Full wwPDB EM Validation Report ⓘ

Nov 13, 2023 – 12:27 pm GMT

PDB ID	:	8OTX
EMDB ID	:	EMD-17186
Title	:	Cryo-EM structure of Strongylocentrotus purpuratus sperm-specific Na+/H+ exchanger SLC9C1 in nanodisc
Authors	:	Yeo, H.; Mehta, V.; Gulati, A.; Drew, D.
Deposited on	:	2023-04-21
Resolution	:	3.08 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:

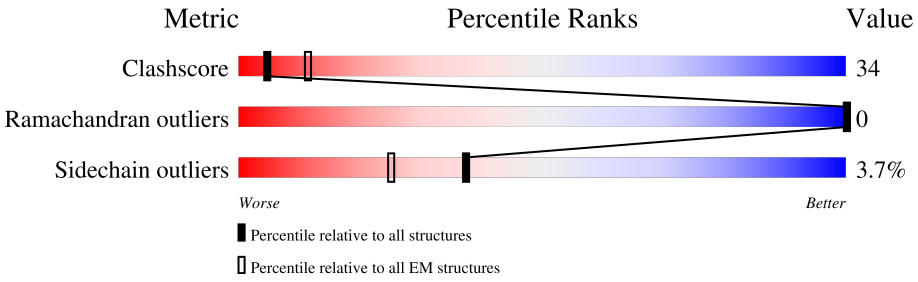
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.08 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	1331	10% 44% 34% · 21%
1	B	1331	10% 45% 33% · 21%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16116 atoms, of which 150 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.

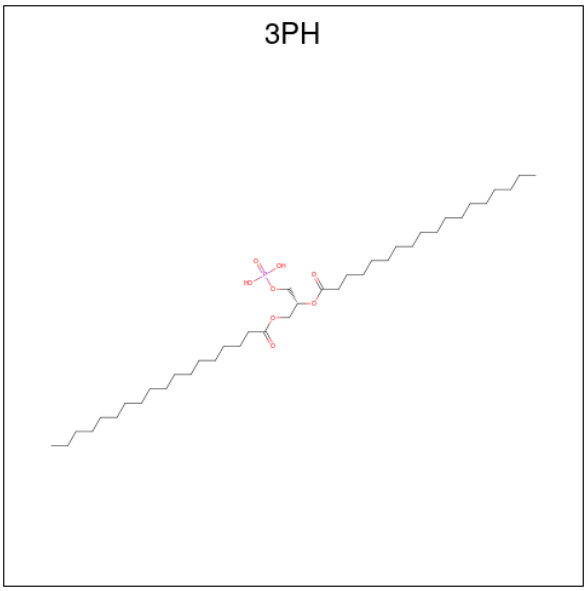
- Molecule 1 is a protein called Sperm-specific sodium proton exchanger.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1054	Total	C	N	O	S	1	0
			7889	5097	1334	1421	37		
1	A	1054	Total	C	N	O	S	1	0
			7889	5097	1334	1421	37		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1326	GLU	-	expression tag	UNP A3RL54
B	1327	ASN	-	expression tag	UNP A3RL54
B	1328	LEU	-	expression tag	UNP A3RL54
B	1329	TYR	-	expression tag	UNP A3RL54
B	1330	PHE	-	expression tag	UNP A3RL54
B	1331	GLN	-	expression tag	UNP A3RL54
A	1326	GLU	-	expression tag	UNP A3RL54
A	1327	ASN	-	expression tag	UNP A3RL54
A	1328	LEU	-	expression tag	UNP A3RL54
A	1329	TYR	-	expression tag	UNP A3RL54
A	1330	PHE	-	expression tag	UNP A3RL54
A	1331	GLN	-	expression tag	UNP A3RL54

- Molecule 2 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
2	B	1	Total C H O P 123 39 75 8 1	0
2	B	1	Total C O P 45 36 8 1	0
2	A	1	Total C H O P 123 39 75 8 1	0
2	A	1	Total C O P 45 36 8 1	0

- Molecule 3 is water.

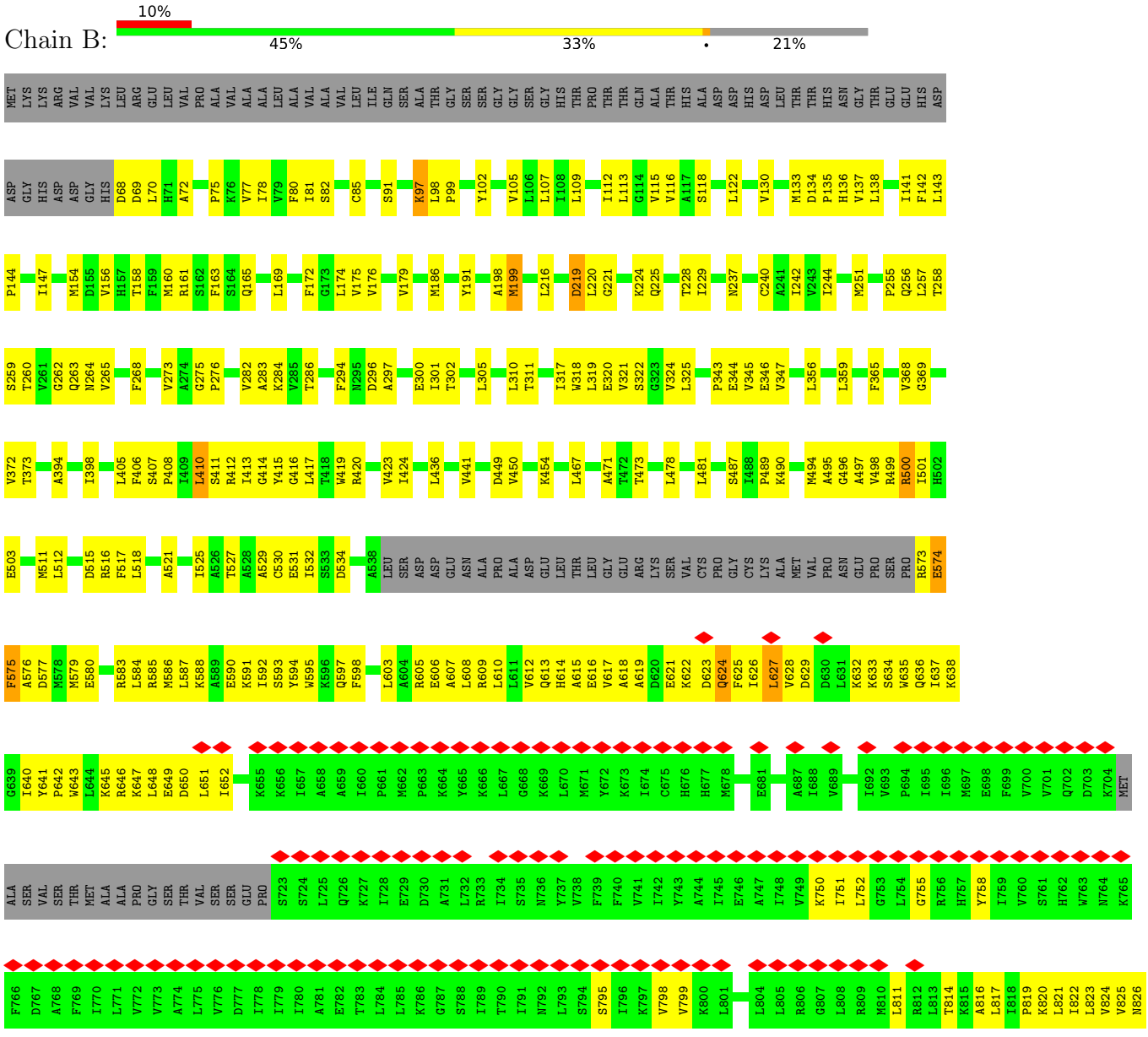
Mol	Chain	Residues	Atoms	AltConf
3	B	1	Total O 1 1	0
3	A	1	Total O 1 1	0

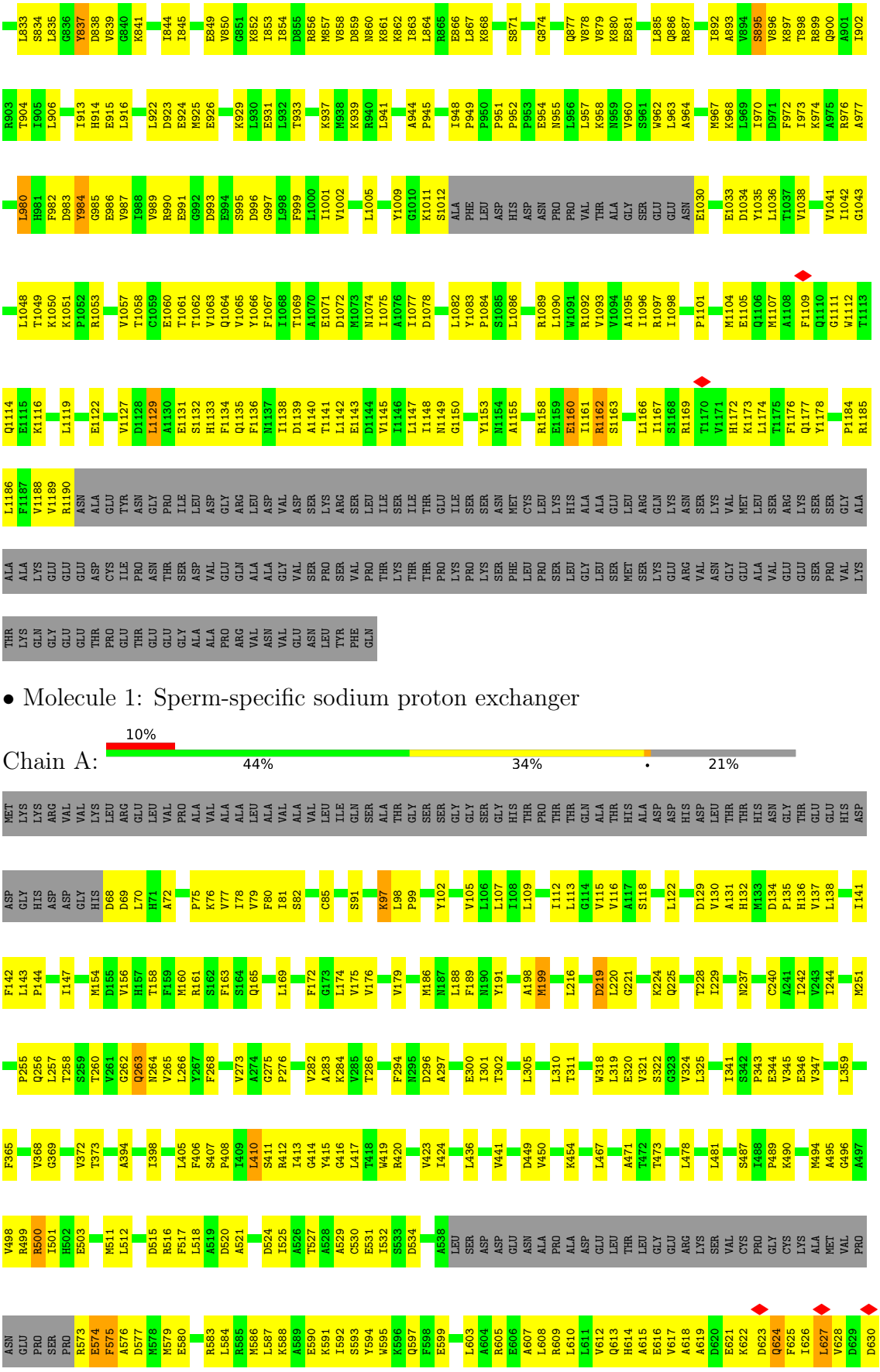
3 Residue-property plots (i)

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.

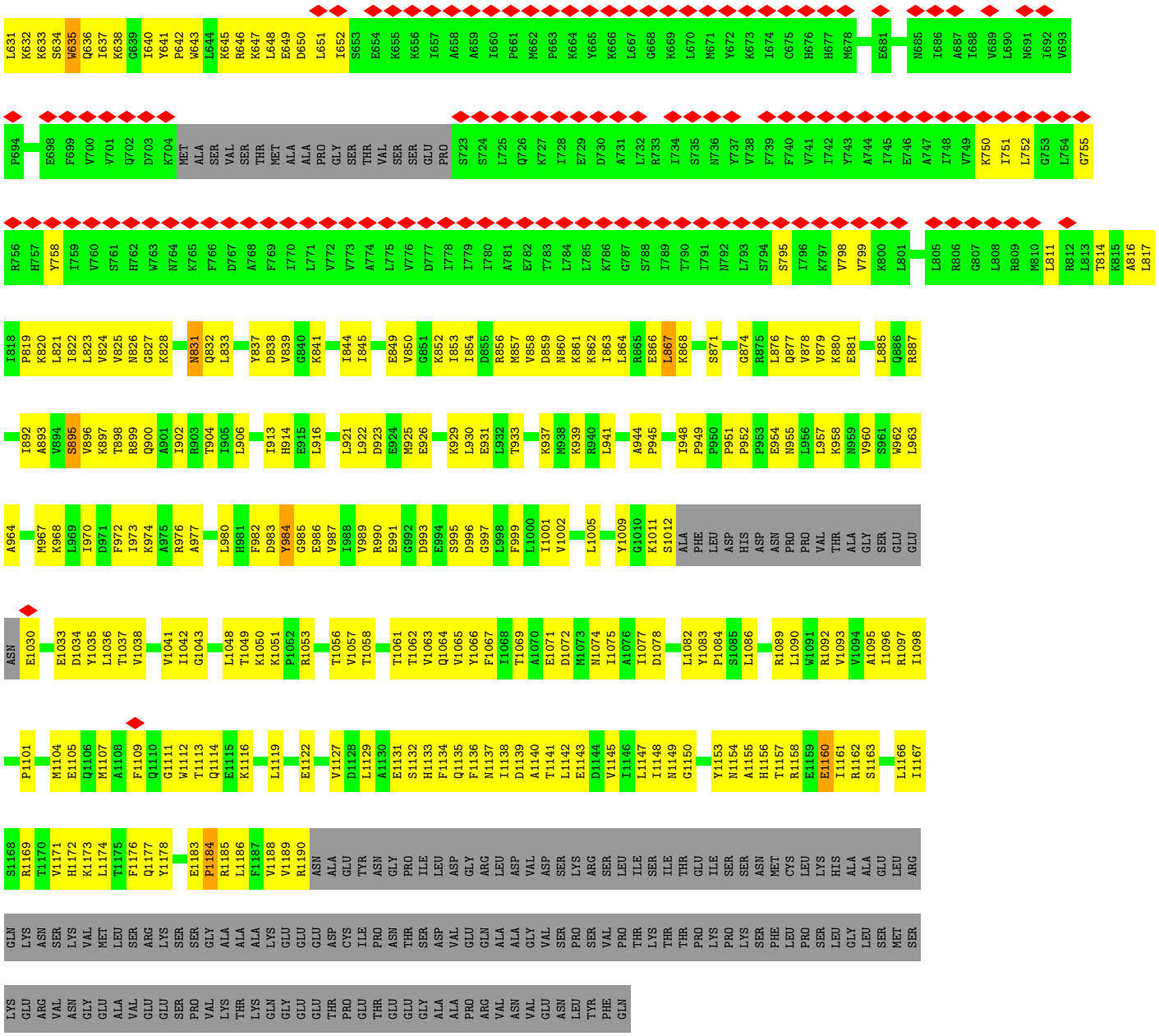
- Molecule 1: Sperm-specific sodium proton exchanger

Chain B:





• Molecule 1: Sperm-specific sodium proton exchanger


L631 K632 K633 S634 W635 Q636 I637 K638 G639 I640 Y641 P642 W643 L644 K645 R646 K647 L648 E649 D650 L651 I652 S653 E654 K655 K656 I657 A658 A659 I660 P661 M662 P663 K664 Y665 K666 L667 G668 K669 L670 M671 Y672 K673 I674 C675 H676 H677 M678 E681 N685 I686 A687 I688 V689 L690 N691 I692 V693
P694 E698 F699 V700 V701 Q702 D703 K704 MET ALA SER VAL SER THR MET ALA ALA PRO GLY SER THR VAL SER SER GLU PRO S723 S724 L725 Q726 K727 I728 E729 D730 A731 L732 R733 I734 S735 N736 Y737 V738 F739 F740 V741 I742 Y743 A744 I745 E746 A747 L748 V749 K750 I751 L752 G753 L754 G755
R756 H757 Y758 I759 V760 S761 H762 W763 N764 K765 F766 D767 A768 F769 I770 L771 V772 V773 A774 L775 V776 D777 I778 I779 I780 A781 E782 T783 L784 L785 K786 G787 S788 I789 T790 I791 N792 L793 S794 S795 I796 K797 V798 V799 K800 L801 L805 R806 G807 L808 R809 M810 L811 R812 L813 T814 K815 A816 L817
I818 P819 K820 L821 I822 L823 V824 V825 N826 G827 K828 N831 Q832 L833 Y837 D838 V839 G840 K841 I844 I845 E849 V850 G851 K852 I853 I854 D855 R856 M857 V858 D859 N860 K861 K862 I863 L864 R865 E866 L867 K868 S871 G874 R875 L876 Q877 V878 V879 K880 E881 L885 Q886 R887
I892 A893 V894 S895 V896 K897 T898 R899 Q900 A901 I902 R903 T904 Y905 L906 I913 H914 E915 L916 L921 L922 D923 E924 M925 E926 K929 L930 E931 L932 T933 K937 N938 K939 R940 L941 A944 P945 I948 P949 P950 P951 P952 P953 E954 N955 L956 L957 K958 N959 V960 S961 W962 L963
A964 M967 K968 L969 I970 D971 F972 I973 K974 A975 R976 A977 L980 H981 F982 D983 Y984 G985 E986 V987 I988 V989 R990 E991 G992 D993 E994 S995 D996 G997 L998 F999 L1000 I1001 V1002 L1005 Y1009 G1010 K1011 S1012 ALA PHE LEU ASP HIS ASP ASN PRO PRO VAL THR ALA GLY SER GLU GLU
ASN E1030 E1033 D1034 Y1035 L1036 T1037 V1038 V1041 I1042 G1043 L1048 T1049 K1050 K1051 P1052 R1053 T1056 V1057 T1058 T1061 T1062 V1063 Q1064 V1065 Y1066 F1067 I1068 T1069 A1070 E1071 D1072 M1073 N1074 I1075 A1076 I1077 D1078 L1082 Y1083 P1084 S1085 L1086 R1089 L1090 W1091 R1092 V1093 V1094 A1095 I1096 R1097 I1098
P1101 M1104 E1105 Q1106 M1107 A1108 F1109 Q1110 G1111 W1112 T1113 Q1114 E1115 K1116 L1119 E1122 V1127 D1128 L1129 A1130 E1131 S1132 H1133 F1134 Q1135 F1136 N1137 I1138 D1139 A1140 T1141 L1142 E1143 D1144 V1145 I1146 L1147 I1148 N1149 G1150 Y1153 N1154 A1155 H1156 T1157 R1158 E1159 E1160 I1161 R1162 S1163 L1166 I1167
S1168 R1169 T1170 V1171 H1172 K1173 L1174 T1175 F1176 Q1177 Y1178 E1183 P1184 R1185 L1186 F1187 V1188 V1189 R1190 ASN ALA GLU TYR ASN GLY PRO ASN THR SER ASP VAL GLU GLN ALA ALA GLY VAL ASP SER LYS ARG SER LEU ILE SER ILE THR GLU ILE SER SER ASN MET CYS LEU LYS HIS ALA ALA GLU LEU ARG
GLN LYS ASN SER LYS VAL MET LEU SER ARG LYS SER SER GLY ALA ALA ALA LYS GLU GLU GLU ASP CYS ILE PRO ASN THR SER ALA VAL GLU GLN ALA ALA GLY VAL SER PRO SER VAL PRO THR LYS THR THR PRO LYS PRO LYS SER SER PHE LEU PRO SER LEU GLY LEU SER MET SER
LYS GLU ARG VAL ASN GLY GLU ALA VAL GLU GLU SER PRO VAL LYS THR LYS GLN GLY GLU GLU THR PRO GLU THR GLU GLU GLY ALA ALA PRO ARG VAL ASN VAL GLU ASN LEU TYR PHE GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1737146	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 ($e^-/Å^2$)	58.45	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.655	Depositor
Minimum map value	-0.333	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	365.47998, 365.47998, 365.47998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9136999, 0.9136999, 0.9136999	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PH

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.26	0/8033	0.47	2/10927 (0.0%)
1	B	0.25	0/8033	0.44	0/10927
All	All	0.25	0/16066	0.45	2/21854 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1184	PRO	CA-N-CD	-14.44	91.29	111.50
1	A	1184	PRO	N-CD-CG	-6.65	93.22	103.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	7889	0	7744	563	0
1	B	7889	0	7744	565	0
2	A	93	75	141	11	0
2	B	93	75	141	9	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	15966	150	15770	1073	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 34.

All (1073) 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:1184:PRO:HD2	1:A:1184:PRO:O	1.54	1.06
1:B:1138:ILE:HA	1:B:1142:LEU:HD21	1.37	1.06
1:A:1142:LEU:HA	1:A:1190:ARG:HA	1.38	1.05
1:A:1138:ILE:HA	1:A:1142:LEU:HD21	1.39	1.03
1:B:1142:LEU:HA	1:B:1190:ARG:HA	1.37	1.02
1:A:819:PRO:HA	1:A:822:ILE:HD12	1.42	1.00
1:B:1147:LEU:HA	1:B:1186:LEU:HD13	1.46	0.98
1:A:1147:LEU:HA	1:A:1186:LEU:HD13	1.46	0.98
1:B:819:PRO:HA	1:B:822:ILE:HD12	1.44	0.96
1:B:530:CYS:HA	1:A:937:LYS:HE2	1.50	0.93
1:A:642:PRO:HB3	1:A:646:ARG:HH21	1.31	0.93
1:A:1183:GLU:OE2	1:A:1184:PRO:HD3	1.68	0.93
1:A:411:SER:HA	1:A:416:GLY:HA2	1.53	0.91
1:B:411:SER:HA	1:B:416:GLY:HA2	1.53	0.90
1:B:937:LYS:HE2	1:A:530:CYS:HA	1.53	0.90
1:B:587:LEU:HD13	1:B:619:ALA:HB2	1.53	0.90
1:A:898:THR:O	1:A:902:ILE:HG13	1.72	0.88
1:B:628:VAL:HG22	1:B:632:LYS:HE3	1.57	0.87
1:A:587:LEU:HD13	1:A:619:ALA:HB2	1.53	0.87
1:B:852:LYS:HE3	1:B:1105:GLU:HG2	1.57	0.87
1:A:615:ALA:HA	1:A:626:ILE:HD13	1.58	0.86
1:B:924:GLU:OE1	1:B:924:GLU:N	2.08	0.85
1:B:898:THR:O	1:B:902:ILE:HG13	1.75	0.85
1:B:407:SER:HA	1:B:410:LEU:HD11	1.56	0.85
1:A:852:LYS:HE3	1:A:1105:GLU:HG2	1.57	0.85
1:B:615:ALA:HA	1:B:626:ILE:HD13	1.58	0.84
1:B:530:CYS:HB3	1:A:937:LYS:HD3	1.58	0.84
1:A:407:SER:HA	1:A:410:LEU:HD11	1.57	0.84
1:A:628:VAL:HG22	1:A:632:LYS:HE3	1.58	0.84
1:B:937:LYS:HD3	1:A:530:CYS:HB3	1.58	0.83
1:B:951:PRO:HB2	1:B:955:ASN:HD21	1.42	0.83
1:A:583:ARG:O	1:A:587:LEU:HG	1.79	0.83
1:A:951:PRO:HB2	1:A:955:ASN:HD21	1.42	0.83
1:A:588:LYS:O	1:A:592:ILE:HG13	1.78	0.83
1:B:863:ILE:O	1:B:867:LEU:HD12	1.79	0.82
1:A:627:LEU:HA	1:A:632:LYS:HD2	1.61	0.82
1:B:583:ARG:O	1:B:587:LEU:HG	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:952:PRO:O	1:A:955:ASN:ND2	2.13	0.81
1:B:224:LYS:H	1:B:224:LYS:HD2	1.46	0.81
1:B:952:PRO:O	1:B:955:ASN:ND2	2.14	0.81
1:A:1135:GLN:HE22	1:A:1155:ALA:HB2	1.46	0.81
1:B:515:ASP:OD1	1:B:516:ARG:N	2.14	0.81
1:B:588:LYS:O	1:B:592:ILE:HG13	1.79	0.81
1:A:515:ASP:OD1	1:A:516:ARG:N	2.15	0.80
1:A:618:ALA:HB3	1:A:626:ILE:HG12	1.63	0.80
1:A:863:ILE:O	1:A:867:LEU:HD12	1.83	0.79
1:B:573:ARG:O	1:B:573:ARG:NH1	2.16	0.79
1:A:1071:GLU:N	1:A:1071:GLU:OE1	2.16	0.79
1:A:628:VAL:H	1:A:632:LYS:HZ2	1.30	0.79
1:A:853:ILE:HG22	1:A:857:MET:CE	2.12	0.79
1:B:1153:TYR:HE1	1:B:1160:GLU:HA	1.48	0.79
1:A:933:THR:O	1:A:937:LYS:HG3	1.83	0.79
1:B:627:LEU:HA	1:B:632:LYS:HD2	1.65	0.78
1:B:628:VAL:H	1:B:632:LYS:HZ2	1.31	0.78
1:B:1162:ARG:O	1:B:1162:ARG:NH1	2.15	0.78
1:A:621:GLU:OE1	1:A:624:GLN:HB3	1.83	0.78
1:B:837:TYR:OH	1:B:886:GLN:HB2	1.83	0.78
1:A:219:ASP:OD1	1:A:220:LEU:HD12	1.82	0.78
1:B:618:ALA:HB3	1:B:626:ILE:HG12	1.64	0.78
1:B:621:GLU:OE1	1:B:624:GLN:HB3	1.83	0.78
1:B:68:ASP:HB2	1:B:72:ALA:CB	2.14	0.78
1:B:219:ASP:OD1	1:B:220:LEU:HD12	1.83	0.78
1:A:1183:GLU:OE1	1:A:1185:ARG:NH1	2.17	0.78
1:B:1071:GLU:OE1	1:B:1071:GLU:N	2.15	0.78
1:A:573:ARG:O	1:A:573:ARG:NH1	2.16	0.77
1:B:525:ILE:CD1	1:A:902:ILE:HG12	2.13	0.77
1:A:77:VAL:O	1:A:81:ILE:HG13	1.85	0.77
1:B:1011:LYS:HD3	1:B:1030:GLU:HG3	1.65	0.77
1:A:1153:TYR:HE1	1:A:1160:GLU:HA	1.50	0.77
1:B:531:GLU:N	1:B:531:GLU:OE1	2.17	0.77
1:B:632:LYS:HA	1:B:635:TRP:CH2	2.20	0.77
1:B:1092:ARG:NH2	1:B:1122:GLU:OE2	2.17	0.77
1:B:933:THR:O	1:B:937:LYS:HG3	1.84	0.77
1:B:1184:PRO:O	1:B:1185:ARG:HD2	1.85	0.77
1:A:1092:ARG:NH2	1:A:1122:GLU:OE2	2.17	0.77
1:B:821:LEU:O	1:B:824:VAL:HG12	1.86	0.76
1:A:319:LEU:HD12	1:A:319:LEU:O	1.86	0.76
1:A:821:LEU:O	1:A:824:VAL:HG12	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:LYS:HD2	1:B:224:LYS:N	2.01	0.74
1:B:77:VAL:O	1:B:81:ILE:HG13	1.88	0.74
1:B:1172:HIS:ND1	1:A:1173:LYS:HE3	2.03	0.74
1:B:1139:ASP:OD1	1:B:1141:THR:OG1	2.06	0.74
1:A:525:ILE:O	1:A:529:ALA:N	2.20	0.74
1:A:583:ARG:HH21	1:A:624:GLN:H	1.35	0.74
1:A:853:ILE:HG22	1:A:857:MET:HE2	1.70	0.74
1:B:645:LYS:O	1:B:648:LEU:HG	1.88	0.73
1:A:531:GLU:OE1	1:A:531:GLU:N	2.18	0.73
1:A:645:LYS:O	1:A:648:LEU:HG	1.88	0.73
1:A:833:LEU:HD13	1:A:885:LEU:HD21	1.70	0.73
1:B:586:MET:CE	1:B:867:LEU:HD23	2.17	0.73
1:B:636:GLN:N	1:B:636:GLN:OE1	2.21	0.73
1:A:987:VAL:HG22	1:A:1058:THR:HG22	1.69	0.73
1:B:853:ILE:HG22	1:B:857:MET:CE	2.18	0.73
1:A:579:MET:CE	1:A:579:MET:HA	2.18	0.73
1:B:849:GLU:OE1	1:B:849:GLU:N	2.22	0.72
1:B:77:VAL:HG13	1:B:130:VAL:CG2	2.19	0.72
1:B:987:VAL:HG22	1:B:1058:THR:HG22	1.68	0.72
1:A:632:LYS:HA	1:A:635:TRP:CZ2	2.24	0.72
1:A:530:CYS:O	1:A:532:ILE:HG12	1.89	0.72
1:B:282:VAL:O	1:B:286:THR:HG22	1.90	0.72
1:B:530:CYS:O	1:B:532:ILE:HG12	1.88	0.72
1:B:587:LEU:HB2	1:B:588:LYS:HZ3	1.54	0.72
1:B:1155:ALA:HB2	1:B:1173:LYS:HB3	1.70	0.72
1:B:1162:ARG:H	1:B:1162:ARG:HD3	1.52	0.71
1:A:282:VAL:O	1:A:286:THR:HG22	1.90	0.71
1:B:583:ARG:HH21	1:B:624:GLN:H	1.35	0.71
1:A:587:LEU:HB2	1:A:588:LYS:HZ3	1.54	0.71
1:A:1074:ASN:HA	1:A:1077:ILE:HG12	1.72	0.71
1:B:530:CYS:SG	1:A:906:LEU:HD21	2.31	0.71
1:B:1145:VAL:HB	1:B:1167:ILE:HD11	1.72	0.71
1:B:625:PHE:CE2	1:B:867:LEU:HA	2.25	0.71
1:B:906:LEU:HD21	1:A:530:CYS:SG	2.30	0.71
1:A:625:PHE:CE2	1:A:867:LEU:HA	2.24	0.71
1:B:219:ASP:OD1	1:B:220:LEU:N	2.24	0.71
1:B:645:LYS:HA	1:B:648:LEU:CD2	2.21	0.71
1:A:68:ASP:HB2	1:A:72:ALA:HB3	1.73	0.70
1:A:494:MET:O	1:A:498:VAL:HG13	1.90	0.70
1:B:960:VAL:HB	1:B:963:LEU:CD2	2.21	0.70
1:B:1131:GLU:OE1	1:B:1132:SER:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:MET:O	1:B:498:VAL:HG13	1.91	0.70
1:B:841:LYS:O	1:B:845:ILE:HG12	1.92	0.69
1:B:1074:ASN:HA	1:B:1077:ILE:HG12	1.72	0.69
1:A:636:GLN:OE1	1:A:636:GLN:N	2.22	0.69
1:A:645:LYS:HA	1:A:648:LEU:CD2	2.22	0.69
1:A:951:PRO:HB2	1:A:955:ASN:ND2	2.06	0.69
1:B:1098:ILE:O	1:B:1101:PRO:HD2	1.92	0.69
1:B:318:TRP:O	1:B:319:LEU:HG	1.92	0.69
1:A:487:SER:OG	1:A:489:PRO:HD2	1.92	0.69
1:A:960:VAL:HB	1:A:963:LEU:CD2	2.22	0.69
1:B:179:VAL:HG22	1:B:199:MET:HE1	1.75	0.69
1:A:179:VAL:HG22	1:A:199:MET:HE1	1.74	0.69
1:B:590:GLU:OE1	1:B:594:TYR:OH	2.11	0.69
1:B:951:PRO:HB2	1:B:955:ASN:ND2	2.07	0.69
1:B:982:PHE:HB2	1:B:1063:VAL:HG12	1.74	0.69
1:A:650:ASP:HB3	1:A:822:ILE:HG12	1.74	0.69
1:A:982:PHE:HB2	1:A:1063:VAL:HG12	1.73	0.69
1:A:1098:ILE:O	1:A:1101:PRO:HD2	1.92	0.69
1:B:650:ASP:HB3	1:B:822:ILE:HG12	1.75	0.69
1:A:224:LYS:HD2	1:A:224:LYS:N	2.07	0.69
1:A:1147:LEU:HA	1:A:1186:LEU:CD1	2.23	0.69
1:B:853:ILE:HG22	1:B:857:MET:HE2	1.73	0.68
1:A:590:GLU:OE1	1:A:594:TYR:OH	2.10	0.68
1:B:858:VAL:HG12	1:B:860:ASN:H	1.59	0.68
1:B:260:THR:HG23	1:B:263:GLN:OE1	1.93	0.68
1:B:172:PHE:O	1:B:176:VAL:HG23	1.94	0.68
1:B:319:LEU:HD12	1:B:319:LEU:O	1.94	0.68
1:B:627:LEU:HD23	1:B:633:LYS:NZ	2.09	0.68
1:A:419:TRP:O	1:A:423:VAL:HG23	1.94	0.68
1:A:877:GLN:O	1:A:881:GLU:HG2	1.94	0.68
1:A:647:LYS:NZ	1:A:822:ILE:O	2.27	0.67
1:A:627:LEU:HD23	1:A:633:LYS:NZ	2.10	0.67
1:B:487:SER:OG	1:B:489:PRO:HD2	1.93	0.67
1:B:647:LYS:NZ	1:B:822:ILE:O	2.27	0.67
1:B:419:TRP:O	1:B:423:VAL:HG23	1.94	0.67
1:A:219:ASP:OD1	1:A:220:LEU:N	2.27	0.67
1:A:633:LYS:HA	1:A:636:GLN:NE2	2.09	0.67
2:B:1402:3PH:H2	2:B:1402:3PH:H322	1.75	0.67
1:B:1132:SER:CB	1:B:1178:TYR:HB2	2.24	0.67
1:A:262:GLY:O	1:A:265:VAL:HG12	1.94	0.67
1:B:902:ILE:CD1	1:A:525:ILE:HD11	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:PHE:O	1:A:176:VAL:HG23	1.94	0.67
1:A:1107:MET:HG2	1:A:1112:TRP:HD1	1.60	0.67
1:A:1132:SER:O	1:A:1176:PHE:HB3	1.94	0.67
1:B:877:GLN:O	1:B:881:GLU:HG2	1.95	0.66
1:B:1131:GLU:HB3	1:B:1134:PHE:HE1	1.59	0.66
1:B:574:GLU:HA	1:B:577:ASP:OD2	1.95	0.66
1:B:948:ILE:HG23	1:B:949:PRO:HD2	1.78	0.66
1:A:574:GLU:HA	1:A:577:ASP:OD2	1.95	0.66
1:A:586:MET:CE	1:A:867:LEU:HD23	2.26	0.66
1:A:1002:VAL:HG23	1:A:1064:GLN:HB2	1.77	0.66
1:B:633:LYS:HA	1:B:636:GLN:NE2	2.11	0.66
1:A:260:THR:N	1:A:263:GLN:OE1	2.26	0.66
1:B:262:GLY:O	1:B:265:VAL:HG12	1.95	0.66
1:B:586:MET:HE3	1:B:867:LEU:HD23	1.77	0.66
1:A:112:ILE:O	1:A:115:VAL:HG12	1.96	0.66
1:B:584:LEU:O	1:B:588:LYS:HG2	1.96	0.66
1:A:1132:SER:CB	1:A:1178:TYR:HB2	2.25	0.66
1:A:1131:GLU:HB3	1:A:1134:PHE:HE2	1.61	0.66
1:B:854:ILE:HD12	1:B:867:LEU:HD22	1.78	0.66
2:A:1402:3PH:H2	2:A:1402:3PH:H322	1.75	0.66
1:B:112:ILE:O	1:B:115:VAL:HG12	1.95	0.66
1:A:221:GLY:HA2	1:A:224:LYS:NZ	2.11	0.66
1:A:853:ILE:O	1:A:857:MET:HE2	1.96	0.66
1:B:645:LYS:HA	1:B:648:LEU:HD23	1.78	0.66
1:B:1002:VAL:HG23	1:B:1064:GLN:HB2	1.78	0.66
1:A:841:LYS:O	1:A:845:ILE:HG12	1.96	0.65
1:A:989:VAL:HG11	1:A:1053:ARG:HD2	1.78	0.65
1:B:1173:LYS:HE2	1:A:1172:HIS:CD2	2.32	0.65
1:B:641:TYR:CD1	1:B:642:PRO:HD2	2.32	0.65
1:A:412:ARG:HG2	1:A:413:ILE:HD13	1.78	0.65
1:B:968:LYS:NZ	1:B:972:PHE:HB2	2.12	0.65
1:A:595:TRP:O	1:A:599:GLU:HG2	1.96	0.65
1:B:530:CYS:CB	1:A:937:LYS:HD3	2.25	0.65
1:A:584:LEU:O	1:A:588:LYS:HG2	1.96	0.65
1:A:1154:ASN:HB2	1:A:1171:VAL:HG13	1.78	0.65
1:A:1145:VAL:HB	1:A:1167:ILE:HD11	1.78	0.65
1:B:613:GLN:HG2	1:B:616:GLU:OE2	1.97	0.65
1:B:989:VAL:HG11	1:B:1053:ARG:HD2	1.77	0.65
1:B:1135:GLN:OE1	1:B:1173:LYS:HG3	1.96	0.65
1:B:1173:LYS:HE2	1:A:1172:HIS:CG	2.32	0.65
1:A:1149:ASN:HA	1:A:1163:SER:OG	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1160:GLU:O	1:B:1161:ILE:HD13	1.98	0.64
1:A:495:ALA:O	1:A:498:VAL:HG22	1.97	0.64
1:B:1131:GLU:HB3	1:B:1134:PHE:CE1	2.32	0.64
1:A:1082:LEU:HG	1:A:1084:PRO:HD2	1.80	0.64
1:B:77:VAL:HG12	1:B:81:ILE:HD11	1.80	0.64
1:A:68:ASP:HB2	1:A:72:ALA:CB	2.26	0.64
1:A:968:LYS:NZ	1:A:972:PHE:HB2	2.12	0.64
1:B:412:ARG:HG2	1:B:413:ILE:HD13	1.80	0.64
1:B:615:ALA:CA	1:B:626:ILE:HD13	2.27	0.64
1:A:849:GLU:N	1:A:849:GLU:OE1	2.30	0.64
1:B:1149:ASN:HA	1:B:1163:SER:OG	1.98	0.64
1:A:573:ARG:NH1	1:A:576:ALA:HB3	2.13	0.64
1:B:449:ASP:OD1	1:B:450:VAL:N	2.31	0.64
1:A:613:GLN:HG2	1:A:616:GLU:OE2	1.97	0.64
1:B:107:LEU:HD21	1:B:368:VAL:HG13	1.80	0.63
1:B:937:LYS:HD3	1:A:530:CYS:CB	2.28	0.63
1:A:175:VAL:O	1:A:179:VAL:HG23	1.98	0.63
1:A:449:ASP:OD1	1:A:450:VAL:N	2.31	0.63
1:A:499:ARG:O	1:A:503:GLU:HG2	1.98	0.63
1:A:615:ALA:CA	1:A:626:ILE:HD13	2.27	0.63
1:A:925:MET:O	1:A:929:LYS:HG2	1.98	0.63
1:A:300:GLU:OE1	1:A:345:VAL:HG11	1.97	0.63
1:A:575:PHE:HE2	1:A:862:LYS:HD2	1.62	0.63
1:B:495:ALA:O	1:B:498:VAL:HG22	1.98	0.63
1:A:172:PHE:HB3	1:A:406:PHE:CZ	2.34	0.63
1:A:1009:TYR:HD1	1:A:1033:GLU:HG2	1.63	0.63
1:A:158:THR:HG22	1:A:228:THR:HG21	1.80	0.63
1:A:816:ALA:O	1:A:819:PRO:HD2	1.99	0.63
1:A:856:ARG:HA	1:A:856:ARG:NH1	2.13	0.63
1:B:172:PHE:HB3	1:B:406:PHE:CZ	2.33	0.63
1:B:175:VAL:O	1:B:179:VAL:HG23	1.98	0.63
1:A:642:PRO:HB3	1:A:646:ARG:NH2	2.09	0.63
1:B:1082:LEU:HG	1:B:1084:PRO:HD2	1.80	0.63
1:A:854:ILE:HD12	1:A:867:LEU:HD22	1.81	0.63
1:A:416:GLY:O	1:A:417:LEU:HD23	1.99	0.63
1:B:499:ARG:O	1:B:503:GLU:HG2	1.99	0.63
1:B:580:GLU:O	1:B:584:LEU:HG	1.99	0.63
1:B:300:GLU:OE1	1:B:345:VAL:HG11	1.98	0.62
1:B:573:ARG:NH1	1:B:576:ALA:HB3	2.14	0.62
1:A:580:GLU:O	1:A:584:LEU:HG	1.99	0.62
1:B:856:ARG:NH1	1:B:856:ARG:HA	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:858:VAL:HG12	1:A:860:ASN:H	1.64	0.62
1:B:525:ILE:HD11	1:A:902:ILE:CD1	2.30	0.62
1:A:224:LYS:HD2	1:A:224:LYS:H	1.61	0.62
1:A:1131:GLU:HB3	1:A:1134:PHE:CE2	2.34	0.62
1:B:413:ILE:HG22	1:B:414:GLY:H	1.63	0.62
1:B:618:ALA:CB	1:B:626:ILE:HG12	2.29	0.62
1:B:1132:SER:O	1:B:1176:PHE:HB3	2.00	0.62
1:A:645:LYS:HA	1:A:648:LEU:HD23	1.81	0.62
1:A:1147:LEU:HG	1:A:1163:SER:HB3	1.81	0.62
1:B:1147:LEU:HA	1:B:1186:LEU:CD1	2.26	0.62
1:B:1172:HIS:CE1	1:A:1173:LYS:HG2	2.34	0.62
1:B:85:CYS:HB3	1:A:302:THR:CG2	2.30	0.62
1:B:302:THR:CG2	1:A:85:CYS:HB3	2.30	0.62
1:B:587:LEU:CD2	1:B:626:ILE:HD11	2.29	0.62
1:B:1145:VAL:CG1	1:B:1188:VAL:HG12	2.30	0.62
1:A:318:TRP:O	1:A:319:LEU:HG	1.99	0.62
1:B:874:GLY:O	1:B:878:VAL:HG23	2.00	0.62
1:B:987:VAL:HG22	1:B:1058:THR:CG2	2.30	0.62
1:B:1173:LYS:HB2	1:A:1172:HIS:HD2	1.64	0.62
2:B:1402:3PH:H221	2:B:1402:3PH:H332	1.82	0.62
2:A:1402:3PH:H362	2:A:1402:3PH:H251	1.81	0.62
1:B:976:ARG:HD3	1:B:1072:ASP:OD1	1.99	0.62
1:A:1145:VAL:CG1	1:A:1188:VAL:HG12	2.29	0.62
1:B:257:LEU:HD12	1:B:258:THR:N	2.15	0.61
1:A:856:ARG:HA	1:A:856:ARG:HH11	1.65	0.61
1:A:579:MET:HA	1:A:579:MET:HE3	1.82	0.61
1:A:987:VAL:HG22	1:A:1058:THR:CG2	2.31	0.61
1:B:158:THR:HG22	1:B:228:THR:HG21	1.82	0.61
2:B:1402:3PH:H362	2:B:1402:3PH:H251	1.81	0.61
1:A:976:ARG:HD3	1:A:1072:ASP:OD1	2.00	0.61
2:A:1402:3PH:H332	2:A:1402:3PH:H221	1.83	0.61
1:B:856:ARG:HA	1:B:856:ARG:HH11	1.64	0.61
1:A:257:LEU:HD12	1:A:258:THR:O	2.00	0.61
1:B:1107:MET:HG2	1:B:1112:TRP:HD1	1.66	0.61
1:A:573:ARG:HH12	1:A:577:ASP:H	1.47	0.61
1:A:1145:VAL:HG13	1:A:1188:VAL:HG12	1.82	0.61
1:B:416:GLY:O	1:B:417:LEU:HD23	2.00	0.61
1:A:413:ILE:HG22	1:A:414:GLY:H	1.66	0.61
1:A:587:LEU:CD2	1:A:626:ILE:HD11	2.30	0.61
1:A:242:ILE:HG21	1:A:324:VAL:HG11	1.83	0.60
1:A:874:GLY:O	1:A:878:VAL:HG23	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:573:ARG:HH12	1:B:577:ASP:H	1.47	0.60
1:B:850:VAL:O	1:B:854:ILE:HG12	2.02	0.60
1:A:1153:TYR:CE1	1:A:1160:GLU:HA	2.35	0.60
1:B:130:VAL:O	1:B:133:MET:HG3	2.02	0.60
1:B:240:CYS:O	1:B:244:ILE:HG13	2.01	0.60
1:B:816:ALA:O	1:B:819:PRO:HD2	2.01	0.60
1:B:1145:VAL:HG13	1:B:1188:VAL:HG12	1.83	0.60
1:A:137:VAL:HG13	1:A:141:ILE:HD12	1.82	0.60
1:A:221:GLY:HA2	1:A:224:LYS:HZ3	1.66	0.60
1:A:618:ALA:CB	1:A:626:ILE:HG12	2.29	0.60
1:B:412:ARG:HG2	1:B:413:ILE:CD1	2.31	0.60
1:A:1148:ILE:O	1:A:1149:ASN:ND2	2.33	0.60
1:B:163:PHE:CZ	2:B:1402:3PH:H272	2.37	0.60
1:B:627:LEU:HD23	1:B:633:LYS:CE	2.32	0.60
1:B:1133:HIS:CE1	1:B:1177:GLN:HA	2.36	0.60
1:A:594:TYR:O	1:A:603:LEU:HD23	2.02	0.60
1:A:647:LYS:HZ1	1:A:826:ASN:N	1.99	0.60
1:A:75:PRO:HB2	1:A:78:ILE:HD12	1.83	0.60
1:A:240:CYS:O	1:A:244:ILE:HG13	2.02	0.60
1:A:627:LEU:HD23	1:A:633:LYS:CE	2.32	0.60
1:A:1071:GLU:O	1:A:1075:ILE:HG12	2.02	0.60
1:B:242:ILE:HG21	1:B:324:VAL:HG11	1.84	0.60
1:A:649:GLU:HA	1:A:652:ILE:HD11	1.84	0.60
1:B:1139:ASP:O	1:B:1142:LEU:HG	2.02	0.59
1:B:1153:TYR:CE1	1:B:1160:GLU:HA	2.33	0.59
1:A:649:GLU:HA	1:A:652:ILE:CD1	2.32	0.59
1:A:850:VAL:O	1:A:854:ILE:HG12	2.01	0.59
1:B:179:VAL:HG22	1:B:199:MET:CE	2.32	0.59
1:B:221:GLY:HA2	1:B:224:LYS:NZ	2.18	0.59
1:B:406:PHE:O	1:B:410:LEU:HG	2.03	0.59
1:A:852:LYS:HE3	1:A:1105:GLU:CG	2.31	0.59
1:A:1142:LEU:HD12	1:A:1143:GLU:N	2.17	0.59
1:A:1132:SER:HB3	1:A:1178:TYR:HB2	1.83	0.59
1:B:1034:ASP:OD1	1:B:1035:TYR:N	2.32	0.59
1:B:628:VAL:HG22	1:B:632:LYS:HG2	1.85	0.59
1:A:622:LYS:HD2	1:A:623:ASP:N	2.17	0.59
1:A:641:TYR:CD1	1:A:642:PRO:HD2	2.37	0.59
1:A:647:LYS:HZ1	1:A:826:ASN:H	1.51	0.59
1:A:575:PHE:CE2	1:A:862:LYS:HD2	2.37	0.59
1:A:587:LEU:HD22	1:A:626:ILE:HD11	1.84	0.59
1:A:1133:HIS:CE1	1:A:1177:GLN:HA	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:586:MET:HE2	1:B:867:LEU:HD23	1.84	0.59
1:B:647:LYS:HZ1	1:B:826:ASN:N	2.00	0.59
1:B:85:CYS:HB3	1:A:302:THR:HG23	1.85	0.58
1:B:964:ALA:O	1:B:1089:ARG:NH1	2.36	0.58
1:A:1131:GLU:OE1	1:A:1132:SER:N	2.31	0.58
1:A:107:LEU:HD21	1:A:368:VAL:HG13	1.86	0.58
1:A:412:ARG:HG2	1:A:413:ILE:CD1	2.33	0.58
1:B:174:LEU:HB2	1:B:237:ASN:OD1	2.03	0.58
1:B:902:ILE:HG12	1:A:525:ILE:CD1	2.33	0.58
1:B:1071:GLU:O	1:B:1075:ILE:HG12	2.02	0.58
1:A:174:LEU:HB2	1:A:237:ASN:OD1	2.03	0.58
1:A:633:LYS:HA	1:A:636:GLN:HE22	1.67	0.58
1:B:525:ILE:HD12	1:A:902:ILE:HG12	1.84	0.58
1:B:91:SER:OG	1:B:102:TYR:HB2	2.03	0.58
1:B:302:THR:HG23	1:A:85:CYS:HB3	1.85	0.58
1:B:369:GLY:O	1:B:372:VAL:HG12	2.03	0.58
1:B:1155:ALA:CB	1:B:1173:LYS:HB3	2.33	0.58
1:A:406:PHE:O	1:A:410:LEU:HG	2.03	0.58
1:A:964:ALA:O	1:A:1089:ARG:NH1	2.36	0.58
1:B:98:LEU:HD13	1:B:99:PRO:HD2	1.86	0.58
1:B:633:LYS:HA	1:B:636:GLN:HE22	1.67	0.58
1:A:625:PHE:HE2	1:A:867:LEU:HA	1.67	0.58
1:B:902:ILE:HG12	1:A:525:ILE:HG12	1.86	0.58
1:A:91:SER:OG	1:A:102:TYR:HB2	2.04	0.58
1:A:107:LEU:HD21	1:A:368:VAL:CG1	2.34	0.58
1:A:179:VAL:HG22	1:A:199:MET:CE	2.33	0.58
1:B:1011:LYS:HE2	1:B:1030:GLU:OE1	2.05	0.57
1:B:1005:LEU:HD12	1:B:1036:LEU:O	2.04	0.57
1:A:163:PHE:CZ	2:A:1402:3PH:H272	2.38	0.57
1:A:982:PHE:HB2	1:A:1063:VAL:CG1	2.34	0.57
1:B:255:PRO:O	1:B:256:GLN:NE2	2.37	0.57
1:B:1140:ALA:HB3	1:A:1169:ARG:NH1	2.19	0.57
1:A:976:ARG:HD3	1:A:1072:ASP:CG	2.24	0.57
1:B:256:GLN:O	1:B:257:LEU:HG	2.04	0.57
1:A:820:LYS:O	1:A:823:LEU:HB2	2.04	0.57
1:B:852:LYS:HE3	1:B:1105:GLU:CG	2.30	0.57
1:B:626:ILE:HG22	1:B:627:LEU:HG	1.87	0.57
1:B:976:ARG:HD3	1:B:1072:ASP:CG	2.25	0.57
1:B:1142:LEU:HD12	1:B:1143:GLU:N	2.20	0.57
1:A:369:GLY:O	1:A:372:VAL:HG12	2.04	0.57
1:B:575:PHE:CE2	1:B:862:LYS:HD2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:820:LYS:O	1:B:823:LEU:HB2	2.04	0.57
1:A:627:LEU:HA	1:A:632:LYS:CD	2.34	0.57
1:A:628:VAL:HG22	1:A:632:LYS:CE	2.33	0.57
1:B:587:LEU:HD22	1:B:626:ILE:HD11	1.86	0.57
1:B:628:VAL:HG22	1:B:632:LYS:CE	2.31	0.57
1:A:613:GLN:O	1:A:617:VAL:HG12	2.05	0.57
1:B:305:LEU:HD22	2:A:1401:3PH:H3G2	1.87	0.56
1:A:368:VAL:HG21	1:A:436:LEU:HD22	1.87	0.56
1:A:586:MET:HE2	1:A:867:LEU:HB3	1.87	0.56
1:B:499:ARG:HG3	1:B:500:ARG:N	2.20	0.56
1:B:525:ILE:HD11	1:A:902:ILE:HG12	1.85	0.56
1:B:613:GLN:O	1:B:617:VAL:HG12	2.05	0.56
1:B:897:LYS:HD3	1:A:518:LEU:HD12	1.88	0.56
1:B:1112:TRP:HA	1:B:1116:LYS:CE	2.35	0.56
1:A:1005:LEU:HD12	1:A:1036:LEU:O	2.06	0.56
1:B:622:LYS:HD2	1:B:623:ASP:N	2.19	0.56
1:B:634:SER:O	1:B:638:LYS:HG2	2.05	0.56
1:B:750:LYS:O	1:B:752:LEU:N	2.39	0.56
1:B:1107:MET:CG	1:B:1112:TRP:HD1	2.18	0.56
1:A:586:MET:CE	1:A:867:LEU:HB3	2.35	0.56
1:B:925:MET:O	1:B:929:LYS:HG2	2.06	0.56
1:A:499:ARG:HG3	1:A:500:ARG:N	2.20	0.56
1:B:632:LYS:O	1:B:633:LYS:HD3	2.06	0.56
1:A:609:ARG:NH1	1:A:610:LEU:HA	2.21	0.56
1:A:98:LEU:HD13	1:A:99:PRO:HD2	1.86	0.56
1:B:518:LEU:HD12	1:A:897:LYS:HD3	1.88	0.56
1:B:833:LEU:HD13	1:B:885:LEU:HD21	1.87	0.56
1:B:982:PHE:HB2	1:B:1063:VAL:CG1	2.34	0.56
1:A:607:ALA:CB	1:A:839:VAL:HG22	2.34	0.56
1:A:628:VAL:HG22	1:A:632:LYS:HG2	1.87	0.56
1:A:1139:ASP:O	1:A:1142:LEU:HG	2.06	0.56
1:B:407:SER:O	1:B:410:LEU:HD12	2.06	0.56
1:B:900:GLN:HA	1:B:900:GLN:OE1	2.05	0.56
1:A:631:LEU:HG	1:A:635:TRP:CH2	2.41	0.56
1:B:80:PHE:CD1	1:B:130:VAL:HG11	2.41	0.55
1:B:648:LEU:HA	1:B:651:LEU:HD12	1.88	0.55
1:A:134:ASP:OD1	1:A:135:PRO:HD2	2.06	0.55
1:A:750:LYS:O	1:A:752:LEU:N	2.39	0.55
1:B:609:ARG:NH1	1:B:610:LEU:HA	2.22	0.55
1:B:1141:THR:HG23	1:A:1169:ARG:NH1	2.21	0.55
1:A:1034:ASP:OD1	1:A:1035:TYR:N	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:VAL:O	1:B:160:MET:HG2	2.07	0.55
1:B:165:GLN:OE1	1:B:415:TYR:HB3	2.06	0.55
1:B:627:LEU:HA	1:B:632:LYS:CD	2.34	0.55
1:A:156:VAL:O	1:A:160:MET:HG2	2.06	0.55
1:A:634:SER:O	1:A:638:LYS:HG2	2.07	0.55
1:A:641:TYR:CD1	1:A:643:TRP:HD1	2.23	0.55
1:B:107:LEU:HD21	1:B:368:VAL:CG1	2.36	0.55
1:A:853:ILE:HG22	1:A:857:MET:HE1	1.86	0.55
1:B:625:PHE:HE2	1:B:867:LEU:HA	1.70	0.55
1:A:260:THR:HG23	1:A:263:GLN:OE1	2.06	0.55
1:A:795:SER:HA	1:A:798:VAL:O	2.06	0.55
1:B:960:VAL:HB	1:B:963:LEU:HD22	1.89	0.55
1:A:1155:ALA:CB	1:A:1173:LYS:HB2	2.37	0.55
1:B:649:GLU:HA	1:B:652:ILE:CD1	2.37	0.55
1:B:1132:SER:HB3	1:B:1178:TYR:HB2	1.89	0.55
1:B:647:LYS:NZ	1:B:825:VAL:HB	2.21	0.55
1:B:957:LEU:HD21	1:B:973:ILE:CG2	2.37	0.55
1:A:957:LEU:HD21	1:A:973:ILE:CG2	2.37	0.55
1:A:976:ARG:NH1	1:A:976:ARG:HB2	2.21	0.55
1:B:862:LYS:HG3	1:B:863:ILE:HD12	1.89	0.55
1:A:138:LEU:HD12	1:A:142:PHE:HD2	1.72	0.55
1:A:255:PRO:O	1:A:256:GLN:NE2	2.40	0.55
1:A:863:ILE:HA	1:A:866:GLU:CD	2.26	0.55
1:A:1107:MET:CG	1:A:1112:TRP:HD1	2.20	0.55
1:A:613:GLN:O	1:A:616:GLU:HG3	2.06	0.54
1:B:525:ILE:O	1:B:529:ALA:N	2.40	0.54
1:B:1169:ARG:NH1	1:A:1140:ALA:HB3	2.23	0.54
1:A:282:VAL:HG11	1:A:311:THR:OG1	2.07	0.54
1:A:627:LEU:CA	1:A:632:LYS:HD2	2.36	0.54
1:A:864:LEU:O	1:A:868:LYS:HG3	2.07	0.54
1:A:1138:ILE:HD13	1:A:1172:HIS:O	2.07	0.54
1:B:368:VAL:HG21	1:B:436:LEU:HD22	1.88	0.54
1:B:1173:LYS:HB2	1:A:1172:HIS:CD2	2.43	0.54
1:A:407:SER:O	1:A:410:LEU:HD12	2.06	0.54
1:A:1135:GLN:NE2	1:A:1155:ALA:HB2	2.19	0.54
1:B:613:GLN:O	1:B:616:GLU:HG3	2.07	0.54
1:A:165:GLN:OE1	1:A:415:TYR:HB3	2.07	0.54
1:A:322:SER:OG	1:A:325:LEU:HB2	2.08	0.54
1:A:948:ILE:CG2	1:A:949:PRO:HD2	2.36	0.54
1:B:621:GLU:CD	1:B:624:GLN:HB3	2.28	0.54
1:A:863:ILE:HG22	1:A:867:LEU:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1030:GLU:OE1	1:A:1030:GLU:N	2.41	0.54
1:B:649:GLU:HA	1:B:652:ILE:HD11	1.90	0.54
1:B:980:LEU:HB2	1:B:1065:VAL:HG23	1.89	0.54
1:A:586:MET:HE2	1:A:867:LEU:HD23	1.89	0.54
1:A:1011:LYS:HD2	1:A:1012:SER:N	2.23	0.54
1:B:138:LEU:HD12	1:B:142:PHE:HD2	1.72	0.54
1:B:405:LEU:O	1:B:408:PRO:HD2	2.08	0.54
1:B:412:ARG:O	1:B:413:ILE:HD13	2.08	0.54
1:A:615:ALA:CB	1:A:626:ILE:HD13	2.38	0.54
1:A:621:GLU:CD	1:A:624:GLN:HB3	2.29	0.54
1:A:853:ILE:HD11	1:A:1107:MET:HE1	1.89	0.54
1:B:322:SER:OG	1:B:325:LEU:HB2	2.08	0.54
1:B:861:LYS:O	1:B:863:ILE:HD12	2.07	0.54
1:B:914:HIS:NE2	1:B:931:GLU:OE2	2.41	0.54
1:B:960:VAL:HB	1:B:963:LEU:HD21	1.89	0.54
1:B:976:ARG:NH1	1:B:976:ARG:HB2	2.22	0.54
1:B:282:VAL:HG11	1:B:311:THR:OG1	2.07	0.54
1:A:343:PRO:O	1:A:346:GLU:HG2	2.09	0.54
1:A:960:VAL:HB	1:A:963:LEU:HD21	1.89	0.54
1:B:904:THR:HG21	1:A:512:LEU:HD21	1.90	0.53
1:B:257:LEU:HD12	1:B:258:THR:H	1.73	0.53
1:B:521:ALA:HB2	1:A:897:LYS:CB	2.37	0.53
1:B:343:PRO:O	1:B:346:GLU:HG2	2.08	0.53
1:A:174:LEU:CD2	1:A:240:CYS:HB2	2.38	0.53
1:B:647:LYS:HZ1	1:B:826:ASN:H	1.54	0.53
1:B:897:LYS:CB	1:A:521:ALA:HB2	2.38	0.53
1:B:989:VAL:HB	1:B:1057:VAL:HG12	1.91	0.53
1:A:586:MET:HE3	1:A:867:LEU:HD23	1.89	0.53
1:A:405:LEU:O	1:A:408:PRO:HD2	2.08	0.53
1:B:275:GLY:HA2	1:B:321:VAL:CG1	2.39	0.53
1:B:980:LEU:HB2	1:B:1065:VAL:CG2	2.39	0.53
1:A:627:LEU:HD23	1:A:633:LYS:HE2	1.90	0.53
1:A:980:LEU:HB2	1:A:1065:VAL:HG23	1.89	0.53
1:B:137:VAL:HG13	1:B:141:ILE:HD12	1.88	0.53
1:B:294:PHE:CE1	1:B:939:LYS:HG2	2.44	0.53
1:B:584:LEU:HA	1:B:587:LEU:CD1	2.38	0.53
1:B:587:LEU:HD13	1:B:619:ALA:CB	2.34	0.53
1:B:1082:LEU:HG	1:B:1084:PRO:CD	2.39	0.53
1:A:275:GLY:HA2	1:A:321:VAL:CG1	2.38	0.53
1:B:407:SER:HA	1:B:410:LEU:CD1	2.34	0.53
1:B:598:PHE:HB2	1:B:603:LEU:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:976:ARG:O	1:A:977:ALA:HB3	2.09	0.53
1:B:296:ASP:O	1:B:300:GLU:HG3	2.09	0.53
1:B:628:VAL:O	1:B:629:ASP:HB3	2.09	0.53
1:B:1184:PRO:C	1:B:1185:ARG:HD2	2.28	0.53
1:B:174:LEU:CD2	1:B:240:CYS:HB2	2.38	0.52
1:B:863:ILE:HA	1:B:866:GLU:CD	2.29	0.52
1:B:996:ASP:OD1	1:B:996:ASP:N	2.41	0.52
1:A:647:LYS:HZ1	1:A:825:VAL:HB	1.74	0.52
1:A:811:LEU:O	1:A:814:THR:HG23	2.10	0.52
1:B:833:LEU:HD23	1:B:892:ILE:HG21	1.91	0.52
1:B:1107:MET:CG	1:B:1111:GLY:H	2.22	0.52
1:A:1174:LEU:HD23	1:A:1174:LEU:O	2.08	0.52
1:B:902:ILE:HB	1:B:941:LEU:CD1	2.39	0.52
1:A:960:VAL:HB	1:A:963:LEU:HD22	1.90	0.52
1:B:923:ASP:OD2	1:B:926:GLU:HG2	2.10	0.52
1:B:1138:ILE:HD13	1:B:1172:HIS:O	2.10	0.52
1:B:1147:LEU:HG	1:B:1163:SER:HB3	1.91	0.52
1:A:75:PRO:HB2	1:A:78:ILE:CD1	2.40	0.52
1:A:294:PHE:CE1	1:A:939:LYS:HG2	2.45	0.52
1:B:645:LYS:HE3	1:B:646:ARG:HH22	1.75	0.52
1:B:902:ILE:HG12	1:A:525:ILE:HD11	1.92	0.52
1:A:615:ALA:HA	1:A:626:ILE:HG21	1.90	0.52
1:A:1082:LEU:HG	1:A:1084:PRO:CD	2.38	0.52
1:B:77:VAL:HG13	1:B:130:VAL:HG22	1.91	0.52
1:A:902:ILE:HB	1:A:941:LEU:CD1	2.40	0.52
1:A:411:SER:HA	1:A:416:GLY:CA	2.34	0.52
1:B:615:ALA:CB	1:B:626:ILE:HD13	2.39	0.52
1:B:864:LEU:O	1:B:868:LYS:HG3	2.09	0.52
1:A:225:GLN:O	1:A:229:ILE:HG13	2.10	0.52
1:A:638:LYS:C	1:A:640:ILE:HD12	2.30	0.52
2:A:1402:3PH:H221	2:A:1402:3PH:H31	1.91	0.52
1:B:225:GLN:O	1:B:229:ILE:HG13	2.09	0.52
1:B:627:LEU:CA	1:B:632:LYS:HD2	2.38	0.51
1:A:584:LEU:HA	1:A:587:LEU:CD1	2.40	0.51
1:A:1153:TYR:HB3	1:A:1158:ARG:CG	2.40	0.51
1:B:186:MET:HG3	1:B:198:ALA:HB2	1.92	0.51
1:B:618:ALA:HB2	1:B:626:ILE:HA	1.93	0.51
1:B:976:ARG:O	1:B:977:ALA:HB3	2.09	0.51
1:A:296:ASP:O	1:A:300:GLU:HG3	2.09	0.51
1:A:643:TRP:HZ3	1:A:828:LYS:CG	2.22	0.51
1:A:980:LEU:HB2	1:A:1065:VAL:CG2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:ASP:OD1	1:B:135:PRO:HD2	2.10	0.51
1:B:179:VAL:HA	1:B:199:MET:HE1	1.93	0.51
2:B:1402:3PH:H221	2:B:1402:3PH:H31	1.91	0.51
1:A:615:ALA:HA	1:A:626:ILE:CG2	2.41	0.51
1:B:1147:LEU:HD11	1:B:1150:GLY:O	2.11	0.51
1:B:1172:HIS:ND1	1:A:1173:LYS:HG2	2.25	0.51
1:A:647:LYS:NZ	1:A:825:VAL:HB	2.25	0.51
1:B:81:ILE:HD13	2:B:1401:3PH:H2C2	1.92	0.51
1:B:647:LYS:HG3	1:B:651:LEU:HD11	1.92	0.51
1:A:863:ILE:O	1:A:866:GLU:HB2	2.11	0.51
1:A:996:ASP:N	1:A:996:ASP:OD1	2.42	0.51
1:A:1011:LYS:NZ	1:A:1030:GLU:HB2	2.26	0.51
1:A:647:LYS:HG3	1:A:651:LEU:HD11	1.93	0.51
1:A:1011:LYS:NZ	1:A:1012:SER:O	2.44	0.51
1:A:1049:THR:OG1	1:A:1051:LYS:HE2	2.11	0.51
1:B:496:GLY:HA2	1:B:499:ARG:NH1	2.26	0.51
1:B:632:LYS:HD3	1:B:633:LYS:HZ2	1.76	0.51
1:B:641:TYR:CG	1:B:642:PRO:HD2	2.46	0.51
1:B:962:TRP:CZ3	1:B:963:LEU:HB3	2.46	0.51
1:A:137:VAL:HG13	1:A:141:ILE:CD1	2.41	0.51
1:A:283:ALA:HA	1:A:286:THR:CG2	2.41	0.51
1:A:861:LYS:O	1:A:862:LYS:HG2	2.11	0.51
1:B:283:ALA:HA	1:B:286:THR:CG2	2.41	0.51
1:B:937:LYS:CD	1:A:530:CYS:HB3	2.35	0.51
1:B:863:ILE:HG22	1:B:867:LEU:HD11	1.93	0.50
1:B:1153:TYR:HB3	1:B:1158:ARG:HA	1.92	0.50
2:B:1401:3PH:H3G2	1:A:305:LEU:HD22	1.93	0.50
1:A:260:THR:OG1	1:A:263:GLN:HB3	2.11	0.50
1:A:424:ILE:HD11	1:A:478:LEU:HD23	1.93	0.50
1:A:751:ILE:O	1:A:755:GLY:N	2.34	0.50
1:A:1011:LYS:HD2	1:A:1012:SER:H	1.75	0.50
1:B:494:MET:SD	1:A:926:GLU:HB3	2.52	0.50
1:B:579:MET:SD	1:B:863:ILE:HG12	2.51	0.50
1:B:609:ARG:HD2	1:B:609:ARG:O	2.11	0.50
1:B:615:ALA:HA	1:B:626:ILE:HG21	1.92	0.50
1:B:633:LYS:O	1:B:637:ILE:HD12	2.12	0.50
1:B:1048:LEU:HD11	1:B:1090:LEU:HB3	1.92	0.50
1:B:1149:ASN:HA	1:B:1163:SER:CB	2.41	0.50
1:A:256:GLN:C	1:A:257:LEU:HG	2.32	0.50
1:A:880:LYS:HD2	1:A:1035:TYR:CZ	2.46	0.50
1:A:960:VAL:O	1:A:963:LEU:HD23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:LEU:HD11	1:A:1090:LEU:HB3	1.92	0.50
1:B:615:ALA:HA	1:B:626:ILE:CG2	2.41	0.50
1:B:1176:PHE:HZ	1:B:1184:PRO:HB2	1.75	0.50
1:A:579:MET:HE2	1:A:863:ILE:HG23	1.92	0.50
1:A:1107:MET:CG	1:A:1111:GLY:H	2.24	0.50
1:A:1154:ASN:CB	1:A:1171:VAL:HG13	2.42	0.50
1:B:649:GLU:O	1:B:652:ILE:HG12	2.11	0.50
1:B:819:PRO:CA	1:B:822:ILE:HD12	2.31	0.50
1:B:1119:LEU:HD12	1:A:511:MET:HG3	1.93	0.50
1:B:960:VAL:O	1:B:963:LEU:HD23	2.11	0.50
1:A:633:LYS:O	1:A:637:ILE:HD12	2.11	0.50
1:A:898:THR:HG22	1:A:902:ILE:HD11	1.93	0.50
1:A:913:ILE:HD12	1:A:930:LEU:HD13	1.94	0.50
1:A:962:TRP:CZ3	1:A:963:LEU:HB3	2.46	0.50
1:B:225:GLN:NE2	1:B:415:TYR:OH	2.43	0.50
1:B:424:ILE:HD11	1:B:478:LEU:HD23	1.94	0.50
1:B:1049:THR:OG1	1:B:1051:LYS:HE2	2.11	0.50
1:A:641:TYR:HD1	1:A:643:TRP:HD1	1.60	0.50
1:A:944:ALA:HB1	1:A:945:PRO:HD2	1.93	0.50
1:B:635:TRP:O	1:B:638:LYS:HB2	2.11	0.50
1:B:638:LYS:HB3	1:B:640:ILE:HD12	1.94	0.50
1:A:407:SER:HA	1:A:410:LEU:CD1	2.34	0.50
1:A:958:LYS:HB2	1:A:974:LYS:NZ	2.27	0.50
1:B:317:ILE:HG22	1:B:318:TRP:CD1	2.47	0.49
1:B:628:VAL:N	1:B:632:LYS:HD2	2.27	0.49
1:B:853:ILE:O	1:B:857:MET:HE2	2.11	0.49
1:A:186:MET:HG3	1:A:198:ALA:HB2	1.92	0.49
1:A:224:LYS:N	1:A:224:LYS:CD	2.75	0.49
1:A:618:ALA:HB2	1:A:626:ILE:HA	1.93	0.49
1:A:626:ILE:HG22	1:A:627:LEU:HG	1.93	0.49
1:A:650:ASP:HB3	1:A:822:ILE:CG1	2.39	0.49
1:B:817:LEU:HD21	1:B:821:LEU:HD12	1.94	0.49
1:B:863:ILE:O	1:B:866:GLU:HB2	2.12	0.49
1:B:937:LYS:HE2	1:A:530:CYS:CA	2.35	0.49
1:A:641:TYR:CG	1:A:642:PRO:HD2	2.47	0.49
1:B:895:SER:HA	1:B:948:ILE:HD13	1.93	0.49
1:B:944:ALA:HB1	1:B:945:PRO:HD2	1.93	0.49
1:A:135:PRO:HB3	1:A:441:VAL:HG22	1.93	0.49
1:A:622:LYS:HD2	1:A:623:ASP:H	1.77	0.49
1:B:579:MET:O	1:B:583:ARG:HG3	2.12	0.49
1:B:795:SER:HA	1:B:798:VAL:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:915:GLU:OE1	1:B:916:LEU:N	2.46	0.49
1:A:81:ILE:HD13	2:A:1401:3PH:H2C2	1.93	0.49
1:A:97:LYS:HG2	1:A:98:LEU:N	2.28	0.49
1:B:530:CYS:SG	1:A:937:LYS:HD3	2.52	0.49
1:B:594:TYR:HB3	1:B:603:LEU:HD21	1.95	0.49
1:B:958:LYS:HB2	1:B:974:LYS:NZ	2.27	0.49
1:A:991:GLU:HB2	1:A:1056:THR:OG1	2.13	0.49
1:B:97:LYS:HG2	1:B:98:LEU:N	2.28	0.49
1:B:650:ASP:HB3	1:B:822:ILE:CG1	2.42	0.49
1:B:880:LYS:HD2	1:B:1035:TYR:CZ	2.47	0.49
1:A:496:GLY:HA2	1:A:499:ARG:NH1	2.27	0.49
1:A:609:ARG:HD2	1:A:609:ARG:O	2.12	0.49
1:A:642:PRO:O	1:A:646:ARG:HG2	2.13	0.49
1:A:344:GLU:OE1	1:A:344:GLU:N	2.36	0.49
1:B:68:ASP:HB2	1:B:72:ALA:HB1	1.91	0.49
1:B:68:ASP:HB2	1:B:72:ALA:HB3	1.91	0.49
1:B:512:LEU:HD21	1:A:904:THR:HG21	1.95	0.49
1:B:573:ARG:HH12	1:B:577:ASP:N	2.09	0.49
1:B:593:SER:O	1:B:597:GLN:HG3	2.13	0.49
1:A:81:ILE:HG22	2:A:1401:3PH:C3I	2.42	0.49
1:A:467:LEU:O	1:A:471:ALA:HB3	2.13	0.49
1:A:751:ILE:HA	1:A:758:TYR:CB	2.43	0.49
1:A:1155:ALA:HB2	1:A:1173:LYS:HB2	1.93	0.49
1:B:135:PRO:HB3	1:B:441:VAL:HG22	1.95	0.49
1:B:584:LEU:HA	1:B:587:LEU:HD12	1.94	0.49
1:B:1136:PHE:O	1:B:1138:ILE:HD12	2.13	0.49
1:A:584:LEU:HA	1:A:587:LEU:HD12	1.95	0.49
1:A:641:TYR:CD1	1:A:643:TRP:CD1	3.01	0.49
1:B:467:LEU:O	1:B:471:ALA:HB3	2.13	0.48
1:B:628:VAL:CG2	1:B:632:LYS:HG2	2.43	0.48
1:B:833:LEU:HD11	1:B:837:TYR:CE2	2.48	0.48
1:A:876:LEU:HD21	1:A:1033:GLU:O	2.12	0.48
1:A:649:GLU:O	1:A:652:ILE:HG12	2.12	0.48
1:B:81:ILE:HG22	2:B:1401:3PH:C3I	2.43	0.48
1:B:751:ILE:HA	1:B:758:TYR:CB	2.44	0.48
1:B:1153:TYR:CE2	1:B:1177:GLN:HG2	2.48	0.48
1:A:613:GLN:HA	1:A:616:GLU:CG	2.44	0.48
1:A:1138:ILE:HD13	1:A:1173:LYS:HA	1.95	0.48
1:B:580:GLU:HB2	1:B:622:LYS:NZ	2.29	0.48
1:B:613:GLN:HA	1:B:616:GLU:CG	2.44	0.48
1:A:579:MET:O	1:A:583:ARG:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:VAL:CG1	1:B:81:ILE:HD11	2.43	0.48
1:B:259:SER:HB2	1:B:264:ASN:OD1	2.13	0.48
1:B:473:THR:HG22	1:B:473:THR:O	2.14	0.48
1:B:1089:ARG:O	1:B:1093:VAL:HG23	2.13	0.48
1:A:473:THR:HG22	1:A:473:THR:O	2.14	0.48
1:A:648:LEU:HA	1:A:651:LEU:HD12	1.94	0.48
1:A:795:SER:HA	1:A:799:VAL:HA	1.95	0.48
1:B:575:PHE:HE2	1:B:862:LYS:HD2	1.75	0.48
1:B:887:ARG:NH2	1:B:1062:THR:HG23	2.28	0.48
1:A:641:TYR:CD1	1:A:642:PRO:CD	2.97	0.48
1:A:1132:SER:HB2	1:A:1178:TYR:N	2.28	0.48
1:B:260:THR:O	1:B:263:GLN:HG2	2.14	0.48
1:B:1077:ILE:HG13	1:B:1078:ASP:N	2.29	0.48
1:B:1153:TYR:HB3	1:B:1158:ARG:CG	2.43	0.48
1:A:636:GLN:HA	1:A:832:GLN:HE22	1.78	0.48
1:A:1112:TRP:O	1:A:1113:THR:OG1	2.26	0.48
1:B:913:ILE:HD13	1:A:501:ILE:HD11	1.96	0.48
1:A:1141:THR:HG22	1:A:1190:ARG:O	2.13	0.48
1:B:586:MET:HE2	1:B:867:LEU:HB3	1.95	0.48
1:B:984:TYR:HD1	1:B:985:GLY:N	2.12	0.48
1:A:105:VAL:O	1:A:109:LEU:HG	2.14	0.48
1:A:1147:LEU:HD11	1:A:1150:GLY:O	2.13	0.48
1:B:902:ILE:HG12	1:A:525:ILE:CG1	2.43	0.48
1:B:1145:VAL:O	1:B:1167:ILE:HG12	2.14	0.48
1:A:1107:MET:HG2	1:A:1111:GLY:H	1.79	0.48
1:B:75:PRO:HB2	1:B:78:ILE:HD12	1.96	0.47
1:B:573:ARG:HH22	1:B:577:ASP:HB3	1.79	0.47
1:B:811:LEU:O	1:B:814:THR:HG23	2.13	0.47
1:A:819:PRO:CA	1:A:822:ILE:HD12	2.30	0.47
1:A:1077:ILE:HG13	1:A:1078:ASP:N	2.29	0.47
1:A:1089:ARG:O	1:A:1093:VAL:HG23	2.13	0.47
1:A:1160:GLU:O	1:A:1161:ILE:HD13	2.14	0.47
1:B:317:ILE:HG22	1:B:318:TRP:HD1	1.79	0.47
1:B:411:SER:HA	1:B:416:GLY:CA	2.37	0.47
1:B:494:MET:CE	1:A:926:GLU:HB3	2.44	0.47
1:B:606:GLU:CD	1:B:606:GLU:H	2.18	0.47
1:B:627:LEU:HD23	1:B:633:LYS:HE2	1.95	0.47
1:B:897:LYS:HB3	1:A:521:ALA:HB2	1.96	0.47
1:A:632:LYS:O	1:A:633:LYS:HD3	2.14	0.47
1:A:853:ILE:HD11	1:A:1107:MET:CE	2.45	0.47
1:A:984:TYR:HD1	1:A:985:GLY:N	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1002:VAL:C	1:A:1038:VAL:HG23	2.34	0.47
2:A:1402:3PH:H31	2:A:1402:3PH:C22	2.43	0.47
1:B:344:GLU:OE1	1:B:344:GLU:N	2.36	0.47
1:B:511:MET:HG3	1:A:1119:LEU:HD12	1.96	0.47
1:B:1127:VAL:HG12	1:B:1186:LEU:H	1.79	0.47
1:A:609:ARG:HA	1:A:612:VAL:HG22	1.95	0.47
1:B:885:LEU:HD12	1:B:885:LEU:O	2.14	0.47
1:A:573:ARG:HH12	1:A:577:ASP:N	2.09	0.47
1:A:1092:ARG:HG3	1:A:1096:ILE:HD12	1.96	0.47
1:A:1145:VAL:O	1:A:1167:ILE:HG12	2.14	0.47
1:B:1049:THR:C	1:B:1050:LYS:HG2	2.34	0.47
1:A:1136:PHE:O	1:A:1138:ILE:HD12	2.14	0.47
1:B:609:ARG:HA	1:B:612:VAL:HG22	1.97	0.47
1:B:853:ILE:HD11	1:B:1107:MET:HE1	1.97	0.47
1:B:1002:VAL:C	1:B:1038:VAL:HG23	2.35	0.47
1:B:105:VAL:O	1:B:109:LEU:HG	2.14	0.47
1:B:224:LYS:N	1:B:224:LYS:CD	2.70	0.47
1:B:413:ILE:HG22	1:B:414:GLY:N	2.30	0.47
1:B:521:ALA:HB2	1:A:897:LYS:HB3	1.95	0.47
1:B:628:VAL:H	1:B:632:LYS:NZ	2.08	0.47
1:B:937:LYS:HD3	1:A:530:CYS:SG	2.55	0.47
1:A:914:HIS:NE2	1:A:931:GLU:OE2	2.47	0.47
1:A:983:ASP:O	1:A:986:GLU:HG3	2.15	0.47
1:B:216:LEU:O	1:B:220:LEU:HD12	2.14	0.47
1:B:320:GLU:O	1:B:321:VAL:HG23	2.15	0.47
1:B:627:LEU:HD23	1:B:633:LYS:HZ1	1.79	0.47
1:B:1145:VAL:HG22	1:B:1188:VAL:HA	1.97	0.47
1:A:1049:THR:C	1:A:1050:LYS:HG2	2.34	0.47
1:B:372:VAL:HG13	1:B:373:THR:N	2.30	0.47
1:B:853:ILE:HG22	1:B:857:MET:HE1	1.96	0.47
1:B:902:ILE:HB	1:B:941:LEU:HD11	1.97	0.47
1:B:983:ASP:O	1:B:986:GLU:HG3	2.15	0.47
1:A:273:VAL:O	1:A:276:PRO:HD2	2.15	0.47
1:A:394:ALA:O	1:A:398:ILE:HG12	2.15	0.47
1:A:637:ILE:HG23	1:A:885:LEU:HD22	1.97	0.47
1:A:1145:VAL:CG2	1:A:1188:VAL:HG12	2.45	0.47
1:B:77:VAL:HG12	1:B:81:ILE:CD1	2.45	0.47
1:B:394:ALA:O	1:B:398:ILE:HG12	2.15	0.47
1:B:525:ILE:HD11	1:A:902:ILE:CG1	2.44	0.47
1:B:161:ARG:HB3	1:B:161:ARG:NH1	2.31	0.46
1:B:641:TYR:CD1	1:B:642:PRO:CD	2.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1092:ARG:HG3	1:B:1096:ILE:HD12	1.96	0.46
1:B:1107:MET:HG2	1:B:1111:GLY:H	1.80	0.46
1:A:372:VAL:HG13	1:A:373:THR:N	2.30	0.46
1:A:957:LEU:HD12	1:A:957:LEU:O	2.15	0.46
1:A:1131:GLU:CB	1:A:1134:PHE:HE2	2.26	0.46
1:B:957:LEU:O	1:B:957:LEU:HD12	2.16	0.46
1:B:1112:TRP:CE3	1:B:1116:LYS:HE3	2.50	0.46
1:B:1131:GLU:CB	1:B:1134:PHE:HE1	2.26	0.46
1:A:161:ARG:NH1	1:A:161:ARG:HB3	2.30	0.46
1:A:885:LEU:HD12	1:A:885:LEU:O	2.15	0.46
1:A:1145:VAL:HG22	1:A:1188:VAL:HA	1.98	0.46
1:B:68:ASP:HB3	1:A:136:HIS:NE2	2.31	0.46
1:B:861:LYS:O	1:B:862:LYS:HG2	2.15	0.46
1:B:1011:LYS:HD2	1:B:1012:SER:N	2.30	0.46
1:B:1145:VAL:CG2	1:B:1188:VAL:HG12	2.45	0.46
1:A:320:GLU:O	1:A:321:VAL:HG23	2.15	0.46
1:A:420:ARG:HB3	1:A:481:LEU:HD13	1.97	0.46
1:A:580:GLU:HB2	1:A:622:LYS:NZ	2.30	0.46
1:A:1001:ILE:O	1:A:1038:VAL:HA	2.16	0.46
1:B:751:ILE:O	1:B:755:GLY:N	2.37	0.46
1:B:922:LEU:HD23	1:B:922:LEU:HA	1.80	0.46
1:A:412:ARG:O	1:A:413:ILE:HD13	2.15	0.46
1:B:365:PHE:O	1:B:368:VAL:HG12	2.16	0.46
1:B:647:LYS:HZ1	1:B:825:VAL:HB	1.78	0.46
1:B:898:THR:CG2	1:A:525:ILE:HD13	2.44	0.46
1:B:1011:LYS:HD2	1:B:1012:SER:H	1.80	0.46
1:A:587:LEU:HD13	1:A:619:ALA:CB	2.34	0.46
1:A:628:VAL:H	1:A:632:LYS:NZ	2.07	0.46
1:A:1154:ASN:HD22	1:A:1157:THR:HG23	1.81	0.46
1:B:638:LYS:HA	1:B:638:LYS:HD3	1.59	0.46
1:B:1001:ILE:O	1:B:1038:VAL:HA	2.15	0.46
1:A:365:PHE:O	1:A:368:VAL:HG12	2.16	0.46
1:A:1127:VAL:HG12	1:A:1186:LEU:H	1.81	0.46
1:B:622:LYS:HD2	1:B:623:ASP:H	1.80	0.46
1:B:626:ILE:HB	1:B:627:LEU:HD12	1.98	0.46
1:B:896:VAL:O	1:B:900:GLN:HG2	2.16	0.46
1:A:413:ILE:HG22	1:A:414:GLY:N	2.30	0.46
1:A:579:MET:HE2	1:A:866:GLU:OE1	2.16	0.46
1:A:587:LEU:O	1:A:591:LYS:HG3	2.15	0.46
1:A:827:GLY:O	1:A:831:ASN:OD1	2.34	0.46
1:A:948:ILE:HG23	1:A:949:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:ILE:O	1:B:529:ALA:HB2	2.16	0.46
1:B:902:ILE:HG21	1:B:941:LEU:HD12	1.98	0.46
1:B:987:VAL:HG11	1:B:990:ARG:HE	1.81	0.46
1:A:517:PHE:O	1:A:518:LEU:HD12	2.16	0.46
1:B:517:PHE:O	1:B:518:LEU:HD12	2.16	0.46
1:B:634:SER:HB3	1:B:638:LYS:HZ1	1.81	0.46
1:A:216:LEU:O	1:A:220:LEU:HD12	2.16	0.46
1:A:632:LYS:HD3	1:A:633:LYS:HZ2	1.79	0.46
1:A:637:ILE:HG23	1:A:885:LEU:CD2	2.46	0.46
1:B:895:SER:O	1:B:899:ARG:HG3	2.16	0.45
1:A:893:ALA:O	1:A:897:LYS:HG3	2.16	0.45
1:A:1176:PHE:HZ	1:A:1184:PRO:HB2	1.81	0.45
1:B:273:VAL:O	1:B:276:PRO:HD2	2.15	0.45
1:A:266:LEU:HD12	1:A:266:LEU:O	2.15	0.45
1:A:638:LYS:HD3	1:A:638:LYS:HA	1.60	0.45
1:A:863:ILE:HA	1:A:866:GLU:OE1	2.15	0.45
1:A:593:SER:O	1:A:597:GLN:HG3	2.16	0.45
1:A:857:MET:O	1:A:858:VAL:HB	2.16	0.45
1:A:989:VAL:HB	1:A:1057:VAL:HG12	1.97	0.45
1:A:1153:TYR:CE2	1:A:1177:GLN:HG2	2.51	0.45
1:B:637:ILE:HG23	1:B:885:LEU:HD22	1.98	0.45
1:B:641:TYR:CD1	1:B:643:TRP:CD1	3.04	0.45
1:A:634:SER:HB3	1:A:638:LYS:HZ1	1.80	0.45
1:A:1104:MET:SD	1:A:1114:GLN:HA	2.56	0.45
1:B:993:ASP:O	1:B:1053:ARG:HG2	2.17	0.45
1:B:527:THR:HA	1:B:531:GLU:OE2	2.17	0.45
1:B:893:ALA:O	1:B:897:LYS:HG3	2.17	0.45
1:B:1166:LEU:HD23	1:B:1167:ILE:N	2.32	0.45
1:A:112:ILE:O	1:A:116:VAL:HG23	2.17	0.45
1:B:833:LEU:CD1	1:B:885:LEU:HD21	2.46	0.45
1:A:628:VAL:N	1:A:632:LYS:HD2	2.32	0.45
1:A:900:GLN:OE1	1:A:900:GLN:HA	2.17	0.45
1:A:962:TRP:CD2	1:A:1090:LEU:HD21	2.52	0.45
1:B:420:ARG:HB3	1:B:481:LEU:HD13	1.98	0.45
1:B:642:PRO:O	1:B:646:ARG:HG2	2.16	0.45
1:A:81:ILE:HG22	2:A:1401:3PH:H3I1	1.98	0.45
1:A:137:VAL:CG1	1:A:141:ILE:HD12	2.47	0.45
1:B:69:ASP:O	1:B:70:LEU:HB2	2.17	0.45
1:B:179:VAL:HA	1:B:199:MET:CE	2.47	0.45
1:B:501:ILE:HG13	1:A:913:ILE:HD11	1.99	0.45
1:B:516:ARG:HG3	1:B:517:PHE:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:892:ILE:HD12	1:B:892:ILE:H	1.81	0.45
1:A:516:ARG:HG3	1:A:517:PHE:CD1	2.52	0.45
1:A:527:THR:HA	1:A:531:GLU:OE2	2.16	0.45
1:A:646:ARG:NH1	1:A:649:GLU:OE1	2.49	0.45
1:A:895:SER:O	1:A:899:ARG:HG3	2.17	0.45
1:A:902:ILE:HB	1:A:941:LEU:HD11	1.97	0.45
1:B:81:ILE:HG22	2:B:1401:3PH:H3I1	1.99	0.45
1:B:587:LEU:O	1:B:591:LYS:HG3	2.16	0.45
1:B:632:LYS:HD3	1:B:633:LYS:NZ	2.31	0.45
1:B:897:LYS:NZ	1:A:520:ASP:OD2	2.27	0.45
1:B:970:ILE:CG2	1:B:974:LYS:HE3	2.48	0.45
1:A:516:ARG:HG3	1:A:517:PHE:N	2.32	0.45
1:A:861:LYS:O	1:A:863:ILE:HD12	2.17	0.45
1:A:970:ILE:HG22	1:A:974:LYS:HE3	2.00	0.45
1:B:821:LEU:O	1:B:825:VAL:HG23	2.17	0.44
1:B:897:LYS:HB2	1:A:521:ALA:HB2	1.99	0.44
1:A:962:TRP:CE3	1:A:963:LEU:HB3	2.52	0.44
1:A:169:LEU:HD13	1:A:410:LEU:HD23	1.99	0.44
1:B:521:ALA:HB2	1:A:897:LYS:HB2	1.98	0.44
1:B:833:LEU:HD23	1:B:892:ILE:CG2	2.47	0.44
1:B:962:TRP:CD2	1:B:1090:LEU:HD21	2.52	0.44
1:A:80:PHE:CD1	1:A:130:VAL:HG11	2.52	0.44
1:A:143:LEU:O	1:A:147:ILE:HG12	2.17	0.44
1:A:638:LYS:O	1:A:640:ILE:HD12	2.17	0.44
1:A:887:ARG:NH2	1:A:1062:THR:HG23	2.32	0.44
1:A:993:ASP:O	1:A:1053:ARG:HG2	2.17	0.44
1:B:143:LEU:O	1:B:147:ILE:HG12	2.17	0.44
1:B:1104:MET:SD	1:B:1114:GLN:HA	2.58	0.44
1:A:77:VAL:HG21	2:A:1401:3PH:H351	1.99	0.44
1:A:573:ARG:HH22	1:A:577:ASP:HB3	1.82	0.44
1:A:643:TRP:HZ3	1:A:828:LYS:HG3	1.81	0.44
1:A:1145:VAL:HB	1:A:1167:ILE:CD1	2.45	0.44
1:B:107:LEU:HD23	1:B:107:LEU:HA	1.83	0.44
1:B:143:LEU:N	1:B:144:PRO:HD2	2.32	0.44
1:A:138:LEU:HD12	1:A:142:PHE:CD2	2.51	0.44
1:A:987:VAL:HG11	1:A:990:ARG:HE	1.82	0.44
1:A:1069:THR:HG22	1:A:1071:GLU:OE1	2.18	0.44
1:A:1082:LEU:HG	1:A:1083:TYR:N	2.32	0.44
1:B:913:ILE:HD11	1:A:501:ILE:HG13	2.00	0.44
1:A:179:VAL:HA	1:A:199:MET:HE1	1.99	0.44
1:A:343:PRO:O	1:A:347:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:PRO:O	1:B:347:VAL:HG23	2.17	0.44
1:B:857:MET:O	1:B:858:VAL:HB	2.16	0.44
1:A:143:LEU:N	1:A:144:PRO:HD2	2.32	0.44
1:A:632:LYS:HD3	1:A:633:LYS:NZ	2.33	0.44
1:A:913:ILE:HD12	1:A:930:LEU:CD1	2.48	0.44
1:A:1074:ASN:O	1:A:1077:ILE:HG13	2.18	0.44
1:B:608:LEU:O	1:B:612:VAL:HG22	2.18	0.44
1:B:613:GLN:HA	1:B:616:GLU:HG3	2.00	0.44
1:B:614:HIS:HA	1:B:617:VAL:HG12	2.00	0.44
1:B:970:ILE:HG22	1:B:974:LYS:HE3	1.99	0.44
1:A:923:ASP:CG	1:A:926:GLU:HG2	2.39	0.44
1:B:137:VAL:CG1	1:B:141:ILE:HD12	2.47	0.44
1:B:525:ILE:CG2	1:B:529:ALA:HB2	2.48	0.44
1:B:647:LYS:HB2	1:B:647:LYS:HE2	1.55	0.44
1:B:795:SER:HA	1:B:799:VAL:HA	1.98	0.44
1:B:898:THR:HG22	1:B:902:ILE:HD11	2.00	0.44
1:B:962:TRP:CE3	1:B:963:LEU:HB3	2.52	0.44
1:A:626:ILE:HB	1:A:627:LEU:HD12	1.99	0.44
1:B:283:ALA:HA	1:B:286:THR:HG22	2.00	0.43
1:B:1009:TYR:HD1	1:B:1033:GLU:CG	2.31	0.43
1:B:1142:LEU:HA	1:B:1190:ARG:HG2	1.99	0.43
1:A:179:VAL:HA	1:A:199:MET:CE	2.48	0.43
1:A:284:LYS:HA	1:A:284:LYS:HD2	1.75	0.43
1:A:902:ILE:HG21	1:A:941:LEU:HD12	2.00	0.43
1:A:1149:ASN:HA	1:A:1163:SER:CB	2.48	0.43
1:B:191:TYR:CE1	1:B:454:LYS:HE3	2.53	0.43
1:B:594:TYR:O	1:B:603:LEU:HD23	2.18	0.43
1:B:1095:ALA:HB1	1:B:1148:ILE:HG13	2.00	0.43
1:B:1160:GLU:C	1:B:1161:ILE:HD13	2.37	0.43
1:A:997:GLY:HA3	1:A:1067:PHE:CE1	2.53	0.43
1:B:169:LEU:HD13	1:B:410:LEU:HD23	2.00	0.43
1:B:516:ARG:HG3	1:B:517:PHE:N	2.33	0.43
1:B:853:ILE:HD11	1:B:1107:MET:CE	2.48	0.43
1:B:853:ILE:HG23	1:B:1109:PHE:CE1	2.53	0.43
1:B:902:ILE:CG1	1:A:525:ILE:HD11	2.47	0.43
1:B:1074:ASN:O	1:B:1077:ILE:HG13	2.17	0.43
1:A:263:GLN:HG2	1:A:264:ASN:N	2.33	0.43
1:A:283:ALA:HA	1:A:286:THR:HG22	2.00	0.43
1:A:1127:VAL:HG11	1:A:1186:LEU:HB2	2.01	0.43
1:B:179:VAL:CG2	1:B:199:MET:HE1	2.45	0.43
1:B:1009:TYR:HD1	1:B:1033:GLU:HG2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1082:LEU:HG	1:B:1083:TYR:N	2.33	0.43
1:A:588:LYS:HA	1:A:591:LYS:HD2	2.00	0.43
1:A:613:GLN:HA	1:A:616:GLU:HG3	2.00	0.43
1:A:1138:ILE:HA	1:A:1142:LEU:CD2	2.29	0.43
1:B:594:TYR:HB3	1:B:603:LEU:CD2	2.48	0.43
1:B:607:ALA:CB	1:B:839:VAL:HG22	2.49	0.43
1:B:221:GLY:HA2	1:B:224:LYS:HZ3	1.82	0.43
1:B:497:ALA:O	1:B:501:ILE:HG12	2.18	0.43
1:B:1142:LEU:O	1:B:1143:GLU:HB2	2.19	0.43
1:B:1162:ARG:HD3	1:B:1162:ARG:N	2.23	0.43
1:A:635:TRP:O	1:A:638:LYS:HB2	2.19	0.43
1:A:868:LYS:HA	1:A:871:SER:OG	2.19	0.43
1:B:137:VAL:HG13	1:B:141:ILE:CD1	2.49	0.43
1:B:310:LEU:HG	1:A:82:SER:HB2	2.01	0.43
1:B:637:ILE:HG23	1:B:885:LEU:CD2	2.49	0.43
1:B:645:LYS:HG3	1:B:648:LEU:HD21	1.99	0.43
1:B:962:TRP:HE3	1:B:1086:LEU:HD11	1.84	0.43
1:B:1127:VAL:CG1	1:B:1186:LEU:H	2.32	0.43
1:B:1176:PHE:CZ	1:B:1184:PRO:HB2	2.52	0.43
1:A:76:LYS:O	1:A:79:VAL:HG12	2.18	0.43
1:A:525:ILE:O	1:A:529:ALA:HB2	2.18	0.43
1:B:294:PHE:HE1	1:B:939:LYS:HG2	1.84	0.43
1:B:579:MET:HE2	1:B:579:MET:N	2.34	0.43
1:A:647:LYS:HB2	1:A:647:LYS:HE2	1.55	0.43
1:A:970:ILE:CG2	1:A:974:LYS:HE3	2.48	0.43
1:A:1129:LEU:O	1:A:1129:LEU:HD23	2.19	0.43
1:B:80:PHE:CE1	1:B:130:VAL:HG11	2.54	0.43
1:B:82:SER:HB2	1:A:310:LEU:HG	2.00	0.43
1:B:122:LEU:HD23	1:B:122:LEU:HA	1.86	0.43
1:B:1083:TYR:HB3	1:B:1084:PRO:HD3	2.00	0.43
1:B:1132:SER:HB2	1:B:1178:TYR:N	2.33	0.43
1:B:1174:LEU:O	1:B:1174:LEU:HD23	2.18	0.43
1:A:69:ASP:O	1:A:70:LEU:HB2	2.18	0.43
1:A:191:TYR:CE1	1:A:454:LYS:HE3	2.53	0.43
1:A:614:HIS:HA	1:A:617:VAL:HG12	2.00	0.43
1:B:976:ARG:HB2	1:B:976:ARG:HH11	1.83	0.42
1:A:916:LEU:HD23	1:A:916:LEU:HA	1.81	0.42
1:A:1074:ASN:HA	1:A:1077:ILE:CG1	2.46	0.42
1:B:136:HIS:NE2	1:A:68:ASP:HB3	2.34	0.42
1:A:297:ALA:O	1:A:301:ILE:HD12	2.19	0.42
1:A:645:LYS:HE3	1:A:646:ARG:HH22	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:833:LEU:CD1	1:A:885:LEU:HD21	2.45	0.42
1:A:1074:ASN:CA	1:A:1077:ILE:HG12	2.47	0.42
1:B:960:VAL:O	1:B:964:ALA:HB2	2.19	0.42
1:B:1069:THR:HG22	1:B:1071:GLU:OE1	2.19	0.42
1:B:1074:ASN:CA	1:B:1077:ILE:HG12	2.47	0.42
1:B:1189:VAL:HG12	1:B:1190:ARG:N	2.34	0.42
1:A:225:GLN:NE2	1:A:415:TYR:OH	2.47	0.42
1:A:579:MET:CE	1:A:863:ILE:HG23	2.49	0.42
1:A:636:GLN:O	1:A:832:GLN:NE2	2.52	0.42
1:A:646:ARG:HA	1:A:646:ARG:HD3	1.90	0.42
1:B:583:ARG:HH21	1:B:624:GLN:N	2.10	0.42
1:B:1127:VAL:HG11	1:B:1186:LEU:HB2	2.01	0.42
1:B:1135:GLN:CD	1:B:1173:LYS:HG3	2.40	0.42
1:A:113:LEU:HD23	1:A:113:LEU:O	2.20	0.42
1:A:603:LEU:HD12	1:A:603:LEU:O	2.20	0.42
1:A:1145:VAL:HG22	1:A:1188:VAL:HG12	2.01	0.42
1:B:112:ILE:O	1:B:116:VAL:HG23	2.18	0.42
1:A:294:PHE:HE1	1:A:939:LYS:HG2	1.84	0.42
1:A:628:VAL:CG2	1:A:632:LYS:HG2	2.48	0.42
1:A:1083:TYR:HB3	1:A:1084:PRO:HD3	2.00	0.42
1:B:297:ALA:O	1:B:301:ILE:HD12	2.19	0.42
1:A:960:VAL:O	1:A:964:ALA:HB2	2.19	0.42
1:A:991:GLU:OE1	1:A:991:GLU:HA	2.18	0.42
1:A:1184:PRO:C	1:A:1185:ARG:HD2	2.40	0.42
1:B:868:LYS:HA	1:B:871:SER:OG	2.20	0.42
1:B:948:ILE:CG2	1:B:949:PRO:HD2	2.47	0.42
1:A:962:TRP:HE3	1:A:1086:LEU:HD11	1.84	0.42
1:A:976:ARG:HB2	1:A:976:ARG:HH11	1.82	0.42
1:A:1166:LEU:HD23	1:A:1167:ILE:N	2.34	0.42
1:B:138:LEU:HD12	1:B:142:PHE:CD2	2.52	0.42
1:A:257:LEU:HD12	1:A:258:THR:N	2.34	0.42
1:A:853:ILE:HG23	1:A:1109:PHE:CE1	2.54	0.42
1:B:957:LEU:HD21	1:B:973:ILE:HG22	2.02	0.42
1:A:1142:LEU:O	1:A:1143:GLU:HB2	2.20	0.42
1:A:1153:TYR:HB3	1:A:1158:ARG:HG3	2.02	0.42
1:B:902:ILE:HG13	1:B:902:ILE:H	1.70	0.42
1:B:1061:THR:HG22	1:B:1062:THR:N	2.35	0.42
1:A:621:GLU:HB3	1:A:624:GLN:OE1	2.19	0.42
1:A:838:ASP:OD1	1:A:838:ASP:N	2.53	0.42
1:B:498:VAL:HG11	1:B:534:ASP:CB	2.50	0.41
1:B:585:ARG:HA	1:B:585:ARG:HD2	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:954:GLU:OE1	1:B:974:LYS:HG2	2.20	0.41
1:B:991:GLU:OE1	1:B:991:GLU:HA	2.19	0.41
1:B:113:LEU:HD23	1:B:113:LEU:O	2.20	0.41
1:B:645:LYS:HB3	1:B:646:ARG:HH21	1.85	0.41
1:A:862:LYS:HG3	1:A:863:ILE:HD12	2.02	0.41
1:A:1189:VAL:HG12	1:A:1190:ARG:N	2.35	0.41
1:B:263:GLN:HG3	1:B:264:ASN:N	2.34	0.41
1:B:284:LYS:HD2	1:B:284:LYS:HA	1.75	0.41
1:B:849:GLU:O	1:B:853:ILE:HG12	2.20	0.41
1:B:1138:ILE:HD13	1:B:1173:LYS:HA	2.02	0.41
1:A:85:CYS:SG	1:A:359:LEU:HD21	2.60	0.41
1:A:122:LEU:HA	1:A:122:LEU:HD23	1.85	0.41
1:A:179:VAL:CG2	1:A:199:MET:HE1	2.45	0.41
1:A:608:LEU:O	1:A:612:VAL:HG22	2.21	0.41
1:A:641:TYR:CD1	1:A:642:PRO:N	2.89	0.41
1:A:817:LEU:HD21	1:A:821:LEU:HD12	2.01	0.41
1:A:864:LEU:HA	1:A:867:LEU:CD1	2.50	0.41
1:B:85:CYS:SG	1:B:359:LEU:HD21	2.60	0.41
1:B:169:LEU:HD12	1:B:169:LEU:HA	1.85	0.41
1:B:359:LEU:HD23	1:B:359:LEU:HA	1.92	0.41
1:B:530:CYS:HB3	1:A:937:LYS:CD	2.38	0.41
1:B:863:ILE:HG23	1:B:866:GLU:OE1	2.20	0.41
1:B:997:GLY:HA3	1:B:1067:PHE:CE1	2.55	0.41
1:A:844:ILE:HD12	1:A:879:VAL:HG23	2.01	0.41
1:A:896:VAL:O	1:A:900:GLN:HG2	2.19	0.41
1:A:1009:TYR:HD1	1:A:1033:GLU:CG	2.31	0.41
1:B:107:LEU:CD2	1:B:368:VAL:HG13	2.48	0.41
1:B:584:LEU:HA	1:B:587:LEU:HG	2.02	0.41
1:B:838:ASP:OD1	1:B:838:ASP:N	2.52	0.41
1:B:1138:ILE:HD12	1:B:1138:ILE:N	2.35	0.41
1:A:188:LEU:HG	1:A:189:PHE:HD1	1.84	0.41
1:A:341:ILE:H	1:A:341:ILE:HG13	1.76	0.41
1:A:824:VAL:HG13	1:A:825:VAL:N	2.36	0.41
1:A:1042:ILE:HG22	1:A:1043:GLY:N	2.35	0.41
1:B:525:ILE:HG23	1:B:529:ALA:HB2	2.02	0.41
1:A:628:VAL:N	1:A:632:LYS:HZ2	2.07	0.41
1:A:999:PHE:O	1:A:1041:VAL:HA	2.20	0.41
1:A:1148:ILE:HD13	1:A:1148:ILE:HA	1.94	0.41
1:A:833:LEU:HD12	1:A:833:LEU:O	2.20	0.41
1:B:621:GLU:HB3	1:B:624:GLN:OE1	2.20	0.41
1:B:834:SER:OG	1:B:835:LEU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1042:ILE:HG22	1:B:1043:GLY:N	2.35	0.41
1:A:107:LEU:HD23	1:A:107:LEU:HA	1.82	0.41
1:A:921:LEU:HD12	1:A:921:LEU:N	2.36	0.41
1:A:999:PHE:HB2	1:A:1042:ILE:HB	2.03	0.41
1:A:1037:THR:OG1	1:A:1038:VAL:N	2.54	0.41
1:B:412:ARG:C	1:B:413:ILE:HD13	2.42	0.41
1:B:819:PRO:O	1:B:823:LEU:HD13	2.21	0.41
1:B:844:ILE:HD12	1:B:879:VAL:HG23	2.01	0.41
1:B:863:ILE:HA	1:B:866:GLU:OE1	2.21	0.41
1:B:999:PHE:HB2	1:B:1042:ILE:HB	2.03	0.41
1:A:584:LEU:HA	1:A:587:LEU:HG	2.03	0.41
1:A:1097:ARG:HH11	1:A:1097:ARG:HG3	1.86	0.41
1:A:1137:ASN:OD1	1:A:1139:ASP:HB3	2.20	0.41
1:B:579:MET:CE	1:B:863:ILE:HG12	2.51	0.41
1:B:590:GLU:HB3	1:B:594:TYR:CZ	2.55	0.41
1:B:880:LYS:NZ	1:B:1060:GLU:OE1	2.39	0.41
1:B:999:PHE:O	1:B:1041:VAL:HA	2.20	0.41
1:A:647:LYS:HD3	1:A:822:ILE:HG23	2.02	0.41
1:A:922:LEU:HA	1:A:922:LEU:HD23	1.79	0.41
1:A:973:ILE:HD13	1:A:973:ILE:HA	1.99	0.41
1:B:588:LYS:HA	1:B:591:LYS:HD2	2.01	0.40
1:B:962:TRP:CE3	1:B:1086:LEU:HD11	2.56	0.40
1:B:1141:THR:HG23	1:A:1169:ARG:HH11	1.86	0.40
1:B:1148:ILE:HD13	1:B:1148:ILE:HA	1.93	0.40
1:A:68:ASP:OD1	1:A:68:ASP:N	2.54	0.40
1:A:131:ALA:O	1:A:132[A]:HIS:ND1	2.55	0.40
1:A:867:LEU:HD12	1:A:867:LEU:H	1.86	0.40
1:A:954:GLU:OE1	1:A:974:LYS:HG2	2.22	0.40
1:A:995:SER:HA	1:A:1053:ARG:NH2	2.36	0.40
1:A:1061:THR:HG22	1:A:1062:THR:N	2.35	0.40
1:B:530:CYS:SG	1:A:906:LEU:HD11	2.61	0.40
1:B:1097:ARG:HH11	1:B:1097:ARG:HG3	1.87	0.40
1:A:990:ARG:CZ	1:A:990:ARG:HB2	2.51	0.40
1:A:816:ALA:C	1:A:819:PRO:HD2	2.42	0.40
1:A:819:PRO:O	1:A:823:LEU:HD13	2.21	0.40
1:A:892:ILE:H	1:A:892:ILE:HD12	1.86	0.40
1:B:356:LEU:HD23	1:B:356:LEU:HA	1.92	0.40
1:B:512:LEU:HD13	1:B:512:LEU:HA	1.97	0.40
1:B:634:SER:HB3	1:B:638:LYS:NZ	2.36	0.40
1:B:816:ALA:C	1:B:819:PRO:HD2	2.41	0.40
1:B:995:SER:HA	1:B:1053:ARG:NH2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1129:LEU:HD23	1:B:1129:LEU:O	2.21	0.40
1:B:1138:ILE:H	1:A:1172:HIS:CE1	2.40	0.40
1:B:1153:TYR:HB3	1:B:1158:ARG:HG3	2.03	0.40
1:A:498:VAL:HG11	1:A:534:ASP:CB	2.51	0.40
1:A:957:LEU:HD11	1:A:973:ILE:HG21	2.04	0.40
1:A:1138:ILE:HD12	1:A:1138:ILE:N	2.36	0.40
1:A:1155:ALA:HB2	1:A:1173:LYS:CB	2.51	0.40
1:B:586:MET:CE	1:B:867:LEU:HB3	2.52	0.40
1:B:641:TYR:O	1:B:643:TRP:N	2.55	0.40
1:B:972:PHE:O	1:B:976:ARG:NH1	2.54	0.40
1:A:1095:ALA:HB1	1:A:1148:ILE:HG13	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	1047/1331 (79%)	982 (94%)	65 (6%)	0	100	100
1	B	1047/1331 (79%)	985 (94%)	62 (6%)	0	100	100
All	All	2094/2662 (79%)	1967 (94%)	127 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	781/1138 (69%)	749 (96%)	32 (4%)	30	62
1	B	781/1138 (69%)	755 (97%)	26 (3%)	38	68
All	All	1562/2276 (69%)	1504 (96%)	58 (4%)	37	65

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	97	LYS
1	B	118	SER
1	B	154	MET
1	B	199	MET
1	B	219	ASP
1	B	251	MET
1	B	268	PHE
1	B	410	LEU
1	B	490	LYS
1	B	500	ARG
1	B	574	GLU
1	B	575	PHE
1	B	595	TRP
1	B	605	ARG
1	B	624	GLN
1	B	627	LEU
1	B	837	TYR
1	B	859	ASP
1	B	895	SER
1	B	967	MET
1	B	980	LEU
1	B	984	TYR
1	B	1066	TYR
1	B	1129	LEU
1	B	1160	GLU
1	B	1162	ARG
1	A	97	LYS
1	A	118	SER
1	A	129	ASP
1	A	154	MET
1	A	199	MET
1	A	219	ASP
1	A	251	MET
1	A	263	GLN
1	A	268	PHE

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Mol	Chain	Res	Type
1	A	410	LEU
1	A	490	LYS
1	A	500	ARG
1	A	524	ASP
1	A	574	GLU
1	A	575	PHE
1	A	605	ARG
1	A	624	GLN
1	A	627	LEU
1	A	630	ASP
1	A	635	TRP
1	A	831	ASN
1	A	837	TYR
1	A	859	ASP
1	A	867	LEU
1	A	895	SER
1	A	967	MET
1	A	984	TYR
1	A	1066	TYR
1	A	1116	LYS
1	A	1156	HIS
1	A	1160	GLU
1	A	1162	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	256	GLN
1	B	955	ASN
1	B	1156	HIS
1	A	256	GLN
1	A	614	HIS
1	A	832	GLN
1	A	955	ASN
1	A	1135	GLN
1	A	1149	ASN
1	A	1154	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	3PH	A	1402	-	44,44,47	0.65	1 (2%)	48,49,52	0.61	1 (2%)
2	3PH	B	1401	-	47,47,47	0.62	1 (2%)	51,52,52	0.61	1 (1%)
2	3PH	B	1402	-	44,44,47	0.65	1 (2%)	48,49,52	0.60	1 (2%)
2	3PH	A	1401	-	47,47,47	0.63	1 (2%)	51,52,52	0.61	1 (1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	3PH	A	1402	-	-	17/46/46/49	-
2	3PH	B	1401	-	-	22/49/49/49	-
2	3PH	B	1402	-	-	17/46/46/49	-
2	3PH	A	1401	-	-	22/49/49/49	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1401	3PH	P-O11	3.29	1.70	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1402	3PH	P-O11	3.26	1.70	1.60
2	B	1401	3PH	P-O11	3.26	1.70	1.60
2	B	1402	3PH	P-O11	3.25	1.70	1.60

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1401	3PH	O13-P-O11	-2.16	100.99	106.73
2	A	1402	3PH	O13-P-O11	-2.16	100.99	106.73
2	A	1401	3PH	O13-P-O11	-2.15	101.00	106.73
2	B	1402	3PH	O13-P-O11	-2.14	101.04	106.73

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1401	3PH	C1-O11-P-O13
2	B	1401	3PH	C1-O11-P-O14
2	B	1401	3PH	O11-C1-C2-O21
2	B	1401	3PH	O22-C21-O21-C2
2	B	1402	3PH	C1-O11-P-O13
2	B	1402	3PH	C1-O11-P-O14
2	B	1402	3PH	C22-C21-O21-C2
2	A	1401	3PH	C1-O11-P-O13
2	A	1401	3PH	C1-O11-P-O14
2	A	1401	3PH	O22-C21-O21-C2
2	A	1401	3PH	C22-C21-O21-C2
2	A	1402	3PH	C1-O11-P-O13
2	A	1402	3PH	C1-O11-P-O14
2	A	1402	3PH	C22-C21-O21-C2
2	B	1402	3PH	O32-C31-O31-C3
2	A	1402	3PH	O32-C31-O31-C3
2	B	1402	3PH	O22-C21-O21-C2
2	A	1402	3PH	O22-C21-O21-C2
2	B	1402	3PH	C32-C31-O31-C3
2	A	1402	3PH	C32-C31-O31-C3
2	B	1401	3PH	C22-C21-O21-C2
2	B	1401	3PH	C32-C31-O31-C3
2	A	1401	3PH	C32-C31-O31-C3
2	B	1401	3PH	O32-C31-O31-C3
2	A	1401	3PH	O32-C31-O31-C3
2	A	1401	3PH	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
2	B	1401	3PH	C21-C22-C23-C24
2	B	1402	3PH	C21-C22-C23-C24
2	A	1402	3PH	C21-C22-C23-C24
2	B	1402	3PH	C38-C39-C3A-C3B
2	A	1401	3PH	C29-C2A-C2B-C2C
2	A	1402	3PH	C38-C39-C3A-C3B
2	B	1402	3PH	C3-C2-O21-C21
2	A	1402	3PH	C3-C2-O21-C21
2	B	1401	3PH	C29-C2A-C2B-C2C
2	B	1401	3PH	C32-C33-C34-C35
2	A	1401	3PH	C32-C33-C34-C35
2	B	1401	3PH	C33-C34-C35-C36
2	B	1401	3PH	C3B-C3C-C3D-C3E
2	A	1401	3PH	C3B-C3C-C3D-C3E
2	B	1401	3PH	C36-C37-C38-C39
2	B	1402	3PH	C2B-C2C-C2D-C2E
2	A	1401	3PH	C36-C37-C38-C39
2	A	1401	3PH	O11-C1-C2-O21
2	A	1402	3PH	C2B-C2C-C2D-C2E
2	A	1401	3PH	C33-C34-C35-C36
2	B	1401	3PH	O11-C1-C2-C3
2	B	1401	3PH	C2-C1-O11-P
2	A	1401	3PH	O11-C1-C2-C3
2	B	1402	3PH	C22-C23-C24-C25
2	A	1402	3PH	C22-C23-C24-C25
2	A	1401	3PH	C2-C1-O11-P
2	B	1401	3PH	C3D-C3E-C3F-C3G
2	A	1401	3PH	C3D-C3E-C3F-C3G
2	A	1401	3PH	C34-C35-C36-C37
2	B	1401	3PH	C34-C35-C36-C37
2	B	1402	3PH	C31-C32-C33-C34
2	A	1402	3PH	C31-C32-C33-C34
2	B	1402	3PH	O21-C2-C3-O31
2	A	1402	3PH	O21-C2-C3-O31
2	B	1401	3PH	C25-C26-C27-C28
2	B	1401	3PH	C2C-C2D-C2E-C2F
2	A	1402	3PH	C28-C29-C2A-C2B
2	B	1402	3PH	C28-C29-C2A-C2B
2	A	1401	3PH	C2C-C2D-C2E-C2F
2	A	1401	3PH	C3F-C3G-C3H-C3I
2	A	1401	3PH	C25-C26-C27-C28
2	B	1401	3PH	C3C-C3D-C3E-C3F

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Mol	Chain	Res	Type	Atoms
2	B	1401	3PH	C3F-C3G-C3H-C3I
2	B	1402	3PH	C33-C34-C35-C36
2	B	1401	3PH	C1-O11-P-O12
2	A	1402	3PH	C33-C34-C35-C36
2	A	1401	3PH	C27-C28-C29-C2A
2	B	1402	3PH	C1-C2-C3-O31
2	A	1402	3PH	C1-C2-C3-O31
2	A	1401	3PH	C3C-C3D-C3E-C3F
2	A	1402	3PH	O31-C31-C32-C33
2	B	1402	3PH	O31-C31-C32-C33

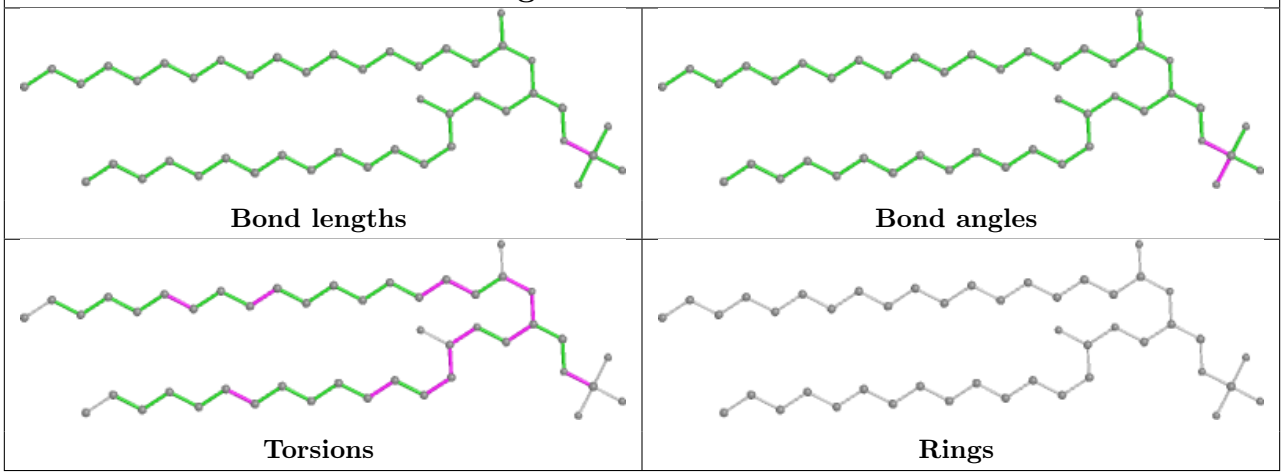
There are no ring outliers.

4 monomers are involved in 20 short contacts:

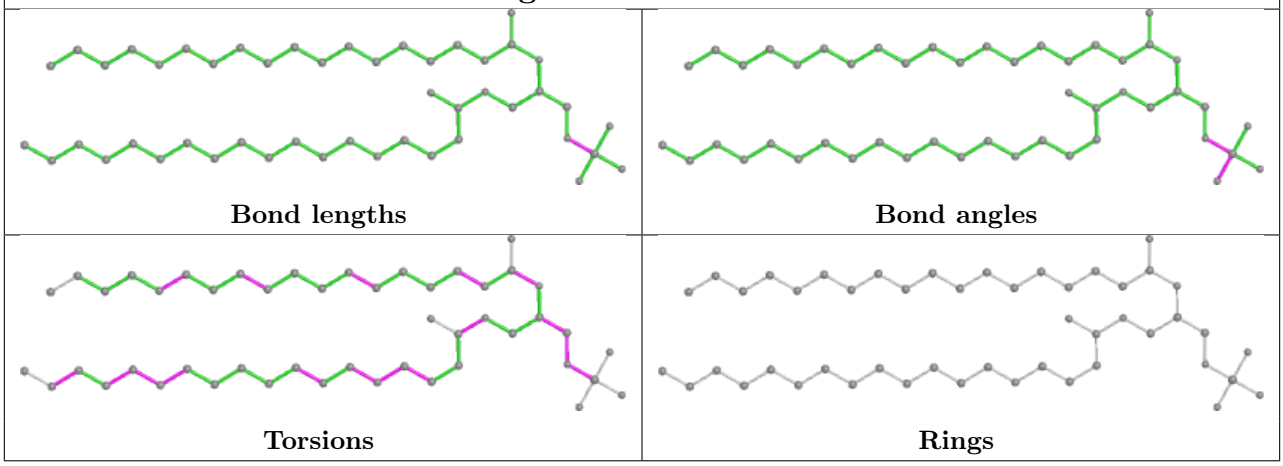
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1402	3PH	6	0
2	B	1401	3PH	4	0
2	B	1402	3PH	5	0
2	A	1401	3PH	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

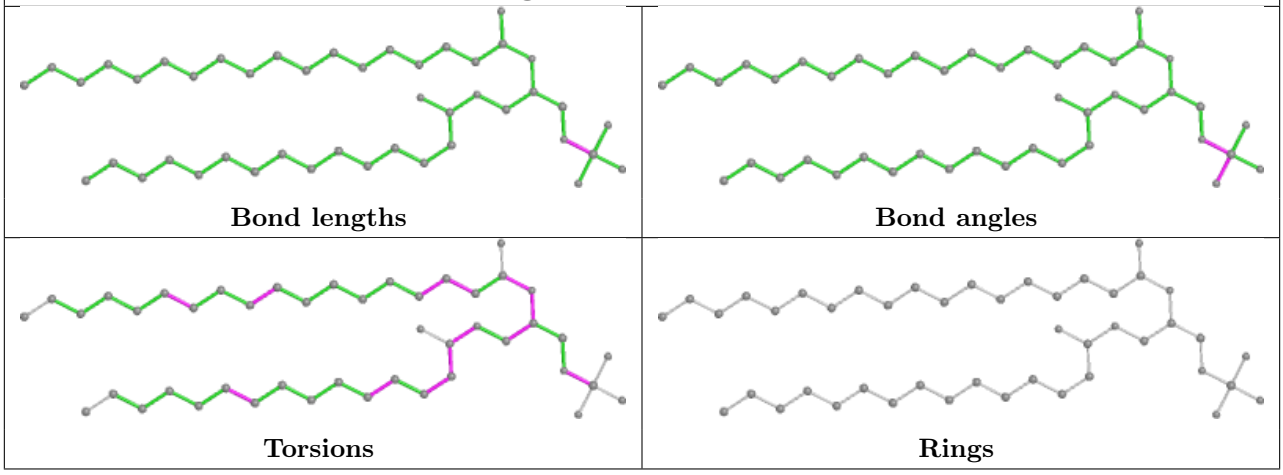
Ligand 3PH A 1402

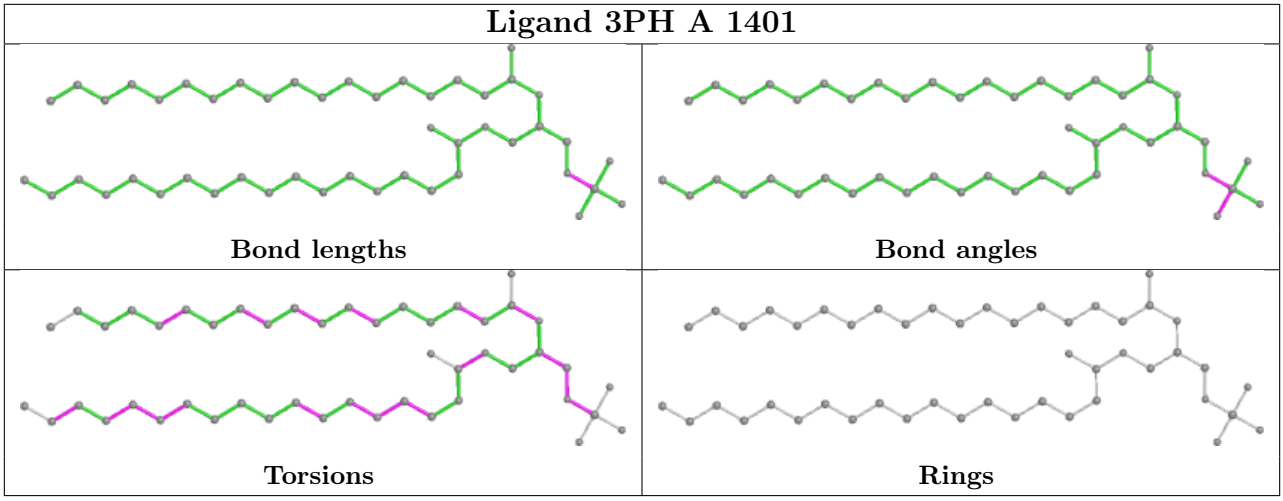


Ligand 3PH B 1401



Ligand 3PH B 1402





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.

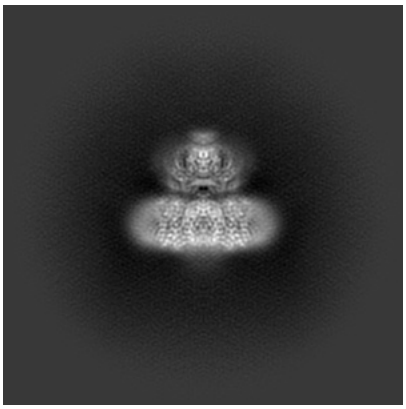
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17186. These allow visual inspection of the internal detail of the map and identification of artifacts.

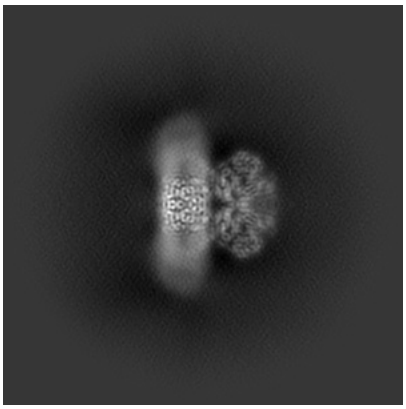
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

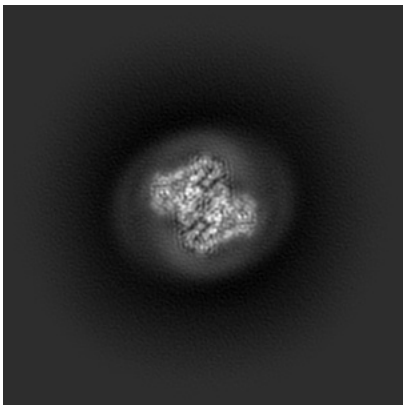
6.1.1 Primary map



X

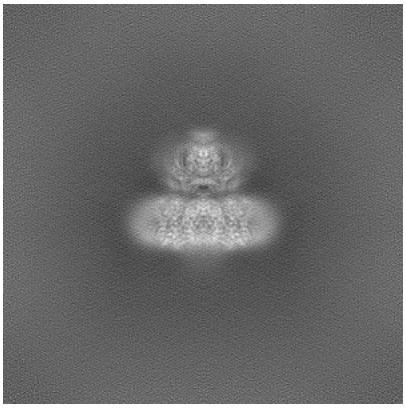


Y

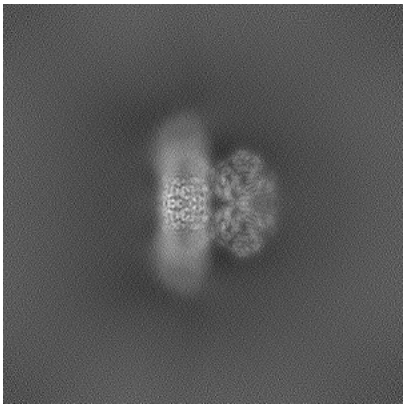


Z

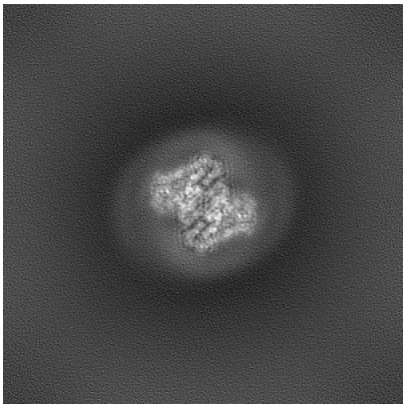
6.1.2 Raw map



X



Y

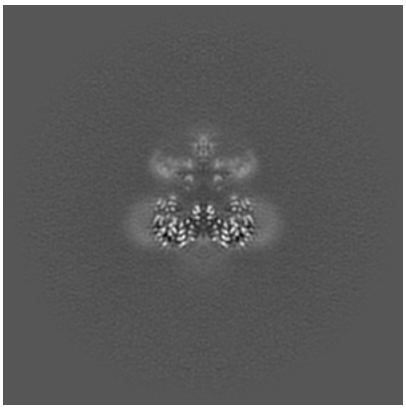


Z

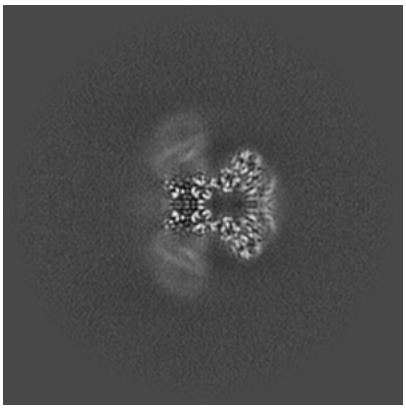
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

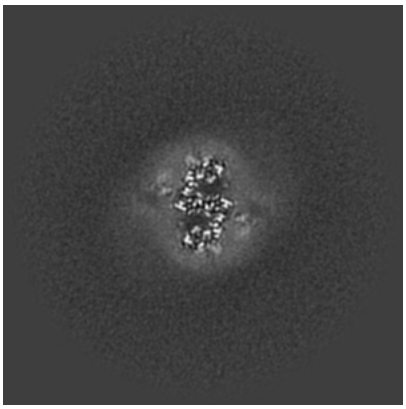
6.2.1 Primary map



X Index: 200

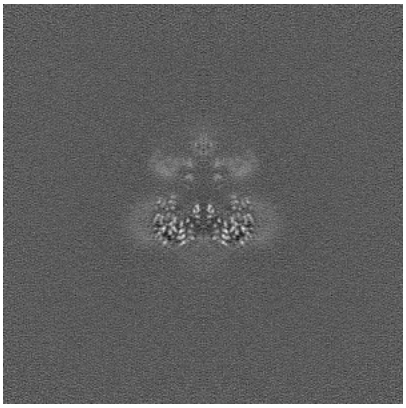


Y Index: 200

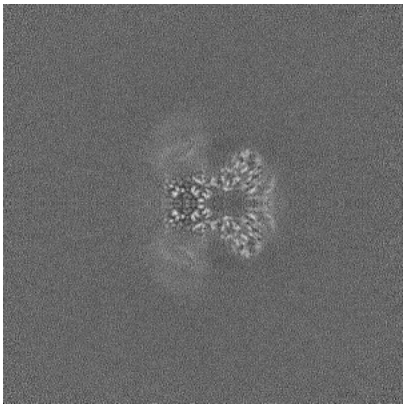


Z Index: 200

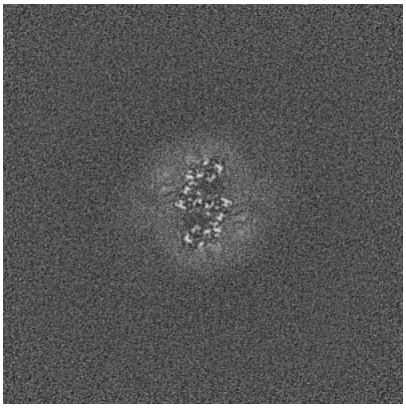
6.2.2 Raw map



X Index: 200



Y Index: 200

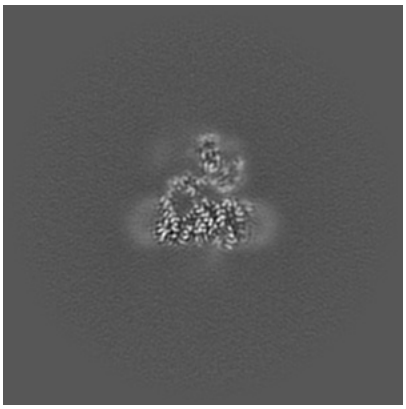


Z Index: 200

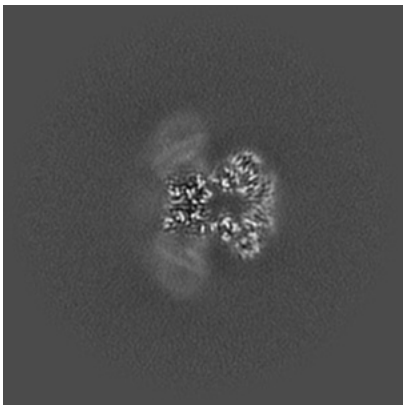
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

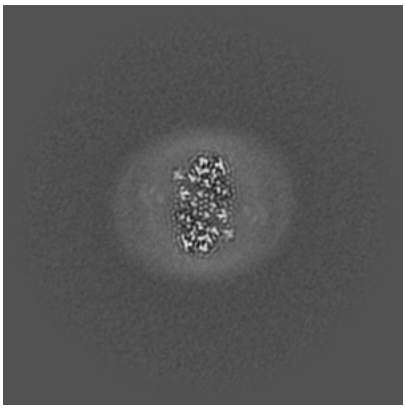
6.3.1 Primary map



X Index: 187

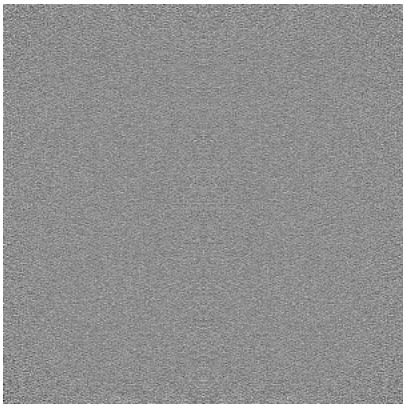


Y Index: 198

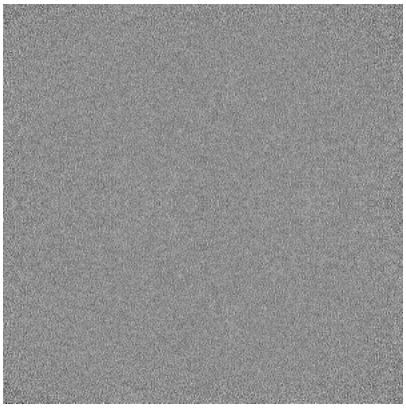


Z Index: 170

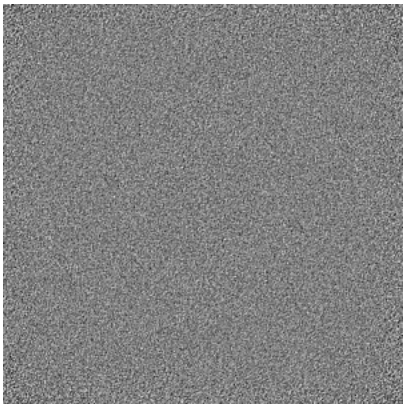
6.3.2 Raw map



X Index: 0



Y Index: 0

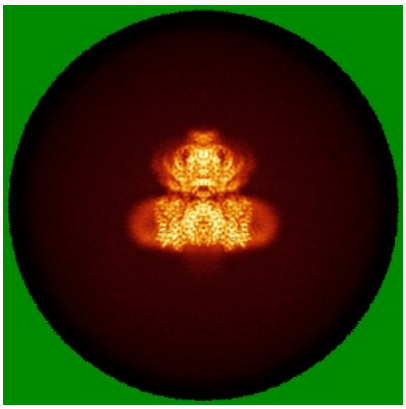


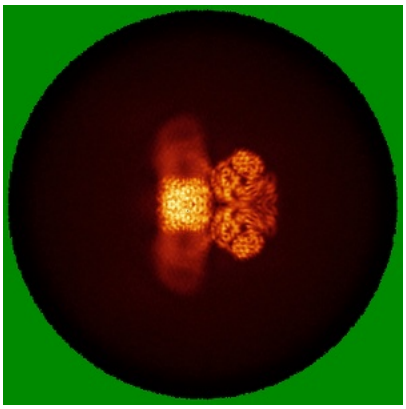
Z Index: 399

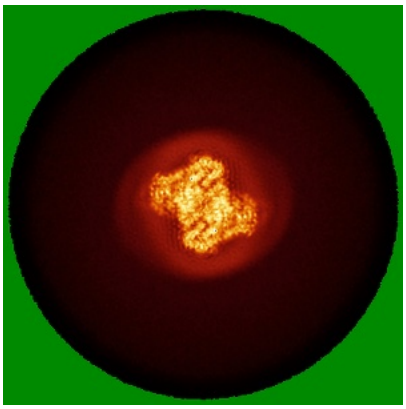
The images above show the largest variance slices of the map in three orthogonal directions.

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

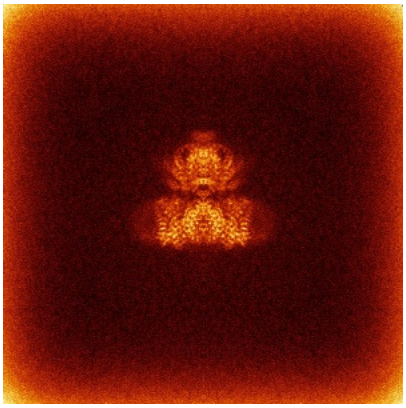
6.4.1 Primary map

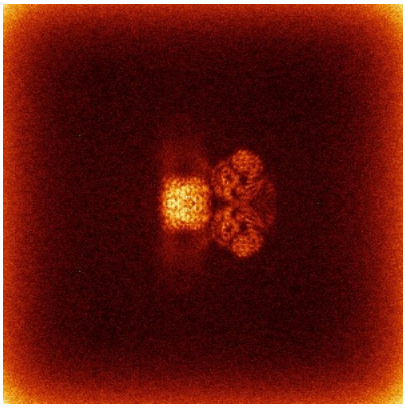

X

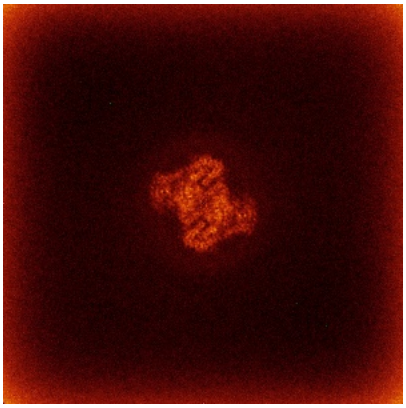

Y


Z

6.4.2 Raw map


X

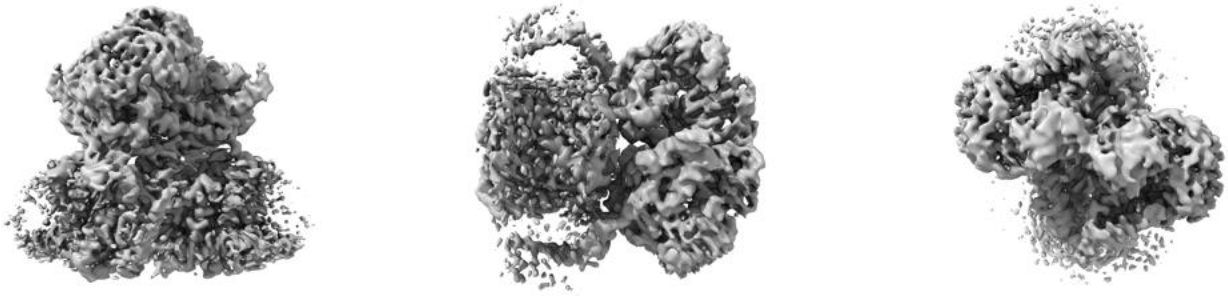

Y


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)

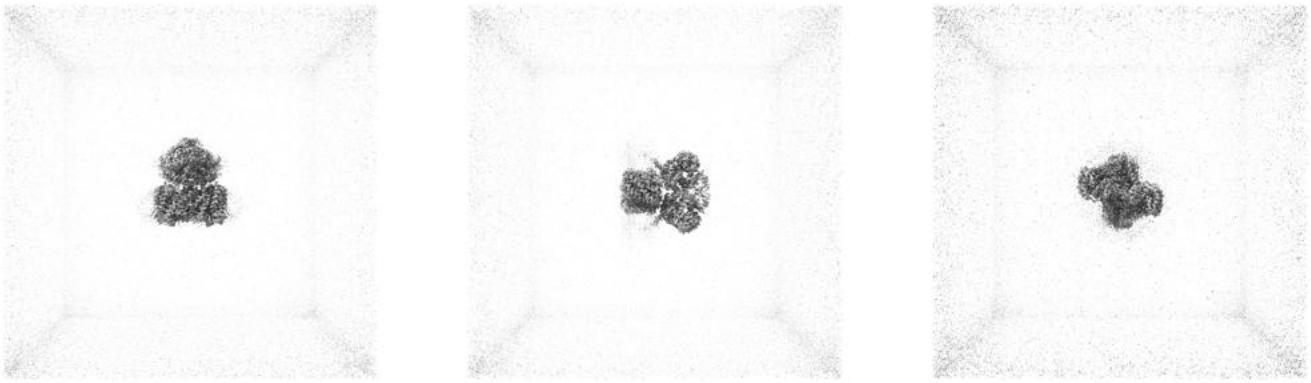
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.11. 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.

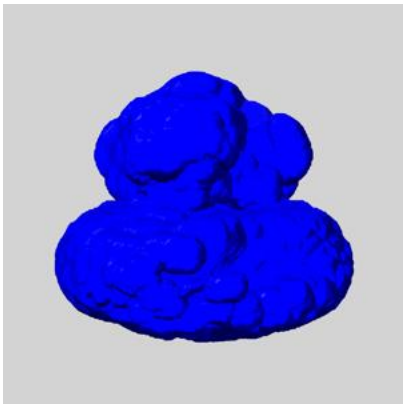
6.6 Mask visualisation (i)

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

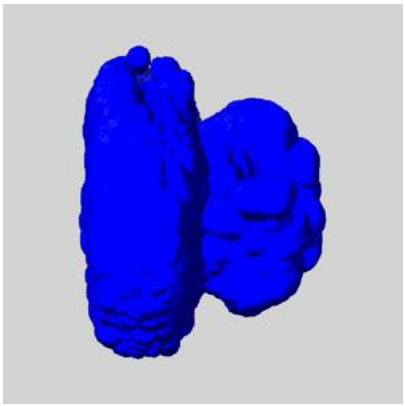
A mask typically either:

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

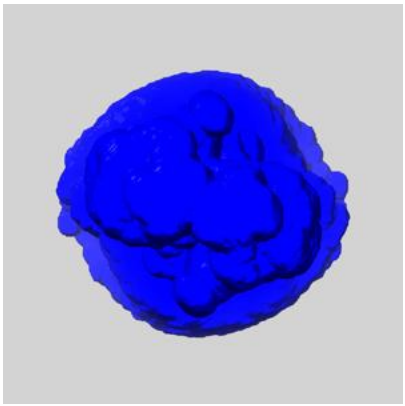
6.6.1 emd_17186_msk_1.map (i)



X



Y

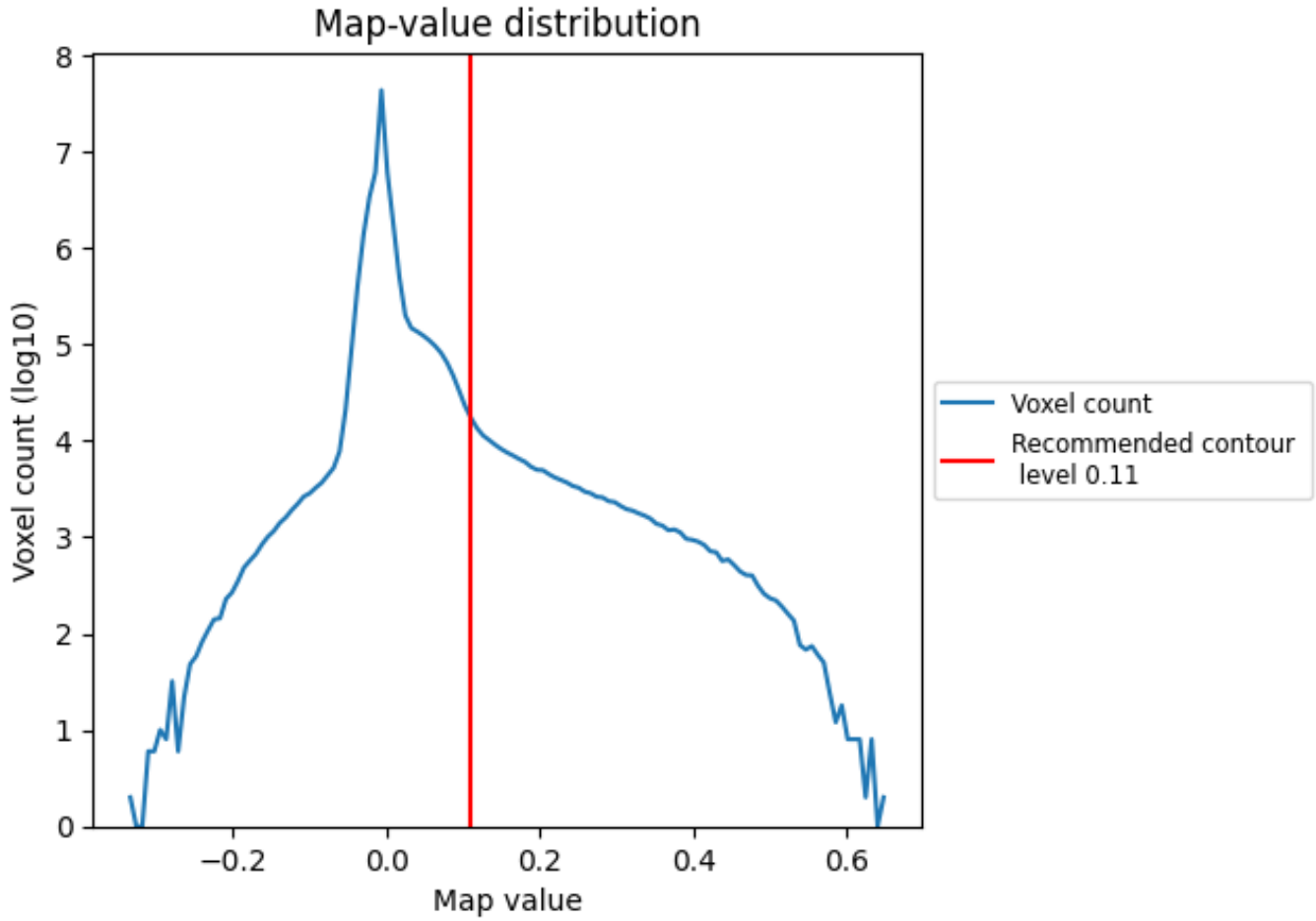


Z

7 Map analysis

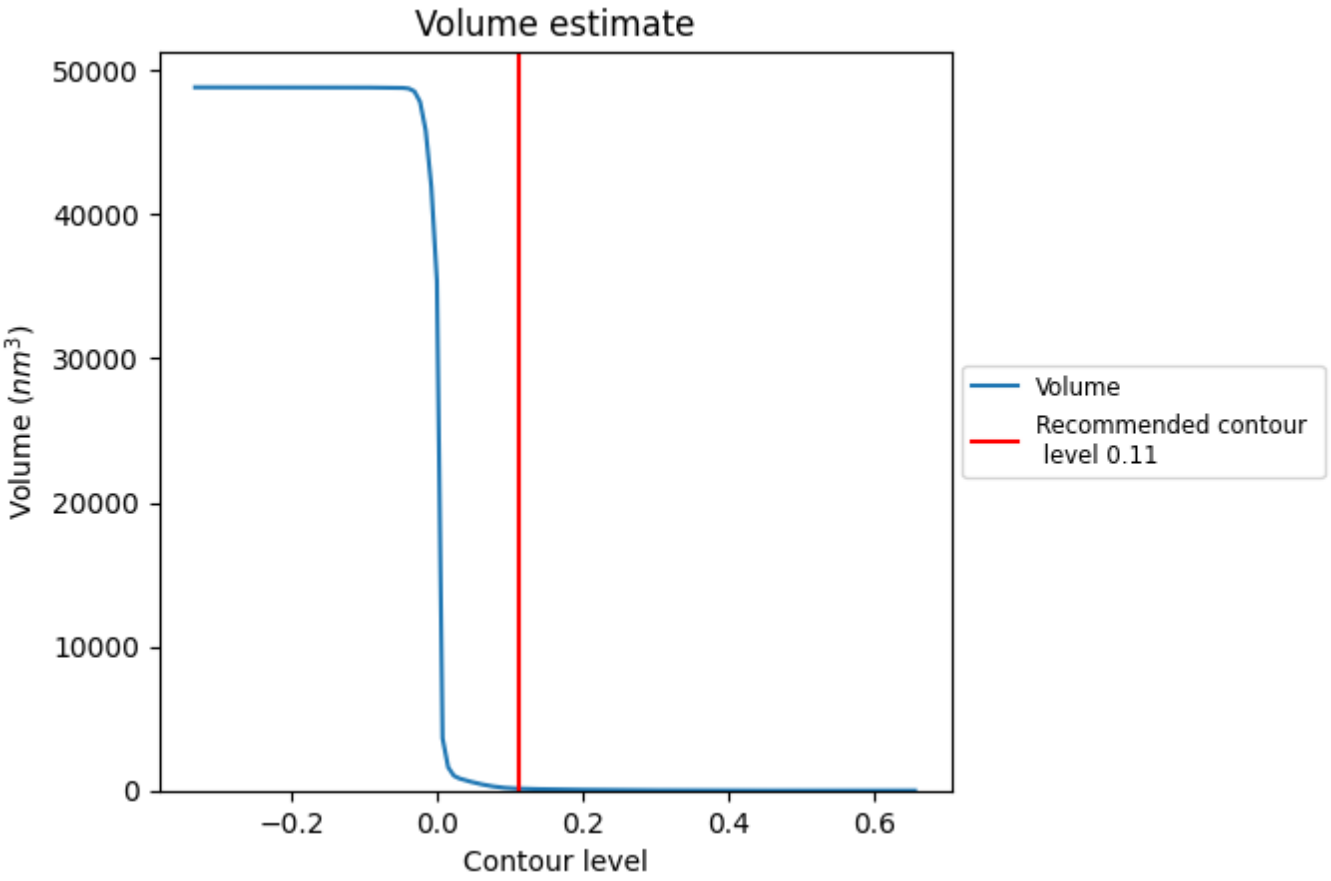
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

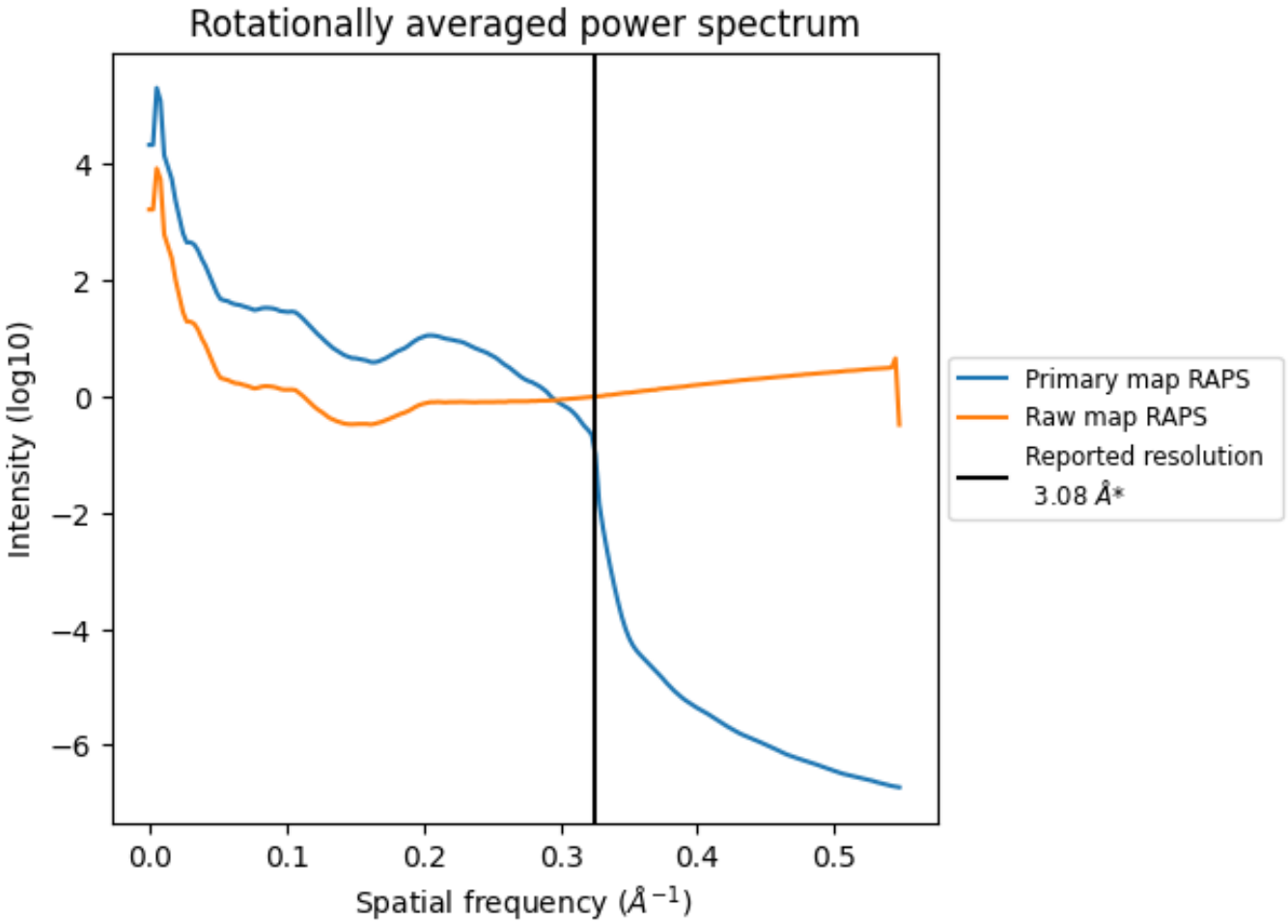
7.2 Volume estimate



The volume at the recommended contour level is 136 nm^3; this corresponds to an approximate mass of 123 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)

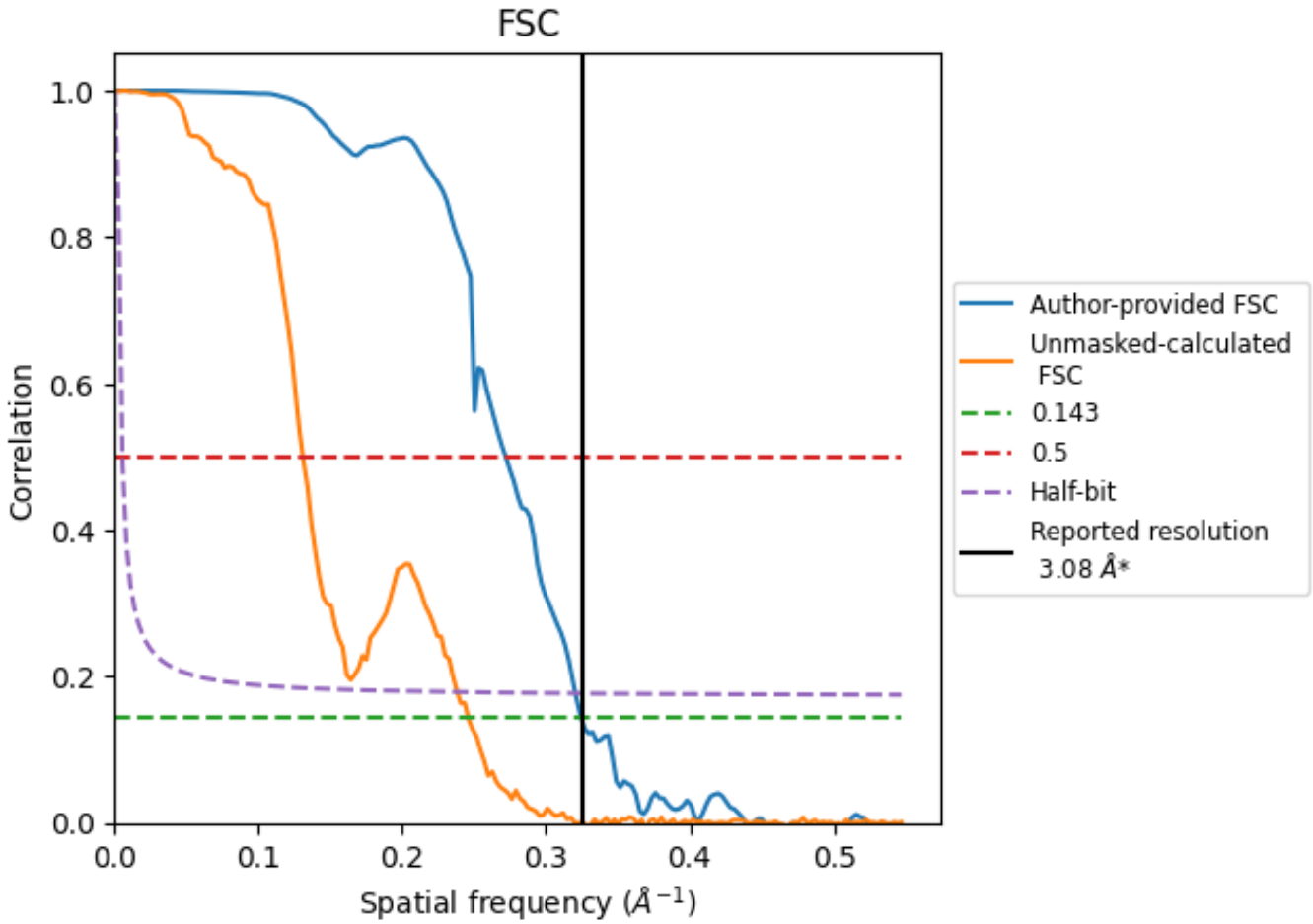


*Reported resolution corresponds to spatial frequency of 0.325 Å^{-1}

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 0.325 Å^{-1}

8.2 Resolution estimates (i)

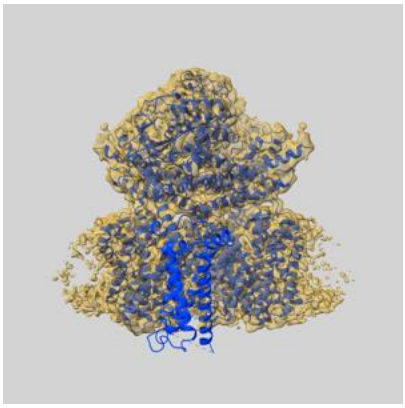
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.08	-	-
Author-provided FSC curve	3.08	3.68	3.12
Unmasked-calculated*	4.07	7.64	4.20

*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 4.07 differs from the reported value 3.08 by more than 10 %

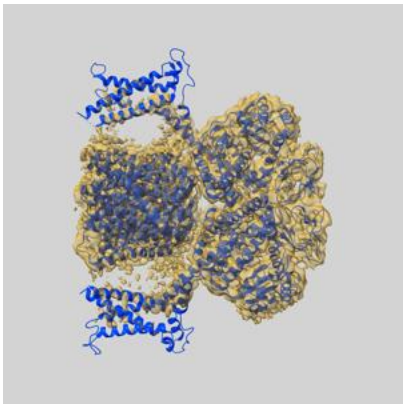
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17186 and PDB model 8OTX. Per-residue inclusion information can be found in section 3 on page 5.

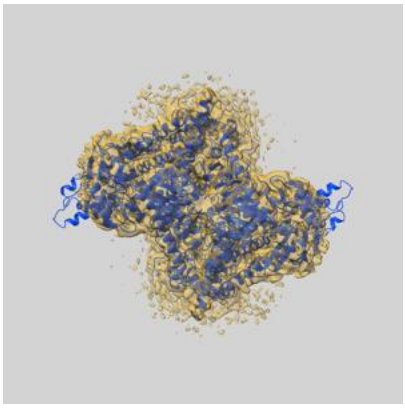
9.1 Map-model overlay



X



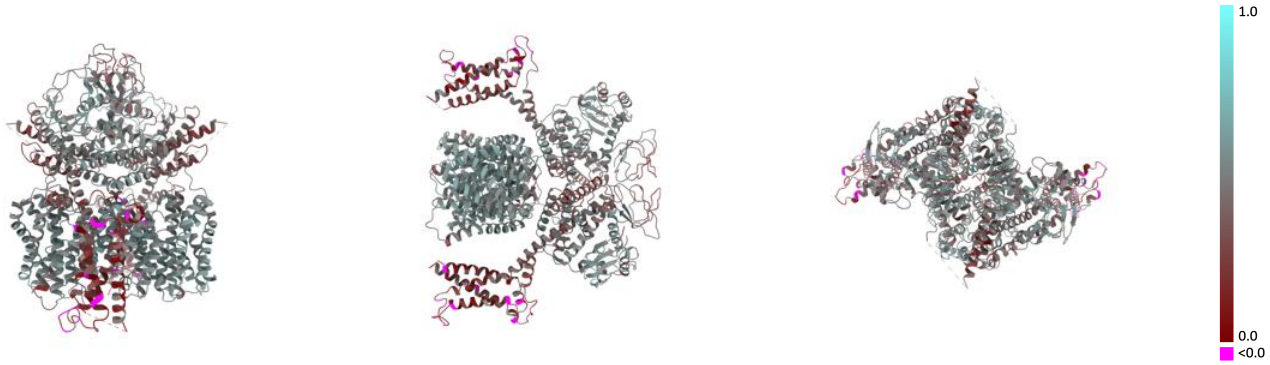
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.11 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.

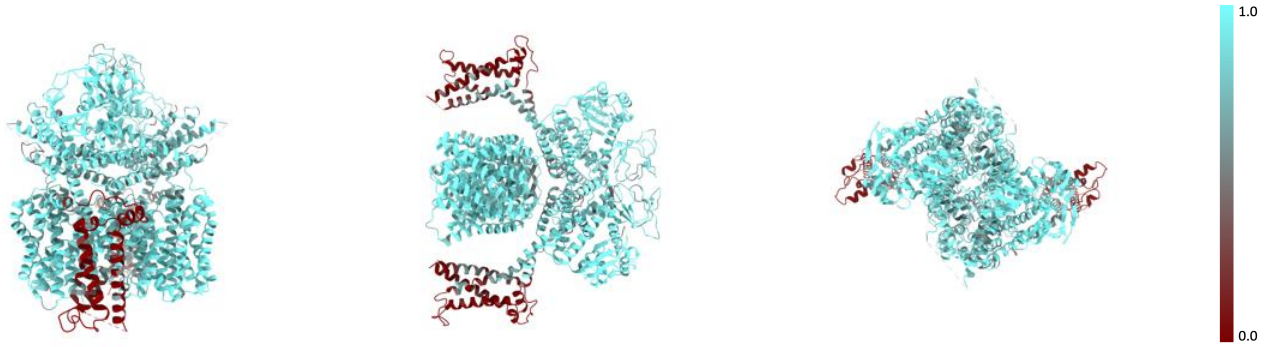
9.2 Q-score mapped to coordinate model (i)



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.

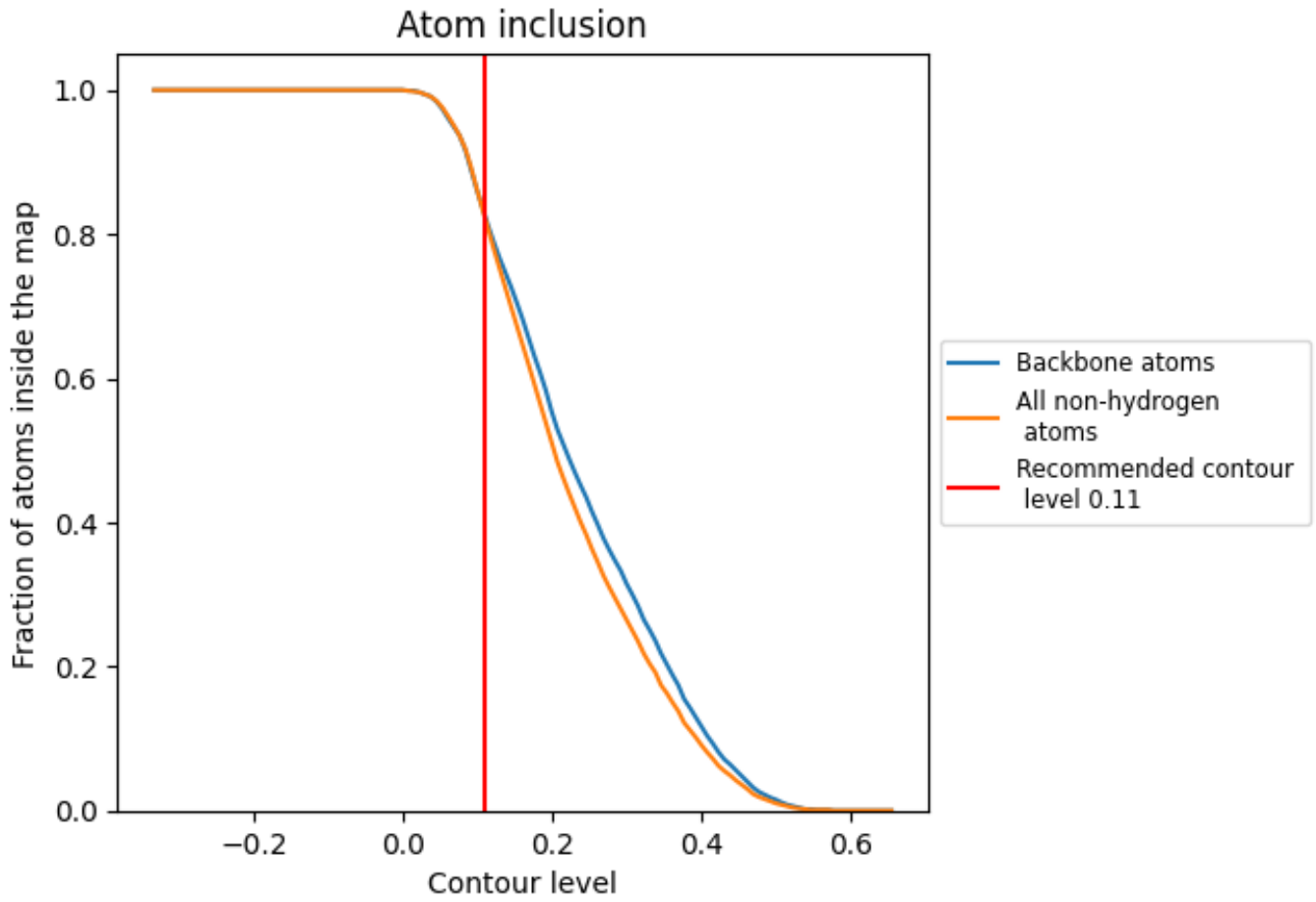
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.11).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 82% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8230	0.4570
A	0.8250	0.4570
B	0.8250	0.4570