Full wwPDB EM Validation Report ⓘ

Apr 22, 2024 – 05:06 pm BST

PDB ID	:	7BLR
EMDB ID	:	EMD-12226
Title	:	Vps35/Vps29 arch of fungal membrane-assembled retromer:Vps5 (SNX-BAR) complex.
Authors	:	Leneva, N.; Kovtun, O.; Morado, D.R.; Briggs, J.A.G.; Owen, D.J.
Deposited on	:	2021-01-18
Resolution	:	9.30 Å(reported)

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

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

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

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

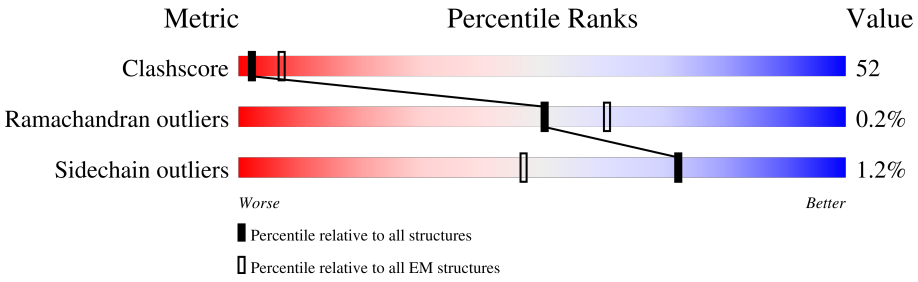
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 9.30 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	869	25% 23% 61% · 14%
1	C	869	25% 26% 59% · 14%
2	B	202	34% 27% 64% · 7%
2	D	202	32% 25% 68% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14950 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 Vacuolar protein sorting-associated protein 35.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	748	Total	C	N	O	S	0	0
			6011	3804	1050	1126	31		
1	C	748	Total	C	N	O	S	0	0
			6011	3804	1050	1126	31		

- Molecule 2 is a protein called Vacuolar protein sorting-associated protein 29.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	187	Total	C	N	O	S	0	0
			1464	946	238	271	9		
2	D	187	Total	C	N	O	S	0	0
			1464	946	238	271	9		

There are 2 discrepancies between the modelled and reference sequences:

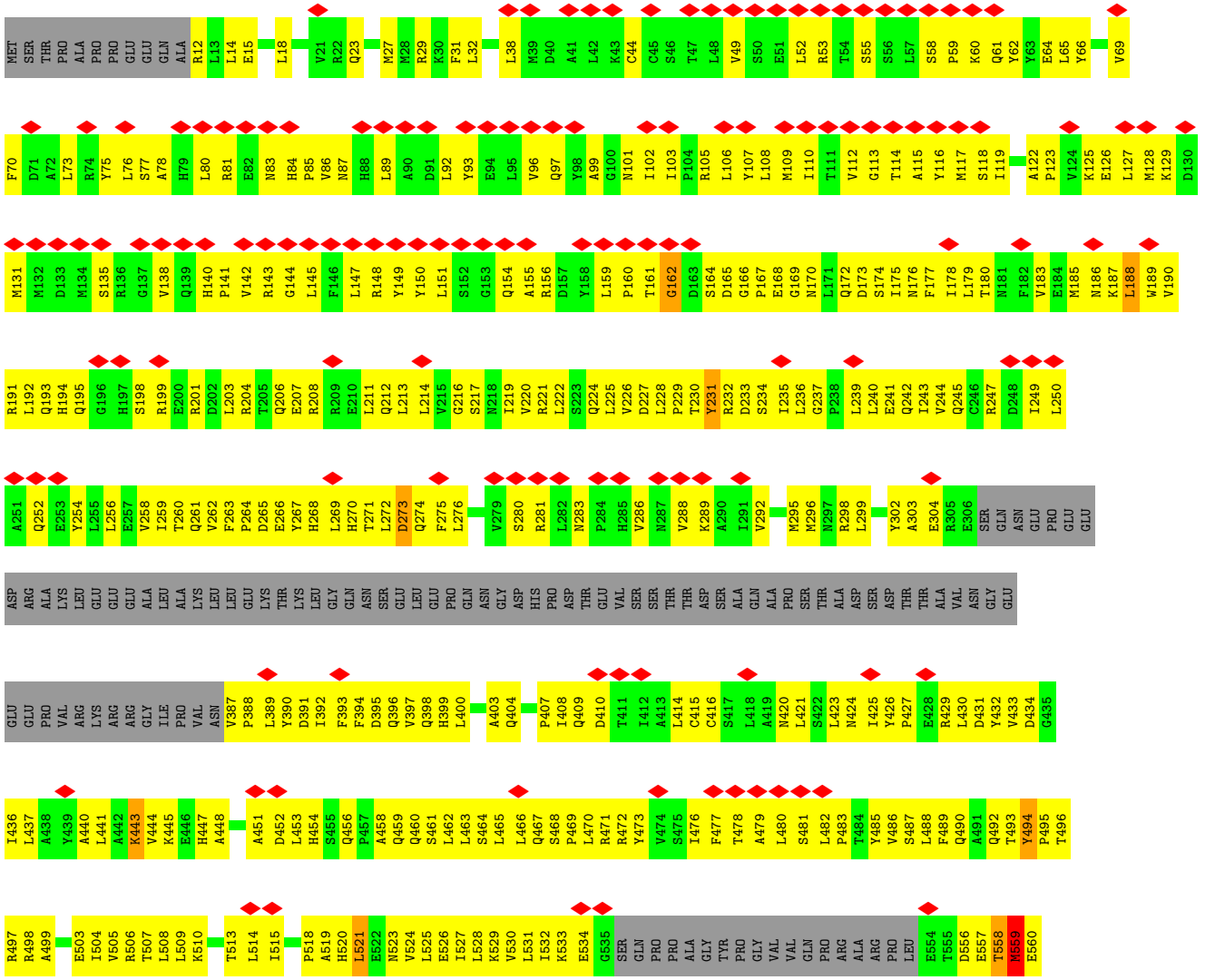
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP G0RZB5
D	0	SER	-	expression tag	UNP G0RZB5

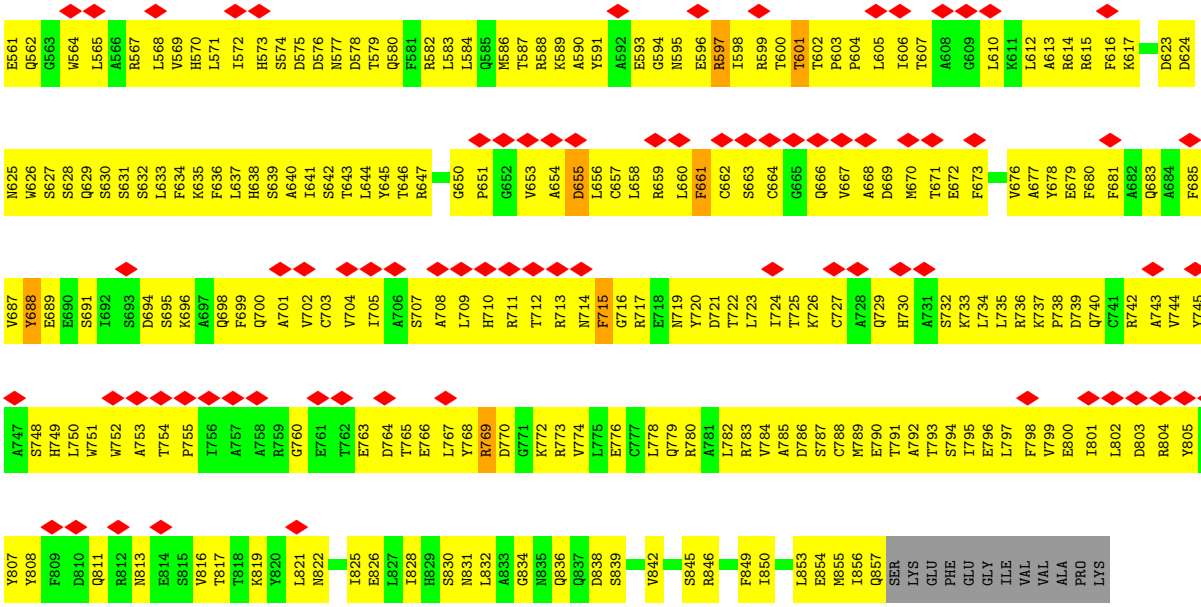
3 Residue-property plots (i)

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: Vacuolar protein sorting-associated protein 35

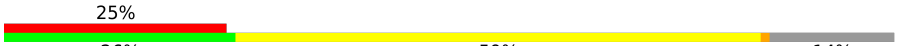
Chain A:

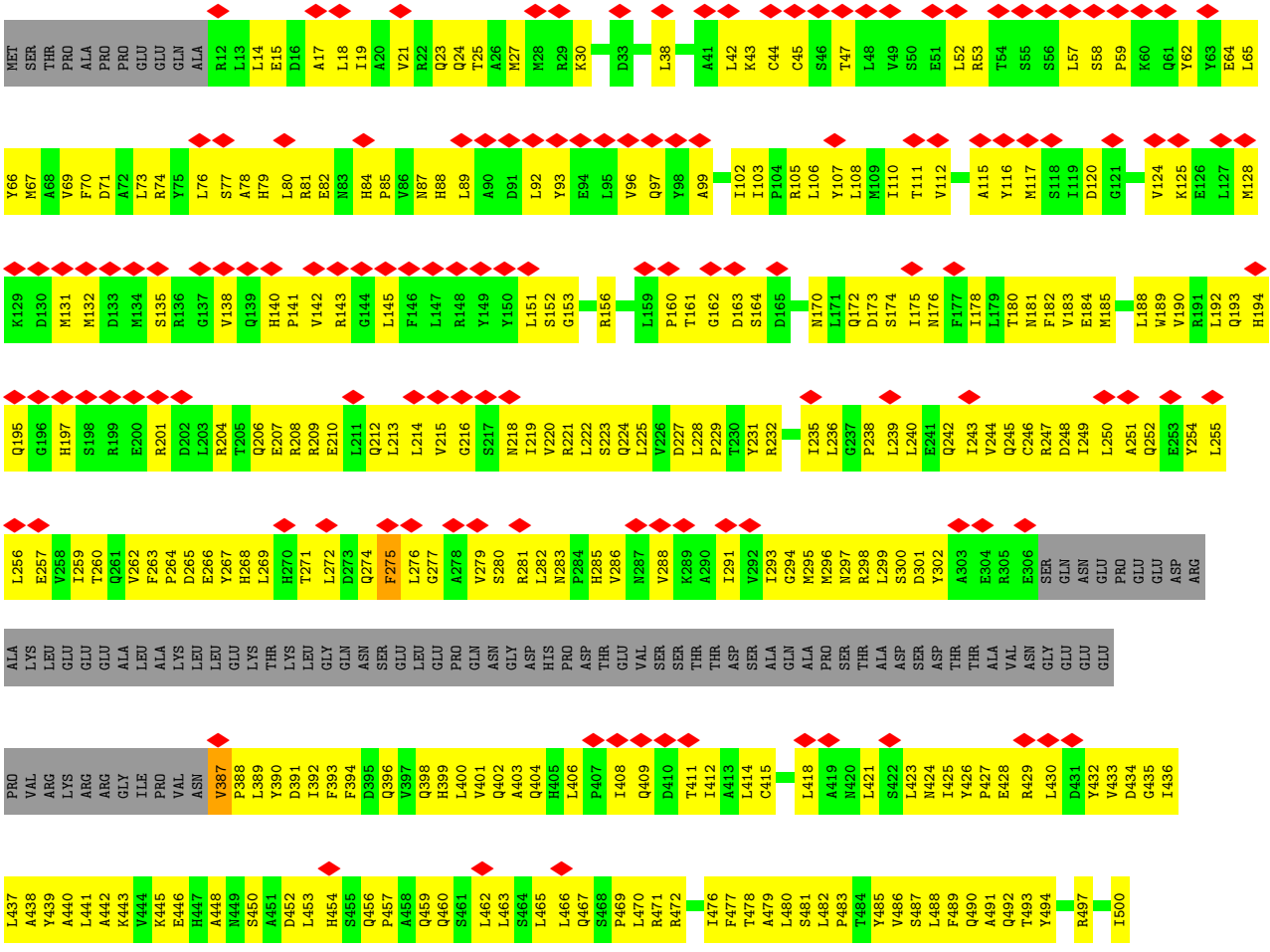


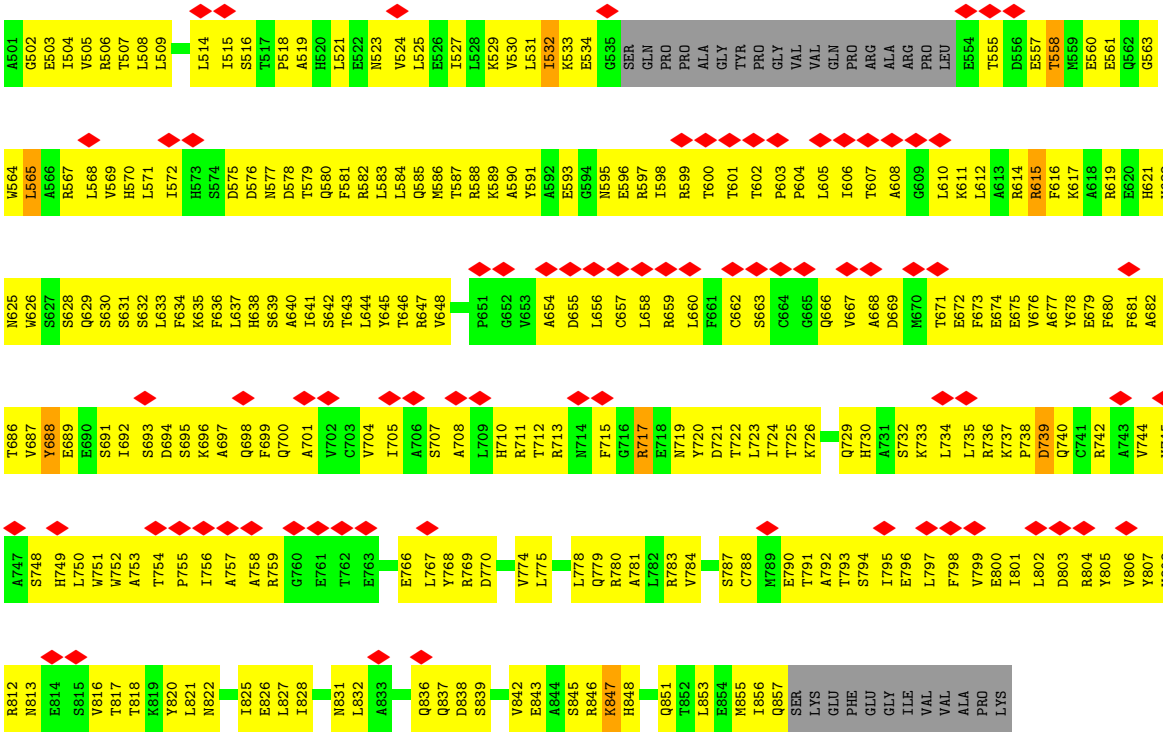


• Molecule 1: Vacuolar protein sorting-associated protein 35

Chain C:

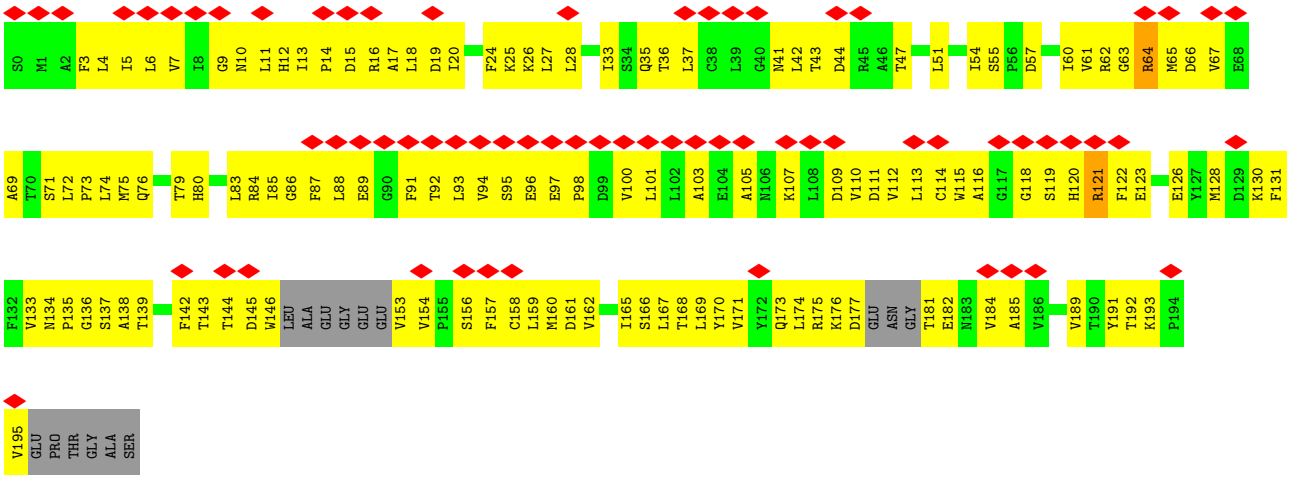






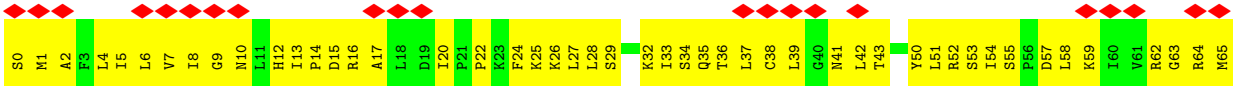
• Molecule 2: Vacuolar protein sorting-associated protein 29

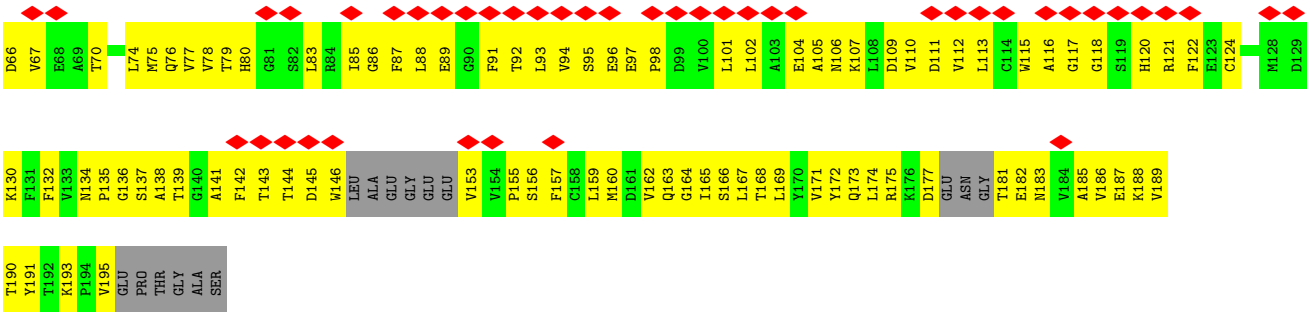
Chain B:



• Molecule 2: Vacuolar protein sorting-associated protein 29

Chain D:




D66 V67 E68 A69 T70 L74 M75 Q76 V77 V78 T79 H80 G81 S82 L83 R84 I85 G86 F87 L88 E89 G90 F91 T92 L93 V94 S95 E96 E97 P98 D99 V100 L101 L102 A103 E104 A105 N106 K107 L108 D109 V110 D111 V112 L113 C114 W115 A116 G117 G118 S119 H120 R121 F122 E123 C124 M128 D129
K130 F131 F132 V133 N134 P135 G136 S137 A138 T139 G140 A141 F142 T143 T144 D145 W146 LEU ALA GLU GLY GLU GLU V153 V154 P155 S156 F157 C158 L159 M160 D161 V162 Q163 G164 I165 S166 L167 T168 L169 Y170 V171 Y172 Q173 L174 R175 K176 D177 GLU ASN GLY T181 E182 N183 V184 A185 V186 E187 K188 V189
T190 Y191 T192 K193 P194 V195 GLU PRO THR GLY ALA SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	18680	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	3.17	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.097	Depositor
Minimum map value	-0.078	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	280.80002, 280.80002, 280.80002	wwPDB
Map dimensions	104, 104, 104	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.7000003, 2.7000003, 2.7000003	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	1.60	6/6125 (0.1%)	0.57	2/8302 (0.0%)
1	C	0.33	0/6125	0.51	0/8302
2	B	0.31	0/1494	0.53	0/2027
2	D	0.32	0/1494	0.54	0/2027
All	All	1.05	6/15238 (0.0%)	0.54	2/20658 (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	3
1	C	0	4
All	All	0	7

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	494	TYR	CD2-CE2	63.05	2.33	1.39
1	A	494	TYR	CD1-CE1	59.46	2.28	1.39
1	A	494	TYR	CE2-CZ	49.11	2.02	1.38
1	A	494	TYR	CE1-CZ	47.99	2.00	1.38
1	A	494	TYR	CG-CD1	36.82	1.87	1.39
1	A	494	TYR	CG-CD2	36.34	1.86	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	521	LEU	CA-CB-CG	-8.59	95.55	115.30
1	A	188	LEU	CA-CB-CG	-5.74	102.09	115.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	558	THR	Peptide
1	A	559	MET	Peptide
1	A	601	THR	Peptide
1	C	387	VAL	Peptide
1	C	428	GLU	Peptide
1	C	532	ILE	Peptide
1	C	558	THR	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	6011	0	5999	676	0
1	C	6011	0	5999	575	0
2	B	1464	0	1484	161	0
2	D	1464	0	1484	168	0
All	All	14950	0	14966	1546	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 52.

All (1546) 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:A:494:TYR:CG	1:A:494:TYR:CD2	1.86	1.62
1:A:494:TYR:CG	1:A:494:TYR:CD1	1.87	1.60
1:A:494:TYR:CE1	1:A:494:TYR:CZ	2.00	1.47
1:A:494:TYR:CZ	1:A:494:TYR:CE2	2.02	1.45
1:A:494:TYR:CD1	1:A:494:TYR:CE1	2.28	1.22
1:A:494:TYR:CD2	1:A:494:TYR:CE2	2.33	1.15
1:C:626:TRP:O	1:C:630:SER:HB3	1.49	1.12
1:A:468:SER:O	1:A:472:ARG:HB2	1.57	1.02
1:A:751:TRP:N	1:A:768:TYR:O	1.97	0.97
1:A:518:PRO:HA	1:A:521:LEU:HD12	1.47	0.96
1:C:751:TRP:HB3	1:C:770:ASP:HB2	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:TYR:HB2	1:A:476:ILE:HG13	1.46	0.94
1:A:191:ARG:HG2	1:A:195:GLN:HB3	1.53	0.91
1:A:443:LYS:O	1:A:447:HIS:HB3	1.71	0.91
1:A:558:THR:HB	1:A:562:GLN:HB2	1.52	0.90
1:C:388:PRO:HB2	1:C:391:ASP:HB2	1.54	0.90
1:A:454:HIS:HA	1:A:459:GLN:HG2	1.54	0.89
2:B:61:VAL:HG12	2:B:75:MET:HA	1.54	0.89
2:B:36:THR:H	2:B:57:ASP:HB3	1.39	0.87
1:C:442:ALA:HB1	1:C:488:LEU:HD11	1.55	0.87
1:C:655:ASP:HA	1:C:658:LEU:HD12	1.56	0.86
1:C:742:ARG:HA	1:C:745:TYR:CE1	2.10	0.85
2:D:115:TRP:H	2:D:135:PRO:HG3	1.38	0.85
1:A:498:ARG:NH1	1:A:531:LEU:O	2.09	0.85
1:A:565:LEU:HD13	1:A:568:LEU:HD23	1.57	0.84
1:C:717:ARG:HA	1:C:720:TYR:HB3	1.59	0.84
2:B:159:LEU:HB2	2:B:170:TYR:HB2	1.60	0.84
1:A:463:LEU:O	1:A:467:GLN:NE2	2.10	0.84
1:A:750:LEU:H	1:A:770:ASP:HB2	1.43	0.83
1:A:470:LEU:HA	1:A:476:ILE:HG12	1.61	0.82
1:A:85:PRO:HB3	1:A:119:ILE:HD13	1.60	0.82
1:A:258:VAL:O	1:A:262:VAL:HB	1.79	0.82
1:A:702:VAL:HA	1:A:705:ILE:HD12	1.61	0.81
1:A:746:LEU:O	1:A:749:HIS:NE2	2.13	0.81
1:C:529:LYS:HD2	1:C:533:LYS:HD2	1.59	0.81
1:A:408:ILE:HD13	1:A:453:LEU:HD22	1.62	0.81
1:A:470:LEU:HD23	1:A:476:ILE:HG21	1.62	0.81
2:B:93:LEU:HG	2:B:95:SER:H	1.44	0.81
2:B:138:ALA:HA	2:B:156:SER:H	1.46	0.81
1:A:639:SER:O	1:A:643:THR:OG1	2.00	0.80
2:B:118:GLY:O	2:B:144:THR:OG1	1.99	0.80
1:A:588:ARG:NH2	1:A:643:THR:OG1	2.12	0.80
1:C:587:THR:O	1:C:591:TYR:N	2.14	0.80
1:C:632:SER:HA	1:C:635:LYS:HD2	1.64	0.80
1:A:426:TYR:HB3	1:A:429:ARG:HB2	1.63	0.80
1:C:467:GLN:OE1	1:C:471:ARG:NH2	2.14	0.80
1:C:532:ILE:HD11	1:C:597:ARG:HB3	1.64	0.80
2:D:120:HIS:ND1	2:D:141:ALA:O	2.14	0.80
1:A:483:PRO:O	1:A:487:SER:N	2.12	0.79
1:C:732:SER:OG	1:C:733:LYS:NZ	2.14	0.79
2:D:173:GLN:HB2	2:D:175:ARG:HE	1.47	0.79
1:C:249:ILE:HG12	1:C:285:HIS:HB3	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:113:LEU:HB3	2:D:115:TRP:HZ3	1.46	0.79
1:A:632:SER:HA	1:A:635:LYS:HD2	1.64	0.79
1:C:726:LYS:O	1:C:730:HIS:ND1	2.13	0.79
1:C:577:ASN:HB2	1:C:615:ARG:HE	1.48	0.79
1:A:742:ARG:HA	1:A:745:TYR:CZ	2.17	0.79
1:A:299:LEU:HB2	1:A:421:LEU:HD11	1.64	0.78
1:C:792:ALA:HA	1:C:795:ILE:HD12	1.63	0.78
1:A:642:SER:O	1:A:646:THR:N	2.16	0.78
2:D:24:PHE:O	2:D:28:LEU:N	2.16	0.78
1:A:268:HIS:O	1:A:272:LEU:N	2.16	0.78
1:C:42:LEU:HD11	1:C:111:THR:HG21	1.64	0.78
2:B:176:LYS:HA	2:B:182:GLU:HA	1.65	0.78
1:C:812:ARG:NH1	1:C:813:ASN:O	2.16	0.78
1:A:601:THR:HG22	1:A:605:LEU:HD11	1.66	0.78
1:A:221:ARG:O	1:A:221:ARG:NH1	2.17	0.77
1:A:737:LYS:HD3	1:A:785:ALA:HA	1.66	0.77
2:D:64:ARG:NH2	2:D:116:ALA:O	2.17	0.77
1:C:99:ALA:O	1:C:105:ARG:NH2	2.17	0.77
1:C:221:ARG:O	1:C:221:ARG:NH1	2.17	0.77
1:A:125:LYS:HD3	1:A:173:ASP:HB3	1.65	0.77
1:A:655:ASP:HA	1:A:658:LEU:HD22	1.65	0.77
2:B:13:ILE:O	2:B:43:THR:N	2.17	0.76
1:A:443:LYS:O	1:A:447:HIS:CB	2.32	0.76
1:A:570:HIS:HA	1:A:573:HIS:CE1	2.21	0.76
1:A:296:MET:HG2	1:A:421:LEU:HD22	1.66	0.76
2:D:83:LEU:HD12	2:D:162:VAL:HG13	1.66	0.76
1:C:390:TYR:OH	1:C:432:TYR:O	2.02	0.76
1:A:156:ARG:HG3	1:A:221:ARG:HD3	1.67	0.76
1:A:161:THR:HG22	1:A:162:GLY:H	1.49	0.76
1:C:485:TYR:O	1:C:489:PHE:N	2.16	0.76
1:A:101:ASN:O	1:A:105:ARG:NH2	2.18	0.76
2:B:121:ARG:NH1	2:B:134:ASN:O	2.17	0.76
1:C:388:PRO:O	1:C:392:ILE:N	2.14	0.76
1:A:533:LYS:HG3	1:A:534:GLU:HA	1.68	0.75
1:C:818:THR:HA	1:C:821:LEU:HD13	1.68	0.75
1:A:715:PHE:HB3	1:A:719:ASN:HB2	1.68	0.75
1:C:52:LEU:HD12	1:C:65:LEU:HB3	1.68	0.75
1:C:682:ALA:HA	1:C:685:PHE:HD2	1.51	0.75
1:C:27:MET:HA	1:C:30:LYS:HD2	1.67	0.75
1:C:643:THR:O	1:C:647:ARG:NH2	2.20	0.75
1:A:473:TYR:HD2	1:A:476:ILE:HA	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:TYR:O	1:A:394:PHE:HB3	1.87	0.75
1:C:569:VAL:HG11	1:C:604:PRO:HB3	1.69	0.75
1:C:681:PHE:HE1	1:C:708:ALA:HB1	1.50	0.75
1:C:800:GLU:O	1:C:804:ARG:NH1	2.19	0.75
1:A:52:LEU:O	1:A:62:TYR:OH	2.05	0.74
1:C:847:LYS:NZ	2:D:106:ASN:O	2.19	0.74
2:D:41:ASN:HD21	2:D:65:MET:H	1.33	0.74
1:A:659:ARG:NH1	1:A:663:SER:OG	2.21	0.74
2:B:167:LEU:N	2:B:191:TYR:O	2.16	0.74
1:A:467:GLN:O	1:A:471:ARG:N	2.17	0.74
1:C:220:VAL:O	1:C:224:GLN:NE2	2.21	0.74
1:C:724:ILE:HG23	1:C:750:LEU:HB3	1.69	0.74
1:C:843:GLU:HA	1:C:846:ARG:HD2	1.69	0.74
1:A:575:ASP:O	1:A:615:ARG:NH1	2.20	0.74
1:C:477:PHE:HA	1:C:480:LEU:HB2	1.69	0.74
1:A:729:GLN:NE2	1:C:692:ILE:O	2.20	0.73
1:A:219:ILE:HG22	1:A:262:VAL:HG21	1.70	0.73
1:A:156:ARG:NH2	1:A:217:SER:O	2.22	0.73
1:C:674:GLU:HA	1:C:677:ALA:HB3	1.69	0.73
1:C:694:ASP:O	1:C:698:GLN:N	2.20	0.73
2:B:173:GLN:O	2:B:185:ALA:N	2.21	0.73
1:A:521:LEU:HD13	1:A:583:LEU:HD22	1.71	0.73
1:A:634:PHE:HA	1:A:637:LEU:HD12	1.69	0.73
1:A:569:VAL:HA	1:A:572:ILE:HD12	1.69	0.73
1:C:610:LEU:O	1:C:614:ARG:NH2	2.22	0.73
1:A:186:ASN:ND2	1:A:242:GLN:OE1	2.21	0.73
1:A:415:CYS:HB3	1:A:441:LEU:HD11	1.71	0.73
1:A:141:PRO:HG3	1:A:191:ARG:HD2	1.70	0.72
1:A:492:GLN:O	1:A:497:ARG:NE	2.21	0.72
1:A:832:LEU:HD11	1:A:842:VAL:HG13	1.70	0.72
1:C:436:ILE:O	1:C:441:LEU:N	2.21	0.72
1:A:170:ASN:H	1:A:173:ASP:HB2	1.53	0.72
1:C:631:SER:HA	1:C:634:PHE:HD2	1.54	0.72
2:D:10:ASN:HD22	2:D:137:SER:HA	1.54	0.72
1:A:602:THR:HG22	1:A:606:ILE:HD11	1.72	0.72
2:B:12:HIS:ND1	2:B:16:ARG:HG3	2.05	0.72
1:C:81:ARG:NH2	1:C:82:GLU:OE2	2.22	0.72
1:C:723:LEU:HA	1:C:726:LYS:HD2	1.69	0.72
1:C:748:SER:HB3	1:C:774:VAL:HG13	1.71	0.72
2:D:24:PHE:HA	2:D:27:LEU:HB2	1.69	0.72
1:A:273:ASP:OD1	1:A:273:ASP:N	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:754:THR:HA	1:C:767:LEU:HD22	1.72	0.72
2:D:113:LEU:HD22	2:D:132:PHE:HA	1.72	0.72
1:A:792:ALA:HA	1:A:795:ILE:HD12	1.71	0.71
1:C:265:ASP:OD1	1:C:298:ARG:NH1	2.21	0.71
1:C:737:LYS:NZ	1:C:784:VAL:O	2.23	0.71
1:A:400:LEU:O	1:A:404:GLN:N	2.18	0.71
1:A:742:ARG:NH2	2:B:92:THR:O	2.23	0.71
1:C:606:ILE:HG13	1:C:660:LEU:HD13	1.72	0.71
1:A:142:VAL:HA	1:A:188:LEU:HD22	1.73	0.71
1:A:421:LEU:HA	1:A:424:ASN:HD22	1.54	0.71
2:B:62:ARG:NE	2:B:72:LEU:O	2.13	0.71
1:C:518:PRO:HA	1:C:521:LEU:HD12	1.70	0.71
2:B:19:ASP:OD1	2:B:25:LYS:NZ	2.24	0.71
2:D:7:VAL:HA	2:D:39:LEU:HD11	1.72	0.71
2:B:33:ILE:HG22	2:B:35:GLN:H	1.56	0.70
1:C:387:VAL:O	1:C:389:LEU:N	2.24	0.70
1:C:584:LEU:HD11	1:C:612:LEU:HD23	1.72	0.70
2:B:85:ILE:HA	2:B:112:VAL:HB	1.71	0.70
1:C:519:ALA:O	1:C:523:ASN:ND2	2.21	0.70
1:A:483:PRO:HA	1:A:486:VAL:HG22	1.72	0.70
1:A:504:ILE:O	1:A:507:THR:OG1	2.08	0.70
1:A:602:THR:HA	1:A:605:LEU:HD12	1.74	0.70
1:A:454:HIS:HE1	1:A:496:THR:HG23	1.57	0.70
2:B:41:ASN:OD1	2:B:65:MET:N	2.25	0.70
2:B:10:ASN:HD21	2:B:116:ALA:HB1	1.57	0.70
1:C:711:ARG:HH22	2:D:143:THR:HG21	1.56	0.70
1:A:228:LEU:HD13	1:A:267:TYR:HA	1.74	0.70
1:A:436:ILE:HG23	1:A:441:LEU:HD23	1.74	0.70
1:C:231:TYR:HA	1:C:235:ILE:HD12	1.73	0.69
1:C:680:PHE:HA	1:C:683:GLN:HG2	1.72	0.69
2:D:51:LEU:HA	2:D:54:ILE:HG12	1.74	0.69
1:A:610:LEU:HB3	1:A:667:VAL:HG21	1.74	0.69
1:C:96:VAL:HB	1:C:105:ARG:HG2	1.74	0.69
2:D:10:ASN:HD21	2:D:39:LEU:HD22	1.58	0.69
1:C:71:ASP:HA	1:C:74:ARG:HD3	1.74	0.69
1:A:465:LEU:O	1:A:468:SER:OG	2.08	0.69
1:A:670:MET:HE1	2:B:146:TRP:HA	1.75	0.69
1:A:752:TRP:HD1	1:A:769:ARG:HH11	1.40	0.69
1:A:416:CYS:HG	1:A:461:SER:HG	1.26	0.69
1:A:617:LYS:NZ	1:A:670:MET:O	2.24	0.69
2:B:41:ASN:HD21	2:B:64:ARG:H	1.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:16:ARG:HD2	2:D:142:PHE:HZ	1.56	0.69
1:C:596:GLU:O	1:C:599:ARG:NH1	2.26	0.69
1:C:524:VAL:HA	1:C:527:ILE:HD12	1.74	0.69
1:A:191:ARG:O	1:A:195:GLN:N	2.26	0.68
1:A:444:VAL:O	1:A:448:ALA:N	2.22	0.68
1:C:736:ARG:O	1:C:740:GLN:HB2	1.92	0.68
2:D:173:GLN:H	2:D:185:ALA:HB3	1.57	0.68
1:C:533:LYS:HE3	1:C:593:GLU:HA	1.75	0.68
1:C:423:LEU:HB3	1:C:472:ARG:HG2	1.74	0.68
2:D:50:TYR:O	2:D:53:SER:OG	2.09	0.68
1:A:276:LEU:HD13	1:A:396:GLN:HG2	1.73	0.68
1:A:579:THR:HG23	1:A:582:ARG:HE	1.58	0.68
1:A:668:ALA:HB3	1:A:677:ALA:HB2	1.76	0.68
1:A:240:LEU:HA	1:A:243:ILE:HD12	1.76	0.68
1:A:641:ILE:HD13	1:A:661:PHE:HE1	1.59	0.68
1:C:478:THR:O	1:C:481:SER:OG	2.10	0.68
1:A:726:LYS:O	1:A:730:HIS:ND1	2.26	0.68
1:C:145:LEU:HD12	1:C:185:MET:HA	1.74	0.68
1:C:766:GLU:HG3	1:C:767:LEU:H	1.59	0.68
1:C:576:ASP:O	1:C:580:GLN:HG3	1.94	0.68
1:C:485:TYR:HA	1:C:488:LEU:HB2	1.75	0.67
1:A:628:SER:O	1:A:631:SER:OG	2.07	0.67
1:C:694:ASP:OD1	1:C:696:LYS:NZ	2.28	0.67
1:A:420:ASN:HA	1:A:423:LEU:HD12	1.75	0.67
1:A:424:ASN:OD1	1:A:472:ARG:NH1	2.27	0.67
1:A:519:ALA:O	1:A:523:ASN:ND2	2.28	0.67
1:C:758:ALA:HB1	1:C:768:TYR:HB2	1.74	0.67
2:D:20:ILE:HB	2:D:25:LYS:HE2	1.74	0.67
2:D:35:GLN:HA	2:D:57:ASP:HB3	1.75	0.67
1:C:808:TYR:HB3	1:C:813:ASN:HB2	1.76	0.67
2:D:12:HIS:HB3	2:D:16:ARG:NE	2.09	0.67
1:A:55:SER:OG	1:A:143:ARG:NH1	2.27	0.67
1:A:468:SER:O	1:A:472:ARG:CB	2.38	0.67
1:C:99:ALA:HB3	1:C:105:ARG:HD2	1.75	0.67
1:C:85:PRO:HG3	1:C:115:ALA:HB1	1.76	0.67
1:A:576:ASP:OD2	1:A:615:ARG:NH2	2.27	0.67
1:A:624:ASP:O	1:A:627:SER:OG	2.12	0.67
1:C:271:THR:HA	1:C:274:GLN:HE22	1.59	0.67
1:A:247:ARG:NH1	1:A:283:ASN:OD1	2.28	0.66
2:B:173:GLN:HB2	2:B:185:ALA:HB3	1.77	0.66
1:A:445:LYS:HE2	1:A:462:LEU:HD21	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:778:LEU:HD11	1:C:801:ILE:HG23	1.78	0.66
2:B:169:LEU:N	2:B:189:VAL:O	2.24	0.66
1:C:667:VAL:O	1:C:671:THR:N	2.18	0.66
1:A:110:ILE:HD13	1:A:147:LEU:HD11	1.77	0.66
1:C:260:THR:O	1:C:298:ARG:NH2	2.29	0.66
1:A:145:LEU:HD13	1:A:188:LEU:HD23	1.77	0.66
1:A:489:PHE:HA	1:A:492:GLN:HE22	1.59	0.66
1:A:579:THR:O	1:A:583:LEU:HG	1.94	0.66
1:A:688:TYR:O	1:A:691:SER:N	2.29	0.66
1:C:588:ARG:HA	1:C:591:TYR:HB2	1.77	0.66
1:C:14:LEU:HD22	1:C:57:LEU:HD13	1.76	0.66
1:C:755:PRO:HB3	2:D:94:VAL:HG22	1.78	0.66
2:D:13:ILE:HG13	2:D:14:PRO:HA	1.77	0.66
2:D:76:GLN:NE2	2:D:77:VAL:O	2.29	0.66
1:A:716:GLY:O	1:A:720:TYR:N	2.27	0.66
2:D:16:ARG:NH2	2:D:65:MET:SD	2.69	0.66
1:A:187:LYS:NZ	1:A:245:GLN:OE1	2.27	0.66
1:A:655:ASP:N	1:A:655:ASP:OD1	2.28	0.66
1:C:423:LEU:HD22	1:C:469:PRO:HA	1.76	0.66
2:B:12:HIS:HB3	2:B:16:ARG:H	1.61	0.65
1:A:303:ALA:HB2	1:A:425:ILE:HD13	1.79	0.65
1:A:567:ARG:NH2	2:B:18:LEU:O	2.29	0.65
1:A:591:TYR:HA	1:A:593:GLU:OE2	1.95	0.65
1:C:769:ARG:NH2	1:C:811:GLN:O	2.25	0.65
2:D:120:HIS:O	2:D:153:VAL:N	2.29	0.65
1:A:751:TRP:HZ3	1:A:772:LYS:HB2	1.62	0.65
1:A:29:ARG:HD3	1:A:32:LEU:HD21	1.78	0.65
1:A:467:GLN:HA	1:A:470:LEU:HD12	1.77	0.65
1:A:125:LYS:HB3	1:A:168:GLU:HB3	1.77	0.65
1:A:219:ILE:HA	1:A:222:LEU:HD12	1.77	0.65
1:A:473:TYR:HE2	1:A:479:ALA:HB2	1.61	0.65
1:A:489:PHE:HA	1:A:492:GLN:NE2	2.12	0.65
1:A:769:ARG:NH2	1:A:807:TYR:O	2.26	0.65
2:B:166:SER:HA	2:B:192:THR:HA	1.79	0.65
1:C:415:CYS:HA	1:C:418:LEU:HD12	1.79	0.65
1:C:739:ASP:OD1	1:C:739:ASP:N	2.26	0.65
2:D:165:ILE:HB	2:D:193:LYS:HB3	1.78	0.65
1:A:778:LEU:O	1:A:782:LEU:HG	1.96	0.65
2:D:117:GLY:N	2:D:145:ASP:HA	2.12	0.65
1:A:521:LEU:O	1:A:525:LEU:HG	1.97	0.65
2:B:121:ARG:HD3	2:B:134:ASN:HD22	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ASP:HB2	1:A:302:TYR:HE1	1.60	0.65
1:C:245:GLN:O	1:C:247:ARG:NH1	2.29	0.65
1:C:626:TRP:O	1:C:630:SER:CB	2.38	0.65
1:C:848:HIS:CD2	2:D:106:ASN:HD22	2.14	0.65
1:A:568:LEU:O	1:A:571:LEU:HG	1.96	0.64
1:C:193:GLN:O	1:C:201:ARG:NH1	2.30	0.64
1:C:780:ARG:HG3	1:C:783:ARG:HH11	1.62	0.64
1:A:521:LEU:HA	1:A:524:VAL:HG22	1.78	0.64
1:C:280:SER:O	1:C:404:GLN:NE2	2.28	0.64
1:C:676:VAL:HA	1:C:679:GLU:HB3	1.77	0.64
2:D:12:HIS:CB	2:D:16:ARG:HB2	2.27	0.64
1:A:737:LYS:NZ	1:A:784:VAL:O	2.31	0.64
1:C:192:LEU:HD13	1:C:208:ARG:HA	1.78	0.64
1:C:252:GLN:HG2	1:C:282:LEU:HD13	1.79	0.64
1:A:599:ARG:HG3	1:A:600:THR:N	2.11	0.64
2:B:10:ASN:O	2:B:139:THR:OG1	2.10	0.64
2:D:4:LEU:HD12	2:D:33:ILE:HG13	1.79	0.64
1:A:504:ILE:O	1:A:508:LEU:HG	1.96	0.64
1:A:804:ARG:NE	1:A:804:ARG:HA	2.12	0.64
1:C:192:LEU:HD23	1:C:195:GLN:HG2	1.80	0.64
1:A:222:LEU:HD23	1:A:225:LEU:HD12	1.80	0.64
1:A:525:LEU:HD11	1:A:586:MET:HE1	1.80	0.64
1:C:488:LEU:O	1:C:492:GLN:N	2.30	0.64
1:C:565:LEU:HD13	1:C:568:LEU:HD23	1.80	0.64
2:D:5:ILE:HA	2:D:37:LEU:HD23	1.78	0.64
1:A:636:PHE:O	1:A:639:SER:OG	2.07	0.64
1:A:724:ILE:HG21	1:A:750:LEU:HD21	1.80	0.64
2:B:89:GLU:HB3	2:B:91:PHE:HD1	1.63	0.64
2:D:105:ALA:O	2:D:109:ASP:N	2.31	0.63
1:A:558:THR:O	1:A:561:GLU:N	2.30	0.63
2:D:193:LYS:HE2	2:D:195:VAL:HB	1.79	0.63
1:C:729:GLN:O	1:C:732:SER:OG	2.15	0.63
1:A:614:ARG:HH11	1:A:670:MET:HB3	1.64	0.63
1:A:420:ASN:O	1:A:424:ASN:ND2	2.32	0.63
1:C:96:VAL:O	1:C:105:ARG:NE	2.32	0.63
1:C:492:GLN:O	1:C:497:ARG:NH1	2.32	0.63
1:C:642:SER:O	1:C:646:THR:N	2.22	0.63
1:A:575:ASP:O	1:A:580:GLN:NE2	2.31	0.63
1:A:748:SER:H	1:A:749:HIS:CD2	2.17	0.63
1:A:774:VAL:O	1:A:778:LEU:HG	1.99	0.63
1:A:599:ARG:HH21	1:A:600:THR:HG22	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:659:ARG:NE	2:D:64:ARG:O	2.32	0.62
1:A:557:GLU:HB2	1:A:559:MET:HG2	1.81	0.62
1:A:729:GLN:NE2	1:C:692:ILE:HG23	2.13	0.62
1:A:49:VAL:HG21	1:A:107:TYR:CD2	2.34	0.62
2:D:12:HIS:HB2	2:D:16:ARG:HB2	1.81	0.62
1:C:185:MET:O	1:C:189:TRP:HB2	2.00	0.62
1:C:424:ASN:HA	1:C:472:ARG:HH11	1.64	0.62
1:C:488:LEU:HA	1:C:491:ALA:HB3	1.80	0.62
1:C:633:LEU:HG	1:C:637:LEU:HD11	1.80	0.62
1:A:80:LEU:HD22	1:A:115:ALA:HB2	1.82	0.62
1:A:189:TRP:CZ2	1:A:212:GLN:HB3	2.34	0.62
1:A:298:ARG:O	1:A:302:TYR:HB2	2.00	0.62
1:A:390:TYR:HE1	1:A:436:ILE:HG12	1.64	0.62
1:A:629:GLN:O	1:A:632:SER:OG	2.09	0.62
2:B:105:ALA:O	2:B:109:ASP:N	2.33	0.62
1:C:673:PHE:HE2	1:C:676:VAL:HG13	1.65	0.62
2:D:4:LEU:HB2	2:D:33:ILE:HG23	1.82	0.62
1:C:615:ARG:O	1:C:615:ARG:NH1	2.33	0.62
1:C:715:PHE:HE2	1:C:719:ASN:HB2	1.64	0.62
1:A:659:ARG:HH22	1:A:666:GLN:HE22	1.45	0.62
2:B:11:LEU:HD22	2:B:42:LEU:HA	1.82	0.62
1:A:657:CYS:HA	1:A:660:LEU:HB2	1.80	0.62
1:C:268:HIS:HB3	1:C:272:LEU:HD21	1.81	0.62
1:C:577:ASN:OD1	1:C:578:ASP:N	2.33	0.62
1:A:564:TRP:CD1	1:A:565:LEU:HD22	2.35	0.62
1:A:748:SER:O	1:A:770:ASP:N	2.32	0.62
1:C:791:THR:O	1:C:794:SER:OG	2.17	0.62
1:A:189:TRP:NE1	1:A:208:ARG:O	2.32	0.61
2:B:177:ASP:OD1	2:B:181:THR:N	2.33	0.61
1:A:29:ARG:HH11	1:A:75:TYR:HD2	1.46	0.61
1:C:602:THR:O	1:C:605:LEU:HG	1.99	0.61
1:C:674:GLU:OE2	1:C:719:ASN:ND2	2.34	0.61
2:D:41:ASN:HD21	2:D:65:MET:N	1.98	0.61
1:A:390:TYR:H	1:A:426:TYR:HE2	1.46	0.61
2:B:95:SER:OG	2:B:96:GLU:N	2.30	0.61
2:B:173:GLN:N	2:B:185:ALA:O	2.32	0.61
1:A:295:MET:O	1:A:299:LEU:HG	1.99	0.61
2:B:103:ALA:O	2:B:107:LYS:HG3	2.00	0.61
2:D:63:GLY:N	2:D:66:ASP:OD2	2.34	0.61
1:A:562:GLN:HG3	1:A:600:THR:HB	1.81	0.61
1:C:710:HIS:CE1	2:D:94:VAL:HG23	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:790:GLU:OE1	1:C:793:THR:N	2.29	0.61
1:A:561:GLU:HA	1:A:564:TRP:HB3	1.81	0.61
1:A:602:THR:O	1:A:605:LEU:N	2.33	0.61
2:B:12:HIS:O	2:B:17:ALA:N	2.32	0.61
1:C:197:HIS:O	1:C:204:ARG:NH1	2.34	0.61
2:D:62:ARG:NH2	2:D:70:THR:O	2.34	0.61
1:A:89:LEU:H	1:A:116:TYR:HH	1.46	0.61
1:A:222:LEU:HA	1:A:225:LEU:HD12	1.83	0.61
1:A:258:VAL:HA	1:A:261:GLN:HE21	1.64	0.61
1:A:750:LEU:N	1:A:770:ASP:HB2	2.13	0.61
1:C:487:SER:HA	1:C:490:GLN:HE21	1.64	0.61
1:C:842:VAL:O	1:C:845:SER:OG	2.16	0.61
1:C:780:ARG:O	1:C:784:VAL:HG23	2.00	0.61
1:C:521:LEU:O	1:C:525:LEU:HG	2.00	0.60
1:C:722:THR:O	1:C:725:THR:OG1	2.17	0.60
2:D:120:HIS:HD2	2:D:145:ASP:HB3	1.66	0.60
1:A:189:TRP:HH2	1:A:250:LEU:HG	1.66	0.60
1:A:272:LEU:HA	1:A:275:PHE:HB3	1.83	0.60
1:A:483:PRO:O	1:A:486:VAL:N	2.34	0.60
1:A:493:THR:O	1:A:497:ARG:N	2.32	0.60
1:C:437:LEU:O	1:C:442:ALA:N	2.29	0.60
1:A:742:ARG:NH1	2:B:92:THR:OG1	2.33	0.60
1:A:66:TYR:O	1:A:70:PHE:HB2	2.01	0.60
1:A:714:ASN:OD1	1:A:714:ASN:N	2.33	0.60
1:C:611:LYS:HA	1:C:614:ARG:NH1	2.16	0.60
1:C:679:GLU:O	1:C:683:GLN:NE2	2.24	0.60
1:C:807:TYR:O	1:C:811:GLN:N	2.31	0.60
2:D:85:ILE:HG23	2:D:112:VAL:HG11	1.84	0.60
1:A:436:ILE:O	1:A:441:LEU:N	2.33	0.60
1:A:513:THR:HB	1:A:571:LEU:HB2	1.83	0.60
1:C:142:VAL:HA	1:C:188:LEU:HD22	1.83	0.60
2:B:11:LEU:HA	2:B:139:THR:HG21	1.83	0.60
1:C:533:LYS:CG	1:C:534:GLU:HA	2.32	0.60
1:C:682:ALA:O	1:C:686:THR:HG23	2.02	0.60
2:D:5:ILE:HG23	2:D:37:LEU:HG	1.82	0.60
1:A:170:ASN:OD1	1:A:173:ASP:N	2.26	0.60
1:A:454:HIS:CE1	1:A:496:THR:HG23	2.36	0.60
1:A:604:PRO:O	1:A:607:THR:OG1	2.18	0.60
1:A:678:TYR:HB3	1:A:679:GLU:OE2	2.02	0.60
1:A:733:LYS:HE3	1:C:693:SER:HA	1.84	0.60
2:D:43:THR:HG21	2:D:65:MET:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:115:TRP:NE1	2:D:146:TRP:O	2.32	0.60
1:A:227:ASP:OD1	1:A:230:THR:OG1	2.17	0.60
1:C:805:TYR:CE2	1:C:821:LEU:HD12	2.37	0.60
1:A:663:SER:HA	1:A:666:GLN:HE21	1.67	0.60
1:A:698:GLN:HA	1:A:701:ALA:HB3	1.84	0.59
1:A:808:TYR:HB3	1:A:813:ASN:HD22	1.66	0.59
1:A:626:TRP:O	1:A:630:SER:HB3	2.02	0.59
2:B:13:ILE:HG23	2:B:18:LEU:HA	1.84	0.59
1:C:808:TYR:HB2	1:C:816:VAL:HG21	1.83	0.59
1:A:299:LEU:HD12	1:A:421:LEU:HD21	1.84	0.59
1:A:584:LEU:O	1:A:587:THR:OG1	2.17	0.59
1:A:602:THR:HA	1:A:605:LEU:CD1	2.33	0.59
1:A:81:ARG:HG2	1:A:118:SER:HB2	1.84	0.59
2:B:24:PHE:HE1	2:B:184:VAL:HG22	1.67	0.59
1:C:392:ILE:O	1:C:396:GLN:HG2	2.02	0.59
2:D:113:LEU:HD11	2:D:130:LYS:HZ1	1.68	0.59
1:A:452:ASP:N	1:A:452:ASP:OD1	2.35	0.59
1:A:631:SER:HA	1:A:634:PHE:CD2	2.38	0.59
1:C:279:VAL:HG11	1:C:295:MET:HE1	1.83	0.59
1:C:681:PHE:CE1	1:C:708:ALA:HB1	2.36	0.59
1:C:796:GLU:O	1:C:800:GLU:HG3	2.03	0.59
1:C:800:GLU:O	1:C:804:ARG:HG2	2.02	0.59
1:C:430:LEU:O	1:C:433:VAL:N	2.36	0.59
1:C:615:ARG:HH22	1:C:619:ARG:HH21	1.51	0.59
1:C:669:ASP:OD2	1:C:712:THR:OG1	2.12	0.59
1:C:710:HIS:O	1:C:757:ALA:N	2.36	0.59
1:A:193:GLN:HA	1:A:204:ARG:HB3	1.84	0.59
1:A:588:ARG:HE	1:A:640:ALA:HA	1.67	0.59
1:A:739:ASP:N	1:A:739:ASP:OD1	2.35	0.59
1:C:673:PHE:HD2	1:C:676:VAL:HG22	1.66	0.59
1:C:676:VAL:O	1:C:680:PHE:N	2.28	0.59
1:A:602:THR:O	1:A:606:ILE:HG12	2.02	0.58
1:A:754:THR:H	1:A:767:LEU:HB3	1.67	0.58
1:C:827:LEU:O	1:C:831:ASN:ND2	2.36	0.58
1:A:477:PHE:HA	1:A:480:LEU:HB3	1.84	0.58
1:C:58:SER:O	1:C:62:TYR:N	2.21	0.58
1:C:775:LEU:O	1:C:779:GLN:HG2	2.03	0.58
1:C:803:ASP:HB2	1:C:804:ARG:NH1	2.18	0.58
1:A:529:LYS:HA	1:A:533:LYS:HB3	1.83	0.58
1:A:586:MET:O	1:A:590:ALA:HB2	2.02	0.58
2:B:84:ARG:O	2:B:111:ASP:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ILE:O	1:C:106:LEU:HG	2.03	0.58
1:A:97:GLN:HA	1:A:105:ARG:NE	2.19	0.58
1:A:454:HIS:CE1	1:A:495:PRO:HB2	2.38	0.58
1:C:581:PHE:HB3	1:C:582:ARG:NH2	2.19	0.58
1:C:808:TYR:O	1:C:812:ARG:N	2.37	0.58
1:A:243:ILE:HD13	1:A:252:GLN:HE22	1.69	0.58
1:A:399:HIS:O	1:A:403:ALA:N	2.28	0.58
1:A:423:LEU:HD22	1:A:472:ARG:HG2	1.84	0.58
2:B:165:ILE:O	2:B:193:LYS:N	2.27	0.58
1:A:423:LEU:O	1:A:427:PRO:HG3	2.04	0.58
1:C:125:LYS:NZ	1:C:173:ASP:O	2.27	0.58
1:C:249:ILE:HG21	1:C:285:HIS:ND1	2.18	0.58
1:C:389:LEU:O	1:C:393:PHE:HB2	2.03	0.58
1:C:756:ILE:HG23	1:C:759:ARG:HE	1.68	0.58
2:D:16:ARG:HD2	2:D:142:PHE:CZ	2.37	0.58
1:A:140:HIS:CE1	1:A:142:VAL:HB	2.38	0.58
1:A:653:VAL:HA	1:A:656:LEU:HD12	1.84	0.58
1:C:813:ASN:HD22	1:C:816:VAL:HG23	1.69	0.58
2:B:63:GLY:HA2	2:B:64:ARG:NH1	2.18	0.58
1:C:700:GLN:O	1:C:704:VAL:HG23	2.04	0.58
1:C:533:LYS:HG2	1:C:534:GLU:HA	1.86	0.58
1:C:606:ILE:HG21	1:C:660:LEU:HD22	1.86	0.58
2:D:120:HIS:CD2	2:D:145:ASP:HB3	2.39	0.58
1:A:125:LYS:HA	1:A:128:MET:HE2	1.86	0.58
1:A:558:THR:O	1:A:562:GLN:NE2	2.37	0.58
1:A:623:ASP:OD1	1:A:625:ASN:N	2.36	0.58
2:B:116:ALA:HA	2:B:134:ASN:OD1	2.04	0.58
1:C:110:ILE:HG23	1:C:151:LEU:HD13	1.86	0.58
1:C:752:TRP:CG	1:C:753:ALA:N	2.72	0.58
2:D:118:GLY:H	2:D:146:TRP:H	1.50	0.58
1:A:440:ALA:O	1:A:444:VAL:HG23	2.04	0.57
1:A:577:ASN:HB2	1:A:616:PHE:CD1	2.39	0.57
1:A:808:TYR:HB3	1:A:813:ASN:HB3	1.85	0.57
1:A:266:GLU:O	1:A:270:HIS:ND1	2.37	0.57
1:A:686:THR:O	1:A:689:GLU:N	2.37	0.57
1:A:727:CYS:HA	1:A:730:HIS:HD1	1.69	0.57
1:C:631:SER:HA	1:C:634:PHE:CD2	2.37	0.57
1:A:93:TYR:HB2	1:A:109:MET:HB2	1.85	0.57
1:A:599:ARG:NH2	1:A:600:THR:HG22	2.19	0.57
1:A:740:GLN:O	1:A:744:VAL:HG23	2.03	0.57
1:A:742:ARG:HA	1:A:745:TYR:CE2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:THR:N	1:A:767:LEU:HB3	2.19	0.57
1:C:637:LEU:O	1:C:641:ILE:HG13	2.05	0.57
2:D:111:ASP:OD1	2:D:191:TYR:OH	2.22	0.57
1:A:737:LYS:NZ	1:A:787:SER:OG	2.34	0.57
1:C:505:VAL:O	1:C:509:LEU:HG	2.05	0.57
1:C:746:LEU:HA	1:C:749:HIS:NE2	2.19	0.57
1:A:528:LEU:O	1:A:531:LEU:N	2.38	0.57
1:A:283:ASN:HB2	1:A:286:VAL:HG23	1.87	0.57
1:A:709:LEU:O	1:A:712:THR:OG1	2.19	0.57
1:A:729:GLN:OE1	1:A:732:SER:OG	2.22	0.57
1:C:673:PHE:CD2	1:C:676:VAL:HG22	2.40	0.57
1:C:189:TRP:HZ3	1:C:251:ALA:HA	1.69	0.57
1:C:595:ASN:OD1	1:C:597:ARG:NH1	2.37	0.57
1:A:409:GLN:HG2	1:A:410:ASP:H	1.70	0.57
2:B:24:PHE:HA	2:B:27:LEU:HD12	1.86	0.57
1:C:172:GLN:HA	1:C:175:ILE:HD12	1.87	0.57
1:A:480:LEU:HD21	1:A:520:HIS:HD2	1.68	0.57
1:A:804:ARG:HH21	1:A:807:TYR:HB2	1.69	0.57
2:B:6:LEU:HD21	2:B:36:THR:HA	1.85	0.57
1:C:438:ALA:O	1:C:443:LYS:NZ	2.24	0.57
2:D:78:VAL:O	2:D:85:ILE:N	2.28	0.57
1:A:707:SER:O	1:A:711:ARG:HG2	2.05	0.57
1:C:125:LYS:HD3	1:C:160:PRO:HG3	1.87	0.57
1:C:832:LEU:HA	1:C:836:GLN:HB2	1.86	0.57
1:C:181:ASN:O	1:C:185:MET:HG2	2.05	0.56
1:C:195:GLN:NE2	1:C:207:GLU:OE1	2.38	0.56
1:C:504:ILE:O	1:C:507:THR:OG1	2.21	0.56
1:A:58:SER:O	1:A:62:TYR:N	2.24	0.56
1:C:433:VAL:O	1:C:437:LEU:HG	2.05	0.56
1:C:506:ARG:HA	1:C:509:LEU:HD12	1.86	0.56
1:C:688:TYR:OH	1:C:730:HIS:HB3	2.05	0.56
1:A:77:SER:OG	1:A:154:GLN:NE2	2.38	0.56
1:A:423:LEU:HD11	1:A:468:SER:HB2	1.85	0.56
1:A:440:ALA:O	1:A:443:LYS:HG3	2.06	0.56
1:A:579:THR:OG1	1:A:582:ARG:NH1	2.39	0.56
1:A:587:THR:O	1:A:590:ALA:HB3	2.05	0.56
1:A:630:SER:HA	1:A:633:LEU:HG	1.88	0.56
1:A:793:THR:O	1:A:797:LEU:HG	2.05	0.56
2:B:51:LEU:HA	2:B:54:ILE:HG22	1.88	0.56
2:B:120:HIS:HE1	2:B:144:THR:HG23	1.71	0.56
2:B:121:ARG:HD3	2:B:134:ASN:ND2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:LEU:HA	1:C:76:LEU:HB3	1.87	0.56
1:C:194:HIS:CD2	1:C:201:ARG:HH12	2.24	0.56
1:C:423:LEU:O	1:C:427:PRO:HG3	2.06	0.56
2:D:29:SER:H	2:D:32:LYS:HZ1	1.53	0.56
2:D:118:GLY:O	2:D:143:THR:OG1	2.19	0.56
1:A:271:THR:HA	1:A:274:GLN:NE2	2.20	0.56
1:A:477:PHE:HD1	1:A:480:LEU:HD13	1.70	0.56
1:C:394:PHE:CD2	1:C:436:ILE:HD12	2.41	0.56
1:A:659:ARG:HD3	1:A:704:VAL:HG11	1.86	0.56
1:C:295:MET:O	1:C:299:LEU:HG	2.06	0.56
1:C:729:GLN:O	1:C:733:LYS:NZ	2.30	0.56
1:A:679:GLU:OE2	1:A:679:GLU:N	2.37	0.56
1:A:795:ILE:O	1:A:799:VAL:HG23	2.06	0.56
1:C:153:GLY:HA2	1:C:156:ARG:HE	1.70	0.56
1:A:249:ILE:HG12	1:A:286:VAL:HA	1.87	0.56
1:A:420:ASN:OD1	1:A:472:ARG:NH2	2.34	0.56
2:B:88:LEU:O	2:B:115:TRP:HA	2.06	0.56
1:C:206:GLN:HB3	1:C:209:ARG:HH11	1.71	0.56
1:C:408:ILE:O	1:C:412:ILE:HG12	2.05	0.56
1:C:560:GLU:N	1:C:561:GLU:OE1	2.36	0.56
2:D:41:ASN:ND2	2:D:65:MET:H	2.03	0.56
2:D:96:GLU:CD	2:D:96:GLU:H	2.09	0.56
2:D:174:LEU:HG	2:D:182:GLU:HB3	1.87	0.56
1:A:203:LEU:O	1:A:207:GLU:HG3	2.05	0.56
2:B:113:LEU:HD11	2:B:130:LYS:HE3	1.86	0.56
1:C:494:TYR:O	1:C:497:ARG:HB2	2.06	0.56
2:D:93:LEU:HD12	2:D:95:SER:O	2.06	0.56
2:B:4:LEU:HD12	2:B:33:ILE:HG12	1.88	0.56
1:C:628:SER:O	1:C:631:SER:OG	2.21	0.56
2:D:155:PRO:HB2	2:D:173:GLN:HA	1.88	0.56
1:A:86:VAL:HG23	1:A:87:ASN:H	1.71	0.55
1:C:504:ILE:HG13	1:C:505:VAL:N	2.21	0.55
1:C:555:THR:HB	1:C:558:THR:HA	1.89	0.55
1:C:602:THR:HG21	1:C:644:LEU:HD11	1.88	0.55
1:A:571:LEU:O	1:A:574:SER:OG	2.16	0.55
1:A:576:ASP:HA	1:A:615:ARG:CZ	2.35	0.55
2:D:25:LYS:O	2:D:29:SER:OG	2.15	0.55
2:B:114:CYS:HA	2:B:133:VAL:HB	1.88	0.55
2:D:113:LEU:HB3	2:D:115:TRP:CZ3	2.36	0.55
1:A:743:ALA:HA	1:A:746:LEU:HD12	1.87	0.55
1:C:488:LEU:O	1:C:492:GLN:NE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:SER:HA	1:A:400:LEU:HD21	1.88	0.55
1:A:720:TYR:O	1:A:724:ILE:HG12	2.07	0.55
1:C:249:ILE:HA	1:C:286:VAL:HG22	1.86	0.55
2:D:51:LEU:HB3	2:D:58:LEU:HD21	1.87	0.55
1:A:187:LYS:HD3	1:A:242:GLN:HE22	1.72	0.55
1:A:201:ARG:HA	1:A:204:ARG:HE	1.70	0.55
1:A:430:LEU:O	1:A:433:VAL:N	2.39	0.55
1:A:750:LEU:H	1:A:770:ASP:CB	2.16	0.55
1:A:126:GLU:O	1:A:129:LYS:HG2	2.07	0.55
1:A:577:ASN:OD1	1:A:578:ASP:N	2.39	0.55
1:A:655:ASP:O	1:A:658:LEU:HB2	2.06	0.55
1:A:773:ARG:O	1:A:776:GLU:HG3	2.07	0.55
2:B:62:ARG:NH2	2:B:71:SER:O	2.40	0.55
2:B:97:GLU:O	2:B:101:LEU:HG	2.07	0.55
1:C:246:CYS:SG	1:C:252:GLN:HG3	2.46	0.55
2:D:4:LEU:HD22	2:D:159:LEU:HD22	1.89	0.55
2:D:9:GLY:O	2:D:138:ALA:N	2.36	0.55
2:D:102:LEU:HD11	2:D:132:PHE:HE2	1.71	0.55
1:A:456:GLN:O	1:A:459:GLN:HG3	2.06	0.55
1:A:659:ARG:NH1	1:A:659:ARG:O	2.35	0.55
1:A:782:LEU:HB2	1:A:783:ARG:NH2	2.22	0.55
1:C:78:ALA:O	1:C:82:GLU:HG2	2.06	0.55
1:C:596:GLU:H	1:C:597:ARG:HH11	1.55	0.55
1:C:740:GLN:O	1:C:744:VAL:HG23	2.06	0.55
2:D:6:LEU:HD21	2:D:36:THR:HG23	1.88	0.55
2:D:78:VAL:HG23	2:D:85:ILE:HB	1.88	0.55
1:A:752:TRP:C	1:A:769:ARG:HB3	2.27	0.55
1:C:193:GLN:HG2	1:C:201:ARG:HH11	1.71	0.55
1:C:454:HIS:HA	1:C:459:GLN:HG3	1.88	0.55
1:A:38:LEU:HD11	1:A:83:ASN:HD21	1.72	0.55
1:A:830:SER:O	1:A:834:GLY:N	2.24	0.55
1:C:797:LEU:O	1:C:801:ILE:HG12	2.07	0.55
2:D:137:SER:OG	2:D:138:ALA:N	2.38	0.55
1:A:804:ARG:HB3	1:A:808:TYR:OH	2.07	0.54
1:C:516:SER:N	1:C:575:ASP:OD1	2.38	0.54
2:D:8:ILE:HG13	2:D:138:ALA:HA	1.88	0.54
2:D:117:GLY:H	2:D:145:ASP:HA	1.72	0.54
1:A:260:THR:O	1:A:298:ARG:NH2	2.40	0.54
2:B:121:ARG:O	2:B:134:ASN:ND2	2.40	0.54
1:C:638:HIS:NE2	1:C:683:GLN:HG3	2.22	0.54
1:C:759:ARG:HA	1:C:767:LEU:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ALA:O	1:A:159:LEU:N	2.41	0.54
1:C:238:PRO:O	1:C:242:GLN:HG2	2.08	0.54
1:C:462:LEU:O	1:C:466:LEU:HG	2.07	0.54
1:C:586:MET:HA	1:C:589:LYS:HD2	1.89	0.54
1:C:633:LEU:O	1:C:637:LEU:HG	2.07	0.54
1:C:737:LYS:NZ	1:C:787:SER:OG	2.38	0.54
2:D:42:LEU:N	2:D:43:THR:HA	2.21	0.54
1:C:161:THR:OG1	1:C:162:GLY:N	2.39	0.54
1:C:656:LEU:O	1:C:660:LEU:HG	2.07	0.54
1:A:77:SER:HA	1:A:80:LEU:HD12	1.89	0.54
1:A:477:PHE:CD1	1:A:480:LEU:HD13	2.43	0.54
2:B:20:ILE:H	2:B:25:LYS:HE3	1.72	0.54
1:C:27:MET:HG3	1:C:44:CYS:SG	2.47	0.54
1:C:401:VAL:HG22	1:C:406:LEU:HD12	1.89	0.54
1:C:603:PRO:HA	1:C:606:ILE:HG12	1.90	0.54
1:C:638:HIS:HB2	1:C:680:PHE:CE2	2.42	0.54
1:C:697:ALA:HA	1:C:700:GLN:OE1	2.07	0.54
1:C:695:SER:OG	1:C:696:LYS:N	2.40	0.54
1:A:175:ILE:HA	1:A:178:ILE:HG22	1.87	0.54
1:A:556:ASP:OD1	1:A:557:GLU:N	2.41	0.54
1:A:801:ILE:HG22	1:A:802:LEU:HD23	1.90	0.54
1:C:264:PRO:HB2	1:C:266:GLU:OE1	2.08	0.54
1:C:688:TYR:O	1:C:692:ILE:N	2.40	0.54
1:C:848:HIS:CE1	2:D:106:ASN:HB2	2.43	0.54
1:A:437:LEU:HD13	1:A:485:TYR:HA	1.89	0.54
1:A:788:CYS:SG	1:A:789:MET:N	2.81	0.54
1:C:116:TYR:O	1:C:120:ASP:N	2.28	0.54
1:C:232:ARG:HA	1:C:236:LEU:HB3	1.90	0.54
1:C:655:ASP:O	1:C:659:ARG:HG3	2.07	0.54
1:C:803:ASP:HB2	1:C:804:ARG:HH12	1.73	0.54
1:A:189:TRP:CE2	1:A:208:ARG:HG2	2.42	0.54
1:A:617:LYS:HD2	1:A:671:THR:HA	1.90	0.54
1:C:607:THR:OG1	2:D:15:ASP:OD1	2.23	0.54
1:C:736:ARG:CZ	1:C:738:PRO:HD2	2.37	0.54
2:D:13:ILE:HG22	2:D:42:LEU:O	2.08	0.54
1:A:802:LEU:HD13	1:A:825:ILE:HG22	1.91	0.54
1:A:387:VAL:HG13	1:A:392:ILE:HD13	1.89	0.53
1:C:847:LYS:O	1:C:851:GLN:HG2	2.08	0.53
2:B:161:ASP:HB2	2:B:168:THR:HB	1.91	0.53
1:C:145:LEU:HD13	1:C:188:LEU:HB3	1.90	0.53
1:C:607:THR:O	1:C:611:LYS:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLY:O	1:A:241:GLU:HG2	2.08	0.53
1:C:256:LEU:HA	1:C:259:ILE:HD12	1.89	0.53
2:D:8:ILE:HD12	2:D:157:PHE:HB3	1.90	0.53
2:D:38:CYS:HB3	2:D:59:LYS:O	2.07	0.53
1:A:108:LEU:O	1:A:112:VAL:HG23	2.09	0.53
1:A:198:SER:OG	1:A:199:ARG:NH1	2.41	0.53
1:A:717:ARG:HG3	1:A:721:ASP:OD1	2.08	0.53
1:A:729:GLN:HE21	1:C:692:ILE:HG23	1.72	0.53
1:C:15:GLU:O	1:C:19:ILE:HG12	2.09	0.53
1:C:293:ILE:HG13	1:C:414:LEU:HD23	1.89	0.53
1:A:231:TYR:CE2	1:A:267:TYR:HB3	2.43	0.53
1:A:232:ARG:HA	1:A:236:LEU:HD13	1.91	0.53
1:A:453:LEU:HB2	1:A:456:GLN:HG3	1.90	0.53
1:A:526:GLU:O	1:A:530:VAL:HG23	2.08	0.53
1:C:736:ARG:HB3	1:C:739:ASP:OD2	2.08	0.53
1:C:744:VAL:HG11	1:C:781:ALA:HB2	1.90	0.53
1:C:799:VAL:HA	1:C:802:LEU:HD12	1.91	0.53
1:A:101:ASN:OD1	1:A:105:ARG:NH1	2.42	0.53
1:A:627:SER:O	1:A:630:SER:OG	2.20	0.53
1:A:641:ILE:HD13	1:A:661:PHE:CE1	2.41	0.53
1:A:798:PHE:HA	1:A:801:ILE:HD12	1.91	0.53
2:B:5:ILE:O	2:B:160:MET:HB2	2.09	0.53
1:C:699:PHE:CE2	1:C:700:GLN:HG3	2.42	0.53
2:D:97:GLU:O	2:D:101:LEU:HG	2.09	0.53
1:A:107:TYR:HA	1:A:110:ILE:HB	1.91	0.53
1:A:469:PRO:HA	1:A:472:ARG:HB3	1.91	0.53
1:A:832:LEU:O	1:A:836:GLN:HB2	2.09	0.53
1:C:70:PHE:HA	1:C:73:LEU:HG	1.91	0.53
1:A:99:ALA:O	1:A:105:ARG:NH1	2.39	0.53
1:A:431:ASP:N	1:A:431:ASP:OD1	2.41	0.53
1:A:494:TYR:HB3	1:A:495:PRO:HD3	1.91	0.53
1:A:838:ASP:OD1	1:A:839:SER:N	2.41	0.53
2:B:42:LEU:N	2:B:43:THR:HA	2.24	0.53
1:C:634:PHE:HA	1:C:637:LEU:HD12	1.90	0.53
1:A:265:ASP:HA	1:A:268:HIS:CD2	2.43	0.53
1:A:387:VAL:O	1:A:389:LEU:N	2.39	0.53
1:A:695:SER:OG	1:A:696:LYS:N	2.41	0.53
1:A:179:LEU:O	1:A:183:VAL:HG13	2.10	0.52
1:A:493:THR:N	1:A:496:THR:OG1	2.41	0.52
2:B:115:TRP:NE1	2:B:134:ASN:HB2	2.24	0.52
1:A:459:GLN:O	1:A:463:LEU:HG	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:LYS:HZ1	1:A:672:GLU:HB2	1.73	0.52
1:A:721:ASP:O	1:A:725:THR:HG23	2.10	0.52
1:C:577:ASN:HB2	1:C:615:ARG:NE	2.21	0.52
1:A:586:MET:O	1:A:590:ALA:CB	2.57	0.52
1:A:790:GLU:OE1	1:A:792:ALA:N	2.42	0.52
1:C:453:LEU:HB2	1:C:456:GLN:HB2	1.90	0.52
1:C:529:LYS:HA	1:C:533:LYS:HB3	1.90	0.52
1:C:678:TYR:CE1	1:C:719:ASN:HB3	2.45	0.52
2:D:12:HIS:HB3	2:D:16:ARG:HB2	1.92	0.52
1:A:388:PRO:O	1:A:391:ASP:N	2.42	0.52
1:A:409:GLN:HA	1:A:458:ALA:HB2	1.90	0.52
2:B:61:VAL:HG13	2:B:87:PHE:CE2	2.44	0.52
1:C:275:PHE:O	1:C:279:VAL:HG23	2.09	0.52
1:A:524:VAL:HA	1:A:527:ILE:HB	1.90	0.52
1:A:614:ARG:NH1	1:A:670:MET:O	2.42	0.52
1:A:656:LEU:HD11	2:B:67:VAL:HG11	1.91	0.52
2:B:12:HIS:CE1	2:B:16:ARG:HG3	2.44	0.52
2:B:75:MET:SD	2:B:76:GLN:N	2.83	0.52
1:C:131:MET:O	1:C:135:SER:OG	2.24	0.52
1:C:163:ASP:OD2	1:C:164:SER:N	2.42	0.52
1:A:14:LEU:HB2	1:A:61:GLN:HB3	1.90	0.52
1:A:742:ARG:HE	1:A:746:LEU:HD11	1.75	0.52
2:B:13:ILE:HA	2:B:17:ALA:O	2.10	0.52
1:C:691:SER:O	1:C:693:SER:OG	2.21	0.52
2:D:89:GLU:HB3	2:D:91:PHE:HD1	1.74	0.52
1:A:623:ASP:OD1	1:A:624:ASP:N	2.43	0.52
1:A:696:LYS:HA	1:A:699:PHE:HB3	1.91	0.52
1:C:813:ASN:HB3	1:C:816:VAL:HG23	1.90	0.52
1:A:769:ARG:NH1	1:A:813:ASN:HB2	2.24	0.52
1:A:779:GLN:HA	1:A:782:LEU:HD12	1.91	0.52
1:C:561:GLU:HA	1:C:564:TRP:CD1	2.44	0.52
1:A:216:GLY:O	1:A:220:VAL:HG23	2.09	0.52
1:A:614:ARG:NH2	1:A:617:LYS:HD3	2.25	0.52
1:C:437:LEU:HA	1:C:441:LEU:HB2	1.92	0.52
1:C:805:TYR:CE1	1:C:816:VAL:HG22	2.44	0.52
1:A:633:LEU:O	1:A:637:LEU:HG	2.10	0.52
1:A:678:TYR:HB2	1:A:715:PHE:CZ	2.44	0.52
1:C:117:MET:HG2	1:C:124:VAL:HG12	1.92	0.52
1:C:240:LEU:HA	1:C:243:ILE:HD12	1.92	0.52
2:D:91:PHE:CE2	2:D:92:THR:HG23	2.45	0.52
1:A:416:CYS:HB3	1:A:465:LEU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:ILE:HB	1:A:644:LEU:HD11	1.92	0.51
1:C:254:TYR:O	1:C:257:GLU:HG3	2.10	0.51
1:C:274:GLN:OE1	1:C:274:GLN:N	2.42	0.51
1:C:753:ALA:HA	1:C:767:LEU:HB2	1.92	0.51
1:A:147:LEU:O	1:A:151:LEU:HG	2.09	0.51
1:A:476:ILE:O	1:A:480:LEU:N	2.36	0.51
1:A:531:LEU:HD23	1:A:532:ILE:HB	1.90	0.51
1:C:423:LEU:CB	1:C:472:ARG:HG2	2.41	0.51
1:C:608:ALA:HA	1:C:611:LYS:HE2	1.91	0.51
1:A:106:LEU:HD21	1:A:147:LEU:HD22	1.90	0.51
1:A:189:TRP:HZ2	1:A:212:GLN:HB3	1.75	0.51
2:B:96:GLU:N	2:B:96:GLU:OE1	2.44	0.51
1:C:92:LEU:O	1:C:96:VAL:HG22	2.10	0.51
1:C:752:TRP:CH2	1:C:813:ASN:HB2	2.46	0.51
1:A:583:LEU:O	1:A:587:THR:HG23	2.10	0.51
1:A:667:VAL:O	1:A:671:THR:HG23	2.11	0.51
1:A:710:HIS:HB3	1:A:711:ARG:HH11	1.75	0.51
1:A:749:HIS:NE2	2:B:94:VAL:HG21	2.26	0.51
1:A:804:ARG:NH2	2:B:100:VAL:HG22	2.25	0.51
2:B:122:PHE:CD2	2:B:135:PRO:HA	2.46	0.51
1:A:160:PRO:HD2	1:A:174:SER:HB3	1.92	0.51
1:A:165:ASP:N	1:A:165:ASP:OD1	2.42	0.51
1:A:498:ARG:NH2	1:A:561:GLU:OE2	2.36	0.51
1:A:580:GLN:HB3	1:A:612:LEU:HD22	1.91	0.51
1:C:189:TRP:HA	1:C:192:LEU:HD12	1.91	0.51
1:C:216:GLY:O	1:C:220:VAL:HG23	2.10	0.51
1:C:235:ILE:HG22	1:C:239:LEU:HG	1.92	0.51
1:C:615:ARG:C	1:C:615:ARG:HH11	2.14	0.51
1:C:724:ILE:HD12	1:C:750:LEU:HB3	1.92	0.51
1:C:804:ARG:HB3	1:C:808:TYR:OH	2.11	0.51
1:A:798:PHE:O	1:A:802:LEU:HG	2.11	0.51
1:C:43:LYS:O	1:C:47:THR:HG23	2.11	0.51
1:C:256:LEU:O	1:C:260:THR:HG23	2.11	0.51
1:C:720:TYR:O	1:C:724:ILE:HG12	2.11	0.51
1:C:729:GLN:O	1:C:733:LYS:HG2	2.10	0.51
2:D:36:THR:O	2:D:58:LEU:HA	2.10	0.51
2:D:115:TRP:CH2	2:D:134:ASN:HA	2.46	0.51
1:A:276:LEU:HB3	1:A:396:GLN:HG2	1.92	0.51
1:A:694:ASP:OD1	1:A:695:SER:N	2.44	0.51
1:A:804:ARG:HB3	1:A:808:TYR:CZ	2.45	0.51
2:B:61:VAL:HG13	2:B:87:PHE:CZ	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:ARG:HB3	2:B:74:LEU:HD23	1.91	0.51
1:C:291:ILE:O	1:C:295:MET:HG3	2.09	0.51
2:D:160:MET:HA	2:D:168:THR:O	2.11	0.51
1:C:23:GLN:O	1:C:27:MET:HG2	2.10	0.51
1:C:579:THR:O	1:C:583:LEU:HG	2.10	0.51
1:C:788:CYS:SG	1:C:794:SER:HB3	2.51	0.51
2:D:86:GLY:HA3	2:D:110:VAL:HG11	1.93	0.51
1:A:80:LEU:O	1:A:85:PRO:HD3	2.11	0.51
1:A:172:GLN:CD	1:A:176:ASN:HD21	2.15	0.51
1:A:240:LEU:O	1:A:244:VAL:HG13	2.11	0.51
1:A:304:GLU:HG2	1:A:424:ASN:HA	1.91	0.51
1:A:575:ASP:OD1	1:A:580:GLN:HG3	2.11	0.51
1:A:831:ASN:OD1	1:A:832:LEU:N	2.44	0.51
1:C:682:ALA:O	1:C:685:PHE:HB2	2.11	0.51
1:C:753:ALA:CA	1:C:767:LEU:HB2	2.41	0.51
1:A:478:THR:O	1:A:481:SER:OG	2.22	0.51
1:C:758:ALA:O	1:C:768:TYR:N	2.44	0.51
1:A:103:ILE:HD13	1:A:106:LEU:HD13	1.93	0.50
1:A:570:HIS:HB2	2:B:18:LEU:HD12	1.93	0.50
2:B:169:LEU:HB3	2:B:189:VAL:HB	1.92	0.50
1:C:222:LEU:HA	1:C:225:LEU:HD12	1.94	0.50
1:A:115:ALA:O	1:A:118:SER:OG	2.19	0.50
1:A:597:ARG:O	1:A:600:THR:OG1	2.18	0.50
1:A:707:SER:HA	1:A:711:ARG:HH12	1.76	0.50
2:B:7:VAL:HG12	2:B:158:CYS:HB2	1.94	0.50
1:C:189:TRP:CH2	1:C:250:LEU:HG	2.47	0.50
1:C:477:PHE:HA	1:C:480:LEU:CB	2.40	0.50
1:C:477:PHE:HZ	1:C:514:LEU:HB3	1.76	0.50
1:A:461:SER:O	1:A:464:SER:OG	2.28	0.50
1:A:513:THR:CB	1:A:571:LEU:HB2	2.42	0.50
1:A:659:ARG:HH22	1:A:666:GLN:NE2	2.09	0.50
1:C:299:LEU:HA	1:C:302:TYR:CD2	2.46	0.50
1:C:805:TYR:OH	1:C:817:THR:N	2.43	0.50
2:D:50:TYR:CZ	2:D:54:ILE:HD11	2.46	0.50
1:A:506:ARG:O	1:A:509:LEU:HG	2.11	0.50
1:A:727:CYS:HA	1:A:730:HIS:ND1	2.26	0.50
1:C:297:ASN:O	1:C:300:SER:OG	2.18	0.50
1:C:443:LYS:HD3	1:C:446:GLU:OE1	2.11	0.50
1:C:527:ILE:O	1:C:531:LEU:HG	2.11	0.50
2:D:102:LEU:HG	2:D:130:LYS:HD3	1.93	0.50
1:A:596:GLU:C	1:A:597:ARG:HD3	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:LEU:HD13	2:B:159:LEU:HD22	1.93	0.50
2:B:12:HIS:HA	2:B:15:ASP:HB2	1.93	0.50
1:C:729:GLN:NE2	1:C:733:LYS:HE2	2.26	0.50
1:A:578:ASP:OD2	1:A:582:ARG:NH1	2.35	0.50
1:C:582:ARG:HA	1:C:585:GLN:OE1	2.12	0.50
1:C:694:ASP:OD1	1:C:695:SER:N	2.45	0.50
1:A:60:LYS:O	1:A:64:GLU:HG2	2.12	0.50
1:A:211:LEU:HA	1:A:214:LEU:HD13	1.93	0.50
1:A:855:MET:HA	1:A:857:GLN:HE21	1.76	0.50
1:C:477:PHE:CZ	1:C:514:LEU:HB3	2.47	0.50
1:A:66:TYR:HA	1:A:69:VAL:HG22	1.92	0.50
1:A:560:GLU:O	1:A:562:GLN:N	2.45	0.50
1:A:683:GLN:O	1:A:687:VAL:HG22	2.10	0.50
1:C:688:TYR:CE2	1:C:689:GLU:HG3	2.46	0.50
1:C:791:THR:OG1	1:C:792:ALA:N	2.44	0.50
2:B:44:ASP:OD1	2:B:47:THR:N	2.45	0.50
1:C:21:VAL:O	1:C:25:THR:HG23	2.12	0.50
1:C:266:GLU:HA	1:C:269:LEU:HG	1.94	0.50
1:C:687:VAL:O	1:C:691:SER:N	2.45	0.50
1:C:756:ILE:HA	1:C:759:ARG:HD3	1.93	0.50
1:A:256:LEU:HD23	1:A:259:ILE:HD12	1.94	0.49
1:A:561:GLU:CA	1:A:564:TRP:HB3	2.42	0.49
1:A:737:LYS:O	1:A:740:GLN:HB2	2.11	0.49
1:A:770:ASP:OD2	1:A:773:ARG:NH1	2.45	0.49
1:C:505:VAL:HG12	1:C:509:LEU:HD11	1.93	0.49
1:C:603:PRO:HA	1:C:606:ILE:CG1	2.42	0.49
1:C:611:LYS:HA	1:C:614:ARG:HH12	1.77	0.49
1:A:533:LYS:CG	1:A:534:GLU:HA	2.39	0.49
1:A:567:ARG:HD2	1:A:567:ARG:N	2.26	0.49
1:A:793:THR:HA	1:A:796:GLU:OE1	2.12	0.49
1:C:201:ARG:HA	1:C:204:ARG:HE	1.76	0.49
1:A:69:VAL:O	1:A:73:LEU:HB2	2.11	0.49
1:A:201:ARG:HE	1:A:204:ARG:NH2	2.10	0.49
1:A:528:LEU:HD13	1:A:531:LEU:HD13	1.94	0.49
1:A:436:ILE:HA	1:A:440:ALA:HB3	1.93	0.49
1:A:659:ARG:NH2	1:A:666:GLN:HE22	2.11	0.49
2:B:121:ARG:NH1	2:B:134:ASN:HD22	2.10	0.49
1:A:23:GLN:O	1:A:27:MET:HG2	2.13	0.49
1:A:140:HIS:HE1	1:A:142:VAL:HB	1.77	0.49
1:A:528:LEU:HD13	1:A:531:LEU:HD22	1.95	0.49
1:C:81:ARG:HA	1:C:85:PRO:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:LEU:HD13	1:C:267:TYR:HA	1.94	0.49
1:C:587:THR:HB	1:C:591:TYR:CE2	2.47	0.49
2:D:173:GLN:CB	2:D:175:ARG:HE	2.22	0.49
1:A:708:ALA:O	1:A:712:THR:HG23	2.12	0.49
1:A:722:THR:O	1:A:726:LYS:HG2	2.11	0.49
1:C:568:LEU:O	1:C:571:LEU:HG	2.13	0.49
1:A:172:GLN:O	1:A:175:ILE:HG22	2.13	0.49
1:A:395:ASP:HA	1:A:398:GLN:HB2	1.95	0.49
1:A:515:ILE:HG13	1:A:515:ILE:O	2.12	0.49
1:A:849:PHE:O	1:A:853:LEU:HG	2.13	0.49
2:B:14:PRO:HD3	2:B:44:ASP:HB3	1.94	0.49
2:D:63:GLY:H	2:D:66:ASP:CG	2.15	0.49
1:A:123:PRO:HA	1:A:126:GLU:OE1	2.12	0.49
1:A:228:LEU:HB2	1:A:267:TYR:CD1	2.48	0.49
1:A:451:ALA:O	1:A:453:LEU:HD23	2.13	0.49
1:A:570:HIS:CG	2:B:18:LEU:HD12	2.48	0.49
1:A:726:LYS:HE3	1:C:735:LEU:HA	1.94	0.49
1:A:805:TYR:HB3	1:A:821:LEU:HD22	1.93	0.49
2:B:41:ASN:ND2	2:B:64:ARG:H	2.07	0.49
1:C:145:LEU:HD22	1:C:188:LEU:HD23	1.95	0.49
1:C:193:GLN:O	1:C:204:ARG:NE	2.46	0.49
1:C:568:LEU:O	1:C:572:ILE:HG12	2.13	0.49
1:C:615:ARG:NH2	1:C:619:ARG:HH21	2.11	0.49
1:C:699:PHE:HZ	2:D:91:PHE:CE2	2.30	0.49
1:C:734:LEU:O	1:C:740:GLN:NE2	2.46	0.49
1:A:263:PHE:HB2	1:A:268:HIS:CE1	2.48	0.49
1:A:396:GLN:HE21	1:A:400:LEU:HD11	1.77	0.49
1:A:503:GLU:O	1:A:507:THR:HG23	2.12	0.49
2:B:5:ILE:HB	2:B:160:MET:HB2	1.95	0.49
1:C:390:TYR:OH	1:C:433:VAL:HA	2.12	0.49
1:C:415:CYS:HB2	1:C:465:LEU:HD22	1.94	0.49
1:C:796:GLU:OE2	1:C:845:SER:HB3	2.13	0.49
1:A:18:LEU:HD21	1:A:65:LEU:HA	1.94	0.49
1:A:243:ILE:HD13	1:A:252:GLN:NE2	2.27	0.49
1:C:595:ASN:OD1	1:C:595:ASN:N	2.46	0.49
2:D:104:GLU:OE2	2:D:107:LYS:HD2	2.12	0.49
1:A:127:LEU:O	1:A:131:MET:HG3	2.12	0.48
1:A:142:VAL:HG22	1:A:192:LEU:HD13	1.94	0.48
1:A:231:TYR:HE2	1:A:271:THR:HG21	1.78	0.48
1:A:769:ARG:CZ	1:A:808:TYR:HA	2.43	0.48
1:C:477:PHE:CD2	1:C:480:LEU:HD12	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ARG:HH22	1:A:220:VAL:HB	1.78	0.48
1:A:528:LEU:C	1:A:531:LEU:H	2.17	0.48
1:A:724:ILE:HG21	1:A:750:LEU:HD11	1.95	0.48
1:A:768:TYR:O	1:A:770:ASP:N	2.46	0.48
2:B:24:PHE:O	2:B:28:LEU:HG	2.12	0.48
2:B:154:VAL:HG21	2:B:175:ARG:HE	1.78	0.48
1:C:59:PRO:HA	1:C:62:TYR:HB3	1.94	0.48
1:C:557:GLU:HB3	1:C:560:GLU:HG2	1.95	0.48
1:C:675:GLU:H	1:C:675:GLU:CD	2.16	0.48
1:C:694:ASP:HB3	1:C:697:ALA:HB3	1.93	0.48
1:A:80:LEU:HD23	1:A:84:HIS:CE1	2.48	0.48
1:A:641:ILE:HG21	1:A:661:PHE:CE1	2.49	0.48
1:C:170:ASN:N	1:C:173:ASP:OD2	2.47	0.48
1:A:230:THR:O	1:A:234:SER:OG	2.18	0.48
1:A:598:ILE:HA	1:A:601:THR:OG1	2.13	0.48
1:A:749:HIS:HB3	1:A:768:TYR:CD2	2.49	0.48
2:B:5:ILE:HG12	2:B:35:GLN:OE1	2.13	0.48
2:B:160:MET:SD	2:B:167:LEU:HD11	2.53	0.48
1:C:117:MET:HA	1:C:124:VAL:HG12	1.95	0.48
1:C:436:ILE:HA	1:C:440:ALA:HB3	1.95	0.48
1:C:521:LEU:O	1:C:524:VAL:HG22	2.13	0.48
1:C:734:LEU:C	1:C:740:GLN:HE22	2.17	0.48
1:A:229:PRO:O	1:A:232:ARG:HG3	2.13	0.48
1:A:244:VAL:HG12	1:A:281:ARG:NE	2.29	0.48
1:A:259:ILE:O	1:A:262:VAL:HG12	2.13	0.48
1:A:591:TYR:HA	1:A:593:GLU:CD	2.33	0.48
1:C:476:ILE:O	1:C:479:ALA:N	2.47	0.48
1:C:570:HIS:CE1	2:D:17:ALA:HA	2.48	0.48
1:C:617:LYS:HD2	1:C:671:THR:HB	1.96	0.48
1:A:89:LEU:N	1:A:116:TYR:OH	2.38	0.48
1:A:160:PRO:HG2	1:A:169:GLY:C	2.33	0.48
1:A:288:VAL:O	1:A:292:VAL:HG23	2.14	0.48
1:C:445:LYS:O	1:C:448:ALA:N	2.46	0.48
1:C:561:GLU:CD	1:C:561:GLU:H	2.17	0.48
1:C:678:TYR:HB2	1:C:715:PHE:HZ	1.78	0.48
1:A:598:ILE:O	1:A:602:THR:OG1	2.29	0.48
1:A:780:ARG:HE	1:A:784:VAL:HG21	1.79	0.48
2:B:176:LYS:HZ2	2:B:181:THR:N	2.11	0.48
1:C:460:GLN:O	1:C:463:LEU:HG	2.14	0.48
1:A:268:HIS:O	1:A:271:THR:N	2.38	0.48
1:A:577:ASN:HB2	1:A:616:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:LEU:O	1:A:613:ALA:HB3	2.13	0.48
1:A:749:HIS:HA	1:A:770:ASP:H	1.77	0.48
1:C:182:PHE:CZ	1:C:255:LEU:HD22	2.49	0.48
1:C:654:ALA:O	1:C:658:LEU:HG	2.13	0.48
1:C:684:ALA:O	1:C:688:TYR:HB3	2.13	0.48
1:C:686:THR:OG1	1:C:687:VAL:N	2.47	0.48
2:D:85:ILE:HA	2:D:112:VAL:HG21	1.95	0.48
1:A:416:CYS:SG	1:A:461:SER:OG	2.48	0.48
1:A:476:ILE:O	1:A:479:ALA:N	2.47	0.48
1:A:499:ALA:O	1:A:503:GLU:HG2	2.13	0.48
1:A:528:LEU:HA	1:A:531:LEU:HB3	1.95	0.48
1:A:664:CYS:O	1:A:667:VAL:HB	2.14	0.48
2:B:115:TRP:CE2	2:B:134:ASN:HB2	2.48	0.48
1:C:580:GLN:O	1:C:584:LEU:HG	2.14	0.48
1:C:657:CYS:HA	1:C:660:LEU:HD12	1.95	0.48
1:C:839:SER:O	1:C:842:VAL:HB	2.14	0.48
1:A:389:LEU:O	1:A:393:PHE:HB2	2.14	0.48
1:A:625:ASN:O	1:A:628:SER:N	2.47	0.48
1:A:804:ARG:HA	1:A:807:TYR:HB3	1.95	0.48
2:B:42:LEU:HB3	2:B:47:THR:HG21	1.96	0.48
2:B:44:ASP:OD1	2:B:47:THR:OG1	2.31	0.48
2:D:120:HIS:N	2:D:145:ASP:O	2.46	0.48
1:A:264:PRO:HB2	1:A:266:GLU:OE1	2.14	0.47
1:A:751:TRP:CH2	1:A:773:ARG:HB2	2.49	0.47
1:A:822:ASN:O	1:A:826:GLU:HG2	2.13	0.47
1:A:832:LEU:HD21	1:A:846:ARG:HE	1.79	0.47
1:C:176:ASN:O	1:C:180:THR:HG23	2.13	0.47
1:C:656:LEU:O	1:C:659:ARG:N	2.47	0.47
1:C:689:GLU:O	1:C:692:ILE:HG22	2.13	0.47
1:C:752:TRP:HB3	1:C:754:THR:HG22	1.96	0.47
1:A:493:THR:HG23	1:A:495:PRO:HD2	1.96	0.47
1:C:182:PHE:HD2	1:C:218:ASN:HB2	1.78	0.47
1:C:509:LEU:HD13	1:C:567:ARG:CZ	2.44	0.47
2:D:10:ASN:ND2	2:D:137:SER:HA	2.25	0.47
2:D:62:ARG:HG3	2:D:66:ASP:HB2	1.95	0.47
2:D:89:GLU:OE1	2:D:116:ALA:HB3	2.14	0.47
1:A:128:MET:HA	1:A:131:MET:HE2	1.96	0.47
1:A:232:ARG:NH2	1:A:233:ASP:OD1	2.43	0.47
1:A:696:LYS:O	1:A:699:PHE:HB3	2.14	0.47
1:A:819:LYS:HA	1:A:819:LYS:HD2	1.73	0.47
1:C:438:ALA:O	1:C:442:ALA:HB3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:ILE:HG22	1:A:528:LEU:HD22	1.96	0.47
1:A:676:VAL:O	1:A:679:GLU:N	2.48	0.47
1:C:408:ILE:HG12	1:C:448:ALA:HB1	1.96	0.47
2:D:117:GLY:HA3	2:D:146:TRP:H	1.78	0.47
1:A:213:LEU:HA	1:A:254:TYR:OH	2.15	0.47
1:A:663:SER:O	1:A:667:VAL:HG23	2.14	0.47
1:A:729:GLN:OE1	1:A:733:LYS:HG2	2.14	0.47
1:A:828:ILE:O	1:A:832:LEU:CB	2.63	0.47
2:B:6:LEU:O	2:B:37:LEU:HB2	2.14	0.47
2:B:121:ARG:O	2:B:136:GLY:N	2.48	0.47
1:C:38:LEU:HD13	1:C:79:HIS:HD2	1.80	0.47
1:C:189:TRP:O	1:C:192:LEU:HB2	2.14	0.47
1:A:503:GLU:CD	1:A:506:ARG:HH11	2.18	0.47
1:A:639:SER:OG	1:A:640:ALA:N	2.46	0.47
1:A:769:ARG:HH22	1:A:811:GLN:HB2	1.80	0.47
2:B:9:GLY:H	2:B:138:ALA:HB3	1.78	0.47
2:B:126:GLU:HG3	2:B:131:PHE:HD1	1.80	0.47
1:C:201:ARG:HA	1:C:204:ARG:NE	2.29	0.47
1:C:388:PRO:HG2	1:C:392:ILE:HG13	1.96	0.47
1:C:529:LYS:HE2	1:C:590:ALA:HA	1.95	0.47
1:C:617:LYS:HG3	1:C:626:TRP:CZ3	2.49	0.47
1:C:749:HIS:CD2	2:D:94:VAL:HB	2.50	0.47
2:D:155:PRO:CB	2:D:174:LEU:H	2.27	0.47
2:D:167:LEU:O	2:D:190:THR:HG23	2.14	0.47
2:D:187:GLU:HG2	2:D:188:LYS:H	1.80	0.47
1:A:73:LEU:HD13	1:A:76:LEU:HD12	1.95	0.47
1:A:78:ALA:N	1:A:81:ARG:HH11	2.11	0.47
1:A:140:HIS:ND1	1:A:143:ARG:HG2	2.29	0.47
1:A:219:ILE:HB	1:A:258:VAL:HG11	1.95	0.47
1:A:268:HIS:C	1:A:272:LEU:HG	2.35	0.47
1:A:423:LEU:CD1	1:A:468:SER:HB2	2.45	0.47
1:A:467:GLN:HG3	1:A:470:LEU:HD12	1.95	0.47
1:A:473:TYR:HB2	1:A:476:ILE:CG1	2.31	0.47
1:A:480:LEU:HD21	1:A:520:HIS:CD2	2.48	0.47
1:A:559:MET:O	1:A:561:GLU:HG3	2.14	0.47
1:A:710:HIS:HB3	1:A:711:ARG:NH1	2.30	0.47
1:A:742:ARG:O	1:A:746:LEU:HG	2.15	0.47
1:A:784:VAL:O	1:A:787:SER:OG	2.28	0.47
1:C:64:GLU:O	1:C:67:MET:HG2	2.14	0.47
1:C:635:LYS:O	1:C:639:SER:OG	2.30	0.47
1:C:742:ARG:HA	1:C:745:TYR:CZ	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:795:ILE:O	1:C:799:VAL:HG23	2.13	0.47
1:C:805:TYR:HH	1:C:820:TYR:HD2	1.60	0.47
2:D:9:GLY:O	2:D:137:SER:OG	2.28	0.47
2:D:12:HIS:HB3	2:D:16:ARG:HE	1.77	0.47
1:A:528:LEU:HA	1:A:531:LEU:CB	2.45	0.47
1:A:642:SER:O	1:A:646:THR:OG1	2.31	0.47
2:B:20:ILE:HD11	2:B:139:THR:HG22	1.96	0.47
2:B:51:LEU:O	2:B:55:SER:N	2.48	0.47
2:B:84:ARG:HB3	2:B:110:VAL:HA	1.96	0.47
2:D:120:HIS:H	2:D:145:ASP:C	2.18	0.47
1:A:145:LEU:HA	1:A:185:MET:HG2	1.96	0.47
1:A:228:LEU:HA	1:A:231:TYR:HB3	1.96	0.47
1:A:634:PHE:HA	1:A:637:LEU:CD1	2.44	0.47
2:B:6:LEU:HA	2:B:158:CYS:O	2.15	0.47
1:C:459:GLN:O	1:C:462:LEU:HB3	2.15	0.47
1:C:597:ARG:HD2	1:C:597:ARG:N	2.29	0.47
1:C:746:LEU:HG	1:C:749:HIS:CD2	2.50	0.47
1:A:842:VAL:O	1:A:845:SER:OG	2.25	0.47
2:B:119:SER:OG	2:B:145:ASP:OD2	2.20	0.47
1:C:593:GLU:O	1:C:597:ARG:HD3	2.14	0.47
1:A:12:ARG:HB2	1:A:15:GLU:OE2	2.15	0.46
1:A:228:LEU:O	1:A:232:ARG:HG2	2.15	0.46
1:A:595:ASN:HA	1:A:647:ARG:HD3	1.96	0.46
1:C:515:ILE:HG22	1:C:575:ASP:HA	1.97	0.46
1:C:565:LEU:CD1	1:C:568:LEU:HD23	2.44	0.46
1:A:289:LYS:HG3	1:A:414:LEU:HG	1.96	0.46
2:B:11:LEU:HD22	2:B:42:LEU:HG	1.98	0.46
1:C:514:LEU:HD23	1:C:515:ILE:O	2.16	0.46
1:C:561:GLU:HB2	1:C:565:LEU:HD23	1.97	0.46
2:D:137:SER:O	2:D:156:SER:OG	2.32	0.46
2:B:14:PRO:HA	2:B:17:ALA:O	2.16	0.46
1:C:21:VAL:HG21	1:C:65:LEU:HD11	1.97	0.46
1:C:66:TYR:O	1:C:70:PHE:HB2	2.16	0.46
1:C:638:HIS:HA	1:C:641:ILE:HD12	1.97	0.46
1:A:221:ARG:HD2	1:A:221:ARG:HA	1.61	0.46
1:A:688:TYR:CG	1:A:689:GLU:N	2.83	0.46
1:A:746:LEU:HD22	2:B:94:VAL:H	1.81	0.46
1:A:764:ASP:O	1:A:766:GLU:HG2	2.15	0.46
1:A:180:THR:HA	1:A:183:VAL:HG22	1.97	0.46
1:A:754:THR:HA	1:A:767:LEU:HD23	1.98	0.46
2:B:193:LYS:HE3	2:B:195:VAL:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:PHE:CD2	1:C:218:ASN:HB2	2.51	0.46
1:C:753:ALA:C	1:C:767:LEU:HB2	2.36	0.46
1:A:186:ASN:O	1:A:190:VAL:HG23	2.16	0.46
1:A:780:ARG:HE	1:A:784:VAL:CG2	2.29	0.46
2:B:12:HIS:O	2:B:16:ARG:N	2.48	0.46
2:B:24:PHE:CE1	2:B:174:LEU:HB2	2.50	0.46
1:A:172:GLN:OE1	1:A:176:ASN:ND2	2.48	0.46
2:B:11:LEU:O	2:B:13:ILE:HG13	2.16	0.46
1:C:443:LYS:HA	1:C:446:GLU:OE1	2.15	0.46
1:C:479:ALA:HA	1:C:482:LEU:HG	1.97	0.46
1:C:712:THR:O	1:C:757:ALA:HA	2.15	0.46
2:D:50:TYR:O	2:D:54:ILE:HG12	2.16	0.46
2:D:177:ASP:OD1	2:D:183:ASN:ND2	2.49	0.46
1:A:224:GLN:N	1:A:224:GLN:OE1	2.49	0.46
1:A:280:SER:HB2	1:A:396:GLN:HE22	1.80	0.46
1:A:434:ASP:HA	1:A:437:LEU:HD12	1.98	0.46
1:A:734:LEU:HB3	1:A:740:GLN:HE21	1.81	0.46
1:C:87:ASN:OD1	1:C:88:HIS:N	2.39	0.46
1:C:240:LEU:O	1:C:244:VAL:HG22	2.15	0.46
1:C:668:ALA:HA	1:C:671:THR:OG1	2.16	0.46
1:A:231:TYR:O	1:A:235:ILE:HD12	2.15	0.46
1:C:141:PRO:HB2	1:C:188:LEU:HB2	1.97	0.46
1:C:477:PHE:CG	1:C:480:LEU:HD12	2.51	0.46
1:C:692:ILE:C	1:C:698:GLN:HE21	2.20	0.46
1:C:755:PRO:O	1:C:767:LEU:HD23	2.16	0.46
2:D:80:HIS:HB2	2:D:162:VAL:HG11	1.98	0.46
2:D:173:GLN:HG3	2:D:175:ARG:HH21	1.80	0.46
1:A:263:PHE:H	1:A:268:HIS:HE2	1.63	0.45
1:A:505:VAL:HG23	1:A:564:TRP:CE3	2.52	0.45
1:A:567:ARG:NH1	2:B:18:LEU:HD22	2.31	0.45
1:A:803:ASP:HB3	1:A:804:ARG:NH1	2.31	0.45
2:B:111:ASP:OD1	2:B:130:LYS:NZ	2.49	0.45
1:C:180:THR:HA	1:C:183:VAL:HG22	1.98	0.45
1:C:221:ARG:NH1	1:C:224:GLN:HB2	2.31	0.45
1:C:737:LYS:HZ1	1:C:787:SER:CB	2.29	0.45
2:D:77:VAL:HG22	2:D:86:GLY:HA2	1.99	0.45
2:D:121:ARG:HE	2:D:122:PHE:N	2.13	0.45
1:A:198:SER:HA	1:A:204:ARG:HH22	1.82	0.45
1:A:505:VAL:HG23	1:A:564:TRP:HE3	1.80	0.45
1:C:248:ASP:HB3	1:C:251:ALA:HB3	1.98	0.45
1:C:398:GLN:O	1:C:402:GLN:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:GLY:O	1:C:439:TYR:HB2	2.16	0.45
1:C:755:PRO:O	1:C:758:ALA:N	2.47	0.45
1:A:148:ARG:HH11	1:A:185:MET:HG3	1.81	0.45
1:A:779:GLN:O	1:A:783:ARG:HG2	2.17	0.45
2:B:9:GLY:O	2:B:139:THR:HG23	2.17	0.45
2:B:161:ASP:N	2:B:168:THR:O	2.46	0.45
1:C:93:TYR:O	1:C:97:GLN:HB2	2.16	0.45
1:C:734:LEU:HD13	1:C:734:LEU:HA	1.76	0.45
2:D:169:LEU:HB3	2:D:189:VAL:O	2.17	0.45
1:A:575:ASP:HB3	1:A:580:GLN:HG3	1.98	0.45
1:A:849:PHE:CZ	1:A:853:LEU:HD11	2.52	0.45
2:B:84:ARG:NH1	2:B:109:ASP:OD2	2.50	0.45
2:B:120:HIS:CE1	2:B:144:THR:HG23	2.50	0.45
1:C:160:PRO:O	1:C:174:SER:N	2.48	0.45
1:C:639:SER:O	1:C:643:THR:OG1	2.25	0.45
1:C:746:LEU:HD23	1:C:746:LEU:O	2.16	0.45
2:D:118:GLY:N	2:D:146:TRP:H	2.14	0.45
2:D:139:THR:O	2:D:139:THR:HG22	2.17	0.45
1:A:441:LEU:HD13	1:A:441:LEU:HA	1.74	0.45
1:A:678:TYR:CZ	1:A:719:ASN:OD1	2.69	0.45
1:A:176:ASN:O	1:A:180:THR:HG22	2.17	0.45
1:A:203:LEU:O	1:A:206:GLN:HB3	2.16	0.45
1:A:531:LEU:HD23	1:A:532:ILE:N	2.30	0.45
1:A:808:TYR:CD2	1:A:816:VAL:HG21	2.51	0.45
1:C:579:THR:HA	1:C:582:ARG:NH1	2.32	0.45
1:C:688:TYR:HE1	1:C:692:ILE:HD13	1.80	0.45
2:D:13:ILE:O	2:D:43:THR:N	2.39	0.45
2:D:13:ILE:CG1	2:D:14:PRO:HA	2.44	0.45
1:A:29:ARG:HA	1:A:32:LEU:HG	1.98	0.45
1:A:164:SER:CB	1:A:170:ASN:HB2	2.46	0.45
1:A:768:TYR:O	1:A:769:ARG:C	2.54	0.45
1:A:853:LEU:HA	1:A:856:ILE:HG23	1.97	0.45
1:C:207:GLU:HA	1:C:210:GLU:OE1	2.17	0.45
1:C:503:GLU:O	1:C:507:THR:HG23	2.16	0.45
1:C:688:TYR:CE1	1:C:692:ILE:HD13	2.51	0.45
1:C:694:ASP:C	1:C:698:GLN:HG3	2.36	0.45
2:D:50:TYR:CE2	2:D:54:ILE:HD11	2.51	0.45
1:A:232:ARG:CA	1:A:236:LEU:HD13	2.46	0.45
1:A:259:ILE:HA	1:A:262:VAL:HG12	1.99	0.45
1:A:459:GLN:NE2	1:A:460:GLN:HG3	2.32	0.45
1:A:583:LEU:O	1:A:586:MET:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:PHE:O	1:A:688:TYR:HB3	2.16	0.45
2:B:24:PHE:HD2	2:B:157:PHE:HE2	1.64	0.45
1:C:178:ILE:HG23	1:C:218:ASN:HB3	1.98	0.45
1:C:212:GLN:O	1:C:254:TYR:OH	2.18	0.45
1:C:411:THR:HA	1:C:414:LEU:HD12	1.99	0.45
2:D:136:GLY:HA3	2:D:156:SER:HB3	1.99	0.45
1:A:113:GLY:HA3	1:A:127:LEU:HD22	1.99	0.45
1:A:236:LEU:O	1:A:240:LEU:HB2	2.17	0.45
1:A:241:GLU:HA	1:A:244:VAL:HG22	1.99	0.45
1:A:265:ASP:HA	1:A:268:HIS:HD2	1.81	0.45
1:A:265:ASP:OD2	1:A:298:ARG:NH1	2.50	0.45
1:C:263:PHE:O	1:C:298:ARG:NH1	2.50	0.45
1:C:486:VAL:HA	1:C:489:PHE:CD2	2.52	0.45
1:C:601:THR:C	1:C:604:PRO:HD2	2.37	0.45
1:C:847:LYS:HZ2	2:D:106:ASN:HB3	1.81	0.45
2:D:89:GLU:HG3	2:D:91:PHE:H	1.82	0.45
2:D:144:THR:HG22	2:D:144:THR:O	2.16	0.45
1:A:443:LYS:O	1:A:447:HIS:HB2	2.17	0.45
1:C:14:LEU:O	1:C:18:LEU:HD23	2.17	0.45
1:C:17:ALA:O	1:C:21:VAL:HG23	2.16	0.45
1:C:408:ILE:HG21	1:C:450:SER:OG	2.17	0.45
2:D:88:LEU:O	2:D:115:TRP:HA	2.17	0.45
2:D:163:GLN:NE2	2:D:166:SER:OG	2.50	0.45
1:A:733:LYS:C	1:A:734:LEU:HD22	2.38	0.44
2:B:79:THR:HA	2:B:83:LEU:O	2.17	0.44
1:C:236:LEU:HD21	1:C:274:GLN:HE21	1.82	0.44
1:C:399:HIS:O	1:C:403:ALA:N	2.28	0.44
1:C:476:ILE:HD13	1:C:508:LEU:HD23	1.98	0.44
1:C:486:VAL:O	1:C:489:PHE:HB2	2.17	0.44
1:C:486:VAL:O	1:C:490:GLN:HG3	2.17	0.44
1:C:660:LEU:O	1:C:663:SER:OG	2.32	0.44
1:C:837:GLN:NE2	1:C:838:ASP:H	2.15	0.44
1:A:14:LEU:HD13	1:A:61:GLN:HB3	1.99	0.44
1:A:78:ALA:HA	1:A:81:ARG:HE	1.83	0.44
1:A:577:ASN:HB3	1:A:615:ARG:HG2	2.00	0.44
1:A:598:ILE:HG22	1:A:602:THR:OG1	2.17	0.44
1:A:769:ARG:NH2	1:A:811:GLN:HB2	2.31	0.44
1:C:152:SER:O	1:C:156:ARG:HG3	2.17	0.44
1:C:486:VAL:HA	1:C:489:PHE:HD2	1.82	0.44
1:C:588:ARG:HH12	1:C:639:SER:HB2	1.82	0.44
1:C:715:PHE:CE2	1:C:719:ASN:HB2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:770:ASP:O	1:C:774:VAL:HG23	2.17	0.44
1:C:778:LEU:HD12	1:C:778:LEU:HA	1.77	0.44
1:A:190:VAL:HG22	1:A:208:ARG:NH2	2.32	0.44
1:A:271:THR:O	1:A:275:PHE:N	2.39	0.44
1:A:726:LYS:C	1:A:730:HIS:HD1	2.19	0.44
1:A:769:ARG:HH11	1:A:813:ASN:HB2	1.82	0.44
2:B:118:GLY:HA2	2:B:120:HIS:CE1	2.52	0.44
1:C:227:ASP:HA	1:C:267:TYR:HE1	1.82	0.44
1:C:247:ARG:C	1:C:283:ASN:HD21	2.21	0.44
1:C:467:GLN:HA	1:C:470:LEU:HD12	1.99	0.44
1:C:563:GLY:C	1:C:567:ARG:HE	2.20	0.44
1:C:564:TRP:CD1	1:C:564:TRP:N	2.86	0.44
1:C:730:HIS:HA	1:C:733:LYS:HG2	1.98	0.44
1:C:805:TYR:HE2	1:C:821:LEU:HD12	1.81	0.44
1:C:822:ASN:HA	1:C:825:ILE:HG12	2.00	0.44
1:C:853:LEU:HA	1:C:856:ILE:HG23	1.98	0.44
2:D:22:PRO:HA	2:D:25:LYS:HB2	1.99	0.44
1:A:397:VAL:HA	1:A:400:LEU:HD12	1.99	0.44
2:B:86:GLY:HA3	2:B:110:VAL:HG21	1.98	0.44
1:C:18:LEU:HD13	1:C:65:LEU:HD13	2.00	0.44
1:C:429:ARG:HD2	1:C:429:ARG:HA	1.78	0.44
1:C:713:ARG:HD3	1:C:759:ARG:HH11	1.82	0.44
1:C:803:ASP:HA	1:C:806:VAL:HG12	1.99	0.44
1:A:470:LEU:CD2	1:A:476:ILE:HG21	2.42	0.44
1:A:588:ARG:O	1:A:591:TYR:N	2.46	0.44
1:A:704:VAL:O	1:A:707:SER:OG	2.33	0.44
1:C:488:LEU:HA	1:C:488:LEU:HD13	1.79	0.44
2:D:75:MET:SD	2:D:76:GLN:N	2.91	0.44
2:D:165:ILE:HD12	2:D:193:LYS:O	2.18	0.44
2:D:177:ASP:OD1	2:D:181:THR:HB	2.17	0.44
1:A:110:ILE:HG12	1:A:131:MET:SD	2.57	0.44
1:A:232:ARG:O	1:A:236:LEU:HB2	2.18	0.44
1:A:808:TYR:HB3	1:A:813:ASN:CB	2.48	0.44
1:C:400:LEU:HD12	1:C:406:LEU:HD11	2.00	0.44
1:C:735:LEU:HD23	1:C:736:ARG:CA	2.48	0.44
2:D:12:HIS:CD2	2:D:142:PHE:CE2	3.05	0.44
2:D:24:PHE:O	2:D:28:LEU:HG	2.18	0.44
2:D:122:PHE:CZ	2:D:124:CYS:HB3	2.53	0.44
1:A:188:LEU:O	1:A:191:ARG:N	2.51	0.44
1:A:532:ILE:HD13	1:A:597:ARG:HG2	2.00	0.44
2:B:137:SER:OG	2:B:153:VAL:HB	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:ILE:HG21	2:B:195:VAL:HB	2.00	0.44
1:C:108:LEU:O	1:C:112:VAL:HG13	2.17	0.44
1:C:145:LEU:HD13	1:C:188:LEU:HD23	1.98	0.44
1:C:430:LEU:HD23	1:C:434:ASP:H	1.83	0.44
1:C:488:LEU:C	1:C:492:GLN:HE21	2.21	0.44
1:C:769:ARG:NH2	1:C:811:GLN:HG3	2.33	0.44
1:A:567:ARG:HH21	2:B:19:ASP:CG	2.21	0.44
1:A:760:GLY:O	1:A:765:THR:N	2.51	0.44
1:C:581:PHE:HB2	1:C:616:PHE:HE2	1.83	0.44
1:A:263:PHE:HD1	1:A:264:PRO:HD2	1.82	0.44
1:A:594:GLY:C	1:A:597:ARG:HH21	2.21	0.44
1:A:700:GLN:O	1:A:703:CYS:HB3	2.18	0.44
1:C:180:THR:O	1:C:184:GLU:HG2	2.18	0.44
2:D:9:GLY:H	2:D:138:ALA:N	2.16	0.44
1:A:462:LEU:O	1:A:465:LEU:HB3	2.17	0.43
1:A:661:PHE:HE2	1:A:683:GLN:HB3	1.83	0.43
2:B:36:THR:HG21	2:B:55:SER:HA	1.99	0.43
1:C:252:GLN:O	1:C:256:LEU:HB2	2.17	0.43
1:C:532:ILE:HG23	1:C:593:GLU:OE1	2.18	0.43
1:C:600:THR:O	1:C:603:PRO:HD2	2.18	0.43
1:C:758:ALA:HB1	1:C:768:TYR:CB	2.47	0.43
1:A:122:ALA:O	1:A:168:GLU:HB2	2.18	0.43
1:A:175:ILE:O	1:A:179:LEU:HB2	2.18	0.43
1:A:258:VAL:HA	1:A:261:GLN:NE2	2.33	0.43
1:A:850:ILE:O	1:A:854:GLU:HG2	2.18	0.43
2:B:35:GLN:HA	2:B:57:ASP:HB2	1.99	0.43
2:B:60:ILE:HG22	2:B:61:VAL:O	2.18	0.43
2:B:62:ARG:NH2	2:B:73:PRO:HA	2.33	0.43
1:C:602:THR:OG1	1:C:603:PRO:HD3	2.18	0.43
1:C:647:ARG:HA	1:C:647:ARG:HD3	1.72	0.43
1:C:701:ALA:O	1:C:705:ILE:HG13	2.18	0.43
1:C:794:SER:HB2	1:C:798:PHE:CZ	2.53	0.43
1:A:114:THR:HG21	1:A:150:TYR:OH	2.19	0.43
1:A:161:THR:HG22	1:A:162:GLY:N	2.28	0.43
1:A:408:ILE:H	1:A:408:ILE:HG13	1.47	0.43
1:A:486:VAL:HA	1:A:489:PHE:CZ	2.52	0.43
1:A:521:LEU:HD11	1:A:583:LEU:HD13	2.00	0.43
1:A:676:VAL:HA	1:A:679:GLU:CD	2.38	0.43
1:C:467:GLN:HE21	1:C:500:ILE:HG12	1.83	0.43
2:D:74:LEU:O	2:D:88:LEU:HA	2.18	0.43
1:A:117:MET:CE	1:A:154:GLN:HB3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:GLY:N	1:A:167:PRO:HD2	2.33	0.43
1:A:240:LEU:HA	1:A:240:LEU:HD23	1.90	0.43
1:A:681:PHE:CE2	1:A:709:LEU:HD13	2.53	0.43
1:A:769:ARG:HH12	1:A:811:GLN:HB2	1.84	0.43
2:B:165:ILE:HB	2:B:193:LYS:HB3	2.01	0.43
1:C:231:TYR:CZ	1:C:236:LEU:HB2	2.53	0.43
1:C:530:VAL:HA	1:C:534:GLU:OE2	2.19	0.43
1:C:647:ARG:HH21	1:C:647:ARG:N	2.16	0.43
1:C:795:ILE:HA	1:C:798:PHE:CD2	2.54	0.43
2:D:38:CYS:HB3	2:D:59:LYS:C	2.39	0.43
2:D:83:LEU:HG	2:D:165:ILE:HA	1.99	0.43
2:D:85:ILE:HA	2:D:112:VAL:CG2	2.48	0.43
1:A:524:VAL:HA	1:A:527:ILE:HD12	2.01	0.43
1:A:671:THR:C	1:A:673:PHE:H	2.21	0.43
1:A:736:ARG:CZ	1:A:738:PRO:HD2	2.49	0.43
2:B:25:LYS:HB3	2:B:26:LYS:NZ	2.33	0.43
1:C:185:MET:HB3	1:C:215:VAL:HG22	2.00	0.43
1:C:296:MET:HA	1:C:299:LEU:HD12	2.00	0.43
1:C:694:ASP:O	1:C:698:GLN:HG3	2.18	0.43
1:C:696:LYS:O	1:C:699:PHE:HB3	2.18	0.43
1:C:739:ASP:O	1:C:742:ARG:HB2	2.18	0.43
2:D:1:MET:SD	2:D:4:LEU:HD21	2.59	0.43
2:D:111:ASP:OD2	2:D:130:LYS:HG2	2.18	0.43
1:A:183:VAL:HG12	1:A:242:GLN:HG3	2.01	0.43
1:A:462:LEU:O	1:A:466:LEU:HG	2.18	0.43
1:A:698:GLN:OE1	1:A:702:VAL:N	2.52	0.43
1:A:734:LEU:HD13	1:A:734:LEU:HA	1.65	0.43
1:A:804:ARG:O	1:A:807:TYR:HB3	2.18	0.43
2:B:122:PHE:HA	2:B:134:ASN:O	2.19	0.43
2:D:187:GLU:HG2	2:D:188:LYS:N	2.34	0.43
1:A:559:MET:H	1:A:559:MET:HG3	1.38	0.43
2:B:158:CYS:HB3	2:B:169:LEU:HG	2.01	0.43
2:B:165:ILE:HD12	2:B:193:LYS:O	2.18	0.43
1:C:45:CYS:SG	1:C:76:LEU:HD22	2.58	0.43
1:C:53:ARG:HD2	1:C:107:TYR:CE2	2.54	0.43
1:C:557:GLU:O	1:C:560:GLU:HA	2.19	0.43
1:C:561:GLU:OE1	1:C:561:GLU:N	2.49	0.43
1:C:855:MET:O	1:C:857:GLN:HG2	2.18	0.43
1:A:580:GLN:OE1	1:A:615:ARG:HD3	2.19	0.43
2:B:64:ARG:C	2:B:66:ASP:H	2.22	0.43
1:C:435:GLY:HA2	1:C:439:TYR:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:83:LEU:HG	2:D:164:GLY:O	2.19	0.43
1:A:409:GLN:HG2	1:A:410:ASP:N	2.32	0.43
1:A:783:ARG:HA	1:A:786:ASP:OD2	2.19	0.43
1:C:103:ILE:HG23	1:C:107:TYR:CE2	2.54	0.43
1:C:298:ARG:HA	1:C:301:ASP:OD2	2.19	0.43
1:C:577:ASN:ND2	1:C:615:ARG:HH21	2.17	0.43
1:C:621:HIS:HB2	1:C:622:TYR:CE2	2.53	0.43
1:A:53:ARG:HD3	1:A:103:ILE:HB	2.00	0.43
1:A:260:THR:CG2	1:A:298:ARG:HE	2.32	0.43
1:A:709:LEU:HD22	1:A:727:CYS:SG	2.59	0.43
2:B:10:ASN:CG	2:B:137:SER:HA	2.40	0.43
1:C:272:LEU:O	1:C:276:LEU:HG	2.18	0.43
1:C:389:LEU:HD22	1:C:393:PHE:HE2	1.84	0.43
1:A:144:GLY:O	1:A:148:ARG:HG3	2.19	0.42
1:A:414:LEU:HD23	1:A:414:LEU:HA	1.81	0.42
1:A:434:ASP:O	1:A:437:LEU:HB2	2.18	0.42
1:A:437:LEU:HB3	1:A:488:LEU:HD11	2.00	0.42
1:A:482:LEU:O	1:A:485:TYR:HB3	2.19	0.42
1:A:514:LEU:HD12	1:A:515:ILE:O	2.18	0.42
1:A:750:LEU:HD12	1:A:773:ARG:HH12	1.84	0.42
2:B:98:PRO:HA	2:B:101:LEU:HD12	2.01	0.42
1:C:231:TYR:HE2	1:C:271:THR:HG21	1.84	0.42
1:C:467:GLN:CD	1:C:470:LEU:HD12	2.39	0.42
1:C:481:SER:O	1:C:483:PRO:HD3	2.19	0.42
1:C:494:TYR:HB2	1:C:497:ARG:NH2	2.33	0.42
1:C:851:GLN:O	1:C:855:MET:HG2	2.19	0.42
2:D:116:ALA:HA	2:D:145:ASP:CG	2.39	0.42
1:A:29:ARG:NH1	1:A:75:TYR:HB2	2.34	0.42
1:A:654:ALA:O	1:A:658:LEU:HD13	2.19	0.42
1:A:749:HIS:HE2	2:B:94:VAL:HG21	1.84	0.42
1:A:791:THR:HG23	1:A:792:ALA:N	2.35	0.42
1:C:128:MET:O	1:C:132:MET:HG3	2.19	0.42
1:A:89:LEU:HD13	1:A:112:VAL:HG22	2.00	0.42
1:A:102:ILE:HD13	1:A:138:VAL:HG23	2.02	0.42
1:A:487:SER:O	1:A:490:GLN:NE2	2.53	0.42
1:A:677:ALA:HA	1:A:680:PHE:CD1	2.54	0.42
2:B:169:LEU:HD22	2:B:189:VAL:HB	2.01	0.42
1:C:825:ILE:HG13	1:C:826:GLU:N	2.35	0.42
1:A:599:ARG:HG3	1:A:600:THR:HG23	2.01	0.42
1:C:206:GLN:OE1	1:C:209:ARG:NE	2.51	0.42
2:D:29:SER:O	2:D:32:LYS:NZ	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:VAL:HA	1:A:52:LEU:HB2	2.01	0.42
1:A:103:ILE:O	1:A:106:LEU:HB3	2.20	0.42
1:A:189:TRP:CZ2	1:A:208:ARG:HG2	2.54	0.42
1:A:521:LEU:HA	1:A:524:VAL:CG2	2.47	0.42
1:A:794:SER:HB2	1:A:798:PHE:CZ	2.55	0.42
1:A:800:GLU:HG3	2:B:107:LYS:NZ	2.35	0.42
2:B:12:HIS:O	2:B:15:ASP:N	2.52	0.42
2:B:13:ILE:HG22	2:B:44:ASP:OD2	2.19	0.42
2:B:24:PHE:HA	2:B:27:LEU:HB2	2.01	0.42
1:C:299:LEU:O	1:C:302:TYR:HB2	2.20	0.42
1:C:409:GLN:HG3	1:C:457:PRO:HG2	2.01	0.42
1:C:578:ASP:N	1:C:578:ASP:OD1	2.52	0.42
1:C:666:GLN:NE2	1:C:707:SER:O	2.52	0.42
1:C:668:ALA:O	1:C:673:PHE:N	2.30	0.42
1:A:15:GLU:OE2	1:A:15:GLU:N	2.53	0.42
1:A:77:SER:O	1:A:80:LEU:HB2	2.19	0.42
1:A:164:SER:HB3	1:A:170:ASN:HB2	2.00	0.42
1:A:387:VAL:O	1:A:389:LEU:HG	2.19	0.42
1:A:638:HIS:HA	1:A:641:ILE:HD12	2.01	0.42
1:A:663:SER:HA	1:A:666:GLN:NE2	2.31	0.42
1:A:755:PRO:O	1:A:767:LEU:HG	2.19	0.42
1:A:763:GLU:O	1:A:766:GLU:HB2	2.20	0.42
1:A:791:THR:HG23	1:A:792:ALA:H	1.85	0.42
1:A:803:ASP:HB3	1:A:804:ARG:HH12	1.85	0.42
2:B:18:LEU:HA	2:B:18:LEU:HD23	1.81	0.42
2:B:69:ALA:HB1	2:B:72:LEU:HG	2.01	0.42
2:B:89:GLU:HG2	2:B:116:ALA:O	2.19	0.42
1:C:190:VAL:HG12	1:C:208:ARG:NH2	2.34	0.42
1:C:277:GLY:O	1:C:281:ARG:NE	2.53	0.42
1:C:518:PRO:O	1:C:521:LEU:HB2	2.20	0.42
1:C:646:THR:HB	1:C:647:ARG:HH22	1.84	0.42
2:D:12:HIS:HB3	2:D:16:ARG:CZ	2.50	0.42
2:D:34:SER:C	2:D:55:SER:HB2	2.39	0.42
2:D:177:ASP:H	2:D:181:THR:N	2.18	0.42
1:A:567:ARG:NH2	2:B:18:LEU:HB3	2.34	0.42
1:A:569:VAL:HG21	1:A:604:PRO:HB3	2.02	0.42
1:A:610:LEU:HD22	1:A:667:VAL:HG11	2.01	0.42
2:B:89:GLU:O	2:B:115:TRP:HB2	2.20	0.42
1:C:213:LEU:HG	1:C:214:LEU:HD12	2.02	0.42
1:C:452:ASP:N	1:C:452:ASP:OD1	2.51	0.42
1:C:790:GLU:OE1	1:C:792:ALA:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:VAL:O	1:A:670:MET:N	2.52	0.42
2:B:121:ARG:NH2	2:B:123:GLU:O	2.48	0.42
1:C:53:ARG:NH2	1:C:103:ILE:HG13	2.35	0.42
1:C:212:GLN:HB2	1:C:254:TYR:CE2	2.54	0.42
1:C:275:PHE:CD2	1:C:276:LEU:HD23	2.55	0.42
1:C:502:GLY:HA2	1:C:564:TRP:CZ3	2.55	0.42
1:C:601:THR:O	1:C:601:THR:OG1	2.35	0.42
1:C:637:LEU:O	1:C:640:ALA:N	2.53	0.42
1:C:668:ALA:O	1:C:672:GLU:N	2.53	0.42
1:C:746:LEU:O	1:C:749:HIS:CD2	2.73	0.42
1:C:853:LEU:O	1:C:856:ILE:HG12	2.19	0.42
1:A:14:LEU:HD22	1:A:61:GLN:HG2	2.00	0.42
1:A:629:GLN:O	1:A:633:LEU:HG	2.20	0.42
1:A:650:GLY:HA2	1:A:651:PRO:HD3	1.92	0.42
1:A:707:SER:HA	1:A:711:ARG:NH1	2.34	0.42
1:A:769:ARG:NH2	1:A:808:TYR:HA	2.34	0.42
1:A:773:ARG:CZ	1:A:773:ARG:HB3	2.49	0.42
2:B:80:HIS:HB2	2:B:162:VAL:HG12	2.00	0.42
1:C:24:GLN:OE1	1:C:47:THR:OG1	2.38	0.42
1:C:89:LEU:O	1:C:116:TYR:OH	2.37	0.42
1:C:467:GLN:NE2	1:C:500:ILE:HG23	2.34	0.42
1:A:92:LEU:O	1:A:96:VAL:HG22	2.20	0.42
1:A:188:LEU:HD21	1:A:192:LEU:HD22	2.01	0.42
1:A:193:GLN:HB3	1:A:194:HIS:CE1	2.54	0.42
1:A:506:ARG:HA	1:A:509:LEU:HG	2.01	0.42
1:A:735:LEU:N	1:A:740:GLN:NE2	2.68	0.42
2:B:3:PHE:CD1	2:B:35:GLN:HB2	2.55	0.42
1:C:77:SER:HA	1:C:80:LEU:HB3	2.02	0.42
1:C:231:TYR:HE1	1:C:239:LEU:HD12	1.85	0.42
1:C:430:LEU:O	1:C:430:LEU:HD23	2.20	0.42
1:C:471:ARG:NE	1:C:471:ARG:HA	2.34	0.42
1:C:656:LEU:HD21	2:D:67:VAL:HG21	2.02	0.42
1:C:723:LEU:HD23	1:C:726:LYS:HZ3	1.85	0.42
1:A:65:LEU:O	1:A:69:VAL:HG13	2.20	0.41
1:A:125:LYS:HZ2	1:A:177:PHE:HB2	1.85	0.41
1:A:179:LEU:HG	1:A:239:LEU:HD21	2.00	0.41
1:A:769:ARG:NH1	1:A:811:GLN:HB2	2.34	0.41
1:A:790:GLU:OE1	1:A:793:THR:HG23	2.20	0.41
2:B:12:HIS:CA	2:B:15:ASP:HB2	2.48	0.41
2:B:121:ARG:NH1	2:B:123:GLU:N	2.68	0.41
1:C:103:ILE:HD13	1:C:103:ILE:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:GLY:HA2	1:C:156:ARG:NE	2.35	0.41
1:C:769:ARG:HH22	1:C:811:GLN:HG3	1.85	0.41
1:C:837:GLN:O	1:C:842:VAL:HG21	2.19	0.41
2:D:10:ASN:ND2	2:D:136:GLY:O	2.53	0.41
2:D:89:GLU:O	2:D:115:TRP:HB2	2.19	0.41
2:D:98:PRO:HA	2:D:101:LEU:HD12	2.02	0.41
1:A:575:ASP:HB3	1:A:580:GLN:CG	2.50	0.41
1:A:676:VAL:HA	1:A:679:GLU:OE1	2.20	0.41
1:A:754:THR:HG22	1:A:769:ARG:HB2	2.02	0.41
2:B:16:ARG:HD3	2:B:142:PHE:CZ	2.55	0.41
2:B:88:LEU:HD23	2:B:114:CYS:O	2.20	0.41
1:C:298:ARG:HG2	1:C:302:TYR:CE1	2.55	0.41
1:C:625:ASN:O	1:C:629:GLN:N	2.45	0.41
1:C:643:THR:O	1:C:646:THR:HB	2.20	0.41
2:D:16:ARG:CD	2:D:142:PHE:HZ	2.29	0.41
2:D:160:MET:HG2	2:D:167:LEU:HD21	2.01	0.41
1:A:31:PHE:HE2	1:A:44:CYS:HB2	1.85	0.41
1:A:226:VAL:HB	1:A:230:THR:OG1	2.20	0.41
1:A:407:PRO:HB2	1:A:409:GLN:CD	2.41	0.41
1:A:482:LEU:HB2	1:A:485:TYR:HB2	2.02	0.41
1:A:521:LEU:HB3	1:A:586:MET:HE2	2.02	0.41
1:A:666:GLN:O	1:A:669:ASP:HB3	2.20	0.41
2:B:111:ASP:HA	2:B:130:LYS:HZ1	1.85	0.41
2:D:76:GLN:HE21	2:D:78:VAL:HG13	1.84	0.41
2:D:171:VAL:HG13	2:D:187:GLU:HB3	2.01	0.41
1:C:598:ILE:H	1:C:598:ILE:HD12	1.85	0.41
2:D:12:HIS:CD2	2:D:141:ALA:HB1	2.55	0.41
1:A:564:TRP:CG	1:A:565:LEU:N	2.88	0.41
1:A:588:ARG:HE	1:A:640:ALA:CA	2.30	0.41
2:B:41:ASN:HA	2:B:66:ASP:OD1	2.21	0.41
1:C:244:VAL:HG12	1:C:282:LEU:HD21	2.02	0.41
1:C:453:LEU:HA	1:C:456:GLN:HB2	2.03	0.41
1:C:756:ILE:HD13	1:C:759:ARG:HD3	2.03	0.41
2:D:8:ILE:CG1	2:D:138:ALA:HA	2.50	0.41
2:D:79:THR:HA	2:D:83:LEU:O	2.21	0.41
1:A:213:LEU:HD23	1:A:213:LEU:H	1.86	0.41
1:A:269:LEU:HA	1:A:272:LEU:HB2	2.02	0.41
2:B:158:CYS:SG	2:B:171:VAL:HB	2.60	0.41
1:C:138:VAL:HG22	1:C:140:HIS:H	1.85	0.41
1:C:582:ARG:O	1:C:586:MET:HG2	2.20	0.41
1:C:606:ILE:HG21	1:C:660:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:692:ILE:HG13	1:C:698:GLN:NE2	2.35	0.41
1:C:744:VAL:CG1	1:C:781:ALA:HB2	2.50	0.41
2:D:52:ARG:HD2	2:D:52:ARG:HA	1.80	0.41
1:A:59:PRO:HG2	1:A:207:GLU:HG2	2.03	0.41
1:A:292:VAL:O	1:A:296:MET:HG3	2.21	0.41
1:A:390:TYR:CE1	1:A:432:TYR:HB3	2.55	0.41
1:C:38:LEU:HD21	1:C:80:LEU:HA	2.02	0.41
1:C:248:ASP:OD2	1:C:251:ALA:N	2.35	0.41
2:D:5:ILE:O	2:D:160:MET:HB2	2.21	0.41
2:D:22:PRO:O	2:D:26:LYS:HG2	2.19	0.41
2:D:76:GLN:HG3	2:D:87:PHE:CZ	2.56	0.41
2:D:111:ASP:HA	2:D:130:LYS:NZ	2.36	0.41
1:A:559:MET:C	1:A:561:GLU:H	2.22	0.41
1:A:723:LEU:HD13	1:A:723:LEU:HA	1.62	0.41
1:A:752:TRP:CG	1:A:753:ALA:N	2.87	0.41
1:A:855:MET:SD	2:B:128:MET:HB3	2.61	0.41
2:B:10:ASN:ND2	2:B:116:ALA:HB1	2.30	0.41
1:C:38:LEU:HB3	1:C:84:HIS:CE1	2.55	0.41
1:C:294:GLY:HA2	1:C:297:ASN:OD1	2.21	0.41
1:C:493:THR:O	1:C:497:ARG:HG3	2.20	0.41
1:C:697:ALA:O	1:C:700:GLN:N	2.54	0.41
1:A:117:MET:HE1	1:A:154:GLN:HB3	2.03	0.41
1:A:192:LEU:HD21	1:A:211:LEU:HD12	2.03	0.41
1:A:526:GLU:OE2	1:A:527:ILE:HG13	2.21	0.41
1:A:587:THR:OG1	1:A:588:ARG:N	2.53	0.41
1:A:625:ASN:O	1:A:629:GLN:HG3	2.21	0.41
1:A:637:LEU:HD13	1:A:664:CYS:SG	2.61	0.41
1:A:749:HIS:CA	1:A:770:ASP:H	2.32	0.41
1:A:817:THR:O	1:A:821:LEU:HG	2.21	0.41
1:A:854:GLU:HB2	1:A:855:MET:HE2	2.03	0.41
2:B:3:PHE:HD1	2:B:35:GLN:HB2	1.86	0.41
2:B:24:PHE:CZ	2:B:174:LEU:HB2	2.56	0.41
2:B:121:ARG:NH1	2:B:123:GLU:H	2.18	0.41
1:C:223:SER:HB2	1:C:262:VAL:CG1	2.51	0.41
1:C:389:LEU:O	1:C:393:PHE:CB	2.69	0.41
1:C:729:GLN:C	1:C:733:LYS:HZ3	2.20	0.41
2:D:89:GLU:HB3	2:D:91:PHE:CD1	2.55	0.41
1:A:183:VAL:CG1	1:A:242:GLN:HG3	2.51	0.41
1:A:254:TYR:O	1:A:258:VAL:HG23	2.20	0.41
1:A:560:GLU:OE2	1:A:564:TRP:N	2.54	0.41
1:A:644:LEU:HD13	1:A:644:LEU:HA	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:678:TYR:CE1	1:A:719:ASN:HA	2.56	0.41
1:A:828:ILE:O	1:A:832:LEU:HB2	2.20	0.41
2:B:143:THR:OG1	2:B:144:THR:N	2.53	0.41
1:C:66:TYR:HA	1:C:69:VAL:HG22	2.03	0.41
1:C:152:SER:O	1:C:156:ARG:N	2.54	0.41
1:C:189:TRP:HE1	1:C:212:GLN:HB3	1.86	0.41
1:C:195:GLN:HG3	1:C:204:ARG:HB2	2.03	0.41
1:C:390:TYR:OH	1:C:436:ILE:HB	2.21	0.41
1:C:532:ILE:HG23	1:C:533:LYS:H	1.84	0.41
1:C:645:TYR:O	1:C:648:VAL:N	2.54	0.41
1:C:756:ILE:HG23	1:C:759:ARG:NE	2.33	0.41
2:D:0:SER:C	2:D:2:ALA:H	2.24	0.41
1:C:38:LEU:HD12	1:C:38:LEU:HA	1.92	0.40
1:C:223:SER:HB3	1:C:224:GLN:NE2	2.36	0.40
1:C:227:ASP:CG	1:C:229:PRO:HD2	2.41	0.40
1:C:288:VAL:HA	1:C:291:ILE:HG22	2.03	0.40
1:C:721:ASP:O	1:C:725:THR:HG23	2.21	0.40
1:C:775:LEU:HG	1:C:779:GLN:HE21	1.85	0.40
2:D:36:THR:HB	2:D:58:LEU:CD1	2.51	0.40
1:A:66:TYR:HE2	1:A:149:TYR:CE2	2.38	0.40
1:A:271:THR:HA	1:A:274:GLN:CD	2.41	0.40
1:A:589:LYS:C	1:A:591:TYR:N	2.73	0.40
1:A:603:PRO:HA	1:A:606:ILE:CG1	2.51	0.40
1:A:659:ARG:NH1	1:A:662:CYS:HB2	2.35	0.40
1:C:38:LEU:HD23	1:C:84:HIS:CD2	2.57	0.40
1:C:57:LEU:O	1:C:62:TYR:HB2	2.21	0.40
1:C:219:ILE:HG23	1:C:263:PHE:CE2	2.56	0.40
1:C:685:PHE:O	1:C:688:TYR:HB3	2.21	0.40
1:C:775:LEU:HD12	1:C:778:LEU:HB3	2.03	0.40
1:C:813:ASN:HB3	1:C:816:VAL:CG2	2.51	0.40
1:C:821:LEU:O	1:C:825:ILE:HG23	2.21	0.40
2:D:139:THR:HA	2:D:155:PRO:HB3	2.03	0.40
1:A:480:LEU:HG	1:A:523:ASN:OD1	2.20	0.40
1:A:642:SER:HA	1:A:645:TYR:HB3	2.03	0.40
1:C:65:LEU:HA	1:C:65:LEU:HD12	1.74	0.40
1:C:280:SER:OG	1:C:399:HIS:HD2	2.05	0.40
1:C:735:LEU:HD23	1:C:736:ARG:N	2.37	0.40
2:D:139:THR:HG21	2:D:182:GLU:OE2	2.21	0.40
2:D:172:TYR:CE1	2:D:186:VAL:HA	2.56	0.40
1:A:131:MET:O	1:A:135:SER:HB3	2.21	0.40
1:A:227:ASP:HA	1:A:267:TYR:OH	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:794:SER:HA	1:A:797:LEU:HG	2.04	0.40
2:B:42:LEU:HD23	2:B:47:THR:HG22	2.04	0.40
2:B:126:GLU:HG2	2:B:131:PHE:HA	2.02	0.40
1:C:221:ARG:HA	1:C:221:ARG:HD2	1.82	0.40
1:C:421:LEU:O	1:C:425:ILE:HG12	2.22	0.40
1:C:441:LEU:HD23	1:C:441:LEU:HA	1.88	0.40
1:C:578:ASP:HA	1:C:616:PHE:CZ	2.57	0.40
1:C:733:LYS:HA	1:C:733:LYS:HD3	1.83	0.40
1:C:798:PHE:HB3	1:C:828:ILE:HD11	2.03	0.40
1:A:224:GLN:O	1:A:225:LEU:HD23	2.22	0.40
1:A:462:LEU:HD12	1:A:465:LEU:HD22	2.03	0.40
1:A:509:LEU:HD12	1:A:510:LYS:N	2.36	0.40
1:C:125:LYS:HD2	1:C:125:LYS:HA	1.73	0.40
1:C:424:ASN:HA	1:C:472:ARG:NH1	2.34	0.40
1:C:426:TYR:HB2	1:C:433:VAL:CG2	2.52	0.40
1:C:588:ARG:HD3	1:C:636:PHE:CZ	2.56	0.40
1:C:662:CYS:SG	1:C:708:ALA:HB2	2.61	0.40
2:D:85:ILE:HG13	2:D:112:VAL:HG21	2.02	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	742/869 (85%)	615 (83%)	124 (17%)	3 (0%)	34 72
1	C	742/869 (85%)	645 (87%)	97 (13%)	0	100 100
2	B	181/202 (90%)	163 (90%)	18 (10%)	0	100 100
2	D	181/202 (90%)	147 (81%)	34 (19%)	0	100 100
All	All	1846/2142 (86%)	1570 (85%)	273 (15%)	3 (0%)	50 81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	769	ARG
1	A	655	ASP
1	A	162	GLY

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	660/762 (87%)	651 (99%)	9 (1%)	67	80
1	C	660/762 (87%)	652 (99%)	8 (1%)	71	83
2	B	165/175 (94%)	163 (99%)	2 (1%)	71	83
2	D	165/175 (94%)	165 (100%)	0	100	100
All	All	1650/1874 (88%)	1631 (99%)	19 (1%)	72	83

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	231	TYR
1	A	273	ASP
1	A	443	LYS
1	A	559	MET
1	A	597	ARG
1	A	661	PHE
1	A	688	TYR
1	A	713	ARG
1	A	715	PHE
2	B	64	ARG
2	B	121	ARG
1	C	143	ARG
1	C	275	PHE
1	C	565	LEU
1	C	615	ARG
1	C	688	TYR
1	C	717	ARG
1	C	739	ASP
1	C	847	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	HIS
1	A	83	ASN
1	A	154	GLN
1	A	176	ASN
1	A	186	ASN
1	A	242	GLN
1	A	261	GLN
1	A	396	GLN
1	A	454	HIS
1	A	490	GLN
1	A	562	GLN
1	A	573	HIS
1	A	638	HIS
1	A	649	ASN
1	A	666	GLN
1	A	740	GLN
1	A	836	GLN
1	A	837	GLN
1	A	857	GLN
2	B	106	ASN
2	B	134	ASN
1	C	84	HIS
1	C	88	HIS
1	C	101	ASN
1	C	194	HIS
1	C	195	GLN
1	C	245	GLN
1	C	268	HIS
1	C	270	HIS
1	C	283	ASN
1	C	399	HIS
1	C	420	ASN
1	C	490	GLN
1	C	492	GLN
1	C	570	HIS
1	C	666	GLN
1	C	698	GLN
1	C	779	GLN
1	C	813	ASN
1	C	837	GLN
1	C	848	HIS

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Mol	Chain	Res	Type
2	D	10	ASN
2	D	35	GLN
2	D	41	ASN
2	D	76	GLN
2	D	163	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

This section contains visualisations of the EMDB entry EMD-12226. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

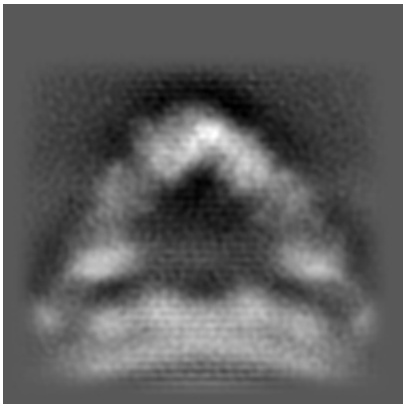
6.1.1 Primary map

X

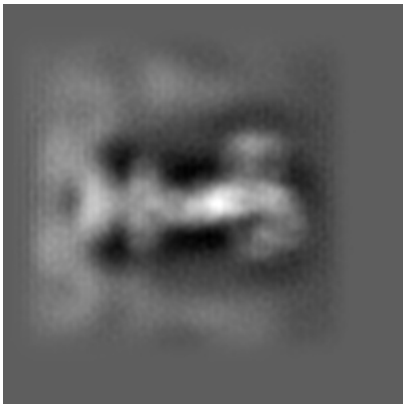
Y

Z

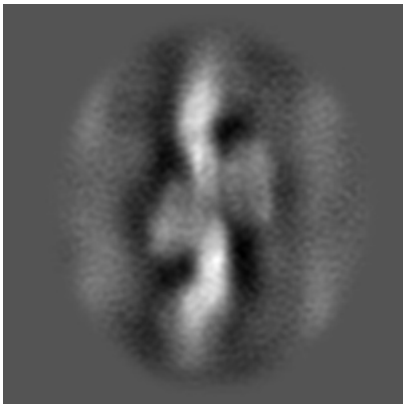
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

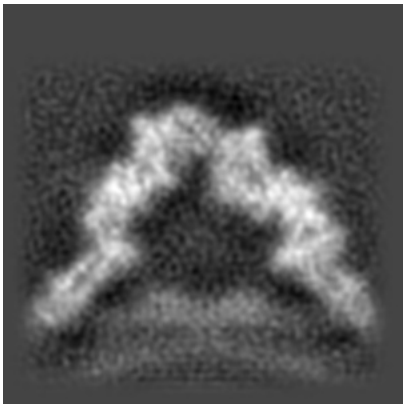
6.2.1 Primary map

X Index: 52

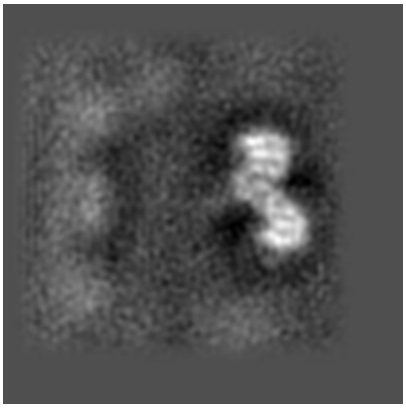
Y Index: 52

Z Index: 52

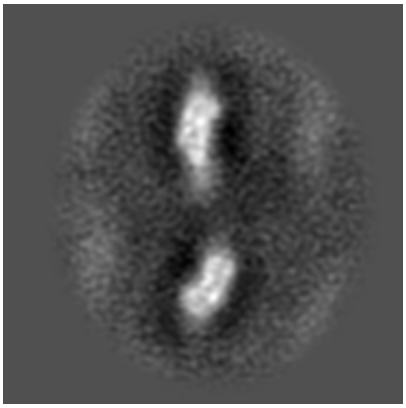
6.2.2 Raw map



X Index: 52



Y Index: 52



Z Index: 52

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

6.3 Largest variance slices (i)

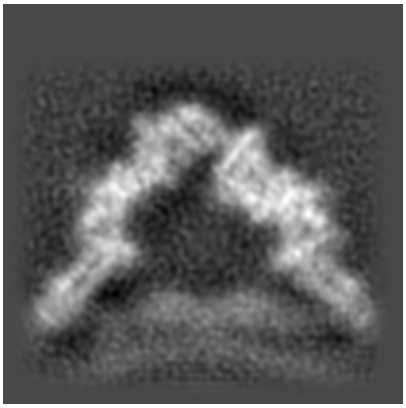
6.3.1 Primary map

X Index: 50

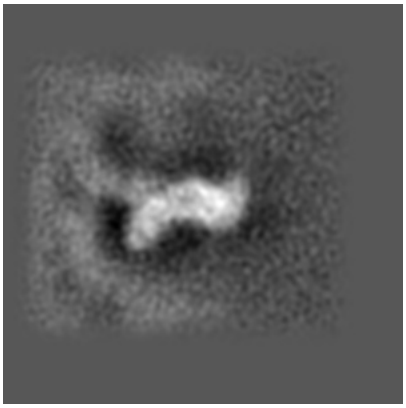
Y Index: 65

Z Index: 60

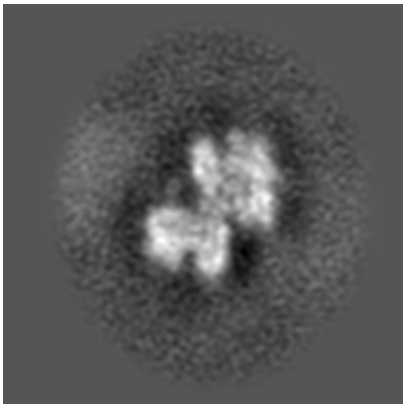
6.3.2 Raw map



X Index: 51



Y Index: 28



Z Index: 65

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

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

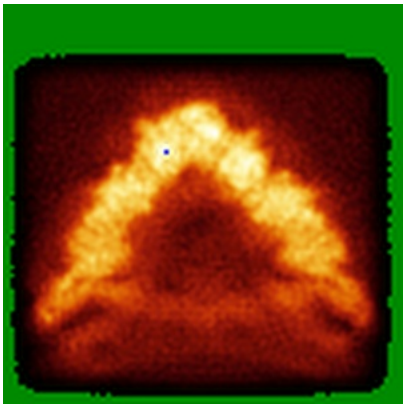
6.4.1 Primary map

X

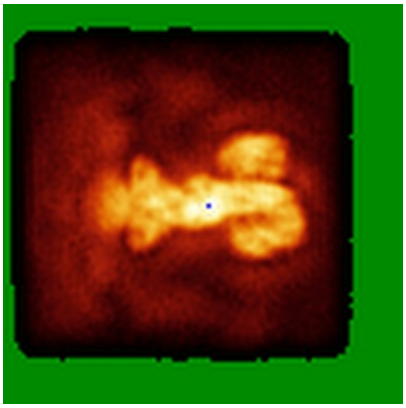
Y

Z

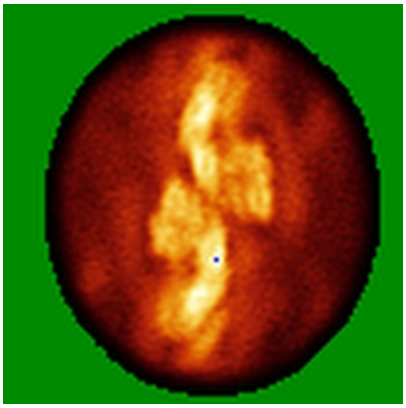
6.4.2 Raw map



X



Y

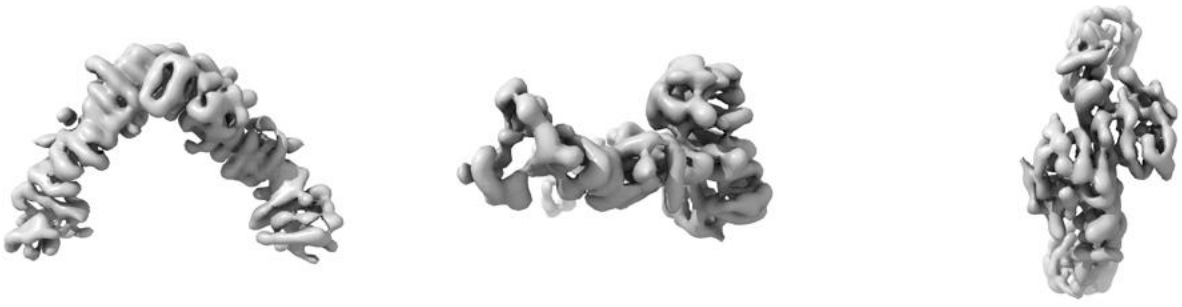


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

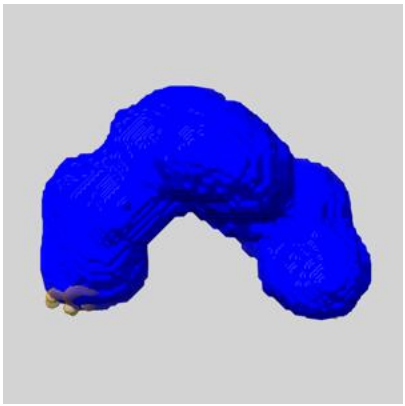
6.6 Mask visualisation

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

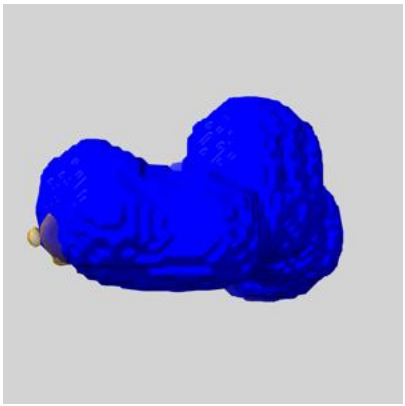
A mask typically either:

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

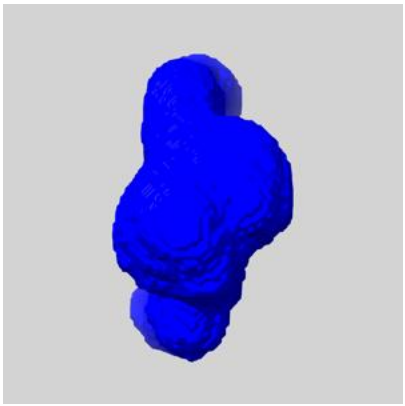
6.6.1 emd_12226_msk_1.map



X



Y

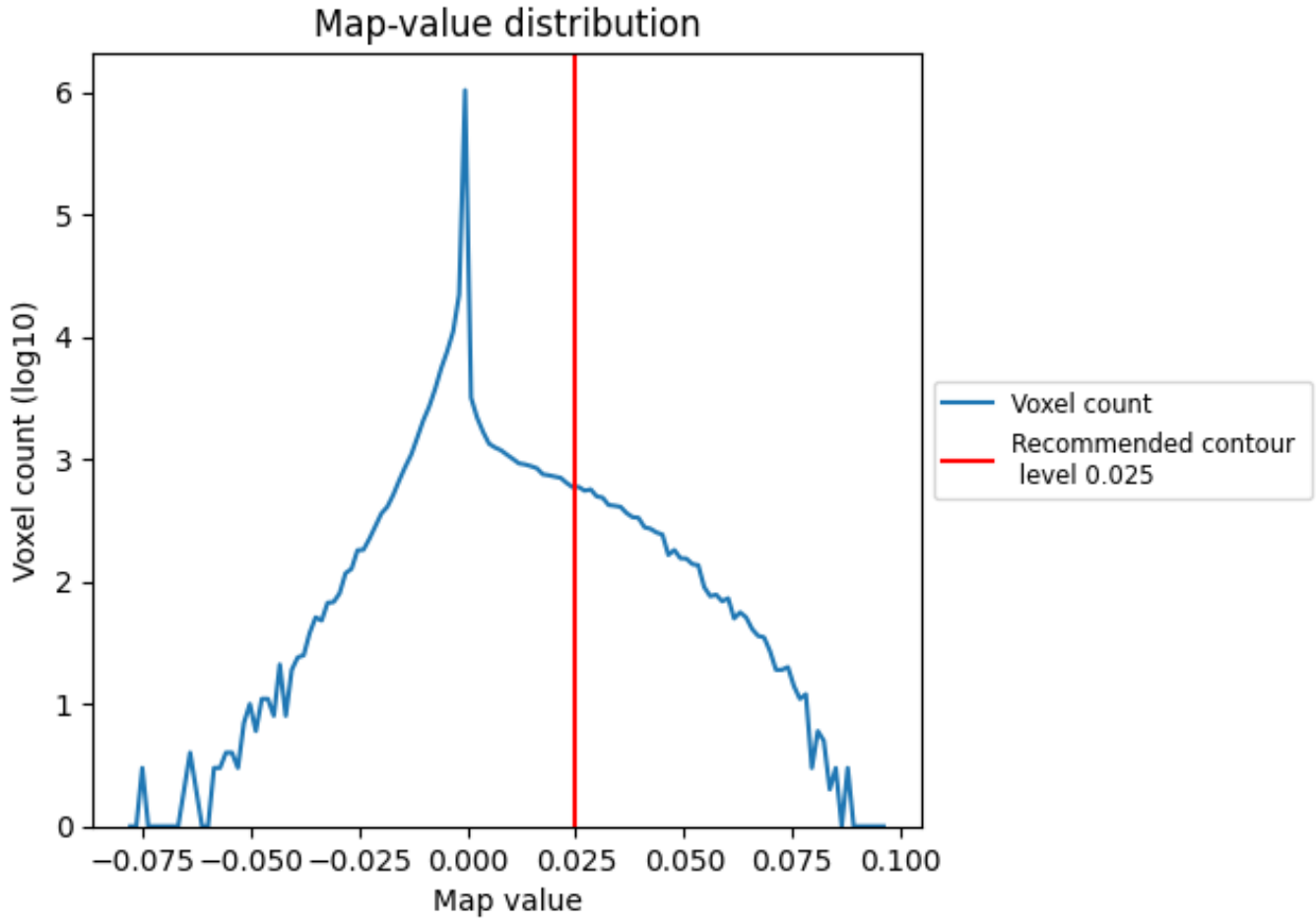


Z

7 Map analysis

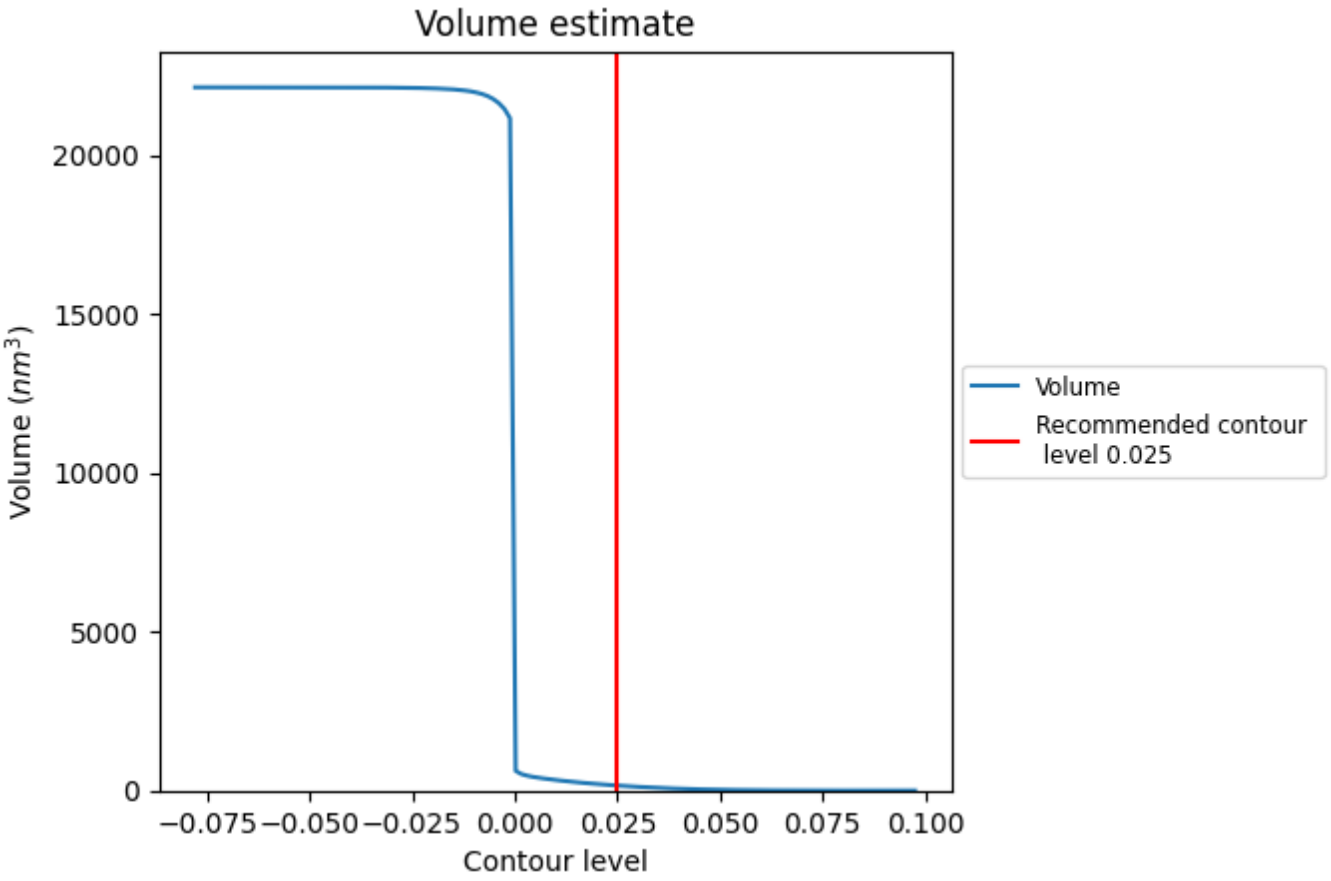
This section contains the results of statistical analysis of the map.

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.

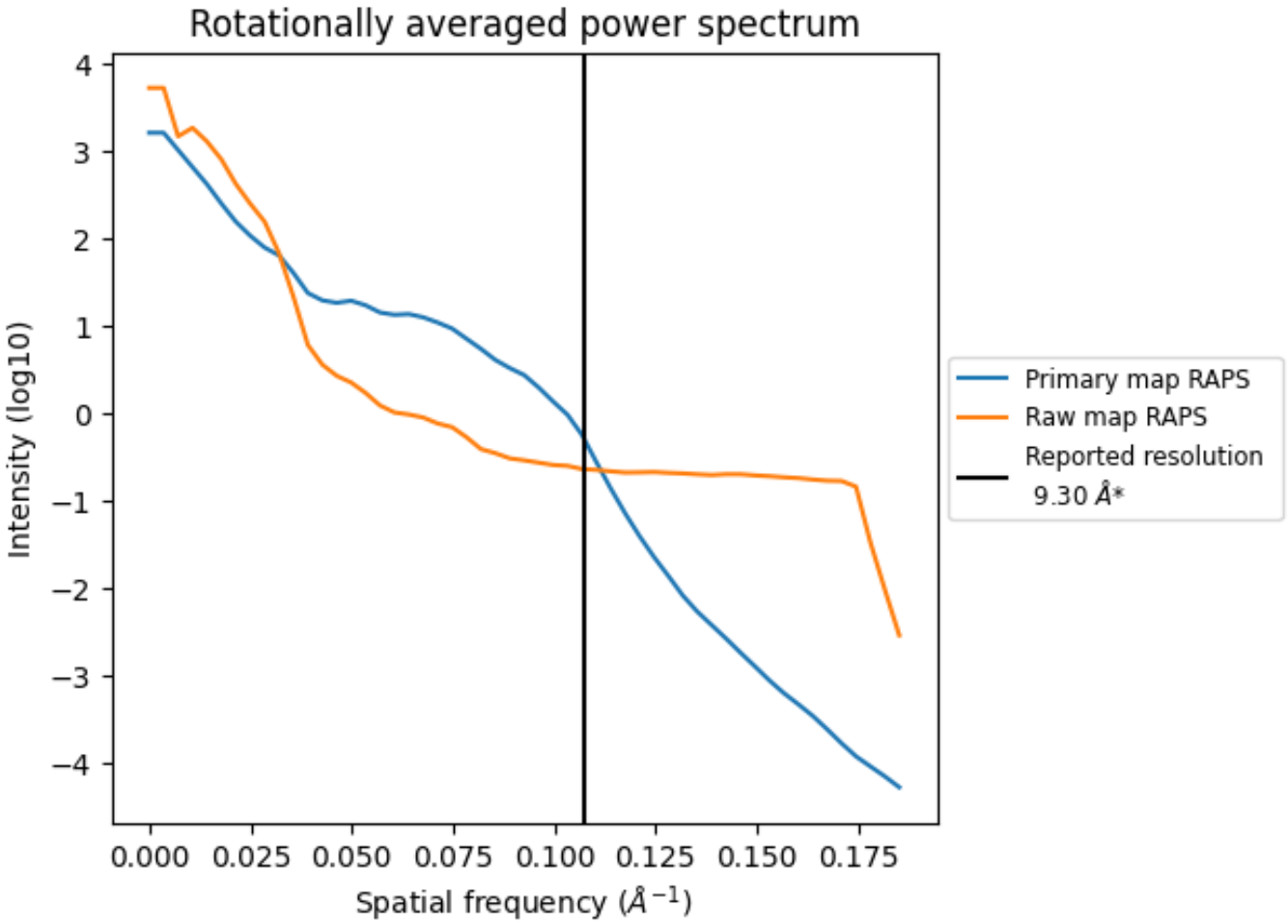
7.2 Volume estimate



The volume at the recommended contour level is 158 nm^3; this corresponds to an approximate mass of 143 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)

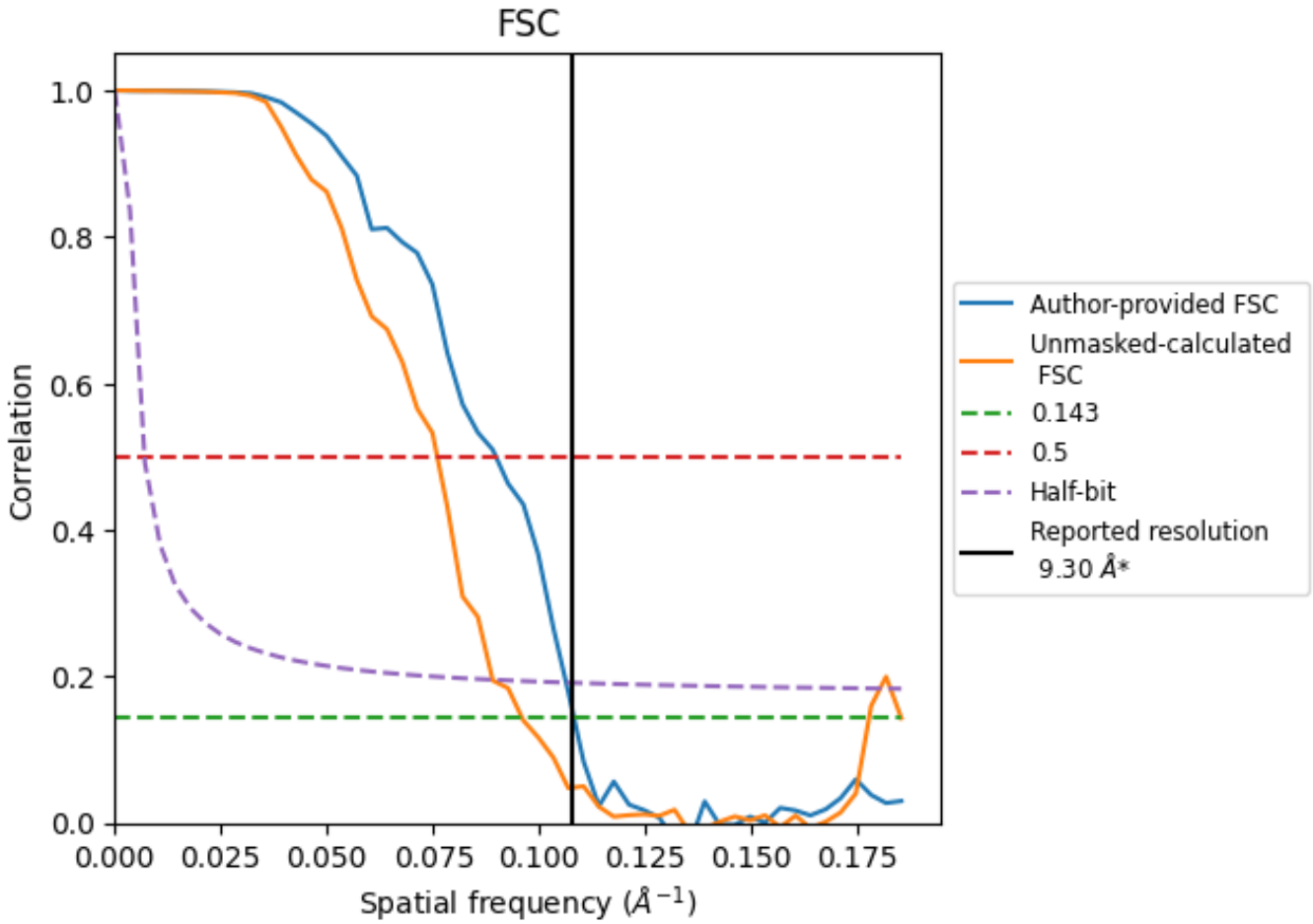


*Reported resolution corresponds to spatial frequency of 0.108 Å^{-1}

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 0.108 Å^{-1}

8.2 Resolution estimates (i)

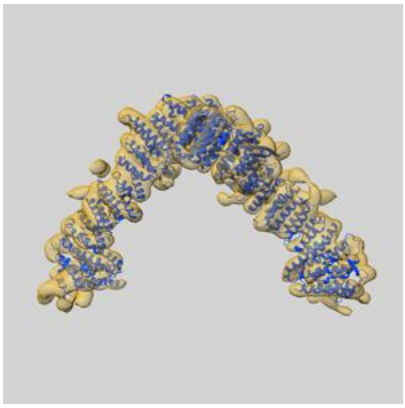
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.30	-	-
Author-provided FSC curve	9.24	11.14	9.41
Unmasked-calculated*	10.43	13.18	11.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 10.43 differs from the reported value 9.3 by more than 10 %

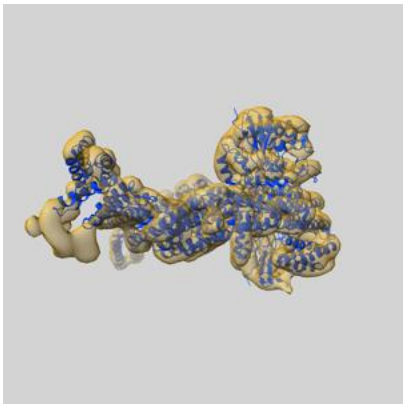
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12226 and PDB model 7BLR. Per-residue inclusion information can be found in section 3 on page 4.

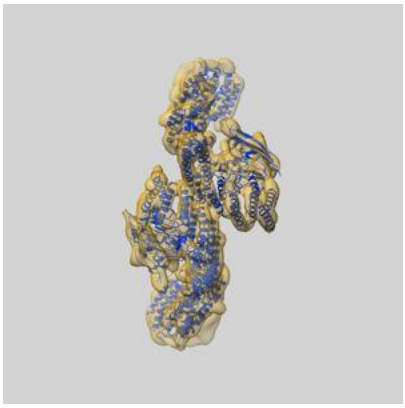
9.1 Map-model overlay



X



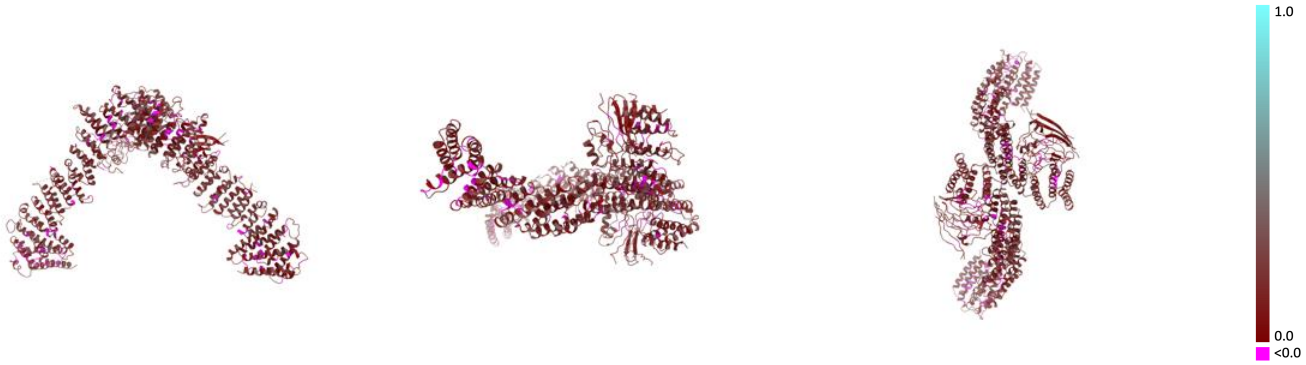
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 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.

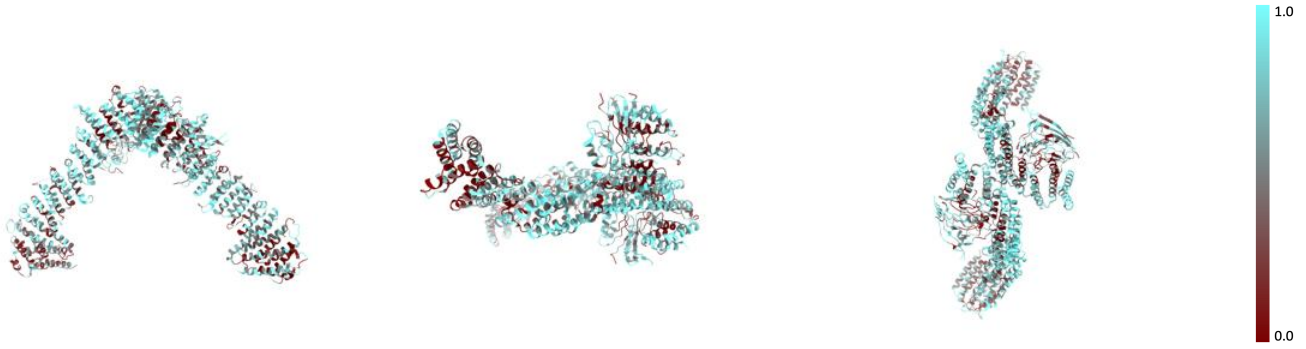
9.2 Q-score mapped to coordinate model (i)



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.

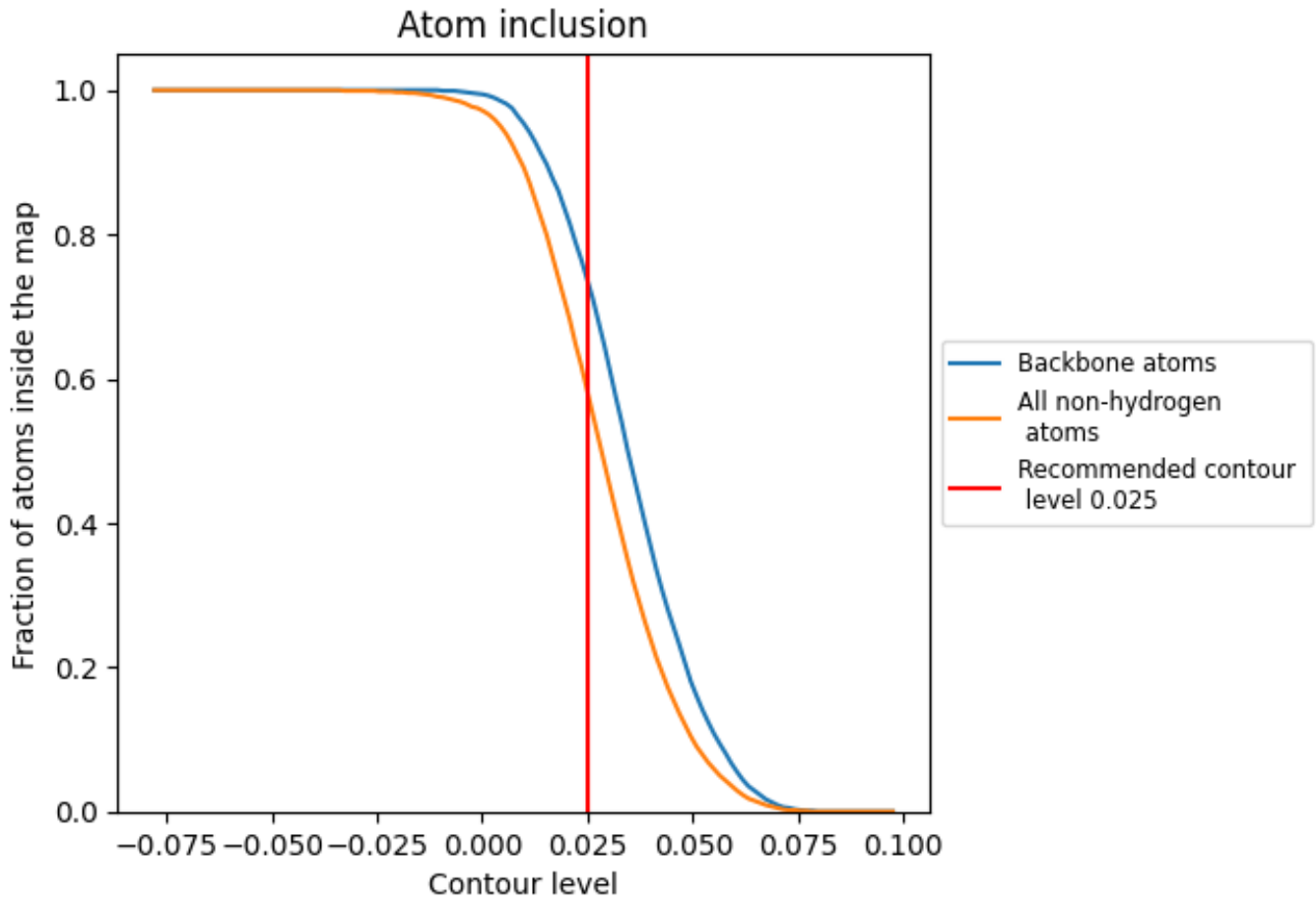
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 58% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5810	0.1530
A	0.5840	0.1580
B	0.5200	0.1360
C	0.6000	0.1580
D	0.5580	0.1260