Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 06:21 PM EST

PDB ID	:	3J3I
EMDB ID	:	EMD-5600
Title	:	Penicillium chrysogenum virus (PcV) capsid structure
Authors	:	Luque, D.; Gomez-Blanco, J.; Garriga, D.; Brilot, A.; Gonzalez, J.M.; Havens, W.H.; Carrascosa, J.L.; Trus, B.L.; Verdaguer, N.; Grigorieff, N.; Ghabrial, S.A.; Caston, J.R.
Deposited on	:	2013-03-08
Resolution	:	4.10 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 (i) symbol.

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

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

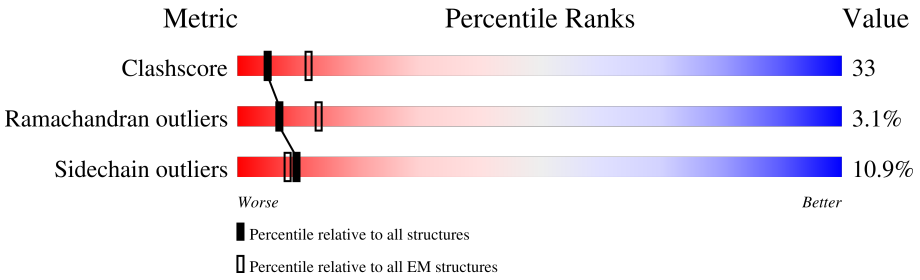
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

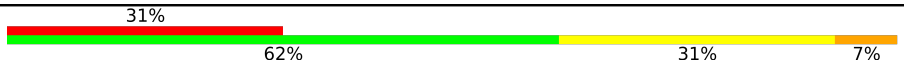
The reported resolution of this entry is 4.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	982	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7515 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 Capsid protein.

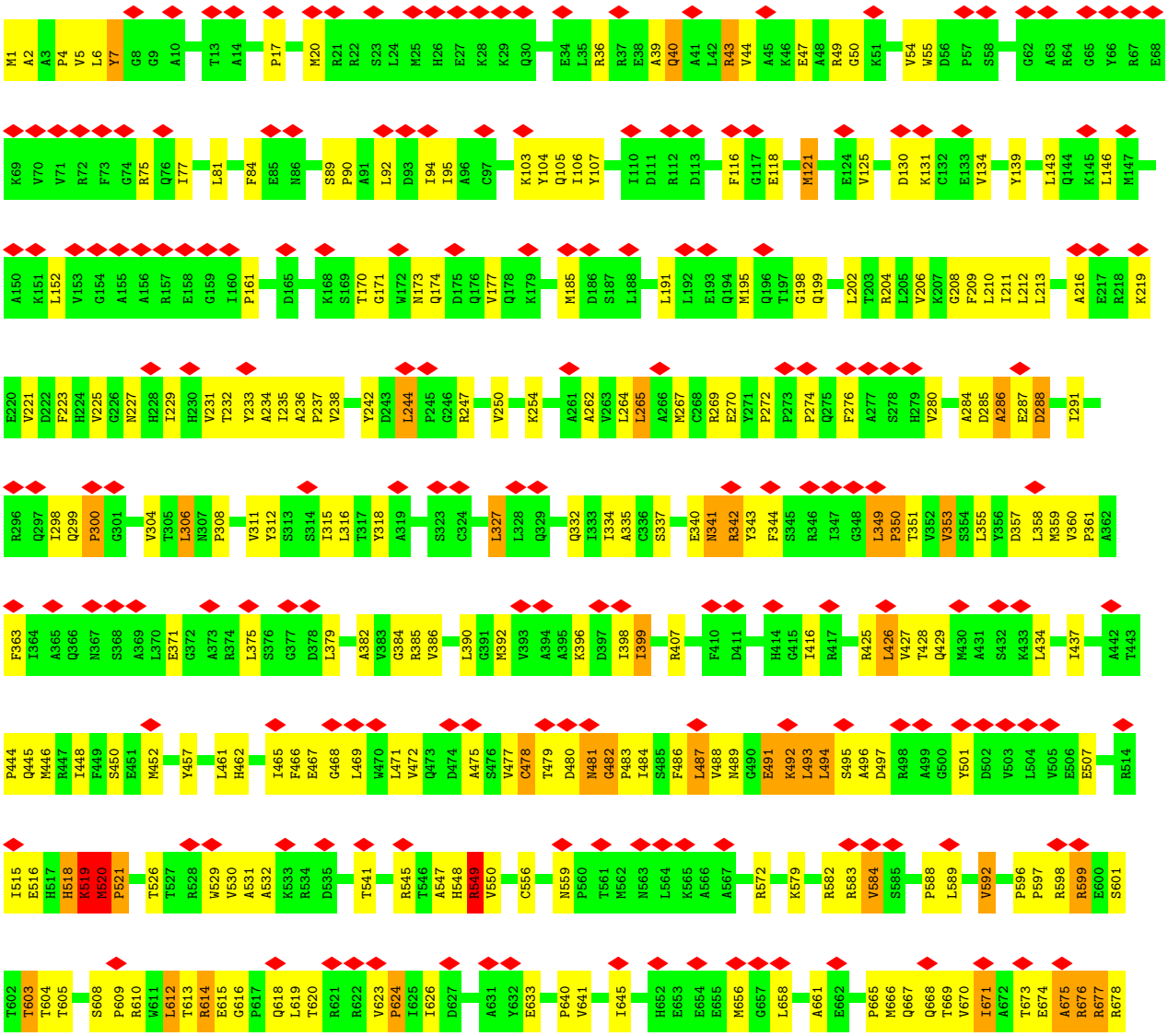
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	982	7515	4685	1369	1417	44	0	17

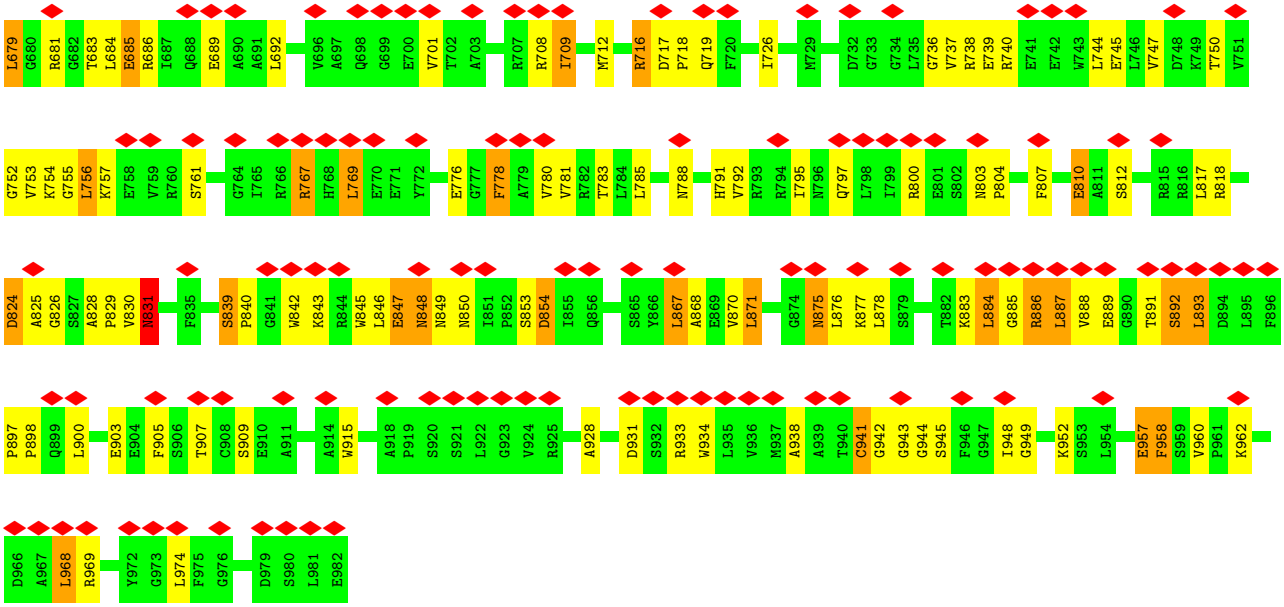
3 Residue-property plots (i)

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: Capsid protein

Chain A:




L679 G680 R681 G682 T683 L684 E685 R686 I687 Q688 E689 A690 A691 L692 V696 A697 Q698 G699 E700 V701 T702 A703 R707 R708 I709 M712 R716 D717 P718 Q719 F720 I726 M729 D732 G733 G734 L735 G736 V737 R738 E739 R740 E741 E742 W743 L744 E745 L746 V747 D748 K749 T750 V751
G752 V753 K754 G755 L756 K757 E758 V759 R760 S761 G764 I765 R766 R767 H768 L769 E770 E771 Y772 E776 G777 F778 A779 V780 V781 R782 T783 L784 L785 N788 H791 V792 R793 R794 I795 N796 Q797 L798 I799 R800 E801 S802 N803 P804 F807 E810 A811 S812 R815 R816 L817 R818
D824 A825 G826 S827 A828 P829 V830 N831 F835 S839 P840 G841 W842 K843 R844 W845 L846 E847 N848 N849 N850 I851 P852 S853 D854 I855 Q856 S865 Y866 L867 A868 E869 V870 L871 G874 N875 L876 K877 L878 S879 T882 K883 L884 G885 R886 L887 V888 E889 G890 T891 S892 L893 D894 L895 F896
P897 P898 Q899 L900 E903 E904 F905 S906 T907 C908 S909 E910 A911 A914 W915 A918 P919 S920 S921 L922 G923 V924 R925 A928 D931 S932 R933 W934 L935 V936 M937 A938 A939 T940 C941 G942 G943 G944 S945 F946 G947 I948 G949 K952 S953 L954 E957 F958 S959 V960 P961 K962
D966 A967 L968 R969 Y972 G973 L974 F975 G976 D979 S980 L981 E982

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	27566	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Phase flipping & amplitude	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	56910	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	0.048	Depositor
Minimum map value	-0.053	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	487.08002, 487.08002, 487.08002	wwPDB
Map dimensions	396, 396, 396	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.23, 1.23, 1.23	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.31	1/7638 (0.0%)	0.52	1/10318 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	521	PRO	N-CD	5.33	1.55	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	482	GLY	N-CA-C	5.21	126.14	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7515	0	7478	491	0
All	All	7515	0	7478	491	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 33.

All (491) 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:507:GLU:CA	1:A:626:ILE:HG23	1.23	1.61
1:A:610:ARG:CZ	1:A:674:GLU:CG	1.79	1.60
1:A:94:ILE:CD1	1:A:496:ALA:HB1	1.39	1.53
1:A:5:VAL:HG21	1:A:17:PRO:CB	1.39	1.52
1:A:610:ARG:NH2	1:A:674:GLU:HG2	1.19	1.50
1:A:610:ARG:NH2	1:A:674:GLU:CG	1.73	1.46
1:A:104:TYR:HA	1:A:493:LEU:CD2	0.96	1.44
1:A:94:ILE:HD13	1:A:496:ALA:CB	1.45	1.42
1:A:104:TYR:CA	1:A:493:LEU:HD21	0.95	1.41
1:A:5:VAL:CG2	1:A:17:PRO:HB3	1.46	1.41
1:A:907:THR:CG2	1:A:943:GLY:HA3	1.51	1.40
1:A:887:LEU:CB	1:A:900:LEU:HD21	1.50	1.37
1:A:94:ILE:CD1	1:A:496:ALA:CB	1.99	1.35
1:A:5:VAL:HG21	1:A:17:PRO:CA	1.56	1.33
1:A:507:GLU:CA	1:A:626:ILE:CG2	2.08	1.29
1:A:610:ARG:CZ	1:A:674:GLU:HG2	1.43	1.28
1:A:610:ARG:CZ	1:A:674:GLU:HG3	1.50	1.28
1:A:887:LEU:HB3	1:A:900:LEU:CD2	1.64	1.28
1:A:103:LYS:O	1:A:493:LEU:CG	1.84	1.24
1:A:550:VAL:CG1	1:A:752:GLY:O	1.85	1.24
1:A:520:MET:CE	1:A:541:THR:HG22	1.67	1.23
1:A:103:LYS:O	1:A:493:LEU:HG	1.31	1.22
1:A:520:MET:CE	1:A:541:THR:CG2	2.19	1.20
1:A:712:MET:HG3	1:A:781:VAL:CG1	1.72	1.20
1:A:426:LEU:HD12	1:A:427:VAL:HG23	1.24	1.17
1:A:618:GLN:HG3	1:A:678:ARG:HB3	1.21	1.17
1:A:4:PRO:HG3	1:A:20:MET:CB	1.74	1.16
1:A:4:PRO:CG	1:A:20:MET:HB2	1.75	1.16
1:A:907:THR:CG2	1:A:943:GLY:CA	2.23	1.15
1:A:495:SER:OG	1:A:849:ASN:ND2	1.80	1.14
1:A:118:GLU:OE2	1:A:484:ILE:HG21	1.46	1.13
1:A:610:ARG:NH1	1:A:674:GLU:OE2	1.80	1.13
1:A:4:PRO:HG3	1:A:20:MET:HB2	1.12	1.12
1:A:103:LYS:O	1:A:493:LEU:CD1	1.99	1.11
1:A:550:VAL:HG13	1:A:752:GLY:O	0.93	1.10
1:A:487:LEU:HD12	1:A:488:VAL:H	1.11	1.09
1:A:610:ARG:NH1	1:A:674:GLU:CG	2.12	1.09
1:A:5:VAL:CG2	1:A:17:PRO:CB	2.12	1.09
1:A:907:THR:HG21	1:A:943:GLY:HA3	1.10	1.09
1:A:104:TYR:HA	1:A:493:LEU:HD23	1.34	1.08
1:A:520:MET:HE2	1:A:541:THR:HG21	1.31	1.07
1:A:103:LYS:C	1:A:493:LEU:HD11	1.74	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:MET:HE3	1:A:541:THR:CG2	1.82	1.06
1:A:520:MET:HE2	1:A:541:THR:CG2	1.81	1.05
1:A:107:TYR:HE2	1:A:491:GLU:HG3	1.17	1.05
1:A:712:MET:CG	1:A:781:VAL:HG13	1.86	1.04
1:A:610:ARG:NH1	1:A:674:GLU:HG2	1.68	1.03
1:A:547:ALA:O	1:A:548:HIS:ND1	1.92	1.03
1:A:957:GLU:HG2	1:A:958:PHE:N	1.74	1.02
1:A:520:MET:HE3	1:A:541:THR:HG22	1.04	1.02
1:A:518:HIS:O	1:A:519:LYS:HB2	1.58	1.02
1:A:487:LEU:HD12	1:A:488:VAL:N	1.74	1.01
1:A:550:VAL:HG13	1:A:752:GLY:C	1.81	1.01
1:A:118:GLU:OE2	1:A:484:ILE:CG2	2.08	1.00
1:A:94:ILE:CD1	1:A:496:ALA:HB3	1.90	0.99
1:A:907:THR:HG22	1:A:943:GLY:CA	1.89	0.99
1:A:340:GLU:HG2	1:A:343:TYR:HB2	1.40	0.99
1:A:94:ILE:HD12	1:A:496:ALA:CB	1.91	0.99
1:A:355:LEU:HD21	1:A:358:LEU:HD12	1.46	0.98
1:A:887:LEU:CB	1:A:900:LEU:CD2	2.31	0.98
1:A:4:PRO:HG3	1:A:20:MET:CG	1.93	0.97
1:A:5:VAL:HG21	1:A:17:PRO:HA	1.46	0.97
1:A:5:VAL:CG2	1:A:17:PRO:CA	2.40	0.97
1:A:107:TYR:CE2	1:A:491:GLU:HG3	2.00	0.96
1:A:104:TYR:C	1:A:493:LEU:HD21	1.87	0.95
1:A:487:LEU:CD1	1:A:488:VAL:H	1.80	0.95
1:A:907:THR:HG22	1:A:943:GLY:HA3	1.42	0.95
1:A:5:VAL:HG21	1:A:17:PRO:HB3	1.02	0.95
1:A:584:VAL:HG13	1:A:645:ILE:HD13	1.47	0.94
1:A:712:MET:HG3	1:A:781:VAL:HG13	0.92	0.92
1:A:94:ILE:HD13	1:A:496:ALA:HB3	1.50	0.92
1:A:828:ALA:HB3	1:A:829:PRO:HD3	1.52	0.91
1:A:94:ILE:HD13	1:A:496:ALA:HB1	0.97	0.91
1:A:668:GLN:O	1:A:671:ILE:HG22	1.71	0.91
1:A:610:ARG:NH1	1:A:674:GLU:CD	2.23	0.91
1:A:104:TYR:N	1:A:493:LEU:HD21	1.86	0.90
1:A:778:PHE:HD2	1:A:780:VAL:HG22	1.33	0.90
1:A:5:VAL:HG22	1:A:17:PRO:HB3	1.53	0.90
1:A:618:GLN:CG	1:A:678:ARG:HB3	2.02	0.89
1:A:675:ALA:HB1	1:A:684:LEU:HG	1.53	0.89
1:A:94:ILE:HD11	1:A:496:ALA:HB1	1.56	0.88
1:A:584:VAL:HG22	1:A:645:ILE:HB	1.52	0.88
1:A:610:ARG:HH22	1:A:674:GLU:HG2	1.06	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:ARG:NE	1:A:677:ARG:O	2.08	0.86
1:A:481:ASN:C	1:A:483:PRO:HD2	1.96	0.86
1:A:712:MET:CE	1:A:781:VAL:HG22	2.06	0.85
1:A:548:HIS:O	1:A:549:ARG:NH2	2.09	0.85
1:A:5:VAL:CG2	1:A:17:PRO:HA	2.02	0.85
1:A:103:LYS:O	1:A:493:LEU:HD11	1.73	0.84
1:A:426:LEU:CD1	1:A:427:VAL:HG23	2.05	0.84
1:A:519:LYS:O	1:A:520:MET:HB2	1.77	0.84
1:A:907:THR:HG21	1:A:943:GLY:CA	2.01	0.84
1:A:515:ILE:CA	1:A:516:GLU:N	2.40	0.84
1:A:493:LEU:CB	1:A:824:ASP:OD2	2.26	0.83
1:A:712:MET:HE2	1:A:781:VAL:CG2	2.09	0.83
1:A:907:THR:HB	1:A:943:GLY:HA2	1.61	0.83
1:A:225:VAL:HG13	1:A:265:LEU:HD12	1.59	0.82
1:A:521:PRO:HB3	1:A:952:LYS:HZ1	1.45	0.82
1:A:121:MET:CE	1:A:481:ASN:O	2.29	0.81
1:A:521:PRO:HB2	1:A:952:LYS:HZ2	1.45	0.81
1:A:883:LYS:HG2	1:A:943:GLY:O	1.81	0.81
1:A:493:LEU:HB2	1:A:824:ASP:OD2	1.80	0.80
1:A:104:TYR:HA	1:A:493:LEU:CG	2.10	0.80
1:A:529:TRP:HZ3	1:A:941:CYS:O	1.65	0.80
1:A:887:LEU:HB3	1:A:900:LEU:HD21	0.80	0.80
1:A:610:ARG:NH2	1:A:674:GLU:CB	2.44	0.80
1:A:610:ARG:NE	1:A:674:GLU:HG3	1.98	0.79
1:A:426:LEU:HD12	1:A:427:VAL:CG2	2.10	0.78
1:A:529:TRP:HB2	1:A:944:GLY:O	1.83	0.78
1:A:615:GLU:CD	1:A:678:ARG:HE	1.87	0.78
1:A:549:ARG:CB	1:A:686:ARG:H	1.97	0.76
1:A:675:ALA:HB1	1:A:684:LEU:CG	2.15	0.76
1:A:529:TRP:HH2	1:A:938:ALA:CB	1.99	0.76
1:A:885:GLY:C	1:A:886:ARG:HG3	2.05	0.76
1:A:887:LEU:CA	1:A:900:LEU:HD21	2.16	0.75
1:A:480:ASP:O	1:A:481:ASN:HB2	1.85	0.75
1:A:231:VAL:HG12	1:A:232:THR:HG23	1.67	0.74
1:A:518:HIS:O	1:A:519:LYS:CB	2.36	0.74
1:A:529:TRP:CB	1:A:944:GLY:O	2.35	0.74
1:A:209:PHE:HB3	1:A:334:ILE:HD13	1.70	0.73
1:A:121:MET:HE3	1:A:481:ASN:O	1.88	0.73
1:A:521:PRO:CB	1:A:952:LYS:NZ	2.52	0.73
1:A:461:LEU:HB3	1:A:471:LEU:HD22	1.70	0.73
1:A:468:GLY:O	1:A:472:VAL:HG23	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:778:PHE:CE2	1:A:781:VAL:HG23	2.24	0.72
1:A:94:ILE:HG21	1:A:496:ALA:HB3	1.71	0.72
1:A:104:TYR:CA	1:A:493:LEU:CD2	1.87	0.72
1:A:545:ARG:HB3	1:A:745:GLU:HG2	1.70	0.72
1:A:618:GLN:HG3	1:A:678:ARG:CB	2.11	0.72
1:A:427:VAL:HG12	1:A:428:THR:H	1.55	0.71
1:A:957:GLU:CG	1:A:958:PHE:N	2.50	0.71
1:A:614:ARG:NH2	1:A:679:LEU:O	2.23	0.71
1:A:907:THR:CB	1:A:943:GLY:HA2	2.21	0.71
1:A:501:TYR:CA	1:A:549:ARG:HH12	2.03	0.71
1:A:104:TYR:C	1:A:493:LEU:CD2	2.51	0.70
1:A:550:VAL:HG11	1:A:753:VAL:HA	1.73	0.70
1:A:817:LEU:HD12	1:A:818:ARG:N	2.06	0.70
1:A:519:LYS:NZ	1:A:679:LEU:HD11	2.07	0.70
1:A:482:GLY:N	1:A:483:PRO:HD2	2.06	0.70
1:A:482:GLY:N	1:A:483:PRO:CD	2.54	0.70
1:A:671:ILE:HA	1:A:689:GLU:OE1	1.92	0.70
1:A:550:VAL:CG1	1:A:753:VAL:HA	2.22	0.69
1:A:75:ARG:NH1	1:A:559:ASN:O	2.24	0.69
1:A:519:LYS:HE3	1:A:679:LEU:HD11	1.74	0.69
1:A:549:ARG:HG3	1:A:686:ARG:CB	2.20	0.69
1:A:883:LYS:HG2	1:A:944:GLY:HA2	1.73	0.69
1:A:739:GLU:HB3	1:A:792:VAL:HG21	1.73	0.68
1:A:5:VAL:CB	1:A:17:PRO:HB3	2.22	0.68
1:A:121:MET:HE1	1:A:481:ASN:O	1.92	0.68
1:A:907:THR:CG2	1:A:943:GLY:HA2	2.20	0.68
1:A:5:VAL:HG22	1:A:17:PRO:CB	2.13	0.68
1:A:549:ARG:HB2	1:A:686:ARG:H	1.56	0.68
1:A:548:HIS:CD2	1:A:549:ARG:H	2.12	0.67
1:A:4:PRO:O	1:A:5:VAL:HG12	1.95	0.67
1:A:521:PRO:HB2	1:A:952:LYS:NZ	2.09	0.67
1:A:583:ARG:O	1:A:584:VAL:HG23	1.95	0.67
1:A:519:LYS:CE	1:A:679:LEU:HD11	2.25	0.67
1:A:548:HIS:CG	1:A:549:ARG:H	2.12	0.67
1:A:712:MET:HE2	1:A:781:VAL:HG21	1.75	0.67
1:A:5:VAL:CG1	1:A:17:PRO:HB3	2.25	0.67
1:A:778:PHE:CD2	1:A:780:VAL:HG22	2.22	0.66
1:A:792:VAL:HA	1:A:795:ILE:HD12	1.77	0.66
1:A:603:THR:HG22	1:A:757:LYS:O	1.95	0.66
1:A:671:ILE:HD13	1:A:671:ILE:C	2.16	0.66
1:A:661:ALA:HB1	1:A:701:VAL:HG11	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:891:THR:O	1:A:892:SER:C	2.33	0.66
1:A:887:LEU:HB3	1:A:900:LEU:CG	2.25	0.65
1:A:712:MET:SD	1:A:781:VAL:HG22	2.36	0.65
1:A:340:GLU:HG2	1:A:343:TYR:CB	2.22	0.65
1:A:675:ALA:HB1	1:A:684:LEU:CD1	2.26	0.65
1:A:4:PRO:HG3	1:A:20:MET:HG3	1.78	0.65
1:A:610:ARG:HH12	1:A:674:GLU:HG2	1.59	0.65
1:A:493:LEU:HG	1:A:493:LEU:O	1.95	0.64
1:A:529:TRP:CZ3	1:A:941:CYS:O	2.49	0.64
1:A:668:GLN:O	1:A:671:ILE:CG2	2.43	0.64
1:A:676:ARG:H	1:A:684:LEU:HD21	1.63	0.64
1:A:477:VAL:O	1:A:478:CYS:HB2	1.95	0.64
1:A:210:LEU:HD21	1:A:337:SER:HB3	1.80	0.64
1:A:549:ARG:HB3	1:A:686:ARG:H	1.63	0.63
1:A:469:LEU:N	1:A:488:VAL:HG21	2.13	0.63
1:A:521:PRO:HB3	1:A:952:LYS:NZ	2.12	0.63
1:A:204:ARG:NH2	1:A:353:VAL:HG11	2.13	0.63
1:A:492:LYS:HE2	1:A:494:LEU:HD21	1.79	0.63
1:A:223:PHE:CE2	1:A:306:LEU:HD21	2.33	0.62
1:A:791:HIS:CE1	1:A:795:ILE:HD11	2.33	0.62
1:A:235:ILE:O	1:A:238:VAL:HG12	2.00	0.62
1:A:398:ILE:HG12	1:A:416:ILE:HD13	1.82	0.62
1:A:209:PHE:CB	1:A:334:ILE:HG21	2.30	0.62
1:A:887:LEU:HB2	1:A:900:LEU:CD2	2.27	0.62
1:A:530:VAL:HG22	1:A:531:ALA:H	1.65	0.61
1:A:390:LEU:HD22	1:A:429:GLN:HE21	1.65	0.61
1:A:907:THR:CB	1:A:943:GLY:CA	2.76	0.61
1:A:495:SER:HG	1:A:849:ASN:ND2	1.99	0.61
1:A:106:ILE:HG23	1:A:489:ASN:O	2.01	0.61
1:A:548:HIS:O	1:A:549:ARG:HD2	2.00	0.61
1:A:493:LEU:HB3	1:A:824:ASP:OD2	2.01	0.60
1:A:549:ARG:HB2	1:A:686:ARG:N	2.16	0.60
1:A:674:GLU:OE1	1:A:685:GLU:O	2.18	0.60
1:A:928:ALA:HB1	1:A:931:ASP:HB2	1.84	0.60
1:A:103:LYS:HB3	1:A:493:LEU:HD11	1.83	0.60
1:A:335:ALA:HB1	1:A:384:GLY:CA	2.32	0.60
1:A:614:ARG:NH2	1:A:684:LEU:HD13	2.16	0.60
1:A:670:VAL:HG22	1:A:689:GLU:OE2	2.01	0.60
1:A:767:ARG:CG	1:A:769:LEU:HD11	2.31	0.60
1:A:797:GLN:HE22	1:A:868:ALA:HB3	1.67	0.60
1:A:355:LEU:CD2	1:A:358:LEU:HD12	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:957:GLU:HG2	1:A:958:PHE:H	1.65	0.60
1:A:94:ILE:HD12	1:A:496:ALA:HB3	1.64	0.59
1:A:610:ARG:NH2	1:A:674:GLU:HG3	1.73	0.59
1:A:171:GLY:HA3	1:A:234:ALA:HB3	1.83	0.59
1:A:5:VAL:HG13	1:A:5:VAL:O	2.02	0.59
1:A:105:GLN:HG2	1:A:493:LEU:HD22	1.83	0.59
1:A:778:PHE:HD2	1:A:780:VAL:CG2	2.11	0.59
1:A:105:GLN:N	1:A:493:LEU:CD2	2.65	0.59
1:A:466:PHE:HD1	1:A:487:LEU:HA	1.68	0.59
1:A:767:ARG:HG3	1:A:769:LEU:HD11	1.84	0.59
1:A:118:GLU:OE2	1:A:484:ILE:HG22	2.00	0.59
1:A:719:GLN:HG2	1:A:726:ILE:HD12	1.84	0.59
1:A:903:GLU:O	1:A:907:THR:HG23	2.03	0.58
1:A:47:GLU:OE2	1:A:49:ARG:N	2.32	0.58
1:A:94:ILE:HD12	1:A:496:ALA:C	2.23	0.58
1:A:549:ARG:CB	1:A:686:ARG:N	2.66	0.58
1:A:233:TYR:CD1	1:A:361:PRO:HG3	2.39	0.58
1:A:462:HIS:O	1:A:488:VAL:HG12	2.02	0.58
1:A:886:ARG:O	1:A:887:LEU:HD22	2.04	0.58
1:A:4:PRO:CD	1:A:20:MET:HB2	2.32	0.58
1:A:235:ILE:HG22	1:A:236:ALA:H	1.67	0.58
1:A:752:GLY:HA2	1:A:846:LEU:HD13	1.85	0.58
1:A:778:PHE:CE2	1:A:781:VAL:CG2	2.86	0.58
1:A:958:PHE:O	1:A:960:VAL:HG23	2.04	0.58
1:A:529:TRP:HH2	1:A:938:ALA:HB1	1.69	0.58
1:A:605:THR:HB	1:A:726:ILE:HG23	1.86	0.58
1:A:5:VAL:CG2	1:A:17:PRO:CG	2.81	0.58
1:A:717:ASP:N	1:A:718:PRO:HD2	2.18	0.57
1:A:529:TRP:HB3	1:A:945:SER:HA	1.86	0.57
1:A:616:GLY:HA3	1:A:785:LEU:HD11	1.85	0.57
1:A:89:SER:HA	1:A:825:ALA:HB1	1.86	0.57
1:A:213:LEU:HD11	1:A:375:LEU:HD23	1.85	0.57
1:A:670:VAL:HG22	1:A:689:GLU:CD	2.25	0.57
1:A:105:GLN:N	1:A:493:LEU:HD22	2.20	0.57
1:A:173:ASN:HB2	1:A:235:ILE:HD12	1.85	0.57
1:A:579:LYS:CG	1:A:641:VAL:HG21	2.34	0.57
1:A:778:PHE:CD2	1:A:781:VAL:HG23	2.39	0.57
1:A:5:VAL:HG22	1:A:17:PRO:HG3	1.85	0.57
1:A:887:LEU:HD12	1:A:888:VAL:H	1.69	0.57
1:A:480:ASP:O	1:A:481:ASN:CB	2.50	0.57
1:A:529:TRP:HB3	1:A:944:GLY:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ILE:HG21	1:A:556:CYS:SG	2.45	0.56
1:A:778:PHE:N	1:A:778:PHE:CD1	2.73	0.56
1:A:548:HIS:CG	1:A:549:ARG:N	2.73	0.56
1:A:579:LYS:CD	1:A:641:VAL:HG21	2.35	0.56
1:A:487:LEU:CG	1:A:488:VAL:H	2.18	0.56
1:A:883:LYS:CG	1:A:943:GLY:O	2.53	0.56
1:A:529:TRP:HH2	1:A:938:ALA:HB2	1.69	0.56
1:A:674:GLU:O	1:A:675:ALA:HB3	2.06	0.56
1:A:270:GLU:HG2	1:A:284:ALA:HB2	1.87	0.56
1:A:737:VAL:HG21	1:A:845:TRP:CE2	2.41	0.56
1:A:5:VAL:HG22	1:A:17:PRO:CG	2.34	0.55
1:A:612:LEU:HD23	1:A:712:MET:SD	2.46	0.55
1:A:675:ALA:CA	1:A:684:LEU:HD11	2.37	0.55
1:A:103:LYS:CB	1:A:493:LEU:HD11	2.36	0.55
1:A:610:ARG:O	1:A:614:ARG:HB2	2.06	0.55
1:A:592:VAL:O	1:A:596:PRO:HD2	2.06	0.55
1:A:604:THR:HG21	1:A:692:LEU:HD21	1.89	0.55
1:A:121:MET:HE1	1:A:481:ASN:C	2.27	0.55
1:A:712:MET:CE	1:A:781:VAL:CG2	2.72	0.55
1:A:716:ARG:NH1	1:A:776:GLU:OE1	2.40	0.55
1:A:316:LEU:HD12	1:A:589:LEU:CD2	2.37	0.54
1:A:826:GLY:O	1:A:830:VAL:HG21	2.07	0.54
1:A:5:VAL:HG23	1:A:17:PRO:HA	1.88	0.54
1:A:884:LEU:HD13	1:A:885:GLY:N	2.21	0.54
1:A:39:ALA:O	1:A:43:ARG:HG3	2.07	0.54
1:A:250:VAL:HG13	1:A:318:TYR:CE1	2.42	0.54
1:A:712:MET:CG	1:A:781:VAL:CG1	2.65	0.54
1:A:583:ARG:C	1:A:584:VAL:HG23	2.28	0.54
1:A:791:HIS:CD2	1:A:968:LEU:HD12	2.42	0.54
1:A:887:LEU:C	1:A:900:LEU:HD21	2.28	0.54
1:A:887:LEU:CD1	1:A:888:VAL:H	2.22	0.53
1:A:143:LEU:HD13	1:A:198:GLY:HA2	1.90	0.53
1:A:549:ARG:HG3	1:A:686:ARG:HB2	1.88	0.53
1:A:891:THR:O	1:A:893:LEU:N	2.41	0.53
1:A:675:ALA:HA	1:A:684:LEU:HD11	1.90	0.53
1:A:712:MET:HE1	1:A:778:PHE:CE2	2.44	0.53
1:A:519:LYS:HZ2	1:A:679:LEU:HD11	1.73	0.53
1:A:234:ALA:HA	1:A:238:VAL:HG11	1.91	0.53
1:A:604:THR:CG2	1:A:692:LEU:HD21	2.38	0.53
1:A:828:ALA:CB	1:A:829:PRO:HD3	2.34	0.52
1:A:584:VAL:HG13	1:A:645:ILE:CD1	2.32	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:PHE:CE1	1:A:92:LEU:HD11	2.44	0.52
1:A:327:LEU:HD12	1:A:371:GLU:HB3	1.92	0.52
1:A:519:LYS:O	1:A:520:MET:CB	2.56	0.52
1:A:81:LEU:HD21	1:A:379:LEU:HD21	1.92	0.52
1:A:616:GLY:O	1:A:620:THR:HG23	2.10	0.52
1:A:618:GLN:NE2	1:A:678:ARG:O	2.42	0.52
1:A:817:LEU:HD12	1:A:818:ARG:H	1.74	0.52
1:A:360:VAL:HG13	1:A:360:VAL:O	2.10	0.52
1:A:675:ALA:CB	1:A:684:LEU:CD1	2.87	0.52
1:A:306:LEU:HD12	1:A:311:VAL:HG22	1.92	0.52
1:A:468:GLY:C	1:A:488:VAL:HG21	2.30	0.52
1:A:526:THR:HG22	1:A:949:GLY:O	2.10	0.52
1:A:957:GLU:CG	1:A:958:PHE:H	2.21	0.52
1:A:107:TYR:HE2	1:A:491:GLU:CG	2.06	0.51
1:A:208:GLY:O	1:A:211:ILE:HG22	2.10	0.51
1:A:209:PHE:HB3	1:A:334:ILE:HG21	1.91	0.51
1:A:466:PHE:HE1	1:A:487:LEU:H	1.59	0.51
1:A:529:TRP:CH2	1:A:938:ALA:HB1	2.45	0.51
1:A:146:LEU:HD21	1:A:357:ASP:HB3	1.91	0.51
1:A:907:THR:HB	1:A:943:GLY:CA	2.35	0.51
1:A:36:ARG:NH1	1:A:810:GLU:O	2.44	0.51
1:A:416:ILE:HG23	1:A:416:ILE:O	2.10	0.51
1:A:466:PHE:CD1	1:A:487:LEU:HA	2.45	0.51
1:A:846:LEU:O	1:A:848:ASN:N	2.44	0.51
1:A:677:ARG:O	1:A:678:ARG:HB2	2.11	0.51
1:A:227:ASN:HD22	1:A:291:ILE:HD12	1.76	0.51
1:A:507:GLU:CA	1:A:626:ILE:HG22	2.30	0.50
1:A:195:MET:HE3	1:A:360:VAL:HG12	1.92	0.50
1:A:225:VAL:CG1	1:A:265:LEU:HD12	2.35	0.50
1:A:871:LEU:HD13	1:A:948:ILE:HG13	1.93	0.50
1:A:106:ILE:HG23	1:A:489:ASN:H	1.75	0.50
1:A:298:ILE:HG22	1:A:300:PRO:HD2	1.94	0.50
1:A:520:MET:CE	1:A:541:THR:CB	2.89	0.50
1:A:238:VAL:HG23	1:A:359:MET:HE2	1.93	0.50
1:A:202:LEU:O	1:A:206:VAL:HG23	2.12	0.50
1:A:216:ALA:HA	1:A:308:PRO:HG3	1.94	0.50
1:A:709:ILE:HG22	1:A:709:ILE:O	2.11	0.50
1:A:285:ASP:O	1:A:286:ALA:C	2.50	0.49
1:A:547:ALA:C	1:A:548:HIS:HD1	2.15	0.49
1:A:2:ALA:HB3	1:A:6:LEU:HD22	1.93	0.49
1:A:238:VAL:HG23	1:A:359:MET:CE	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:TYR:CA	1:A:549:ARG:NH1	2.75	0.49
1:A:7:TYR:CD1	1:A:7:TYR:N	2.78	0.49
1:A:6:LEU:HD12	1:A:7:TYR:H	1.78	0.49
1:A:486:PHE:O	1:A:487:LEU:HB3	2.13	0.49
1:A:487:LEU:CD1	1:A:488:VAL:N	2.54	0.49
1:A:618:GLN:HE21	1:A:679:LEU:HG	1.76	0.49
1:A:623:VAL:HB	1:A:624:PRO:HD3	1.95	0.49
1:A:191:LEU:HD12	1:A:242:TYR:HB2	1.94	0.49
1:A:342:ARG:O	1:A:343:TYR:HD1	1.96	0.49
1:A:465:ILE:HG22	1:A:467:GLU:H	1.77	0.49
1:A:870:VAL:HG22	1:A:915:TRP:HH2	1.78	0.49
1:A:549:ARG:HG2	1:A:550:VAL:N	2.28	0.48
1:A:134:VAL:HB	1:A:280:VAL:HA	1.94	0.48
1:A:448:ILE:HG23	1:A:448:ILE:O	2.13	0.48
1:A:209:PHE:HB2	1:A:334:ILE:HG21	1.94	0.48
1:A:426:LEU:CD1	1:A:427:VAL:CG2	2.80	0.48
1:A:678:ARG:HG3	1:A:678:ARG:HH11	1.78	0.48
1:A:342:ARG:HD3	1:A:444:PRO:HG3	1.96	0.48
1:A:236:ALA:HB3	1:A:237:PRO:HD3	1.95	0.48
1:A:803:ASN:N	1:A:804:PRO:HD2	2.29	0.48
1:A:40:GLN:O	1:A:44:VAL:HG12	2.14	0.48
1:A:437:ILE:O	1:A:437:ILE:HG22	2.13	0.48
1:A:549:ARG:HG2	1:A:550:VAL:H	1.79	0.48
1:A:614:ARG:CZ	1:A:677:ARG:O	2.61	0.48
1:A:210:LEU:HD21	1:A:337:SER:CB	2.43	0.48
1:A:712:MET:HE2	1:A:781:VAL:HG22	1.71	0.48
1:A:548:HIS:O	1:A:549:ARG:HB3	2.14	0.47
1:A:747:VAL:HG11	1:A:853:SER:HB2	1.96	0.47
1:A:960:VAL:HG12	1:A:960:VAL:O	2.13	0.47
1:A:530:VAL:HG13	1:A:532:ALA:H	1.77	0.47
1:A:661:ALA:HB1	1:A:701:VAL:CG1	2.43	0.47
1:A:549:ARG:CB	1:A:686:ARG:CA	2.92	0.47
1:A:744:LEU:HD12	1:A:854:ASP:OD2	2.15	0.47
1:A:134:VAL:HG22	1:A:340:GLU:OE2	2.15	0.47
1:A:244:LEU:HD12	1:A:247:ARG:NH1	2.30	0.47
1:A:262:ALA:HB2	1:A:304:VAL:HG21	1.96	0.47
1:A:520:MET:H	1:A:521:PRO:CD	2.28	0.47
1:A:584:VAL:HG21	1:A:645:ILE:N	2.29	0.47
1:A:675:ALA:HB1	1:A:684:LEU:HD11	1.96	0.47
1:A:712:MET:CE	1:A:778:PHE:CZ	2.97	0.47
1:A:209:PHE:CE1	1:A:315:ILE:HG21	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:LEU:HD12	1:A:427:VAL:H	1.80	0.47
1:A:426:LEU:HD21	1:A:450:SER:HB2	1.96	0.47
1:A:579:LYS:HD2	1:A:641:VAL:HG21	1.96	0.47
1:A:871:LEU:HD23	1:A:871:LEU:C	2.36	0.47
1:A:382:ALA:O	1:A:386:VAL:HG23	2.14	0.46
1:A:426:LEU:HD23	1:A:452:MET:HB2	1.97	0.46
1:A:708:ARG:HD3	1:A:709:ILE:H	1.79	0.46
1:A:676:ARG:H	1:A:684:LEU:HD11	1.80	0.46
1:A:519:LYS:HZ1	1:A:679:LEU:HD21	1.79	0.46
1:A:477:VAL:O	1:A:478:CYS:CB	2.63	0.46
1:A:50:GLY:O	1:A:54:VAL:HG23	2.16	0.46
1:A:312:TYR:CE2	1:A:316:LEU:HD11	2.51	0.46
1:A:426:LEU:HD11	1:A:450:SER:HB3	1.98	0.46
1:A:94:ILE:HG21	1:A:496:ALA:CB	2.45	0.46
1:A:341:ASN:HD22	1:A:341:ASN:HA	1.61	0.46
1:A:334:ILE:CD1	1:A:375:LEU:HD21	2.45	0.46
1:A:744:LEU:HD21	1:A:850:ASN:HB2	1.98	0.46
1:A:492:LYS:CE	1:A:494:LEU:HD21	2.46	0.46
1:A:1:MET:HG2	1:A:1:MET:O	2.16	0.45
1:A:174:GLN:HA	1:A:177:VAL:HG22	1.97	0.45
1:A:596:PRO:HB2	1:A:597:PRO:HD3	1.98	0.45
1:A:6:LEU:HD12	1:A:7:TYR:N	2.31	0.45
1:A:486:PHE:CD1	1:A:487:LEU:N	2.85	0.45
1:A:229:ILE:HD12	1:A:291:ILE:O	2.16	0.45
1:A:588:PRO:O	1:A:592:VAL:HG23	2.16	0.45
1:A:665:PRO:O	1:A:669:THR:HG23	2.17	0.45
1:A:92:LEU:HD22	1:A:386:VAL:CG2	2.47	0.45
1:A:355:LEU:HD11	1:A:358:LEU:HG	1.99	0.45
1:A:877:LYS:O	1:A:878:LEU:HB2	2.17	0.45
1:A:335:ALA:HB1	1:A:384:GLY:HA3	1.98	0.45
1:A:885:GLY:O	1:A:886:ARG:HG3	2.16	0.45
1:A:349:LEU:HD22	1:A:349:LEU:O	2.16	0.44
1:A:327:LEU:O	1:A:327:LEU:HD13	2.18	0.44
1:A:807:PHE:CB	1:A:817:LEU:HD21	2.48	0.44
1:A:675:ALA:CB	1:A:684:LEU:HD11	2.48	0.44
1:A:549:ARG:C	1:A:549:ARG:CD	2.86	0.44
1:A:350:PRO:O	1:A:351:THR:HG23	2.18	0.44
1:A:287:GLU:O	1:A:288:ASP:CB	2.66	0.44
1:A:609:PRO:O	1:A:613:THR:HG22	2.17	0.44
1:A:103:LYS:C	1:A:493:LEU:CD1	2.50	0.44
1:A:125:VAL:HG13	1:A:445:GLN:HE21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:778:PHE:CD2	1:A:780:VAL:CG2	2.93	0.44
1:A:867:LEU:HD12	1:A:868:ALA:H	1.81	0.44
1:A:90:PRO:HG3	1:A:846:LEU:HD11	2.00	0.43
1:A:379:LEU:HD23	1:A:556:CYS:SG	2.57	0.43
1:A:549:ARG:CG	1:A:550:VAL:N	2.80	0.43
1:A:875:ASN:C	1:A:876:LEU:HD22	2.39	0.43
1:A:545:ARG:HD3	1:A:545:ARG:HA	1.59	0.43
1:A:755:GLY:C	1:A:756:LEU:HD22	2.38	0.43
1:A:830:VAL:O	1:A:831:ASN:ND2	2.42	0.43
1:A:227:ASN:HB3	1:A:265:LEU:HD11	2.00	0.43
1:A:342:ARG:HG2	1:A:392:MET:SD	2.58	0.43
1:A:461:LEU:HD21	1:A:467:GLU:HB2	2.00	0.43
1:A:399:ILE:HD13	1:A:399:ILE:O	2.18	0.43
1:A:583:ARG:O	1:A:584:VAL:CG2	2.65	0.43
1:A:737:VAL:HG21	1:A:845:TRP:NE1	2.34	0.43
1:A:907:THR:HG22	1:A:943:GLY:C	2.38	0.43
1:A:957:GLU:HG2	1:A:958:PHE:HB2	2.00	0.43
1:A:146:LEU:HD22	1:A:199:GLN:HB2	2.00	0.43
1:A:202:LEU:HB2	1:A:351:THR:HG21	2.00	0.43
1:A:212:LEU:HD13	1:A:212:LEU:C	2.39	0.43
1:A:355:LEU:HD12	1:A:357:ASP:OD1	2.19	0.43
1:A:633:GLU:HG3	1:A:668:GLN:HB3	2.01	0.43
1:A:270:GLU:CG	1:A:284:ALA:HB2	2.47	0.43
1:A:847:GLU:O	1:A:849:ASN:N	2.52	0.43
1:A:5:VAL:HG11	1:A:17:PRO:HB3	1.99	0.43
1:A:103:LYS:C	1:A:493:LEU:HD21	2.39	0.43
1:A:396:LYS:HA	1:A:399:ILE:HG22	2.01	0.42
1:A:461:LEU:HD23	1:A:461:LEU:O	2.19	0.42
1:A:812:SER:O	1:A:817:LEU:HD23	2.19	0.42
1:A:897:PRO:N	1:A:898:PRO:HD2	2.34	0.42
1:A:125:VAL:CG1	1:A:445:GLN:HE21	2.31	0.42
1:A:529:TRP:CH2	1:A:938:ALA:CB	2.89	0.42
1:A:299:GLN:HB3	1:A:300:PRO:HD3	2.01	0.42
1:A:487:LEU:CG	1:A:488:VAL:N	2.80	0.42
1:A:202:LEU:HD12	1:A:349:LEU:HD23	2.01	0.42
1:A:615:GLU:OE2	1:A:678:ARG:NH2	2.46	0.42
1:A:676:ARG:N	1:A:684:LEU:HD11	2.34	0.42
1:A:152:LEU:HD11	1:A:170:THR:CG2	2.50	0.42
1:A:529:TRP:CZ3	1:A:942:GLY:HA2	2.54	0.42
1:A:684:LEU:HD12	1:A:684:LEU:HA	1.93	0.42
1:A:264:LEU:HA	1:A:267:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:LEU:HD22	1:A:681:ARG:O	2.19	0.42
1:A:306:LEU:HD23	1:A:306:LEU:N	2.35	0.42
1:A:740:ARG:CD	1:A:795:ILE:HG21	2.49	0.42
1:A:671:ILE:HD13	1:A:671:ILE:O	2.20	0.42
1:A:250:VAL:O	1:A:291:ILE:HG23	2.19	0.41
1:A:667:GLN:O	1:A:670:VAL:HG12	2.20	0.41
1:A:678:ARG:HG3	1:A:678:ARG:NH1	2.35	0.41
1:A:826:GLY:N	1:A:848:ASN:HD22	2.17	0.41
1:A:592:VAL:HG13	1:A:596:PRO:HG2	2.02	0.41
1:A:106:ILE:CG2	1:A:489:ASN:H	2.33	0.41
1:A:250:VAL:HG13	1:A:318:TYR:HE1	1.85	0.41
1:A:445:GLN:HB3	1:A:475:ALA:O	2.20	0.41
1:A:526:THR:HG23	1:A:526:THR:O	2.20	0.41
1:A:608:SER:O	1:A:612:LEU:HD13	2.20	0.41
1:A:5:VAL:HG22	1:A:5:VAL:O	2.21	0.41
1:A:583:ARG:O	1:A:584:VAL:CB	2.69	0.41
1:A:828:ALA:HB3	1:A:829:PRO:CD	2.36	0.41
1:A:95:ILE:O	1:A:385:ARG:NH2	2.50	0.41
1:A:671:ILE:C	1:A:671:ILE:CD1	2.86	0.41
1:A:139:TYR:CE2	1:A:350:PRO:HB3	2.55	0.41
1:A:191:LEU:C	1:A:191:LEU:HD23	2.41	0.41
1:A:221:VAL:HG13	1:A:221:VAL:O	2.21	0.41
1:A:736:GLY:N	1:A:788:ASN:OD1	2.54	0.41
1:A:871:LEU:HB3	1:A:948:ILE:HD12	2.01	0.41
1:A:550:VAL:CG1	1:A:753:VAL:CA	2.97	0.41
1:A:675:ALA:CB	1:A:684:LEU:HG	2.39	0.41
1:A:893:LEU:HD22	1:A:893:LEU:O	2.20	0.41
1:A:445:GLN:CB	1:A:475:ALA:O	2.69	0.41
1:A:548:HIS:CE1	1:A:685:GLU:HB3	2.56	0.41
1:A:719:GLN:CG	1:A:726:ILE:HD12	2.51	0.41
1:A:683:THR:OG1	1:A:738:ARG:NH1	2.54	0.41
1:A:717:ASP:N	1:A:718:PRO:CD	2.83	0.41
1:A:791:HIS:O	1:A:795:ILE:HD12	2.21	0.41
1:A:598:ARG:O	1:A:599:ARG:HB3	2.20	0.40
1:A:960:VAL:CG1	1:A:962:LYS:HD2	2.51	0.40
1:A:719:GLN:NE2	1:A:726:ILE:HG21	2.37	0.40
1:A:807:PHE:CG	1:A:817:LEU:HD21	2.57	0.40
1:A:94:ILE:HD12	1:A:496:ALA:O	2.20	0.40
1:A:667:GLN:O	1:A:670:VAL:CG1	2.70	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	961/982 (98%)	781 (81%)	150 (16%)	30 (3%)	4 31

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	PHE
1	A	288	ASP
1	A	481	ASN
1	A	519	LYS
1	A	520	MET
1	A	847	GLU
1	A	848	ASN
1	A	892	SER
1	A	286	ALA
1	A	353	VAL
1	A	584	VAL
1	A	709	ILE
1	A	831	ASN
1	A	272	PRO
1	A	457	TYR
1	A	549	ARG
1	A	675	ALA
1	A	750	THR
1	A	839	SER
1	A	161	PRO
1	A	274	PRO
1	A	300	PRO
1	A	761	SER
1	A	871	LEU
1	A	244	LEU
1	A	957	GLU
1	A	624	PRO
1	A	350	PRO

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Mol	Chain	Res	Type
1	A	640	PRO
1	A	592	VAL

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	806/821 (98%)	718 (89%)	88 (11%)	6 26

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	TYR
1	A	40	GLN
1	A	43	ARG
1	A	55	TRP
1	A	116	PHE
1	A	121	MET
1	A	130	ASP
1	A	131	LYS
1	A	185	MET
1	A	219	LYS
1	A	254	LYS
1	A	265	LEU
1	A	269	ARG
1	A	306	LEU
1	A	327	LEU
1	A	332	GLN
1	A	341	ASN
1	A	342	ARG
1	A	344	PHE
1	A	349	LEU
1	A	363	PHE
1	A	399	ILE
1	A	407	ARG
1	A	425	ARG

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Mol	Chain	Res	Type
1	A	426	LEU
1	A	434	LEU
1	A	446	MET
1	A	478	CYS
1	A	479	THR
1	A	487	LEU
1	A	491	GLU
1	A	492	LYS
1	A	493	LEU
1	A	494	LEU
1	A	497	ASP
1	A	518	HIS
1	A	519	LYS
1	A	520	MET
1	A	549	ARG
1	A	572	ARG
1	A	582	ARG
1	A	599	ARG
1	A	601	SER
1	A	603	THR
1	A	612	LEU
1	A	614	ARG
1	A	619	LEU
1	A	656	MET
1	A	658	LEU
1	A	666	MET
1	A	671	ILE
1	A	673	THR
1	A	676	ARG
1	A	677	ARG
1	A	679	LEU
1	A	685	GLU
1	A	716	ARG
1	A	754	LYS
1	A	756	LEU
1	A	767	ARG
1	A	769	LEU
1	A	778	PHE
1	A	783	THR
1	A	800	ARG
1	A	810	GLU
1	A	824	ASP

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Mol	Chain	Res	Type
1	A	831	ASN
1	A	839	SER
1	A	840	PRO
1	A	842	TRP
1	A	843	LYS
1	A	854	ASP
1	A	867	LEU
1	A	875	ASN
1	A	884	LEU
1	A	886	ARG
1	A	887	LEU
1	A	889	GLU
1	A	893	LEU
1	A	905	PHE
1	A	909	SER
1	A	933	ARG
1	A	934	TRP
1	A	941	CYS
1	A	958	PHE
1	A	968	LEU
1	A	969	ARG
1	A	974	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	105	GLN
1	A	174	GLN
1	A	230	HIS
1	A	279	HIS
1	A	299	GLN
1	A	329	GLN
1	A	341	ASN
1	A	387	HIS
1	A	388	GLN
1	A	405	GLN
1	A	429	GLN
1	A	489	ASN
1	A	618	GLN
1	A	695	GLN
1	A	719	GLN

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Mol	Chain	Res	Type
1	A	791	HIS
1	A	797	GLN
1	A	849	ASN
1	A	875	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

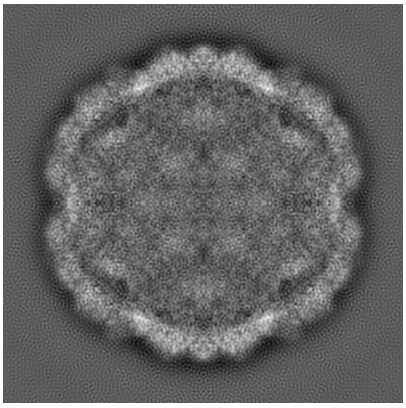
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-5600. These allow visual inspection of the internal detail of the map and identification of artifacts.

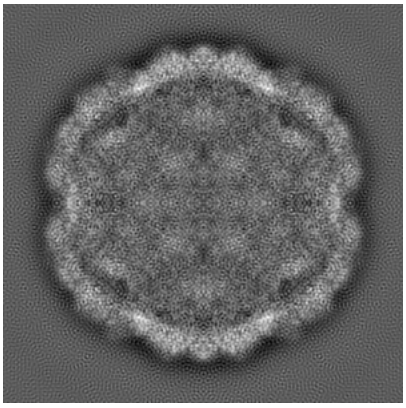
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

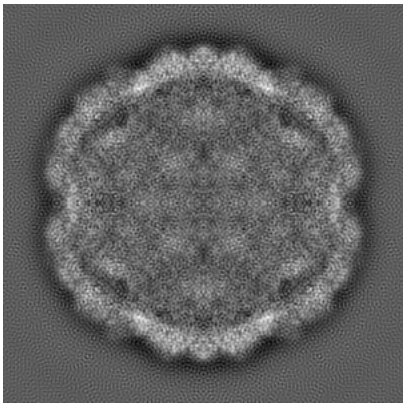
6.1.1 Primary map



X



Y

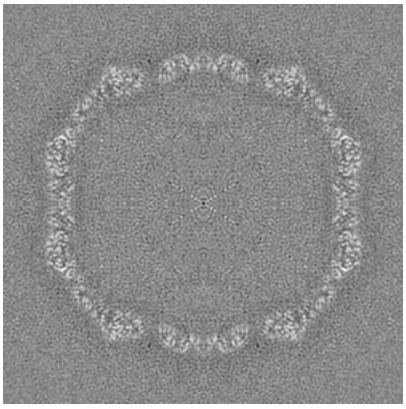


Z

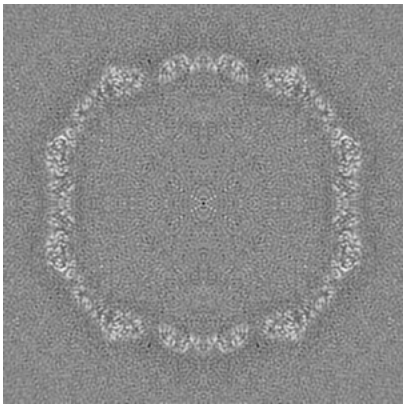
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

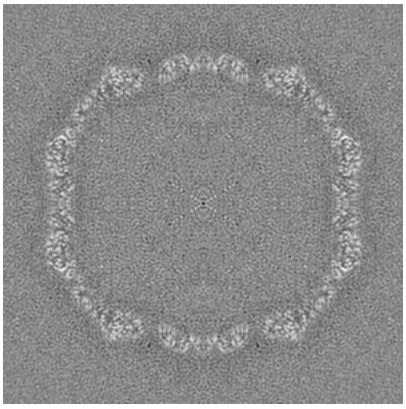
6.2.1 Primary map



X Index: 198



Y Index: 198

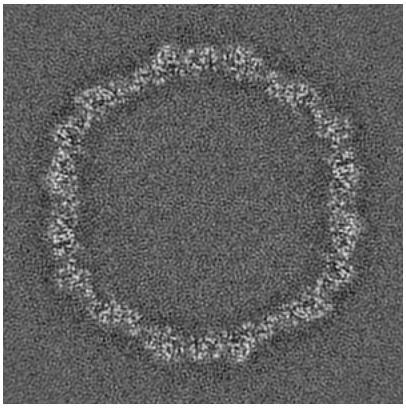


Z Index: 198

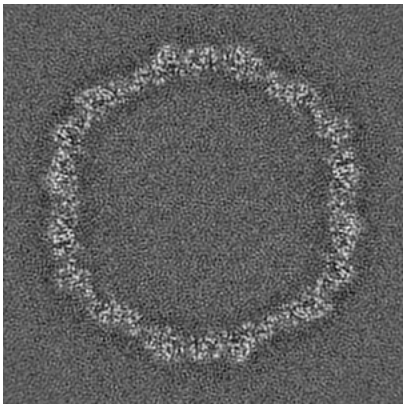
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

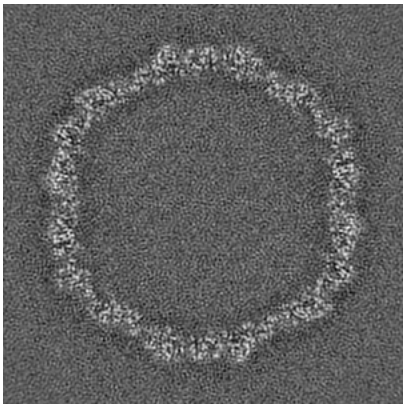
6.3.1 Primary map



X Index: 227



Y Index: 227

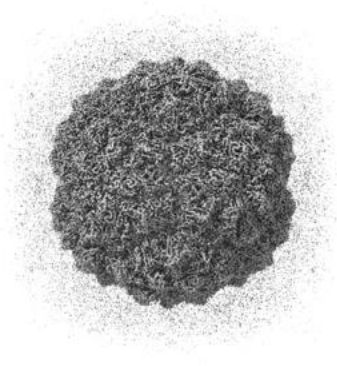


Z Index: 227

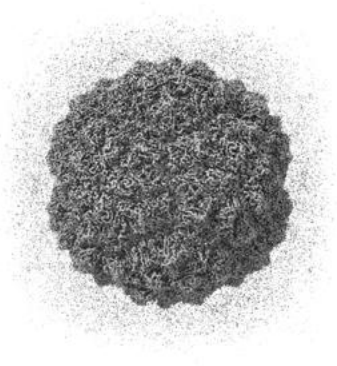
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

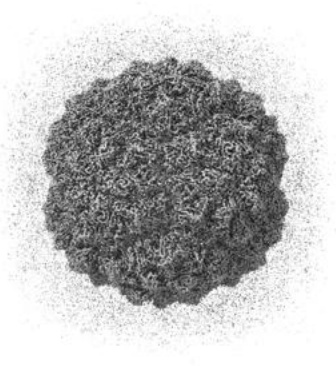
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

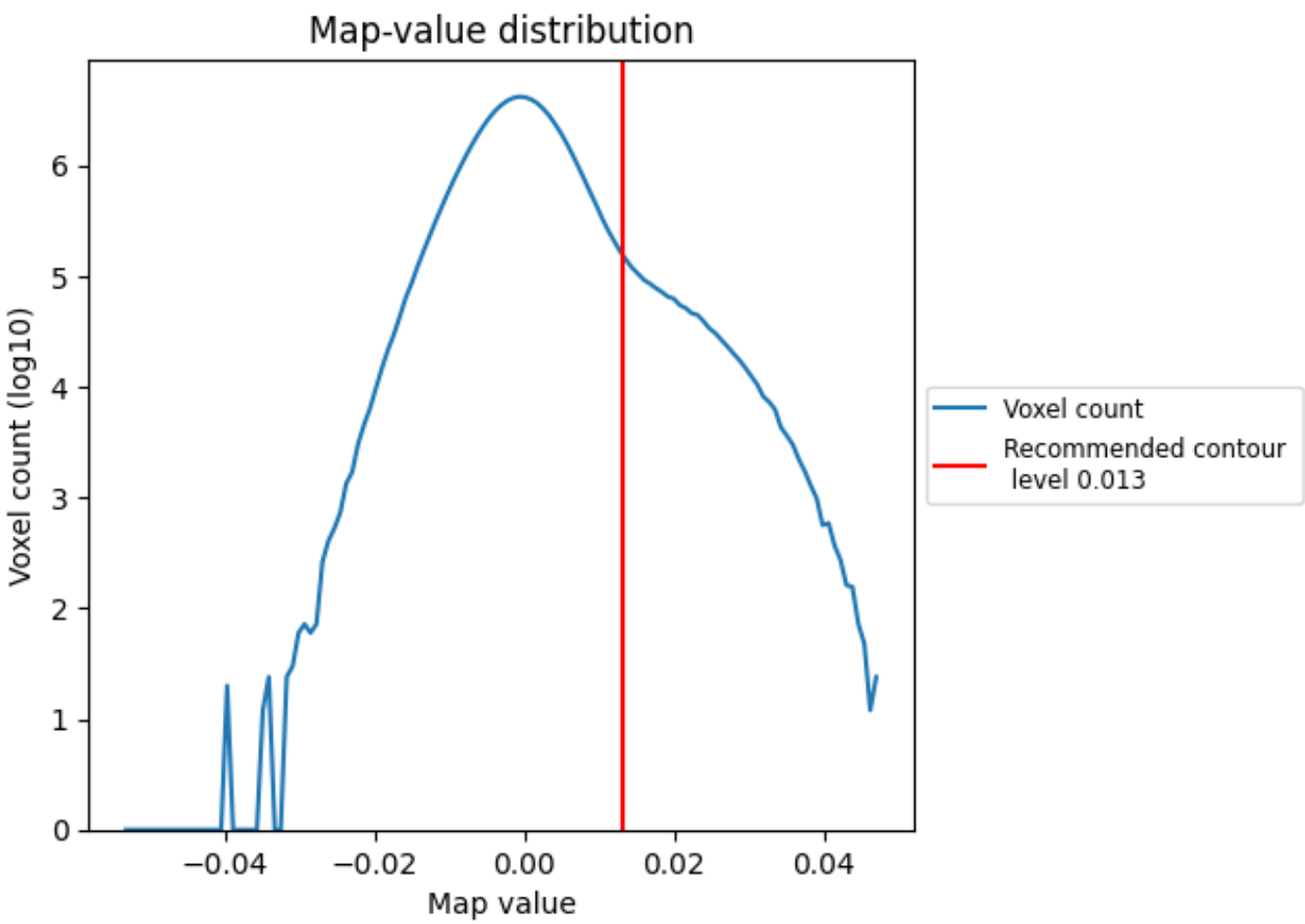
6.5 Mask visualisation (i)

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

7 Map analysis (i)

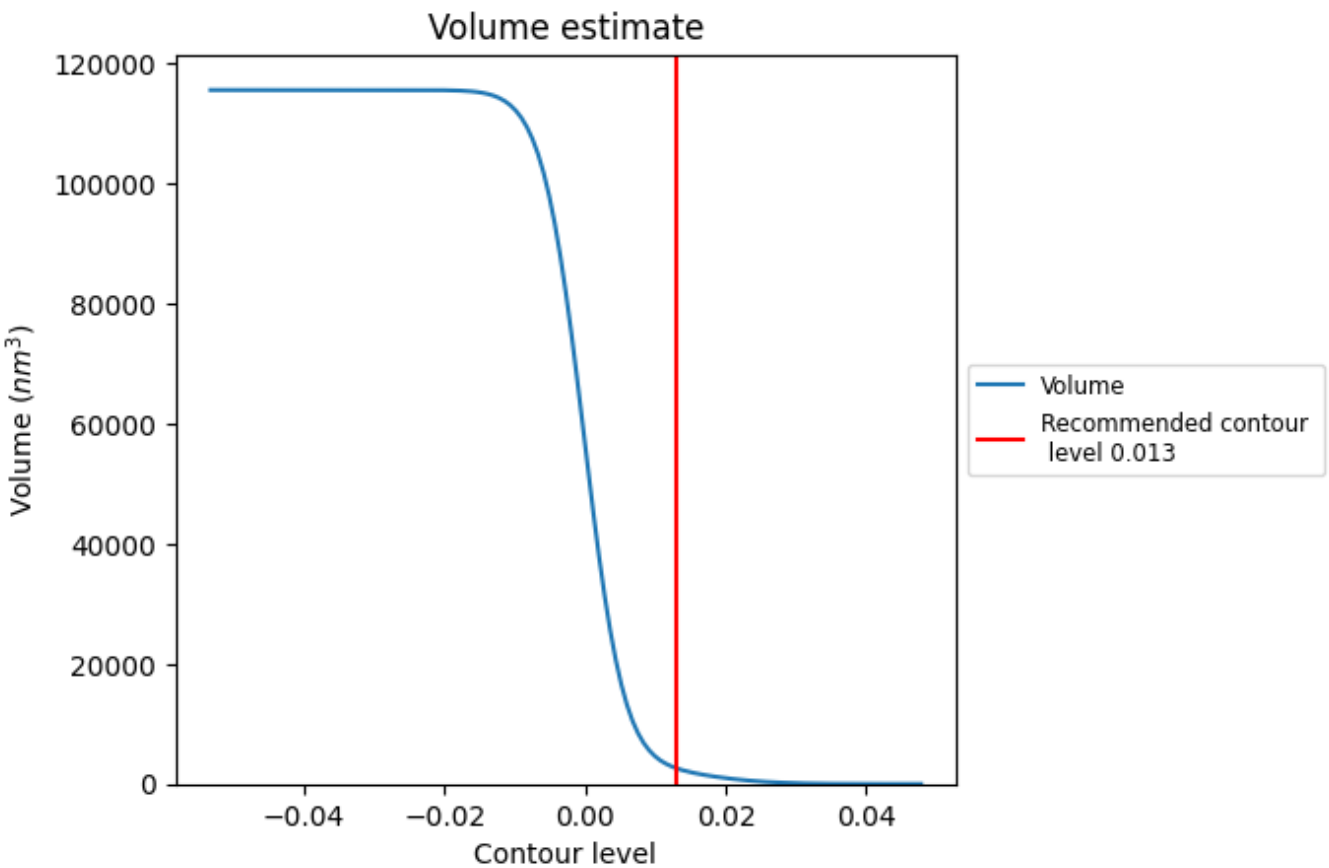
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

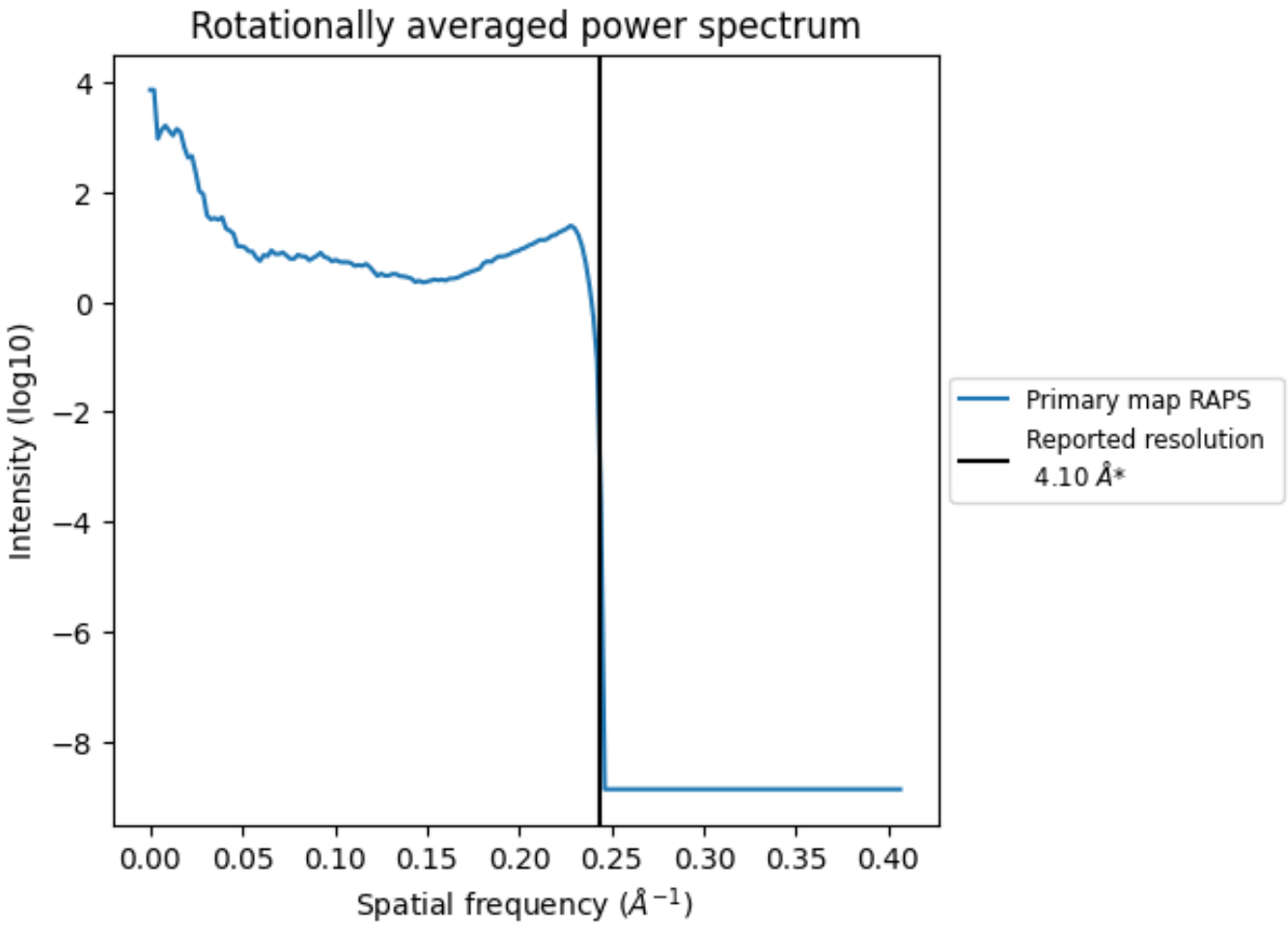
7.2 Volume estimate (i)



The volume at the recommended contour level is 2622 nm^3; this corresponds to an approximate mass of 2368 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 0.244 Å^{-1}

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

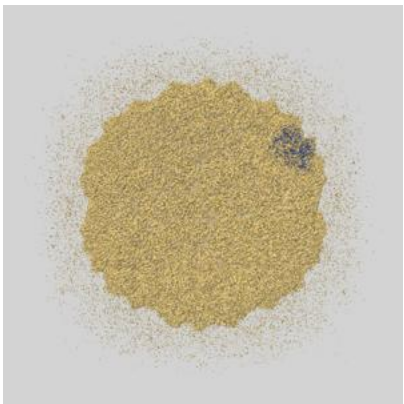
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-5600 and PDB model 3J3I. Per-residue inclusion information can be found in section 3 on page 4.

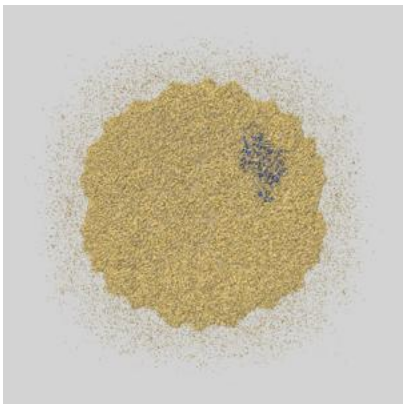
9.1 Map-model overlays

9.1.1 Map-model overlay (i)

X

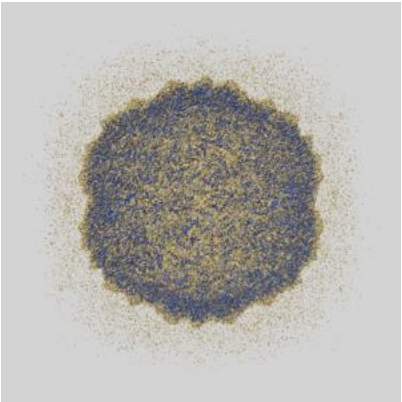


Y

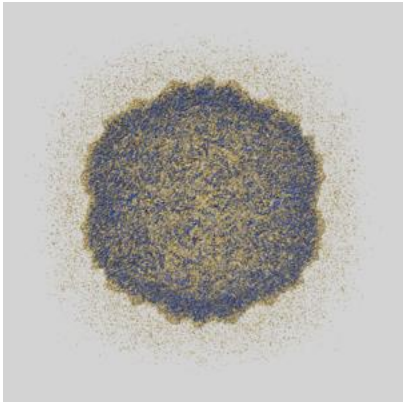


Z

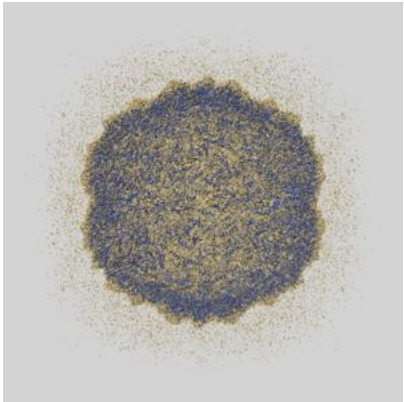
9.1.2 Map-model assembly overlay (i)



X



Y



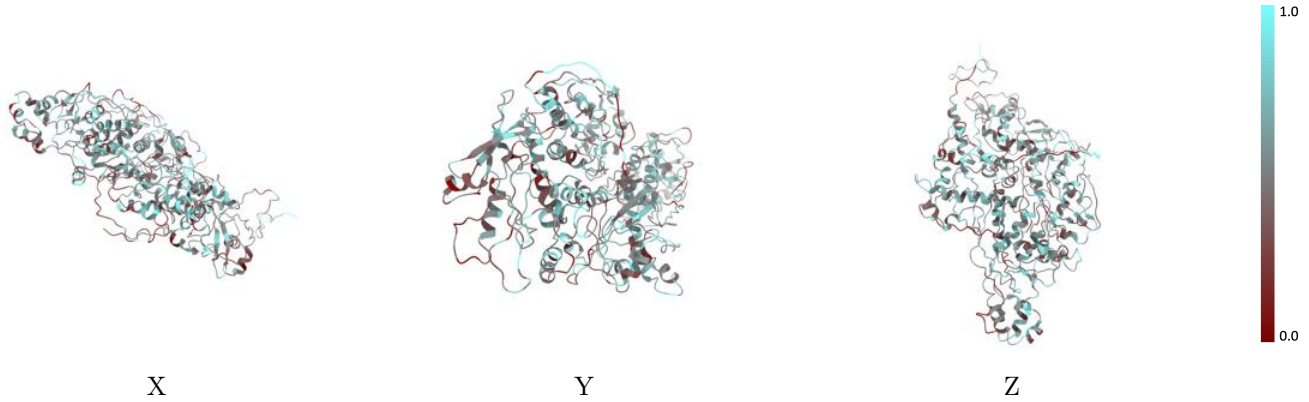
Z

The images above show the 3D surface view of the map at the recommended contour level 0.013 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)

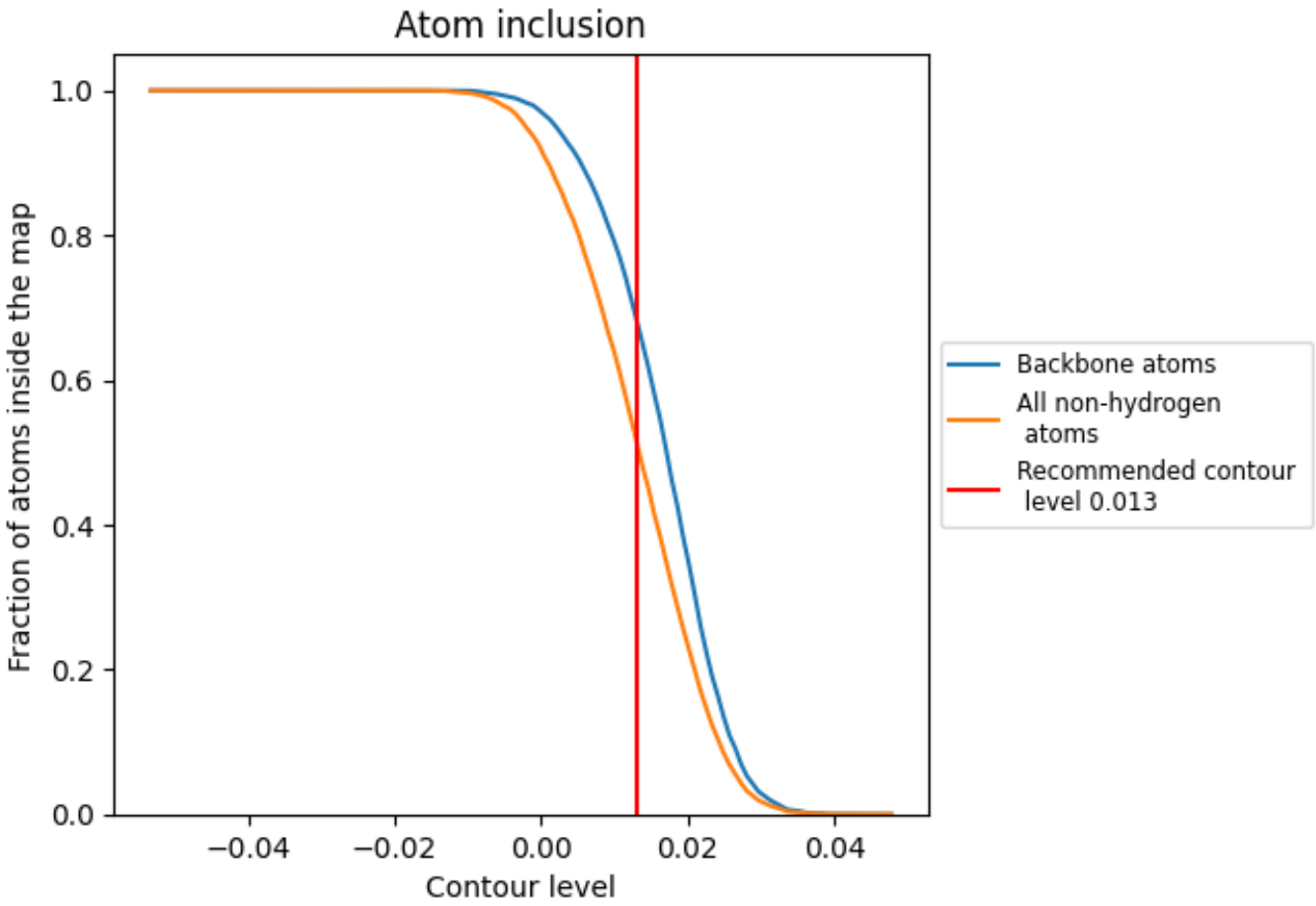
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)



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 (0.013).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 52% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5154	0.3080
A	0.5154	0.3080