Full wwPDB EM Validation Report ⓘ

Dec 10, 2022 – 09:24 am GMT

PDB ID	:	5FJ5
EMDB ID	:	EMD-3185
Title	:	Structure of the in vitro assembled bacteriophage phi6 polymerase complex
Authors	:	Ilca, S.; Kotecha, A.; Sun, X.; Poranen, M.P.; Stuart, D.I.; Huiskonen, J.T.
Deposited on	:	2015-10-06
Resolution	:	4.80 Å(reported)
Based on initial model	:	4K7H

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

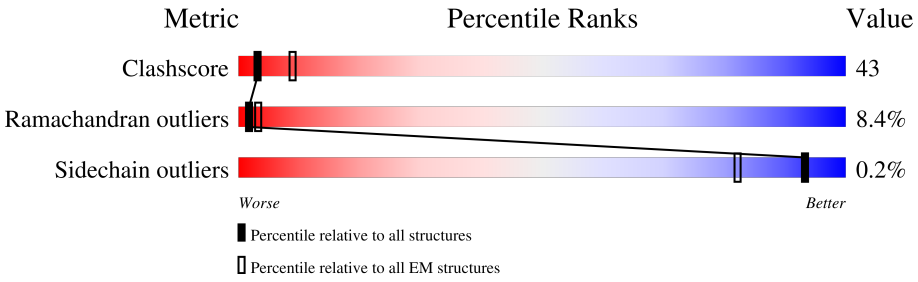
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.80 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	761	30% 33% 59% 7% .
1	B	761	51% 36% 59% 5%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 11840 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 MAJOR INNER PROTEIN P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	761	Total	C	N	O	S	0	0
			5920	3741	1048	1109	22		
1	B	761	Total	C	N	O	S	0	0
			5920	3741	1048	1109	22		

There are 2 discrepancies between the modelled and reference sequences:

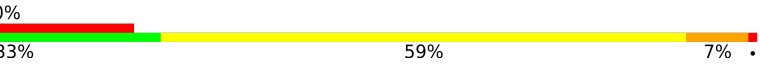
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P11126
B	1	GLY	-	expression tag	UNP P11126

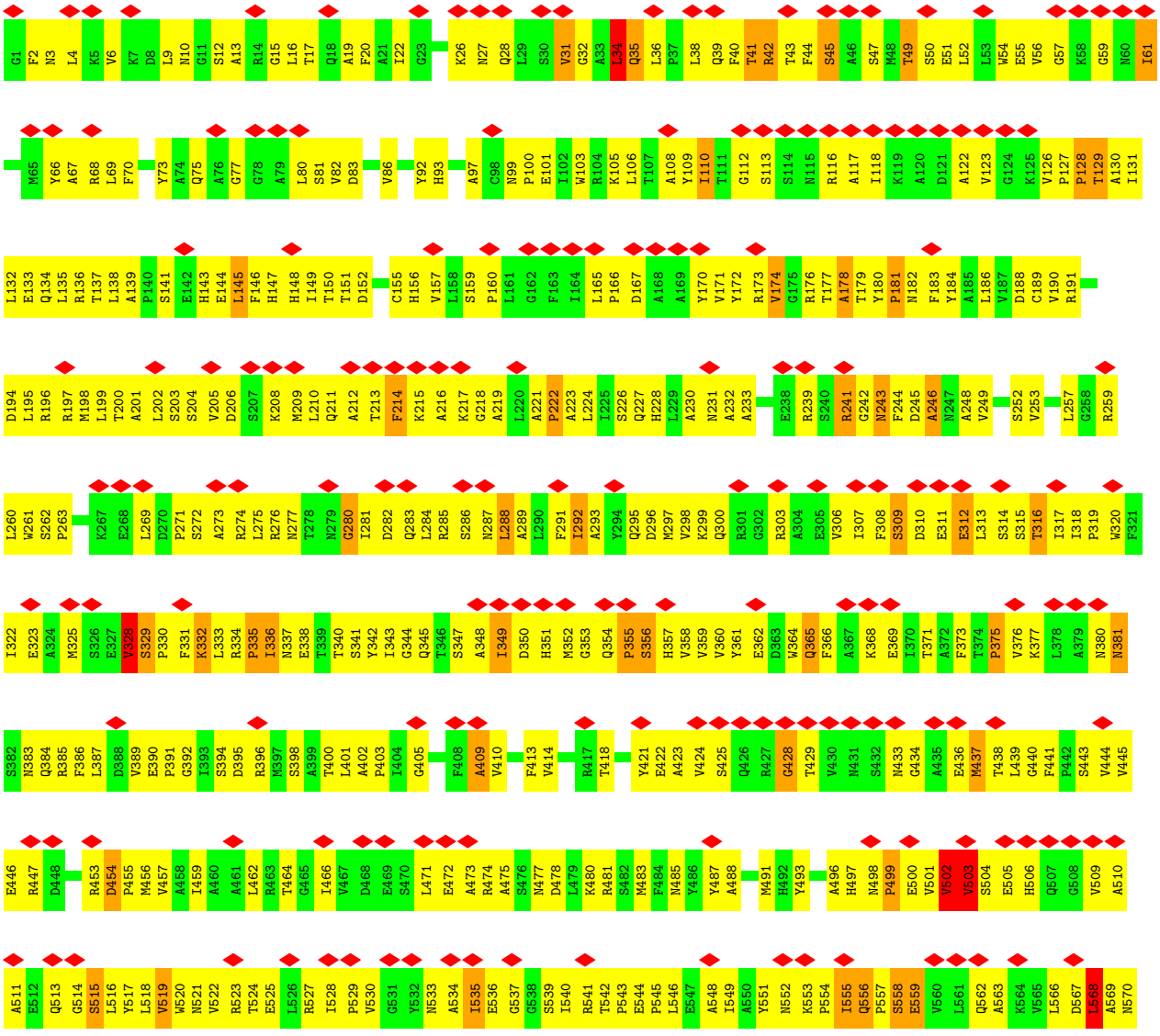
3 Residue-property plots (i)

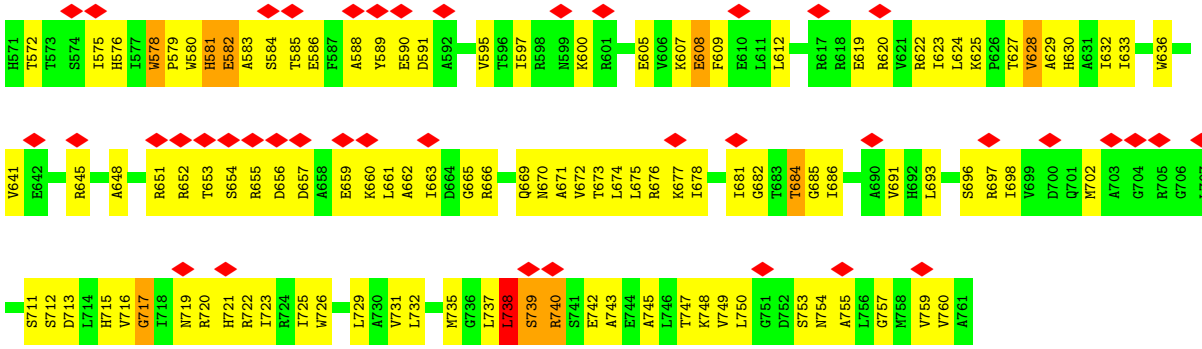
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: MAJOR INNER PROTEIN P1

Chain A:

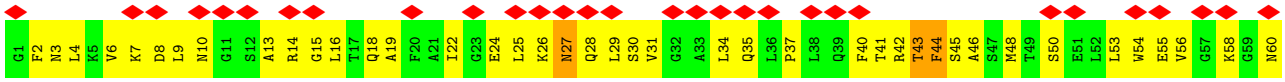


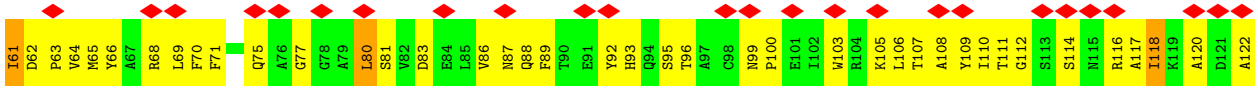


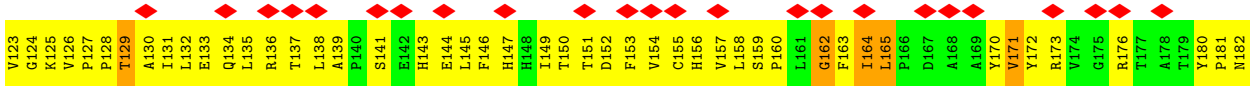


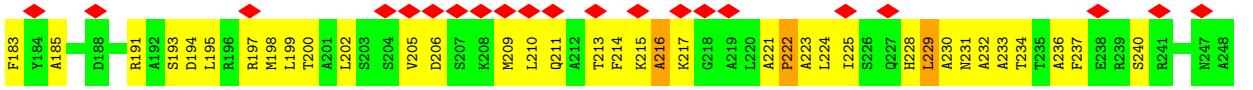
• Molecule 1: MAJOR INNER PROTEIN P1

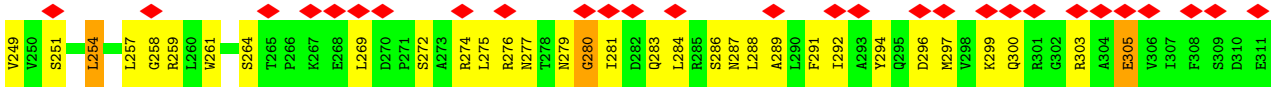
Chain B:

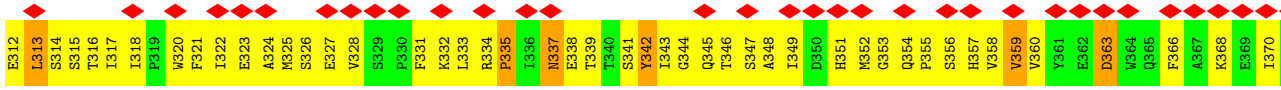


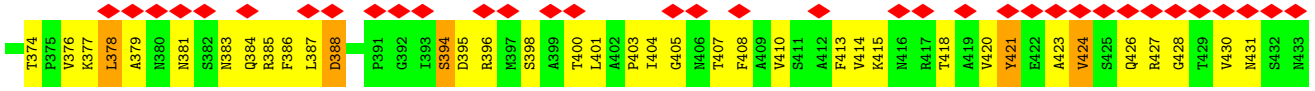


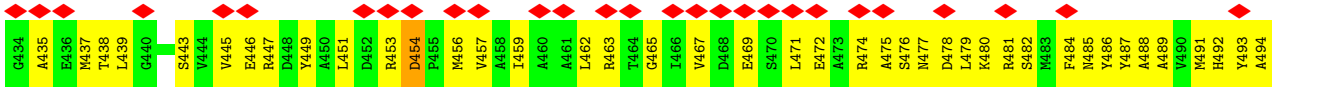


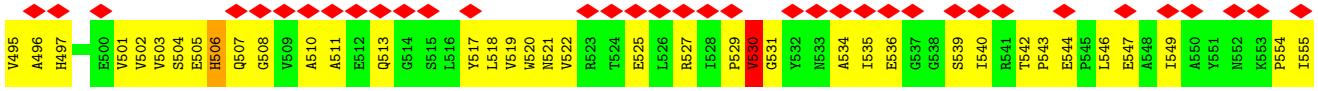


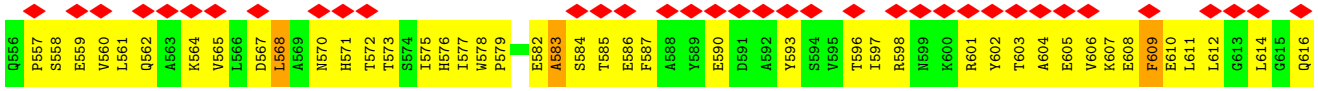


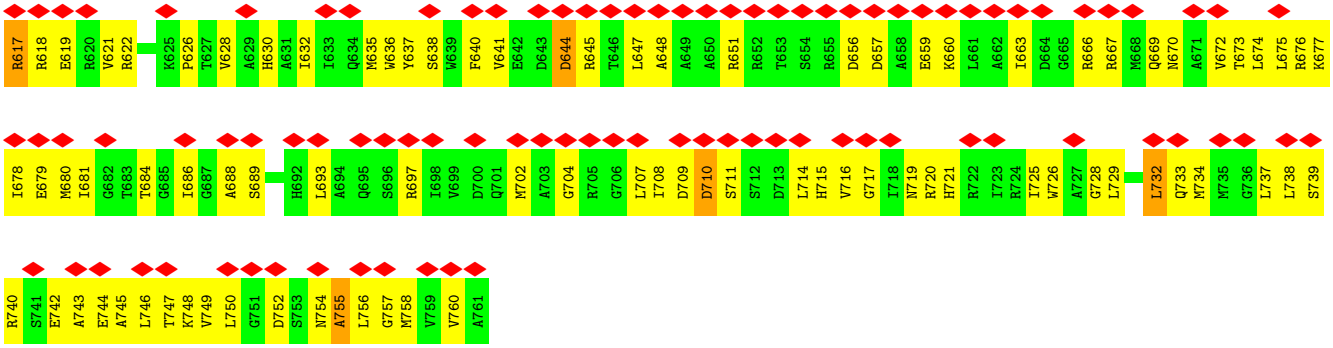











R617 R618 E619 R620 V621 R622 K625 P626 T627 V628 A629 H630 A631 I632 I633 Q634 M635 W636 Y637 S638 W639 F640 V641 E642 D643 D644 R645 T646 L647 A648 A649 A650 R651 R652 T653 S654 R655 D656 D657 A658 E659 K660 L661 A662 I663 D664 G665 R666 R667 M668 Q669 N670 A671 V672 T673 L674 L675 R676 K677
I678 E679 M680 I681 G682 T683 T684 G685 I686 G687 A688 S689 H692 L693 A694 Q695 S696 R697 I698 V699 D700 Q701 M702 A703 G704 R705 G706 L707 I708 D709 D710 S711 S712 D713 L714 H715 V716 G717 I718 N719 R720 H721 R722 I723 R724 I725 W726 A727 G728 L729 L732 Q733 M734 W735 G736 L737 L738 S739
R740 S741 E742 A743 E744 A745 L746 T747 K748 V749 L750 G751 D752 S753 N754 A755 L756 G757 M758 V759 V760 A761

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	4379	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	16	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	37037	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.056	Depositor
Minimum map value	-0.049	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	648.0, 648.0, 648.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality

5.1 Standard geometry

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	0.43	0/6040	0.70	7/8206 (0.1%)
1	B	0.40	0/6040	0.68	1/8206 (0.0%)
All	All	0.41	0/12080	0.69	8/16412 (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	5
1	B	0	3
All	All	0	8

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	128	PRO	CA-C-N	6.74	132.03	117.20
1	A	128	PRO	C-N-CA	6.09	136.93	121.70
1	A	568	LEU	CA-CB-CG	5.92	128.90	115.30
1	A	502	VAL	C-N-CA	5.79	136.19	121.70
1	B	313	LEU	CA-CB-CG	5.67	128.35	115.30
1	A	128	PRO	N-CA-C	5.33	125.97	112.10
1	A	738	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	128	PRO	CA-C-O	-5.16	107.83	120.20

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	328	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	A	34	LEU	Peptide
1	A	35	GLN	Peptide
1	A	365	GLN	Peptide
1	A	437	MET	Peptide
1	B	165	LEU	Peptide
1	B	171	VAL	Peptide
1	B	508	GLY	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	5920	0	5913	515	0
1	B	5920	0	5913	504	0
All	All	11840	0	11826	1011	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 43.

All (1011) 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:42:ARG:HD2	1:B:339:THR:H	1.30	0.96
1:A:117:ALA:H	1:A:221:ALA:H	1.10	0.93
1:B:117:ALA:HB1	1:B:221:ALA:HB1	1.50	0.91
1:B:80:LEU:HD12	1:B:81:SER:H	1.36	0.88
1:A:342:TYR:HA	1:A:559:GLU:HG3	1.57	0.86
1:B:259:ARG:HG2	1:B:269:LEU:HG	1.56	0.85
1:A:108:ALA:HA	1:A:112:GLY:HA3	1.59	0.85
1:B:103:TRP:HE1	1:B:230:ALA:H	1.23	0.85
1:B:400:THR:HG21	1:B:686:ILE:HG12	1.59	0.84
1:B:63:PRO:HB3	1:B:199:LEU:HB2	1.60	0.83
1:B:128:PRO:O	1:B:132:LEU:N	2.12	0.83
1:B:172:TYR:HD1	1:B:578:TRP:HB2	1.42	0.83
1:B:254:LEU:HD11	1:B:294:TYR:HA	1.60	0.82
1:B:733:GLN:HG3	1:B:734:MET:HG2	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:THR:HG21	1:B:547:GLU:HB2	1.62	0.82
1:A:502:VAL:HA	1:A:503:VAL:HG12	1.62	0.81
1:A:4:LEU:HG	1:A:436:GLU:HB2	1.60	0.81
1:A:527:ARG:HG3	1:A:529:PRO:HD3	1.61	0.81
1:B:281:ILE:HA	1:B:284:LEU:HB3	1.63	0.80
1:A:44:PHE:HA	1:A:333:LEU:HA	1.64	0.80
1:B:42:ARG:HD3	1:B:337:ASN:H	1.45	0.80
1:A:582:GLU:O	1:A:625:LYS:NZ	2.15	0.80
1:A:715:HIS:HD2	1:A:716:VAL:HG22	1.43	0.80
1:A:16:LEU:HA	1:A:487:TYR:HE1	1.46	0.80
1:B:135:LEU:O	1:B:139:ALA:N	2.15	0.80
1:A:651:ARG:HB2	1:A:663:ILE:HD11	1.63	0.80
1:B:93:HIS:O	1:B:96:THR:OG1	1.99	0.80
1:A:436:GLU:OE2	1:A:439:LEU:N	2.12	0.80
1:A:528:ILE:HG12	1:A:536:GLU:HB3	1.65	0.79
1:A:173:ARG:HB2	1:A:579:PRO:HG2	1.64	0.79
1:B:53:LEU:HD21	1:B:171:VAL:HG23	1.64	0.79
1:B:756:LEU:HG	1:B:757:GLY:H	1.48	0.79
1:A:117:ALA:N	1:A:221:ALA:H	1.81	0.78
1:A:197:ARG:HA	1:A:200:THR:HG22	1.66	0.78
1:B:407:THR:OG1	1:B:680:MET:SD	2.42	0.77
1:A:581:HIS:O	1:A:583:ALA:N	2.17	0.77
1:A:195:LEU:HA	1:A:198:MET:HB3	1.67	0.77
1:B:408:PHE:HD1	1:B:413:PHE:HZ	1.33	0.77
1:B:609:PHE:HB3	1:B:611:LEU:H	1.49	0.77
1:B:106:LEU:HD13	1:B:154:VAL:HG21	1.67	0.76
1:A:189:CYS:HB3	1:A:323:GLU:HG3	1.67	0.76
1:B:7:LYS:HD3	1:B:531:GLY:H	1.51	0.76
1:A:176:ARG:HH12	1:A:447:ARG:HA	1.49	0.75
1:B:451:LEU:O	1:B:453:ARG:NH1	2.19	0.75
1:A:387:LEU:HG	1:A:572:THR:HG21	1.66	0.75
1:B:647:LEU:HD23	1:B:667:ARG:HG3	1.67	0.75
1:A:588:ALA:HB1	1:A:589:TYR:HB2	1.67	0.75
1:A:200:THR:HA	1:A:203:SER:HB3	1.67	0.75
1:A:480:LYS:HA	1:A:483:MET:HG2	1.68	0.75
1:B:608:GLU:N	1:B:609:PHE:HB2	2.01	0.75
1:B:575:ILE:HA	1:B:576:HIS:HB2	1.68	0.75
1:A:410:VAL:HA	1:A:413:PHE:HB3	1.66	0.74
1:A:148:HIS:O	1:A:151:THR:OG1	2.04	0.74
1:A:208:LYS:O	1:A:211:GLN:NE2	2.19	0.74
1:B:75:GLN:OE1	1:B:447:ARG:NH2	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:ILE:HD13	1:A:738:LEU:HB3	1.69	0.74
1:B:182:ASN:ND2	1:B:296:ASP:OD2	2.21	0.74
1:A:134:GLN:O	1:A:137:THR:OG1	2.06	0.74
1:A:347:SER:HA	1:A:358:VAL:HG13	1.70	0.73
1:A:717:GLY:O	1:A:721:HIS:N	2.16	0.73
1:B:95:SER:OG	1:B:99:ASN:ND2	2.21	0.73
1:B:134:GLN:O	1:B:137:THR:OG1	2.06	0.73
1:A:530:VAL:O	1:A:551:TYR:OH	2.07	0.73
1:A:619:GLU:OE2	1:A:620:ARG:NH1	2.21	0.72
1:B:323:GLU:O	1:B:326:SER:OG	2.05	0.72
1:A:359:VAL:HA	1:A:438:THR:HA	1.71	0.72
1:B:14:ARG:HB2	1:B:465:GLY:HA3	1.70	0.72
1:B:46:ALA:HA	1:B:331:PHE:HA	1.71	0.72
1:B:342:TYR:HB3	1:B:559:GLU:HG2	1.72	0.72
1:A:55:GLU:HG3	1:A:171:VAL:HG22	1.70	0.72
1:A:365:GLN:HA	1:A:562:GLN:HB2	1.70	0.72
1:B:348:ALA:HB3	1:B:356:SER:H	1.55	0.72
1:A:352:MET:N	1:A:353:GLY:HA2	2.05	0.72
1:A:533:ASN:HD22	1:A:543:PRO:HD2	1.55	0.72
1:B:152:ASP:O	1:B:156:HIS:N	2.23	0.72
1:B:714:LEU:HB3	1:B:719:ASN:HD22	1.54	0.72
1:A:132:LEU:HD21	1:A:136:ARG:HH21	1.53	0.72
1:B:644:ASP:OD2	1:B:748:LYS:NZ	2.23	0.71
1:A:272:SER:HB2	1:A:275:LEU:HB3	1.72	0.71
1:B:42:ARG:HD2	1:B:339:THR:N	2.05	0.71
1:A:40:PHE:HB2	1:A:288:LEU:HB3	1.73	0.71
1:B:224:LEU:O	1:B:228:HIS:N	2.24	0.71
1:A:630:HIS:HB2	1:A:737:LEU:HD22	1.73	0.71
1:A:334:ARG:HD3	1:A:338:GLU:HB2	1.72	0.71
1:B:35:GLN:NE2	1:B:504:SER:OG	2.24	0.71
1:A:392:GLY:O	1:A:396:ARG:NH1	2.24	0.70
1:B:231:ASN:O	1:B:234:THR:OG1	2.08	0.70
1:A:172:TYR:CD1	1:A:578:TRP:HB2	2.26	0.70
1:A:73:TYR:O	1:A:77:GLY:N	2.25	0.70
1:B:4:LEU:HD21	1:B:13:ALA:HB3	1.73	0.70
1:B:584:SER:H	1:B:622:ARG:NH1	1.90	0.70
1:A:385:ARG:HD2	1:A:580:TRP:HE1	1.57	0.70
1:A:242:GLY:O	1:A:244:PHE:N	2.24	0.70
1:B:182:ASN:OD1	1:B:183:PHE:N	2.25	0.70
1:A:655:ARG:N	1:A:656:ASP:HB2	2.07	0.69
1:B:163:PHE:HA	1:B:164:ILE:HB	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:ALA:H	1:B:536:GLU:HG3	1.57	0.69
1:B:213:THR:O	1:B:215:LYS:N	2.25	0.69
1:A:31:VAL:HG22	1:A:32:GLY:H	1.58	0.69
1:A:453:ARG:NH2	1:A:474:ARG:O	2.26	0.69
1:A:534:ALA:O	1:A:536:GLU:N	2.26	0.69
1:A:40:PHE:HD2	1:A:289:ALA:HA	1.57	0.69
1:A:97:ALA:HA	1:A:103:TRP:HZ2	1.58	0.69
1:A:45:SER:OG	1:A:332:LYS:HB2	1.93	0.68
1:B:46:ALA:O	1:B:334:ARG:NH2	2.27	0.68
1:A:368:LYS:HG2	1:A:402:ALA:HA	1.76	0.68
1:A:126:VAL:HG13	1:A:166:PRO:HD3	1.75	0.67
1:B:678:ILE:HA	1:B:681:ILE:HD12	1.76	0.67
1:A:51:GLU:HA	1:A:174:VAL:HG21	1.75	0.67
1:A:194:ASP:O	1:A:198:MET:N	2.25	0.67
1:A:315:SER:O	1:A:317:ILE:N	2.28	0.67
1:A:580:TRP:HA	1:A:581:HIS:O	1.95	0.67
1:A:712:SER:O	1:A:715:HIS:ND1	2.22	0.67
1:A:739:SER:OG	1:A:740:ARG:N	2.28	0.67
1:A:283:GLN:O	1:A:286:SER:OG	2.09	0.67
1:B:15:GLY:HA3	1:B:462:LEU:HG	1.76	0.67
1:B:10:ASN:HD22	1:B:29:LEU:HD21	1.59	0.66
1:B:337:ASN:OD1	1:B:338:GLU:N	2.28	0.66
1:B:237:PHE:O	1:B:240:SER:OG	2.14	0.66
1:B:334:ARG:HD3	1:B:335:PRO:HD2	1.77	0.66
1:A:179:THR:N	1:A:180:TYR:HA	2.11	0.66
1:A:456:MET:HA	1:A:459:ILE:HD12	1.78	0.66
1:A:627:THR:O	1:A:629:ALA:N	2.29	0.66
1:A:112:GLY:HA2	1:A:116:ARG:HD3	1.76	0.66
1:B:667:ARG:NH2	1:B:752:ASP:OD2	2.29	0.66
1:B:30:SER:HB2	1:B:517:TYR:CZ	2.31	0.65
1:A:296:ASP:O	1:A:300:GLN:N	2.19	0.65
1:B:349:ILE:HG13	1:B:351:HIS:H	1.61	0.65
1:B:275:LEU:HB2	1:B:312:GLU:HG2	1.78	0.65
1:A:92:TYR:HE2	1:A:150:THR:HG21	1.62	0.65
1:A:283:GLN:NE2	1:A:286:SER:OG	2.30	0.65
1:A:395:ASP:OD1	1:A:396:ARG:N	2.30	0.65
1:B:45:SER:OG	1:B:46:ALA:N	2.29	0.65
1:A:505:GLU:HG2	1:A:515:SER:H	1.61	0.65
1:B:274:ARG:HB3	1:B:312:GLU:HG3	1.79	0.65
1:A:306:VAL:O	1:A:308:PHE:N	2.30	0.65
1:A:655:ARG:H	1:A:656:ASP:HB2	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:TYR:HA	1:B:576:HIS:CD2	2.31	0.65
1:A:358:VAL:H	1:A:437:MET:HB3	1.60	0.65
1:A:691:VAL:HG12	1:A:723:ILE:HG12	1.77	0.65
1:B:18:GLN:HE22	1:B:518:LEU:HB2	1.62	0.64
1:A:535:ILE:HD12	1:A:541:ARG:H	1.61	0.64
1:A:729:LEU:HD21	1:A:743:ALA:HB1	1.79	0.64
1:A:501:VAL:HG23	1:A:502:VAL:HG12	1.78	0.64
1:B:125:LYS:HE2	1:B:163:PHE:HB2	1.80	0.64
1:A:45:SER:HB3	1:A:334:ARG:HB2	1.80	0.64
1:B:66:TYR:HD1	1:B:69:LEU:HD12	1.63	0.64
1:B:506:HIS:HB2	1:B:517:TYR:HE2	1.62	0.64
1:A:57:GLY:H	1:A:170:TYR:HB2	1.62	0.64
1:A:315:SER:OG	1:A:316:THR:N	2.30	0.64
1:B:156:HIS:NE2	1:B:206:ASP:OD2	2.16	0.64
1:B:233:ALA:O	1:B:237:PHE:N	2.30	0.64
1:B:606:VAL:HB	1:B:697:ARG:NH2	2.12	0.64
1:A:520:TRP:H	1:A:542:THR:H	1.46	0.64
1:B:44:PHE:HE2	1:B:181:PRO:HG3	1.63	0.64
1:A:580:TRP:CD2	1:A:581:HIS:HA	2.33	0.64
1:B:420:VAL:HG13	1:B:669:GLN:HE22	1.62	0.64
1:B:132:LEU:HD13	1:B:151:THR:HG22	1.80	0.64
1:A:77:GLY:O	1:A:474:ARG:NH1	2.28	0.64
1:A:358:VAL:N	1:A:437:MET:SD	2.71	0.64
1:A:178:ALA:O	1:A:332:LYS:NZ	2.31	0.63
1:B:83:ASP:HA	1:B:191:ARG:HG2	1.79	0.63
1:B:205:VAL:O	1:B:209:MET:HG2	1.98	0.63
1:A:144:GLU:HG2	1:A:145:LEU:H	1.63	0.63
1:A:554:PRO:O	1:A:556:GLN:N	2.22	0.63
1:B:616:GLN:HG3	1:B:617:ARG:HG2	1.78	0.63
1:A:42:ARG:NH2	1:A:283:GLN:HE21	1.96	0.63
1:B:225:ILE:HA	1:B:228:HIS:HB3	1.79	0.63
1:B:449:TYR:HH	1:B:630:HIS:HD1	0.65	0.63
1:B:485:ASN:OD1	1:B:486:TYR:N	2.32	0.63
1:B:593:TYR:HB3	1:B:604:ALA:HB3	1.80	0.63
1:A:597:ILE:HD11	1:A:600:LYS:HE3	1.81	0.63
1:A:498:ASN:HD22	1:A:500:GLU:HG2	1.64	0.63
1:B:312:GLU:O	1:B:315:SER:N	2.24	0.63
1:B:317:ILE:HG12	1:B:320:TRP:CZ2	2.34	0.63
1:B:370:ILE:HG12	1:B:626:PRO:HG3	1.80	0.63
1:A:4:LEU:H	1:A:436:GLU:HB2	1.64	0.63
1:B:35:GLN:HE21	1:B:502:VAL:HG23	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ARG:HB2	1:B:147:HIS:NE2	2.14	0.63
1:A:375:PRO:HG3	1:A:622:ARG:HE	1.63	0.62
1:B:77:GLY:HA3	1:B:474:ARG:HH22	1.63	0.62
1:B:608:GLU:HA	1:B:609:PHE:O	1.99	0.62
1:A:10:ASN:HA	1:A:17:THR:HG21	1.81	0.62
1:A:666:ARG:HD3	1:A:669:GLN:NE2	2.14	0.62
1:B:2:PHE:O	1:B:439:LEU:N	2.30	0.62
1:B:153:PHE:HB3	1:B:229:LEU:HD21	1.80	0.62
1:B:635:MET:O	1:B:638:SER:OG	2.10	0.62
1:B:408:PHE:HD1	1:B:413:PHE:CZ	2.16	0.62
1:B:472:GLU:O	1:B:476:SER:N	2.30	0.62
1:A:607:LYS:O	1:A:609:PHE:N	2.32	0.62
1:A:715:HIS:CD2	1:A:716:VAL:HG22	2.31	0.62
1:B:123:VAL:HG23	1:B:164:ILE:HG12	1.80	0.62
1:A:360:VAL:HG22	1:A:438:THR:HG22	1.80	0.62
1:B:16:LEU:HD23	1:B:546:LEU:HD21	1.81	0.62
1:B:132:LEU:HA	1:B:135:LEU:HB2	1.82	0.62
1:A:61:ILE:HD11	1:A:199:LEU:HD21	1.80	0.62
1:A:173:ARG:HD3	1:A:579:PRO:HG2	1.82	0.62
1:A:172:TYR:HD1	1:A:578:TRP:HB2	1.65	0.62
1:B:41:THR:N	1:B:286:SER:OG	2.32	0.62
1:B:128:PRO:HA	1:B:131:ILE:HG22	1.81	0.62
1:B:136:ARG:HB2	1:B:147:HIS:CD2	2.35	0.62
1:B:209:MET:O	1:B:213:THR:OG1	2.09	0.62
1:B:421:TYR:HE2	1:B:427:ARG:HH22	1.47	0.62
1:B:637:TYR:HA	1:B:640:PHE:CD2	2.34	0.62
1:A:40:PHE:CD2	1:A:289:ALA:HA	2.35	0.62
1:B:61:ILE:HG12	1:B:152:ASP:HB2	1.82	0.62
1:A:100:PRO:HA	1:A:103:TRP:HD1	1.63	0.61
1:A:190:VAL:HG12	1:A:323:GLU:HB2	1.81	0.61
1:A:502:VAL:HA	1:A:503:VAL:CG1	2.28	0.61
1:B:481:ARG:HA	1:B:484:PHE:CE2	2.34	0.61
1:A:287:ASN:O	1:A:289:ALA:N	2.33	0.61
1:A:349:ILE:HG13	1:A:350:ASP:H	1.65	0.61
1:A:666:ARG:HG3	1:A:670:ASN:HD21	1.65	0.61
1:B:630:HIS:NE2	1:B:738:LEU:HA	2.15	0.61
1:A:173:ARG:HE	1:A:566:LEU:HD21	1.65	0.61
1:A:183:PHE:HA	1:A:186:LEU:HD13	1.82	0.61
1:B:153:PHE:CZ	1:B:202:LEU:HB3	2.36	0.61
1:B:745:ALA:O	1:B:748:LYS:HG2	2.01	0.61
1:A:128:PRO:N	1:A:129:THR:HB	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:GLU:HA	1:A:516:LEU:HB3	1.83	0.61
1:A:713:ASP:HA	1:A:715:HIS:CE1	2.36	0.61
1:B:231:ASN:OD1	1:B:232:ALA:N	2.34	0.61
1:A:296:ASP:HA	1:A:299:LYS:HB3	1.82	0.60
1:B:388:ASP:HA	1:B:572:THR:HG21	1.82	0.60
1:A:9:LEU:HA	1:A:12:SER:HB3	1.84	0.60
1:A:127:PRO:HG2	1:A:130:ALA:HB2	1.83	0.60
1:A:176:ARG:NH2	1:A:447:ARG:HD2	2.17	0.60
1:B:75:GLN:HB3	1:B:447:ARG:HH22	1.66	0.60
1:A:135:LEU:HD12	1:A:151:THR:HG22	1.84	0.60
1:A:214:PHE:HA	1:A:215:LYS:O	2.02	0.60
1:A:666:ARG:HA	1:A:669:GLN:HE22	1.65	0.60
1:A:754:ASN:N	1:A:755:ALA:HA	2.16	0.60
1:B:163:PHE:HB3	1:B:164:ILE:HG22	1.84	0.60
1:A:493:TYR:CE2	1:A:549:ILE:HG12	2.36	0.60
1:B:543:PRO:HG2	1:B:544:GLU:HG3	1.83	0.60
1:B:636:TRP:HB3	1:B:640:PHE:CZ	2.37	0.60
1:A:13:ALA:HB1	1:A:16:LEU:HD12	1.83	0.60
1:A:4:LEU:N	1:A:436:GLU:HB2	2.17	0.60
1:B:37:PRO:HA	1:B:502:VAL:HG12	1.84	0.60
1:B:131:ILE:O	1:B:134:GLN:HB3	2.02	0.60
1:B:715:HIS:HB3	1:B:720:ARG:NH2	2.17	0.60
1:B:744:GLU:O	1:B:747:THR:OG1	2.17	0.60
1:A:472:GLU:HB3	1:A:475:ALA:HB3	1.83	0.60
1:B:598:ARG:NH1	1:B:710:ASP:OD1	2.35	0.60
1:A:116:ARG:HB2	1:A:222:PRO:HA	1.83	0.59
1:A:181:PRO:HD3	1:A:485:ASN:HD21	1.67	0.59
1:A:360:VAL:HG13	1:A:438:THR:HG23	1.84	0.59
1:A:671:ALA:O	1:A:674:LEU:HG	2.01	0.59
1:B:583:ALA:N	1:B:584:SER:HA	2.16	0.59
1:A:715:HIS:CD2	1:A:716:VAL:H	2.21	0.59
1:B:521:ASN:HA	1:B:540:ILE:HB	1.84	0.59
1:B:732:LEU:HG	1:B:738:LEU:HD22	1.83	0.59
1:A:660:LYS:O	1:A:663:ILE:HG13	2.02	0.59
1:A:678:ILE:HG21	1:A:725:ILE:HG23	1.85	0.59
1:B:8:ASP:OD1	1:B:9:LEU:N	2.35	0.59
1:B:288:LEU:O	1:B:291:PHE:HB3	2.03	0.59
1:B:159:SER:OG	1:B:162:GLY:O	2.21	0.59
1:B:656:ASP:HB3	1:B:659:GLU:HG2	1.84	0.59
1:B:264:SER:HB3	1:B:269:LEU:HD22	1.85	0.59
1:B:279:ASN:O	1:B:281:ILE:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:ASP:OD1	1:B:561:LEU:HD22	2.03	0.59
1:B:471:LEU:HB3	1:B:475:ALA:HB3	1.85	0.59
1:A:173:ARG:HB2	1:A:579:PRO:CG	2.33	0.59
1:A:306:VAL:HG12	1:A:309:SER:HA	1.85	0.59
1:B:145:LEU:HD12	1:B:146:PHE:N	2.18	0.59
1:B:332:LYS:HE2	1:B:334:ARG:HH12	1.67	0.59
1:B:478:ASP:OD1	1:B:479:LEU:N	2.36	0.59
1:A:505:GLU:OE2	1:A:515:SER:OG	2.15	0.58
1:A:661:LEU:O	1:A:665:GLY:N	2.35	0.58
1:A:144:GLU:O	1:A:146:PHE:N	2.36	0.58
1:A:445:VAL:HG13	1:A:455:PRO:HG3	1.85	0.58
1:A:61:ILE:HG13	1:A:66:TYR:HE2	1.68	0.58
1:A:347:SER:H	1:A:554:PRO:HB3	1.68	0.58
1:A:589:TYR:OH	1:A:740:ARG:NE	2.26	0.58
1:B:479:LEU:O	1:B:482:SER:OG	2.18	0.58
1:A:395:ASP:O	1:A:398:SER:OG	2.14	0.58
1:A:669:GLN:HA	1:A:672:VAL:HB	1.86	0.58
1:B:562:GLN:HG2	1:B:564:LYS:H	1.68	0.58
1:B:746:LEU:HA	1:B:749:VAL:HG22	1.85	0.58
1:A:180:TYR:CE1	1:A:331:PHE:HA	2.38	0.58
1:A:740:ARG:N	1:A:742:GLU:OE1	2.36	0.58
1:B:476:SER:O	1:B:480:LYS:HG2	2.04	0.58
1:A:530:VAL:HG13	1:A:551:TYR:CZ	2.38	0.58
1:A:568:LEU:HD12	1:A:569:ALA:N	2.19	0.58
1:B:407:THR:HG23	1:B:408:PHE:CD2	2.39	0.58
1:B:424:VAL:HG23	1:B:430:VAL:HA	1.85	0.58
1:B:617:ARG:N	1:B:618:ARG:HA	2.18	0.58
1:A:284:LEU:HG	1:A:287:ASN:ND2	2.19	0.58
1:B:170:TYR:HA	1:B:576:HIS:CG	2.39	0.58
1:B:506:HIS:HB2	1:B:517:TYR:CE2	2.39	0.58
1:B:506:HIS:HA	1:B:507:GLN:HB3	1.86	0.58
1:A:47:SER:HB3	1:A:332:LYS:HD3	1.84	0.58
1:A:358:VAL:H	1:A:437:MET:CB	2.17	0.58
1:B:443:SER:HA	1:B:446:GLU:HG2	1.85	0.58
1:B:587:PHE:HB3	1:B:621:VAL:HG23	1.85	0.58
1:A:210:LEU:HD22	1:A:228:HIS:ND1	2.18	0.57
1:A:343:ILE:N	1:A:559:GLU:OE2	2.34	0.57
1:B:182:ASN:H	1:B:185:ALA:HB3	1.69	0.57
1:B:467:VAL:HG13	1:B:469:GLU:HB2	1.86	0.57
1:A:4:LEU:O	1:A:436:GLU:N	2.37	0.57
1:B:194:ASP:OD1	1:B:195:LEU:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:669:GLN:HA	1:B:672:VAL:HG12	1.85	0.57
1:A:661:LEU:HD22	1:B:105:LYS:HD2	1.84	0.57
1:B:75:GLN:OE1	1:B:481:ARG:NH1	2.37	0.57
1:B:560:VAL:O	1:B:561:LEU:HG	2.04	0.57
1:B:324:ALA:HB1	1:B:333:LEU:HB2	1.86	0.57
1:A:97:ALA:HA	1:A:103:TRP:CZ2	2.37	0.57
1:A:375:PRO:HB2	1:A:385:ARG:HD3	1.86	0.57
1:A:702:MET:HG3	1:A:711:SER:HB3	1.86	0.57
1:A:732:LEU:HG	1:A:738:LEU:HD11	1.86	0.57
1:B:216:ALA:HA	1:B:217:LYS:C	2.25	0.57
1:A:433:ASN:HB3	1:A:434:GLY:CA	2.35	0.57
1:A:200:THR:O	1:A:204:SER:N	2.37	0.57
1:B:607:LYS:HB2	1:B:608:GLU:O	2.05	0.57
1:B:693:LEU:HD23	1:B:697:ARG:HH11	1.70	0.57
1:B:707:LEU:HD12	1:B:708:ILE:HG23	1.86	0.57
1:B:56:VAL:HG23	1:B:170:TYR:HB3	1.86	0.57
1:B:87:ASN:OD1	1:B:88:GLN:N	2.37	0.57
1:B:609:PHE:HB3	1:B:611:LEU:N	2.19	0.57
1:A:67:ALA:HA	1:A:70:PHE:HD2	1.68	0.56
1:A:179:THR:HG21	1:A:488:ALA:HB1	1.87	0.56
1:A:544:GLU:CD	1:A:546:LEU:H	2.08	0.56
1:B:489:ALA:HA	1:B:492:HIS:CE1	2.40	0.56
1:A:354:GLN:NE2	1:A:525:GLU:OE1	2.38	0.56
1:A:400:THR:HG21	1:A:731:VAL:HG21	1.87	0.56
1:B:70:PHE:CE1	1:B:145:LEU:HD13	2.40	0.56
1:A:52:LEU:O	1:A:174:VAL:HG13	2.05	0.56
1:A:342:TYR:O	1:A:362:GLU:HG2	2.05	0.56
1:B:153:PHE:HZ	1:B:202:LEU:HD23	1.70	0.56
1:B:345:GLN:HB2	1:B:554:PRO:HA	1.87	0.56
1:B:377:LYS:HB2	1:B:385:ARG:HG2	1.86	0.56
1:B:586:GLU:O	1:B:622:ARG:NH2	2.38	0.56
1:B:647:LEU:HD21	1:B:663:ILE:HA	1.88	0.56
1:B:199:LEU:HD23	1:B:202:LEU:HD22	1.88	0.56
1:A:557:PRO:HB2	1:A:559:GLU:HB2	1.87	0.56
1:A:591:ASP:OD2	1:A:726:TRP:NE1	2.38	0.56
1:B:738:LEU:HD23	1:B:742:GLU:HG2	1.86	0.56
1:B:651:ARG:HG2	1:B:663:ILE:HD13	1.88	0.56
1:B:125:LYS:NZ	1:B:158:LEU:O	2.38	0.56
1:B:291:PHE:O	1:B:294:TYR:HB3	2.05	0.56
1:A:422:GLU:OE2	1:B:116:ARG:HB3	2.06	0.56
1:A:473:ALA:O	1:A:477:ASN:ND2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:ASP:OD1	1:B:568:LEU:N	2.34	0.56
1:A:93:HIS:NE2	1:A:202:LEU:HD13	2.21	0.56
1:A:337:ASN:ND2	1:A:496:ALA:HB2	2.21	0.56
1:B:43:THR:HG21	1:B:289:ALA:H	1.70	0.56
1:A:558:SER:N	1:A:559:GLU:OE1	2.39	0.55
1:B:43:THR:OG1	1:B:288:LEU:N	2.35	0.55
1:A:274:ARG:HH12	1:A:312:GLU:HG3	1.71	0.55
1:A:344:GLY:N	1:A:361:TYR:O	2.27	0.55
1:A:196:ARG:HD3	1:A:328:VAL:HG12	1.89	0.55
1:B:344:GLY:HA2	1:B:555:ILE:HG13	1.88	0.55
1:B:456:MET:HA	1:B:459:ILE:HD12	1.87	0.55
1:B:640:PHE:CZ	1:B:674:LEU:HD21	2.41	0.55
1:A:291:PHE:HZ	1:A:517:TYR:HA	1.71	0.55
1:A:568:LEU:HD12	1:A:569:ALA:H	1.71	0.55
1:B:93:HIS:CE1	1:B:96:THR:HA	2.41	0.55
1:B:597:ILE:O	1:B:602:TYR:OH	2.17	0.55
1:B:4:LEU:O	1:B:437:MET:N	2.40	0.55
1:A:196:ARG:HH11	1:A:328:VAL:HG12	1.72	0.55
1:A:210:LEU:HG	1:A:213:THR:HA	1.88	0.55
1:A:585:THR:N	1:A:586:GLU:HB2	2.22	0.55
1:B:68:ARG:NH1	1:B:327:GLU:O	2.38	0.55
1:B:272:SER:O	1:B:276:ARG:HG3	2.06	0.55
1:A:533:ASN:ND2	1:A:543:PRO:HD2	2.21	0.55
1:A:605:GLU:N	1:A:605:GLU:OE1	2.40	0.55
1:B:3:ASN:HB3	1:B:438:THR:HA	1.88	0.55
1:A:42:ARG:NH2	1:A:283:GLN:O	2.40	0.54
1:A:42:ARG:CZ	1:A:283:GLN:HE21	2.20	0.54
1:A:45:SER:HB2	1:A:334:ARG:CZ	2.38	0.54
1:A:586:GLU:HB3	1:A:623:ILE:HG22	1.89	0.54
1:A:693:LEU:O	1:A:697:ARG:HG2	2.08	0.54
1:B:193:SER:HA	1:B:328:VAL:HG11	1.89	0.54
1:B:249:VAL:HG23	1:B:318:ILE:HG23	1.90	0.54
1:B:347:SER:HB3	1:B:355:PRO:HB3	1.88	0.54
1:A:42:ARG:NH2	1:A:286:SER:OG	2.40	0.54
1:A:214:PHE:HA	1:A:215:LYS:C	2.28	0.54
1:B:312:GLU:C	1:B:315:SER:H	2.10	0.54
1:B:358:VAL:HG11	1:B:437:MET:SD	2.47	0.54
1:B:666:ARG:O	1:B:669:GLN:HG2	2.07	0.54
1:A:446:GLU:HG3	1:A:627:THR:HB	1.90	0.54
1:B:467:VAL:HG22	1:B:469:GLU:H	1.71	0.54
1:A:22:ILE:HG21	1:A:515:SER:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:PHE:HE1	1:A:629:ALA:HB2	1.73	0.54
1:B:132:LEU:O	1:B:136:ARG:N	2.40	0.54
1:A:15:GLY:HA2	1:A:20:PHE:CG	2.42	0.54
1:A:350:ASP:O	1:A:352:MET:N	2.36	0.54
1:A:558:SER:OG	1:A:559:GLU:N	2.40	0.54
1:B:35:GLN:HB3	1:B:502:VAL:HB	1.88	0.54
1:B:42:ARG:NH1	1:B:339:THR:O	2.40	0.54
1:A:272:SER:HB2	1:A:275:LEU:CB	2.38	0.54
1:B:501:VAL:HG11	1:B:518:LEU:HD13	1.89	0.54
1:B:702:MET:HA	1:B:708:ILE:HD12	1.90	0.54
1:A:349:ILE:HD13	1:A:357:HIS:H	1.71	0.54
1:A:572:THR:HA	1:A:575:ILE:O	2.08	0.54
1:B:100:PRO:HA	1:B:103:TRP:CE3	2.43	0.54
1:B:354:GLN:HE21	1:B:431:ASN:HB3	1.73	0.53
1:A:144:GLU:HB2	1:A:147:HIS:HB3	1.90	0.53
1:A:165:LEU:N	1:A:166:PRO:HD2	2.23	0.53
1:B:143:HIS:HB2	1:B:146:PHE:CE2	2.43	0.53
1:A:99:ASN:ND2	1:A:101:GLU:OE2	2.41	0.53
1:B:443:SER:O	1:B:446:GLU:HG2	2.08	0.53
1:B:50:SER:H	1:B:176:ARG:HB3	1.74	0.53
1:B:124:GLY:H	1:B:164:ILE:HG21	1.73	0.53
1:A:42:ARG:HH21	1:A:286:SER:HG	1.55	0.53
1:B:272:SER:O	1:B:276:ARG:N	2.42	0.53
1:B:354:GLN:HE22	1:B:431:ASN:HD22	1.57	0.53
1:A:42:ARG:H	1:A:336:ILE:HD13	1.73	0.53
1:A:383:ASN:O	1:A:385:ARG:N	2.38	0.53
1:B:394:SER:OG	1:B:395:ASP:N	2.41	0.53
1:B:404:ILE:HG23	1:B:408:PHE:CD2	2.44	0.53
1:A:26:LYS:HE3	1:A:509:VAL:HG22	1.91	0.53
1:A:527:ARG:HH11	1:A:528:ILE:H	1.56	0.53
1:B:275:LEU:HD13	1:B:315:SER:HB2	1.91	0.53
1:A:170:TYR:HD1	1:A:576:HIS:CE1	2.27	0.53
1:A:285:ARG:O	1:A:288:LEU:HD13	2.09	0.53
1:A:310:ASP:OD2	1:A:313:LEU:N	2.42	0.53
1:B:42:ARG:HB2	1:B:339:THR:HA	1.91	0.53
1:B:86:VAL:HG21	1:B:191:ARG:HG3	1.90	0.53
1:B:345:GLN:CB	1:B:554:PRO:HA	2.39	0.53
1:A:182:ASN:ND2	1:A:184:TYR:HB2	2.23	0.53
1:B:128:PRO:O	1:B:131:ILE:N	2.42	0.53
1:B:709:ASP:O	1:B:711:SER:N	2.41	0.53
1:B:733:GLN:OE1	1:B:740:ARG:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:PHE:H	1:A:439:LEU:HD11	1.74	0.53
1:A:44:PHE:HE1	1:A:180:TYR:H	1.57	0.53
1:A:365:GLN:OE1	1:A:563:ALA:HB3	2.09	0.53
1:A:368:LYS:HE2	1:A:402:ALA:HA	1.91	0.53
1:A:702:MET:HB3	1:A:708:ILE:HA	1.91	0.53
1:B:467:VAL:HG22	1:B:469:GLU:N	2.24	0.53
1:B:570:ASN:O	1:B:573:THR:HG22	2.08	0.53
1:B:616:GLN:O	1:B:617:ARG:HB2	2.08	0.53
1:A:143:HIS:CD2	1:A:146:PHE:HE2	2.26	0.52
1:A:585:THR:HB	1:A:586:GLU:HA	1.91	0.52
1:A:641:VAL:O	1:A:645:ARG:HG2	2.08	0.52
1:B:16:LEU:HD13	1:B:462:LEU:HD21	1.91	0.52
1:B:459:ILE:O	1:B:463:ARG:HG3	2.09	0.52
1:B:571:HIS:O	1:B:575:ILE:HG23	2.09	0.52
1:B:610:GLU:C	1:B:612:LEU:H	2.12	0.52
1:A:34:LEU:HG	1:A:35:GLN:HG3	1.89	0.52
1:A:231:ASN:OD1	1:A:232:ALA:N	2.42	0.52
1:A:287:ASN:C	1:A:289:ALA:H	2.13	0.52
1:A:630:HIS:N	1:A:737:LEU:HD13	2.24	0.52
1:B:377:LYS:HG3	1:B:384:GLN:O	2.10	0.52
1:B:487:TYR:O	1:B:491:MET:HG2	2.10	0.52
1:A:519:VAL:HG22	1:A:542:THR:N	2.25	0.52
1:A:223:ALA:O	1:A:227:GLN:N	2.34	0.52
1:A:472:GLU:HB3	1:A:475:ALA:CB	2.40	0.52
1:B:80:LEU:CD1	1:B:81:SER:H	2.14	0.52
1:B:133:GLU:OE2	1:B:136:ARG:HD2	2.09	0.52
1:B:114:SER:HB2	1:B:223:ALA:HB2	1.90	0.52
1:B:610:GLU:OE2	1:B:614:LEU:N	2.40	0.52
1:A:345:GLN:HG2	1:A:555:ILE:HG12	1.91	0.52
1:A:732:LEU:HD21	1:A:738:LEU:HD21	1.91	0.52
1:A:38:LEU:H	1:A:501:VAL:HG21	1.73	0.52
1:B:42:ARG:HH11	1:B:339:THR:N	2.07	0.52
1:B:378:LEU:HD12	1:B:379:ALA:N	2.24	0.52
1:B:400:THR:O	1:B:403:PRO:HD2	2.10	0.52
1:B:575:ILE:HB	1:B:576:HIS:O	2.09	0.52
1:A:524:THR:HG21	1:A:540:ILE:HG12	1.92	0.52
1:B:346:THR:OG1	1:B:359:VAL:HG11	2.10	0.52
1:B:445:VAL:O	1:B:449:TYR:HB3	2.09	0.52
1:B:35:GLN:NE2	1:B:503:VAL:O	2.42	0.52
1:A:713:ASP:HA	1:A:715:HIS:ND1	2.24	0.52
1:B:587:PHE:HA	1:B:622:ARG:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:PRO:O	1:A:130:ALA:N	2.36	0.51
1:A:159:SER:OG	1:A:160:PRO:HD3	2.09	0.51
1:B:42:ARG:CZ	1:B:334:ARG:HG3	2.39	0.51
1:B:107:THR:HA	1:B:110:ILE:HD12	1.92	0.51
1:B:110:ILE:O	1:B:111:THR:OG1	2.28	0.51
1:B:152:ASP:OD1	1:B:153:PHE:N	2.43	0.51
1:B:408:PHE:CD1	1:B:413:PHE:HZ	2.22	0.51
1:A:100:PRO:HA	1:A:103:TRP:CD1	2.45	0.51
1:B:338:GLU:OE2	1:B:341:SER:N	2.43	0.51
1:B:387:LEU:HD23	1:B:578:TRP:HH2	1.75	0.51
1:A:105:LYS:HE2	1:A:138:LEU:HD11	1.91	0.51
1:A:296:ASP:HB2	1:A:300:GLN:HG2	1.92	0.51
1:B:482:SER:HA	1:B:485:ASN:HD21	1.76	0.51
1:A:32:GLY:H	1:A:541:ARG:HH21	1.59	0.51
1:A:245:ASP:HB2	1:A:248:ALA:HB3	1.93	0.51
1:A:580:TRP:CH2	1:A:622:ARG:HD3	2.45	0.51
1:B:326:SER:HB2	1:B:328:VAL:HG22	1.92	0.51
1:A:39:GLN:HA	1:A:501:VAL:HG11	1.92	0.51
1:A:144:GLU:HG2	1:A:145:LEU:N	2.26	0.51
1:A:157:VAL:O	1:A:160:PRO:HD2	2.10	0.51
1:B:132:LEU:HG	1:B:135:LEU:HB2	1.91	0.51
1:B:198:MET:O	1:B:202:LEU:HD13	2.11	0.51
1:A:252:SER:HB3	1:A:306:VAL:HG13	1.93	0.51
1:B:25:LEU:O	1:B:27:ASN:ND2	2.44	0.51
1:B:154:VAL:HA	1:B:229:LEU:HD11	1.92	0.51
1:B:343:ILE:HB	1:B:493:TYR:OH	2.10	0.51
1:B:568:LEU:O	1:B:572:THR:N	2.38	0.51
1:A:103:TRP:O	1:A:226:SER:OG	2.26	0.51
1:A:106:LEU:O	1:A:110:ILE:HG12	2.10	0.51
1:A:720:ARG:HD2	1:A:760:VAL:HG21	1.91	0.51
1:B:100:PRO:HA	1:B:103:TRP:HE3	1.74	0.51
1:A:284:LEU:C	1:A:287:ASN:H	2.14	0.51
1:B:7:LYS:HA	1:B:531:GLY:HA2	1.93	0.51
1:B:145:LEU:HD12	1:B:146:PHE:H	1.76	0.51
1:B:363:ASP:OD2	1:B:557:PRO:HB2	2.11	0.51
1:A:196:ARG:O	1:A:197:ARG:NH1	2.40	0.51
1:A:698:ILE:O	1:A:702:MET:HE2	2.11	0.51
1:B:45:SER:HG	1:B:180:TYR:HE1	1.57	0.51
1:B:387:LEU:H	1:B:575:ILE:HD11	1.76	0.51
1:A:54:TRP:CZ3	1:A:174:VAL:HG12	2.46	0.50
1:A:261:TRP:CE2	1:A:288:LEU:HG	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:GLN:O	1:A:673:THR:N	2.39	0.50
1:B:42:ARG:HE	1:B:335:PRO:C	2.15	0.50
1:B:183:PHE:HB2	1:B:297:MET:HB3	1.92	0.50
1:A:276:ARG:HB2	1:A:281:ILE:HD11	1.93	0.50
1:B:114:SER:HB3	1:B:222:PRO:HG2	1.92	0.50
1:B:321:PHE:HA	1:B:325:MET:SD	2.51	0.50
1:A:340:THR:O	1:A:343:ILE:HG22	2.12	0.50
1:A:369:GLU:HA	1:A:398:SER:HB2	1.94	0.50
1:A:387:LEU:H	1:A:572:THR:HG22	1.76	0.50
1:B:4:LEU:H	1:B:437:MET:HB3	1.76	0.50
1:B:16:LEU:HB3	1:B:546:LEU:HD11	1.94	0.50
1:A:409:ALA:O	1:A:413:PHE:N	2.38	0.50
1:B:18:GLN:O	1:B:22:ILE:HG12	2.11	0.50
1:B:413:PHE:HB3	1:B:636:TRP:HZ2	1.76	0.50
1:A:715:HIS:CG	1:A:716:VAL:H	2.29	0.50
1:B:597:ILE:HG22	1:B:602:TYR:CE2	2.47	0.50
1:A:347:SER:O	1:A:358:VAL:HG22	2.11	0.50
1:A:352:MET:SD	1:A:355:PRO:HD2	2.51	0.50
1:B:352:MET:H	1:B:353:GLY:HA2	1.75	0.50
1:A:366:PHE:HD2	1:A:405:GLY:HA2	1.77	0.50
1:B:24:GLU:OE2	1:B:28:GLN:N	2.45	0.50
1:B:71:PHE:O	1:B:75:GLN:HG2	2.12	0.50
1:B:342:TYR:HB3	1:B:559:GLU:CG	2.42	0.50
1:B:586:GLU:C	1:B:622:ARG:HE	2.15	0.50
1:A:502:VAL:HA	1:A:503:VAL:CB	2.42	0.50
1:A:745:ALA:O	1:A:749:VAL:HG23	2.12	0.50
1:B:560:VAL:O	1:B:562:GLN:N	2.45	0.50
1:A:16:LEU:HD11	1:A:462:LEU:HB3	1.94	0.49
1:B:352:MET:H	1:B:353:GLY:CA	2.26	0.49
1:B:58:LYS:HE2	1:B:60:ASN:HD22	1.77	0.49
1:B:666:ARG:HA	1:B:669:GLN:HG2	1.93	0.49
1:A:128:PRO:HG2	1:A:129:THR:OG1	2.13	0.49
1:A:196:ARG:HB3	1:A:197:ARG:NH1	2.27	0.49
1:A:81:SER:HB2	1:A:188:ASP:OD2	2.12	0.49
1:A:42:ARG:H	1:A:336:ILE:CD1	2.25	0.49
1:A:127:PRO:C	1:A:129:THR:HB	2.33	0.49
1:A:477:ASN:OD1	1:A:478:ASP:N	2.45	0.49
1:B:45:SER:O	1:B:332:LYS:N	2.45	0.49
1:B:199:LEU:HA	1:B:202:LEU:HB2	1.93	0.49
1:B:209:MET:SD	1:B:228:HIS:HE1	2.35	0.49
1:A:567:ASP:O	1:A:569:ALA:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:PHE:CZ	1:B:405:GLY:HA2	2.47	0.49
1:B:676:ARG:O	1:B:679:GLU:HB3	2.12	0.49
1:A:253:VAL:HG11	1:A:322:ILE:HD13	1.95	0.49
1:B:232:ALA:O	1:B:236:ALA:N	2.43	0.49
1:A:156:HIS:O	1:A:159:SER:OG	2.30	0.49
1:A:585:THR:O	1:A:622:ARG:HG2	2.12	0.49
1:B:379:ALA:O	1:B:381:ASN:N	2.45	0.49
1:B:403:PRO:O	1:B:407:THR:HG22	2.13	0.49
1:A:365:GLN:CA	1:A:562:GLN:HB2	2.41	0.49
1:A:433:ASN:HB3	1:A:434:GLY:HA3	1.95	0.49
1:A:433:ASN:HB3	1:A:434:GLY:C	2.33	0.49
1:A:443:SER:O	1:A:447:ARG:HG2	2.11	0.49
1:A:716:VAL:HG21	1:B:386:PHE:CE2	2.48	0.49
1:B:296:ASP:O	1:B:299:LYS:HB3	2.13	0.49
1:B:415:LYS:O	1:B:418:THR:OG1	2.28	0.49
1:A:155:CYS:O	1:A:159:SER:N	2.45	0.49
1:B:42:ARG:HD3	1:B:337:ASN:N	2.21	0.49
1:A:15:GLY:O	1:A:487:TYR:OH	2.21	0.48
1:A:396:ARG:HE	1:A:612:LEU:HB3	1.78	0.48
1:B:125:LYS:HZ2	1:B:155:CYS:HA	1.78	0.48
1:B:136:ARG:HE	1:B:147:HIS:CD2	2.31	0.48
1:B:726:TRP:HA	1:B:729:LEU:HD12	1.95	0.48
1:B:737:LEU:HB3	1:B:738:LEU:HD12	1.95	0.48
1:A:391:PRO:HA	1:A:394:SER:HB2	1.93	0.48
1:B:30:SER:HB2	1:B:517:TYR:CE2	2.47	0.48
1:B:396:ARG:HD2	1:B:612:LEU:HD13	1.95	0.48
1:A:16:LEU:HA	1:A:487:TYR:CE1	2.36	0.48
1:B:610:GLU:CD	1:B:614:LEU:H	2.15	0.48
1:A:556:GLN:OE1	1:A:557:PRO:HD2	2.13	0.48
1:A:747:THR:HA	1:A:750:LEU:HG	1.96	0.48
1:B:743:ALA:O	1:B:747:THR:N	2.36	0.48
1:A:61:ILE:HG13	1:A:66:TYR:CE2	2.47	0.48
1:A:418:THR:O	1:A:421:TYR:CD1	2.66	0.48
1:A:719:ASN:OD1	1:A:720:ARG:N	2.46	0.48
1:B:30:SER:O	1:B:543:PRO:HG3	2.13	0.48
1:B:41:THR:O	1:B:42:ARG:HG2	2.14	0.48
1:A:729:LEU:O	1:A:732:LEU:HB3	2.14	0.48
1:A:66:TYR:HA	1:A:69:LEU:HD12	1.95	0.48
1:A:355:PRO:O	1:A:356:SER:OG	2.28	0.48
1:A:477:ASN:O	1:A:481:ARG:N	2.47	0.48
1:A:516:LEU:O	1:A:516:LEU:HD12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:GLY:HA2	1:B:261:TRP:HD1	1.78	0.48
1:B:314:SER:OG	1:B:317:ILE:N	2.31	0.48
1:A:696:SER:OG	1:A:697:ARG:NH1	2.47	0.48
1:B:660:LYS:O	1:B:663:ILE:HG13	2.13	0.48
1:A:335:PRO:HB2	1:A:338:GLU:OE2	2.14	0.48
1:A:648:ALA:O	1:A:652:ARG:HG3	2.14	0.48
1:A:16:LEU:HD21	1:A:462:LEU:HD13	1.96	0.48
1:A:109:TYR:OH	1:A:130:ALA:HB1	2.14	0.48
1:A:257:LEU:HB3	1:A:261:TRP:CZ2	2.48	0.48
1:B:164:ILE:HG13	1:B:165:LEU:H	1.79	0.48
1:B:254:LEU:HD22	1:B:297:MET:SD	2.54	0.48
1:B:747:THR:O	1:B:750:LEU:HG	2.13	0.48
1:A:533:ASN:ND2	1:A:542:THR:OG1	2.47	0.47
1:A:672:VAL:HA	1:A:675:LEU:HD12	1.96	0.47
1:B:132:LEU:HA	1:B:135:LEU:HD13	1.95	0.47
1:B:357:HIS:O	1:B:359:VAL:HG23	2.14	0.47
1:B:510:ALA:HB1	1:B:513:GLN:H	1.79	0.47
1:A:4:LEU:HG	1:A:436:GLU:CB	2.37	0.47
1:A:362:GLU:HB2	1:A:364:TRP:HE1	1.79	0.47
1:B:197:ARG:NH2	1:B:240:SER:HA	2.29	0.47
1:B:288:LEU:O	1:B:292:ILE:HD12	2.14	0.47
1:B:356:SER:HA	1:B:435:ALA:HB1	1.96	0.47
1:B:719:ASN:OD1	1:B:720:ARG:N	2.47	0.47
1:A:334:ARG:HD3	1:A:338:GLU:CB	2.41	0.47
1:B:525:GLU:OE2	1:B:535:ILE:HG12	2.14	0.47
1:A:83:ASP:OD1	1:A:191:ARG:NE	2.47	0.47
1:B:345:GLN:OE1	1:B:360:VAL:HG12	2.14	0.47
1:B:449:TYR:OH	1:B:630:HIS:ND1	2.13	0.47
1:A:375:PRO:CG	1:A:622:ARG:HE	2.26	0.47
1:A:441:PHE:HB2	1:A:444:VAL:HG22	1.96	0.47
1:B:379:ALA:C	1:B:381:ASN:H	2.17	0.47
1:A:282:ASP:O	1:A:285:ARG:HB3	2.14	0.47
1:A:308:PHE:HE2	1:A:318:ILE:HG13	1.80	0.47
1:A:745:ALA:O	1:A:748:LYS:HB3	2.15	0.47
1:B:111:THR:HA	1:B:112:GLY:HA3	1.65	0.47
1:B:725:ILE:O	1:B:729:LEU:HG	2.15	0.47
1:A:80:LEU:HD21	1:A:477:ASN:HD21	1.79	0.47
1:A:344:GLY:HA2	1:A:557:PRO:HB3	1.96	0.47
1:A:376:VAL:O	1:A:386:PHE:N	2.47	0.47
1:A:580:TRP:CE3	1:A:581:HIS:HA	2.49	0.47
1:A:739:SER:OG	1:A:742:GLU:OE1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:757:GLY:HA3	1:A:759:VAL:H	1.79	0.47
1:B:145:LEU:O	1:B:149:ILE:HG12	2.14	0.47
1:B:195:LEU:O	1:B:198:MET:HB3	2.14	0.47
1:B:585:THR:C	1:B:622:ARG:HB2	2.35	0.47
1:A:6:VAL:HG11	1:A:530:VAL:HG23	1.96	0.47
1:B:437:MET:HE2	1:B:546:LEU:HD22	1.96	0.47
1:B:474:ARG:O	1:B:477:ASN:HB3	2.15	0.47
1:A:56:VAL:HG13	1:A:66:TYR:CE1	2.50	0.47
1:A:493:TYR:CZ	1:A:549:ILE:HG12	2.49	0.47
1:A:712:SER:C	1:A:715:HIS:HD1	2.16	0.47
1:B:7:LYS:HD3	1:B:531:GLY:N	2.22	0.47
1:B:54:TRP:CZ3	1:B:65:MET:HG2	2.50	0.47
1:B:125:LYS:NZ	1:B:155:CYS:HA	2.29	0.47
1:B:144:GLU:OE1	1:B:144:GLU:N	2.45	0.47
1:B:619:GLU:N	1:B:619:GLU:OE1	2.48	0.47
1:B:630:HIS:HE1	1:B:739:SER:HB3	1.80	0.47
1:A:280:GLY:N	1:A:282:ASP:OD1	2.48	0.47
1:B:9:LEU:HD22	1:B:546:LEU:HD12	1.97	0.47
1:B:136:ARG:HH21	1:B:147:HIS:CG	2.33	0.47
1:B:686:ILE:O	1:B:689:SER:OG	2.21	0.47
1:A:149:ILE:HA	1:A:152:ASP:OD2	2.15	0.46
1:A:535:ILE:HG13	1:A:540:ILE:HG23	1.96	0.46
1:B:41:THR:C	1:B:43:THR:H	2.17	0.46
1:B:129:THR:HG22	1:B:151:THR:HG21	1.96	0.46
1:B:297:MET:HA	1:B:300:GLN:OE1	2.15	0.46
1:B:414:VAL:O	1:B:418:THR:HG23	2.15	0.46
1:B:449:TYR:HH	1:B:630:HIS:CE1	2.19	0.46
1:B:154:VAL:HG22	1:B:229:LEU:HD13	1.97	0.46
1:B:176:ARG:NH2	1:B:446:GLU:O	2.44	0.46
1:B:317:ILE:HA	1:B:320:TRP:CE2	2.50	0.46
1:B:354:GLN:NE2	1:B:431:ASN:HD22	2.12	0.46
1:B:677:LYS:O	1:B:680:MET:HG2	2.15	0.46
1:A:212:ALA:HB3	1:A:219:ALA:HB3	1.97	0.46
1:B:386:PHE:CE1	1:B:576:HIS:N	2.83	0.46
1:B:427:ARG:HB3	1:B:428:GLY:HA3	1.97	0.46
1:B:481:ARG:O	1:B:485:ASN:ND2	2.48	0.46
1:B:577:ILE:HG13	1:B:578:TRP:H	1.80	0.46
1:B:673:THR:O	1:B:677:LYS:HD3	2.14	0.46
1:A:337:ASN:HD21	1:A:496:ALA:HB2	1.80	0.46
1:B:529:PRO:O	1:B:530:VAL:HG13	2.16	0.46
1:B:606:VAL:HB	1:B:697:ARG:CZ	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:610:GLU:OE1	1:B:610:GLU:N	2.42	0.46
1:B:648:ALA:HA	1:B:651:ARG:HD3	1.98	0.46
1:B:657:ASP:O	1:B:660:LYS:HB3	2.15	0.46
1:A:176:ARG:C	1:A:447:ARG:HH12	2.19	0.46
1:A:282:ASP:OD1	1:A:282:ASP:N	2.48	0.46
1:A:418:THR:O	1:A:421:TYR:HD1	1.99	0.46
1:B:53:LEU:HD22	1:B:571:HIS:ND1	2.30	0.46
1:A:36:LEU:C	1:A:502:VAL:HG11	2.36	0.46
1:B:318:ILE:HD12	1:B:318:ILE:H	1.80	0.46
1:B:368:LYS:O	1:B:398:SER:OG	2.32	0.46
1:A:210:LEU:HB3	1:A:212:ALA:O	2.16	0.46
1:A:281:ILE:HG22	1:A:319:PRO:HB2	1.98	0.46
1:A:329:SER:HB3	1:A:331:PHE:HB3	1.98	0.46
1:A:349:ILE:HD11	1:A:356:SER:HB2	1.96	0.46
1:A:678:ILE:HA	1:A:681:ILE:HG12	1.97	0.46
1:B:18:GLN:OE1	1:B:517:TYR:HB2	2.16	0.46
1:B:164:ILE:HG23	1:B:165:LEU:N	2.31	0.46
1:B:374:THR:N	1:B:387:LEU:O	2.43	0.46
1:A:45:SER:C	1:A:332:LYS:HD2	2.37	0.46
1:A:261:TRP:HE1	1:A:288:LEU:HD11	1.81	0.46
1:A:303:ARG:HB2	1:A:513:GLN:OE1	2.15	0.46
1:B:10:ASN:HB2	1:B:14:ARG:HH11	1.81	0.46
1:B:62:ASP:CG	1:B:64:VAL:HG22	2.37	0.46
1:B:376:VAL:HG12	1:B:378:LEU:HD23	1.98	0.46
1:B:641:VAL:HG23	1:B:645:ARG:HH12	1.80	0.46
1:B:677:LYS:O	1:B:681:ILE:HG13	2.15	0.46
1:A:328:VAL:HG23	1:A:329:SER:CB	2.46	0.46
1:A:350:ASP:OD1	1:A:350:ASP:N	2.49	0.46
1:A:371:THR:O	1:A:623:ILE:HD12	2.16	0.46
1:A:559:GLU:OE1	1:A:559:GLU:N	2.49	0.46
1:A:666:ARG:O	1:A:670:ASN:ND2	2.49	0.46
1:B:317:ILE:HA	1:B:320:TRP:CD2	2.51	0.46
1:B:584:SER:C	1:B:622:ARG:HG2	2.35	0.46
1:B:590:GLU:HB2	1:B:606:VAL:O	2.16	0.46
1:B:596:THR:HG22	1:B:601:ARG:HD2	1.97	0.46
1:A:3:ASN:HA	1:A:436:GLU:HB3	1.98	0.45
1:A:328:VAL:HG23	1:A:329:SER:HB2	1.97	0.45
1:A:685:GLY:HA2	1:A:686:ILE:HA	1.53	0.45
1:B:63:PRO:HG3	1:B:200:THR:HB	1.98	0.45
1:B:754:ASN:OD1	1:B:755:ALA:N	2.49	0.45
1:A:17:THR:O	1:A:19:ALA:N	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:VAL:CA	1:A:413:PHE:HB3	2.41	0.45
1:B:334:ARG:HA	1:B:335:PRO:HD3	1.80	0.45
1:A:263:PRO:HG3	1:A:504:SER:HA	1.97	0.45
1:A:317:ILE:O	1:A:320:TRP:HB3	2.16	0.45
1:A:662:ALA:HA	1:B:108:ALA:O	2.17	0.45
1:B:10:ASN:ND2	1:B:29:LEU:HD21	2.30	0.45
1:B:413:PHE:HB3	1:B:636:TRP:CZ2	2.51	0.45
1:A:69:LEU:HD22	1:A:172:TYR:HD2	1.80	0.45
1:A:146:PHE:HA	1:A:149:ILE:HB	1.97	0.45
1:A:498:ASN:OD1	1:A:499:PRO:HD2	2.15	0.45
1:A:298:VAL:HG21	1:A:514:GLY:O	2.17	0.45
1:A:315:SER:O	1:A:319:PRO:HD2	2.16	0.45
1:A:371:THR:HB	1:A:389:VAL:HG23	1.96	0.45
1:A:497:HIS:HE2	1:A:548:ALA:C	2.20	0.45
1:A:502:VAL:HG23	1:A:503:VAL:HG12	1.97	0.45
1:A:566:LEU:HD12	1:A:568:LEU:HD23	1.98	0.45
1:B:89:PHE:O	1:B:92:TYR:HB3	2.16	0.45
1:A:16:LEU:HD21	1:A:462:LEU:HB3	1.99	0.45
1:A:75:GLN:HE22	1:A:447:ARG:NH2	2.14	0.45
1:A:410:VAL:O	1:A:414:VAL:HG23	2.16	0.45
1:A:428:GLY:HA3	1:A:429:THR:HA	1.59	0.45
1:A:652:ARG:O	1:A:653:THR:OG1	2.30	0.45
1:B:55:GLU:O	1:B:58:LYS:NZ	2.49	0.45
1:B:254:LEU:O	1:B:257:LEU:HB3	2.17	0.45
1:A:201:ALA:HB1	1:A:239:ARG:HD3	1.98	0.45
1:A:209:MET:O	1:A:210:LEU:HB2	2.16	0.45
1:A:320:TRP:HA	1:A:325:MET:HE1	1.99	0.45
1:A:503:VAL:HG11	1:A:517:TYR:O	2.16	0.45
1:A:595:VAL:HG12	1:A:597:ILE:HG23	1.99	0.45
1:B:25:LEU:O	1:B:27:ASN:N	2.49	0.45
1:B:42:ARG:HG2	1:B:335:PRO:O	2.17	0.45
1:B:326:SER:CB	1:B:328:VAL:HG22	2.47	0.45
1:B:560:VAL:C	1:B:561:LEU:HG	2.36	0.45
1:A:138:LEU:HB3	1:A:139:ALA:H	1.69	0.45
1:A:674:LEU:HA	1:A:677:LYS:NZ	2.32	0.45
1:B:607:LYS:C	1:B:609:PHE:HB2	2.36	0.45
1:B:628:VAL:O	1:B:632:ILE:HG22	2.17	0.45
1:A:224:LEU:HA	1:A:227:GLN:HB3	1.99	0.45
1:A:503:VAL:HG22	1:A:504:SER:H	1.81	0.45
1:B:42:ARG:HH11	1:B:339:THR:CA	2.30	0.45
1:B:426:GLN:HA	1:B:427:ARG:HA	1.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:HIS:HE1	1:B:555:ILE:HD13	1.82	0.45
1:A:211:GLN:O	1:A:218:GLY:HA3	2.18	0.44
1:B:143:HIS:HB3	1:B:145:LEU:HG	1.98	0.44
1:B:321:PHE:CE1	1:B:325:MET:HG3	2.52	0.44
1:B:346:THR:OG1	1:B:359:VAL:HG21	2.17	0.44
1:A:503:VAL:HG21	1:A:517:TYR:C	2.36	0.44
1:B:125:LYS:HB2	1:B:163:PHE:HB3	1.98	0.44
1:B:454:ASP:O	1:B:457:VAL:HG22	2.17	0.44
1:A:313:LEU:HB3	1:A:314:SER:HB3	1.99	0.44
1:A:366:PHE:O	1:A:368:LYS:HD2	2.17	0.44
1:A:500:GLU:HB3	1:A:521:ASN:H	1.83	0.44
1:B:125:LYS:HB3	1:B:165:LEU:O	2.18	0.44
1:B:609:PHE:HA	1:B:616:GLN:OE1	2.18	0.44
1:A:51:GLU:CA	1:A:174:VAL:HG21	2.44	0.44
1:A:57:GLY:N	1:A:170:TYR:HB2	2.30	0.44
1:A:271:PRO:HA	1:A:276:ARG:HD3	2.00	0.44
1:B:122:ALA:H	1:B:163:PHE:HE1	1.64	0.44
1:B:125:LYS:HE2	1:B:163:PHE:CB	2.47	0.44
1:A:55:GLU:N	1:A:55:GLU:OE1	2.51	0.44
1:A:580:TRP:HA	1:A:581:HIS:C	2.36	0.44
1:A:719:ASN:O	1:A:722:ARG:HB3	2.18	0.44
1:B:61:ILE:HD13	1:B:156:HIS:HB3	1.99	0.44
1:B:274:ARG:CB	1:B:312:GLU:HG3	2.46	0.44
1:B:332:LYS:HE2	1:B:334:ARG:NH1	2.30	0.44
1:A:66:TYR:HD1	1:A:69:LEU:HD12	1.83	0.44
1:A:423:ALA:HA	1:A:424:VAL:HA	1.48	0.44
1:B:233:ALA:HA	1:B:236:ALA:HB3	1.98	0.44
1:B:280:GLY:HA2	1:B:283:GLN:HE22	1.83	0.44
1:B:292:ILE:HG21	1:B:488:ALA:HB2	1.98	0.44
1:B:577:ILE:HG13	1:B:578:TRP:N	2.33	0.44
1:A:366:PHE:CD2	1:A:405:GLY:HA2	2.52	0.44
1:A:549:ILE:HA	1:A:552:ASN:HB2	2.00	0.44
1:A:590:GLU:OE1	1:A:607:LYS:HD3	2.18	0.44
1:B:56:VAL:O	1:B:170:TYR:N	2.50	0.44
1:B:106:LEU:O	1:B:109:TYR:HB3	2.17	0.44
1:A:260:LEU:HD11	1:A:285:ARG:HH12	1.82	0.44
1:A:337:ASN:O	1:A:341:SER:N	2.50	0.44
1:B:172:TYR:CE1	1:B:579:PRO:HG2	2.51	0.44
1:B:225:ILE:O	1:B:228:HIS:HB3	2.18	0.44
1:B:387:LEU:HD23	1:B:578:TRP:CH2	2.53	0.44
1:A:56:VAL:HB	1:A:170:TYR:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LEU:HD23	1:A:203:SER:HB2	1.99	0.44
1:A:385:ARG:HD2	1:A:580:TRP:NE1	2.29	0.44
1:A:737:LEU:O	1:A:738:LEU:HG	2.18	0.44
1:B:14:ARG:CZ	1:B:26:LYS:HA	2.48	0.44
1:B:321:PHE:CD1	1:B:325:MET:HG3	2.53	0.44
1:B:656:ASP:HB3	1:B:659:GLU:CG	2.48	0.44
1:A:116:ARG:HA	1:A:118:ILE:H	1.82	0.43
1:A:348:ALA:O	1:A:349:ILE:HG22	2.18	0.43
1:B:9:LEU:HD12	1:B:10:ASN:N	2.33	0.43
1:B:251:SER:O	1:B:254:LEU:HB3	2.18	0.43
1:B:610:GLU:HG2	1:B:612:LEU:N	2.33	0.43
1:B:675:LEU:HD21	1:B:757:GLY:O	2.18	0.43
1:A:293:ALA:O	1:A:297:MET:HB2	2.19	0.43
1:A:402:ALA:HB3	1:A:403:PRO:HD3	2.00	0.43
1:A:454:ASP:O	1:A:457:VAL:HG12	2.18	0.43
1:B:66:TYR:CD1	1:B:69:LEU:HD12	2.49	0.43
1:A:68:ARG:CZ	1:A:330:PRO:HG3	2.49	0.43
1:A:389:VAL:HG13	1:A:391:PRO:HD3	1.99	0.43
1:A:655:ARG:H	1:A:656:ASP:CB	2.30	0.43
1:B:228:HIS:O	1:B:230:ALA:N	2.51	0.43
1:B:349:ILE:HD12	1:B:353:GLY:HA3	2.00	0.43
1:A:259:ARG:O	1:A:262:SER:OG	2.23	0.43
1:A:359:VAL:HG22	1:A:437:MET:O	2.19	0.43
1:A:590:GLU:OE2	1:A:607:LYS:HA	2.18	0.43
1:A:682:GLY:O	1:A:684:THR:N	2.51	0.43
1:B:133:GLU:O	1:B:136:ARG:HB3	2.18	0.43
1:B:209:MET:HG3	1:B:228:HIS:CE1	2.54	0.43
1:B:230:ALA:HB1	1:B:233:ALA:HB3	2.00	0.43
1:B:225:ILE:O	1:B:229:LEU:N	2.23	0.43
1:B:234:THR:O	1:B:237:PHE:HB3	2.17	0.43
1:B:313:LEU:HD12	1:B:313:LEU:O	2.18	0.43
1:B:681:ILE:HG21	1:B:728:GLY:HA2	1.99	0.43
1:A:59:GLY:HA3	1:A:155:CYS:HB3	2.00	0.43
1:A:204:SER:O	1:A:206:ASP:N	2.52	0.43
1:A:221:ALA:HB1	1:A:224:LEU:HB3	1.99	0.43
1:A:362:GLU:OE1	1:A:443:SER:OG	2.35	0.43
1:A:424:VAL:HG12	1:A:425:SER:O	2.18	0.43
1:A:754:ASN:HB3	1:A:755:ALA:C	2.39	0.43
1:B:604:ALA:HB1	1:B:697:ARG:NH2	2.32	0.43
1:A:49:THR:OG1	1:A:50:SER:N	2.44	0.43
1:A:349:ILE:HD12	1:A:349:ILE:HA	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:LEU:HA	1:A:677:LYS:HG2	2.00	0.43
1:B:675:LEU:O	1:B:678:ILE:HG13	2.19	0.43
1:A:241:ARG:HG3	1:A:243:ASN:H	1.84	0.43
1:A:345:GLN:HE22	1:A:549:ILE:HG23	1.83	0.43
1:A:368:LYS:HE2	1:A:402:ALA:O	2.18	0.43
1:A:369:GLU:HA	1:A:398:SER:CB	2.49	0.43
1:A:544:GLU:HG2	1:A:545:PRO:HD2	2.01	0.43
1:A:715:HIS:HB2	1:A:716:VAL:HG13	2.01	0.43
1:A:754:ASN:H	1:A:755:ALA:HA	1.82	0.43
1:B:521:ASN:OD1	1:B:539:SER:HB3	2.18	0.43
1:B:721:HIS:CD2	1:B:757:GLY:HA2	2.54	0.43
1:B:732:LEU:HD13	1:B:743:ALA:HB2	2.00	0.43
1:A:177:THR:HA	1:A:447:ARG:HH22	1.83	0.43
1:A:368:LYS:HA	1:A:401:LEU:HD23	2.01	0.43
1:B:2:PHE:N	1:B:439:LEU:O	2.50	0.43
1:B:160:PRO:HG3	1:B:210:LEU:HD22	2.00	0.43
1:B:604:ALA:HB1	1:B:697:ARG:HH21	1.83	0.43
1:A:54:TRP:CH2	1:A:174:VAL:HG12	2.54	0.43
1:A:176:ARG:NH1	1:A:447:ARG:HA	2.26	0.43
1:A:566:LEU:CD1	1:A:568:LEU:HB3	2.49	0.43
1:B:3:ASN:HA	1:B:437:MET:O	2.19	0.43
1:B:153:PHE:CZ	1:B:202:LEU:HD23	2.51	0.43
1:B:359:VAL:HG22	1:B:418:THR:HG22	2.00	0.43
1:B:360:VAL:HG23	1:B:439:LEU:HB3	2.00	0.43
1:B:376:VAL:N	1:B:386:PHE:O	2.50	0.43
1:A:41:THR:OG1	1:A:42:ARG:N	2.51	0.42
1:A:182:ASN:HD21	1:A:184:TYR:HD2	1.67	0.42
1:A:536:GLU:N	1:A:536:GLU:OE1	2.40	0.42
1:A:628:VAL:O	1:A:632:ILE:HD12	2.19	0.42
1:A:666:ARG:HA	1:A:669:GLN:NE2	2.31	0.42
1:A:732:LEU:O	1:A:735:MET:HB3	2.18	0.42
1:B:13:ALA:HA	1:B:463:ARG:O	2.19	0.42
1:B:423:ALA:O	1:B:430:VAL:HG22	2.19	0.42
1:A:80:LEU:HA	1:A:81:SER:HA	1.78	0.42
1:A:289:ALA:C	1:A:291:PHE:H	2.22	0.42
1:A:520:TRP:CH2	1:A:545:PRO:HG3	2.54	0.42
1:A:716:VAL:HG21	1:B:386:PHE:CD2	2.54	0.42
1:B:257:LEU:HG	1:B:261:TRP:HE1	1.84	0.42
1:B:316:THR:HG22	1:B:320:TRP:CD1	2.53	0.42
1:B:675:LEU:HD21	1:B:758:MET:N	2.34	0.42
1:A:521:ASN:O	1:A:539:SER:OG	2.10	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:HIS:HD2	1:A:633:ILE:HD11	1.83	0.42
1:A:246:ALA:O	1:A:249:VAL:HG22	2.19	0.42
1:A:292:ILE:HD11	1:A:491:MET:HG3	2.02	0.42
1:A:523:ARG:HA	1:A:539:SER:HB2	2.01	0.42
1:B:130:ALA:O	1:B:133:GLU:HB3	2.20	0.42
1:B:345:GLN:O	1:B:554:PRO:HB3	2.20	0.42
1:B:606:VAL:HG22	1:B:607:LYS:O	2.20	0.42
1:A:2:PHE:HE2	1:A:4:LEU:HD23	1.85	0.42
1:A:43:THR:HA	1:A:289:ALA:CB	2.50	0.42
1:A:212:ALA:H	1:A:218:GLY:C	2.23	0.42
1:A:259:ARG:HG3	1:A:269:LEU:HD13	2.01	0.42
1:A:291:PHE:O	1:A:292:ILE:HB	2.19	0.42
1:B:40:PHE:CZ	1:B:495:VAL:HG13	2.54	0.42
1:A:474:ARG:HA	1:A:474:ARG:HD3	1.82	0.42
1:A:498:ASN:ND2	1:A:500:GLU:HG2	2.33	0.42
1:A:510:ALA:HA	1:A:511:ALA:HA	1.72	0.42
1:B:43:THR:HG21	1:B:289:ALA:N	2.34	0.42
1:B:518:LEU:O	1:B:543:PRO:HA	2.19	0.42
1:A:608:GLU:HG3	1:A:609:PHE:N	2.35	0.42
1:A:676:ARG:NH1	1:B:165:LEU:HD23	2.34	0.42
1:B:684:THR:O	1:B:688:ALA:N	2.51	0.42
1:A:331:PHE:O	1:A:332:LYS:HG2	2.19	0.42
1:A:373:PHE:CE1	1:A:387:LEU:HD22	2.54	0.42
1:B:2:PHE:CZ	1:B:463:ARG:HG2	2.55	0.42
1:B:19:ALA:HB1	1:B:24:GLU:HB3	2.02	0.42
1:B:494:ALA:HB2	1:B:549:ILE:HD11	2.02	0.42
1:A:41:THR:HG23	1:A:286:SER:O	2.20	0.42
1:A:82:VAL:O	1:A:86:VAL:HG23	2.19	0.42
1:A:101:GLU:OE1	1:A:101:GLU:N	2.49	0.42
1:A:133:GLU:O	1:A:137:THR:HG23	2.20	0.42
1:A:292:ILE:HA	1:A:295:GLN:CG	2.50	0.42
1:A:331:PHE:C	1:A:332:LYS:HG2	2.40	0.42
1:A:377:LYS:HD2	1:A:380:ASN:HA	2.01	0.42
1:A:436:GLU:CD	1:A:438:THR:H	2.23	0.42
1:A:629:ALA:HA	1:A:632:ILE:HD13	2.02	0.42
1:B:257:LEU:HG	1:B:261:TRP:NE1	2.34	0.42
1:B:387:LEU:HD11	1:B:568:LEU:HD13	2.02	0.42
1:B:522:VAL:HB	1:B:540:ILE:HD11	2.02	0.42
1:B:546:LEU:O	1:B:549:ILE:HB	2.19	0.42
1:B:610:GLU:CG	1:B:614:LEU:H	2.33	0.42
1:A:117:ALA:H	1:A:221:ALA:N	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:PRO:HB2	1:A:182:ASN:H	1.43	0.41
1:A:386:PHE:HE1	1:A:576:HIS:H	1.68	0.41
1:A:413:PHE:CZ	1:A:636:TRP:HA	2.54	0.41
1:B:19:ALA:HB1	1:B:24:GLU:CB	2.50	0.41
1:B:43:THR:HG21	1:B:289:ALA:HB3	2.02	0.41
1:B:610:GLU:HG3	1:B:614:LEU:H	1.85	0.41
1:B:640:PHE:HA	1:B:670:ASN:HD21	1.85	0.41
1:B:757:GLY:N	1:B:758:MET:HA	2.35	0.41
1:A:358:VAL:N	1:A:437:MET:HB3	2.31	0.41
1:A:753:SER:HA	1:A:754:ASN:HA	1.85	0.41
1:B:313:LEU:HA	1:B:314:SER:HA	1.32	0.41
1:B:384:GLN:HA	1:B:577:ILE:HG21	2.01	0.41
1:A:38:LEU:HD23	1:A:39:GLN:O	2.19	0.41
1:A:230:ALA:HA	1:A:233:ALA:HB3	2.03	0.41
1:A:349:ILE:HG21	1:A:354:GLN:O	2.20	0.41
1:A:708:ILE:O	1:A:711:SER:OG	2.22	0.41
1:B:401:LEU:O	1:B:405:GLY:N	2.53	0.41
1:A:314:SER:HA	1:A:315:SER:C	2.41	0.41
1:A:349:ILE:HG13	1:A:353:GLY:O	2.21	0.41
1:A:383:ASN:C	1:A:385:ARG:H	2.22	0.41
1:A:553:LYS:O	1:A:555:ILE:HG23	2.20	0.41
1:B:118:ILE:H	1:B:222:PRO:HD2	1.85	0.41
1:B:284:LEU:HA	1:B:287:ASN:HD22	1.86	0.41
1:B:410:VAL:HA	1:B:413:PHE:HD2	1.85	0.41
1:B:522:VAL:O	1:B:540:ILE:HG13	2.20	0.41
1:A:281:ILE:O	1:A:284:LEU:HB2	2.21	0.41
1:A:366:PHE:CE1	1:A:629:ALA:HB2	2.54	0.41
1:B:198:MET:HG3	1:B:202:LEU:HD22	2.02	0.41
1:B:289:ALA:HA	1:B:292:ILE:HD13	2.02	0.41
1:B:637:TYR:O	1:B:641:VAL:HG22	2.20	0.41
1:A:44:PHE:HE1	1:A:180:TYR:N	2.18	0.41
1:A:128:PRO:O	1:A:131:ILE:HB	2.21	0.41
1:A:128:PRO:HD3	1:A:166:PRO:HB2	2.03	0.41
1:A:357:HIS:HA	1:A:437:MET:HG2	2.02	0.41
1:A:657:ASP:O	1:A:660:LYS:HG2	2.20	0.41
1:B:13:ALA:HB1	1:B:462:LEU:HD23	2.03	0.41
1:B:62:ASP:HB3	1:B:65:MET:HG3	2.03	0.41
1:B:669:GLN:O	1:B:672:VAL:HG12	2.21	0.41
1:B:43:THR:HG22	1:B:44:PHE:O	2.21	0.41
1:B:92:TYR:OH	1:B:150:THR:HG21	2.21	0.41
1:B:132:LEU:HD23	1:B:147:HIS:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:ASN:O	1:B:577:ILE:HG12	2.20	0.41
1:B:427:ARG:H	1:B:428:GLY:HA3	1.86	0.41
1:A:173:ARG:HH11	1:A:579:PRO:HG2	1.86	0.41
1:A:186:LEU:O	1:A:190:VAL:HG13	2.21	0.41
1:A:257:LEU:O	1:A:260:LEU:HB3	2.21	0.41
1:A:334:ARG:HG3	1:A:335:PRO:HD2	2.03	0.41
1:A:349:ILE:CD1	1:A:356:SER:HB2	2.51	0.41
1:A:521:ASN:HA	1:A:540:ILE:O	2.21	0.41
1:A:659:GLU:O	1:A:662:ALA:HB3	2.20	0.41
1:B:35:GLN:HE21	1:B:502:VAL:CG2	2.32	0.41
1:B:171:VAL:HG12	1:B:576:HIS:HB3	2.03	0.41
1:B:342:TYR:HA	1:B:558:SER:H	1.86	0.41
1:B:505:GLU:HB2	1:B:506:HIS:O	2.20	0.41
1:B:674:LEU:HA	1:B:674:LEU:HD23	1.82	0.41
1:B:676:ARG:HA	1:B:679:GLU:OE1	2.21	0.41
1:A:27:ASN:OD1	1:A:28:GLN:N	2.54	0.41
1:A:216:ALA:HA	1:A:217:LYS:HA	1.72	0.41
1:A:436:GLU:O	1:A:438:THR:N	2.54	0.41
1:A:657:ASP:HA	1:A:660:LYS:HE3	2.03	0.41
1:B:135:LEU:HG	1:B:138:LEU:HD12	2.02	0.41
1:B:210:LEU:HD12	1:B:211:GLN:N	2.36	0.41
1:A:141:SER:HB3	1:A:144:GLU:HA	2.03	0.41
1:A:310:ASP:CG	1:A:311:GLU:H	2.25	0.41
1:A:506:HIS:CD2	1:A:517:TYR:CE2	3.09	0.41
1:B:68:ARG:NH1	1:B:328:VAL:O	2.54	0.41
1:B:132:LEU:CA	1:B:135:LEU:HB2	2.49	0.41
1:B:141:SER:CB	1:B:147:HIS:HB2	2.50	0.41
1:B:173:ARG:CZ	1:B:578:TRP:HE1	2.34	0.41
1:B:451:LEU:HG	1:B:453:ARG:CZ	2.51	0.41
1:B:510:ALA:N	1:B:511:ALA:HA	2.35	0.41
1:B:607:LYS:HB2	1:B:608:GLU:C	2.40	0.41
1:A:674:LEU:O	1:A:678:ILE:HG13	2.22	0.40
1:B:303:ARG:HB2	1:B:305:GLU:OE2	2.20	0.40
1:B:519:VAL:HG12	1:B:543:PRO:HA	2.03	0.40
1:A:517:TYR:HD1	1:A:518:LEU:H	1.69	0.40
1:B:103:TRP:HH2	1:B:234:THR:HG21	1.86	0.40
1:B:493:TYR:O	1:B:496:ALA:HB3	2.22	0.40
1:B:747:THR:HA	1:B:750:LEU:HG	2.02	0.40
1:A:3:ASN:HA	1:A:436:GLU:CB	2.50	0.40
1:A:381:ASN:N	1:A:381:ASN:OD1	2.54	0.40
1:A:464:THR:HG23	1:A:466:ILE:HG13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:ASP:OD2	1:A:570:ASN:ND2	2.31	0.40
1:B:6:VAL:HG12	1:B:435:ALA:N	2.36	0.40
1:B:118:ILE:O	1:B:120:ALA:N	2.54	0.40
1:B:321:PHE:CZ	1:B:326:SER:HB3	2.57	0.40
1:B:501:VAL:HG22	1:B:520:TRP:CD1	2.56	0.40
1:A:361:TYR:CD1	1:A:414:VAL:HG21	2.57	0.40
1:A:666:ARG:HD3	1:A:669:GLN:HE22	1.87	0.40
1:B:497:HIS:HE1	1:B:555:ILE:CD1	2.35	0.40
1:A:361:TYR:CG	1:A:414:VAL:HG21	2.56	0.40
1:A:389:VAL:HG22	1:A:390:GLU:N	2.37	0.40
1:A:425:SER:CB	1:B:116:ARG:HE	2.35	0.40
1:A:716:VAL:HG11	1:B:386:PHE:CD2	2.56	0.40
1:B:230:ALA:O	1:B:234:THR:HG23	2.22	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	759/761 (100%)	593 (78%)	92 (12%)	74 (10%)	0	10
1	B	759/761 (100%)	597 (79%)	108 (14%)	54 (7%)	1	16
All	All	1518/1522 (100%)	1190 (78%)	200 (13%)	128 (8%)	2	13

All (128) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	VAL
1	A	41	THR
1	A	129	THR
1	A	145	LEU
1	A	174	VAL

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Mol	Chain	Res	Type
1	A	222	PRO
1	A	243	ASN
1	A	288	LEU
1	A	292	ILE
1	A	307	ILE
1	A	349	ILE
1	A	503	VAL
1	A	535	ILE
1	A	568	LEU
1	A	581	HIS
1	A	582	GLU
1	A	608	GLU
1	A	684	THR
1	A	738	LEU
1	B	27	ASN
1	B	31	VAL
1	B	126	VAL
1	B	127	PRO
1	B	164	ILE
1	B	280	GLY
1	B	335	PRO
1	B	337	ASN
1	B	359	VAL
1	B	424	VAL
1	B	582	GLU
1	A	45	SER
1	A	61	ILE
1	A	110	ILE
1	A	122	ALA
1	A	181	PRO
1	A	241	ARG
1	A	277	ASN
1	A	309	SER
1	A	316	THR
1	A	332	LYS
1	A	355	PRO
1	A	356	SER
1	A	381	ASN
1	A	502	VAL
1	A	522	VAL
1	A	537	GLY
1	A	555	ILE

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Mol	Chain	Res	Type
1	A	558	SER
1	A	559	GLU
1	A	717	GLY
1	A	740	ARG
1	B	43	THR
1	B	44	PHE
1	B	48	MET
1	B	61	ILE
1	B	80	LEU
1	B	129	THR
1	B	229	LEU
1	B	342	TYR
1	B	388	ASP
1	B	394	SER
1	B	421	TYR
1	B	565	VAL
1	B	583	ALA
1	B	605	GLU
1	B	609	PHE
1	B	717	GLY
1	B	732	LEU
1	A	34	LEU
1	A	167	ASP
1	A	205	VAL
1	A	214	PHE
1	A	335	PRO
1	A	351	HIS
1	A	384	GLN
1	A	409	ALA
1	A	584	SER
1	A	654	SER
1	A	739	SER
1	B	216	ALA
1	B	710	ASP
1	B	755	ALA
1	B	760	VAL
1	A	49	THR
1	A	113	SER
1	A	178	ALA
1	A	273	ALA
1	A	312	GLU
1	A	375	PRO

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Mol	Chain	Res	Type
1	A	556	GLN
1	B	157	VAL
1	B	254	LEU
1	B	363	ASP
1	B	378	LEU
1	B	506	HIS
1	B	527	ARG
1	B	530	VAL
1	B	603	THR
1	B	617	ARG
1	B	644	ASP
1	A	42	ARG
1	A	123	VAL
1	A	328	VAL
1	A	454	ASP
1	A	499	PRO
1	A	515	SER
1	A	624	LEU
1	A	628	VAL
1	B	34	LEU
1	B	214	PHE
1	B	277	ASN
1	B	454	ASP
1	B	704	GLY
1	A	246	ALA
1	A	329	SER
1	A	471	LEU
1	A	578	TRP
1	B	305	GLU
1	B	568	LEU
1	A	336	ILE
1	A	440	GLY
1	A	428	GLY
1	B	162	GLY
1	B	222	PRO
1	A	280	GLY
1	B	322	ILE
1	B	716	VAL
1	B	118	ILE

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	629/629 (100%)	627 (100%)	2 (0%)	92 95
1	B	629/629 (100%)	628 (100%)	1 (0%)	93 96
All	All	1258/1258 (100%)	1255 (100%)	3 (0%)	93 96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	503	VAL
1	A	519	VAL
1	B	530	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	HIS
1	A	283	GLN
1	A	337	ASN
1	A	345	GLN
1	A	485	ASN
1	A	492	HIS
1	A	506	HIS
1	A	670	ASN
1	A	695	GLN
1	B	27	ASN
1	B	35	GLN
1	B	39	GLN
1	B	72	GLN
1	B	93	HIS
1	B	228	HIS
1	B	384	GLN
1	B	431	ASN
1	B	492	HIS
1	B	497	HIS

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Mol	Chain	Res	Type
1	B	507	GLN
1	B	634	GLN
1	B	669	GLN
1	B	670	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

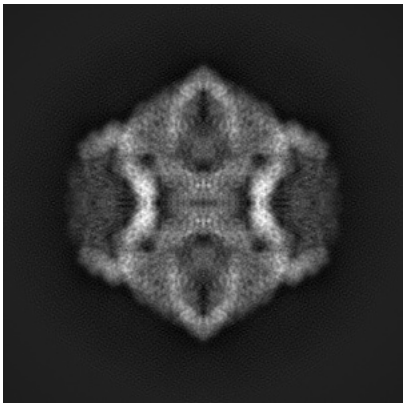
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3185. These allow visual inspection of the internal detail of the map and identification of artifacts.

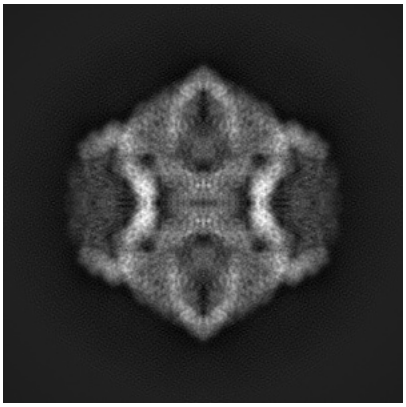
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

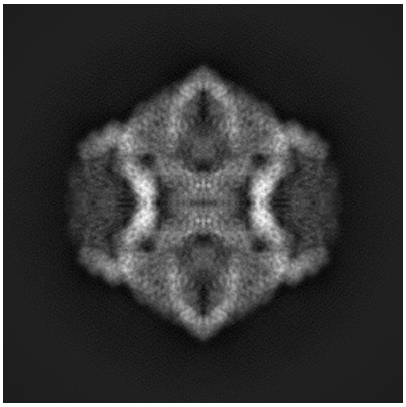
6.1.1 Primary map



X



Y

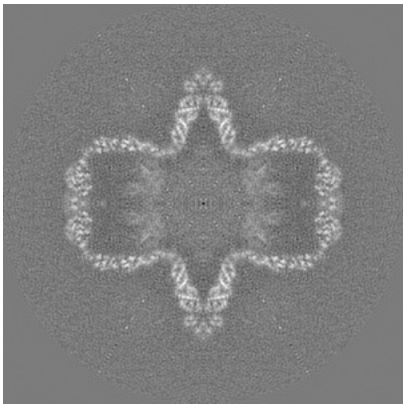


Z

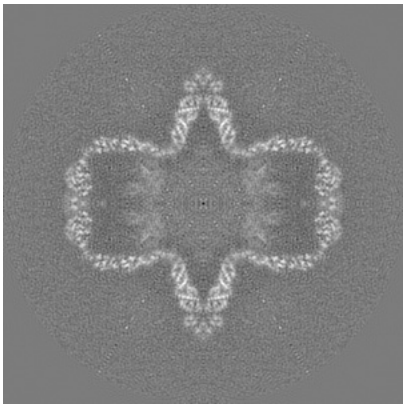
The images above show the map projected in three orthogonal directions.

6.2 Central slices

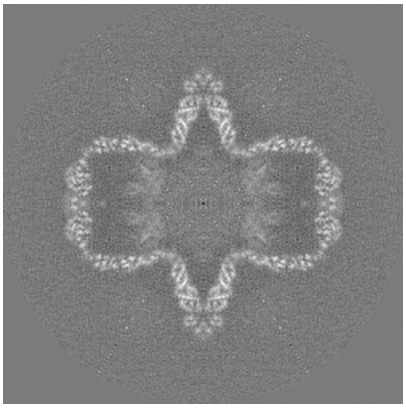
6.2.1 Primary map



X Index: 240



Y Index: 240

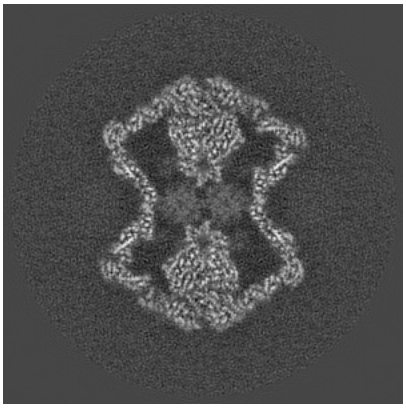


Z Index: 240

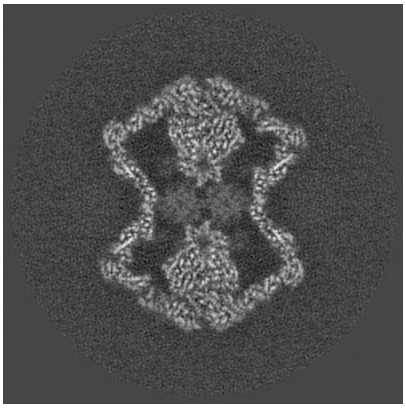
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

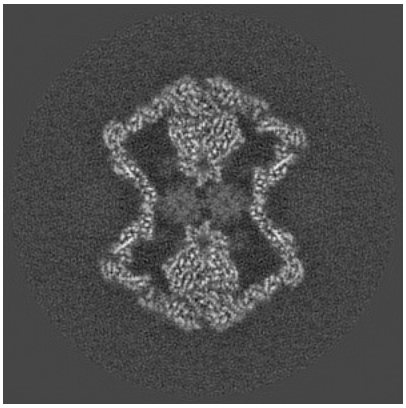
6.3.1 Primary map



X Index: 309



Y Index: 309

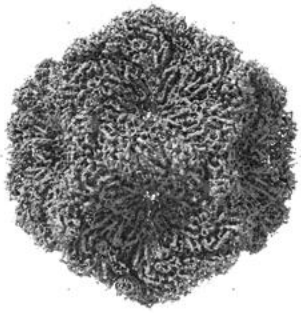


Z Index: 309

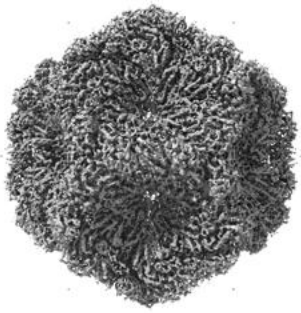
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

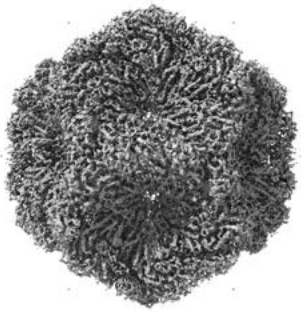
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

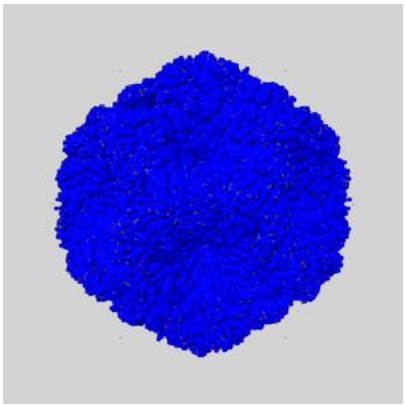
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

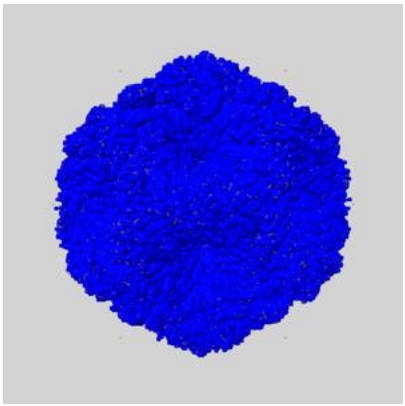
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

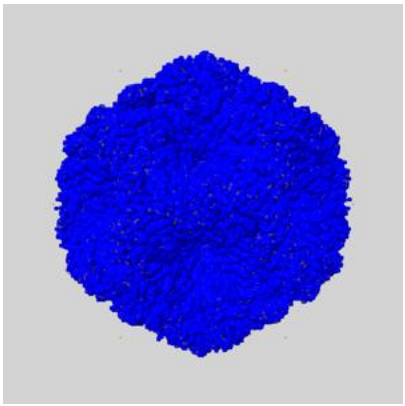
6.5.1 emd_3185_msk.map (i)



X



Y

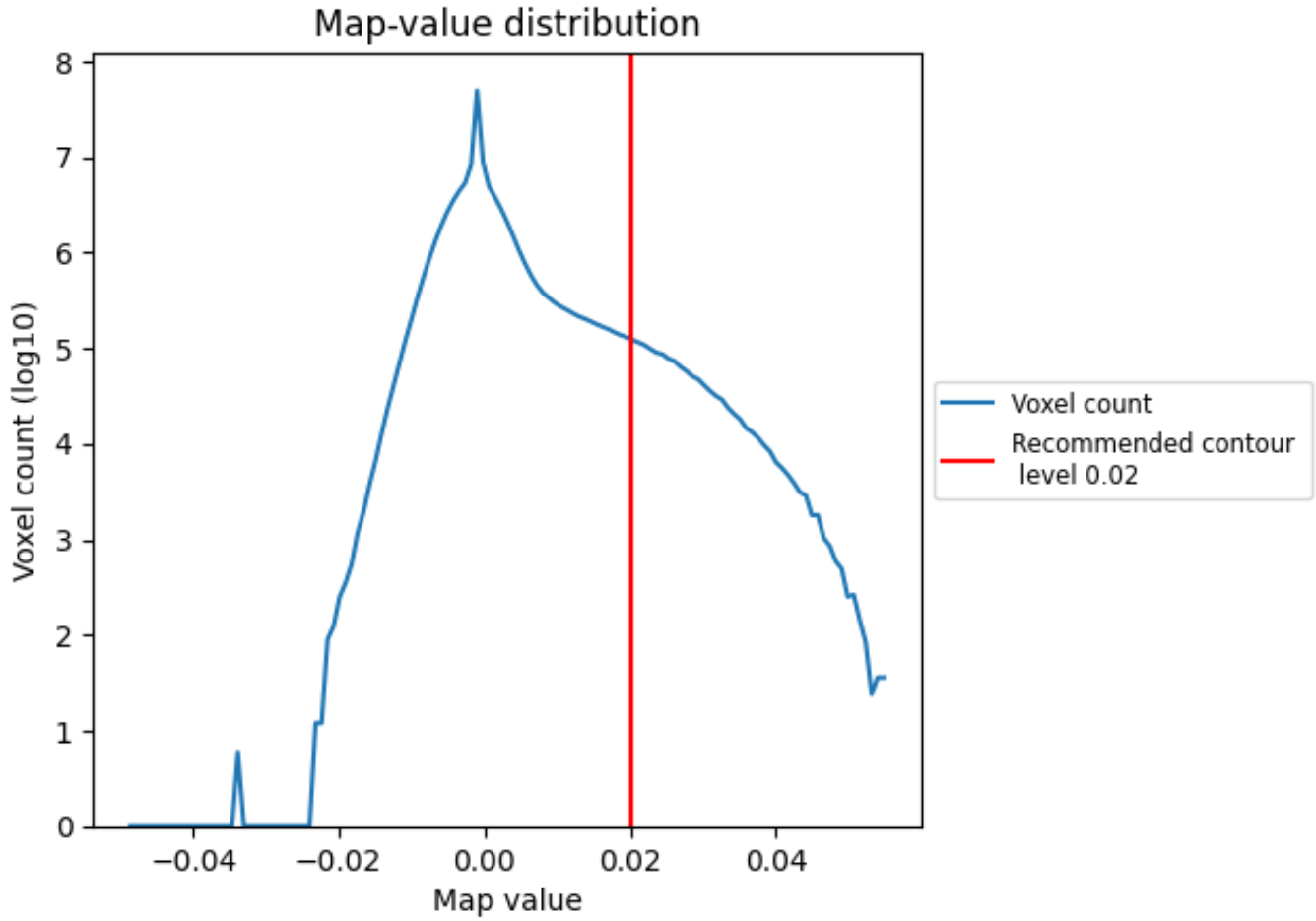


Z

7 Map analysis

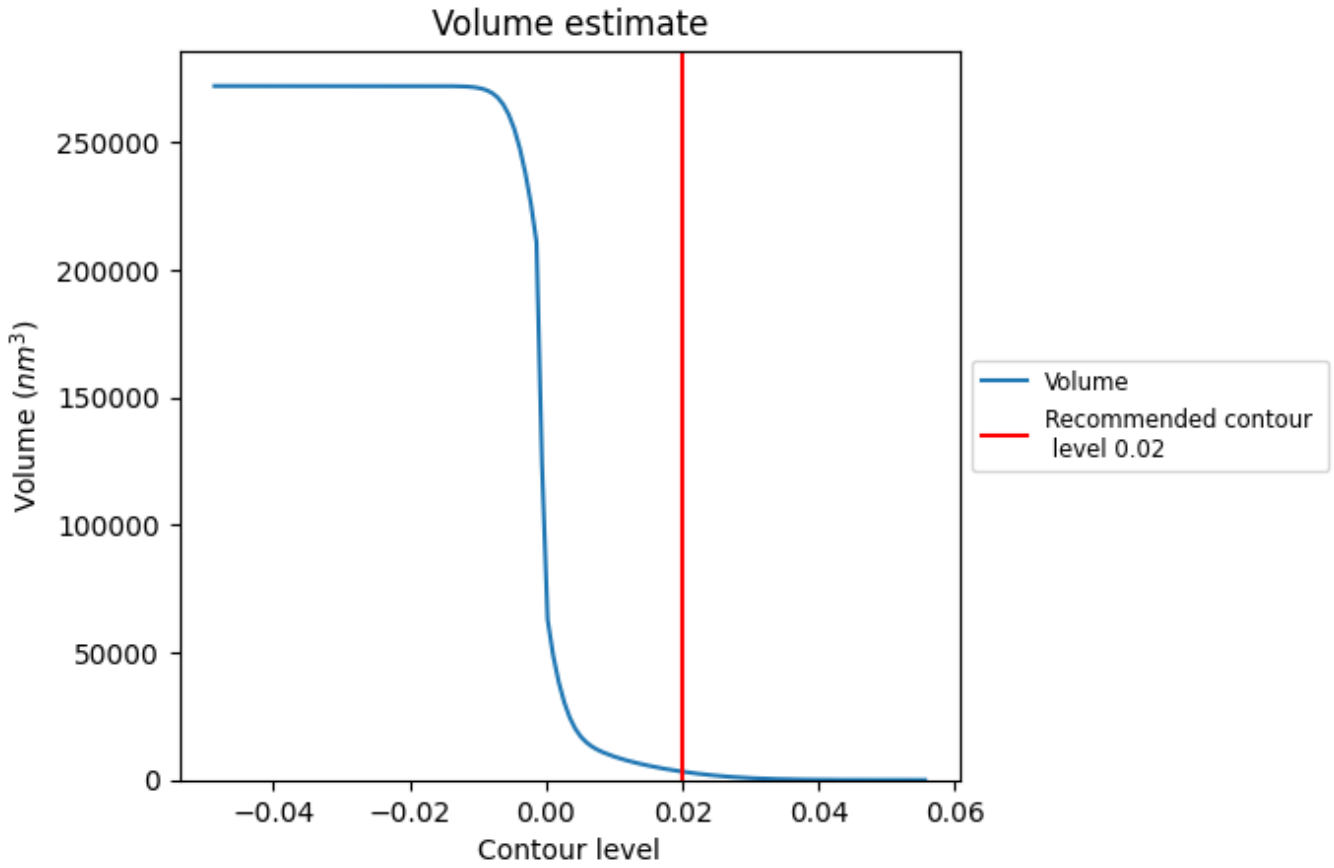
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

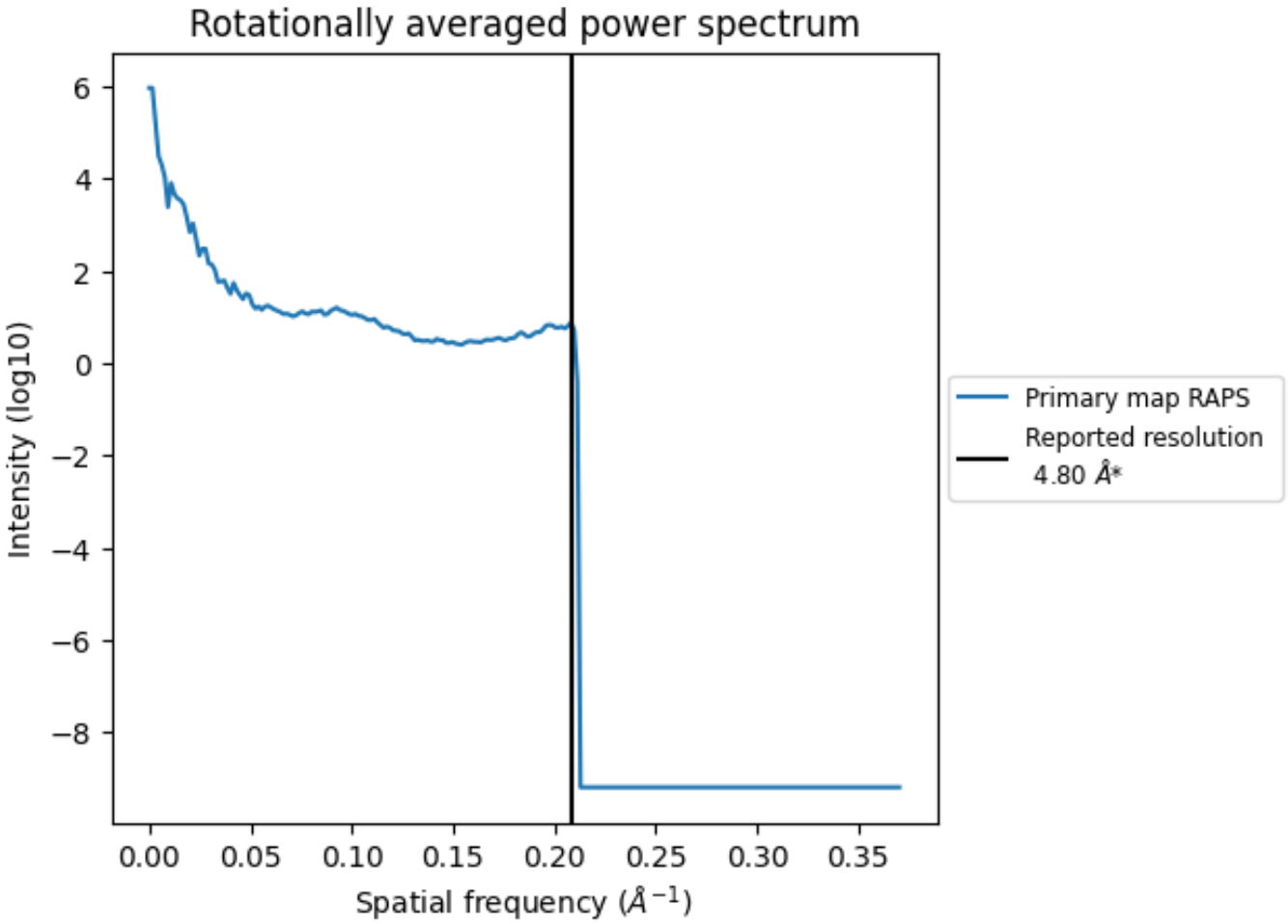
7.2 Volume estimate



The volume at the recommended contour level is 3274 nm^3; this corresponds to an approximate mass of 2957 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)

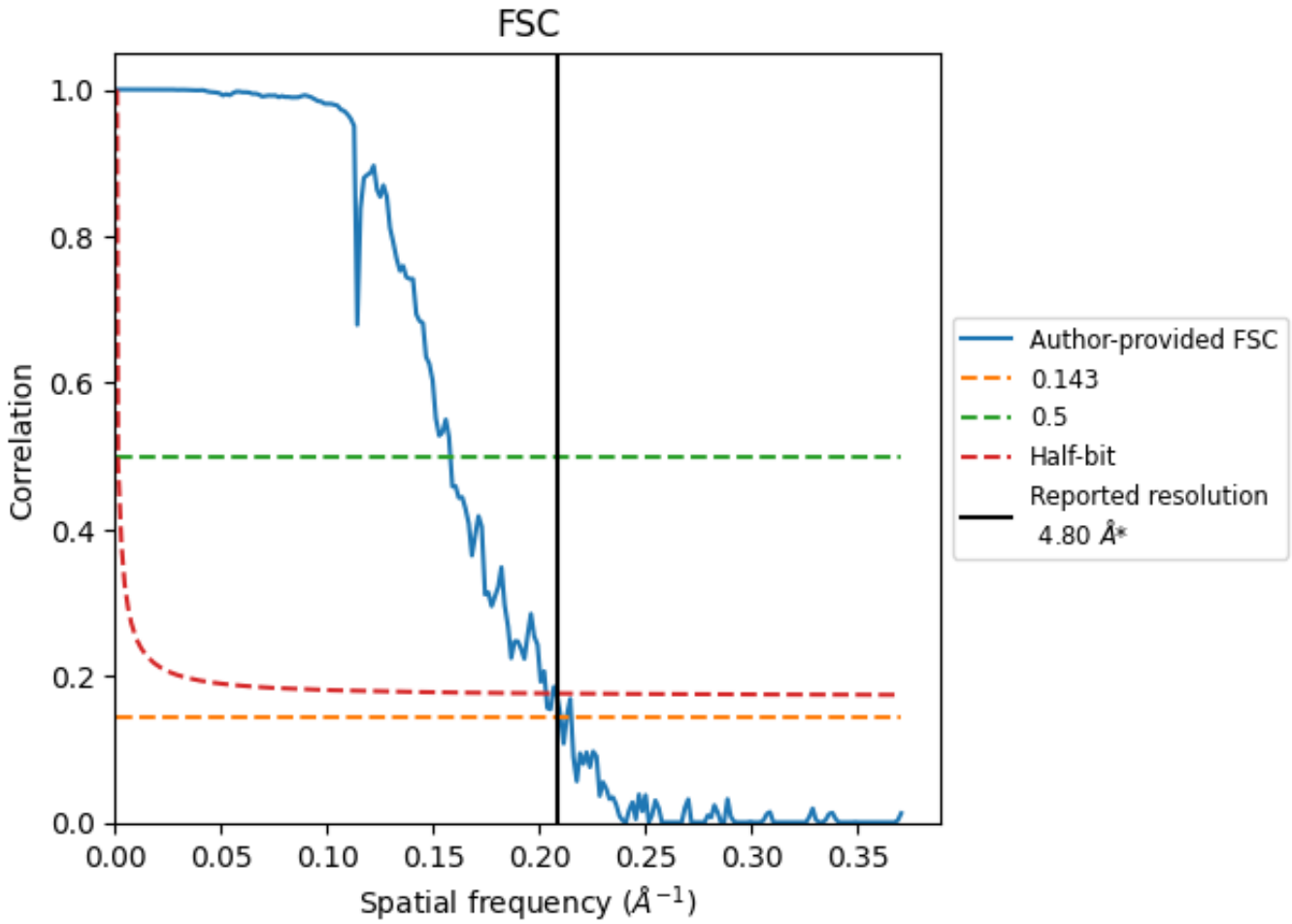


*Reported resolution corresponds to spatial frequency of 0.208 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.208 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	4.76	6.33	4.92
Unmasked-calculated*	-	-	-

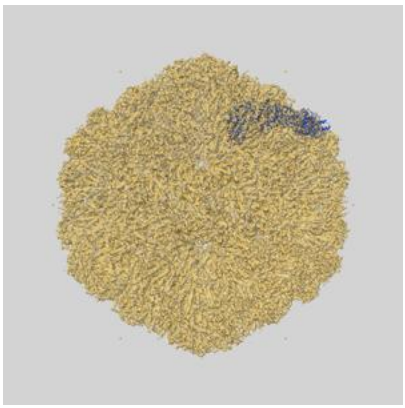
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit

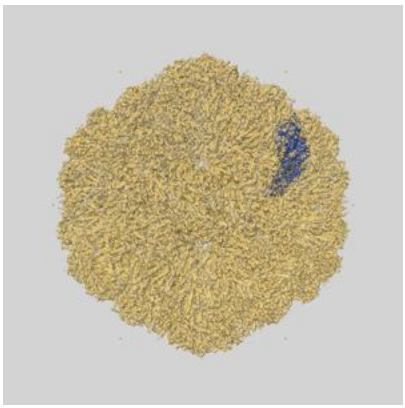
This section contains information regarding the fit between EMDB map EMD-3185 and PDB model 5FJ5. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlays

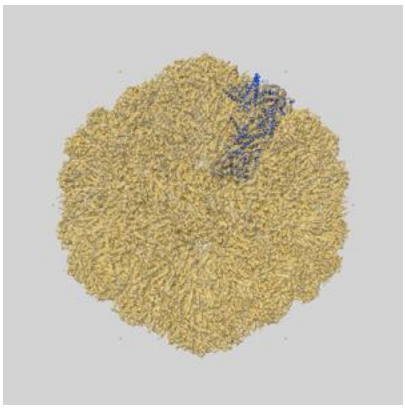
9.1.1 Map-model overlay



X

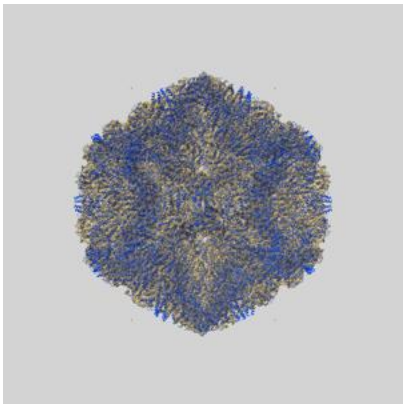


Y

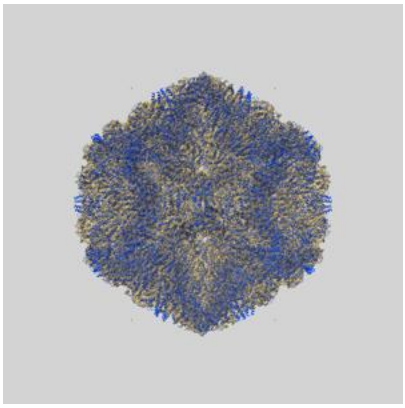


Z

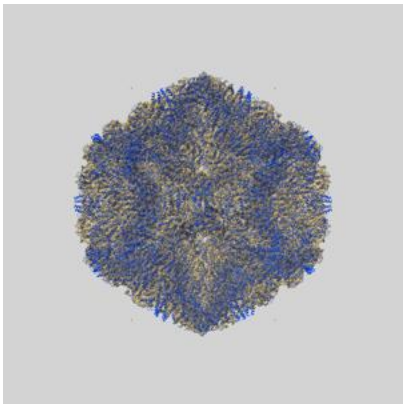
9.1.2 Map-model assembly overlay



X



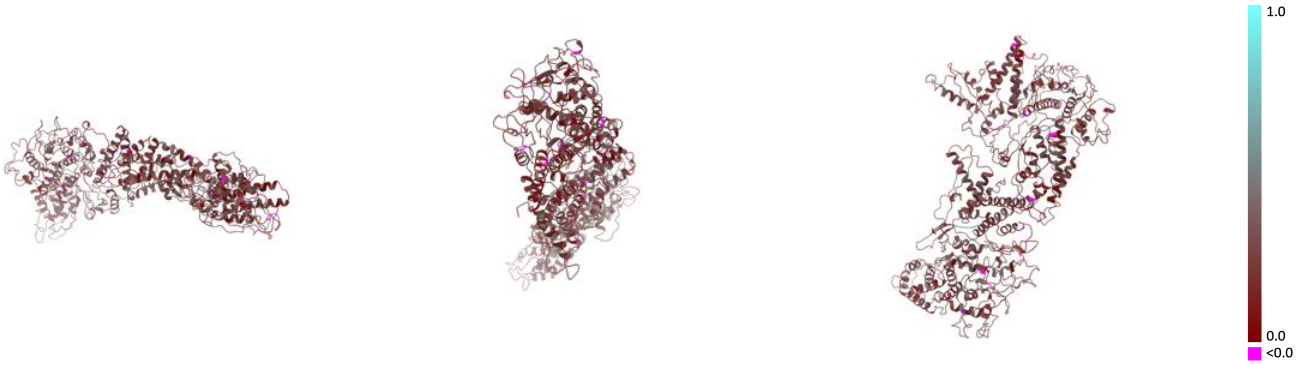
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

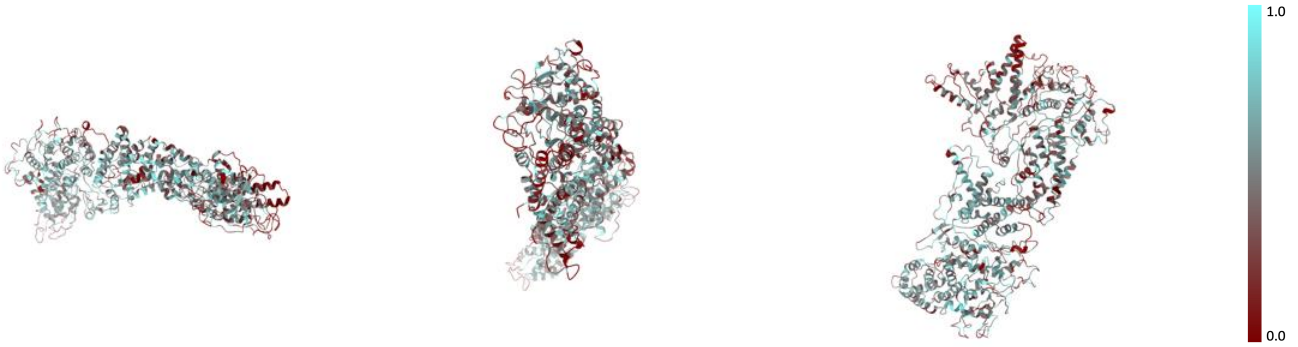
9.2 Q-score mapped to coordinate model (i)



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.

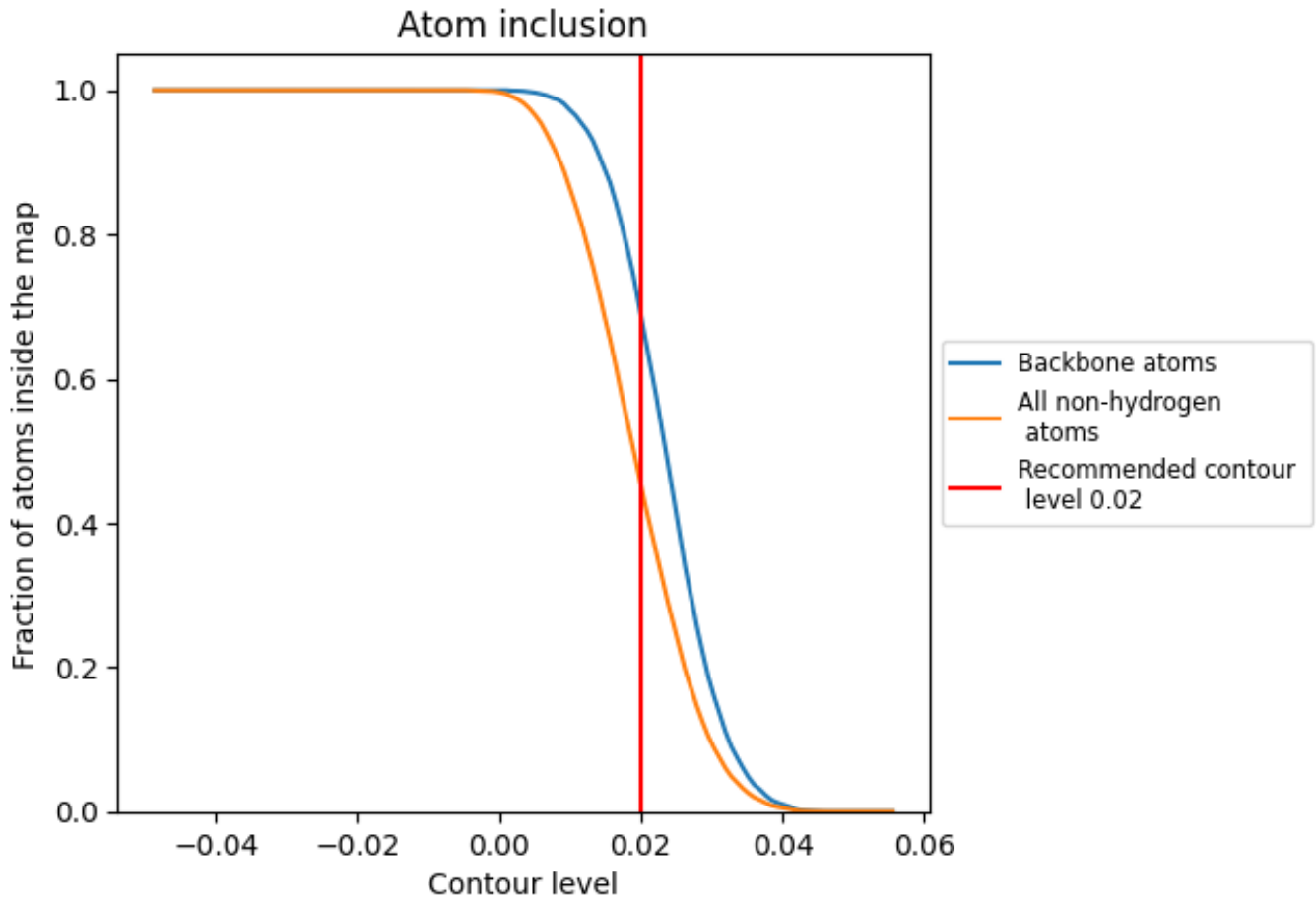
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 69% of all backbone atoms, 46% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4569	0.2720
A	0.5097	0.2860
B	0.4040	0.2590