:PHE:CZ	1:B:399:LEU:HG	2.52	0.45
1:B:700:LEU:HA	1:B:701:ASP:HB2	1.99	0.45
1:C:138:GLU:HG3	1:C:139:GLY:N	2.32	0.45
1:C:701:ASP:HB3	1:C:704:GLU:HB2	1.99	0.45
1:A:193:PRO:HB2	1:A:195:GLU:HG3	1.99	0.44
1:A:615:GLY:N	1:A:627:ARG:HE	2.15	0.44
1:B:429:TYR:HD2	1:B:432:THR:HB	1.81	0.44
1:B:685:PRO:HB2	1:B:690:THR:HG21	1.98	0.44
1:C:189:ARG:HE	1:C:189:ARG:HB3	1.47	0.44
1:C:546:ASN:OD1	1:C:549:ALA:N	2.30	0.44
1:C:708:ARG:C	1:C:715:ARG:HH22	2.13	0.44
1:A:374:GLU:OE2	1:A:390:ALA:N	2.50	0.44
1:A:562:ARG:HG2	1:A:569:ALA:HB3	1.98	0.44
1:B:326:TYR:CD2	1:B:335:ARG:HG3	2.53	0.44
1:B:710:GLN:HG3	1:B:714:LEU:HD11	1.98	0.44
1:C:424:ILE:HD13	1:C:427:ARG:CZ	2.48	0.44
1:C:651:GLU:HG2	1:C:651:GLU:O	2.16	0.44
1:B:124:VAL:HA	1:C:665:THR:OG1	2.17	0.44
1:C:117:PRO:HG3	1:C:242:ARG:HH22	1.83	0.44
1:C:208:ARG:H	1:C:208:ARG:HG3	1.55	0.44
1:C:712:HIS:ND1	1:C:715:ARG:HB2	2.33	0.44
1:A:197:VAL:HA	1:A:201:ILE:HB	1.99	0.44
1:A:696:ASP:O	1:A:697:SER:OG	2.34	0.44
1:B:119:PRO:O	1:B:562:ARG:NE	2.49	0.44
1:B:550:ILE:O	1:B:554:THR:OG1	2.32	0.44
1:C:194:PHE:HB2	1:C:320:LYS:HE3	2.00	0.44
1:C:208:ARG:HB3	1:C:229:GLU:CG	2.46	0.44
1:C:412:CYS:SG	1:C:413:ILE:N	2.91	0.44
1:A:146:ILE:HG23	1:A:453:GLN:HB3	1.98	0.44
1:A:225:ARG:HA	1:A:254:TYR:CG	2.53	0.44
1:A:463:LEU:HD21	1:A:506:LEU:HB3	1.99	0.44
1:A:655:TYR:CZ	1:A:657:HIS:HA	2.52	0.44
1:B:132:ARG:HH11	1:B:133:CYS:H	1.65	0.44
1:B:325:PHE:HD2	1:B:342:ARG:HB2	1.83	0.44
1:B:345:LEU:O	1:B:351:THR:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:THR:HB	1:B:501:ILE:HD13	1.99	0.44
1:C:116:CYS:SG	1:C:623:LEU:N	2.90	0.44
1:C:588:ARG:NH2	1:C:594:GLY:H	2.16	0.44
1:A:402:TYR:CE2	1:A:406:ARG:HB2	2.52	0.44
1:A:687:GLU:O	1:A:688:VAL:HG23	2.18	0.44
1:B:151:LYS:CE	1:C:669:THR:H	2.31	0.44
1:B:276:VAL:HG11	1:C:681:HIS:CD2	2.51	0.44
1:B:710:GLN:NE2	1:B:710:GLN:O	2.50	0.44
1:C:176:GLY:HA3	1:C:179:TYR:CZ	2.53	0.44
1:C:302:GLY:HA3	1:C:356:TRP:NE1	2.33	0.44
1:C:527:ALA:O	1:C:531:LEU:HG	2.17	0.44
1:C:620:ASN:OD1	1:C:642:THR:HG21	2.17	0.44
1:A:158:LYS:CD	1:A:279:ARG:HG3	2.47	0.44
1:A:197:VAL:HG11	1:A:344:LEU:HD21	2.00	0.44
1:A:318:ARG:HH12	1:A:348:PRO:HD3	1.82	0.44
1:A:676:THR:OG1	1:A:677:MET:N	2.51	0.44
1:B:165:TYR:CA	1:B:192:VAL:HG23	2.48	0.44
1:B:335:ARG:HH12	1:B:339:PRO:HD3	1.83	0.44
1:B:565:GLY:N	1:C:639:ARG:NH1	2.66	0.44
1:C:201:ILE:O	1:C:328:ARG:HD2	2.17	0.44
1:C:322:VAL:O	1:C:322:VAL:HG13	2.17	0.44
1:C:345:LEU:HB2	1:C:354:TRP:HH2	1.83	0.44
1:C:701:ASP:CG	1:C:704:GLU:HG2	2.37	0.44
1:A:105:LYS:HG3	1:A:107:GLU:OE2	2.18	0.44
1:A:686:LEU:HD23	1:A:690:THR:HA	2.00	0.44
1:B:144:GLU:OE2	1:B:456:LEU:HA	2.17	0.44
1:B:198:ILE:HD13	1:B:325:PHE:CE1	2.52	0.44
1:B:289:LEU:HD22	1:B:293:ASP:HB3	1.98	0.44
1:B:341:THR:HG23	1:B:356:TRP:H	1.83	0.44
1:B:604:PHE:O	1:B:612:LEU:CA	2.37	0.44
1:B:681:HIS:CG	1:B:682:GLU:N	2.86	0.44
1:C:666:THR:HG22	1:C:667:VAL:N	2.33	0.44
1:B:254:TYR:CE2	1:B:256:PRO:HA	2.53	0.44
1:C:117:PRO:HG3	1:C:242:ARG:NH2	2.32	0.44
1:C:203:ALA:HA	1:C:335:ARG:NH1	2.33	0.44
1:C:256:PRO:HB2	1:C:264:ARG:HE	1.82	0.44
1:C:320:LYS:NZ	1:C:346:THR:OG1	2.50	0.44
1:C:439:PRO:O	1:C:475:LYS:NZ	2.50	0.44
1:C:466:ARG:NH1	1:C:470:ARG:HG3	2.33	0.44
1:A:178:ARG:NE	1:A:258:ARG:HH22	2.15	0.43
1:A:208:ARG:HB3	1:A:229:GLU:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:TYR:HB3	1:A:385:ARG:HD2	2.00	0.43
1:B:164:TYR:CD1	1:B:273:VAL:HG22	2.46	0.43
1:B:281:VAL:N	1:B:286:GLU:OE2	2.26	0.43
1:B:587:MET:HE3	1:B:654:ALA:HA	1.98	0.43
1:A:124:VAL:HG22	1:B:665:THR:HG23	2.00	0.43
1:A:499:SER:HG	1:A:503:PHE:HE1	1.65	0.43
1:A:501:ILE:O	1:A:505:ARG:HG3	2.18	0.43
1:B:168:VAL:HG11	1:B:211:ALA:HB3	2.00	0.43
1:B:326:TYR:CE2	1:B:335:ARG:HG3	2.53	0.43
1:C:175:PHE:CD1	1:C:180:SER:HB2	2.52	0.43
1:A:473:SER:HG	1:A:474:ARG:NH1	2.15	0.43
1:A:616:GLN:HB2	1:A:626:THR:OG1	2.17	0.43
1:B:175:PHE:HB3	1:B:260:GLU:HA	1.99	0.43
1:B:385:ARG:N	1:B:385:ARG:HD2	2.33	0.43
1:B:449:LEU:HD12	1:B:450:ILE:H	1.82	0.43
1:C:277:ASP:O	1:C:279:ARG:NH1	2.51	0.43
1:C:314:TYR:HB3	1:C:318:ARG:HH12	1.83	0.43
1:C:616:GLN:HE21	1:C:627:ARG:HA	1.84	0.43
1:A:226:ASP:H	1:A:267:THR:HG22	1.82	0.43
1:A:368:LYS:NZ	1:A:416:ASP:HB3	2.32	0.43
1:A:383:SER:OG	1:A:396:THR:HG23	2.18	0.43
1:A:463:LEU:HD13	1:A:466:ARG:NH1	2.30	0.43
1:A:494:ARG:O	1:A:496:LYS:HG2	2.18	0.43
1:A:531:LEU:O	1:A:535:GLU:HG2	2.18	0.43
1:A:592:ARG:NH1	1:A:593:PRO:O	2.52	0.43
1:B:129:GLN:O	1:B:131:ARG:NE	2.50	0.43
1:B:189:ARG:HG3	1:C:684:VAL:CG1	2.48	0.43
1:B:553:VAL:HG13	1:B:554:THR:N	2.33	0.43
1:C:105:LYS:HA	1:C:578:ALA:HB3	2.00	0.43
1:C:193:PRO:HB2	1:C:195:GLU:OE2	2.18	0.43
1:C:304:ARG:HB2	1:C:356:TRP:CH2	2.54	0.43
1:A:150:PHE:CD2	1:A:366:MET:HG3	2.53	0.43
1:B:564:LEU:O	1:B:567:VAL:HG12	2.18	0.43
1:B:601:LEU:HD12	1:B:616:GLN:HG3	2.00	0.43
1:C:210:THR:HG22	1:C:223:PHE:HA	1.99	0.43
1:A:165:TYR:CD2	1:A:350:PHE:HB3	2.54	0.43
1:A:568:MET:N	1:A:568:MET:SD	2.92	0.43
1:A:666:THR:HG21	1:C:446:GLY:C	2.38	0.43
1:A:675:ILE:HD13	1:C:570:VAL:HG11	2.01	0.43
1:B:221:THR:HG1	1:B:223:PHE:HE2	1.65	0.43
1:B:529:CYS:SG	1:B:533:ASN:ND2	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:536:LEU:HA	1:B:539:TRP:CD1	2.53	0.43
1:C:300:PHE:HB2	1:C:310:GLU:CD	2.39	0.43
1:C:384:PHE:CZ	1:C:474:ARG:HB3	2.52	0.43
1:C:468:HIS:CG	1:C:469:LEU:N	2.86	0.43
1:C:507:GLN:NE2	1:C:511:ASN:OD1	2.52	0.43
1:C:636:GLY:CA	1:C:638:ARG:HH21	2.31	0.43
1:A:114:TYR:CZ	1:A:558:ARG:HA	2.53	0.43
1:A:153:ASN:OD1	1:B:671:ILE:HD13	2.18	0.43
1:A:402:TYR:CD1	1:A:443:LEU:HB2	2.53	0.43
1:A:592:ARG:HD2	1:A:592:ARG:HA	1.75	0.43
1:B:128:GLU:HB2	1:B:131:ARG:HH21	1.83	0.43
1:B:377:ARG:HD3	1:B:379:GLU:HB3	2.01	0.43
1:B:616:GLN:HB3	1:B:624:ARG:HH21	1.83	0.43
1:C:274:GLU:N	1:C:274:GLU:OE2	2.51	0.43
1:C:377:ARG:HD2	1:C:384:PHE:CE1	2.53	0.43
1:C:402:TYR:CE2	1:C:406:ARG:HB2	2.54	0.43
1:A:280:SER:OG	1:A:281:VAL:N	2.52	0.43
1:A:402:TYR:H	1:A:441:TYR:HB2	1.83	0.43
1:A:493:GLU:OE2	1:A:495:ILE:HA	2.19	0.43
1:A:498:THR:O	1:A:500:SER:N	2.52	0.43
1:A:584:GLN:HG2	1:A:601:LEU:HB3	2.00	0.43
1:B:147:ALA:CB	1:B:375:MET:HG3	2.49	0.43
1:B:174:TRP:CE3	1:B:181:GLN:HB2	2.50	0.43
1:B:377:ARG:HH11	1:B:379:GLU:HG2	1.84	0.43
1:B:440:GLN:OE1	1:B:452:TYR:HB3	2.19	0.43
1:B:466:ARG:NH1	1:B:467:GLU:HG2	2.34	0.43
1:B:564:LEU:HD23	1:B:569:ALA:HB2	2.00	0.43
1:C:144:GLU:HA	1:C:375:MET:O	2.19	0.43
1:C:275:GLU:OE2	1:C:330:LEU:HB2	2.19	0.43
1:C:342:ARG:HD3	1:C:342:ARG:HA	1.73	0.43
1:C:466:ARG:O	1:C:469:LEU:CB	2.65	0.43
1:C:634:THR:H	1:C:653:TYR:HE2	1.66	0.43
1:A:106:ALA:O	1:A:579:ASP:HA	2.19	0.43
1:A:138:GLU:HB3	1:A:139:GLY:H	1.70	0.43
1:A:201:ILE:O	1:A:205:GLY:N	2.51	0.43
1:A:320:LYS:NZ	1:A:346:THR:OG1	2.31	0.43
1:B:589:ILE:HD12	1:B:589:ILE:HA	1.88	0.43
1:B:635:VAL:HG22	1:B:693:GLU:OE1	2.19	0.43
1:C:401:GLU:HG2	1:C:442:TYR:CE1	2.54	0.43
1:A:146:ILE:HA	1:A:373:ASP:HA	2.01	0.43
1:A:200:LYS:O	1:A:205:GLY:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:SER:HB3	1:A:230:THR:HB	2.01	0.43
1:A:711:LEU:HD21	1:C:631:GLU:OE1	2.19	0.43
1:B:104:ILE:N	1:B:582:ILE:HG23	2.33	0.43
1:B:202:ASN:O	1:B:328:ARG:HB2	2.18	0.43
1:B:412:CYS:SG	1:B:413:ILE:N	2.92	0.43
1:B:515:ARG:HE	1:B:515:ARG:HB2	1.63	0.43
1:B:641:PHE:O	1:B:648:VAL:HG12	2.19	0.43
1:C:230:THR:O	1:C:232:MET:HG3	2.19	0.43
1:A:132:ARG:HH11	1:A:133:CYS:H	1.67	0.42
1:A:162:THR:HB	1:A:164:TYR:OH	2.18	0.42
1:A:183:MET:HG3	1:A:263:HIS:CE1	2.54	0.42
1:A:581:VAL:HG13	1:A:604:PHE:HB3	2.00	0.42
1:A:599:ARG:HD3	1:A:624:ARG:HH12	1.84	0.42
1:B:194:PHE:CG	1:B:320:LYS:HG2	2.54	0.42
1:B:551:ALA:O	1:B:555:VAL:CB	2.63	0.42
1:B:561:ALA:CA	1:B:569:ALA:O	2.61	0.42
1:A:704:GLU:HA	1:A:707:ARG:HB2	2.00	0.42
1:B:119:PRO:HD2	1:B:562:ARG:CZ	2.49	0.42
1:B:160:LYS:HA	1:B:160:LYS:HD3	1.79	0.42
1:B:200:LYS:O	1:B:204:LYS:HB2	2.19	0.42
1:B:325:PHE:C	1:B:340:THR:H	2.23	0.42
1:B:342:ARG:NH2	1:B:354:TRP:HA	2.33	0.42
1:B:672:ASP:CA	1:B:673:LEU:HB3	2.35	0.42
1:C:162:THR:HA	1:C:275:GLU:HA	2.00	0.42
1:C:242:ARG:HH12	1:C:573:CYS:HA	1.84	0.42
1:C:600:PRO:O	1:C:602:VAL:HG13	2.19	0.42
1:C:690:THR:OG1	1:C:691:ARG:N	2.52	0.42
1:A:193:PRO:O	1:A:197:VAL:HG23	2.20	0.42
1:A:289:LEU:HB2	1:A:293:ASP:O	2.20	0.42
1:A:384:PHE:HB3	1:A:386:PHE:CZ	2.53	0.42
1:A:466:ARG:NE	1:A:507:GLN:HB2	2.34	0.42
1:B:631:GLU:OE1	1:B:695:LYS:HE2	2.19	0.42
1:C:150:PHE:CB	1:C:366:MET:HB3	2.48	0.42
1:C:307:SER:O	1:C:310:GLU:HB2	2.19	0.42
1:C:321:GLN:HA	1:C:343:ASN:HA	2.00	0.42
1:C:425:PHE:O	1:C:429:TYR:N	2.38	0.42
1:C:552:SER:OG	1:C:558:ARG:NH1	2.52	0.42
1:C:599:ARG:NH1	1:C:619:GLU:OE2	2.52	0.42
1:A:150:PHE:O	1:A:151:LYS:HG2	2.20	0.42
1:A:190:ALA:HB1	1:A:213:TYR:CB	2.49	0.42
1:A:233:GLU:O	1:A:249:THR:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:VAL:HG12	1:A:294:PHE:CE2	2.55	0.42
1:B:121:GLY:HA2	1:B:570:VAL:HG12	2.01	0.42
1:B:127:PHE:CE1	1:B:568:MET:HG2	2.54	0.42
1:B:189:ARG:HG3	1:C:684:VAL:HB	2.00	0.42
1:B:424:ILE:HD13	1:B:427:ARG:CZ	2.49	0.42
1:B:605:ARG:CZ	1:B:612:LEU:HG	2.49	0.42
1:B:695:LYS:HD2	1:B:695:LYS:O	2.19	0.42
1:C:224:HIS:HE1	1:C:268:THR:HG23	1.78	0.42
1:C:371:GLU:CD	1:C:420:ALA:HB1	2.40	0.42
1:A:159:PHE:CE2	1:A:354:TRP:HB2	2.54	0.42
1:A:168:VAL:N	1:A:187:GLU:OE2	2.53	0.42
1:A:460:LEU:HD22	1:A:506:LEU:HD22	2.01	0.42
1:A:500:SER:HB3	1:A:503:PHE:CZ	2.54	0.42
1:A:703:THR:HG21	1:C:545:LEU:CD1	2.48	0.42
1:B:498:THR:HG21	1:B:503:PHE:HB2	2.01	0.42
1:B:570:VAL:HG11	1:C:677:MET:HG2	2.01	0.42
1:C:115:VAL:O	1:C:625:LEU:HD21	2.20	0.42
1:C:509:THR:O	1:C:513:ILE:HG12	2.19	0.42
1:A:164:TYR:HB3	1:A:192:VAL:HB	2.01	0.42
1:A:289:LEU:HD13	1:A:294:PHE:HA	2.01	0.42
1:C:329:ASP:O	1:C:333:LYS:N	2.52	0.42
1:C:599:ARG:NE	1:C:618:GLY:HA2	2.35	0.42
1:C:707:ARG:HD2	1:C:708:ARG:N	2.34	0.42
1:A:392:SER:OG	1:A:528:TRP:HD1	2.00	0.42
1:A:401:GLU:OE2	1:A:440:GLN:HB3	2.19	0.42
1:B:700:LEU:HA	1:B:700:LEU:HD23	1.80	0.42
1:C:165:TYR:HA	1:C:192:VAL:HG23	2.01	0.42
1:A:154:ILE:HG22	1:B:671:ILE:HD11	2.01	0.42
1:A:302:GLY:HA2	1:A:319:PHE:HZ	1.85	0.42
1:A:412:CYS:SG	1:A:413:ILE:N	2.92	0.42
1:A:699:LEU:HD11	1:C:626:THR:HG22	2.02	0.42
1:A:699:LEU:N	1:A:700:LEU:HB2	2.35	0.42
1:B:128:GLU:OE1	1:B:131:ARG:NH2	2.51	0.42
1:B:146:ILE:CG2	1:B:453:GLN:HB3	2.50	0.42
1:B:290:ALA:O	1:C:679:GLU:HG2	2.19	0.42
1:C:104:ILE:N	1:C:579:ASP:HA	2.35	0.42
1:C:280:SER:HB2	1:C:299:PRO:HB3	2.02	0.42
1:C:327:ALA:H	1:C:337:THR:HG21	1.85	0.42
1:A:141:ASN:ND2	1:A:471:GLU:OE2	2.53	0.42
1:A:178:ARG:NE	1:A:258:ARG:HH12	2.17	0.42
1:A:209:SER:O	1:A:269:VAL:HB	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:LEU:HD22	1:A:410:GLY:HA3	2.01	0.42
1:A:588:ARG:HB3	1:A:596:CYS:SG	2.60	0.42
1:A:630:ILE:HG13	1:B:711:LEU:HD21	2.02	0.42
1:A:666:THR:O	1:A:666:THR:HG22	2.19	0.42
1:A:700:LEU:HG	1:A:705:VAL:HG22	2.02	0.42
1:B:369:TRP:HE1	1:C:669:THR:HG23	1.84	0.42
1:B:502:GLU:CA	1:B:505:ARG:HB2	2.41	0.42
1:B:580:ASN:ND2	1:B:608:ASP:HA	2.35	0.42
1:B:648:VAL:HG23	1:B:658:GLN:HE22	1.84	0.42
1:B:648:VAL:HG23	1:B:658:GLN:NE2	2.34	0.42
1:C:236:PRO:HA	1:C:247:TRP:CD1	2.54	0.42
1:C:286:GLU:OE1	1:C:296:TYR:HB3	2.20	0.42
1:C:635:VAL:HG23	1:C:635:VAL:O	2.20	0.42
1:A:224:HIS:HE2	1:A:252:LEU:HD21	1.85	0.42
1:A:514:GLN:O	1:A:518:ASN:ND2	2.53	0.42
1:A:626:THR:HA	1:B:689:TYR:OH	2.20	0.42
1:B:355:ASP:OD1	1:B:355:ASP:N	2.51	0.42
1:B:381:GLY:HA3	1:B:385:ARG:NH2	2.35	0.42
1:B:700:LEU:CD2	1:B:701:ASP:HB2	2.50	0.42
1:C:392:SER:HB2	1:C:528:TRP:CD1	2.55	0.42
1:A:257:SER:HB2	1:A:264:ARG:NH1	2.35	0.41
1:B:352:VAL:HB	1:B:354:TRP:CZ3	2.55	0.41
1:B:392:SER:HA	1:B:528:TRP:NE1	2.30	0.41
1:B:704:GLU:HA	1:B:707:ARG:HB3	2.01	0.41
1:C:155:ALA:HA	1:C:156:PRO:HD3	1.93	0.41
1:C:178:ARG:NE	1:C:178:ARG:HA	2.35	0.41
1:C:440:GLN:H	1:C:452:TYR:H	1.66	0.41
1:A:154:ILE:HD12	1:A:282:TYR:HD2	1.83	0.41
1:A:155:ALA:O	1:A:281:VAL:HA	2.20	0.41
1:A:497:THR:HB	1:A:501:ILE:HD13	2.02	0.41
1:B:173:VAL:HA	1:B:182:PHE:HA	2.02	0.41
1:B:298:SER:HB2	1:B:311:HIS:HB3	2.01	0.41
1:B:342:ARG:HA	1:B:342:ARG:HD2	1.69	0.41
1:B:365:THR:O	1:B:367:THR:HG23	2.20	0.41
1:B:620:ASN:O	1:B:622:GLU:HG2	2.20	0.41
1:B:701:ASP:HB3	1:B:704:GLU:HG3	2.01	0.41
1:C:441:TYR:HA	1:C:450:ILE:O	2.20	0.41
1:C:463:LEU:HD11	1:C:506:LEU:O	2.20	0.41
1:C:633:CYS:HA	1:C:653:TYR:HE2	1.84	0.41
1:A:141:ASN:ND2	1:A:470:ARG:HH12	2.19	0.41
1:A:360:ARG:HA	1:A:360:ARG:NE	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:LEU:HD21	1:A:569:ALA:HB2	2.02	0.41
1:B:119:PRO:HG2	1:B:562:ARG:HG2	2.02	0.41
1:B:183:MET:HG3	1:B:263:HIS:HE1	1.83	0.41
1:B:385:ARG:HG3	1:B:396:THR:HG23	2.02	0.41
1:C:138:GLU:CG	1:C:139:GLY:N	2.82	0.41
1:C:193:PRO:O	1:C:197:VAL:HG23	2.20	0.41
1:C:280:SER:HA	1:C:287:PHE:CB	2.49	0.41
1:C:692:HIS:HD2	1:C:695:LYS:NZ	2.18	0.41
1:A:257:SER:HB2	1:A:264:ARG:HH12	1.85	0.41
1:A:635:VAL:HG22	1:A:692:HIS:CB	2.50	0.41
1:B:188:ASP:O	1:C:684:VAL:HG21	2.19	0.41
1:B:194:PHE:CE1	1:B:198:ILE:HD11	2.56	0.41
1:B:297:MET:HB2	1:B:314:TYR:CD2	2.55	0.41
1:B:317:ASP:O	1:B:318:ARG:HD2	2.19	0.41
1:B:327:ALA:N	1:B:337:THR:OG1	2.33	0.41
1:B:369:TRP:HD1	1:C:669:THR:OG1	2.03	0.41
1:B:419:ASP:HA	1:B:422:ASP:OD1	2.20	0.41
1:B:574:VAL:HG12	1:B:576:VAL:HG23	2.03	0.41
1:C:140:GLN:HB3	1:C:379:GLU:N	2.36	0.41
1:C:167:ASP:HB3	1:C:187:GLU:OE1	2.20	0.41
1:C:167:ASP:HB2	1:C:270:ASN:HD21	1.85	0.41
1:C:308:HIS:CE1	1:C:309:THR:HG23	2.56	0.41
1:C:469:LEU:HA	1:C:472:GLN:OE1	2.21	0.41
1:C:515:ARG:HB3	1:C:516:PRO:HD3	2.02	0.41
1:A:111:ALA:HB3	1:A:644:GLY:O	2.20	0.41
1:A:200:LYS:HA	1:A:204:LYS:HB2	2.01	0.41
1:A:494:ARG:HB3	1:A:496:LYS:HZ3	1.85	0.41
1:A:639:ARG:NH1	1:C:565:GLY:H	2.19	0.41
1:A:649:TYR:CD2	1:A:656:SER:HB3	2.55	0.41
1:B:328:ARG:HG2	1:B:330:LEU:HD22	2.02	0.41
1:B:376:LEU:HA	1:B:376:LEU:HD23	1.79	0.41
1:B:634:THR:OG1	1:B:696:ASP:OD1	2.39	0.41
1:C:167:ASP:OD2	1:C:189:ARG:HG2	2.20	0.41
1:C:300:PHE:HD1	1:C:357:VAL:HG13	1.84	0.41
1:C:365:THR:OG1	1:C:408:ASP:HB2	2.21	0.41
1:C:709:ASN:OD1	1:C:710:GLN:N	2.54	0.41
1:A:178:ARG:HE	1:A:258:ARG:NH2	2.15	0.41
1:A:208:ARG:NH1	1:A:210:THR:O	2.54	0.41
1:A:323:ASP:OD2	1:A:324:GLY:N	2.49	0.41
1:A:372:VAL:HG22	1:A:390:ALA:HB3	2.03	0.41
1:A:694:ILE:HA	1:A:698:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702:TYR:O	1:A:705:VAL:HB	2.20	0.41
1:B:285:ASP:HA	1:B:311:HIS:HB3	2.02	0.41
1:B:424:ILE:HD13	1:B:427:ARG:NE	2.35	0.41
1:B:543:ARG:HG2	1:B:547:PRO:HA	2.01	0.41
1:B:583:VAL:HA	1:B:602:VAL:HG22	2.03	0.41
1:B:599:ARG:HB3	1:B:616:GLN:CG	2.50	0.41
1:B:640:TYR:CD1	1:B:649:TYR:HB2	2.55	0.41
1:B:640:TYR:HB3	1:B:647:TYR:HB3	2.01	0.41
1:B:701:ASP:HB3	1:B:704:GLU:CG	2.51	0.41
1:C:119:PRO:HD2	1:C:562:ARG:HG2	2.02	0.41
1:C:560:SER:N	1:C:571:SER:O	2.33	0.41
1:A:115:VAL:HG13	1:A:242:ARG:HD2	2.02	0.41
1:A:126:GLN:OE1	1:A:126:GLN:N	2.54	0.41
1:A:234:LEU:HD21	1:A:271:CYS:SG	2.61	0.41
1:A:413:ILE:H	1:A:413:ILE:HD12	1.85	0.41
1:B:116:CYS:SG	1:B:622:GLU:HB3	2.60	0.41
1:B:128:GLU:OE1	1:B:131:ARG:NE	2.51	0.41
1:B:237:ALA:HB2	1:B:248:HIS:CG	2.55	0.41
1:B:375:MET:HB3	1:B:452:TYR:HE1	1.85	0.41
1:B:391:ILE:O	1:B:392:SER:OG	2.37	0.41
1:B:436:VAL:HG11	1:B:456:LEU:HD11	2.02	0.41
1:B:558:ARG:CD	1:B:559:VAL:H	2.33	0.41
1:B:611:PRO:O	1:B:613:VAL:HG23	2.21	0.41
1:C:385:ARG:NE	1:C:396:THR:HG23	2.36	0.41
1:C:671:ILE:HD12	1:C:675:ILE:HD13	2.03	0.41
1:C:712:HIS:CD2	1:C:715:ARG:HD2	2.56	0.41
1:A:254:TYR:CE2	1:A:256:PRO:HA	2.56	0.41
1:A:722:VAL:O	1:B:181:GLN:HG3	2.21	0.41
1:B:130:PRO:N	1:B:536:LEU:HD22	2.36	0.41
1:C:171:SER:O	1:C:171:SER:OG	2.33	0.41
1:C:191:PRO:HB3	1:C:350:PHE:O	2.21	0.41
1:C:234:LEU:HB3	1:C:247:TRP:CB	2.49	0.41
1:A:177:HIS:CD2	1:A:179:TYR:CE1	3.09	0.41
1:A:237:ALA:HB3	1:A:240:ALA:HB2	2.02	0.41
1:A:320:LYS:HB2	1:A:320:LYS:HE2	1.88	0.41
1:A:343:ASN:HB2	1:A:354:TRP:CZ2	2.56	0.41
1:A:602:VAL:C	1:A:627:ARG:HH21	2.24	0.41
1:B:116:CYS:HB2	1:B:624:ARG:HA	2.02	0.41
1:B:158:LYS:CD	1:B:279:ARG:HG2	2.51	0.41
1:B:160:LYS:HD2	1:B:244:SER:OG	2.21	0.41
1:B:177:HIS:CE1	1:B:178:ARG:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:VAL:O	1:B:202:ASN:N	2.48	0.41
1:B:198:ILE:HA	1:B:325:PHE:HZ	1.86	0.41
1:B:224:HIS:HE2	1:B:252:LEU:HD13	1.86	0.41
1:B:245:ARG:HH12	1:B:329:ASP:CG	2.24	0.41
1:B:323:ASP:OD2	1:B:324:GLY:N	2.54	0.41
1:B:404:LEU:HD22	1:B:410:GLY:O	2.21	0.41
1:C:150:PHE:HD2	1:C:366:MET:C	2.25	0.41
1:C:172:GLN:HG3	1:C:265:TYR:CE1	2.55	0.41
1:C:321:GLN:HG3	1:C:343:ASN:OD1	2.20	0.41
1:C:404:LEU:HB2	1:C:410:GLY:CA	2.44	0.41
1:A:288:VAL:C	1:A:289:LEU:HD12	2.40	0.41
1:A:321:GLN:HG3	1:A:343:ASN:OD1	2.21	0.41
1:A:699:LEU:HD12	1:A:699:LEU:O	2.21	0.41
1:A:704:GLU:CA	1:A:707:ARG:HE	2.31	0.41
1:B:149:VAL:HG21	1:B:369:TRP:HE3	1.84	0.41
1:B:541:GLU:O	1:B:544:LYS:HB2	2.20	0.41
1:C:552:SER:O	1:C:558:ARG:NH2	2.54	0.41
1:C:690:THR:HG23	1:C:692:HIS:H	1.86	0.41
1:A:121:GLY:CA	1:A:570:VAL:H	2.34	0.40
1:A:136:ARG:NH2	1:A:526:ILE:HD12	2.37	0.40
1:A:208:ARG:HH22	1:A:212:LYS:HG2	1.86	0.40
1:A:359:LYS:H	1:A:359:LYS:HG2	1.72	0.40
1:B:104:ILE:O	1:B:582:ILE:HA	2.21	0.40
1:B:392:SER:HB3	1:B:528:TRP:CZ2	2.55	0.40
1:B:543:ARG:HD3	1:B:568:MET:HE1	2.03	0.40
1:B:553:VAL:HG13	1:B:554:THR:H	1.86	0.40
1:C:136:ARG:HB3	1:C:137:PRO:HD2	2.03	0.40
1:C:318:ARG:O	1:C:320:LYS:NZ	2.46	0.40
1:C:551:ALA:O	1:C:555:VAL:HG13	2.20	0.40
1:A:114:TYR:HE2	1:A:552:SER:OG	2.04	0.40
1:A:628:ASP:O	1:A:630:ILE:HG12	2.22	0.40
1:B:117:PRO:O	1:B:119:PRO:HD3	2.21	0.40
1:B:193:PRO:O	1:B:197:VAL:HG23	2.21	0.40
1:B:196:GLU:CD	1:B:200:LYS:HD2	2.42	0.40
1:B:469:LEU:HA	1:B:472:GLN:NE2	2.37	0.40
1:C:119:PRO:HG2	1:C:569:ALA:O	2.22	0.40
1:C:199:ASP:O	1:C:204:LYS:N	2.55	0.40
1:C:297:MET:HE1	1:C:314:TYR:H	1.86	0.40
1:C:330:LEU:HA	1:C:333:LYS:HA	2.03	0.40
1:C:529:CYS:O	1:C:532:GLN:HG3	2.21	0.40
1:C:637:HIS:N	1:C:652:GLU:OE1	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:690:THR:OG1	1:C:691:ARG:HD3	2.21	0.40
1:A:326:TYR:HE1	1:A:339:PRO:HB3	1.85	0.40
1:A:535:GLU:HB3	1:A:539:TRP:CE2	2.56	0.40
1:A:661:ARG:NH1	1:C:129:GLN:OE1	2.55	0.40
1:B:158:LYS:HD3	1:B:279:ARG:HG2	2.03	0.40
1:B:413:ILE:H	1:B:413:ILE:HD12	1.87	0.40
1:B:465:VAL:HA	1:B:468:HIS:NE2	2.35	0.40
1:C:128:GLU:O	1:C:536:LEU:HD11	2.21	0.40
1:C:192:VAL:HA	1:C:193:PRO:HD3	1.91	0.40
1:C:214:VAL:HA	1:C:219:GLU:HA	2.03	0.40
1:A:166:LYS:HE3	1:A:211:ALA:HB2	2.03	0.40
1:A:191:PRO:HD3	1:A:349:LYS:HA	2.04	0.40
1:A:318:ARG:CZ	1:A:347:THR:HA	2.52	0.40
1:A:349:LYS:HE2	1:A:350:PHE:CE2	2.56	0.40
1:A:604:PHE:O	1:A:612:LEU:HD12	2.21	0.40
1:A:614:GLU:HB2	1:A:627:ARG:CZ	2.51	0.40
1:A:672:ASP:HA	1:A:673:LEU:CB	2.51	0.40
1:B:140:GLN:OE1	1:B:140:GLN:HA	2.22	0.40
1:B:226:ASP:HB2	1:B:254:TYR:CZ	2.57	0.40
1:B:320:LYS:HB2	1:B:320:LYS:HE2	1.91	0.40
1:C:521:LEU:O	1:C:524:VAL:HG22	2.22	0.40
1:A:123:THR:HG21	1:A:568:MET:H	1.87	0.40
1:A:140:GLN:C	1:A:379:GLU:HG2	2.42	0.40
1:A:286:GLU:HB2	1:A:294:PHE:HZ	1.86	0.40
1:B:105:LYS:NZ	1:B:612:LEU:HD21	2.36	0.40
1:B:194:PHE:CE1	1:B:344:LEU:HD13	2.57	0.40
1:B:258:ARG:NH1	1:B:260:GLU:OE2	2.45	0.40
1:B:297:MET:CG	1:B:312:THR:HA	2.52	0.40
1:B:466:ARG:CD	1:B:507:GLN:HB2	2.50	0.40
1:B:469:LEU:HA	1:B:472:GLN:CD	2.42	0.40
1:B:691:ARG:HD3	1:B:691:ARG:H	1.86	0.40
1:C:141:ASN:HB2	1:C:379:GLU:HB2	2.04	0.40
1:C:349:LYS:HE2	1:C:350:PHE:HE2	1.86	0.40
1:C:709:ASN:C	1:C:715:ARG:HH12	2.25	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	602/904 (67%)	513 (85%)	85 (14%)	4 (1%)	22	63
1	B	602/904 (67%)	484 (80%)	115 (19%)	3 (0%)	29	69
1	C	602/904 (67%)	494 (82%)	102 (17%)	6 (1%)	15	55
All	All	1806/2712 (67%)	1491 (83%)	302 (17%)	13 (1%)	26	63

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	PRO
1	A	671	ILE
1	C	137	PRO
1	C	687	GLU
1	C	688	VAL
1	C	138	GLU
1	B	700	LEU
1	A	138	GLU
1	C	689	TYR
1	B	139	GLY
1	B	685	PRO
1	C	139	GLY
1	A	136	ARG

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	529/746 (71%)	522 (99%)	7 (1%)	69	81
1	B	529/746 (71%)	520 (98%)	9 (2%)	60	78
1	C	529/746 (71%)	523 (99%)	6 (1%)	73	84
All	All	1587/2238 (71%)	1565 (99%)	22 (1%)	68	80

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	276	VAL
1	A	279	ARG
1	A	282	TYR
1	A	335	ARG
1	A	412	CYS
1	A	528	TRP
1	A	667	VAL
1	B	177	HIS
1	B	394	THR
1	B	412	CYS
1	B	505	ARG
1	B	599	ARG
1	B	624	ARG
1	B	656	SER
1	B	691	ARG
1	B	715	ARG
1	C	136	ARG
1	C	279	ARG
1	C	335	ARG
1	C	592	ARG
1	C	633	CYS
1	C	691	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	A	177	HIS
1	A	255	ASN
1	A	674	ASN
1	A	692	HIS
1	A	706	GLN
1	A	712	HIS

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Mol	Chain	Res	Type
1	B	172	GLN
1	B	216	ASN
1	B	514	GLN
1	B	532	GLN
1	B	580	ASN
1	B	692	HIS
1	B	710	GLN
1	C	153	ASN
1	C	172	GLN
1	C	177	HIS
1	C	181	GLN
1	C	216	ASN
1	C	308	HIS
1	C	311	HIS
1	C	370	GLN
1	C	468	HIS
1	C	507	GLN
1	C	511	ASN
1	C	514	GLN
1	C	518	ASN
1	C	692	HIS

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

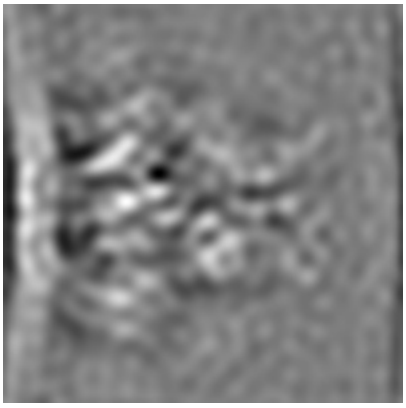
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11123. These allow visual inspection of the internal detail of the map and identification of artifacts.

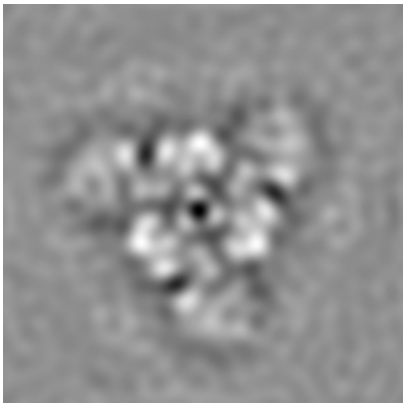
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

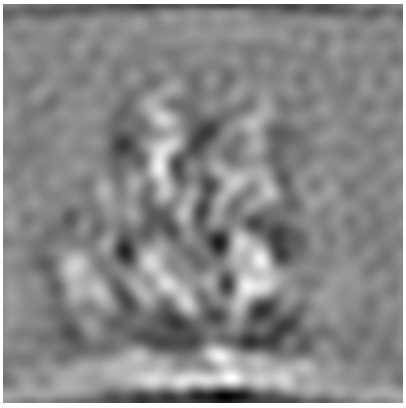
6.1.1 Primary map



X



Y

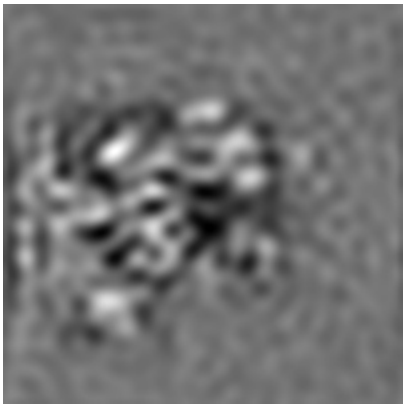


Z

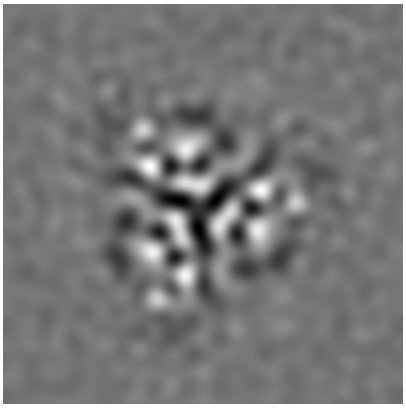
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 50



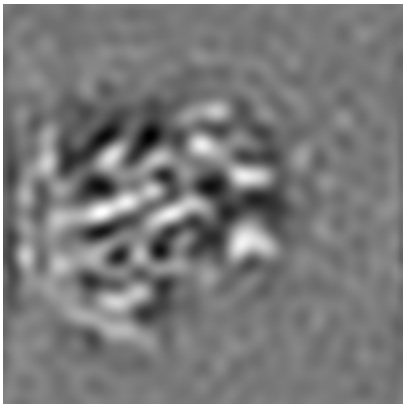
Y Index: 50

Z Index: 50

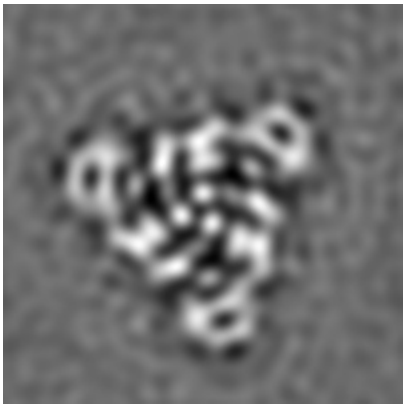
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

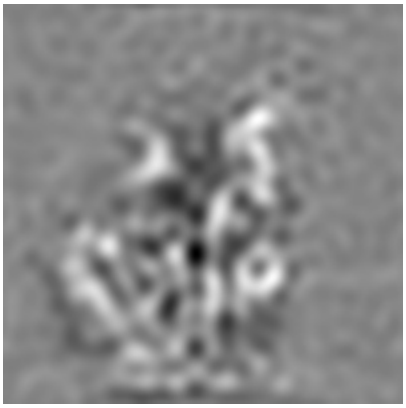
6.3.1 Primary map



X Index: 52



Y Index: 29

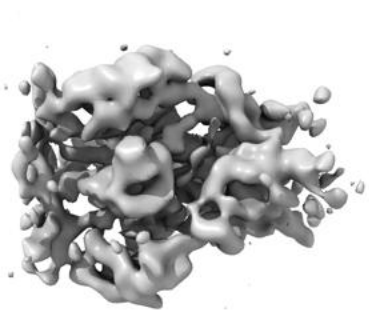


Z Index: 49

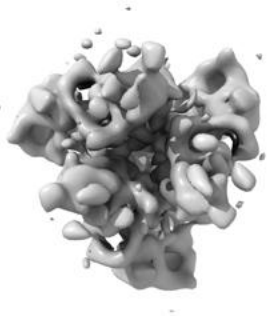
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.056. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

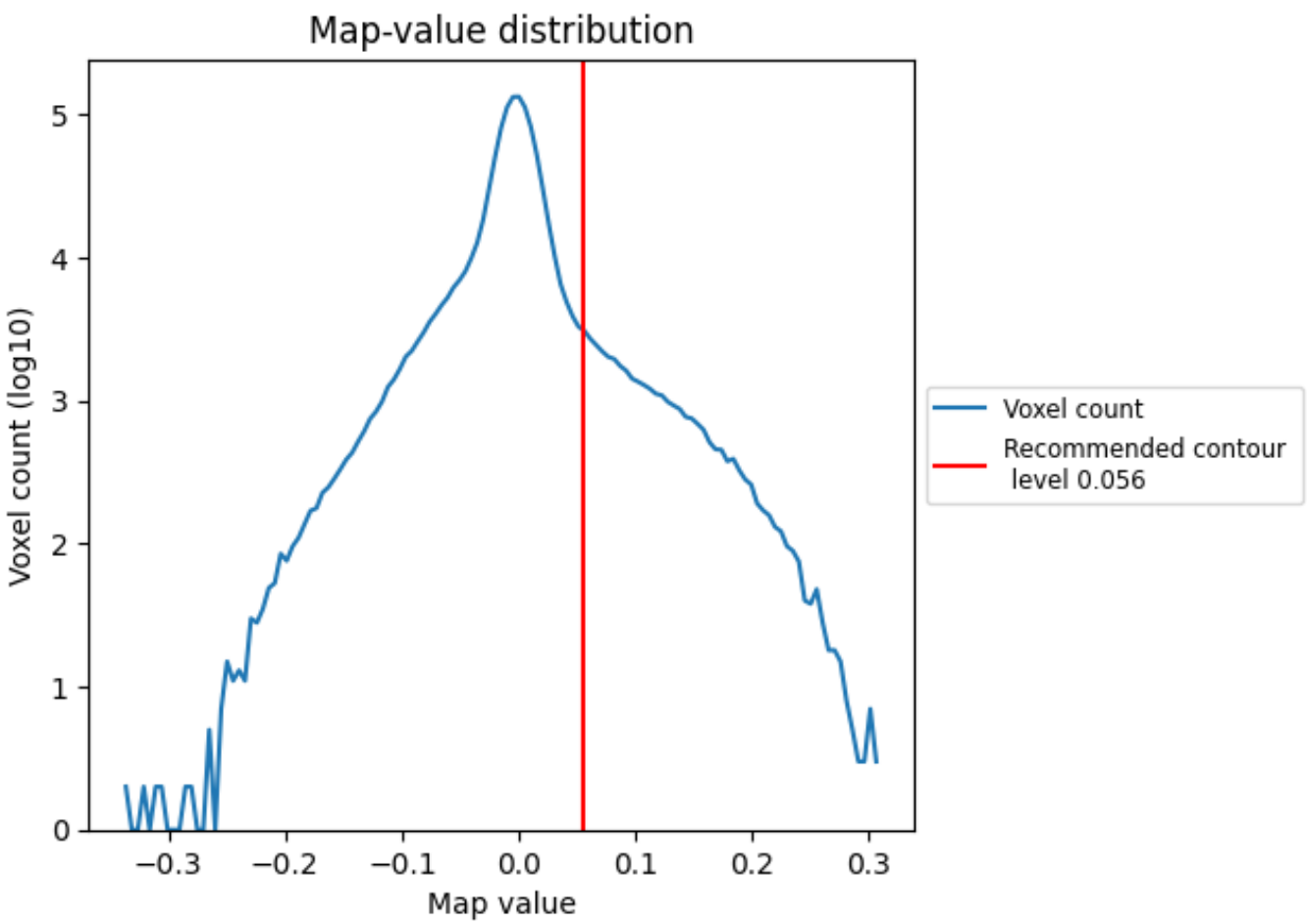
6.5 Mask visualisation (i)

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

7 Map analysis (i)

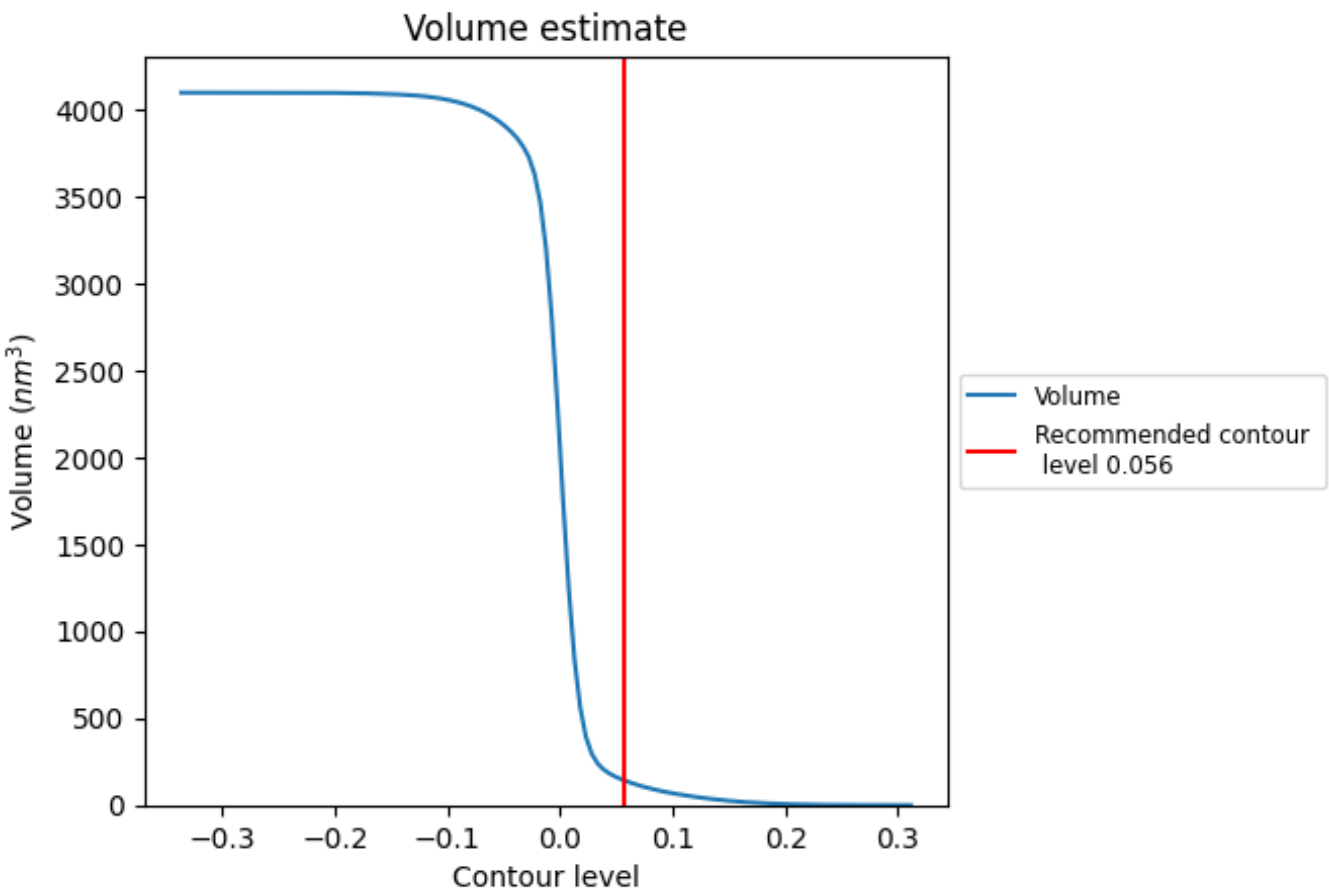
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

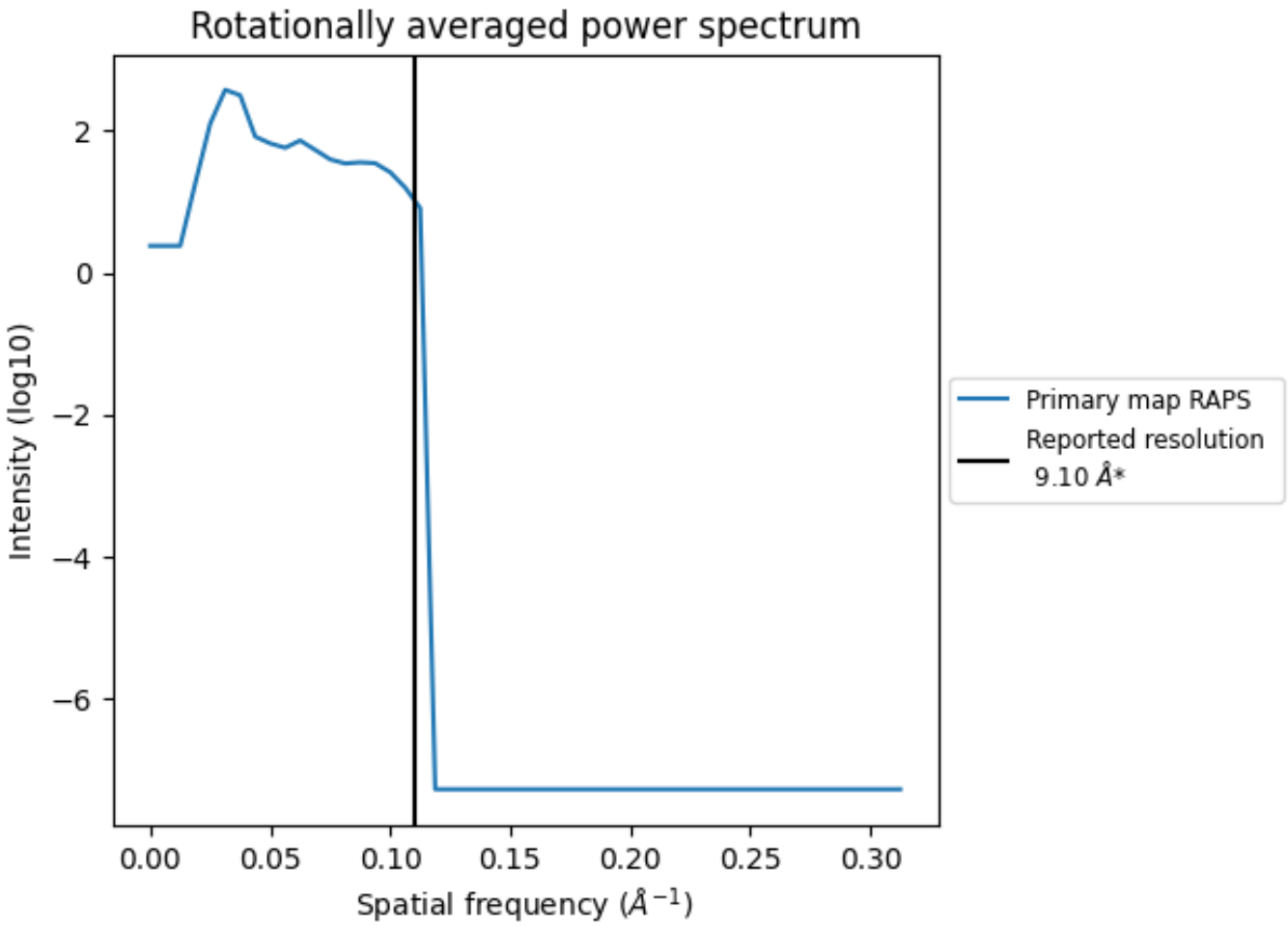
7.2 Volume estimate (i)



The volume at the recommended contour level is 145 nm^3; this corresponds to an approximate mass of 131 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)

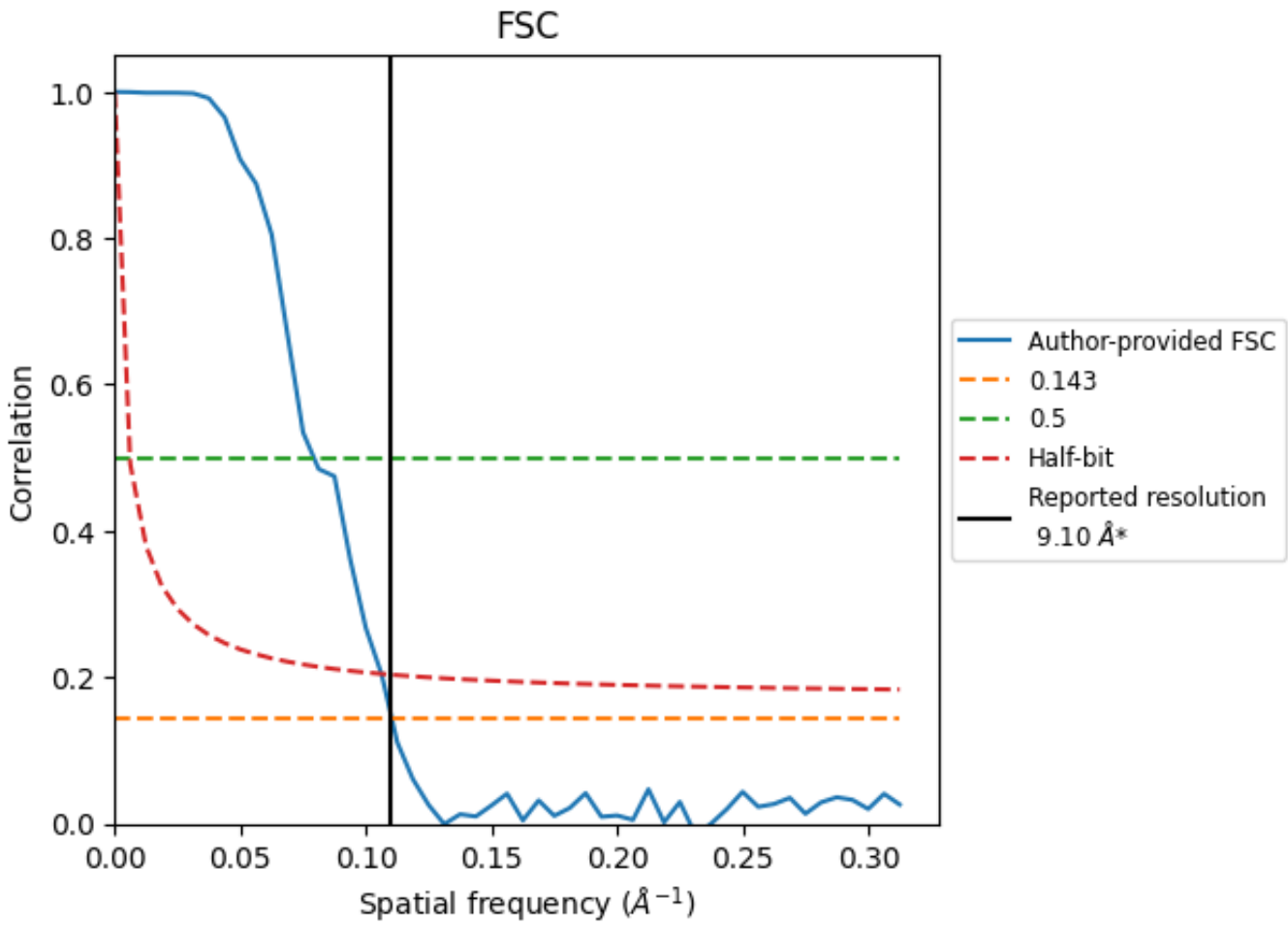


*Reported resolution corresponds to spatial frequency of 0.110 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.110 Å^{-1}

8.2 Resolution estimates (i)

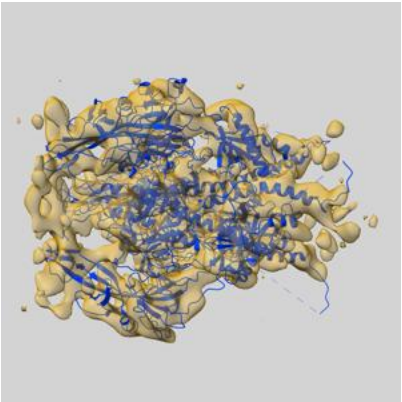
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.10	-	-
Author-provided FSC curve	9.07	12.61	9.43
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

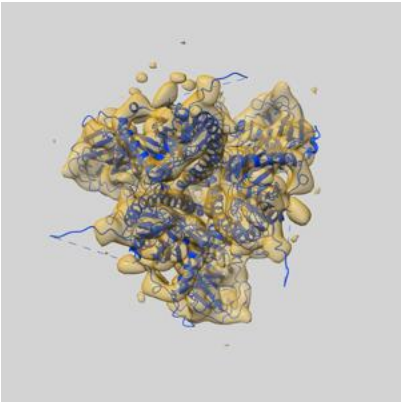
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11123 and PDB model 6Z9M. Per-residue inclusion information can be found in section 3 on page 4.

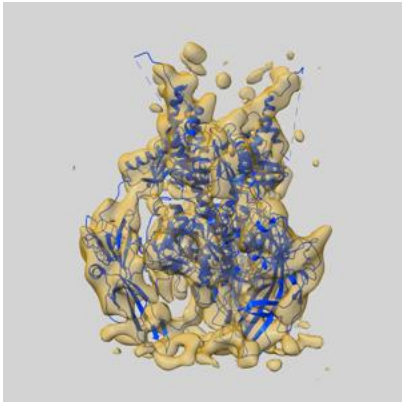
9.1 Map-model overlay (i)



X



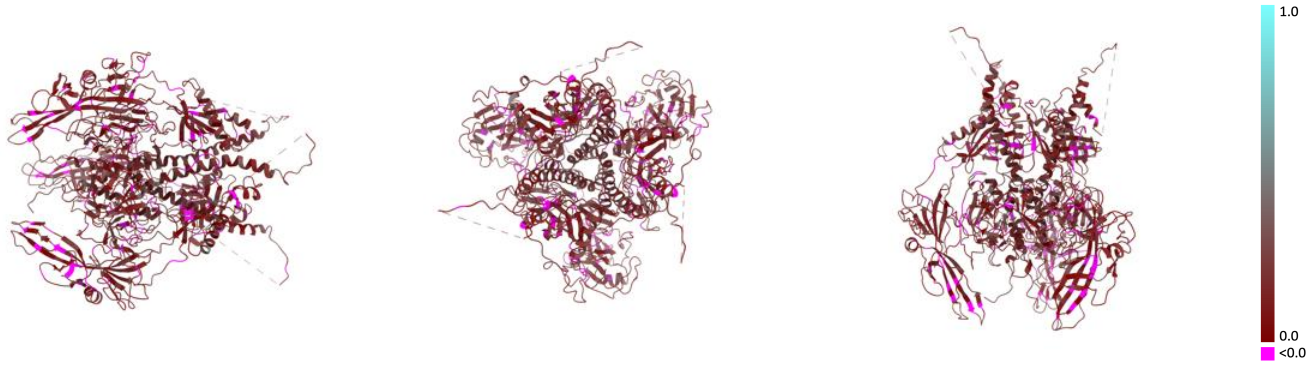
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.056 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.

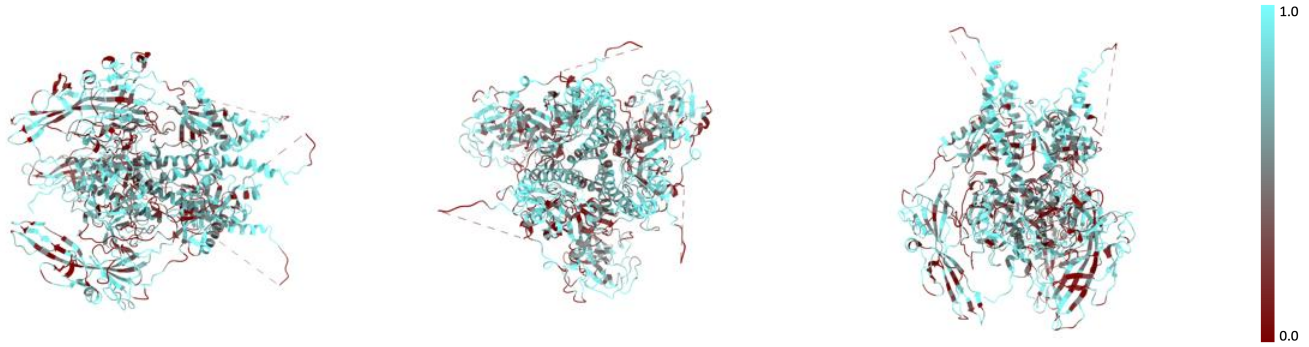
9.2 Q-score mapped to coordinate model (i)



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.

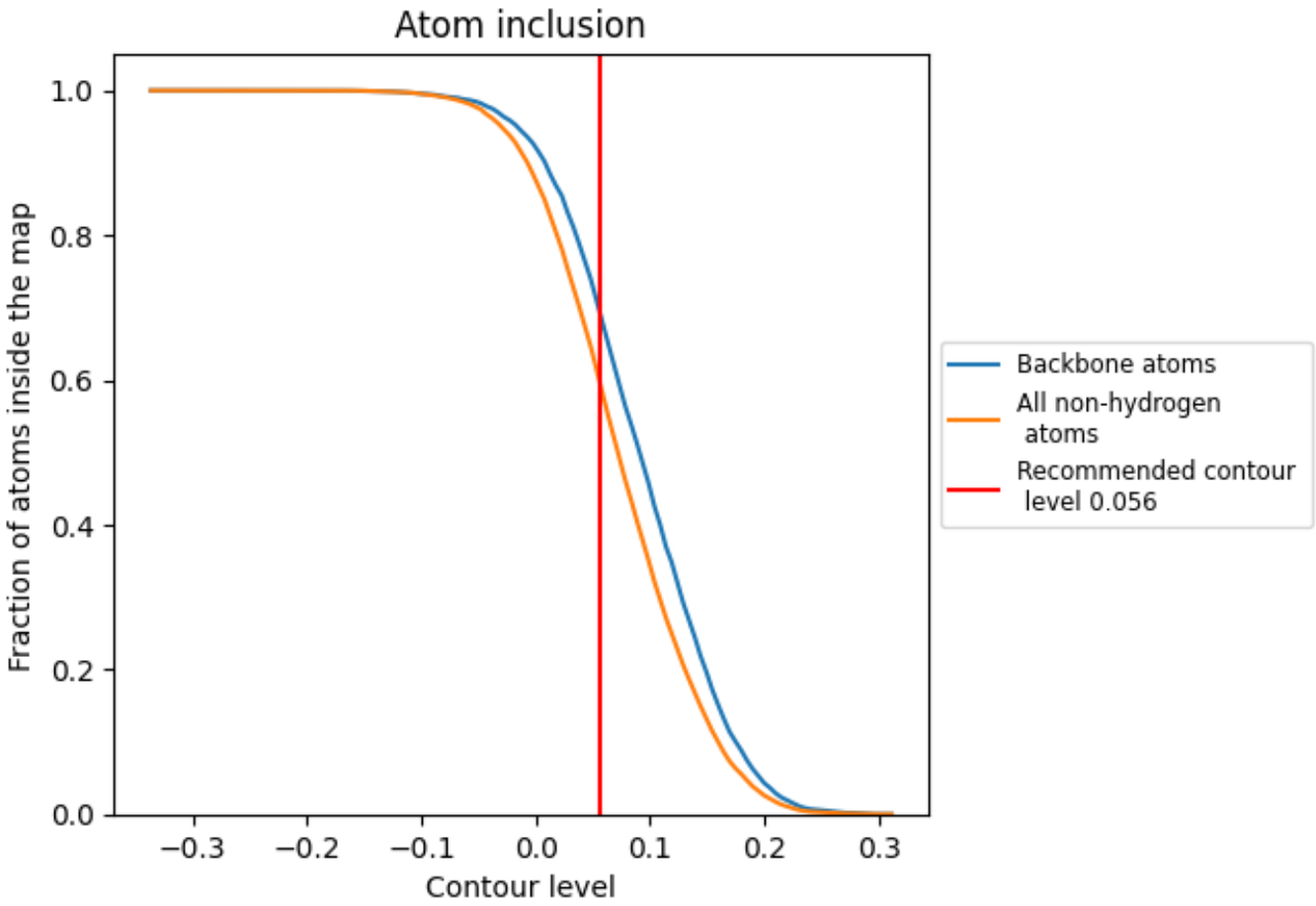
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.056).

9.4 Atom inclusion (i)



At the recommended contour level, 69% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.056) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5972	0.1550
A	0.5998	0.1540
B	0.6024	0.1540
C	0.5895	0.1580