Full wwPDB EM Validation Report ⓘ

Apr 23, 2024 – 12:39 PM JST

PDB ID	:	8XCI
EMDB ID	:	EMD-38244
Title	:	Open state of central tail fiber of bacteriophage lambda upon binding to LamB
Authors	:	Ge, X.F.; Wang, J.W.
Deposited on	:	2023-12-09
Resolution	:	3.57 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:

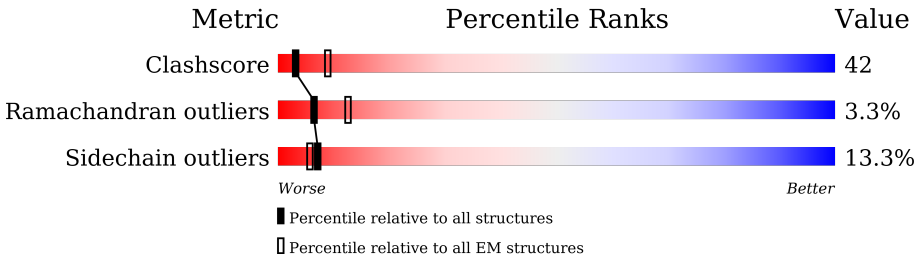
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.57 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	F	1132	7% 15% 15% 66%
1	J	1132	6% 15% 16% 66%
1	Z	1132	14% 17% 66%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8842 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.

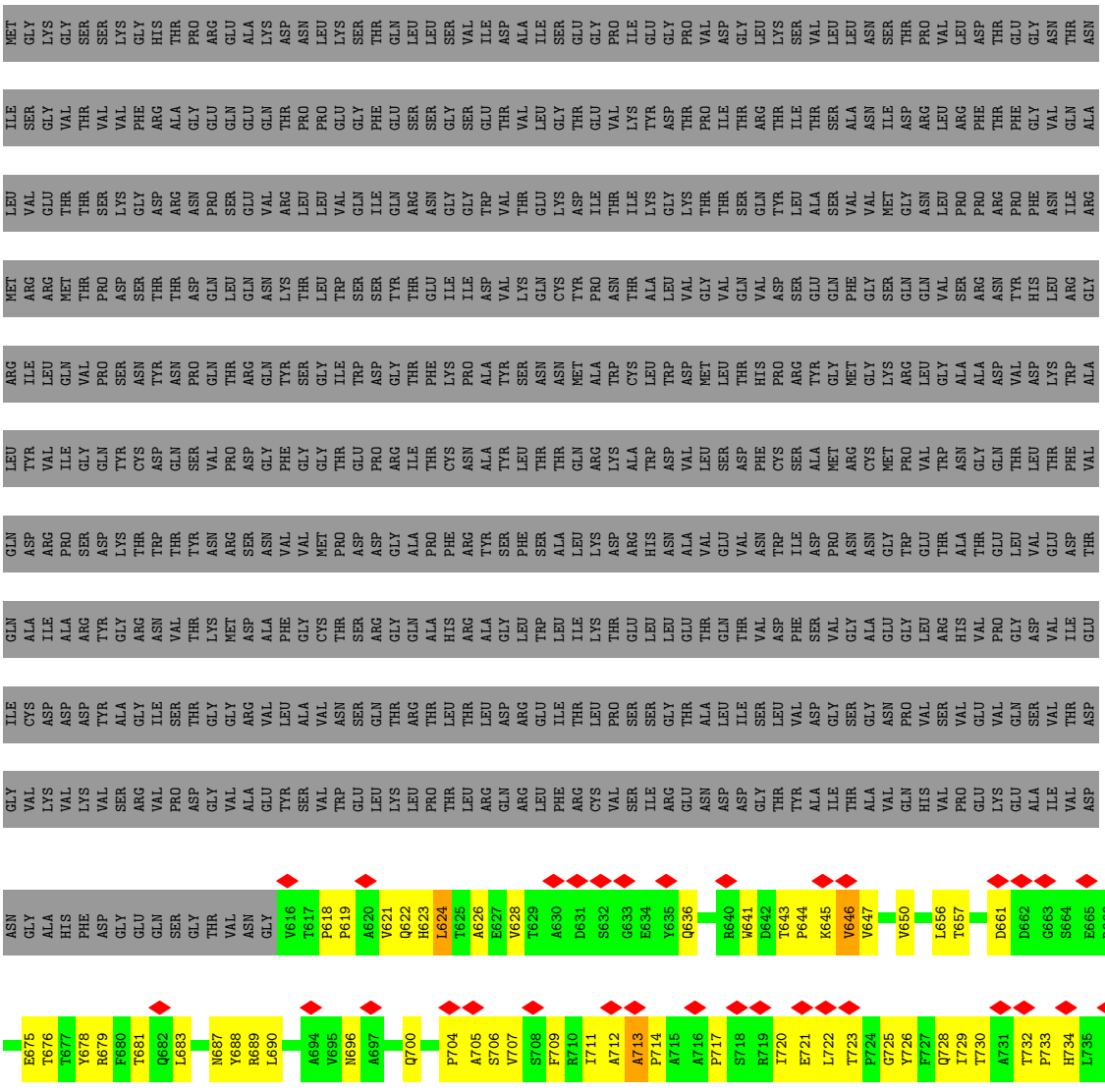
- Molecule 1 is a protein called Tip attachment protein J.

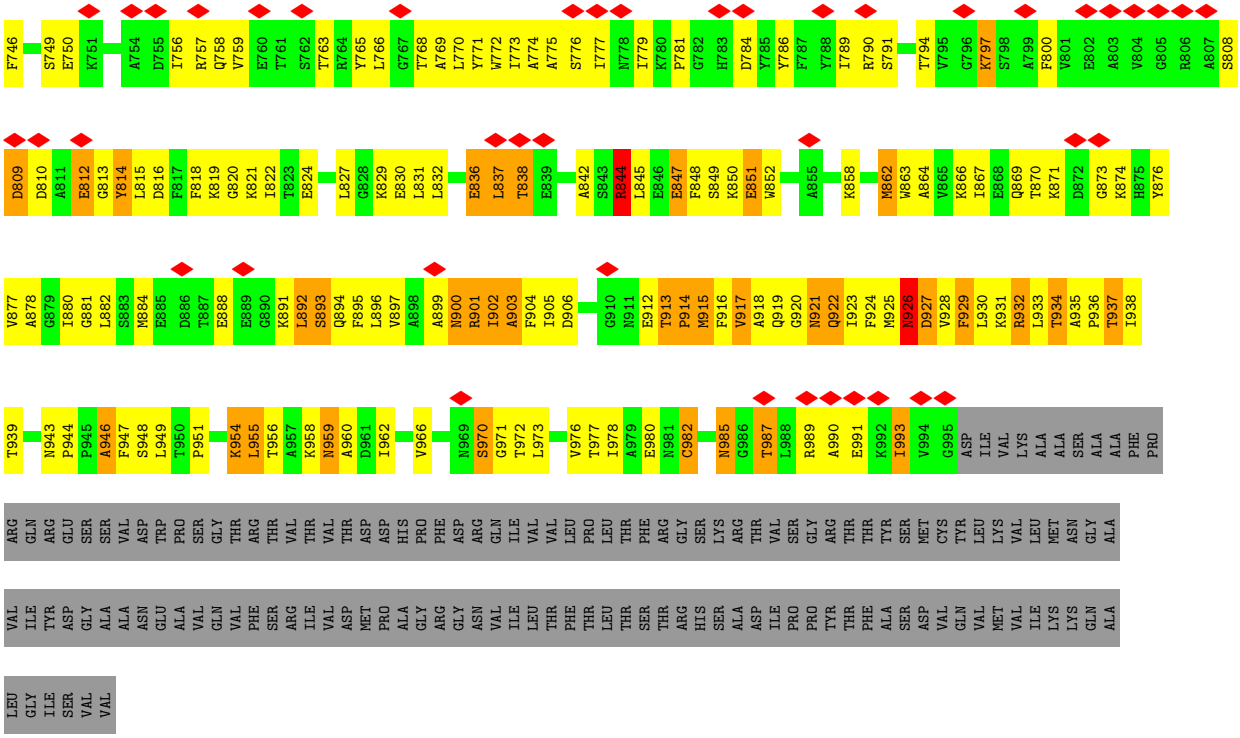
Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	380	Total	C	N	O	S	0	0
			2941	1864	499	573	5		
1	J	380	Total	C	N	O	S	0	0
			2941	1864	499	573	5		
1	Z	383	Total	C	N	O	S	0	0
			2960	1875	503	577	5		

3 Residue-property plots (i)

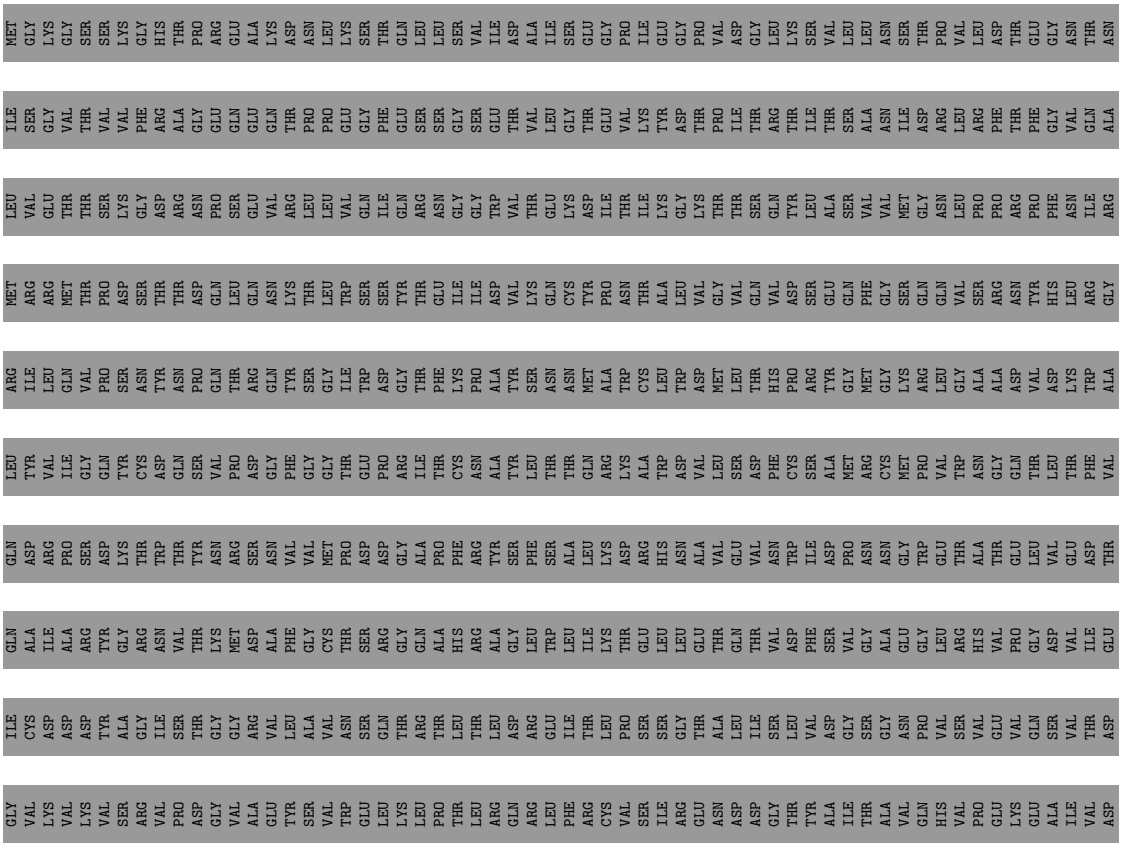
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

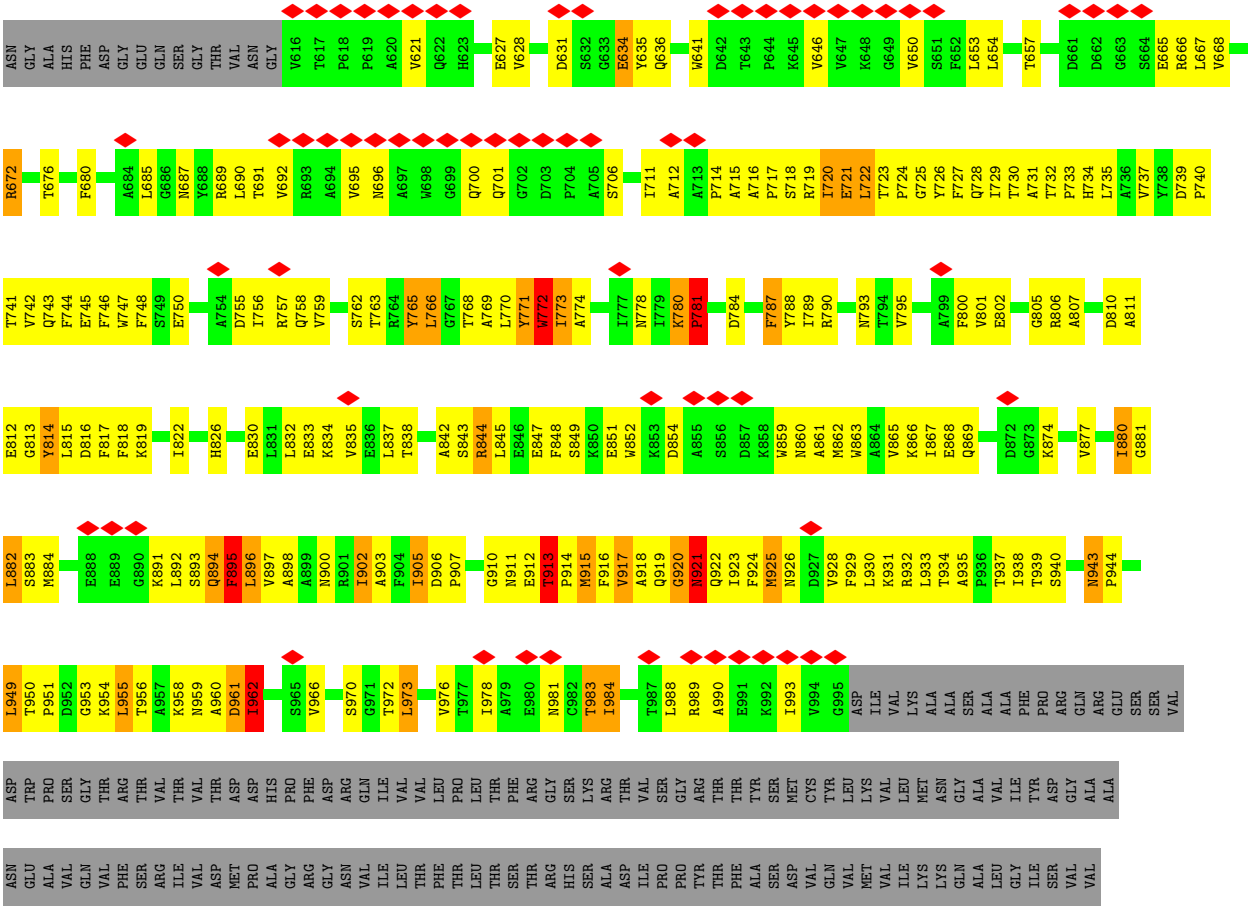
- Molecule 1: Tip attachment protein J





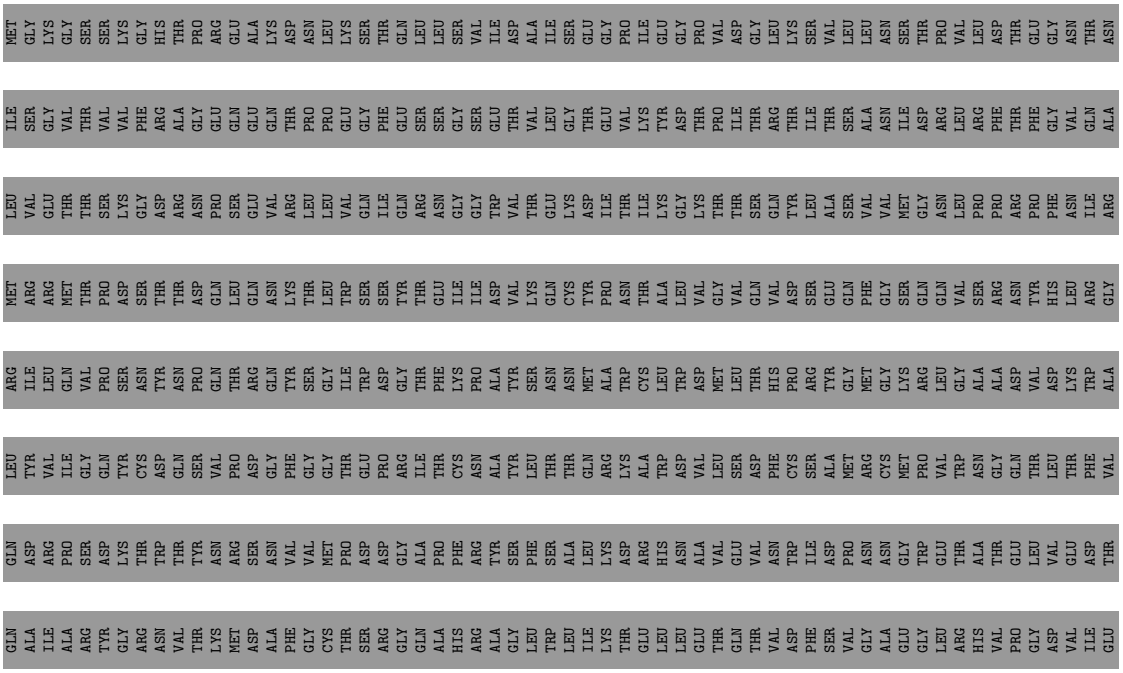
• Molecule 1: Tip attachment protein J

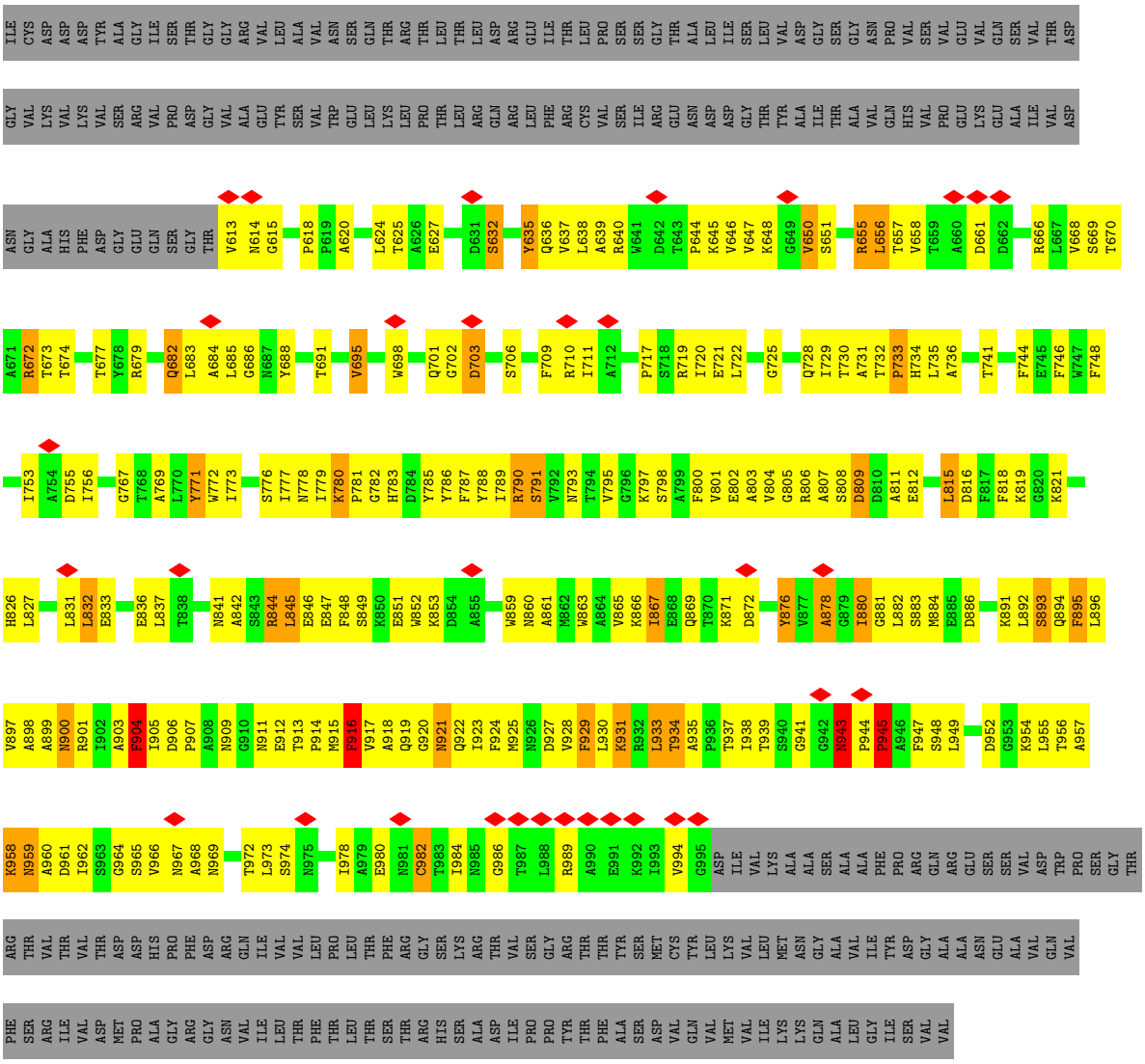




• Molecule 1: Tip attachment protein J

Chain Z:




ILE CYS ASP ASP ASP TYR ALA GLY ILE SER THR GLY GLY ARG VAL LEU ALA VAL ASN SER GLN THR ARG THR LEU THR LEU ASP ARG GLU ILE THR LEU PRO SER SER GLY THR ALA LEU ILE SER LEU VAL ASP GLY SER GLY ASN PRO VAL SER VAL GLU VAL GLN SER VAL THR ASP
GLY VAL LYS VAL LYS VAL SER ARG VAL PRO ASP GLY VAL ALA GLU TYR SER VAL TRP GLU LEU LYS LEU PRO THR LEU ARG GLN ARG LEU PHE ARG CYS VAL SER ILE ARG GLU ASN ASP GLY THR TYR ALA ILE THR ALA VAL GLN HIS VAL PRO GLU LYS GLU ALA ILE VAL ASP
ASN GLY ALA HIS PHE ASP GLY GLU GLN SER GLY THR V613 N614 G615 P618 P619 A620 L624 T625 A626 E627 D631 S632 Y635 Q636 V637 L638 A639 R640 W641 D642 T643 P644 K645 V646 V647 K648 G649 V650 S651 R655 L656 T657 V658 T659 A660 D661 D662 R666 L667 V668 S669 T670
A671 R672 T673 T674 T677 Y678 R679 Q682 L683 A684 L685 G686 N687 Y688 T691 V695 W698 Q701 G702 D703 S706 F709 R710 I711 A712 P717 S718 R719 I720 E721 L722 G725 Q728 I729 T730 A731 T732 P733 H734 L735 A736 T741 F744 E745 F746 W747 F748
I753 A754 D755 I756 G767 T768 A769 L770 Y771 W772 I773 S776 I777 N778 I779 K780 P781 G782 H783 D784 Y785 Y786 F787 Y788 I789 R790 S791 V792 N793 T794 V795 G796 K797 S798 A799 F800 V801 E802 A803 V804 G805 R806 A807 S808 D809 D810 A811 E812 L815 D816 F817 F818 K819 G820 K821
H826 L827 L831 L832 E833 E836 L837 T938 N841 A842 S843 R844 L845 E846 E847 F848 S849 K850 E851 W852 K853 D854 A855 W859 N860 A861 M862 W863 A864 V865 K866 I867 E868 Q869 Y870 K871 D872 Y876 V877 A878 G879 I880 G881 L882 S883 M884 E885 D886 K891 L892 S893 Q894 F895 L896
V897 A898 A899 N900 R901 I902 A903 F904 I905 D906 P907 A908 N909 G910 N911 E912 T913 P914 M915 F916 V917 A918 Q919 G920 N921 Q922 I923 F924 M925 N926 D927 V928 F929 L930 K931 R932 L933 T934 A935 P936 T937 I938 T939 S940 G941 G942 N943 P944 F945 A946 F947 S948 L949 D952 G953 K954 L955 T956 A957
K958 N959 A960 D961 I962 S963 G964 S965 V966 N967 A968 N969 T972 L973 S974 N975 I978 A979 E980 N981 C982 T983 I984 N985 G986 T987 L988 R989 A990 E991 K992 I993 V994 G995 ASP ILE VAL LYS ALA ALA SER ALA ALA PHE PRO ARG GLN ARG GLU SER SER VAL ASP TRP PRO SER GLY THR
ARG THR VAL THR VAL THR ASP ASP HIS PRO PHE ASP ARG GLN ILE VAL VAL LEU PRO LEU THR PHE ARG GLY SER LYS ARG THR VAL SER GLY ARG THR THR TYR SER MET CYS TYR LEU LYS VAL LEU MET ASN GLY ALA ALA VAL ILE TYR ASP GLY ALA ALA ASN GLU ALA VAL GLN VAL
PHE SER ARG ILE VAL ASP MET PRO ALA GLY ARG GLY ASN VAL ILE LEU THR PHE THR LEU THR SER THR ARG HIS SER ALA ASP ILE PRO PRO TYR THR PHE ALA SER ASP VAL GLN VAL MET VAL ILE LYS LYS GLN ALA ALA LEU GLY ILE SER VAL VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	358235	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.839	Depositor
Minimum map value	-1.114	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	343.74402, 343.74402, 343.74402	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	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	F	0.83	0/3005	1.05	5/4089 (0.1%)
1	J	0.87	0/3005	1.14	5/4089 (0.1%)
1	Z	0.88	0/3024	1.19	14/4115 (0.3%)
All	All	0.86	0/9034	1.13	24/12293 (0.2%)

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	F	0	3
1	J	0	3
1	Z	0	3
All	All	0	9

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	814	TYR	CB-CG-CD2	-9.10	115.54	121.00
1	Z	916	PHE	CB-CA-C	7.49	125.37	110.40
1	Z	672	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	Z	900	ASN	CB-CA-C	6.92	124.25	110.40
1	Z	904	PHE	CB-CG-CD1	-6.88	115.98	120.80
1	Z	916	PHE	CB-CG-CD1	6.71	125.50	120.80
1	Z	682	GLN	CB-CA-C	6.22	122.84	110.40
1	Z	895	PHE	CB-CA-C	-6.02	98.36	110.40
1	Z	904	PHE	CB-CA-C	-6.02	98.37	110.40
1	J	913	THR	CA-CB-OG1	-5.97	96.46	109.00
1	F	922	GLN	CB-CA-C	-5.67	99.06	110.40
1	Z	666	ARG	NE-CZ-NH2	-5.66	117.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Z	672	ARG	CG-CD-NE	5.65	123.67	111.80
1	F	901	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	Z	733	PRO	N-CD-CG	-5.59	94.81	103.20
1	F	844	ARG	CG-CD-NE	5.56	123.47	111.80
1	J	814	TYR	CA-CB-CG	-5.55	102.85	113.40
1	Z	876	TYR	CB-CA-C	-5.39	99.62	110.40
1	F	903	ALA	N-CA-CB	-5.39	102.56	110.10
1	Z	657	THR	CA-CB-OG1	-5.33	97.82	109.00
1	J	895	PHE	C-N-CA	-5.27	108.53	121.70
1	F	903	ALA	CB-CA-C	5.26	117.98	110.10
1	Z	956	THR	CA-CB-OG1	-5.10	98.30	109.00
1	J	773	ILE	C-N-CA	5.03	134.28	121.70

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	713	ALA	Peptide
1	F	929	PHE	Peptide
1	F	934	THR	Peptide
1	J	722	LEU	Peptide
1	J	772	TRP	Peptide
1	J	781	PRO	Peptide
1	Z	878	ALA	Peptide
1	Z	943	ASN	Peptide
1	Z	959	ASN	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	F	2941	0	2886	317	0
1	J	2941	0	2885	308	0
1	Z	2960	0	2903	328	0
All	All	8842	0	8674	741	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 42.

All (741) 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:F:902:ILE:CD1	1:J:895:PHE:HB2	1.65	1.24
1:Z:905:ILE:HD13	1:Z:912:GLU:O	1.47	1.15
1:F:928:VAL:HG23	1:J:923:ILE:CG2	1.75	1.14
1:F:902:ILE:HD12	1:J:895:PHE:CB	1.80	1.11
1:F:902:ILE:HD12	1:J:895:PHE:HB2	1.19	1.09
1:F:925:MET:HE1	1:J:923:ILE:HG21	1.32	1.07
1:F:928:VAL:CG2	1:J:923:ILE:HG22	1.87	1.03
1:Z:722:LEU:CD1	1:Z:804:VAL:O	2.07	1.02
1:F:923:ILE:HG22	1:Z:928:VAL:HG23	1.39	1.01
1:Z:827:LEU:HD22	1:Z:896:LEU:HB3	1.38	1.00
1:F:899:ALA:O	1:Z:906:ASP:HA	1.61	0.99
1:J:746:PHE:HD2	1:J:772:TRP:HB2	1.28	0.98
1:Z:722:LEU:HD13	1:Z:804:VAL:O	1.62	0.98
1:J:859:TRP:O	1:J:891:LYS:NZ	1.99	0.96
1:F:955:LEU:HD23	1:F:956:THR:N	1.81	0.95
1:J:720:ILE:HD13	1:J:789:ILE:HD13	1.45	0.95
1:J:960:ALA:O	1:J:962:ILE:HD12	1.69	0.93
1:F:970:SER:O	1:Z:973:LEU:HD23	1.70	0.92
1:J:730:THR:HG23	1:J:773:ILE:HD11	1.50	0.91
1:J:746:PHE:CD2	1:J:772:TRP:HB2	2.06	0.91
1:Z:720:ILE:HG22	1:Z:733:PRO:HB3	1.51	0.91
1:Z:685:LEU:HB2	1:Z:711:ILE:HD13	1.53	0.90
1:J:766:LEU:HD11	1:J:774:ALA:HB2	1.53	0.90
1:F:884:MET:HE3	1:Z:867:ILE:HD11	1.55	0.89
1:F:928:VAL:HG23	1:J:923:ILE:HG22	0.91	0.88
1:Z:613:VAL:HG11	1:Z:698:TRP:HZ2	1.39	0.87
1:J:628:VAL:HG21	1:J:711:ILE:HD11	1.57	0.87
1:Z:955:LEU:HD13	1:Z:955:LEU:O	1.74	0.86
1:J:772:TRP:C	1:J:773:ILE:HD12	1.96	0.86
1:Z:613:VAL:HG11	1:Z:698:TRP:CZ2	2.11	0.86
1:J:914:PRO:HD3	1:Z:819:LYS:HB2	1.59	0.85
1:F:900:ASN:OD1	1:J:893:SER:N	2.10	0.84
1:F:901:ARG:HG2	1:F:919:GLN:HB2	1.59	0.84
1:F:966:VAL:HG12	1:F:966:VAL:O	1.78	0.84
1:F:897:VAL:O	1:Z:904:PHE:HA	1.77	0.84
1:F:618:PRO:HB3	1:F:647:VAL:HG21	1.59	0.84
1:F:657:THR:HG22	1:F:667:LEU:HA	1.60	0.83
1:F:781:PRO:HB3	1:F:809:ASP:HA	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:624:LEU:HD11	1:F:707:VAL:CG2	2.09	0.83
1:F:917:VAL:HG12	1:F:924:PHE:HD2	1.42	0.83
1:Z:827:LEU:HB3	1:Z:896:LEU:HD23	1.59	0.82
1:Z:776:SER:OG	1:Z:778:ASN:OD1	1.97	0.82
1:Z:905:ILE:HG12	1:Z:914:PRO:HA	1.61	0.82
1:F:814:TYR:CD1	1:Z:924:PHE:CE2	2.68	0.81
1:J:772:TRP:O	1:J:773:ILE:HD12	1.79	0.81
1:F:893:SER:CB	1:Z:878:ALA:HB2	2.10	0.81
1:Z:779:ILE:HG23	1:Z:785:TYR:HE2	1.45	0.81
1:Z:720:ILE:CG2	1:Z:733:PRO:HB3	2.10	0.81
1:F:902:ILE:CD1	1:J:895:PHE:CB	2.45	0.80
1:Z:635:TYR:O	1:Z:683:LEU:HB2	1.80	0.80
1:J:720:ILE:CD1	1:J:789:ILE:HD13	2.11	0.79
1:Z:684:ALA:O	1:Z:688:TYR:OH	2.01	0.79
1:J:863:TRP:CH2	1:J:865:VAL:HG23	2.19	0.78
1:J:961:ASP:OD2	1:Z:954:LYS:HD2	1.84	0.78
1:Z:673:THR:OG1	1:Z:674:THR:N	2.13	0.78
1:F:893:SER:OG	1:Z:899:ALA:HA	1.84	0.78
1:Z:955:LEU:O	1:Z:955:LEU:CD1	2.31	0.78
1:J:931:LYS:O	1:J:931:LYS:NZ	2.14	0.78
1:Z:779:ILE:HG23	1:Z:785:TYR:CE2	2.19	0.78
1:F:901:ARG:NH2	1:J:894:GLN:HE22	1.82	0.77
1:F:937:THR:HG23	1:F:951:PRO:HD3	1.66	0.76
1:F:628:VAL:HG13	1:F:711:ILE:HD12	1.66	0.76
1:Z:978:ILE:HG22	1:Z:980:GLU:O	1.84	0.75
1:F:947:PHE:CD1	1:J:949:LEU:HD22	2.22	0.75
1:J:726:TYR:CZ	1:J:813:GLY:HA3	2.21	0.75
1:F:728:GLN:HA	1:F:774:ALA:O	1.87	0.74
1:Z:656:LEU:HD23	1:Z:668:VAL:HB	1.68	0.74
1:Z:729:ILE:HD12	1:Z:806:ARG:O	1.88	0.74
1:J:972:THR:HG22	1:J:972:THR:O	1.87	0.74
1:J:962:ILE:HG22	1:Z:958:LYS:O	1.88	0.74
1:F:720:ILE:HD11	1:F:789:ILE:HD11	1.70	0.74
1:F:930:LEU:HD22	1:Z:933:LEU:HD11	1.70	0.74
1:J:973:LEU:H	1:J:973:LEU:HD12	1.51	0.73
1:Z:721:GLU:OE2	1:Z:732:THR:OG1	2.03	0.73
1:F:667:LEU:HD11	1:F:670:THR:HG23	1.70	0.73
1:F:902:ILE:HD11	1:J:895:PHE:HB2	1.68	0.73
1:J:715:ALA:HB3	1:J:735:LEU:HD21	1.69	0.73
1:J:955:LEU:HD23	1:J:956:THR:N	2.04	0.72
1:F:924:PHE:CE1	1:Z:929:PHE:CE2	2.77	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:905:ILE:HG23	1:Z:913:THR:O	1.89	0.72
1:F:858:LYS:HE2	1:Z:871:LYS:HD3	1.72	0.71
1:J:925:MET:HG2	1:Z:923:ILE:HD13	1.72	0.71
1:J:780:LYS:O	1:J:781:PRO:O	2.08	0.71
1:Z:904:PHE:CE2	1:Z:916:PHE:CD1	2.77	0.71
1:F:884:MET:HE3	1:Z:867:ILE:CD1	2.20	0.71
1:J:730:THR:HG23	1:J:773:ILE:CD1	2.20	0.71
1:J:913:THR:HG23	1:Z:819:LYS:HD2	1.72	0.71
1:Z:722:LEU:HD12	1:Z:804:VAL:O	1.90	0.71
1:J:863:TRP:CH2	1:J:865:VAL:CG2	2.74	0.71
1:J:868:GLU:HG3	1:J:877:VAL:HG23	1.73	0.71
1:F:893:SER:HB2	1:Z:878:ALA:HB2	1.73	0.71
1:Z:685:LEU:HA	1:Z:711:ILE:HG12	1.73	0.71
1:J:717:PRO:HG3	1:J:744:PHE:CE1	2.25	0.70
1:F:914:PRO:HB2	1:J:815:LEU:CD2	2.20	0.70
1:J:781:PRO:HG2	1:Z:929:PHE:CE2	2.26	0.70
1:Z:725:GLY:O	1:Z:808:SER:OG	2.08	0.70
1:Z:788:TYR:HE1	1:Z:802:GLU:HB2	1.56	0.70
1:F:901:ARG:O	1:J:894:GLN:HA	1.92	0.70
1:Z:933:LEU:O	1:Z:934:THR:OG1	2.04	0.70
1:J:722:LEU:HD12	1:J:722:LEU:N	2.07	0.69
1:J:930:LEU:CD1	1:Z:925:MET:HB2	2.22	0.69
1:F:920:GLY:O	1:F:921:ASN:ND2	2.25	0.69
1:Z:837:LEU:HD21	1:Z:842:ALA:HB3	1.74	0.69
1:F:925:MET:HE1	1:J:923:ILE:CG2	2.16	0.69
1:F:893:SER:HB3	1:Z:900:ASN:OD1	1.92	0.69
1:Z:729:ILE:HD11	1:Z:805:GLY:HA3	1.73	0.69
1:F:893:SER:HB2	1:Z:878:ALA:CB	2.22	0.69
1:F:924:PHE:HE1	1:Z:929:PHE:CE2	2.11	0.69
1:J:863:TRP:HB3	1:J:882:LEU:HD21	1.74	0.69
1:Z:720:ILE:HG22	1:Z:733:PRO:CB	2.22	0.69
1:J:920:GLY:C	1:J:922:GLN:H	1.96	0.68
1:F:914:PRO:HB2	1:J:815:LEU:HD21	1.75	0.68
1:Z:788:TYR:CE1	1:Z:802:GLU:HB2	2.28	0.68
1:J:646:VAL:HG21	1:J:650:VAL:HB	1.75	0.68
1:F:899:ALA:HB1	1:J:893:SER:O	1.94	0.68
1:J:744:PHE:O	1:J:768:THR:HA	1.92	0.68
1:J:867:ILE:CD1	1:Z:882:LEU:CD2	2.72	0.68
1:F:720:ILE:CD1	1:F:789:ILE:HD11	2.23	0.68
1:F:704:PRO:O	1:J:743:GLN:NE2	2.20	0.68
1:J:922:GLN:NE2	1:Z:780:LYS:HB3	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:773:ILE:HD12	1:J:773:ILE:N	2.08	0.67
1:F:893:SER:HG	1:Z:899:ALA:HA	1.60	0.67
1:J:939:THR:O	1:Z:934:THR:HG23	1.94	0.67
1:F:982:CYS:SG	1:Z:984:ILE:HG12	2.34	0.66
1:Z:636:GLN:HA	1:Z:683:LEU:HD12	1.76	0.66
1:Z:916:PHE:O	1:Z:917:VAL:HG22	1.95	0.66
1:J:920:GLY:O	1:J:922:GLN:N	2.29	0.66
1:J:771:TYR:HD1	1:J:771:TYR:H	1.43	0.66
1:F:925:MET:CE	1:J:923:ILE:HG21	2.19	0.66
1:F:905:ILE:HD11	1:J:822:ILE:HD13	1.77	0.66
1:F:946:ALA:O	1:J:953:GLY:HA3	1.95	0.65
1:F:845:LEU:HD12	1:F:867:ILE:HD11	1.79	0.65
1:Z:921:ASN:OD1	1:Z:921:ASN:N	2.29	0.65
1:F:906:ASP:OD2	1:J:900:ASN:HA	1.97	0.65
1:J:746:PHE:CD1	1:J:789:ILE:HG22	2.31	0.65
1:J:930:LEU:HD13	1:Z:925:MET:HB2	1.77	0.65
1:Z:895:PHE:CG	1:Z:895:PHE:O	2.43	0.65
1:J:911:ASN:OD1	1:J:912:GLU:N	2.30	0.65
1:F:917:VAL:HG12	1:F:924:PHE:CD2	2.29	0.65
1:J:924:PHE:N	1:J:924:PHE:CD1	2.60	0.65
1:Z:871:LYS:NZ	1:Z:872:ASP:OD2	2.30	0.64
1:J:933:LEU:HD11	1:J:935:ALA:HB2	1.78	0.64
1:J:960:ALA:O	1:J:962:ILE:CD1	2.43	0.64
1:J:726:TYR:OH	1:J:813:GLY:HA3	1.98	0.64
1:J:733:PRO:O	1:J:734:HIS:ND1	2.30	0.64
1:J:880:ILE:HG22	1:J:897:VAL:HA	1.80	0.64
1:F:924:PHE:CE1	1:Z:929:PHE:HE2	2.15	0.64
1:F:958:LYS:O	1:F:959:ASN:HB2	1.97	0.64
1:J:717:PRO:HG3	1:J:744:PHE:CZ	2.33	0.64
1:J:917:VAL:HG11	1:Z:818:PHE:CG	2.33	0.64
1:J:988:LEU:HD23	1:J:989:ARG:N	2.13	0.64
1:Z:897:VAL:HG12	1:Z:897:VAL:O	1.97	0.64
1:F:771:TYR:CE1	1:Z:909:ASN:OD1	2.51	0.64
1:F:814:TYR:CD1	1:Z:924:PHE:HE2	2.16	0.64
1:Z:916:PHE:O	1:Z:917:VAL:CG2	2.46	0.64
1:Z:948:SER:C	1:Z:949:LEU:HD12	2.18	0.63
1:F:814:TYR:CG	1:Z:924:PHE:HE2	2.17	0.63
1:F:896:LEU:HD12	1:Z:903:ALA:O	1.97	0.63
1:Z:904:PHE:HE2	1:Z:916:PHE:CD1	2.16	0.63
1:Z:903:ALA:HB1	1:Z:914:PRO:HB3	1.81	0.63
1:Z:978:ILE:HD13	1:Z:982:CYS:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:722:LEU:HA	1:F:730:THR:O	1.98	0.63
1:F:931:LYS:O	1:F:932:ARG:HB2	1.98	0.63
1:Z:613:VAL:CG1	1:Z:698:TRP:CZ2	2.82	0.62
1:F:876:TYR:HB3	1:J:884:MET:CE	2.29	0.62
1:J:905:ILE:O	1:Z:898:ALA:HA	1.99	0.62
1:Z:918:ALA:CB	1:Z:923:ILE:HG13	2.29	0.62
1:F:618:PRO:HA	1:F:647:VAL:HG11	1.81	0.62
1:F:819:LYS:HD3	1:Z:913:THR:OG1	2.00	0.62
1:F:884:MET:HE3	1:Z:867:ILE:CG1	2.28	0.62
1:F:905:ILE:HD13	1:F:914:PRO:HA	1.80	0.62
1:F:933:LEU:CD1	1:J:930:LEU:HD23	2.29	0.62
1:J:880:ILE:CG2	1:J:897:VAL:HA	2.30	0.62
1:F:845:LEU:HD11	1:J:849:SER:HB2	1.81	0.62
1:F:882:LEU:HD13	1:Z:880:ILE:HD13	1.82	0.62
1:Z:753:ILE:HD12	1:Z:753:ILE:O	2.00	0.62
1:Z:982:CYS:O	1:Z:982:CYS:SG	2.58	0.62
1:Z:904:PHE:O	1:Z:915:MET:N	2.33	0.61
1:J:814:TYR:O	1:J:817:PHE:HB3	1.99	0.61
1:J:922:GLN:O	1:J:923:ILE:HD12	2.00	0.61
1:F:728:GLN:HB3	1:F:775:ALA:HB2	1.82	0.61
1:F:949:LEU:HD22	1:Z:947:PHE:CD1	2.35	0.61
1:F:978:ILE:HD13	1:J:976:VAL:HG11	1.81	0.61
1:J:906:ASP:OD1	1:J:907:PRO:HD2	2.00	0.61
1:F:924:PHE:CE1	1:Z:929:PHE:CD2	2.88	0.61
1:F:643:THR:HG22	1:F:646:VAL:H	1.65	0.61
1:F:881:GLY:O	1:F:895:PHE:HA	2.00	0.61
1:F:749:SER:OG	1:F:786:TYR:HB2	2.01	0.61
1:J:773:ILE:CD1	1:J:773:ILE:N	2.64	0.61
1:Z:827:LEU:HD21	1:Z:881:GLY:C	2.22	0.61
1:F:928:VAL:CG1	1:Z:930:LEU:HD13	2.30	0.60
1:J:657:THR:HG22	1:J:667:LEU:HA	1.82	0.60
1:F:902:ILE:CG1	1:J:895:PHE:CB	2.79	0.60
1:F:626:ALA:HB1	1:F:709:PHE:HB3	1.82	0.60
1:F:706:SER:O	1:J:768:THR:OG1	2.19	0.60
1:Z:636:GLN:HG3	1:Z:679:ARG:HH22	1.65	0.60
1:J:990:ALA:HB3	1:J:993:ILE:HD11	1.84	0.60
1:Z:837:LEU:HD11	1:Z:842:ALA:CB	2.32	0.60
1:F:922:GLN:O	1:F:923:ILE:HD12	2.02	0.60
1:Z:933:LEU:HD12	1:Z:934:THR:H	1.67	0.60
1:F:624:LEU:HD11	1:F:707:VAL:HG21	1.84	0.60
1:Z:683:LEU:HD22	1:Z:688:TYR:CZ	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:782:GLY:O	1:Z:783:HIS:ND1	2.35	0.60
1:Z:656:LEU:HD21	1:Z:668:VAL:HG11	1.83	0.59
1:J:635:TYR:OH	1:J:795:VAL:HG22	2.03	0.59
1:J:880:ILE:HG21	1:J:897:VAL:HG13	1.84	0.59
1:F:746:PHE:HA	1:F:789:ILE:HG22	1.85	0.59
1:Z:656:LEU:CD2	1:Z:668:VAL:CG1	2.80	0.59
1:F:838:THR:HA	1:F:870:THR:HG21	1.84	0.59
1:F:848:PHE:HE2	1:F:850:LYS:HG2	1.65	0.59
1:F:954:LYS:HD2	1:Z:959:ASN:HB2	1.84	0.59
1:Z:786:TYR:HA	1:Z:803:ALA:O	2.02	0.59
1:F:933:LEU:HD12	1:J:930:LEU:HD23	1.83	0.59
1:Z:904:PHE:O	1:Z:914:PRO:HA	2.03	0.59
1:Z:848:PHE:O	1:Z:863:TRP:CD1	2.55	0.59
1:Z:837:LEU:HD11	1:Z:842:ALA:HB1	1.85	0.58
1:F:959:ASN:HB3	1:J:954:LYS:HA	1.85	0.58
1:Z:769:ALA:HB3	1:Z:771:TYR:O	2.04	0.58
1:Z:808:SER:O	1:Z:809:ASP:HB3	2.03	0.58
1:Z:656:LEU:O	1:Z:668:VAL:HB	2.04	0.58
1:F:962:ILE:HD12	1:F:962:ILE:N	2.19	0.58
1:Z:756:ILE:HG22	1:Z:800:PHE:HB2	1.84	0.58
1:J:905:ILE:CG2	1:Z:898:ALA:HB2	2.33	0.58
1:Z:636:GLN:HG3	1:Z:679:ARG:NH2	2.19	0.58
1:Z:656:LEU:HD23	1:Z:668:VAL:CB	2.34	0.58
1:Z:685:LEU:HD23	1:Z:685:LEU:H	1.68	0.58
1:Z:744:PHE:N	1:Z:744:PHE:CD2	2.70	0.58
1:F:891:LYS:O	1:Z:876:TYR:CE2	2.57	0.57
1:Z:720:ILE:HD11	1:Z:803:ALA:HB3	1.86	0.57
1:Z:741:THR:O	1:Z:741:THR:OG1	2.19	0.57
1:Z:949:LEU:HD12	1:Z:949:LEU:N	2.19	0.57
1:J:725:GLY:HA3	1:J:728:GLN:NE2	2.19	0.57
1:J:746:PHE:HD2	1:J:772:TRP:CB	2.11	0.57
1:Z:656:LEU:HD23	1:Z:668:VAL:CG1	2.34	0.57
1:F:901:ARG:HD3	1:F:919:GLN:OE1	2.05	0.57
1:J:938:ILE:HG12	1:Z:933:LEU:HB3	1.86	0.57
1:Z:831:LEU:C	1:Z:832:LEU:HD23	2.25	0.57
1:F:902:ILE:CG2	1:F:904:PHE:HE1	2.16	0.57
1:F:893:SER:OG	1:Z:878:ALA:HB2	2.04	0.57
1:F:970:SER:OG	1:F:971:GLY:N	2.38	0.57
1:J:845:LEU:N	1:J:845:LEU:HD12	2.20	0.57
1:Z:827:LEU:CD2	1:Z:896:LEU:HB3	2.26	0.57
1:F:696:ASN:OD1	1:F:700:GLN:N	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:902:ILE:CG1	1:J:895:PHE:HB2	2.34	0.57
1:J:771:TYR:CD1	1:J:771:TYR:O	2.57	0.57
1:J:837:LEU:HD13	1:J:842:ALA:HB1	1.85	0.57
1:J:851:GLU:HA	1:J:860:ASN:O	2.04	0.57
1:Z:613:VAL:HG12	1:Z:614:ASN:N	2.19	0.57
1:Z:710:ARG:HB2	1:Z:710:ARG:CZ	2.34	0.57
1:F:932:ARG:HG3	1:Z:937:THR:HB	1.87	0.57
1:J:744:PHE:HB2	1:J:769:ALA:O	2.03	0.57
1:Z:918:ALA:HB2	1:Z:923:ILE:CG1	2.35	0.57
1:F:837:LEU:HG	1:F:844:ARG:HB2	1.87	0.57
1:F:893:SER:OG	1:Z:899:ALA:CA	2.53	0.57
1:Z:613:VAL:CG1	1:Z:698:TRP:CH2	2.88	0.56
1:F:744:PHE:O	1:F:768:THR:HA	2.05	0.56
1:F:848:PHE:CE2	1:F:850:LYS:HG2	2.38	0.56
1:Z:787:PHE:HB3	1:Z:789:ILE:CD1	2.35	0.56
1:F:647:VAL:HG22	1:F:650:VAL:HB	1.87	0.56
1:F:730:THR:HG23	1:F:773:ILE:HG22	1.86	0.56
1:F:902:ILE:HD12	1:J:895:PHE:N	2.19	0.56
1:F:922:GLN:C	1:F:923:ILE:HD12	2.26	0.56
1:F:947:PHE:CG	1:J:949:LEU:HD22	2.41	0.56
1:J:810:ASP:O	1:J:814:TYR:HD2	1.89	0.56
1:F:902:ILE:HG13	1:J:895:PHE:CD2	2.40	0.56
1:J:973:LEU:HD12	1:J:973:LEU:N	2.21	0.56
1:Z:620:ALA:HB2	1:Z:703:ASP:O	2.06	0.56
1:Z:720:ILE:HA	1:Z:733:PRO:HA	1.86	0.56
1:F:836:GLU:HB2	1:F:844:ARG:NH2	2.20	0.56
1:J:766:LEU:HD11	1:J:774:ALA:CB	2.32	0.56
1:F:905:ILE:HD11	1:J:822:ILE:CD1	2.36	0.56
1:J:880:ILE:HG22	1:J:898:ALA:H	1.71	0.56
1:Z:638:LEU:HD11	1:Z:679:ARG:HH21	1.70	0.56
1:J:744:PHE:HB3	1:J:746:PHE:CE1	2.40	0.56
1:J:657:THR:HA	1:J:668:VAL:HG23	1.88	0.55
1:J:771:TYR:CD1	1:J:771:TYR:N	2.74	0.55
1:Z:907:PRO:HA	1:Z:911:ASN:O	2.06	0.55
1:F:641:TRP:O	1:F:676:THR:HB	2.06	0.55
1:F:882:LEU:HD23	1:Z:865:VAL:HG12	1.89	0.55
1:F:923:ILE:CG2	1:Z:928:VAL:HG23	2.27	0.55
1:F:933:LEU:HD23	1:Z:938:ILE:HG23	1.88	0.55
1:F:628:VAL:CG1	1:F:711:ILE:HD12	2.36	0.55
1:J:842:ALA:O	1:J:869:GLN:HA	2.07	0.55
1:F:771:TYR:O	1:Z:909:ASN:ND2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:849:SER:HB2	1:Z:845:LEU:HD21	1.88	0.55
1:J:732:THR:HG22	1:J:771:TYR:HB2	1.89	0.55
1:F:928:VAL:HG11	1:Z:930:LEU:HD13	1.89	0.55
1:J:865:VAL:HG21	1:Z:863:TRP:CZ3	2.42	0.55
1:Z:827:LEU:CB	1:Z:896:LEU:HD23	2.36	0.55
1:F:717:PRO:HG3	1:F:744:PHE:HE2	1.72	0.55
1:F:955:LEU:HD23	1:F:955:LEU:C	2.27	0.55
1:F:831:LEU:HD21	1:F:864:ALA:HB1	1.88	0.55
1:F:918:ALA:HA	1:F:922:GLN:O	2.07	0.55
1:F:765:TYR:OH	1:F:873:GLY:O	2.23	0.54
1:J:830:GLU:HG2	1:J:848:PHE:CZ	2.42	0.54
1:J:867:ILE:CD1	1:Z:882:LEU:HD21	2.38	0.54
1:Z:781:PRO:HA	1:Z:807:ALA:HB3	1.89	0.54
1:F:641:TRP:HH2	1:F:678:TYR:HB2	1.72	0.54
1:J:746:PHE:HE2	1:J:772:TRP:N	2.05	0.54
1:F:619:PRO:HD3	1:F:647:VAL:CG1	2.38	0.54
1:J:869:GLN:HG3	1:Z:884:MET:SD	2.48	0.54
1:Z:639:ALA:O	1:Z:677:THR:HA	2.07	0.54
1:Z:748:PHE:HD1	1:Z:787:PHE:CE1	2.26	0.54
1:J:722:LEU:O	1:J:724:PRO:HD3	2.08	0.54
1:F:894:GLN:N	1:Z:899:ALA:HB1	2.23	0.54
1:J:843:SER:HB2	1:Z:859:TRP:HE3	1.72	0.54
1:J:922:GLN:OE1	1:Z:781:PRO:HD2	2.08	0.54
1:F:622:GLN:HG3	1:F:644:PRO:HG3	1.90	0.54
1:F:902:ILE:HG13	1:J:895:PHE:CB	2.38	0.54
1:F:966:VAL:O	1:F:966:VAL:CG1	2.47	0.54
1:J:722:LEU:HD22	1:J:805:GLY:HA3	1.89	0.54
1:J:759:VAL:O	1:J:763:THR:OG1	2.13	0.54
1:Z:658:VAL:HG13	1:Z:658:VAL:O	2.08	0.54
1:F:628:VAL:HG12	1:F:794:THR:HG21	1.90	0.54
1:F:893:SER:CB	1:Z:878:ALA:CB	2.81	0.54
1:Z:827:LEU:HD21	1:Z:881:GLY:O	2.07	0.54
1:J:924:PHE:N	1:J:924:PHE:HD1	2.06	0.54
1:Z:847:GLU:HB2	1:Z:865:VAL:HG22	1.90	0.54
1:F:814:TYR:CG	1:Z:924:PHE:CE2	2.95	0.54
1:F:882:LEU:HD11	1:Z:878:ALA:C	2.28	0.54
1:Z:827:LEU:HD23	1:Z:831:LEU:HD22	1.90	0.53
1:F:949:LEU:HD22	1:Z:947:PHE:CG	2.43	0.53
1:J:961:ASP:N	1:J:961:ASP:OD1	2.39	0.53
1:Z:955:LEU:HD13	1:Z:955:LEU:C	2.28	0.53
1:F:619:PRO:HD3	1:F:647:VAL:HG11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:688:TYR:HB2	1:Z:709:PHE:CE1	2.43	0.53
1:J:835:VAL:O	1:J:835:VAL:HG22	2.08	0.53
1:J:925:MET:CE	1:Z:925:MET:CE	2.87	0.53
1:F:880:ILE:O	1:F:880:ILE:HG13	2.09	0.53
1:F:876:TYR:HB3	1:J:884:MET:HE2	1.91	0.53
1:J:916:PHE:CD1	1:J:916:PHE:C	2.81	0.53
1:Z:918:ALA:HB1	1:Z:923:ILE:HG13	1.90	0.53
1:J:730:THR:HG23	1:J:773:ILE:CG1	2.39	0.53
1:J:816:ASP:OD1	1:J:817:PHE:N	2.42	0.53
1:J:849:SER:HB3	1:J:863:TRP:HD1	1.74	0.53
1:F:818:PHE:O	1:F:822:ILE:HG12	2.09	0.53
1:J:718:SER:O	1:J:719:ARG:HG2	2.09	0.53
1:F:814:TYR:CE1	1:Z:924:PHE:CE2	2.97	0.52
1:F:902:ILE:HG13	1:J:895:PHE:HD2	1.72	0.52
1:F:906:ASP:HB2	1:F:915:MET:HE1	1.91	0.52
1:J:817:PHE:C	1:J:817:PHE:CD2	2.83	0.52
1:J:695:VAL:HG22	1:J:701:GLN:HG2	1.90	0.52
1:Z:916:PHE:C	1:Z:917:VAL:HG23	2.29	0.52
1:F:931:LYS:O	1:F:932:ARG:CB	2.58	0.52
1:Z:837:LEU:HD13	1:Z:844:ARG:HB2	1.91	0.52
1:F:973:LEU:O	1:Z:978:ILE:HA	2.09	0.52
1:J:641:TRP:O	1:J:676:THR:OG1	2.27	0.52
1:J:868:GLU:CG	1:J:877:VAL:HG23	2.38	0.52
1:J:937:THR:C	1:J:938:ILE:HG13	2.29	0.52
1:Z:656:LEU:CD2	1:Z:668:VAL:HG11	2.40	0.52
1:J:918:ALA:CB	1:J:923:ILE:HD11	2.39	0.52
1:J:790:ARG:CZ	1:J:800:PHE:CZ	2.93	0.52
1:Z:686:GLY:N	1:Z:711:ILE:HD11	2.24	0.52
1:F:901:ARG:NH1	1:J:894:GLN:OE1	2.43	0.52
1:F:930:LEU:HB3	1:Z:935:ALA:HB2	1.92	0.52
1:Z:918:ALA:HB2	1:Z:923:ILE:HG13	1.91	0.52
1:J:726:TYR:O	1:J:727:PHE:HB2	2.10	0.51
1:J:925:MET:SD	1:Z:925:MET:HE1	2.49	0.51
1:Z:701:GLN:N	1:Z:701:GLN:OE1	2.43	0.51
1:J:771:TYR:HD1	1:J:771:TYR:N	2.06	0.51
1:J:866:LYS:HG2	1:J:868:GLU:OE1	2.10	0.51
1:F:858:LYS:CE	1:Z:871:LYS:HD3	2.40	0.51
1:F:915:MET:O	1:F:925:MET:HA	2.10	0.51
1:J:720:ILE:HD11	1:J:731:ALA:HB1	1.91	0.51
1:Z:720:ILE:HD11	1:Z:803:ALA:CB	2.40	0.51
1:J:717:PRO:CG	1:J:744:PHE:CE1	2.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:923:ILE:C	1:J:924:PHE:CD1	2.84	0.51
1:J:810:ASP:O	1:J:814:TYR:CD2	2.63	0.51
1:Z:669:SER:OG	1:Z:670:THR:N	2.44	0.51
1:Z:895:PHE:O	1:Z:895:PHE:CD2	2.63	0.51
1:Z:962:ILE:HD13	1:Z:966:VAL:HG22	1.93	0.51
1:Z:650:VAL:HG12	1:Z:650:VAL:O	2.11	0.51
1:F:928:VAL:HG22	1:F:929:PHE:N	2.26	0.51
1:F:985:ASN:OD1	1:F:985:ASN:N	2.43	0.51
1:J:781:PRO:HA	1:J:807:ALA:HB3	1.93	0.51
1:J:810:ASP:OD1	1:J:811:ALA:N	2.43	0.51
1:Z:982:CYS:SG	1:Z:984:ILE:HD11	2.51	0.51
1:F:791:SER:O	1:F:797:LYS:HA	2.11	0.51
1:J:922:GLN:OE1	1:J:924:PHE:CZ	2.64	0.51
1:Z:919:GLN:HE22	1:Z:922:GLN:HB2	1.75	0.51
1:F:729:ILE:HG23	1:F:774:ALA:HB3	1.93	0.51
1:F:900:ASN:OD1	1:J:892:LEU:HG	2.10	0.51
1:F:960:ALA:O	1:Z:966:VAL:HA	2.11	0.51
1:J:925:MET:SD	1:Z:925:MET:CE	2.99	0.51
1:F:978:ILE:HD13	1:J:976:VAL:CG1	2.41	0.50
1:J:920:GLY:C	1:J:922:GLN:N	2.64	0.50
1:Z:853:LYS:HE3	1:Z:859:TRP:CD1	2.45	0.50
1:Z:933:LEU:O	1:Z:934:THR:CB	2.58	0.50
1:F:619:PRO:HG3	1:F:645:LYS:HG2	1.92	0.50
1:F:851:GLU:HB2	1:Z:845:LEU:HD23	1.93	0.50
1:F:906:ASP:OD2	1:J:900:ASN:O	2.28	0.50
1:J:843:SER:HB2	1:Z:859:TRP:CE3	2.46	0.50
1:J:928:VAL:HG23	1:J:930:LEU:CD2	2.42	0.50
1:F:917:VAL:HG11	1:J:818:PHE:CD2	2.47	0.50
1:J:628:VAL:HG21	1:J:711:ILE:CD1	2.35	0.50
1:F:624:LEU:HD11	1:F:707:VAL:CB	2.42	0.50
1:J:854:ASP:OD2	1:J:860:ASN:ND2	2.45	0.50
1:Z:916:PHE:C	1:Z:917:VAL:CG2	2.80	0.50
1:F:726:TYR:HD1	1:F:810:ASP:HA	1.77	0.50
1:F:863:TRP:CD2	1:Z:865:VAL:HG21	2.47	0.50
1:J:739:ASP:OD1	1:J:741:THR:HG22	2.11	0.50
1:J:880:ILE:HD13	1:J:895:PHE:CZ	2.47	0.50
1:J:955:LEU:HD23	1:J:956:THR:O	2.11	0.50
1:F:618:PRO:HD3	1:F:696:ASN:HB3	1.94	0.50
1:F:902:ILE:CG1	1:J:895:PHE:HB3	2.41	0.50
1:Z:861:ALA:O	1:Z:883:SER:HB2	2.11	0.50
1:F:924:PHE:HE1	1:Z:929:PHE:CD2	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:780:LYS:CB	1:Z:780:LYS:NZ	2.74	0.50
1:F:790:ARG:HD3	1:F:800:PHE:CE1	2.47	0.50
1:F:917:VAL:CG1	1:F:924:PHE:HD2	2.18	0.50
1:Z:722:LEU:HD23	1:Z:731:ALA:HA	1.94	0.50
1:Z:837:LEU:CD2	1:Z:842:ALA:HB3	2.42	0.50
1:Z:845:LEU:O	1:Z:845:LEU:HG	2.12	0.50
1:J:845:LEU:HD21	1:Z:861:ALA:HB1	1.94	0.50
1:J:778:ASN:O	1:J:780:LYS:HG3	2.12	0.49
1:Z:618:PRO:O	1:Z:702:GLY:HA3	2.12	0.49
1:Z:802:GLU:CG	1:Z:803:ALA:N	2.73	0.49
1:Z:831:LEU:O	1:Z:832:LEU:HD23	2.11	0.49
1:J:729:ILE:HG21	1:J:787:PHE:HE2	1.77	0.49
1:J:926:ASN:OD1	1:Z:921:ASN:HB3	2.13	0.49
1:Z:647:VAL:H	1:Z:650:VAL:HG23	1.78	0.49
1:Z:846:GLU:HB3	1:Z:866:LYS:O	2.11	0.49
1:Z:884:MET:HG3	1:Z:884:MET:O	2.13	0.49
1:F:690:LEU:C	1:F:690:LEU:HD13	2.33	0.49
1:Z:711:ILE:HD12	1:Z:711:ILE:C	2.32	0.49
1:F:893:SER:CB	1:Z:900:ASN:OD1	2.58	0.49
1:J:689:ARG:NH2	1:J:706:SER:O	2.46	0.49
1:J:759:VAL:HG13	1:J:763:THR:HG21	1.94	0.49
1:Z:919:GLN:O	1:Z:920:GLY:C	2.51	0.49
1:F:689:ARG:NH1	1:F:689:ARG:HB2	2.28	0.49
1:F:933:LEU:HD21	1:F:935:ALA:CB	2.43	0.49
1:J:635:TYR:CE1	1:J:711:ILE:HD13	2.48	0.49
1:Z:773:ILE:HD12	1:Z:773:ILE:O	2.13	0.49
1:F:621:VAL:CG2	1:F:705:ALA:HB3	2.43	0.49
1:J:880:ILE:HD13	1:J:895:PHE:CE1	2.47	0.49
1:F:746:PHE:O	1:F:766:LEU:HB2	2.13	0.49
1:J:844:ARG:C	1:J:845:LEU:HD12	2.33	0.49
1:J:742:VAL:HG12	1:J:793:ASN:HB3	1.95	0.48
1:J:938:ILE:HG12	1:Z:933:LEU:CB	2.42	0.48
1:J:978:ILE:HG23	1:Z:974:SER:O	2.13	0.48
1:Z:625:THR:HG22	1:Z:640:ARG:O	2.13	0.48
1:F:902:ILE:HG22	1:F:904:PHE:HE1	1.78	0.48
1:F:913:THR:O	1:F:914:PRO:O	2.30	0.48
1:Z:717:PRO:O	1:Z:801:VAL:HG21	2.13	0.48
1:F:759:VAL:O	1:F:763:THR:OG1	2.30	0.48
1:F:842:ALA:HA	1:J:859:TRP:CZ3	2.48	0.48
1:F:978:ILE:CD1	1:J:976:VAL:HG11	2.43	0.48
1:J:938:ILE:HG12	1:Z:933:LEU:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:733:PRO:HG3	1:F:744:PHE:CE1	2.48	0.48
1:J:918:ALA:HB2	1:J:923:ILE:HD11	1.95	0.48
1:Z:767:GLY:HA3	1:Z:772:TRP:CH2	2.47	0.48
1:Z:816:ASP:OD1	1:Z:816:ASP:N	2.46	0.48
1:F:905:ILE:HG22	1:F:906:ASP:N	2.29	0.48
1:F:926:ASN:HB3	1:J:921:ASN:O	2.14	0.48
1:J:758:GLN:OE1	1:J:758:GLN:N	2.46	0.48
1:F:777:ILE:HD13	1:F:829:LYS:HG2	1.94	0.48
1:F:936:PRO:O	1:F:951:PRO:HG3	2.14	0.48
1:F:725:GLY:N	1:F:808:SER:HB3	2.28	0.48
1:F:897:VAL:O	1:Z:904:PHE:CA	2.58	0.48
1:F:900:ASN:HA	1:Z:906:ASP:CG	2.34	0.48
1:J:722:LEU:N	1:J:722:LEU:CD1	2.76	0.48
1:J:724:PRO:HB3	1:J:806:ARG:O	2.14	0.48
1:Z:624:LEU:HD23	1:Z:625:THR:N	2.29	0.48
1:Z:730:THR:HG23	1:Z:773:ILE:HG22	1.96	0.48
1:F:675:GLU:OE2	1:F:678:TYR:HD1	1.96	0.48
1:F:884:MET:HE2	1:F:893:SER:HB2	1.96	0.48
1:F:928:VAL:HG12	1:Z:930:LEU:HD13	1.95	0.48
1:J:867:ILE:HD11	1:Z:882:LEU:CD2	2.42	0.48
1:Z:918:ALA:CB	1:Z:923:ILE:CG1	2.92	0.48
1:F:821:LYS:HE3	1:Z:901:ARG:HH22	1.78	0.47
1:F:914:PRO:CB	1:J:815:LEU:CD2	2.90	0.47
1:F:925:MET:HE2	1:F:928:VAL:HB	1.96	0.47
1:F:930:LEU:O	1:Z:811:ALA:CB	2.61	0.47
1:J:937:THR:O	1:J:938:ILE:HG13	2.14	0.47
1:F:884:MET:CE	1:Z:867:ILE:CG1	2.92	0.47
1:Z:753:ILE:HG13	1:Z:788:TYR:CE2	2.49	0.47
1:F:882:LEU:HD23	1:Z:865:VAL:CG1	2.45	0.47
1:F:884:MET:HA	1:F:892:LEU:O	2.14	0.47
1:J:959:ASN:HB2	1:Z:954:LYS:HA	1.96	0.47
1:Z:624:LEU:HD23	1:Z:624:LEU:C	2.34	0.47
1:F:902:ILE:HD12	1:J:895:PHE:CA	2.43	0.47
1:F:946:ALA:O	1:J:953:GLY:CA	2.60	0.47
1:Z:717:PRO:HG3	1:Z:789:ILE:HG22	1.96	0.47
1:F:980:GLU:HA	1:Z:986:GLY:HA3	1.96	0.47
1:F:987:THR:OG1	1:F:989:ARG:NH2	2.47	0.47
1:F:619:PRO:HB2	1:F:644:PRO:HG2	1.96	0.47
1:Z:683:LEU:CD2	1:Z:688:TYR:CZ	2.97	0.47
1:Z:919:GLN:NE2	1:Z:922:GLN:HB2	2.29	0.47
1:F:624:LEU:HD11	1:F:707:VAL:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:746:PHE:CD2	1:F:772:TRP:HB3	2.49	0.47
1:F:756:ILE:HD12	1:F:757:ARG:N	2.30	0.47
1:F:884:MET:CE	1:Z:867:ILE:HD11	2.36	0.47
1:J:770:LEU:HD23	1:J:770:LEU:HA	1.77	0.47
1:F:626:ALA:HB2	1:F:707:VAL:CG1	2.45	0.47
1:F:656:LEU:HD21	1:F:688:TYR:HB3	1.95	0.47
1:F:812:GLU:O	1:F:816:ASP:HB2	2.14	0.47
1:F:827:LEU:CD2	1:F:881:GLY:HA3	2.45	0.47
1:F:913:THR:C	1:F:914:PRO:O	2.51	0.47
1:J:635:TYR:OH	1:J:795:VAL:HA	2.13	0.47
1:F:900:ASN:O	1:F:919:GLN:HG3	2.15	0.47
1:F:904:PHE:CD1	1:F:904:PHE:N	2.83	0.47
1:J:880:ILE:HB	1:J:897:VAL:HA	1.97	0.47
1:J:913:THR:HG23	1:Z:819:LYS:CD	2.43	0.47
1:F:643:THR:CG2	1:F:646:VAL:H	2.27	0.47
1:F:832:LEU:HD22	1:Z:912:GLU:HG3	1.97	0.47
1:F:904:PHE:CD1	1:F:916:PHE:HD2	2.33	0.47
1:J:745:GLU:HG2	1:J:768:THR:HG22	1.97	0.47
1:J:919:GLN:O	1:J:920:GLY:O	2.33	0.47
1:F:619:PRO:CG	1:F:645:LYS:HG2	2.44	0.46
1:F:790:ARG:HD2	1:F:797:LYS:HB3	1.97	0.46
1:F:863:TRP:CD1	1:Z:847:GLU:OE1	2.68	0.46
1:J:925:MET:CE	1:Z:925:MET:HE3	2.45	0.46
1:J:933:LEU:HD12	1:J:934:THR:H	1.79	0.46
1:Z:753:ILE:HD13	1:Z:755:ASP:O	2.15	0.46
1:F:928:VAL:HG11	1:Z:930:LEU:CD1	2.46	0.46
1:J:816:ASP:OD1	1:J:816:ASP:C	2.54	0.46
1:Z:725:GLY:HA3	1:Z:728:GLN:CG	2.45	0.46
1:F:869:GLN:HE22	1:F:871:LYS:HB2	1.80	0.46
1:J:861:ALA:O	1:J:883:SER:OG	2.31	0.46
1:F:776:SER:N	1:F:779:ILE:HD12	2.30	0.46
1:J:653:LEU:O	1:J:692:VAL:HA	2.14	0.46
1:Z:849:SER:HB3	1:Z:863:TRP:HD1	1.80	0.46
1:F:888:GLU:HA	1:F:888:GLU:OE1	2.14	0.46
1:J:812:GLU:OE1	1:Z:931:LYS:NZ	2.47	0.46
1:F:858:LYS:NZ	1:Z:841:ASN:OD1	2.45	0.46
1:F:980:GLU:C	1:Z:986:GLY:HA3	2.35	0.46
1:J:712:ALA:C	1:J:795:VAL:HG11	2.35	0.46
1:J:880:ILE:HG22	1:J:898:ALA:N	2.31	0.46
1:Z:735:LEU:HD23	1:Z:736:ALA:N	2.31	0.46
1:F:722:LEU:CD1	1:F:729:ILE:HD11	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:814:TYR:CE1	1:Z:924:PHE:CZ	3.04	0.46
1:F:928:VAL:CG2	1:J:923:ILE:CG2	2.68	0.46
1:J:962:ILE:HG12	1:Z:960:ALA:HB2	1.98	0.46
1:F:847:GLU:OE2	1:J:847:GLU:OE2	2.34	0.46
1:J:756:ILE:HD11	1:J:802:GLU:OE2	2.16	0.46
1:F:933:LEU:HD11	1:J:930:LEU:HD23	1.98	0.46
1:J:636:GLN:HA	1:J:680:PHE:O	2.15	0.46
1:J:745:GLU:HA	1:J:768:THR:HG22	1.97	0.46
1:F:720:ILE:HD13	1:F:733:PRO:HA	1.99	0.45
1:J:902:ILE:C	1:J:902:ILE:HD12	2.36	0.45
1:J:925:MET:HE2	1:J:925:MET:HB2	1.73	0.45
1:F:733:PRO:O	1:F:734:HIS:ND1	2.48	0.45
1:F:884:MET:HB3	1:F:893:SER:HA	1.97	0.45
1:F:776:SER:OG	1:F:777:ILE:N	2.49	0.45
1:F:902:ILE:CG2	1:F:904:PHE:CE1	2.98	0.45
1:J:918:ALA:CB	1:J:923:ILE:CD1	2.93	0.45
1:F:728:GLN:CB	1:F:775:ALA:HB2	2.46	0.45
1:F:757:ARG:HH11	1:F:758:GLN:HB3	1.80	0.45
1:F:821:LYS:HE3	1:Z:901:ARG:NH2	2.31	0.45
1:F:880:ILE:O	1:F:880:ILE:CG1	2.65	0.45
1:J:905:ILE:HG22	1:Z:898:ALA:HB2	1.97	0.45
1:F:899:ALA:O	1:Z:907:PRO:HD2	2.16	0.45
1:F:932:ARG:CG	1:Z:937:THR:HB	2.46	0.45
1:J:917:VAL:HG21	1:Z:818:PHE:CD2	2.51	0.45
1:Z:785:TYR:O	1:Z:805:GLY:N	2.50	0.45
1:F:901:ARG:NH2	1:J:894:GLN:NE2	2.59	0.45
1:Z:955:LEU:CD1	1:Z:957:ALA:HB2	2.47	0.45
1:J:714:PRO:HB3	1:J:742:VAL:HG11	1.99	0.45
1:J:863:TRP:CZ3	1:J:865:VAL:HG23	2.51	0.45
1:J:880:ILE:HD12	1:J:881:GLY:N	2.32	0.45
1:Z:934:THR:HG22	1:Z:934:THR:O	2.17	0.45
1:F:901:ARG:CD	1:F:919:GLN:OE1	2.64	0.45
1:J:747:TRP:CE3	1:J:765:TYR:HA	2.52	0.45
1:Z:637:VAL:HG13	1:Z:637:VAL:O	2.17	0.45
1:F:924:PHE:CD1	1:Z:929:PHE:HD2	2.35	0.45
1:J:755:ASP:OD2	1:J:757:ARG:NH2	2.50	0.45
1:J:845:LEU:N	1:J:845:LEU:CD1	2.80	0.45
1:Z:691:THR:HG22	1:Z:706:SER:OG	2.16	0.45
1:Z:849:SER:HB3	1:Z:863:TRP:CD1	2.52	0.45
1:J:966:VAL:HG12	1:J:966:VAL:O	2.18	0.44
1:F:726:TYR:HE2	1:F:820:GLY:HA3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:757:ARG:NH1	1:F:758:GLN:HB3	2.32	0.44
1:J:917:VAL:HB	1:Z:818:PHE:CE2	2.53	0.44
1:F:624:LEU:HD11	1:F:707:VAL:HG23	1.94	0.44
1:F:934:THR:HG21	1:J:929:PHE:CE2	2.53	0.44
1:J:832:LEU:O	1:J:834:LYS:N	2.49	0.44
1:J:880:ILE:CB	1:J:897:VAL:HA	2.47	0.44
1:J:913:THR:CG2	1:Z:819:LYS:CD	2.95	0.44
1:Z:790:ARG:HB3	1:Z:800:PHE:CD1	2.53	0.44
1:Z:802:GLU:HG2	1:Z:803:ALA:N	2.31	0.44
1:J:746:PHE:CD2	1:J:772:TRP:CD1	3.05	0.44
1:Z:939:THR:HG22	1:Z:941:GLY:H	1.82	0.44
1:F:905:ILE:HD13	1:F:914:PRO:CA	2.45	0.44
1:F:954:LYS:HD2	1:Z:959:ASN:O	2.17	0.44
1:J:720:ILE:HB	1:J:789:ILE:CD1	2.48	0.44
1:F:706:SER:OG	1:J:768:THR:OG1	2.17	0.44
1:Z:720:ILE:O	1:Z:720:ILE:HG13	2.17	0.44
1:F:990:ALA:HB2	1:J:984:ILE:HD12	2.00	0.44
1:J:621:VAL:HG13	1:J:641:TRP:HB2	2.00	0.44
1:J:932:ARG:HB2	1:Z:927:ASP:CG	2.38	0.44
1:F:636:GLN:HG3	1:F:681:THR:HA	1.98	0.44
1:F:656:LEU:HD22	1:F:657:THR:N	2.33	0.44
1:Z:790:ARG:HD2	1:Z:797:LYS:HB3	2.00	0.44
1:Z:904:PHE:O	1:Z:914:PRO:CA	2.65	0.44
1:F:819:LYS:HG3	1:Z:913:THR:HA	1.99	0.43
1:J:958:LYS:O	1:J:959:ASN:OD1	2.36	0.43
1:F:877:VAL:HG22	1:F:878:ALA:N	2.33	0.43
1:F:880:ILE:HG22	1:F:897:VAL:HG13	1.99	0.43
1:J:844:ARG:O	1:J:844:ARG:HG3	2.18	0.43
1:Z:632:SER:O	1:Z:632:SER:OG	2.27	0.43
1:F:733:PRO:HG3	1:F:744:PHE:CD1	2.53	0.43
1:F:827:LEU:HD22	1:F:881:GLY:HA3	2.00	0.43
1:F:827:LEU:HD23	1:F:862:MET:CE	2.47	0.43
1:F:893:SER:HG	1:Z:899:ALA:CA	2.30	0.43
1:J:739:ASP:OD1	1:J:740:PRO:HD2	2.19	0.43
1:J:867:ILE:HD13	1:Z:882:LEU:CD2	2.48	0.43
1:J:970:SER:HB3	1:Z:965:SER:HA	2.00	0.43
1:Z:638:LEU:HD11	1:Z:679:ARG:NH2	2.32	0.43
1:F:893:SER:OG	1:Z:878:ALA:CB	2.66	0.43
1:J:918:ALA:HB2	1:J:923:ILE:CD1	2.49	0.43
1:J:962:ILE:HG21	1:Z:960:ALA:HB2	2.00	0.43
1:Z:746:PHE:CD2	1:Z:789:ILE:HG13	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:899:ALA:N	1:Z:905:ILE:O	2.40	0.43
1:J:737:VAL:HG13	1:J:737:VAL:O	2.19	0.43
1:F:845:LEU:HA	1:F:867:ILE:HD13	2.01	0.43
1:F:917:VAL:HG11	1:J:818:PHE:CG	2.53	0.43
1:F:955:LEU:C	1:F:955:LEU:CD2	2.87	0.43
1:J:750:GLU:N	1:J:750:GLU:OE1	2.52	0.43
1:J:822:ILE:HG23	1:J:896:LEU:HD11	2.01	0.43
1:J:932:ARG:HG3	1:J:932:ARG:HH11	1.84	0.43
1:Z:933:LEU:HD12	1:Z:934:THR:N	2.31	0.43
1:F:901:ARG:HG2	1:F:919:GLN:CB	2.37	0.43
1:F:914:PRO:HG3	1:J:822:ILE:HD12	2.01	0.43
1:Z:711:ILE:C	1:Z:711:ILE:CD1	2.87	0.43
1:Z:928:VAL:HG22	1:Z:930:LEU:HD23	2.01	0.43
1:F:902:ILE:HD12	1:J:895:PHE:H	1.80	0.43
1:J:739:ASP:OD2	1:J:742:VAL:HG13	2.18	0.43
1:J:943:ASN:HB2	1:J:944:PRO:HD3	2.01	0.43
1:F:904:PHE:O	1:F:914:PRO:HA	2.18	0.42
1:F:946:ALA:CB	1:J:951:PRO:O	2.67	0.42
1:Z:831:LEU:HA	1:Z:866:LYS:HD3	2.01	0.42
1:F:976:VAL:HG12	1:F:977:THR:N	2.34	0.42
1:J:962:ILE:HD12	1:J:962:ILE:H	1.83	0.42
1:Z:837:LEU:CG	1:Z:842:ALA:HB3	2.49	0.42
1:F:745:GLU:OE2	1:F:790:ARG:NH2	2.45	0.42
1:F:830:GLU:O	1:F:866:LYS:HE2	2.20	0.42
1:F:845:LEU:CD1	1:J:849:SER:HB2	2.49	0.42
1:J:722:LEU:HD23	1:J:729:ILE:CG2	2.49	0.42
1:Z:836:GLU:HB2	1:Z:844:ARG:CZ	2.49	0.42
1:J:744:PHE:O	1:J:768:THR:CA	2.62	0.42
1:Z:945:PRO:HB3	1:Z:948:SER:HG	1.85	0.42
1:Z:945:PRO:HB3	1:Z:948:SER:OG	2.19	0.42
1:F:683:LEU:HD12	1:F:683:LEU:HA	1.90	0.42
1:F:832:LEU:CD2	1:Z:912:GLU:HG3	2.49	0.42
1:F:882:LEU:HD21	1:Z:878:ALA:O	2.19	0.42
1:F:884:MET:SD	1:Z:869:GLN:OE1	2.78	0.42
1:F:895:PHE:CE1	1:Z:880:ILE:HG12	2.54	0.42
1:F:924:PHE:CE1	1:Z:929:PHE:HD2	2.36	0.42
1:F:938:ILE:HG22	1:F:939:THR:N	2.35	0.42
1:J:903:ALA:HB2	1:J:917:VAL:HG13	2.00	0.42
1:F:621:VAL:HG23	1:F:705:ALA:HB3	2.01	0.42
1:F:809:ASP:O	1:F:810:ASP:OD1	2.36	0.42
1:J:910:GLY:O	1:J:912:GLU:OE1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:913:THR:HG22	1:Z:819:LYS:HD3	2.02	0.42
1:Z:722:LEU:HD21	1:Z:731:ALA:HB2	2.01	0.42
1:J:721:GLU:C	1:J:722:LEU:HD12	2.40	0.42
1:J:962:ILE:HG12	1:Z:960:ALA:CB	2.49	0.42
1:Z:780:LYS:CB	1:Z:780:LYS:HZ3	2.31	0.42
1:F:842:ALA:HA	1:J:859:TRP:CE3	2.55	0.42
1:F:903:ALA:CB	1:F:917:VAL:HG23	2.49	0.42
1:F:913:THR:CA	1:J:819:LYS:HD3	2.49	0.42
1:F:914:PRO:HG2	1:J:815:LEU:HD23	2.01	0.42
1:J:727:PHE:HE1	1:J:780:LYS:HA	1.84	0.42
1:Z:791:SER:H	1:Z:798:SER:HG	1.68	0.42
1:F:927:ASP:OD2	1:F:927:ASP:C	2.59	0.42
1:J:913:THR:HA	1:Z:819:LYS:HB2	2.01	0.42
1:Z:615:GLY:HA2	1:Z:698:TRP:CZ3	2.54	0.42
1:Z:746:PHE:CD1	1:Z:746:PHE:N	2.88	0.42
1:Z:771:TYR:N	1:Z:771:TYR:CD1	2.88	0.42
1:F:946:ALA:HB1	1:J:951:PRO:O	2.20	0.42
1:J:691:THR:HG23	1:J:706:SER:HB3	2.02	0.42
1:J:915:MET:O	1:Z:923:ILE:HD11	2.20	0.42
1:Z:695:VAL:HG12	1:Z:701:GLN:HG3	2.01	0.42
1:Z:826:HIS:CE1	1:Z:852:TRP:CZ2	3.08	0.42
1:F:902:ILE:O	1:F:903:ALA:HB2	2.20	0.41
1:J:680:PHE:CE1	1:J:690:LEU:HD11	2.55	0.41
1:J:720:ILE:HD13	1:J:789:ILE:HG21	2.02	0.41
1:Z:683:LEU:HD22	1:Z:688:TYR:CE2	2.55	0.41
1:Z:832:LEU:HD23	1:Z:832:LEU:N	2.35	0.41
1:F:722:LEU:HD12	1:F:729:ILE:HD11	2.02	0.41
1:F:895:PHE:CE1	1:Z:880:ILE:CG1	3.03	0.41
1:Z:928:VAL:CG2	1:Z:930:LEU:HD23	2.50	0.41
1:F:930:LEU:O	1:Z:811:ALA:HB2	2.21	0.41
1:J:972:THR:O	1:J:972:THR:CG2	2.54	0.41
1:Z:916:PHE:HA	1:Z:924:PHE:O	2.19	0.41
1:F:683:LEU:HD11	1:F:688:TYR:CE2	2.55	0.41
1:J:843:SER:HA	1:J:868:GLU:O	2.21	0.41
1:F:882:LEU:HD12	1:F:894:GLN:O	2.20	0.41
1:Z:962:ILE:HG22	1:Z:964:GLY:O	2.20	0.41
1:F:871:LYS:O	1:F:874:LYS:HG2	2.20	0.41
1:F:989:ARG:HB2	1:J:983:THR:HA	2.02	0.41
1:J:634:GLU:OE1	1:J:634:GLU:HA	2.20	0.41
1:J:665:GLU:CD	1:J:689:ARG:HG3	2.41	0.41
1:J:928:VAL:HG23	1:J:930:LEU:HD22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:696:ASN:HD21	1:J:700:GLN:HB3	1.86	0.41
1:J:766:LEU:HA	1:J:766:LEU:HD23	1.85	0.41
1:J:916:PHE:HD1	1:J:916:PHE:O	2.03	0.41
1:Z:719:ARG:NH2	1:Z:734:HIS:ND1	2.68	0.41
1:F:827:LEU:HD23	1:F:862:MET:HE3	2.03	0.41
1:F:966:VAL:HG23	1:Z:968:ALA:HB1	2.02	0.41
1:J:729:ILE:O	1:J:773:ILE:HG23	2.21	0.41
1:J:742:VAL:HG23	1:J:742:VAL:O	2.20	0.41
1:J:902:ILE:HG13	1:J:918:ALA:HB3	2.02	0.41
1:J:922:GLN:HG3	1:Z:780:LYS:HE2	2.02	0.41
1:F:832:LEU:HD13	1:Z:912:GLU:OE1	2.21	0.41
1:F:891:LYS:O	1:Z:876:TYR:HE2	2.01	0.41
1:F:900:ASN:ND2	1:J:893:SER:OG	2.54	0.41
1:F:993:ILE:CD1	1:J:988:LEU:HD22	2.51	0.41
1:J:657:THR:HG22	1:J:667:LEU:HD12	2.02	0.41
1:J:716:ALA:O	1:J:717:PRO:C	2.58	0.41
1:J:747:TRP:CH2	1:J:765:TYR:CG	3.09	0.41
1:Z:892:LEU:C	1:Z:893:SER:O	2.59	0.41
1:F:626:ALA:HB2	1:F:707:VAL:HG12	2.02	0.41
1:F:641:TRP:CH2	1:F:678:TYR:HB2	2.55	0.41
1:F:993:ILE:HD13	1:J:988:LEU:HD22	2.03	0.41
1:J:747:TRP:HB2	1:J:788:TYR:HB2	2.02	0.41
1:Z:655:ARG:HA	1:Z:670:THR:HA	2.02	0.41
1:Z:905:ILE:HG12	1:Z:914:PRO:CA	2.40	0.41
1:J:746:PHE:CD2	1:J:772:TRP:HD1	2.40	0.40
1:J:817:PHE:CD2	1:J:818:PHE:N	2.89	0.40
1:J:863:TRP:HH2	1:J:865:VAL:CG2	2.33	0.40
1:Z:793:ASN:OD1	1:Z:795:VAL:HG22	2.21	0.40
1:Z:815:LEU:HD13	1:Z:815:LEU:HA	1.65	0.40
1:F:914:PRO:CG	1:J:815:LEU:CD2	2.99	0.40
1:J:826:HIS:C	1:J:862:MET:HE1	2.41	0.40
1:Z:624:LEU:C	1:Z:624:LEU:CD2	2.89	0.40
1:F:721:GLU:HB2	1:F:732:THR:OG1	2.21	0.40
1:F:814:TYR:HD1	1:F:814:TYR:O	2.04	0.40
1:F:905:ILE:HB	1:J:898:ALA:HB2	2.02	0.40
1:F:912:GLU:O	1:J:819:LYS:HG3	2.20	0.40
1:J:756:ILE:O	1:J:759:VAL:HG23	2.21	0.40
1:J:788:TYR:HA	1:J:801:VAL:O	2.21	0.40
1:Z:860:ASN:OD1	1:Z:886:ASP:N	2.54	0.40
1:Z:903:ALA:HB1	1:Z:914:PRO:CB	2.49	0.40
1:F:750:GLU:H	1:F:750:GLU:CD	2.23	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:882:LEU:HD11	1:Z:878:ALA:CB	2.51	0.40
1:F:932:ARG:CD	1:Z:937:THR:HG21	2.52	0.40
1:J:672:ARG:NH1	1:J:672:ARG:O	2.54	0.40
1:F:882:LEU:CD2	1:Z:865:VAL:HG12	2.51	0.40
1:Z:833:GLU:O	1:Z:833:GLU:HG2	2.22	0.40
1:Z:905:ILE:HG21	1:Z:912:GLU:C	2.42	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	F	378/1132 (33%)	311 (82%)	50 (13%)	17 (4%)	2	23
1	J	378/1132 (33%)	317 (84%)	53 (14%)	8 (2%)	7	40
1	Z	381/1132 (34%)	311 (82%)	57 (15%)	13 (3%)	3	31
All	All	1137/3396 (34%)	939 (83%)	160 (14%)	38 (3%)	6	31

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	713	ALA
1	J	920	GLY
1	Z	651	SER
1	Z	893	SER
1	Z	934	THR
1	F	926	ASN
1	F	932	ARG
1	F	946	ALA
1	F	959	ASN
1	J	781	PRO
1	Z	809	ASP

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Mol	Chain	Res	Type
1	Z	967	ASN
1	Z	969	ASN
1	F	646	VAL
1	F	812	GLU
1	F	948	SER
1	J	962	ILE
1	Z	648	LYS
1	Z	894	GLN
1	Z	944	PRO
1	F	769	ALA
1	F	809	ASP
1	F	862	MET
1	F	991	GLU
1	J	838	THR
1	J	921	ASN
1	Z	650	VAL
1	F	714	PRO
1	F	944	PRO
1	J	723	THR
1	F	712	ALA
1	J	833	GLU
1	Z	943	ASN
1	F	813	GLY
1	F	914	PRO
1	Z	644	PRO
1	Z	945	PRO
1	J	984	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	312/958 (33%)	273 (88%)	39 (12%)	4 25
1	J	312/958 (33%)	268 (86%)	44 (14%)	3 21
1	Z	314/958 (33%)	272 (87%)	42 (13%)	4 23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	938/2874 (33%)	813 (87%)	125 (13%)	7 23

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	623	HIS
1	F	624	LEU
1	F	661	ASP
1	F	679	ARG
1	F	687	ASN
1	F	723	THR
1	F	770	LEU
1	F	784	ASP
1	F	797	LYS
1	F	814	TYR
1	F	815	LEU
1	F	824	GLU
1	F	836	GLU
1	F	837	LEU
1	F	838	THR
1	F	844	ARG
1	F	847	GLU
1	F	851	GLU
1	F	852	TRP
1	F	892	LEU
1	F	893	SER
1	F	900	ASN
1	F	902	ILE
1	F	913	THR
1	F	915	MET
1	F	917	VAL
1	F	921	ASN
1	F	926	ASN
1	F	927	ASP
1	F	937	THR
1	F	943	ASN
1	F	954	LYS
1	F	955	LEU
1	F	970	SER
1	F	972	THR
1	F	982	CYS
1	F	985	ASN

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Mol	Chain	Res	Type
1	F	987	THR
1	F	993	ILE
1	J	627	GLU
1	J	631	ASP
1	J	634	GLU
1	J	654	LEU
1	J	666	ARG
1	J	672	ARG
1	J	685	LEU
1	J	687	ASN
1	J	720	ILE
1	J	721	GLU
1	J	748	PHE
1	J	762	SER
1	J	765	TYR
1	J	766	LEU
1	J	771	TYR
1	J	772	TRP
1	J	780	LYS
1	J	784	ASP
1	J	787	PHE
1	J	844	ARG
1	J	852	TRP
1	J	874	LYS
1	J	880	ILE
1	J	882	LEU
1	J	894	GLN
1	J	895	PHE
1	J	896	LEU
1	J	902	ILE
1	J	905	ILE
1	J	913	THR
1	J	915	MET
1	J	917	VAL
1	J	921	ASN
1	J	925	MET
1	J	940	SER
1	J	943	ASN
1	J	949	LEU
1	J	950	THR
1	J	955	LEU
1	J	961	ASP

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Mol	Chain	Res	Type
1	J	962	ILE
1	J	973	LEU
1	J	981	ASN
1	J	983	THR
1	Z	627	GLU
1	Z	632	SER
1	Z	635	TYR
1	Z	645	LYS
1	Z	646	VAL
1	Z	655	ARG
1	Z	656	LEU
1	Z	661	ASP
1	Z	672	ARG
1	Z	682	GLN
1	Z	695	VAL
1	Z	703	ASP
1	Z	771	TYR
1	Z	777	ILE
1	Z	780	LYS
1	Z	790	ARG
1	Z	791	SER
1	Z	812	GLU
1	Z	815	LEU
1	Z	821	LYS
1	Z	832	LEU
1	Z	844	ARG
1	Z	845	LEU
1	Z	851	GLU
1	Z	867	ILE
1	Z	880	ILE
1	Z	891	LYS
1	Z	904	PHE
1	Z	916	PHE
1	Z	921	ASN
1	Z	929	PHE
1	Z	931	LYS
1	Z	933	LEU
1	Z	943	ASN
1	Z	945	PRO
1	Z	952	ASP
1	Z	958	LYS
1	Z	961	ASP

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Mol	Chain	Res	Type
1	Z	972	THR
1	Z	982	CYS
1	Z	989	ARG
1	Z	994	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	921	ASN
1	F	943	ASN
1	J	981	ASN
1	Z	909	ASN
1	Z	919	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.

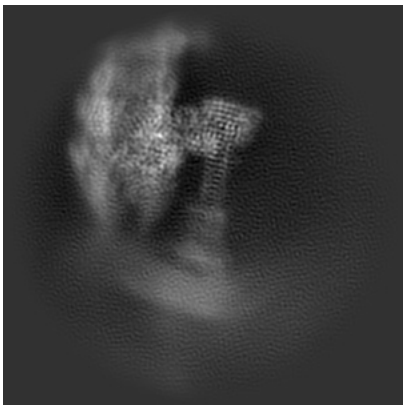
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38244. These allow visual inspection of the internal detail of the map and identification of artifacts.

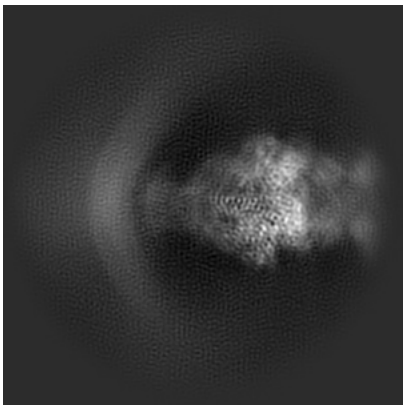
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

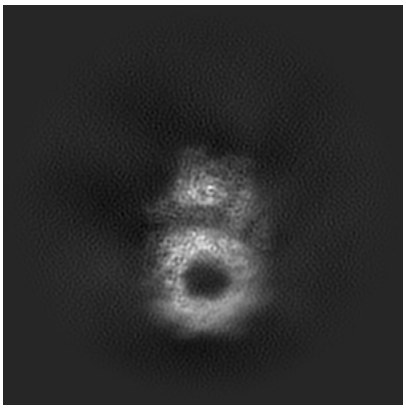
6.1.1 Primary map



X

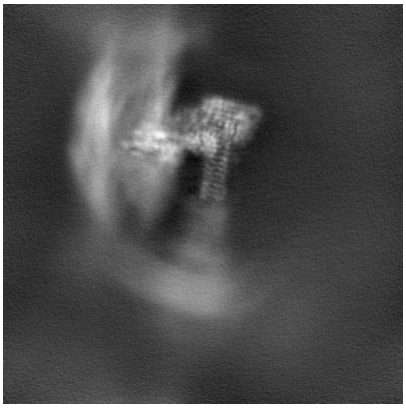


Y

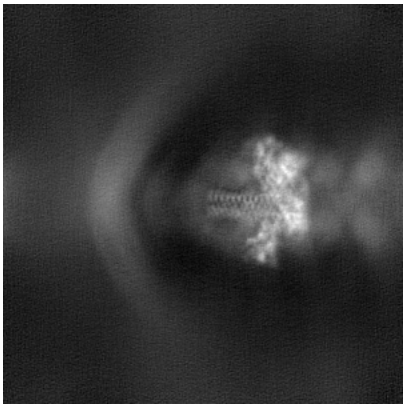


Z

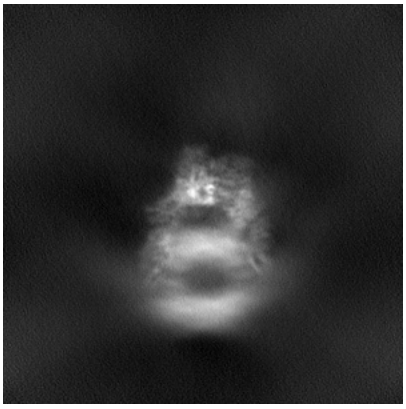
6.1.2 Raw map



X



Y

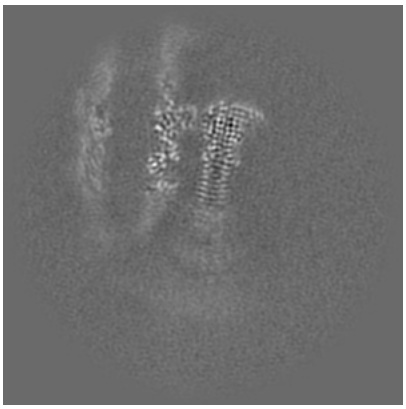


Z

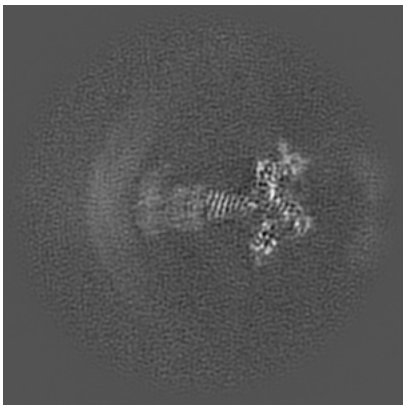
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

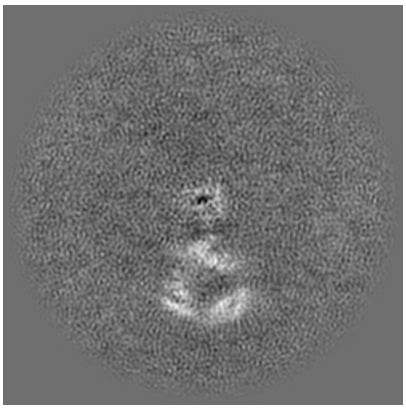
6.2.1 Primary map



X Index: 160

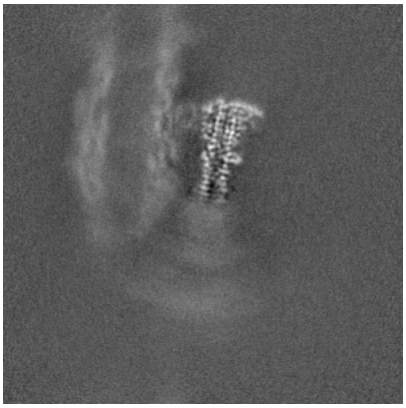


Y Index: 160

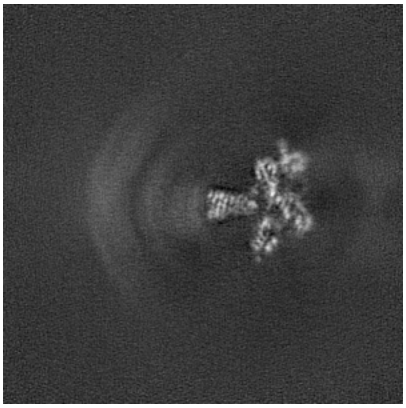


Z Index: 160

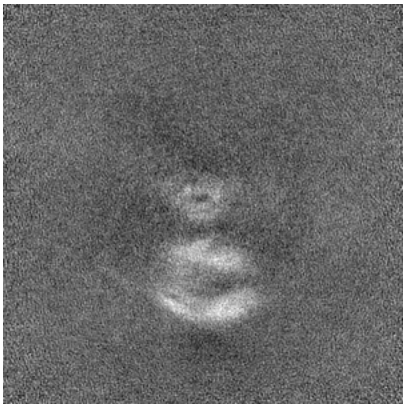
6.2.2 Raw map



X Index: 160



Y Index: 160

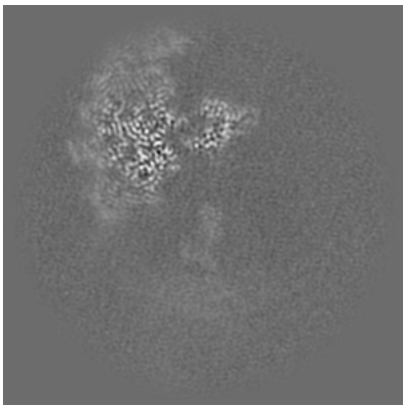


Z Index: 160

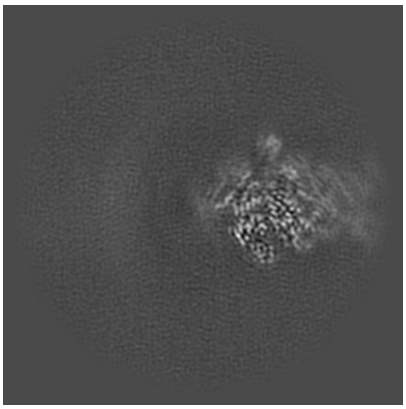
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

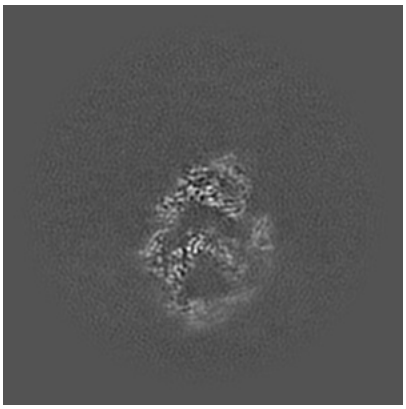
6.3.1 Primary map



X Index: 141

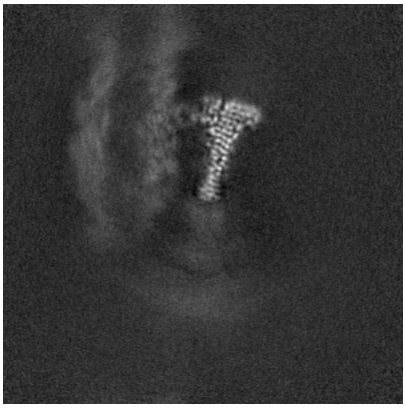


Y Index: 126

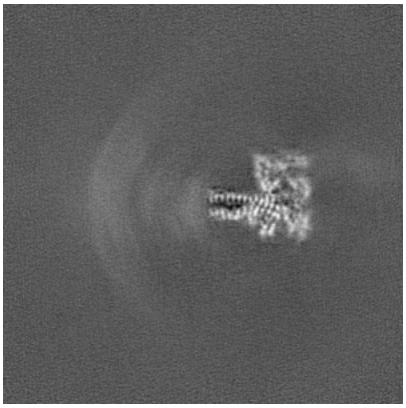


Z Index: 215

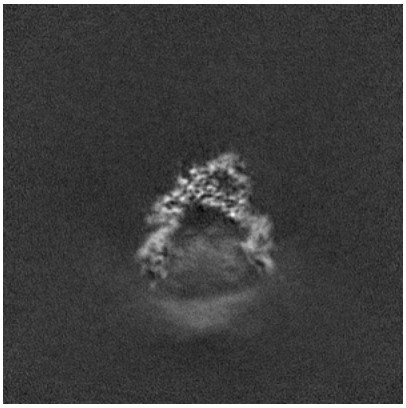
6.3.2 Raw map



X Index: 151



Y Index: 168

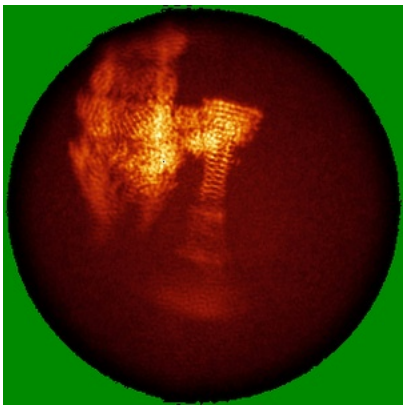


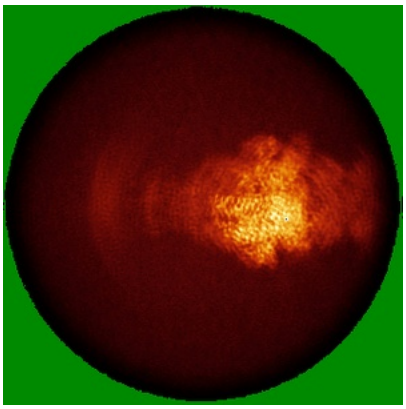
Z Index: 214

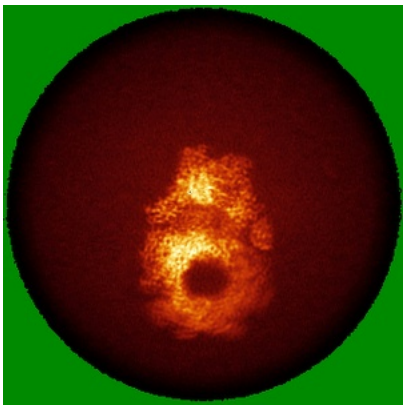
The images above show the largest variance slices of the map in three orthogonal directions.

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

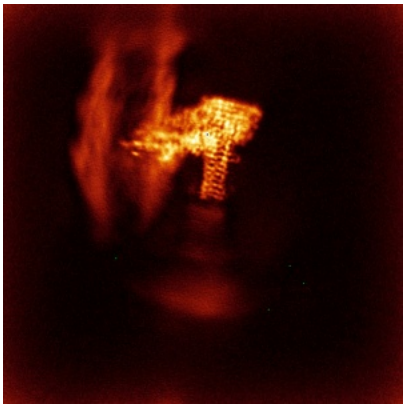
6.4.1 Primary map

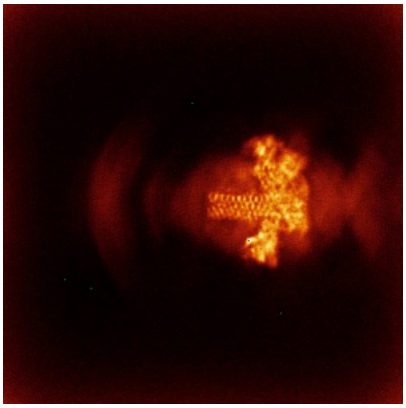

X

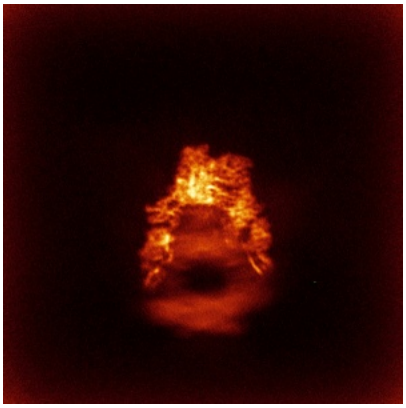

Y


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 0.3. 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.

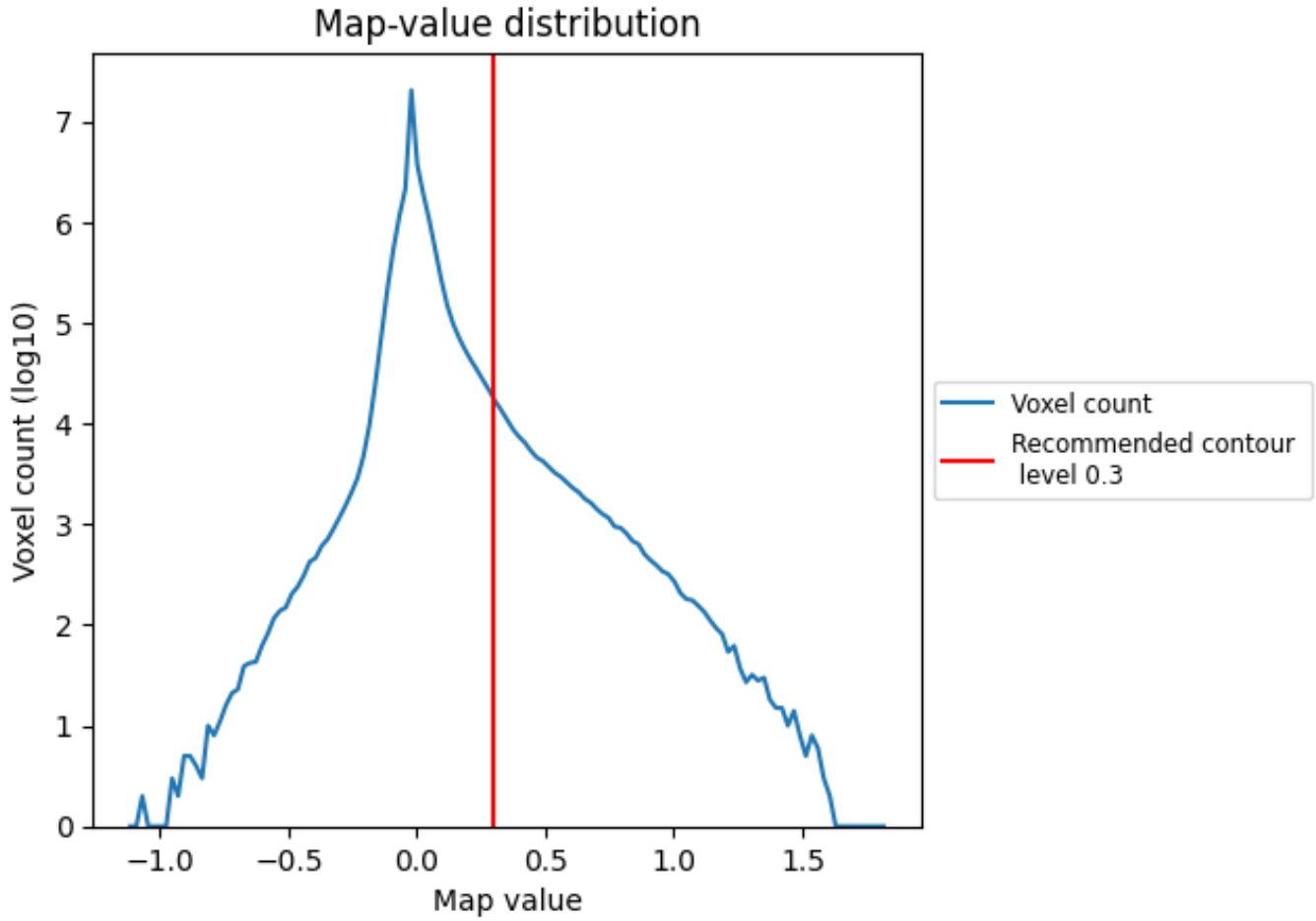
6.6 Mask visualisation (i)

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

7 Map analysis

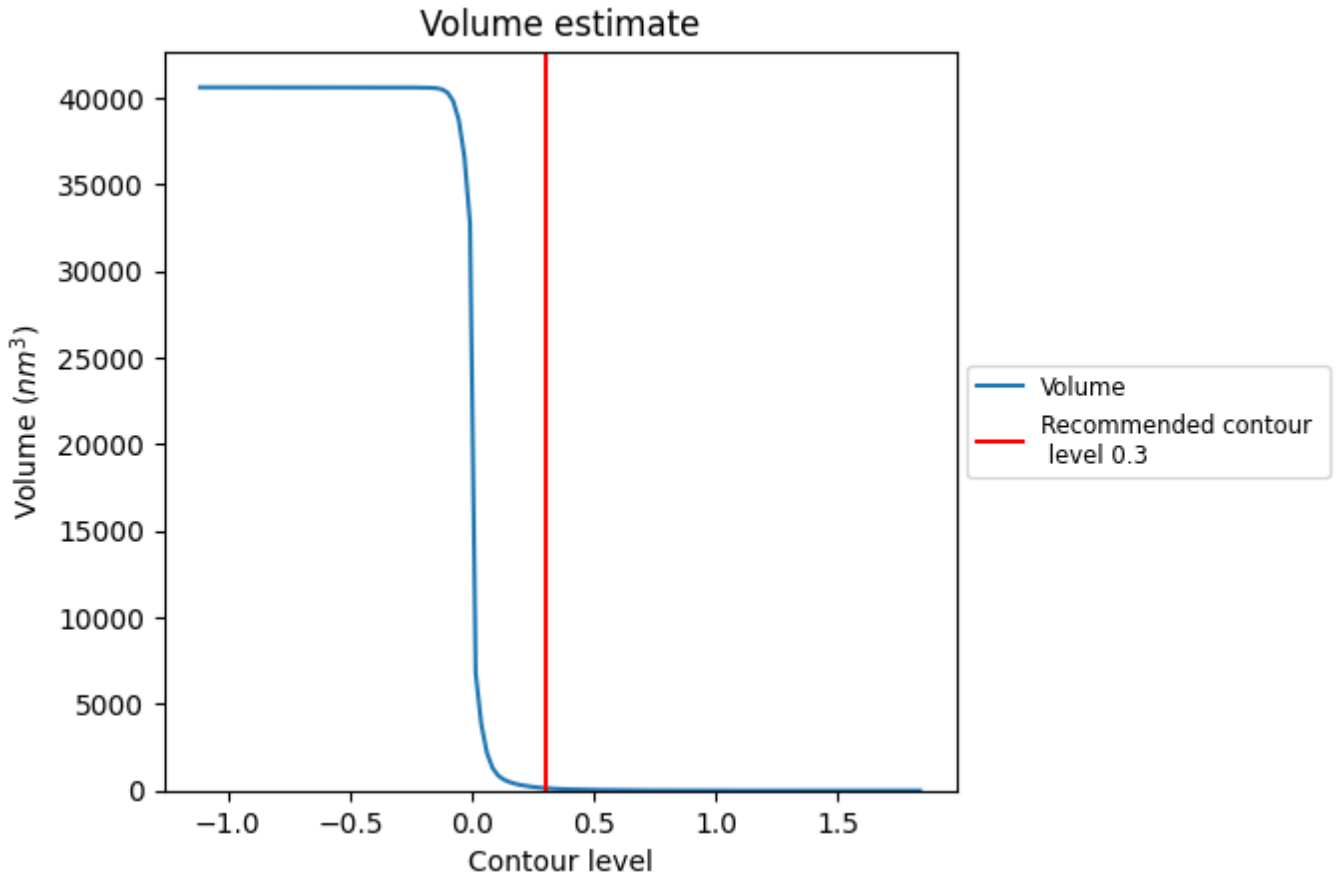
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

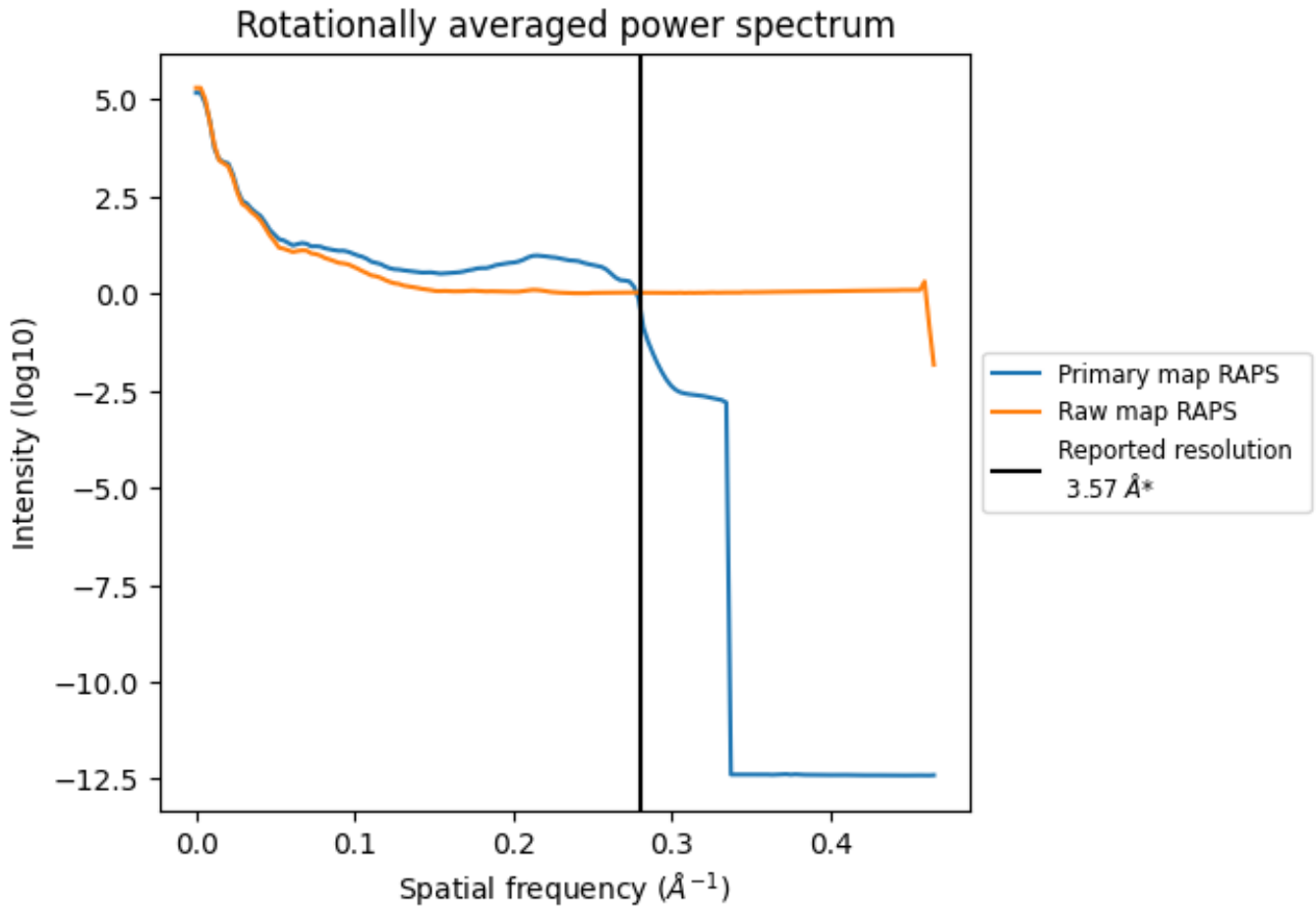
7.2 Volume estimate



The volume at the recommended contour level is 142 nm^3; this corresponds to an approximate mass of 128 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)

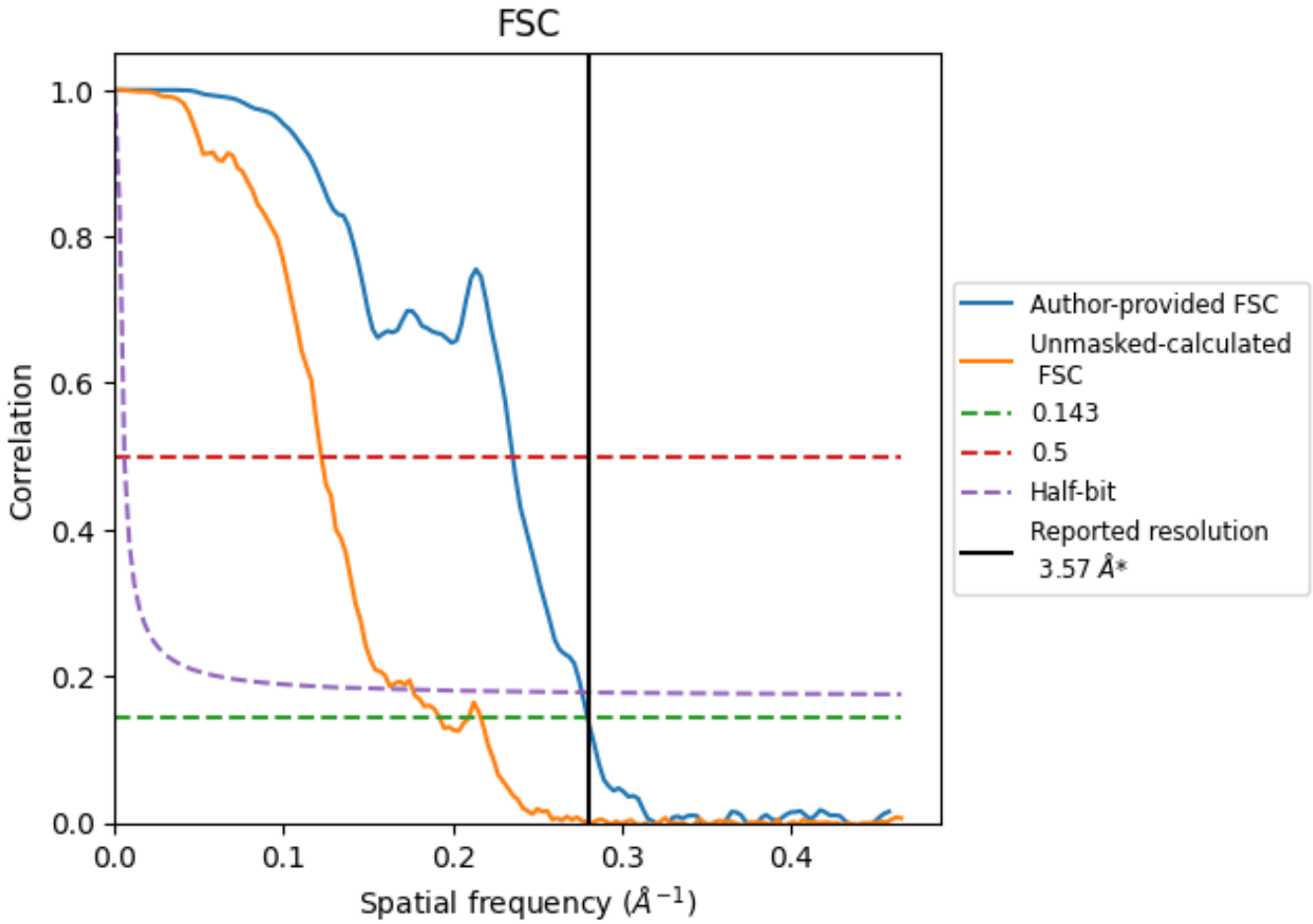


*Reported resolution corresponds to spatial frequency of 0.280 $Å^{-1}$

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 0.280 Å^{-1}

8.2 Resolution estimates (i)

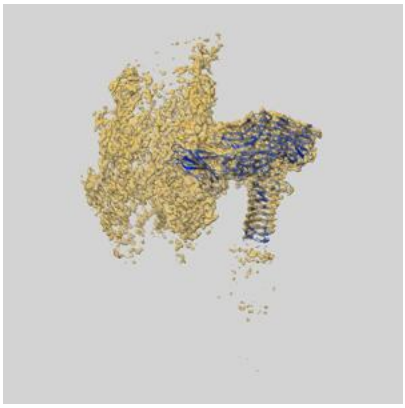
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.57	-	-
Author-provided FSC curve	3.57	4.25	3.62
Unmasked-calculated*	5.20	8.18	5.67

*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 5.20 differs from the reported value 3.57 by more than 10 %

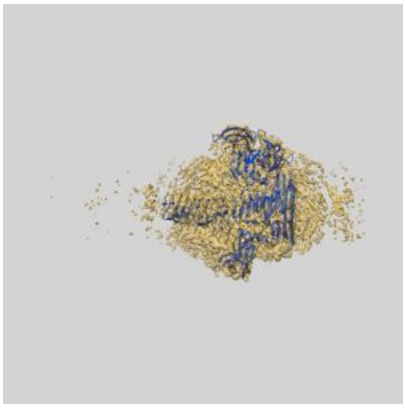
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38244 and PDB model 8XCI. Per-residue inclusion information can be found in section 3 on page 4.

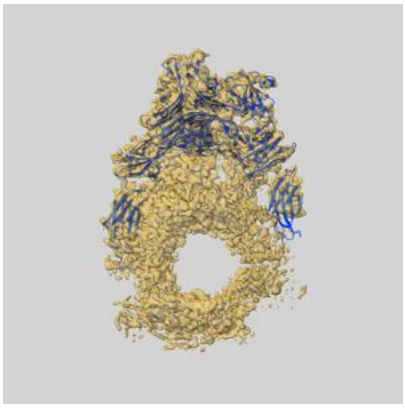
9.1 Map-model overlay



X



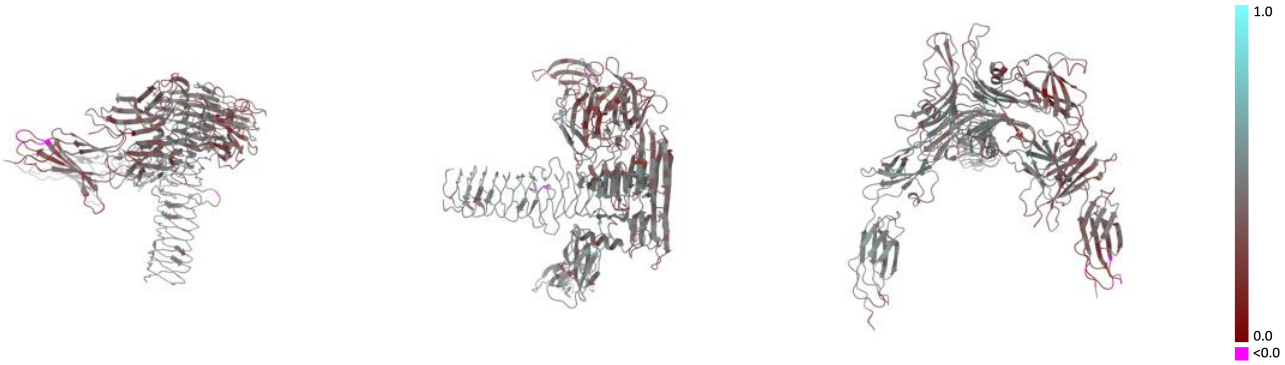
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 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.

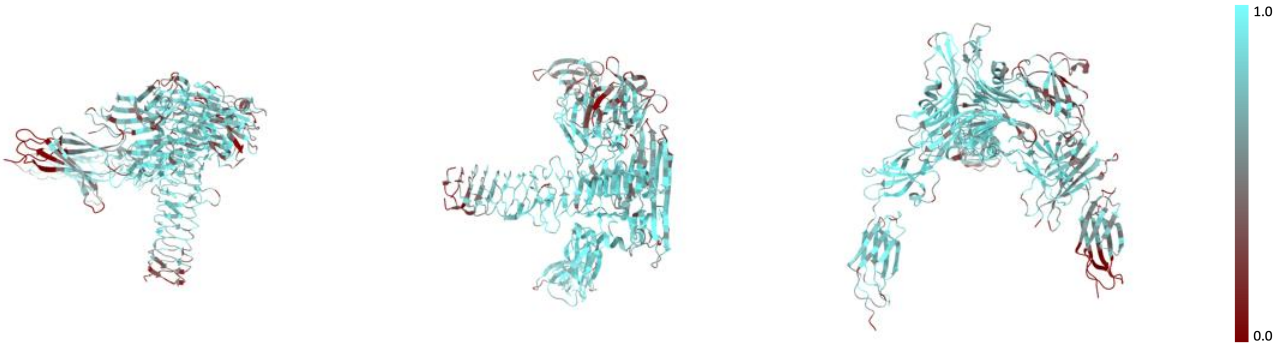
9.2 Q-score mapped to coordinate model



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.

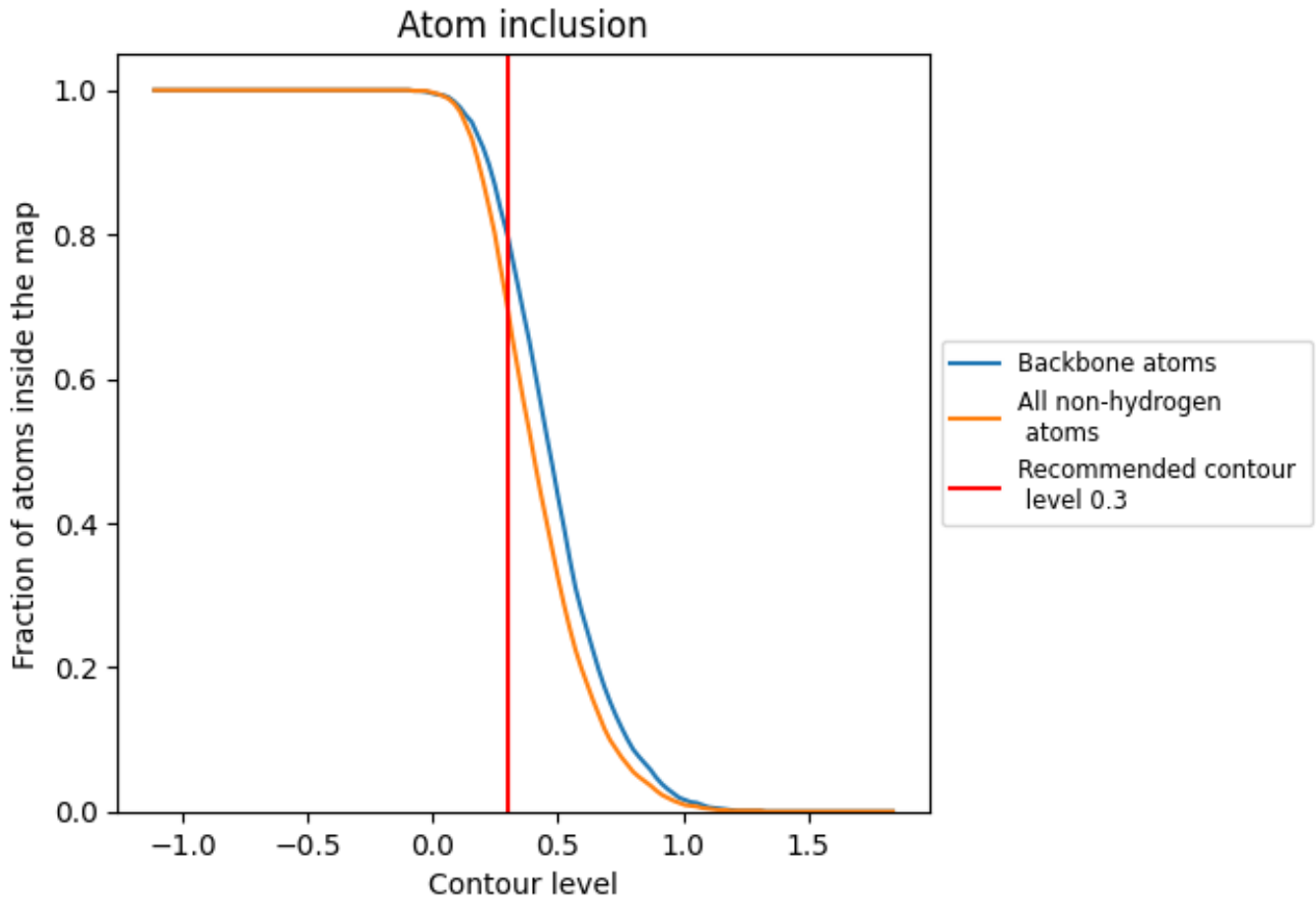
9.3 Atom inclusion mapped to coordinate model



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 (0.3).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6950	0.4240
F	0.6530	0.4030
J	0.6650	0.4090
Z	0.7680	0.4610