Full wwPDB EM Validation Report ⓘ

May 15, 2024 – 05:19 PM EDT

PDB ID	:	7K0S
EMDB ID	:	EMD-22615
Title	:	Cryo-EM structure of rabbit RyR1 in the presence of Mg2+ and AMP-PCP in nanodisc
Authors	:	Nayak, A.R.; Samso, M.
Deposited on	:	2020-09-05
Resolution	:	4.50 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:

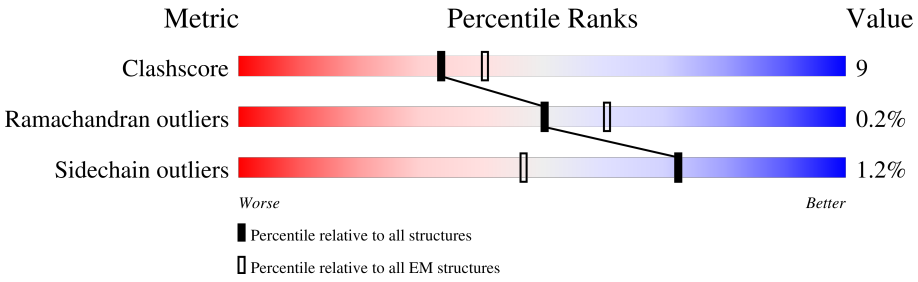
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 4.50 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	5037	69% 12% 18%
1	B	5037	68% 13% 18%
1	C	5037	68% 13% 18%
1	D	5037	69% 13% 18%

2 Entry composition

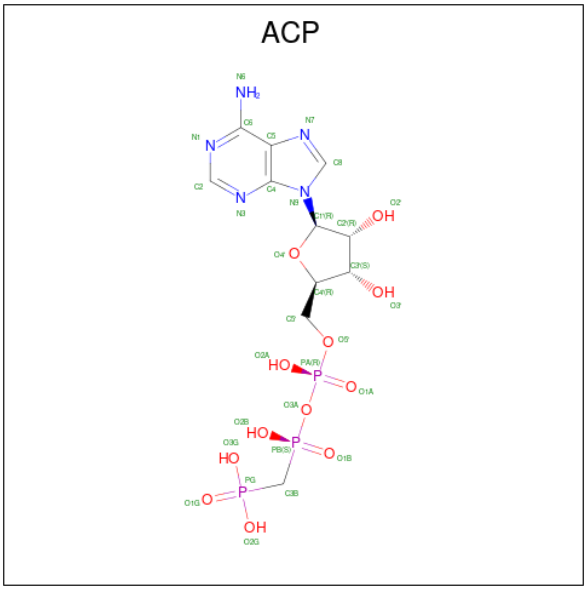
There are 4 unique types of molecules in this entry. The entry contains 115935 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RyR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4110	Total	C	N	O	S	0	0
			28941	18335	5131	5318	157		
1	B	4110	Total	C	N	O	S	0	0
			28940	18334	5135	5315	156		
1	D	4110	Total	C	N	O	S	0	0
			28963	18348	5134	5324	157		
1	C	4110	Total	C	N	O	S	0	0
			28958	18354	5132	5317	155		

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			31	11	5	12	3	
2	B	1	Total	C	N	O	P	0
			31	11	5	12	3	

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Mol	Chain	Residues	Atoms					AltConf
2	D	1	Total	C	N	O	P	0
			31	11	5	12	3	
2	C	1	Total	C	N	O	P	0
			31	11	5	12	3	

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

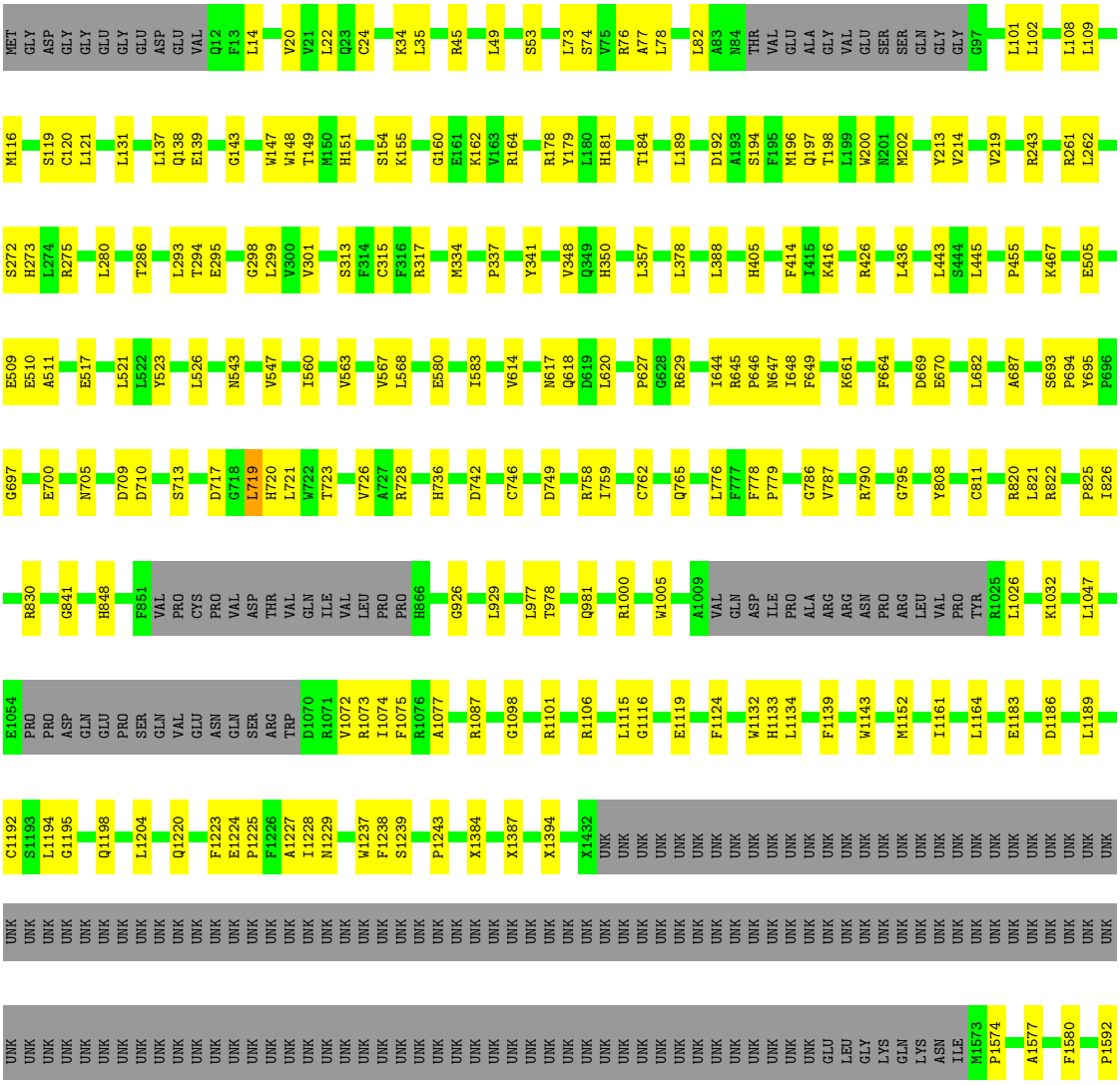
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	B	2	Total	Mg	0
			2	2	
4	D	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	

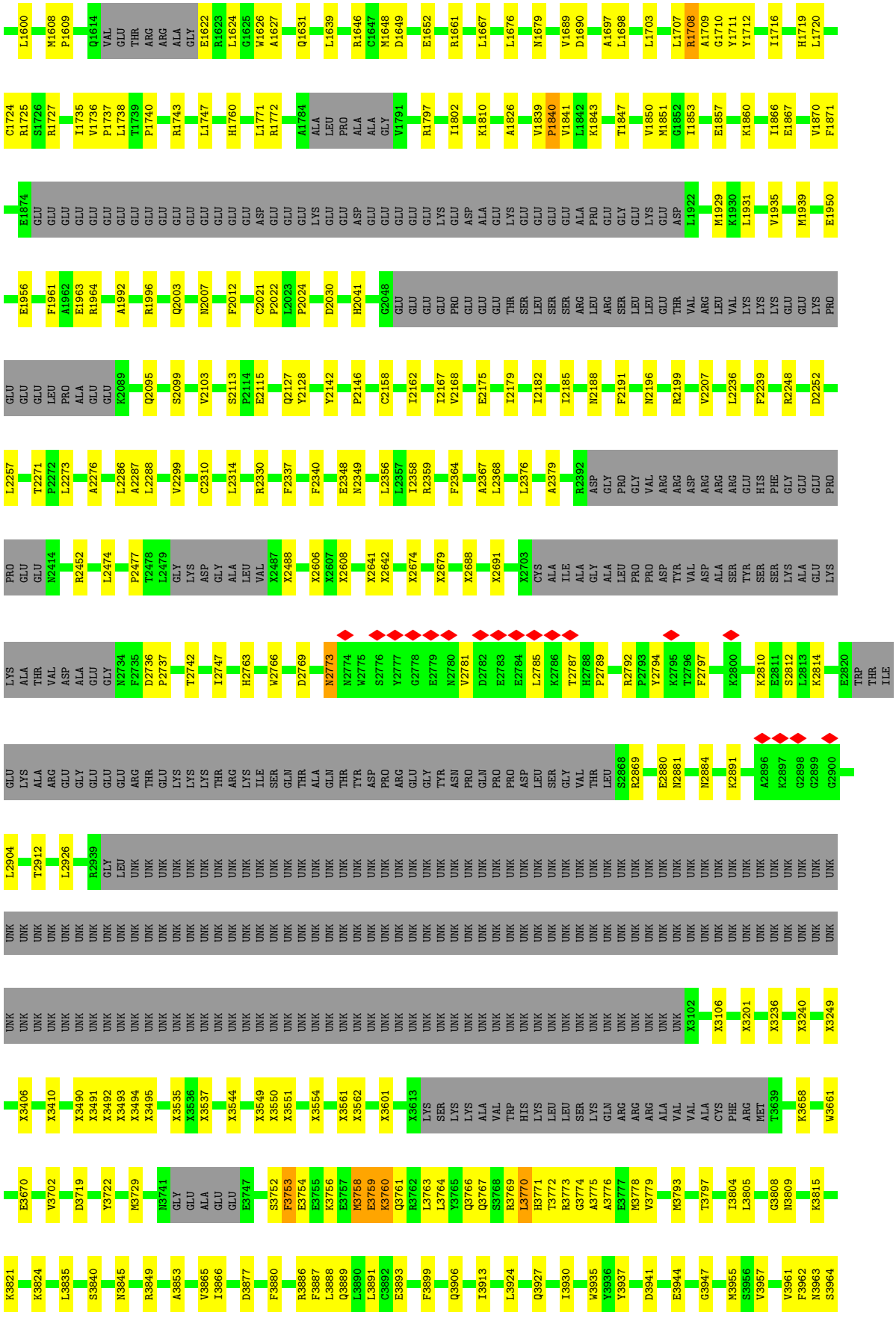
3 Residue-property plots (i)

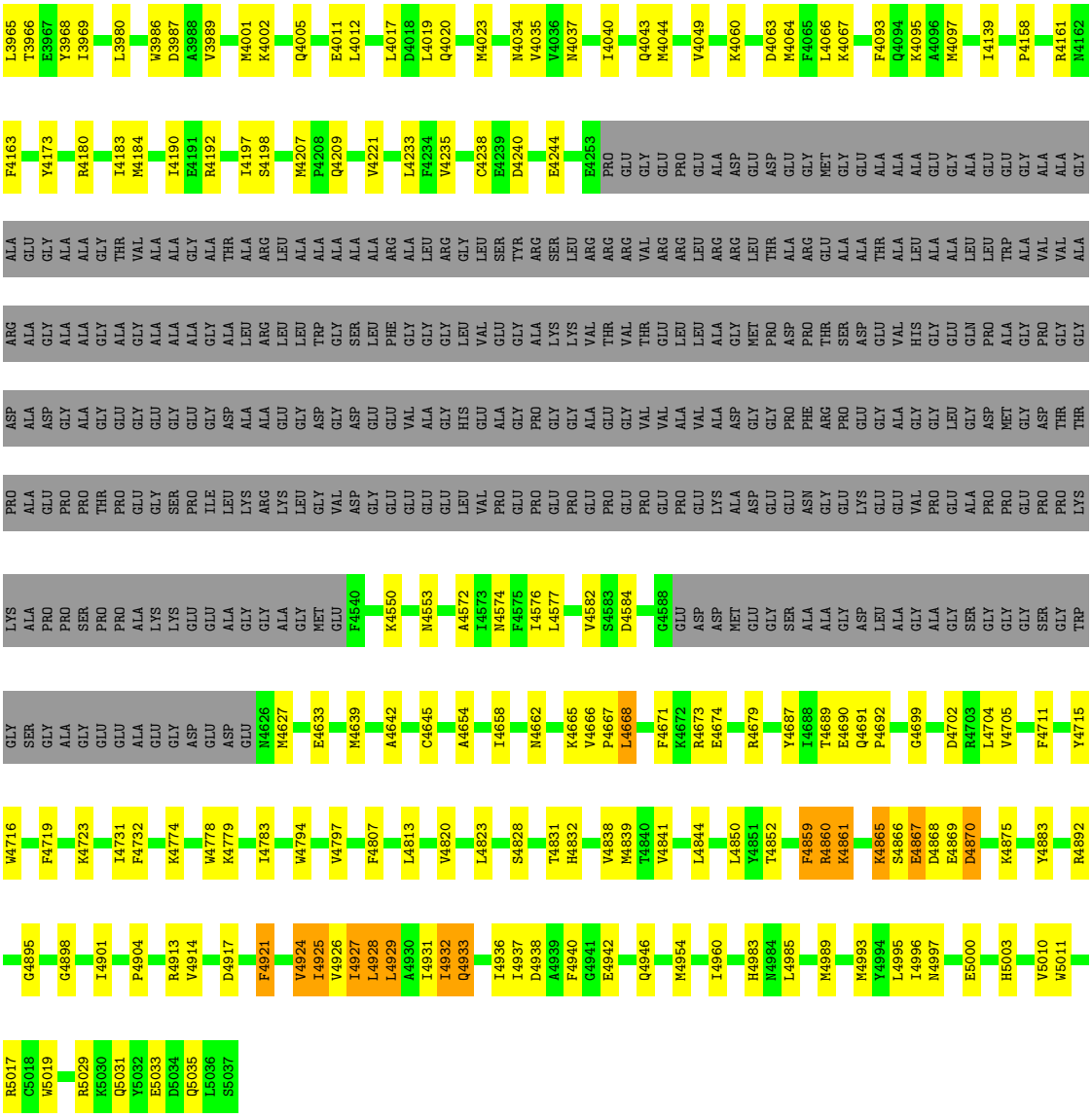
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: RyR1

Chain A:

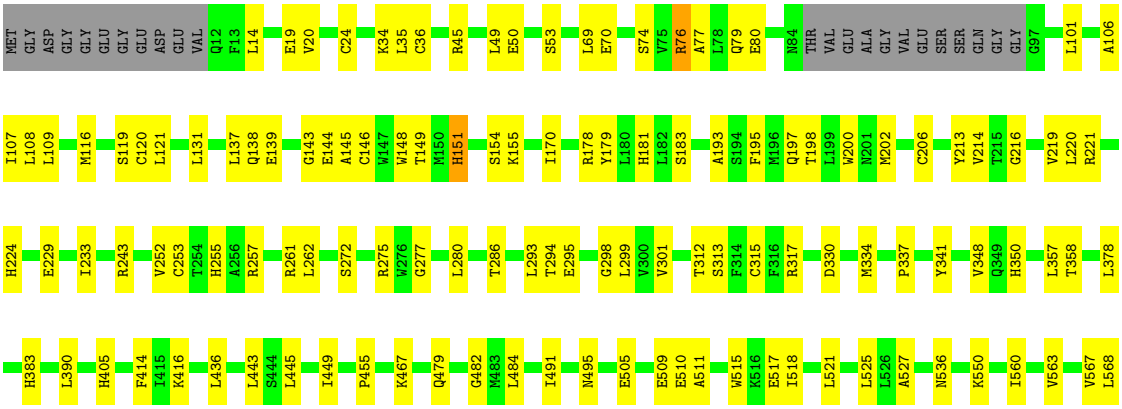


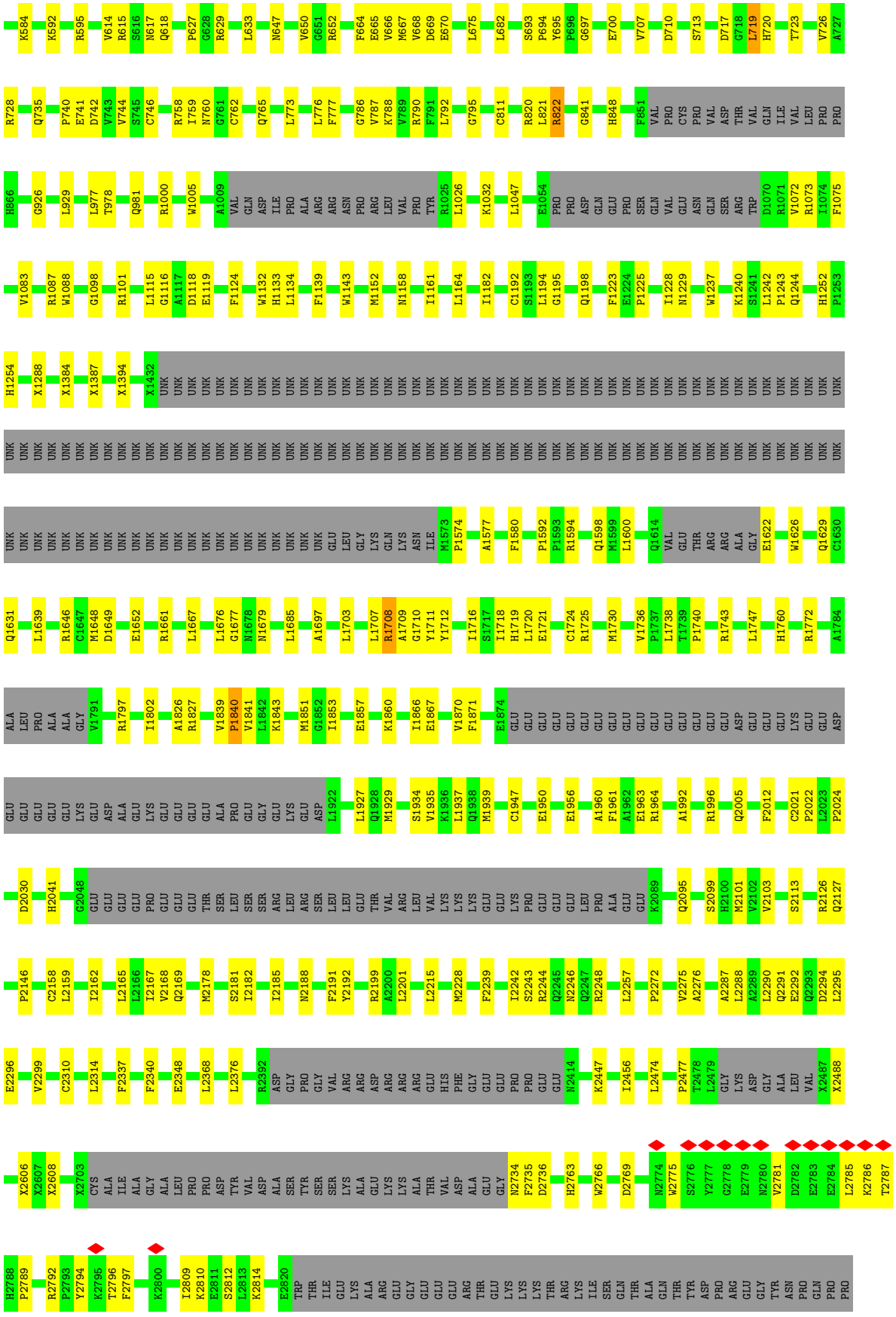


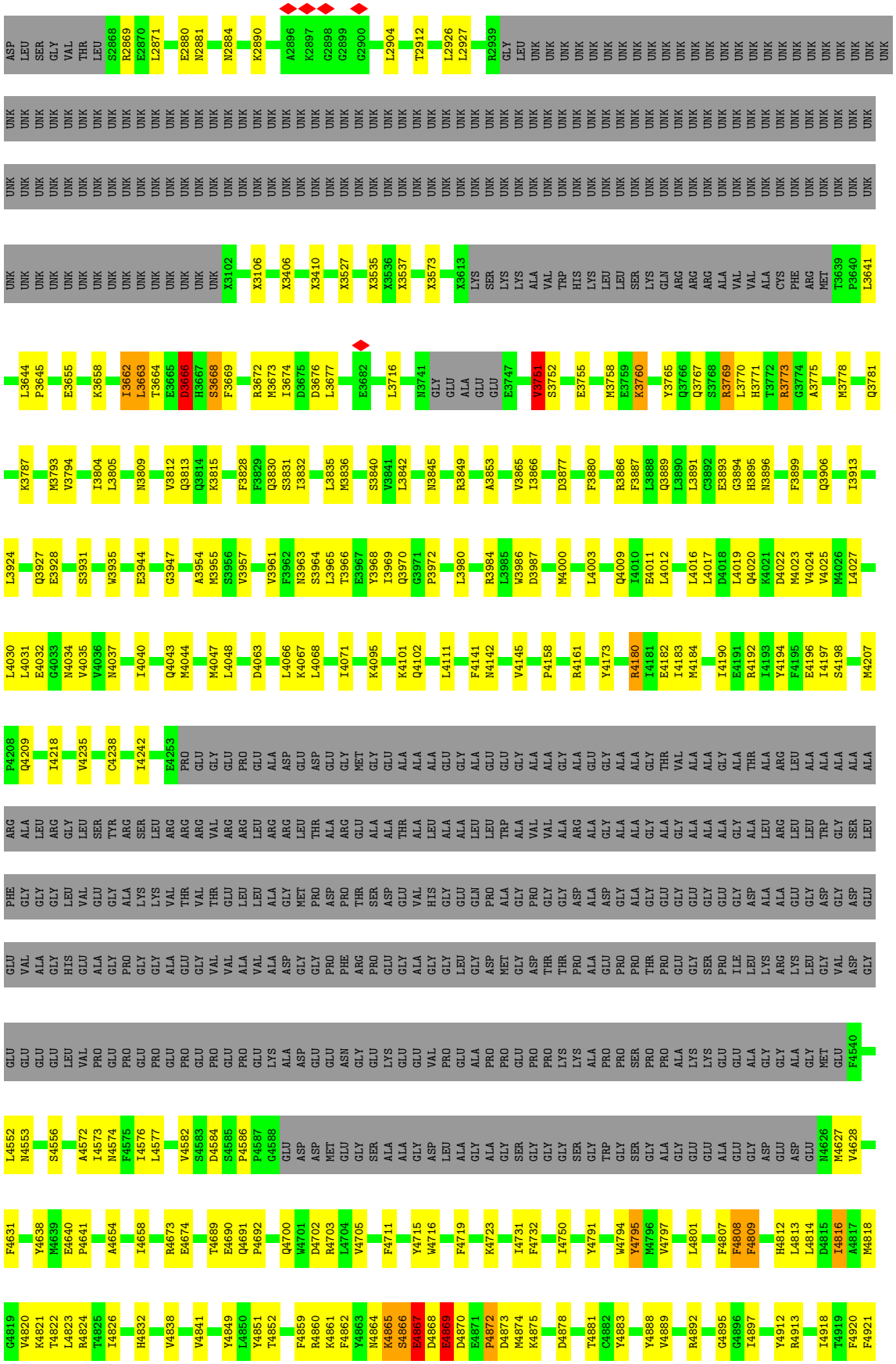


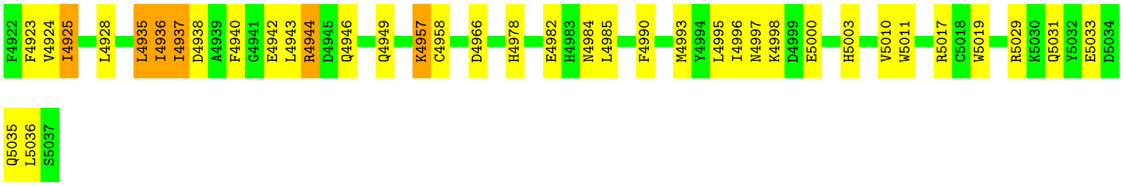
• Molecule 1: RyR1

Chain B:

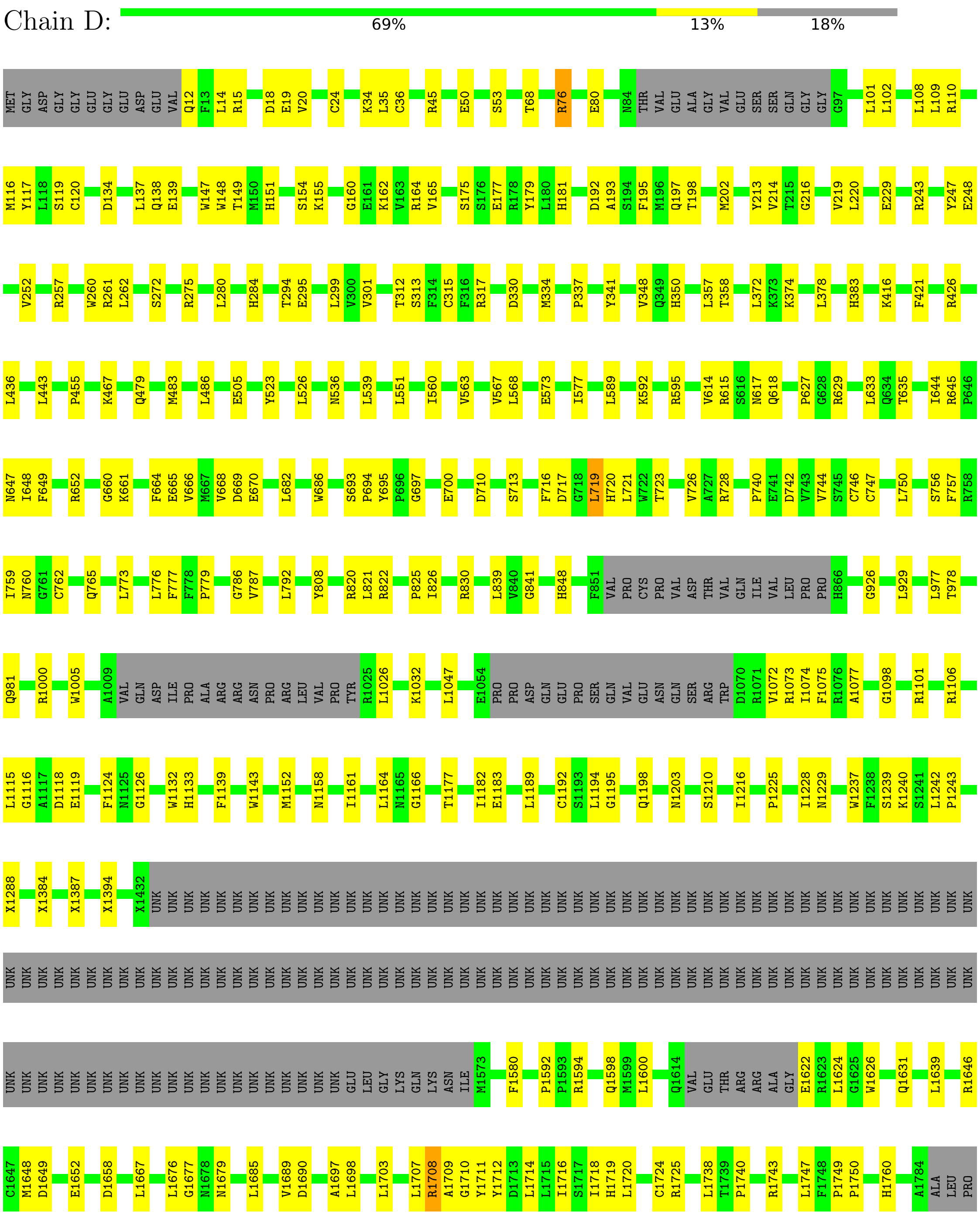


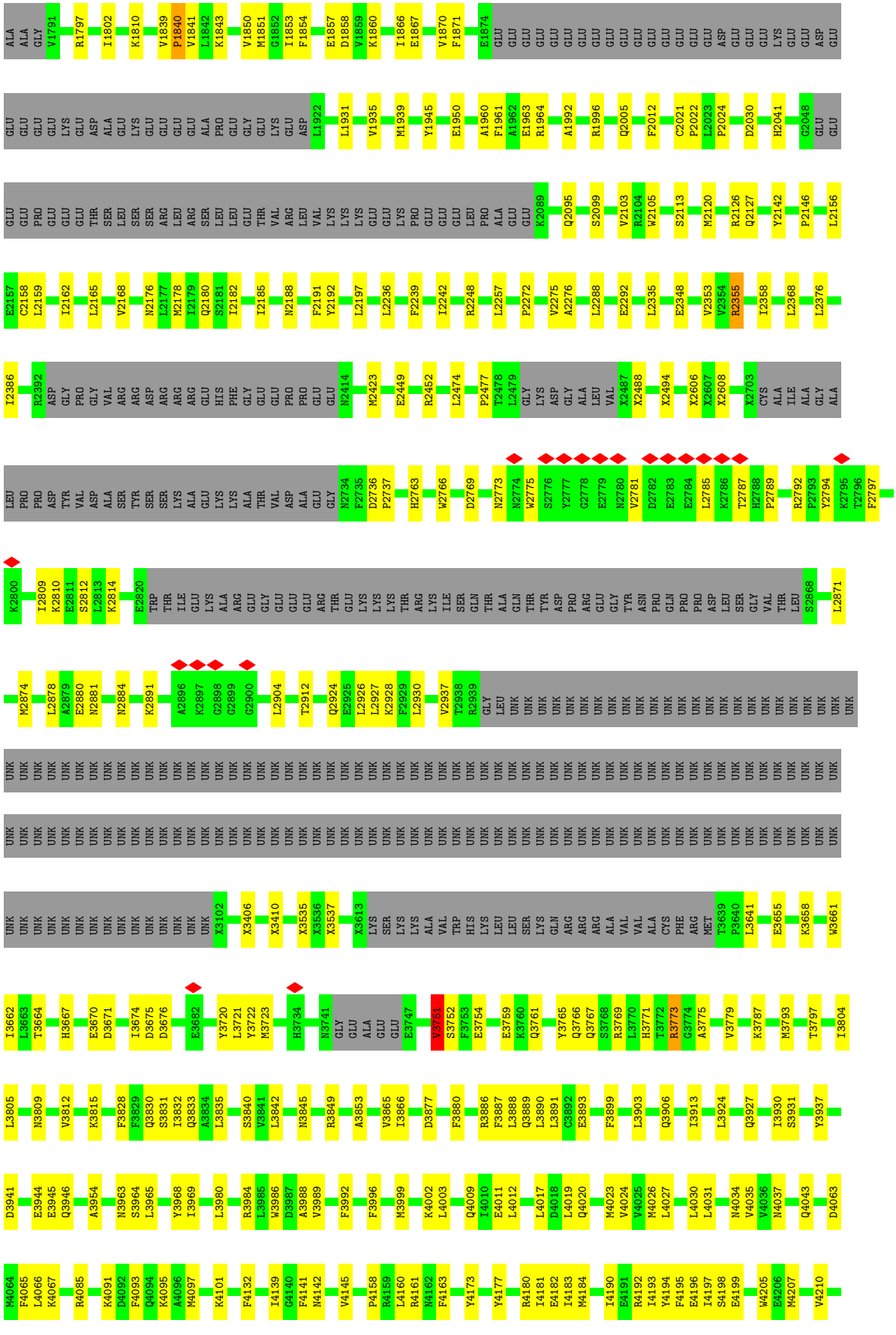


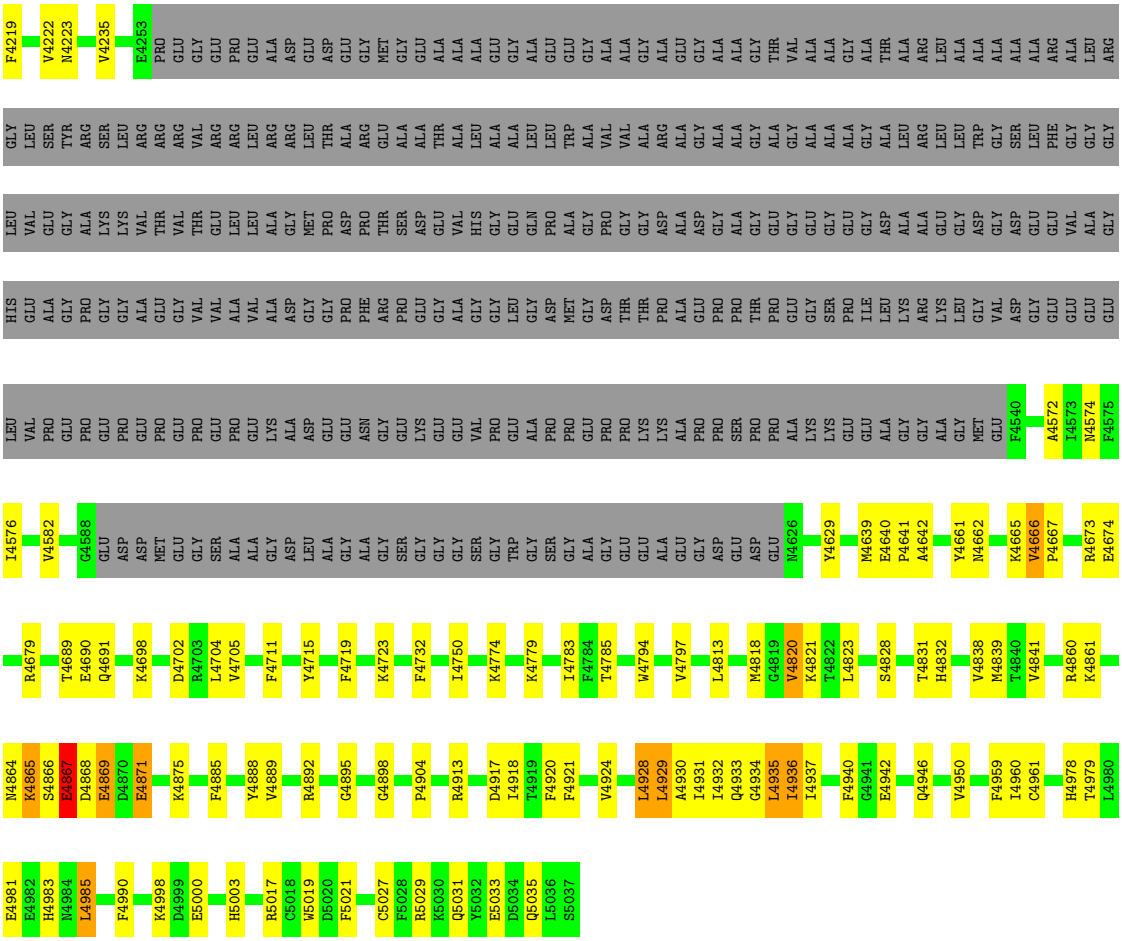




- Molecule 1: RyR1

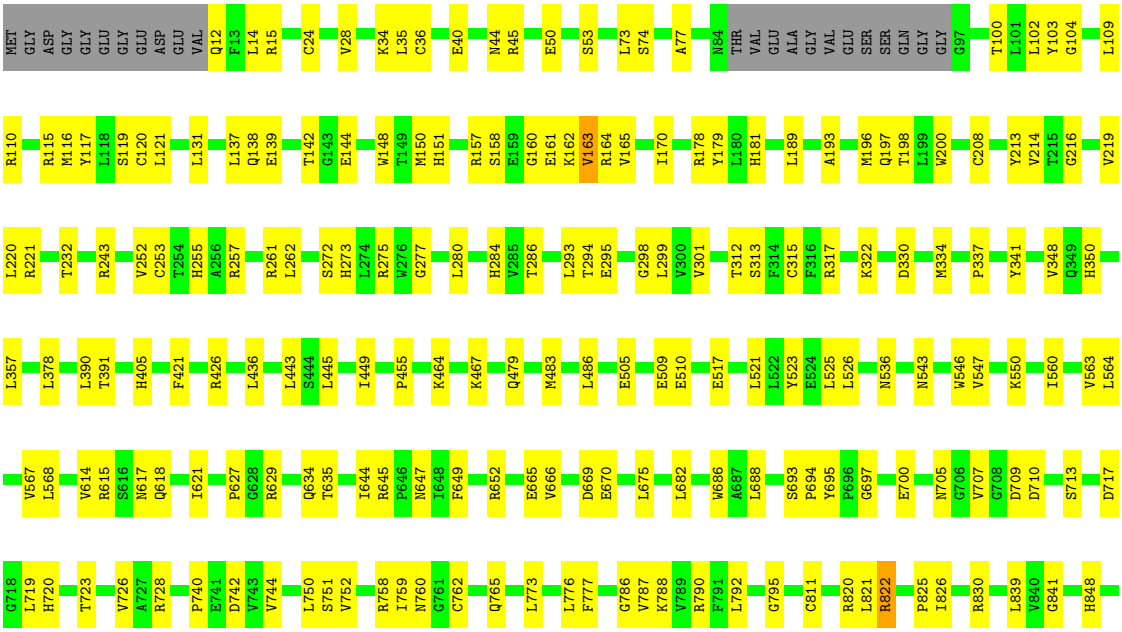


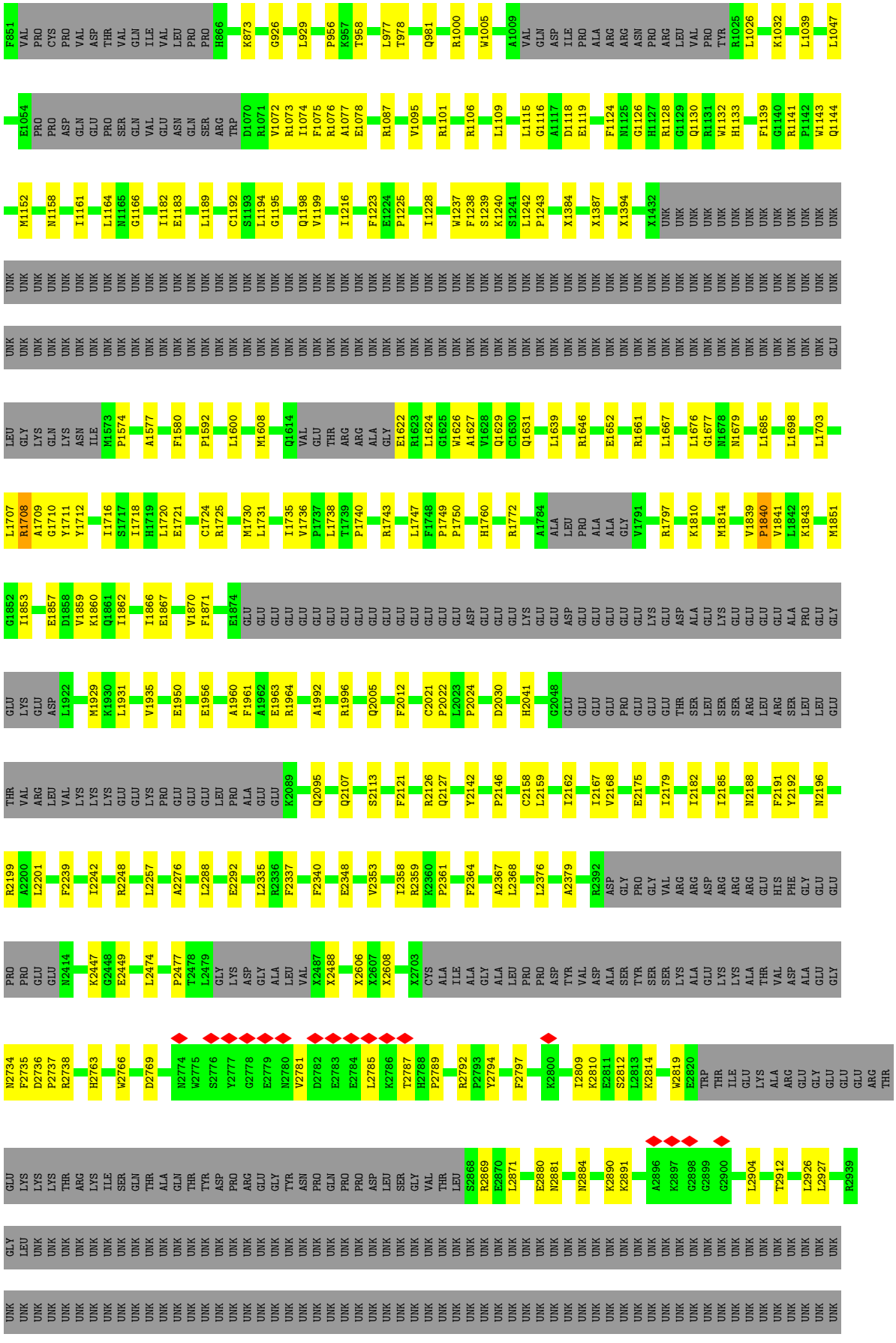


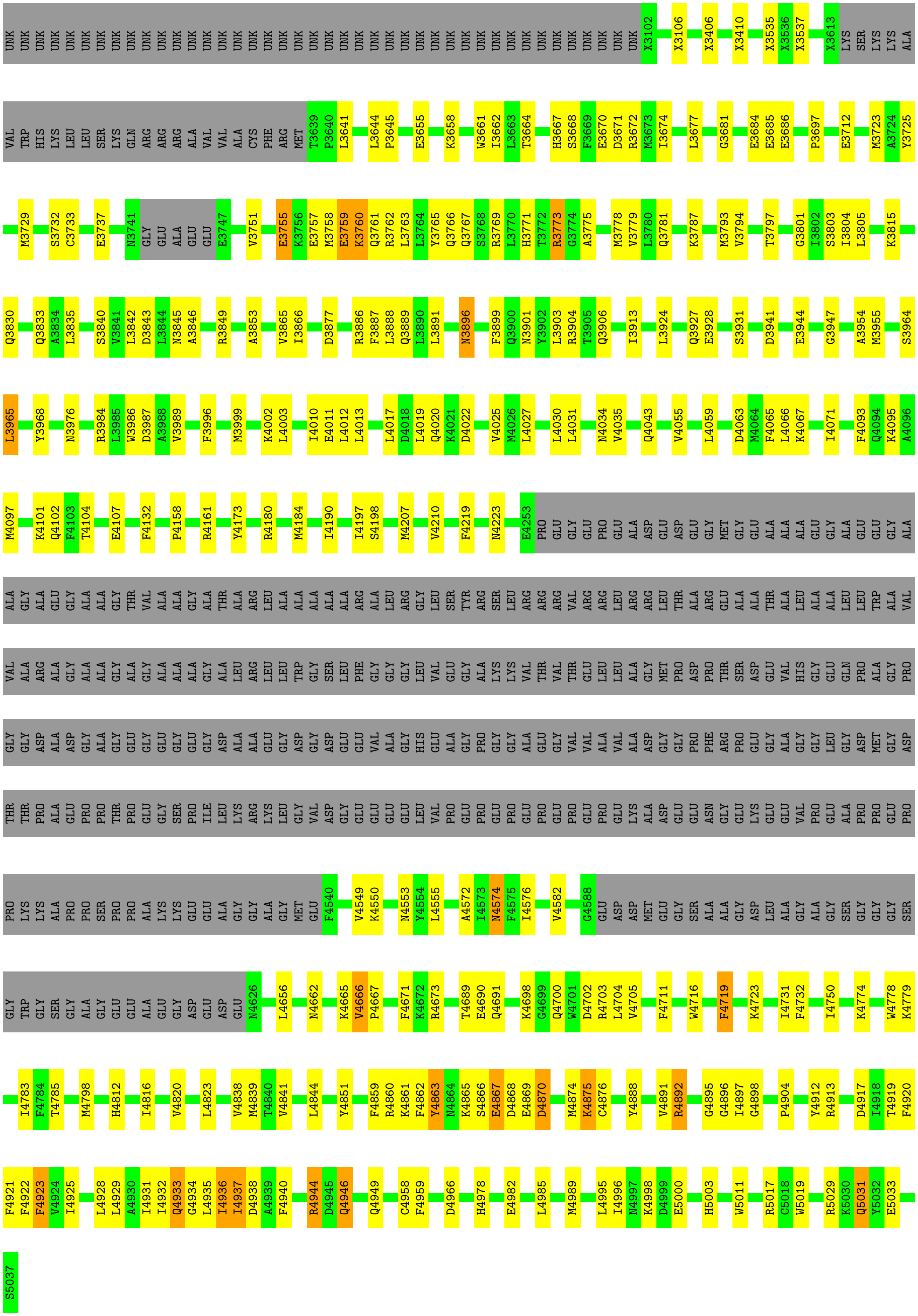


• Molecule 1: RyR1

Chain C:



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VAL TRP HIS LYS LEU LEU SER LYS GLN ARG ARG ARG ALA VAL VAL ALA CYS PHE ARG MET T3639 P3640 L3641 L3644 P3645 E3655 K3658 W3661 I3662 L3663 T3664 H3667 S3668 F3669 E3670 D3671 R3672 M3673 I3674 L3677 G3681 E3684 E3685 E3686 P3697 E3712 M3723 A3724 Y3725
M3729 S3732 C3733 E3737 N3741 GLY GLU ALA GLU GLU E3747 V3751 E3755 K3756 E3757 M3758 E3759 K3760 Q3761 R3762 L3763 L3764 Y3765 Q3766 Q3767 S3768 R3769 L3770 H3771 T3772 R3773 G3774 A3775 M3778 V3779 L3780 Q3781 K3787 M3793 V3794 T3797 G3801 I3802 S3803 I3804 L3805 K3815
Q3830 Q3833 A3834 L3835 S3840 V3841 L3842 D3843 L3844 N3845 A3846 R3849 A3853 V3865 I3866 D3877 R3886 F3887 L3888 Q3889 L3890 L3891 N3896 F3899 Q3900 N3901 Y3902 L3903 R3904 T3905 Q3906 I3913 L3924 Q3927 E3928 S3931 D3941 E3944 G3947 A3954 M3955 S3964
L3965 Y3968 N3976 R3984 L3985 W3986 D3987 A3988 V3989 F3996 M3999 K4002 L4003 I4010 E4011 L4012 L4013 L4017 D4018 L4019 Q4020 K4021 D4022 V4025 M4026 L4027 L4030 L4031 N4034 V4035 Q4043 V4055 L4059 D4063 M4064 F4065 L4066 K4067 I4071 F4093 Q4094 K4095 A4096
M4097 K4101 Q4102 F4103 T4104 E4107 F4132 P4158 R4161 Y4173 R4180 M4184 I4190 I4197 S4198 M4207 V4210 F4219 N4223 E4253 PRO GLU GLY GLU PRO GLU ALA ASP GLU ASP GLU GLY MET GLY GLU ALA ALA ALA GLU GLY ALA GLU GLU GLY ALA
ALA GLY ALA GLU GLY ALA ALA GLY THR VAL ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ALA ALA ARG ALA LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG VAL ARG ARG LEU ARG ARG LEU THR ALA ARG GLU ALA ALA THR ALA LEU ALA ALA LEU LEU TRP ALA VAL
VAL ALA ARG ALA GLY ALA ALA GLY ALA GLY ALA ALA ALA GLY ALA LEU ARG LEU LEU TRP GLY SER LEU PHE GLY GLY GLY LEU VAL GLU GLY ALA LYS LYS VAL THR VAL THR GLU LEU LEU ALA GLY MET PRO ASP PRO THR SER ASP GLU VAL HIS GLY GLU GLN PRO ALA GLY PRO
GLY GLY ASP ALA ASP GLY ALA GLY GLU GLY GLU GLY GLU GLY ASP ALA ALA GLU GLY ASP GLY ASP GLU GLU VAL ALA GLY HIS GLU ALA GLY PRO GLY GLY ALA GLU GLY VAL VAL ALA VAL ALA ASP GLY GLY PRO PHE ARG PRO GLU GLY ALA GLY GLY LEU GLY ASP MET GLY ASP
THR THR PRO ALA GLU PRO PRO THR PRO GLU GLY GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU GLU LEU VAL PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU LYS ALA ASP GLU GLU ASN GLY GLU LYS GLU GLU VAL PRO GLU ALA PRO PRO GLU PRO
PRO LYS LYS ALA PRO PRO SER PRO PRO ALA LYS LYS GLU GLU ALA GLY GLY ALA GLY MET GLU F4540 V4549 K4550 N4553 Y4554 L4555 A4572 I4573 N4574 F4575 I4576 V4582 G4588 GLU ASP ASP MET GLU GLY SER ALA ALA GLY ASP LEU ALA GLY ALA GLY SER GLY GLY GLY SER
GLY TRP GLY SER GLY ALA GLY GLU GLU ALA GLU GLY ASP GLU ASP GLU N4626 L4656 N4662 K4665 V4666 P4667 F4671 K4672 R4673 T4689 E4690 Q4691 K4698 G4699 Q4700 W4701 D4702 R4703 L4704 V4705 F4711 W4716 F4719 K4723 I4731 F4732 I4750 K4774 W4778 K4779
I4783 F4784 T4785 M4798 H4812 I4816 V4820 L4823 V4838 M4839 T4840 V4841 L4844 Y4851 F4859 R4860 K4861 F4862 Y4863 N4864 K4865 S4866 E4867 D4868 E4869 D4870 M4874 K4875 C4876 Y4888 V4891 R4892 G4895 G4896 I4897 G4898 P4904 Y4912 R4913 D4917 I4918 T4919 F4920
F4921 F4922 F4923 V4924 I4925 L4928 L4929 A4930 I4931 I4932 Q4933 G4934 L4935 I4936 I4937 D4938 A4939 F4940 R4944 D4945 Q4946 Q4949 C4958 F4959 D4966 H4978 E4982 L4985 M4989 L4995 I4996 N4997 K4998 D4999 E5000 H5003 W5011 R5017 C5018 W5019 R5029 K5030 Q5031 Y5032 E5033
S5037

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	68155	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.200	Depositor
Minimum map value	-0.126	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	478.72, 478.72, 478.72	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, ACP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.26	0/25057	0.50	1/34021 (0.0%)
1	B	0.27	0/25055	0.50	3/34016 (0.0%)
1	C	0.26	0/25076	0.50	2/34047 (0.0%)
1	D	0.26	0/25078	0.50	2/34045 (0.0%)
All	All	0.26	0/100266	0.50	8/136129 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	3751	VAL	C-N-CA	-5.77	107.27	121.70
1	B	719	LEU	CA-CB-CG	5.62	128.23	115.30
1	D	3751	VAL	C-N-CA	-5.62	107.66	121.70
1	D	719	LEU	CA-CB-CG	5.56	128.08	115.30
1	C	4891	VAL	O-C-N	5.30	131.18	122.70
1	C	4862	PHE	O-C-N	5.27	131.13	122.70
1	B	4872	PRO	CA-N-CD	-5.26	104.13	111.50
1	A	3753	PHE	CB-CA-C	-5.21	99.97	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	4892	ARG	Sidechain

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	28941	0	24397	483	0
1	B	28940	0	24404	519	0
1	C	28958	0	24429	510	0
1	D	28963	0	24439	493	0
2	A	31	0	14	7	0
2	B	31	0	14	4	0
2	C	31	0	14	3	0
2	D	31	0	14	8	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	115935	0	97725	1937	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 9.

All (1937) 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:3773:ARG:CB	1:A:3815:LYS:HE3	1.46	1.45
1:C:3765:TYR:CE1	1:C:4750:ILE:HG23	1.52	1.40
1:A:4921:PHE:O	1:A:4925:ILE:HG22	1.27	1.30
1:A:3767:GLN:O	1:A:3772:THR:HB	1.29	1.28
1:D:3674:ILE:HG12	1:D:3769:ARG:CD	1.64	1.28
1:B:3765:TYR:CE1	1:B:4750:ILE:CG2	2.20	1.24
1:C:3757:GLU:O	1:C:3760:LYS:HG3	1.40	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3674:ILE:CG1	1:D:3769:ARG:HD2	1.71	1.20
1:A:3702:VAL:HG11	1:A:3775:ALA:HB1	1.28	1.15
1:B:4935:LEU:HD23	1:C:4940:PHE:HE2	1.03	1.15
1:B:4573:ILE:HD13	1:B:4809:PHE:CE2	1.83	1.13
1:A:4904:PRO:HG3	1:A:4913:ARG:NH1	1.65	1.11
1:D:3674:ILE:O	1:D:3769:ARG:HD3	1.52	1.09
1:B:3765:TYR:CE1	1:B:4750:ILE:HG23	1.87	1.08
1:B:4573:ILE:CD1	1:B:4809:PHE:HE2	1.67	1.08
1:A:3773:ARG:CB	1:A:3815:LYS:CE	2.33	1.07
1:B:4577:LEU:HD21	1:B:4807:PHE:CE1	1.90	1.07
1:D:4985:LEU:HG	2:D:5101:ACP:HN61	1.12	1.07
1:C:3765:TYR:CE1	1:C:4750:ILE:CG2	2.38	1.06
1:B:4935:LEU:HD23	1:C:4940:PHE:CE2	1.90	1.06
1:A:4985:LEU:HD23	2:A:5101:ACP:HN61	1.19	1.05
1:B:4865:LYS:HA	1:B:4865:LYS:HE3	1.37	1.02
1:A:3702:VAL:HG11	1:A:3775:ALA:CB	1.88	1.01
1:B:4866:SER:O	1:B:4867:GLU:CG	2.07	1.01
1:D:4985:LEU:CG	2:D:5101:ACP:HN61	1.71	1.01
1:C:100:THR:HG21	1:C:162:LYS:HE3	1.42	1.00
1:B:4577:LEU:HD21	1:B:4807:PHE:CD1	1.97	0.99
1:A:3201:UNK:CB	1:A:3249:UNK:CB	2.41	0.98
1:C:3765:TYR:CZ	1:C:4750:ILE:HG23	1.98	0.97
1:D:3674:ILE:HG12	1:D:3769:ARG:HD2	0.98	0.97
1:B:4801:LEU:HD23	1:B:4808:PHE:CE2	2.01	0.96
1:C:3765:TYR:HE1	1:C:4750:ILE:HG23	1.18	0.95
1:B:3765:TYR:HE1	1:B:4750:ILE:HG21	1.31	0.95
1:B:4573:ILE:HD13	1:B:4809:PHE:HE2	1.14	0.95
1:B:3765:TYR:CE1	1:B:4750:ILE:HG21	2.01	0.94
1:B:3674:ILE:CG2	1:B:3769:ARG:HD2	1.97	0.94
1:B:4574:ASN:HD22	1:B:4813:LEU:HD22	1.31	0.94
1:C:162:LYS:HB2	1:C:164:ARG:HH11	1.33	0.94
1:B:3674:ILE:HG22	1:B:3769:ARG:CD	1.98	0.93
1:B:4866:SER:O	1:B:4867:GLU:HG3	1.67	0.93
1:B:4801:LEU:CD2	1:B:4808:PHE:HE2	1.81	0.92
1:D:4820:VAL:HG11	1:D:4823:LEU:HD23	1.51	0.91
1:B:4865:LYS:HB3	1:B:4875:LYS:HG2	1.49	0.91
1:A:4860:ARG:HH11	1:A:4860:ARG:HG3	1.35	0.91
1:A:3702:VAL:CG1	1:A:3775:ALA:HB1	2.00	0.90
1:A:4932:ILE:O	1:A:4936:ILE:HD13	1.71	0.90
1:A:3549:UNK:O	1:A:3550:UNK:C	2.18	0.90
1:D:3767:GLN:HE22	1:D:3804:ILE:HA	1.36	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:LEU:HD12	1:C:163:VAL:O	1.72	0.89
1:C:3765:TYR:HE2	1:C:3769:ARG:NH2	1.71	0.89
1:D:4940:PHE:CE2	1:C:4935:LEU:CD2	2.54	0.89
1:D:5029:ARG:O	1:D:5033:GLU:HB3	1.72	0.89
1:B:4921:PHE:O	1:B:4925:ILE:HG22	1.71	0.88
1:D:4961:CYS:SG	1:D:4983:HIS:CE1	2.67	0.88
1:B:3765:TYR:CD1	1:B:4750:ILE:HG23	2.08	0.88
1:B:4573:ILE:CD1	1:B:4809:PHE:CE2	2.51	0.88
1:A:4921:PHE:O	1:A:4925:ILE:CG2	2.20	0.88
1:B:4016:LEU:HD23	1:B:4020:GLN:HE22	1.38	0.87
1:D:4662:ASN:HA	1:D:4666:VAL:HG21	1.55	0.86
1:B:4801:LEU:HD23	1:B:4808:PHE:HE2	1.36	0.85
1:A:759:ILE:HG22	1:A:762:CYS:HB2	1.57	0.85
1:A:4666:VAL:N	1:A:4667:PRO:HD2	1.91	0.85
1:C:3765:TYR:OH	1:C:4750:ILE:CG2	2.24	0.85
1:C:5029:ARG:O	1:C:5033:GLU:HB3	1.77	0.85
1:A:3760:LYS:HA	1:A:3760:LYS:HZ2	1.42	0.84
1:C:3765:TYR:CZ	1:C:4750:ILE:CG2	2.58	0.84
1:C:2107:GLN:HE22	1:C:3681:GLY:HA2	1.40	0.84
1:B:4921:PHE:O	1:B:4925:ILE:CG2	2.24	0.84
1:C:74:SER:H	1:C:77:ALA:HB3	1.41	0.84
1:D:4985:LEU:HG	2:D:5101:ACP:N6	1.91	0.84
1:C:4944:ARG:HG3	1:C:4944:ARG:HH11	1.40	0.84
1:C:3964:SER:O	1:C:3968:TYR:CE1	2.30	0.84
1:D:4985:LEU:CD2	2:D:5101:ACP:HN61	1.91	0.84
1:B:5029:ARG:O	1:B:5033:GLU:HB3	1.78	0.84
1:A:4940:PHE:CE2	1:D:4935:LEU:CD2	2.61	0.83
1:B:4862:PHE:CE2	1:B:4913:ARG:HD2	2.11	0.83
1:C:4662:ASN:HA	1:C:4666:VAL:HG21	1.59	0.83
1:B:4818:MET:HA	1:B:4823:LEU:HG	1.60	0.83
1:C:162:LYS:HB2	1:C:164:ARG:NH1	1.93	0.83
1:B:4574:ASN:HD22	1:B:4813:LEU:CD2	1.89	0.83
1:C:3765:TYR:HE1	1:C:4750:ILE:CG2	1.85	0.83
1:A:3760:LYS:O	1:A:3760:LYS:HD3	1.79	0.82
1:A:5029:ARG:O	1:A:5033:GLU:HB3	1.79	0.82
1:B:4574:ASN:ND2	1:B:4813:LEU:HD22	1.93	0.82
1:A:4985:LEU:CD2	2:A:5101:ACP:HN61	1.92	0.82
1:B:4812:HIS:ND1	1:B:4812:HIS:O	2.13	0.82
1:B:3674:ILE:HG21	1:B:3769:ARG:HD2	1.60	0.81
1:A:4904:PRO:HG3	1:A:4913:ARG:HH11	1.45	0.81
1:B:4795:TYR:C	1:B:4795:TYR:HD1	1.82	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3965:LEU:HD12	1:C:3965:LEU:O	1.78	0.81
1:B:3674:ILE:CG2	1:B:3769:ARG:CD	2.57	0.81
1:B:4944:ARG:HH11	1:B:4944:ARG:HG3	1.44	0.81
1:D:4865:LYS:HA	1:D:4865:LYS:HZ2	1.46	0.80
1:B:4866:SER:C	1:B:4867:GLU:HG3	2.02	0.80
1:A:4985:LEU:HD23	2:A:5101:ACP:N6	1.97	0.80
1:B:759:ILE:HG22	1:B:762:CYS:HB2	1.62	0.80
1:A:4892:ARG:NH2	1:D:4898:GLY:H	1.79	0.80
1:C:759:ILE:HG22	1:C:762:CYS:HB2	1.63	0.79
1:B:4795:TYR:C	1:B:4795:TYR:CD1	2.54	0.79
1:C:2107:GLN:NE2	1:C:3681:GLY:HA2	1.97	0.79
1:D:4985:LEU:CD2	2:D:5101:ACP:N6	2.45	0.79
1:A:4925:ILE:HD12	1:A:4925:ILE:O	1.83	0.79
1:B:4791:TYR:OH	1:B:4816:ILE:HD13	1.81	0.79
1:A:3544:UNK:CB	1:A:3554:UNK:CB	2.62	0.78
1:A:4823:LEU:HD22	1:D:4839:MET:HE3	1.63	0.78
1:C:742:ASP:HB3	1:C:759:ILE:HD11	1.65	0.78
1:A:4892:ARG:HH22	1:D:4898:GLY:H	1.26	0.78
1:C:2447:LYS:HE2	1:C:2449:GLU:HB2	1.65	0.78
1:A:121:LEU:HD11	1:A:138:GLN:HE22	1.47	0.78
1:A:3729:MET:HG3	1:A:3770:LEU:HD11	1.65	0.78
1:D:4662:ASN:HA	1:D:4666:VAL:CG2	2.13	0.78
1:B:4574:ASN:ND2	1:B:4813:LEU:CD2	2.47	0.77
1:A:4820:VAL:HB	1:A:4823:LEU:HD23	1.66	0.77
1:B:4820:VAL:HB	1:B:4823:LEU:HD23	1.64	0.77
1:B:4866:SER:O	1:B:4867:GLU:HG2	1.83	0.77
1:A:4860:ARG:NH1	1:B:4582:VAL:HG11	1.99	0.77
1:A:2641:UNK:O	1:A:2642:UNK:CB	2.32	0.77
1:A:3490:UNK:CB	1:A:3601:UNK:CB	2.63	0.77
1:C:4919:THR:O	1:C:4923:PHE:HB2	1.85	0.76
1:D:4937:ILE:CD1	1:C:4934:GLY:HA2	2.16	0.76
1:C:4666:VAL:N	1:C:4667:PRO:CD	2.49	0.76
1:A:4240:ASP:OD1	1:A:4668:LEU:HD21	1.86	0.76
1:B:3674:ILE:HG22	1:B:3769:ARG:HD3	1.68	0.76
1:D:3787:LYS:HG3	1:D:3831:SER:HA	1.66	0.75
1:C:4662:ASN:HA	1:C:4666:VAL:CG2	2.15	0.75
1:A:74:SER:H	1:A:77:ALA:HB3	1.52	0.75
1:D:3761:GLN:NE2	1:D:3761:GLN:HA	2.01	0.75
1:D:4871:GLU:HG2	1:D:4871:GLU:O	1.86	0.75
1:B:4865:LYS:HE3	1:B:4865:LYS:CA	2.16	0.75
1:A:4904:PRO:CG	1:A:4913:ARG:NH1	2.49	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3674:ILE:HG21	1:D:3766:GLN:OE1	1.87	0.75
1:D:3767:GLN:NE2	1:D:3804:ILE:HG23	2.01	0.75
1:A:4666:VAL:N	1:A:4667:PRO:CD	2.49	0.74
1:B:3787:LYS:HG3	1:B:3831:SER:HA	1.67	0.74
1:D:4666:VAL:N	1:D:4667:PRO:CD	2.50	0.74
1:B:4865:LYS:CB	1:B:4875:LYS:HG2	2.17	0.74
1:A:4898:GLY:H	1:B:4892:ARG:HH22	1.36	0.74
1:A:76:ARG:NH1	1:B:3935:TRP:O	2.21	0.74
1:C:1152:MET:HB3	1:C:1161:ILE:HB	1.70	0.74
1:A:2452:ARG:NH2	1:D:177:GLU:OE1	2.21	0.74
1:A:1707:LEU:HG	1:A:1708:ARG:H	1.53	0.74
1:A:3761:GLN:OE1	1:A:3761:GLN:HA	1.87	0.74
1:D:1707:LEU:HG	1:D:1708:ARG:H	1.53	0.74
1:C:121:LEU:HD11	1:C:138:GLN:HE22	1.53	0.73
1:D:3674:ILE:HG12	1:D:3769:ARG:CG	2.18	0.73
1:A:1152:MET:HB3	1:A:1161:ILE:HB	1.71	0.73
1:C:645:ARG:HD3	1:C:826:ILE:HG22	1.70	0.73
1:C:1707:LEU:HG	1:C:1708:ARG:H	1.54	0.73
1:B:121:LEU:HD11	1:B:138:GLN:HE22	1.54	0.73
1:B:1152:MET:HB3	1:B:1161:ILE:HB	1.70	0.72
1:A:3773:ARG:CA	1:A:3815:LYS:HE3	2.18	0.72
1:D:759:ILE:HG22	1:D:762:CYS:HB2	1.69	0.72
1:A:3760:LYS:HA	1:A:3760:LYS:NZ	2.04	0.72
1:A:4860:ARG:HG3	1:A:4860:ARG:NH1	2.05	0.72
1:C:103:TYR:CE1	1:C:163:VAL:HG13	2.25	0.72
1:A:3544:UNK:C	1:A:3551:UNK:CB	2.67	0.72
1:A:4860:ARG:HH12	1:B:4582:VAL:HG11	1.51	0.72
1:B:4984:ASN:HA	2:B:5101:ACP:N6	2.04	0.72
1:C:151:HIS:HB2	1:C:170:ILE:HB	1.71	0.72
1:C:162:LYS:CB	1:C:164:ARG:HH11	2.02	0.72
1:C:4223:ASN:HD21	1:C:4946:GLN:HE22	1.38	0.72
1:D:4034:ASN:OD1	1:D:4035:VAL:N	2.23	0.72
1:D:4865:LYS:HA	1:D:4865:LYS:NZ	2.03	0.72
1:C:977:LEU:HB3	1:C:1047:LEU:HD11	1.72	0.72
1:D:1152:MET:HB3	1:D:1161:ILE:HB	1.72	0.72
1:B:977:LEU:HB3	1:B:1047:LEU:HD11	1.72	0.72
2:C:5101:ACP:O2G	2:C:5101:ACP:O2B	2.07	0.72
1:A:3935:TRP:HD1	1:D:76:ARG:HH12	1.38	0.71
1:B:3666:ASP:OD1	1:B:3666:ASP:N	2.20	0.71
1:C:3755:GLU:OE1	1:C:3755:GLU:HA	1.90	0.71
1:D:977:LEU:HB3	1:D:1047:LEU:HD11	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:742:ASP:HB3	1:B:759:ILE:HD11	1.71	0.71
1:D:4892:ARG:NH2	1:C:4917:ASP:OD1	2.23	0.71
1:C:4197:ILE:HG13	1:C:4198:SER:H	1.56	0.71
1:D:645:ARG:HD3	1:D:826:ILE:HG22	1.72	0.71
1:A:977:LEU:HB3	1:A:1047:LEU:HD11	1.71	0.70
1:D:3773:ARG:HA	1:D:3815:LYS:HE3	1.72	0.70
1:C:3765:TYR:CE1	1:C:4750:ILE:HD12	2.26	0.70
1:B:2095:GLN:NE2	1:B:2127:GLN:O	2.25	0.70
1:B:1707:LEU:HG	1:B:1708:ARG:H	1.55	0.70
1:B:479:GLN:OE1	1:B:536:ASN:ND2	2.25	0.70
1:B:4995:LEU:HD21	1:B:5011:TRP:HB2	1.73	0.69
1:D:479:GLN:OE1	1:D:536:ASN:ND2	2.25	0.69
1:D:4197:ILE:HG21	1:D:4990:PHE:HB3	1.73	0.69
1:D:4913:ARG:NH2	1:D:4917:ASP:OD2	2.24	0.69
1:B:3969:ILE:HD11	1:B:3980:LEU:HD12	1.74	0.69
1:B:4577:LEU:CD2	1:B:4807:PHE:CE1	2.72	0.69
1:D:3767:GLN:HE22	1:D:3804:ILE:CA	2.05	0.68
1:C:158:SER:N	1:C:161:GLU:OE1	2.24	0.68
1:C:4936:ILE:HD13	1:C:4936:ILE:N	2.08	0.68
1:D:3751:VAL:O	1:D:3752:SER:C	2.29	0.68
1:D:1116:GLY:HA3	1:D:1132:TRP:HB3	1.74	0.68
1:C:2095:GLN:NE2	1:C:2127:GLN:O	2.27	0.68
1:D:4574:ASN:HD22	1:D:4813:LEU:HD13	1.59	0.68
1:C:4995:LEU:HD21	1:C:5011:TRP:HB2	1.76	0.68
1:A:4197:ILE:HG13	1:A:4198:SER:H	1.57	0.68
1:C:2107:GLN:HE22	1:C:3681:GLY:CA	2.07	0.68
1:D:179:TYR:HB3	1:D:197:GLN:HB2	1.76	0.68
1:B:4182:GLU:OE2	1:B:4192:ARG:NH2	2.25	0.67
1:C:220:LEU:HD22	1:C:262:LEU:HD23	1.76	0.67
1:C:670:GLU:HG3	1:C:788:LYS:H	1.59	0.67
1:A:4244:GLU:CG	1:A:4668:LEU:HD11	2.25	0.67
1:A:4936:ILE:N	1:A:4936:ILE:HD12	2.09	0.67
1:C:4034:ASN:OD1	1:C:4035:VAL:N	2.27	0.67
1:D:2095:GLN:NE2	1:D:2127:GLN:O	2.27	0.67
1:B:1116:GLY:HA3	1:B:1132:TRP:HB3	1.77	0.67
1:D:742:ASP:HB3	1:D:759:ILE:HD11	1.76	0.67
1:A:4839:MET:HE3	1:B:4823:LEU:HD22	1.76	0.67
1:A:4865:LYS:HA	1:A:4865:LYS:HE3	1.77	0.67
1:C:3964:SER:O	1:C:3968:TYR:HE1	1.77	0.67
1:B:664:PHE:HB2	1:B:746:CYS:HB2	1.77	0.66
1:D:4985:LEU:CG	2:D:5101:ACP:N6	2.53	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4820:VAL:CG1	1:D:4823:LEU:HD23	2.24	0.66
1:C:4888:TYR:CE2	1:C:4892:ARG:NH1	2.58	0.66
1:B:131:LEU:HD22	1:B:178:ARG:HH22	1.61	0.66
1:B:4935:LEU:CD2	1:C:4940:PHE:HE2	1.94	0.66
1:A:3767:GLN:HG3	1:A:3809:ASN:HD21	1.61	0.66
1:A:1116:GLY:HA3	1:A:1132:TRP:HB3	1.77	0.66
1:C:3757:GLU:O	1:C:3760:LYS:CG	2.31	0.66
1:B:4020:GLN:HA	1:B:4023:MET:SD	2.34	0.66
1:D:2176:ASN:O	1:D:2180:GLN:NE2	2.29	0.66
1:C:158:SER:H	1:C:161:GLU:CD	1.99	0.66
1:C:3765:TYR:OH	1:C:4750:ILE:HG22	1.96	0.66
1:A:3969:ILE:HD11	1:A:3980:LEU:HD12	1.78	0.66
1:A:4665:LYS:C	1:A:4667:PRO:HD2	2.16	0.65
1:B:3668:SER:O	1:B:3672:ARG:NH2	2.28	0.65
1:D:4892:ARG:HH22	1:C:4898:GLY:H	1.42	0.65
1:C:1243:PRO:HB2	1:C:1600:LEU:HD12	1.78	0.65
1:C:3658:LYS:HA	1:C:3661:TRP:HZ3	1.62	0.65
1:B:719:LEU:O	1:B:720:HIS:ND1	2.30	0.65
1:B:4197:ILE:HG13	1:B:4198:SER:H	1.61	0.65
1:A:2095:GLN:NE2	1:A:2127:GLN:O	2.29	0.65
1:C:4892:ARG:O	1:C:4892:ARG:HG2	1.96	0.65
1:A:4839:MET:HE1	1:B:4826:ILE:HD13	1.78	0.65
1:C:4944:ARG:HG3	1:C:4944:ARG:NH1	2.09	0.65
1:A:3493:UNK:O	1:A:3494:UNK:CB	2.41	0.65
1:C:3674:ILE:HD12	1:C:3769:ARG:HD2	1.79	0.65
1:A:1679:ASN:ND2	1:A:1797:ARG:O	2.30	0.64
1:B:14:LEU:HB3	1:B:101:LEU:HD12	1.78	0.64
1:C:4223:ASN:HD21	1:C:4946:GLN:NE2	1.95	0.64
1:B:4944:ARG:HG3	1:B:4944:ARG:NH1	2.11	0.64
1:A:1229:ASN:HB3	1:A:1826:ALA:HB1	1.79	0.64
1:B:4573:ILE:HD11	1:B:4809:PHE:HE2	1.60	0.64
1:B:4832:HIS:CD2	1:B:4942:GLU:OE1	2.49	0.64
1:A:4240:ASP:CG	1:A:4668:LEU:HD21	2.18	0.64
1:D:4892:ARG:CZ	1:C:4896:GLY:HA3	2.27	0.64
1:C:4937:ILE:HD13	1:C:4937:ILE:N	2.12	0.64
1:D:216:GLY:HA2	1:D:262:LEU:HD11	1.80	0.64
1:A:3729:MET:CG	1:A:3770:LEU:HD11	2.26	0.64
1:D:3986:TRP:NE1	1:D:4043:GLN:OE1	2.29	0.64
1:D:4865:LYS:HZ3	1:D:4865:LYS:HB2	1.62	0.64
1:B:179:TYR:HB3	1:B:197:GLN:HB2	1.80	0.64
1:B:3767:GLN:OE1	1:B:3804:ILE:HA	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3674:ILE:CG2	1:D:3769:ARG:HD2	2.28	0.64
1:A:4844:LEU:HD12	1:A:4928:LEU:HD12	1.79	0.64
1:D:1679:ASN:ND2	1:D:1797:ARG:O	2.31	0.64
1:D:1931:LEU:HB3	1:D:1935:VAL:HB	1.80	0.64
1:A:3763:LEU:C	1:A:3763:LEU:HD13	2.18	0.64
1:A:4197:ILE:HG13	1:A:4198:SER:N	2.13	0.64
1:B:3927:GLN:NE2	1:B:3931:SER:OG	2.31	0.64
1:D:45:ARG:HG2	1:D:443:LEU:HD21	1.78	0.64
1:D:1074:ILE:HG22	1:D:1239:SER:HB2	1.80	0.64
1:D:4885:PHE:O	1:D:4889:VAL:HG12	1.98	0.64
1:C:150:MET:CE	1:C:163:VAL:HG11	2.28	0.64
1:A:4869:GLU:OE1	1:A:4869:GLU:HA	1.98	0.63
1:B:627:PRO:O	1:B:629:ARG:NH1	2.31	0.63
1:D:4959:PHE:CD2	1:D:4985:LEU:CD1	2.82	0.63
1:C:12:GLN:HG2	1:C:165:VAL:HG12	1.80	0.63
1:C:4869:GLU:O	1:C:4870:ASP:O	2.16	0.63
1:D:1724:CYS:SG	1:D:1725:ARG:N	2.70	0.63
1:C:3763:LEU:HD13	1:C:3763:LEU:C	2.19	0.63
1:A:1243:PRO:HB2	1:A:1600:LEU:HD12	1.79	0.63
1:B:34:LYS:HE2	1:B:53:SER:HA	1.79	0.63
1:C:3763:LEU:HD13	1:C:3763:LEU:O	1.97	0.63
1:D:3765:TYR:CD1	1:D:4750:ILE:HG23	2.34	0.63
1:C:3794:VAL:HG11	1:C:3835:LEU:HD21	1.79	0.63
1:C:4869:GLU:HA	1:C:4869:GLU:OE1	1.97	0.63
1:A:647:ASN:HD21	1:A:821:LEU:HA	1.63	0.63
1:B:4865:LYS:HG3	1:B:4875:LYS:CG	2.29	0.63
1:C:1708:ARG:HA	1:C:1711:TYR:HB2	1.79	0.63
1:A:4662:ASN:O	1:A:4666:VAL:HG12	1.98	0.63
1:B:567:VAL:HG13	1:B:568:LEU:HD12	1.81	0.63
1:D:1243:PRO:HB2	1:D:1600:LEU:HD12	1.80	0.63
1:C:4197:ILE:HG13	1:C:4198:SER:N	2.14	0.63
1:D:2185:ILE:O	1:D:2188:ASN:ND2	2.32	0.62
1:D:4892:ARG:HG2	1:C:4895:GLY:O	1.99	0.62
1:C:34:LYS:HE2	1:C:53:SER:HA	1.80	0.62
1:C:4958:CYS:SG	1:C:4978:HIS:CD2	2.91	0.62
1:A:3986:TRP:NE1	1:A:4043:GLN:OE1	2.32	0.62
1:A:4954:MET:HG3	2:A:5101:ACP:H1'	1.81	0.62
1:D:3830:GLN:HA	1:D:3833:GLN:HG2	1.80	0.62
1:A:4020:GLN:HA	1:A:4023:MET:HG2	1.81	0.62
1:B:221:ARG:HH22	1:B:253:CYS:HA	1.64	0.62
1:B:1679:ASN:ND2	1:B:1797:ARG:O	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1724:CYS:SG	1:B:1725:ARG:N	2.72	0.62
1:B:4034:ASN:OD1	1:B:4035:VAL:N	2.32	0.62
1:C:348:VAL:HB	1:C:357:LEU:HD22	1.81	0.62
1:A:647:ASN:ND2	1:A:820:ARG:O	2.33	0.62
1:D:4940:PHE:HE2	1:C:4935:LEU:CD2	2.10	0.62
1:A:4940:PHE:CE2	1:D:4935:LEU:HD23	2.33	0.62
1:B:647:ASN:ND2	1:B:820:ARG:O	2.32	0.62
1:D:3674:ILE:O	1:D:3769:ARG:CD	2.39	0.62
1:D:4940:PHE:CZ	1:C:4935:LEU:HD21	2.34	0.62
1:A:243:ARG:NH1	1:A:301:VAL:O	2.32	0.62
1:B:4865:LYS:HD3	1:B:4865:LYS:C	2.20	0.62
1:D:4027:LEU:HD13	1:D:4030:LEU:HD12	1.82	0.62
1:D:4832:HIS:NE2	1:D:4942:GLU:OE2	2.32	0.62
1:C:719:LEU:O	1:C:720:HIS:ND1	2.32	0.62
1:A:3767:GLN:O	1:A:3772:THR:CB	2.25	0.62
1:B:4860:ARG:HE	1:C:4582:VAL:HG11	1.64	0.62
1:D:4020:GLN:HG3	1:D:4023:MET:HE3	1.81	0.62
1:A:4779:LYS:HE2	1:A:4783:ILE:HD11	1.80	0.62
1:B:4197:ILE:HG13	1:B:4198:SER:N	2.14	0.62
1:D:660:GLY:HA3	1:D:750:LEU:HD13	1.82	0.62
1:D:4183:ILE:HD12	1:D:4193:ILE:HD12	1.82	0.61
1:D:4985:LEU:HD21	2:D:5101:ACP:N6	2.15	0.61
1:C:3986:TRP:NE1	1:C:4043:GLN:OE1	2.32	0.61
1:A:1708:ARG:HA	1:A:1711:TYR:HB2	1.82	0.61
1:D:647:ASN:HD21	1:D:821:LEU:HA	1.65	0.61
1:D:716:PHE:HE1	1:D:720:HIS:H	1.48	0.61
1:C:3766:GLN:OE1	1:C:3766:GLN:HA	2.00	0.61
1:B:3891:LEU:HB3	1:B:3899:PHE:HE2	1.65	0.61
1:D:1240:LYS:NZ	1:D:1242:LEU:O	2.31	0.61
1:A:2688:UNK:CB	1:A:2691:UNK:O	2.48	0.61
1:C:131:LEU:HD22	1:C:178:ARG:HH22	1.64	0.61
1:C:3765:TYR:CE2	1:C:3769:ARG:NH2	2.62	0.61
1:C:4067:LYS:HD2	1:C:4102:GLN:HG3	1.83	0.61
1:A:3941:ASP:HA	1:A:4002:LYS:HE3	1.82	0.61
1:D:3658:LYS:HA	1:D:3661:TRP:HZ3	1.65	0.61
1:A:348:VAL:HB	1:A:357:LEU:HD22	1.82	0.61
1:D:110:ARG:HA	1:D:117:TYR:HA	1.82	0.61
1:C:3941:ASP:HA	1:C:4002:LYS:HE3	1.83	0.61
1:A:3760:LYS:HB2	1:A:3760:LYS:HZ3	1.64	0.61
1:D:2248:ARG:HH21	1:D:3866:ILE:HA	1.65	0.61
1:D:3924:LEU:HD22	1:D:3984:ARG:HE	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4871:GLU:O	1:D:4871:GLU:CG	2.49	0.61
1:C:286:THR:HA	1:C:405:HIS:HB2	1.82	0.61
1:A:1074:ILE:HG22	1:A:1239:SER:HB2	1.82	0.61
1:A:4946:GLN:OE1	1:A:4946:GLN:HA	2.00	0.61
1:A:4995:LEU:HD21	1:A:5011:TRP:HB2	1.82	0.61
1:B:1708:ARG:HA	1:B:1711:TYR:HB2	1.83	0.61
1:C:3684:GLU:C	1:C:3686:GLU:H	2.04	0.61
1:A:4240:ASP:OD1	1:A:4668:LEU:CD2	2.48	0.61
1:B:4719:PHE:O	1:B:4723:LYS:NZ	2.34	0.61
1:A:3658:LYS:HA	1:A:3661:TRP:HZ3	1.64	0.61
1:A:4904:PRO:CG	1:A:4913:ARG:HH11	2.11	0.61
2:A:5101:ACP:H3B1	2:A:5101:ACP:O1A	2.00	0.61
1:B:181:HIS:H	1:B:193:ALA:HA	1.66	0.61
1:D:1708:ARG:HA	1:D:1711:TYR:HB2	1.81	0.61
1:C:1724:CYS:SG	1:C:1725:ARG:N	2.74	0.61
1:A:2196:ASN:OD1	1:A:2199:ARG:NH1	2.34	0.60
1:C:1387:UNK:HA	1:C:1394:UNK:HA	1.82	0.60
1:C:3737:GLU:HA	1:C:3763:LEU:HD23	1.82	0.60
1:C:4666:VAL:N	1:C:4667:PRO:HD3	2.16	0.60
1:A:4901:ILE:CB	1:A:4913:ARG:NH2	2.64	0.60
1:A:4985:LEU:CD2	2:A:5101:ACP:N6	2.62	0.60
1:A:649:PHE:HB3	1:A:776:LEU:HD13	1.83	0.60
1:A:1387:UNK:HA	1:A:1394:UNK:HA	1.84	0.60
1:C:647:ASN:ND2	1:C:820:ARG:O	2.34	0.60
1:C:4958:CYS:HA	2:C:5101:ACP:H2	1.83	0.60
1:B:2291:GLN:OE1	1:B:2294:ASP:N	2.35	0.60
1:B:3986:TRP:NE1	1:B:4043:GLN:OE1	2.35	0.60
1:B:4184:MET:HB2	1:B:4190:ILE:HG22	1.82	0.60
1:B:4801:LEU:HD21	1:B:4808:PHE:HE2	1.63	0.60
1:D:3969:ILE:HD11	1:D:3980:LEU:HD12	1.81	0.60
1:A:4034:ASN:OD1	1:A:4035:VAL:N	2.34	0.60
1:A:4832:HIS:NE2	1:A:4942:GLU:OE1	2.35	0.60
1:A:4865:LYS:HG2	1:A:4875:LYS:HG2	1.83	0.60
1:B:272:SER:HA	1:B:334:MET:HG2	1.82	0.60
1:C:1867:GLU:HA	1:C:1870:VAL:HB	1.84	0.60
1:B:2288:LEU:O	1:B:3849:ARG:NH1	2.34	0.60
1:A:567:VAL:HG13	1:A:568:LEU:HD12	1.84	0.60
1:B:348:VAL:HB	1:B:357:LEU:HD22	1.82	0.60
1:D:4940:PHE:CE2	1:C:4935:LEU:HD21	2.36	0.60
1:D:1387:UNK:HA	1:D:1394:UNK:HA	1.84	0.59
1:A:719:LEU:O	1:A:720:HIS:ND1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:644:ILE:HA	1:D:825:PRO:HA	1.84	0.59
1:C:243:ARG:NH1	1:C:301:VAL:O	2.35	0.59
1:C:647:ASN:HD21	1:C:821:LEU:HA	1.67	0.59
1:C:1679:ASN:ND2	1:C:1797:ARG:O	2.34	0.59
1:B:2248:ARG:HH21	1:B:3866:ILE:HA	1.67	0.59
1:D:647:ASN:ND2	1:D:820:ARG:O	2.36	0.59
1:C:4820:VAL:HB	1:C:4823:LEU:HD23	1.84	0.59
1:B:4801:LEU:CD2	1:B:4808:PHE:CE2	2.66	0.59
1:A:2207:VAL:HG21	1:A:2236:LEU:HD21	1.84	0.59
1:D:3767:GLN:HE21	1:D:3804:ILE:HG23	1.67	0.59
1:D:4892:ARG:NH2	1:C:4898:GLY:H	2.01	0.59
1:C:3758:MET:HE1	1:C:3762:ARG:HH21	1.68	0.59
1:A:3760:LYS:HD3	1:A:3760:LYS:C	2.22	0.59
1:D:567:VAL:HG13	1:D:568:LEU:HD12	1.85	0.59
1:D:765:GLN:O	1:D:1387:UNK:N	2.36	0.59
1:D:3674:ILE:CB	1:D:3769:ARG:HD2	2.32	0.59
1:A:3756:LYS:O	1:A:3760:LYS:N	2.31	0.59
1:B:74:SER:H	1:B:77:ALA:HB3	1.67	0.59
1:C:776:LEU:HG	1:C:848:HIS:HA	1.85	0.59
1:A:3702:VAL:HG21	1:A:3775:ALA:CB	2.33	0.58
1:A:4704:LEU:HB2	1:A:4774:LYS:HE3	1.85	0.58
1:B:1387:UNK:HA	1:B:1394:UNK:HA	1.86	0.58
1:B:3755:GLU:HA	1:B:3755:GLU:OE1	2.02	0.58
1:B:3804:ILE:O	1:B:3809:ASN:ND2	2.36	0.58
1:D:1143:TRP:HD1	1:D:1164:LEU:HD13	1.68	0.58
1:C:2248:ARG:HH21	1:C:3866:ILE:HA	1.67	0.58
1:A:4924:VAL:O	1:A:4924:VAL:HG13	2.03	0.58
1:B:286:THR:HA	1:B:405:HIS:HB2	1.85	0.58
1:D:776:LEU:HG	1:D:848:HIS:HA	1.83	0.58
1:D:4779:LYS:HE2	1:D:4783:ILE:HD11	1.84	0.58
1:D:4959:PHE:CD2	1:D:4985:LEU:HD11	2.38	0.58
1:A:645:ARG:HD3	1:A:826:ILE:HG22	1.84	0.58
1:A:3891:LEU:HB3	1:A:3899:PHE:HE2	1.68	0.58
1:B:3886:ARG:NH1	1:B:3889:GLN:OE1	2.36	0.58
1:D:4719:PHE:O	1:D:4723:LYS:NZ	2.36	0.58
1:C:315:CYS:SG	1:C:317:ARG:NH1	2.76	0.58
1:C:1931:LEU:HB3	1:C:1935:VAL:HB	1.85	0.58
1:C:4704:LEU:HB2	1:C:4774:LYS:HE3	1.86	0.58
1:D:1738:LEU:HB2	1:D:2146:PRO:HD3	1.86	0.58
1:C:2196:ASN:OD1	1:C:2199:ARG:NH1	2.35	0.58
1:A:4852:THR:HG21	1:A:4883:TYR:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4932:ILE:O	1:A:4936:ILE:CD1	2.49	0.58
1:B:315:CYS:SG	1:B:317:ARG:NH1	2.76	0.58
1:D:3667:HIS:NE2	1:D:3671:ASP:OD2	2.36	0.58
1:C:1074:ILE:HG22	1:C:1239:SER:HB2	1.85	0.58
1:C:2257:LEU:HD11	1:C:2276:ALA:HB2	1.86	0.58
1:A:1931:LEU:HB3	1:A:1935:VAL:HB	1.84	0.58
1:D:4666:VAL:N	1:D:4667:PRO:HD3	2.18	0.58
1:C:73:LEU:HD12	1:C:77:ALA:HB1	1.86	0.58
1:C:4665:LYS:C	1:C:4667:PRO:HD2	2.24	0.58
1:A:1724:CYS:SG	1:A:1725:ARG:N	2.76	0.58
1:A:2248:ARG:HH21	1:A:3866:ILE:HA	1.68	0.58
1:B:149:THR:HG23	1:B:151:HIS:HE1	1.68	0.58
1:B:3662:ILE:O	1:B:3662:ILE:HG23	2.03	0.58
1:B:4978:HIS:ND1	1:B:4982:GLU:OE1	2.37	0.58
1:D:315:CYS:SG	1:D:317:ARG:NH1	2.76	0.58
1:D:4820:VAL:HG12	1:D:4823:LEU:HB2	1.85	0.58
1:A:3763:LEU:HD13	1:A:3763:LEU:O	2.04	0.58
1:D:4665:LYS:C	1:D:4667:PRO:HD2	2.24	0.58
1:A:272:SER:HB2	1:A:334:MET:HA	1.84	0.58
1:A:644:ILE:HA	1:A:825:PRO:HA	1.86	0.58
1:D:34:LYS:HE2	1:D:53:SER:HA	1.85	0.58
1:D:294:THR:HG23	1:D:295:GLU:H	1.68	0.58
1:C:4673:ARG:NH1	1:C:4702:ASP:OD2	2.37	0.58
1:B:262:LEU:HB2	1:B:280:LEU:HD23	1.86	0.58
1:D:3941:ASP:HA	1:D:4002:LYS:HE3	1.86	0.58
1:A:315:CYS:SG	1:A:317:ARG:NH1	2.77	0.57
1:A:2358:ILE:HA	1:A:2364:PHE:HZ	1.68	0.57
1:D:12:GLN:HG2	1:D:165:VAL:HG12	1.85	0.57
1:D:2810:LYS:HG2	1:D:2814:LYS:HE3	1.86	0.57
1:B:1738:LEU:HB2	1:B:2146:PRO:HD3	1.84	0.57
1:B:3955:MET:HG3	1:B:4019:LEU:HD22	1.86	0.57
1:C:3891:LEU:HB3	1:C:3899:PHE:HE2	1.67	0.57
1:C:4719:PHE:O	1:C:4723:LYS:NZ	2.37	0.57
1:A:34:LYS:HE2	1:A:53:SER:HA	1.85	0.57
1:B:4872:PRO:HD2	1:B:4873:ASP:N	2.19	0.57
1:C:765:GLN:O	1:C:1387:UNK:N	2.38	0.57
1:C:2185:ILE:O	1:C:2188:ASN:ND2	2.37	0.57
1:A:1238:PHE:HE1	1:A:1608:MET:HB3	1.68	0.57
1:A:3955:MET:HG3	1:A:4019:LEU:HD22	1.86	0.57
1:B:45:ARG:HG2	1:B:443:LEU:HD21	1.84	0.57
1:C:109:LEU:HD23	1:C:148:TRP:HD1	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:MET:HE2	1:C:163:VAL:HG11	1.85	0.57
1:C:1116:GLY:HA3	1:C:1132:TRP:HB3	1.85	0.57
1:A:509:GLU:O	1:A:510:GLU:HG3	2.05	0.57
1:B:2869:ARG:NH1	1:B:3106:UNK:O	2.37	0.57
1:B:4690:GLU:HG2	1:B:4691:GLN:N	2.20	0.57
1:C:3765:TYR:HE1	1:C:4750:ILE:HD12	1.66	0.57
1:A:1143:TRP:HD1	1:A:1164:LEU:HD13	1.68	0.57
1:C:116:MET:HG3	1:C:137:LEU:HD12	1.87	0.57
1:C:272:SER:HA	1:C:334:MET:HG2	1.86	0.57
1:A:2773:ASN:O	1:A:2773:ASN:ND2	2.37	0.57
1:A:3770:LEU:HD23	1:A:3770:LEU:O	2.05	0.57
1:A:4940:PHE:CE2	1:D:4935:LEU:HD21	2.40	0.57
1:B:243:ARG:NH1	1:B:301:VAL:O	2.38	0.57
1:B:4795:TYR:HD1	1:B:4795:TYR:O	1.88	0.57
1:D:3828:PHE:CZ	1:D:3832:ILE:HD11	2.39	0.57
1:B:2257:LEU:HD11	1:B:2276:ALA:HB2	1.87	0.57
1:B:4016:LEU:HD23	1:B:4020:GLN:NE2	2.13	0.57
1:B:4673:ARG:NH1	1:B:4702:ASP:OD2	2.38	0.57
1:C:45:ARG:HG2	1:C:443:LEU:HD21	1.86	0.57
1:C:1101:ARG:HE	1:C:1115:LEU:HD12	1.69	0.57
1:A:4719:PHE:O	1:A:4723:LYS:NZ	2.37	0.57
1:D:3765:TYR:CE1	1:D:4750:ILE:CG2	2.87	0.57
1:D:3891:LEU:HB3	1:D:3899:PHE:HE2	1.69	0.57
1:A:3924:LEU:O	1:A:3927:GLN:HG3	2.04	0.57
1:A:4633:GLU:HA	1:A:4639:MET:HG3	1.87	0.57
1:B:788:LYS:HD3	1:B:1629:GLN:HA	1.85	0.56
1:B:1229:ASN:HD21	1:B:1827:ARG:HD3	1.69	0.56
1:B:4037:ASN:HD22	1:B:5035:GLN:HE21	1.51	0.56
1:D:4940:PHE:CE2	1:C:4935:LEU:HD23	2.40	0.56
1:C:3984:ARG:HG2	1:C:3987:ASP:HB2	1.86	0.56
1:A:4993:MET:SD	1:A:4997:ASN:ND2	2.77	0.56
1:B:670:GLU:HG3	1:B:788:LYS:H	1.70	0.56
1:B:2291:GLN:HG3	1:B:2292:GLU:H	1.70	0.56
1:D:4197:ILE:HG13	1:D:4198:SER:H	1.70	0.56
1:A:78:LEU:HD21	1:A:147:TRP:CE2	2.40	0.56
1:A:2288:LEU:O	1:A:3849:ARG:NH1	2.34	0.56
1:A:4244:GLU:HG2	1:A:4668:LEU:HD11	1.87	0.56
1:A:4690:GLU:HG2	1:A:4691:GLN:N	2.20	0.56
1:B:666:VAL:HB	1:B:744:VAL:HB	1.87	0.56
1:B:1243:PRO:HB2	1:B:1600:LEU:HD12	1.87	0.56
1:B:4047:MET:SD	1:B:4048:LEU:HD22	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:MET:HG2	1:D:137:LEU:HD13	1.85	0.56
1:C:262:LEU:HB2	1:C:280:LEU:HD23	1.87	0.56
1:C:1735:ILE:HG22	1:C:2142:TYR:HB3	1.86	0.56
1:C:2869:ARG:NH1	1:C:3106:UNK:O	2.36	0.56
1:C:3804:ILE:HG23	1:C:3805:LEU:HD12	1.87	0.56
1:B:4016:LEU:O	1:B:4020:GLN:NE2	2.37	0.56
1:B:4866:SER:C	1:B:4867:GLU:CG	2.64	0.56
1:D:1124:PHE:HE1	1:D:1139:PHE:HB3	1.70	0.56
1:A:627:PRO:O	1:A:629:ARG:NH1	2.39	0.56
1:A:4940:PHE:CZ	1:D:4935:LEU:HD21	2.41	0.56
1:D:220:LEU:HD22	1:D:262:LEU:HD23	1.87	0.56
1:D:3674:ILE:HG23	1:D:3769:ARG:HD2	1.88	0.56
1:C:179:TYR:HB3	1:C:197:GLN:HB2	1.87	0.56
1:C:1240:LYS:NZ	1:C:1242:LEU:O	2.31	0.56
1:B:3751:VAL:O	1:B:3752:SER:C	2.41	0.56
1:D:1101:ARG:HE	1:D:1115:LEU:HD12	1.71	0.56
1:D:4690:GLU:HG2	1:D:4691:GLN:N	2.21	0.56
1:D:4704:LEU:HB2	1:D:4774:LYS:HE3	1.88	0.56
1:C:1866:ILE:HG22	1:C:1870:VAL:HG23	1.88	0.56
1:D:1106:ARG:NH2	1:D:1183:GLU:OE2	2.38	0.56
1:C:103:TYR:OH	1:C:157:ARG:HG2	2.06	0.56
1:C:2763:HIS:NE2	1:C:2792:ARG:O	2.34	0.56
1:C:4690:GLU:HG2	1:C:4691:GLN:N	2.20	0.56
1:A:1580:PHE:HE2	1:A:1592:PRO:HG2	1.71	0.56
1:A:2257:LEU:HD11	1:A:2276:ALA:HB2	1.87	0.56
1:D:4959:PHE:CD2	1:D:4985:LEU:HD13	2.41	0.56
1:C:216:GLY:HA2	1:C:262:LEU:HD11	1.87	0.56
1:C:1703:LEU:HB2	1:C:1707:LEU:HB3	1.88	0.56
1:D:4219:PHE:O	1:D:4223:ASN:ND2	2.38	0.56
1:C:841:GLY:HA2	1:C:1073:ARG:HD2	1.88	0.56
1:C:4223:ASN:ND2	1:C:4946:GLN:OE1	2.39	0.56
1:A:116:MET:HG3	1:A:137:LEU:HD12	1.88	0.55
1:D:4979:THR:HG21	2:D:5101:ACP:H2'	1.88	0.55
1:C:1238:PHE:HE1	1:C:1608:MET:HB3	1.72	0.55
1:C:4067:LYS:O	1:C:4071:ILE:HG12	2.06	0.55
1:A:294:THR:HG23	1:A:295:GLU:H	1.71	0.55
1:A:682:LEU:HD13	1:A:787:VAL:HG11	1.88	0.55
1:A:742:ASP:HB3	1:A:759:ILE:HD11	1.89	0.55
1:B:647:ASN:HD21	1:B:821:LEU:HA	1.70	0.55
1:C:4017:LEU:HD13	1:C:4020:GLN:NE2	2.21	0.55
1:A:131:LEU:HD22	1:A:178:ARG:HH22	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4795:TYR:CD1	1:B:4795:TYR:O	2.59	0.55
1:C:3955:MET:HG3	1:C:4019:LEU:HD22	1.88	0.55
1:B:1676:LEU:HD13	1:B:2168:VAL:HG22	1.88	0.55
1:B:3828:PHE:CZ	1:B:3832:ILE:HD11	2.42	0.55
1:D:728:ARG:NH1	1:D:1384:UNK:O	2.39	0.55
1:A:1735:ILE:HG22	1:A:2142:TYR:HB3	1.88	0.55
1:B:4872:PRO:HD2	1:B:4873:ASP:H	1.72	0.55
1:D:665:GLU:HB3	1:D:792:LEU:HD12	1.88	0.55
1:D:1851:MET:HB2	1:D:1853:ILE:HG12	1.89	0.55
1:C:627:PRO:O	1:C:629:ARG:NH1	2.40	0.55
1:C:4666:VAL:O	1:C:4666:VAL:HG12	2.07	0.55
1:A:445:LEU:HD13	1:A:521:LEU:HB3	1.88	0.55
1:A:765:GLN:O	1:A:1387:UNK:N	2.40	0.55
1:B:195:PHE:O	1:C:2359:ARG:NH1	2.37	0.55
1:B:294:THR:HG23	1:B:295:GLU:H	1.72	0.55
1:D:4936:ILE:HD13	1:D:4936:ILE:N	2.20	0.55
1:A:728:ARG:NH1	1:A:1384:UNK:O	2.40	0.55
1:A:3776:ALA:O	1:A:3778:MET:N	2.40	0.55
1:A:4895:GLY:O	1:B:4892:ARG:NE	2.39	0.55
1:B:4849:TYR:HB2	1:B:4883:TYR:HE1	1.71	0.55
1:D:262:LEU:HB2	1:D:280:LEU:HD23	1.88	0.55
1:D:4673:ARG:NH1	1:D:4702:ASP:OD2	2.38	0.55
1:B:3813:GLN:OE1	1:B:3896:ASN:ND2	2.40	0.55
1:D:1992:ALA:O	1:D:1996:ARG:NH1	2.39	0.55
1:D:2423:MET:HE1	1:D:2494:UNK:HA	1.88	0.55
1:C:1143:TRP:HD1	1:C:1164:LEU:HD13	1.72	0.55
1:C:1950:GLU:OE2	1:C:2041:HIS:NE2	2.40	0.55
1:A:2869:ARG:NH1	1:A:3106:UNK:O	2.35	0.54
1:A:3544:UNK:O	1:A:3551:UNK:CB	2.55	0.54
1:B:4197:ILE:HG21	1:B:4990:PHE:HB3	1.87	0.54
1:D:2763:HIS:NE2	1:D:2792:ARG:O	2.33	0.54
1:C:615:ARG:NH1	1:C:1677:GLY:O	2.38	0.54
1:C:666:VAL:HB	1:C:744:VAL:HG23	1.89	0.54
1:C:3758:MET:CE	1:C:3762:ARG:HH21	2.21	0.54
1:A:73:LEU:HD12	1:A:77:ALA:HB1	1.89	0.54
1:A:3804:ILE:O	1:A:3809:ASN:OD1	2.25	0.54
1:B:841:GLY:HA2	1:B:1073:ARG:HD2	1.89	0.54
1:C:100:THR:CG2	1:C:162:LYS:HE3	2.26	0.54
1:A:4936:ILE:HD12	1:A:4936:ILE:H	1.72	0.54
1:D:670:GLU:HG3	1:D:787:VAL:HA	1.89	0.54
1:D:1950:GLU:OE2	1:D:2041:HIS:NE2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3886:ARG:NH1	1:C:3889:GLN:OE1	2.40	0.54
1:A:286:THR:HA	1:A:405:HIS:HB2	1.89	0.54
1:B:4864:ASN:HA	1:B:4874:MET:CE	2.37	0.54
1:D:4066:LEU:HD21	1:D:4173:TYR:CZ	2.43	0.54
1:B:151:HIS:HB2	1:B:170:ILE:HB	1.89	0.54
1:D:4182:GLU:OE2	1:D:4192:ARG:NE	2.31	0.54
1:C:294:THR:HG23	1:C:295:GLU:H	1.73	0.54
1:A:3758:MET:HG3	1:A:3759:GLU:N	2.22	0.54
1:A:4859:PHE:N	1:A:4859:PHE:CD1	2.73	0.54
1:B:4067:LYS:HD2	1:B:4102:GLN:HG3	1.89	0.54
1:C:4851:TYR:HD2	1:C:4920:PHE:HD1	1.56	0.54
1:B:759:ILE:HG13	1:B:760:ASN:H	1.73	0.54
1:C:232:THR:HG21	1:C:252:VAL:HG11	1.88	0.54
1:C:644:ILE:HA	1:C:825:PRO:HA	1.90	0.54
1:A:4673:ARG:NH1	1:A:4702:ASP:OD2	2.39	0.54
1:D:3674:ILE:HG23	1:D:3769:ARG:CD	2.37	0.54
1:D:4940:PHE:CZ	1:C:4935:LEU:CD2	2.90	0.54
1:B:4924:VAL:HA	1:B:4928:LEU:HD23	1.90	0.54
1:D:668:VAL:HG23	1:D:740:PRO:HA	1.90	0.54
1:D:786:GLY:HA2	1:D:1631:GLN:HA	1.89	0.54
1:B:2904:LEU:HD21	1:B:2912:THR:HG23	1.90	0.54
1:D:2904:LEU:HD21	1:D:2912:THR:HG23	1.90	0.54
1:C:445:LEU:HD13	1:C:521:LEU:HB3	1.89	0.54
1:C:546:TRP:O	1:C:550:LYS:NZ	2.41	0.54
1:C:4779:LYS:HE2	1:C:4783:ILE:HD11	1.90	0.54
1:A:2185:ILE:O	1:A:2188:ASN:ND2	2.41	0.53
1:A:4898:GLY:N	1:B:4892:ARG:HH22	2.04	0.53
1:D:14:LEU:HB3	1:D:101:LEU:HD12	1.90	0.53
1:C:1676:LEU:HD13	1:C:2168:VAL:HG22	1.90	0.53
1:B:665:GLU:HB2	1:B:792:LEU:HB2	1.90	0.53
1:B:786:GLY:HA2	1:B:1631:GLN:HA	1.91	0.53
1:D:109:LEU:HD23	1:D:148:TRP:HD1	1.73	0.53
1:C:786:GLY:HA2	1:C:1631:GLN:HA	1.90	0.53
1:B:3773:ARG:HA	1:B:3815:LYS:HE3	1.90	0.53
1:B:4180:ARG:HG3	1:B:4194:TYR:CE1	2.42	0.53
1:A:14:LEU:HB3	1:A:101:LEU:HD12	1.89	0.53
1:A:4940:PHE:CZ	1:D:4935:LEU:CD2	2.92	0.53
1:B:509:GLU:O	1:B:510:GLU:HG3	2.09	0.53
1:B:3963:ASN:O	1:B:3966:THR:OG1	2.26	0.53
1:D:120:CYS:SG	1:D:175:SER:OG	2.66	0.53
1:D:1697:ALA:HB1	1:D:1708:ARG:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:ARG:HH21	1:C:208:CYS:HB3	1.73	0.53
1:A:3779:VAL:HG23	1:A:3797:THR:HG22	1.90	0.53
1:B:2199:ARG:NE	1:B:2246:ASN:OD1	2.40	0.53
1:B:3794:VAL:HG21	1:B:3835:LEU:HD11	1.90	0.53
1:B:4577:LEU:CD2	1:B:4807:PHE:HE1	2.19	0.53
1:D:4666:VAL:O	1:D:4666:VAL:HG12	2.07	0.53
1:D:4865:LYS:O	1:D:4865:LYS:HG3	2.07	0.53
1:D:4895:GLY:HA2	1:D:4921:PHE:CE1	2.43	0.53
1:A:3840:SER:OG	1:A:3877:ASP:OD2	2.26	0.53
1:B:4869:GLU:OE2	1:B:4870:ASP:N	2.41	0.53
1:B:4913:ARG:NH1	1:C:4888:TYR:OH	2.42	0.53
1:D:1240:LYS:NZ	1:D:1242:LEU:HB3	2.23	0.53
1:C:1738:LEU:HB2	1:C:2146:PRO:HD3	1.89	0.53
1:C:4874:MET:O	1:C:4876:CYS:N	2.42	0.53
1:C:4958:CYS:O	2:C:5101:ACP:N1	2.42	0.53
1:A:2904:LEU:HD21	1:A:2912:THR:HG23	1.91	0.53
1:B:36:CYS:HB3	1:B:50:GLU:HB3	1.90	0.53
1:B:2185:ILE:O	1:B:2188:ASN:ND2	2.41	0.53
1:C:1106:ARG:NH2	1:C:1183:GLU:OE2	2.41	0.53
1:C:2368:LEU:HD22	1:C:2376:LEU:HD21	1.91	0.53
1:C:665:GLU:HB3	1:C:792:LEU:HD12	1.91	0.53
1:C:788:LYS:HD3	1:C:1629:GLN:HA	1.91	0.53
1:C:3684:GLU:C	1:C:3686:GLU:N	2.63	0.53
1:A:4936:ILE:CD1	1:A:4936:ILE:H	2.21	0.53
1:B:1992:ALA:O	1:B:1996:ARG:NH1	2.42	0.53
1:D:4892:ARG:NH2	1:C:4896:GLY:HA3	2.24	0.53
1:D:4940:PHE:HE2	1:C:4935:LEU:HD22	1.74	0.53
1:C:617:ASN:OD1	1:C:618:GLN:N	2.42	0.53
1:C:1124:PHE:HE1	1:C:1139:PHE:HB3	1.73	0.53
1:C:2288:LEU:HD12	1:C:3853:ALA:HB2	1.91	0.53
1:A:3760:LYS:O	1:A:3763:LEU:HB3	2.09	0.53
1:A:4063:ASP:OD2	1:A:4067:LYS:NZ	2.39	0.53
1:B:2809:ILE:HD11	1:B:2926:LEU:HD13	1.91	0.53
1:B:3663:LEU:N	1:B:3663:LEU:CD1	2.72	0.53
1:D:2156:LEU:HD12	1:D:2159:LEU:HD11	1.91	0.53
1:D:4639:MET:SD	1:D:4639:MET:N	2.80	0.53
1:B:220:LEU:HD12	1:B:390:LEU:HB3	1.91	0.52
1:B:560:ILE:HA	1:B:563:VAL:HG12	1.90	0.52
1:B:765:GLN:O	1:B:1387:UNK:N	2.42	0.52
1:B:1867:GLU:HA	1:B:1870:VAL:HB	1.90	0.52
1:B:2288:LEU:HD12	1:B:3853:ALA:HB2	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1950:GLU:OE2	1:A:2041:HIS:NE2	2.42	0.52
1:A:2785:LEU:HB3	1:A:2787:THR:HG22	1.92	0.52
1:D:4928:LEU:CD2	1:D:4928:LEU:N	2.72	0.52
1:A:4731:ILE:HA	1:B:4101:LYS:HG3	1.91	0.52
1:D:627:PRO:O	1:D:629:ARG:NH1	2.43	0.52
1:D:4865:LYS:NZ	1:D:4865:LYS:CB	2.72	0.52
1:C:157:ARG:HA	1:C:161:GLU:OE1	2.08	0.52
1:D:1143:TRP:CD1	1:D:1164:LEU:HD13	2.44	0.52
1:C:479:GLN:HE22	1:C:536:ASN:HA	1.74	0.52
1:C:670:GLU:OE2	1:C:788:LYS:HB2	2.10	0.52
1:C:1867:GLU:O	1:C:1871:PHE:N	2.34	0.52
1:A:1738:LEU:HB2	1:A:2146:PRO:HD3	1.91	0.52
1:A:4662:ASN:O	1:A:4666:VAL:CG1	2.57	0.52
1:B:1697:ALA:HB1	1:B:1708:ARG:HD3	1.90	0.52
1:B:4238:CYS:O	1:B:4242:ILE:HG12	2.09	0.52
1:D:2288:LEU:HD12	1:D:3853:ALA:HB2	1.91	0.52
1:C:103:TYR:CZ	1:C:163:VAL:HG13	2.44	0.52
1:C:181:HIS:H	1:C:193:ALA:HA	1.74	0.52
1:C:652:ARG:HD2	1:C:750:LEU:HB3	1.92	0.52
1:B:4731:ILE:HA	1:C:4101:LYS:HG3	1.92	0.52
1:D:682:LEU:HD13	1:D:787:VAL:HG11	1.92	0.52
1:D:1676:LEU:HD13	1:D:2168:VAL:HG22	1.92	0.52
1:D:1697:ALA:HB1	1:D:1708:ARG:HH11	1.74	0.52
1:C:2904:LEU:HD21	1:C:2912:THR:HG23	1.91	0.52
1:A:3760:LYS:NZ	1:A:3760:LYS:CB	2.72	0.52
1:A:4066:LEU:HD21	1:A:4173:TYR:CZ	2.45	0.52
1:A:4933:GLN:O	1:A:4937:ILE:HG12	2.09	0.52
1:A:4940:PHE:HE2	1:D:4935:LEU:CD2	2.17	0.52
1:B:1950:GLU:OE2	1:B:2041:HIS:NE2	2.42	0.52
1:B:4985:LEU:HB2	2:B:5101:ACP:N1	2.25	0.52
1:C:3684:GLU:O	1:C:3686:GLU:N	2.43	0.52
1:C:4937:ILE:N	1:C:4937:ILE:CD1	2.73	0.52
1:A:1101:ARG:HE	1:A:1115:LEU:HD12	1.75	0.52
1:B:449:ILE:HG13	1:B:525:LEU:HD12	1.91	0.52
1:B:2785:LEU:HB3	1:B:2787:THR:HG22	1.92	0.52
1:D:181:HIS:H	1:D:193:ALA:HA	1.75	0.52
1:D:4920:PHE:O	1:D:4924:VAL:HG12	2.10	0.52
1:B:445:LEU:HD13	1:B:521:LEU:HB3	1.92	0.52
1:D:4063:ASP:OD2	1:D:4067:LYS:NZ	2.41	0.52
1:C:728:ARG:NH1	1:C:1384:UNK:O	2.43	0.52
1:C:1237:TRP:HH2	1:C:1652:GLU:HA	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2785:LEU:HB3	1:C:2787:THR:HG22	1.92	0.52
1:A:617:ASN:OD1	1:A:618:GLN:N	2.43	0.52
1:A:3760:LYS:NZ	1:A:3760:LYS:CA	2.71	0.52
1:A:4933:GLN:NE2	1:D:4930:ALA:HA	2.25	0.52
1:B:617:ASN:OD1	1:B:618:GLN:N	2.43	0.52
1:D:3754:GLU:HA	1:D:3754:GLU:OE2	2.10	0.52
1:D:4864:ASN:OD1	1:D:4871:GLU:OE1	2.28	0.52
1:C:3667:HIS:NE2	1:C:3671:ASP:OD2	2.43	0.52
1:A:45:ARG:HG2	1:A:443:LEU:HD21	1.92	0.51
1:A:1697:ALA:HB1	1:A:1708:ARG:HD3	1.92	0.51
1:B:220:LEU:HD22	1:B:262:LEU:HD23	1.92	0.51
1:B:1927:LEU:HD13	1:B:2101:MET:HG3	1.91	0.51
1:B:4003:LEU:HD11	1:B:4009:GLN:HG2	1.92	0.51
1:C:2337:PHE:HA	1:C:2340:PHE:HB2	1.91	0.51
1:C:4207:MET:HE3	1:C:4210:VAL:HG23	1.91	0.51
1:B:1839:VAL:HG13	1:B:1841:VAL:HG22	1.93	0.51
1:D:197:GLN:NE2	1:D:198:THR:O	2.43	0.51
1:D:666:VAL:HB	1:D:744:VAL:HB	1.91	0.51
1:D:2881:ASN:HA	1:D:2884:ASN:HD21	1.75	0.51
1:C:509:GLU:O	1:C:510:GLU:HG3	2.10	0.51
1:C:3758:MET:HE3	1:C:3762:ARG:NH2	2.24	0.51
1:B:3716:LEU:HD23	1:B:3793:MET:HG3	1.92	0.51
1:B:3770:LEU:HD13	1:B:3804:ILE:HD11	1.91	0.51
1:C:4698:LYS:HE3	1:C:4785:THR:HB	1.93	0.51
1:C:4936:ILE:N	1:C:4936:ILE:CD1	2.73	0.51
1:A:2763:HIS:NE2	1:A:2792:ARG:O	2.34	0.51
1:B:1101:ARG:HE	1:B:1115:LEU:HD12	1.76	0.51
1:B:4801:LEU:HD23	1:B:4808:PHE:CD2	2.43	0.51
1:D:617:ASN:OD1	1:D:618:GLN:N	2.43	0.51
1:D:1126:GLY:HA3	1:D:1143:TRP:CZ3	2.45	0.51
1:D:3906:GLN:HE22	1:D:3913:ILE:HB	1.75	0.51
1:C:24:CYS:HB3	1:C:200:TRP:CE3	2.46	0.51
1:C:1240:LYS:NZ	1:C:1242:LEU:HB3	2.26	0.51
1:C:3787:LYS:N	1:C:3787:LYS:HD2	2.25	0.51
1:B:4689:THR:HA	1:B:4732:PHE:HE2	1.75	0.51
1:D:1960:ALA:O	1:D:1963:GLU:HG3	2.10	0.51
1:D:2785:LEU:HB3	1:D:2787:THR:HG22	1.92	0.51
1:C:1126:GLY:HA3	1:C:1143:TRP:CZ3	2.46	0.51
1:A:841:GLY:HA2	1:A:1073:ARG:HD2	1.93	0.51
1:A:2368:LEU:HD22	1:A:2376:LEU:HD21	1.92	0.51
1:B:4865:LYS:HG3	1:B:4875:LYS:HG3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4639:MET:HB2	1:D:4642:ALA:HB3	1.91	0.51
1:C:102:LEU:HD13	1:C:160:GLY:HA2	1.93	0.51
1:C:157:ARG:NH2	1:C:164:ARG:NH2	2.59	0.51
1:A:4860:ARG:NH1	1:A:4860:ARG:CG	2.73	0.51
1:A:4921:PHE:CD2	1:B:4892:ARG:HD2	2.46	0.51
1:B:682:LEU:HD13	1:B:787:VAL:HG11	1.93	0.51
1:D:348:VAL:HB	1:D:357:LEU:HD22	1.91	0.51
1:D:4865:LYS:HG2	1:D:4875:LYS:HG2	1.92	0.51
1:C:102:LEU:HB2	1:C:161:GLU:O	2.11	0.51
1:A:2022:PRO:HB2	1:A:2024:PRO:HD2	1.93	0.51
1:A:2359:ARG:NH1	1:D:195:PHE:O	2.37	0.51
1:A:3753:PHE:C	1:A:3753:PHE:CD2	2.84	0.51
1:A:4584:ASP:HA	1:A:4627:MET:HA	1.93	0.51
1:A:4936:ILE:N	1:A:4936:ILE:CD1	2.73	0.51
1:B:1685:LEU:HD23	1:B:1718:ILE:HD12	1.91	0.51
1:B:4573:ILE:HD11	1:B:4809:PHE:CE2	2.40	0.51
1:C:36:CYS:HB3	1:C:50:GLU:HB3	1.91	0.51
1:C:1076:ARG:HD3	1:C:1109:LEU:HD12	1.92	0.51
1:A:776:LEU:HG	1:A:848:HIS:HA	1.93	0.51
1:A:2688:UNK:O	1:A:2691:UNK:C	2.58	0.51
1:A:2881:ASN:HA	1:A:2884:ASN:HD21	1.76	0.51
1:A:4689:THR:HA	1:A:4732:PHE:HE2	1.75	0.51
1:B:2881:ASN:HA	1:B:2884:ASN:HD21	1.76	0.51
1:D:3751:VAL:O	1:D:3751:VAL:HG23	2.10	0.51
1:D:4865:LYS:NZ	1:D:4865:LYS:CA	2.72	0.51
1:C:682:LEU:HD13	1:C:787:VAL:HG11	1.93	0.51
1:A:414:PHE:HE1	1:A:436:LEU:HD12	1.75	0.50
1:B:69:LEU:HB3	1:B:107:ILE:HD11	1.92	0.50
1:B:76:ARG:O	1:B:79:GLN:HG2	2.11	0.50
1:B:1947:CYS:SG	1:B:2126:ARG:NH2	2.77	0.50
1:B:3984:ARG:HG2	1:B:3987:ASP:HB2	1.91	0.50
1:B:4935:LEU:CD2	1:C:4940:PHE:CE2	2.79	0.50
1:D:3769:ARG:O	1:D:3771:HIS:ND1	2.45	0.50
1:C:2358:ILE:HA	1:C:2364:PHE:HZ	1.75	0.50
1:C:2871:LEU:HD12	1:C:2927:LEU:HD21	1.93	0.50
1:C:3758:MET:CE	1:C:3762:ARG:NH2	2.74	0.50
1:A:455:PRO:HG3	1:A:467:LYS:HB3	1.92	0.50
1:A:687:ALA:HB3	1:A:778:PHE:HB2	1.94	0.50
1:A:1075:PHE:HB2	1:A:1192:CYS:SG	2.51	0.50
1:A:2288:LEU:HD12	1:A:3853:ALA:HB2	1.93	0.50
1:B:710:ASP:OD1	1:B:713:SER:OG	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4141:PHE:CZ	1:B:4196:GLU:HB3	2.46	0.50
1:D:1703:LEU:HB2	1:D:1707:LEU:HB3	1.92	0.50
1:D:2924:GLN:O	1:D:2928:LYS:HG2	2.10	0.50
1:D:4181:ILE:HG12	1:D:4195:PHE:HE1	1.77	0.50
1:A:149:THR:HG23	1:A:151:HIS:CE1	2.46	0.50
1:A:4001:MET:O	1:A:4005:GLN:NE2	2.44	0.50
1:B:1840:PRO:HB3	1:B:1843:LYS:HD3	1.93	0.50
1:D:1698:LEU:HD23	1:D:1810:LYS:HD2	1.93	0.50
1:D:4026:MET:O	1:D:4030:LEU:HG	2.11	0.50
1:D:4661:TYR:O	1:D:4666:VAL:HG23	2.11	0.50
1:D:4888:TYR:OH	1:C:4913:ARG:NH1	2.43	0.50
1:C:1574:PRO:HD2	1:C:1577:ALA:HB2	1.94	0.50
1:C:3965:LEU:O	1:C:3968:TYR:HD1	1.94	0.50
1:B:2810:LYS:HG2	1:B:2814:LYS:HE3	1.93	0.50
1:D:102:LEU:HD13	1:D:160:GLY:HA2	1.93	0.50
1:D:4640:GLU:HB2	1:D:4641:PRO:HD3	1.92	0.50
1:D:4690:GLU:HG2	1:D:4691:GLN:H	1.77	0.50
1:C:3751:VAL:CG2	1:C:3755:GLU:HB3	2.40	0.50
1:C:3773:ARG:HA	1:C:3815:LYS:HE3	1.92	0.50
1:C:3999:MET:HB2	1:C:4003:LEU:HD13	1.94	0.50
1:A:4921:PHE:CD1	1:A:4921:PHE:C	2.85	0.50
1:B:1960:ALA:O	1:B:1963:GLU:HG3	2.12	0.50
1:C:2881:ASN:HA	1:C:2884:ASN:HD21	1.76	0.50
1:C:3889:GLN:HB2	1:C:3964:SER:HA	1.94	0.50
1:C:3927:GLN:NE2	1:C:3931:SER:OG	2.44	0.50
1:A:1851:MET:HB2	1:A:1853:ILE:HG12	1.94	0.50
1:A:4582:VAL:HG11	1:D:4860:ARG:HE	1.76	0.50
1:B:776:LEU:HG	1:B:848:HIS:HA	1.93	0.50
1:B:2022:PRO:HB2	1:B:2024:PRO:HD2	1.94	0.50
1:B:3760:LYS:HD2	1:B:3760:LYS:C	2.31	0.50
1:B:4985:LEU:HD23	1:B:4985:LEU:O	2.12	0.50
1:D:4823:LEU:HD22	1:C:4839:MET:HE3	1.93	0.50
1:D:4865:LYS:C	1:D:4865:LYS:HD3	2.32	0.50
1:C:2113:SER:O	1:C:2113:SER:OG	2.29	0.50
1:B:2165:LEU:HD13	1:B:2178:MET:HB3	1.94	0.50
1:D:560:ILE:HA	1:D:563:VAL:HG12	1.93	0.50
1:D:3840:SER:OG	1:D:3877:ASP:OD2	2.30	0.50
1:D:3888:LEU:HD13	1:D:3891:LEU:HD12	1.94	0.50
1:D:4698:LYS:HE3	1:D:4785:THR:HB	1.93	0.50
1:C:2107:GLN:NE2	1:C:3681:GLY:CA	2.69	0.50
1:C:2812:SER:HB2	1:C:2926:LEU:HD22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:710:ASP:OD1	1:D:713:SER:OG	2.26	0.50
1:A:1676:LEU:HD22	1:A:2167:ILE:HG22	1.94	0.50
1:A:1698:LEU:HD23	1:A:1810:LYS:HD2	1.94	0.50
1:A:3702:VAL:HG11	1:A:3775:ALA:HB2	1.89	0.50
1:A:4011:GLU:HG2	1:A:4012:LEU:HD12	1.92	0.50
1:A:4240:ASP:OD2	1:A:4668:LEU:HD21	2.12	0.50
1:B:1075:PHE:HB2	1:B:1192:CYS:SG	2.52	0.50
1:B:3804:ILE:HG22	1:B:3805:LEU:HD12	1.94	0.50
1:D:686:TRP:CZ3	1:D:777:PHE:HB3	2.47	0.50
1:D:1867:GLU:HA	1:D:1870:VAL:HB	1.92	0.50
1:A:1106:ARG:NH2	1:A:1183:GLU:OE2	2.44	0.49
1:A:1676:LEU:HD13	1:A:2168:VAL:HG22	1.94	0.49
1:B:299:LEU:HG	1:B:378:LEU:HG	1.94	0.49
1:B:2248:ARG:NH2	1:B:3865:VAL:O	2.45	0.49
1:B:2871:LEU:HD12	1:B:2927:LEU:HD21	1.94	0.49
1:D:1166:GLY:HA3	1:D:1216:ILE:HD13	1.93	0.49
1:D:4223:ASN:OD1	1:D:4946:GLN:NE2	2.42	0.49
1:A:109:LEU:HD23	1:A:148:TRP:HD1	1.76	0.49
1:A:197:GLN:NE2	1:A:198:THR:O	2.44	0.49
1:B:3787:LYS:NZ	1:B:3830:GLN:HG3	2.27	0.49
1:B:4865:LYS:CB	1:B:4875:LYS:CG	2.88	0.49
1:D:214:VAL:HG22	1:D:341:TYR:HE1	1.77	0.49
1:D:1667:LEU:HD21	1:D:1710:GLY:HA3	1.93	0.49
1:D:3761:GLN:HA	1:D:3761:GLN:HE21	1.72	0.49
1:C:1143:TRP:CD1	1:C:1164:LEU:HD13	2.47	0.49
1:C:4892:ARG:O	1:C:4892:ARG:CG	2.60	0.49
1:A:4574:ASN:HD22	1:A:4813:LEU:HD13	1.77	0.49
1:A:4927:ILE:N	1:A:4927:ILE:CD1	2.75	0.49
1:B:2192:TYR:HD1	1:B:2242:ILE:HD13	1.77	0.49
1:B:4849:TYR:OH	1:C:4574:ASN:ND2	2.46	0.49
1:D:719:LEU:HD12	1:D:719:LEU:O	2.13	0.49
1:D:841:GLY:HA2	1:D:1073:ARG:HD2	1.93	0.49
1:D:3767:GLN:NE2	1:D:3804:ILE:HD12	2.27	0.49
1:D:3927:GLN:NE2	1:D:3931:SER:OG	2.44	0.49
1:C:4690:GLU:HG2	1:C:4691:GLN:H	1.78	0.49
1:A:2248:ARG:NH2	1:A:3865:VAL:O	2.46	0.49
1:A:2812:SER:HB2	1:A:2926:LEU:HD22	1.93	0.49
1:B:1229:ASN:HB2	1:B:1826:ALA:HB1	1.95	0.49
1:B:1747:LEU:HB3	1:B:1760:HIS:HB3	1.93	0.49
1:B:3669:PHE:O	1:B:3673:MET:HG2	2.12	0.49
1:B:4812:HIS:HD1	1:B:4812:HIS:C	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4985:LEU:HD13	2:B:5101:ACP:H2	1.92	0.49
1:D:483:MET:HA	1:D:486:LEU:HD13	1.93	0.49
1:C:759:ILE:HG13	1:C:760:ASN:H	1.76	0.49
1:A:648:ILE:HD13	1:A:779:PRO:HG2	1.93	0.49
1:A:1867:GLU:HA	1:A:1870:VAL:HB	1.94	0.49
1:B:3924:LEU:HD22	1:B:3984:ARG:HD2	1.95	0.49
1:D:717:ASP:OD1	1:D:717:ASP:N	2.45	0.49
1:D:2477:PRO:HB2	1:D:2488:UNK:HA	1.93	0.49
1:D:3887:PHE:O	1:D:3891:LEU:HG	2.12	0.49
1:C:669:ASP:OD1	1:C:669:ASP:N	2.44	0.49
1:C:790:ARG:HD3	1:C:1627:ALA:HB2	1.94	0.49
1:C:1859:VAL:HA	1:C:1862:ILE:HG22	1.93	0.49
1:C:2477:PRO:HB2	1:C:2488:UNK:HA	1.95	0.49
1:A:4850:LEU:HD13	1:B:4814:LEU:HD22	1.94	0.49
1:B:2477:PRO:HB2	1:B:2488:UNK:HA	1.95	0.49
1:B:4066:LEU:HD21	1:B:4173:TYR:CZ	2.48	0.49
1:D:1840:PRO:HB3	1:D:1843:LYS:HD3	1.95	0.49
1:D:2812:SER:HB2	1:D:2926:LEU:HD22	1.94	0.49
1:D:3779:VAL:HG23	1:D:3797:THR:HG22	1.94	0.49
1:C:214:VAL:HG22	1:C:341:TYR:HE1	1.77	0.49
1:C:3737:GLU:CA	1:C:3763:LEU:HD23	2.42	0.49
1:A:1929:MET:N	1:A:1929:MET:SD	2.86	0.49
1:A:3886:ARG:NH1	1:A:3889:GLN:OE1	2.45	0.49
1:A:3987:ASP:OD1	1:D:162:LYS:NZ	2.46	0.49
1:B:719:LEU:O	1:B:719:LEU:HD12	2.11	0.49
1:B:5017:ARG:HH21	1:B:5019:TRP:HE1	1.60	0.49
1:D:36:CYS:HB3	1:D:50:GLU:HB3	1.94	0.49
1:D:2809:ILE:HD11	1:D:2926:LEU:HD13	1.94	0.49
1:D:3767:GLN:NE2	1:D:3804:ILE:CD1	2.75	0.49
1:C:652:ARG:HD3	1:C:773:LEU:HD12	1.94	0.49
1:C:1075:PHE:HB2	1:C:1192:CYS:SG	2.53	0.49
1:C:3840:SER:OG	1:C:3877:ASP:OD2	2.30	0.49
1:A:154:SER:OG	1:A:155:LYS:N	2.46	0.49
1:A:1143:TRP:CD1	1:A:1164:LEU:HD13	2.48	0.49
1:A:3561:UNK:O	1:A:3562:UNK:CB	2.61	0.49
1:A:4550:LYS:HA	1:A:4553:ASN:ND2	2.27	0.49
1:B:667:MET:HB2	1:B:790:ARG:HB2	1.95	0.49
1:B:728:ARG:NH1	1:B:1384:UNK:O	2.46	0.49
1:B:2337:PHE:HA	1:B:2340:PHE:HB2	1.94	0.49
1:B:2763:HIS:NE2	1:B:2792:ARG:O	2.34	0.49
1:B:4066:LEU:HD21	1:B:4173:TYR:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1228:ILE:HG23	1:D:1229:ASN:H	1.77	0.49
1:D:1740:PRO:HA	1:D:1743:ARG:HG2	1.95	0.49
1:D:1747:LEU:HB3	1:D:1760:HIS:HB3	1.95	0.49
1:C:4689:THR:HA	1:C:4732:PHE:HE2	1.78	0.49
1:A:4244:GLU:HG2	1:A:4668:LEU:CD1	2.43	0.49
1:B:24:CYS:HB3	1:B:200:TRP:CE3	2.48	0.49
1:B:2178:MET:SD	1:B:2228:MET:HE1	2.53	0.49
1:B:4872:PRO:CD	1:B:4873:ASP:N	2.76	0.49
1:D:1580:PHE:HE2	1:D:1592:PRO:HG2	1.78	0.49
1:D:3886:ARG:NH1	1:D:3889:GLN:OE1	2.46	0.49
1:C:2810:LYS:HG2	1:C:2814:LYS:HE3	1.94	0.49
1:C:4066:LEU:HD21	1:C:4173:TYR:CE2	2.48	0.49
1:B:1639:LEU:N	1:B:1648:MET:O	2.44	0.48
1:B:4812:HIS:ND1	1:B:4812:HIS:C	2.67	0.48
1:C:483:MET:HA	1:C:486:LEU:HD13	1.95	0.48
1:C:1698:LEU:HD22	1:C:1810:LYS:HG2	1.93	0.48
1:C:4944:ARG:NH1	1:C:4944:ARG:CG	2.76	0.48
1:A:786:GLY:HA2	1:A:1631:GLN:HA	1.95	0.48
1:A:3889:GLN:HG3	1:A:3964:SER:HA	1.95	0.48
1:D:154:SER:OG	1:D:155:LYS:N	2.45	0.48
1:C:567:VAL:HG13	1:C:568:LEU:HD12	1.94	0.48
1:C:3723:MET:HE1	1:C:3793:MET:HA	1.94	0.48
1:A:790:ARG:HD3	1:A:1627:ALA:HB2	1.96	0.48
1:A:1649:ASP:N	1:A:1649:ASP:OD1	2.45	0.48
1:A:1703:LEU:HB2	1:A:1707:LEU:HB3	1.94	0.48
1:A:2736:ASP:N	1:A:2736:ASP:OD1	2.46	0.48
1:B:650:VAL:HB	1:B:777:PHE:HD2	1.77	0.48
1:D:19:GLU:HB3	1:D:68:THR:HG22	1.95	0.48
1:D:1240:LYS:HZ1	1:D:1242:LEU:HB3	1.77	0.48
1:D:2248:ARG:NH2	1:D:3865:VAL:O	2.46	0.48
1:D:3670:GLU:OE1	1:D:3670:GLU:N	2.44	0.48
1:D:4003:LEU:HD11	1:D:4009:GLN:HG2	1.96	0.48
1:D:4141:PHE:CE2	1:D:4196:GLU:HB2	2.48	0.48
1:C:426:ARG:NE	1:C:505:GLU:O	2.41	0.48
1:C:1857:GLU:HA	1:C:1860:LYS:HE2	1.95	0.48
1:C:2022:PRO:HB2	1:C:2024:PRO:HD2	1.95	0.48
1:C:3778:MET:HA	1:C:3781:GLN:HG2	1.96	0.48
1:B:116:MET:HG3	1:B:137:LEU:HD12	1.94	0.48
1:D:149:THR:HG23	1:D:151:HIS:HE1	1.78	0.48
1:D:1075:PHE:HB2	1:D:1192:CYS:SG	2.53	0.48
1:D:2022:PRO:HB2	1:D:2024:PRO:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3968:TYR:O	1:C:3976:ASN:ND2	2.46	0.48
1:A:4238:CYS:HA	1:A:4989:MET:HE1	1.94	0.48
1:B:149:THR:HG23	1:B:151:HIS:CE1	2.49	0.48
1:B:1676:LEU:HD22	1:B:2167:ILE:HG22	1.95	0.48
1:B:1740:PRO:HA	1:B:1743:ARG:HG2	1.95	0.48
1:B:2368:LEU:HD13	1:B:2376:LEU:HD21	1.94	0.48
1:B:4852:THR:HG21	1:B:4883:TYR:HA	1.95	0.48
1:D:248:GLU:HG2	1:D:252:VAL:HG23	1.96	0.48
1:D:1237:TRP:HH2	1:D:1652:GLU:HA	1.78	0.48
1:D:3805:LEU:O	1:D:3890:LEU:HD23	2.14	0.48
1:B:3972:PRO:HB3	1:B:4032:GLU:HG3	1.96	0.48
1:B:4865:LYS:CG	1:B:4875:LYS:CG	2.91	0.48
1:D:1707:LEU:O	1:D:1709:ALA:N	2.47	0.48
1:D:3767:GLN:HE22	1:D:3804:ILE:CD1	2.27	0.48
1:D:4095:LYS:HE2	1:D:4095:LYS:HB3	1.68	0.48
1:C:138:GLN:HG2	1:C:139:GLU:H	1.78	0.48
1:B:138:GLN:HG2	1:B:139:GLU:H	1.78	0.48
1:B:143:GLY:HA2	1:B:146:CYS:SG	2.54	0.48
1:D:455:PRO:HG3	1:D:467:LYS:HB3	1.95	0.48
1:D:1689:VAL:HG13	1:D:1690:ASP:N	2.28	0.48
1:B:2736:ASP:OD1	1:B:2736:ASP:N	2.46	0.48
1:B:4851:TYR:HD2	1:B:4920:PHE:HD1	1.61	0.48
1:D:243:ARG:NH1	1:D:301:VAL:O	2.47	0.48
1:D:1712:TYR:O	1:D:1716:ILE:HG12	2.13	0.48
1:C:3944:GLU:HG2	1:C:3947:GLY:H	1.79	0.48
1:A:664:PHE:CZ	1:A:779:PRO:HG3	2.49	0.48
1:A:1697:ALA:HB1	1:A:1708:ARG:HH11	1.78	0.48
1:A:1712:TYR:O	1:A:1716:ILE:HG12	2.14	0.48
1:A:1747:LEU:HB3	1:A:1760:HIS:HB3	1.94	0.48
1:A:4183:ILE:HD13	1:A:5010:VAL:HG21	1.96	0.48
1:A:4927:ILE:N	1:A:4927:ILE:HD13	2.29	0.48
1:B:700:GLU:HA	1:B:1646:ARG:HA	1.96	0.48
1:C:220:LEU:HD12	1:C:390:LEU:HB3	1.95	0.48
1:A:1689:VAL:HG13	1:A:1690:ASP:N	2.29	0.48
1:A:1740:PRO:HA	1:A:1743:ARG:HG2	1.96	0.48
1:D:2113:SER:OG	1:D:2113:SER:O	2.31	0.48
1:D:2871:LEU:HD12	1:D:2927:LEU:HD21	1.95	0.48
1:C:1698:LEU:HD21	1:C:1814:MET:HB2	1.95	0.48
1:C:3765:TYR:CD1	1:C:4750:ILE:HD12	2.49	0.48
1:B:216:GLY:HA2	1:B:262:LEU:HD11	1.96	0.47
1:B:3835:LEU:HD21	1:B:3880:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1580:PHE:HE2	1:C:1592:PRO:HG2	1.78	0.47
1:C:1929:MET:N	1:C:1929:MET:SD	2.87	0.47
1:C:2248:ARG:NH2	1:C:3865:VAL:O	2.47	0.47
1:A:24:CYS:HB3	1:A:200:TRP:CE3	2.49	0.47
1:A:273:HIS:H	1:A:334:MET:HB3	1.80	0.47
1:A:978:THR:HG22	1:A:981:GLN:H	1.79	0.47
1:A:2477:PRO:HB2	1:A:2488:UNK:HA	1.95	0.47
1:A:4244:GLU:HG3	1:A:4668:LEU:HD11	1.96	0.47
1:B:213:TYR:CG	1:B:337:PRO:HB2	2.49	0.47
1:D:3945:GLU:OE1	1:D:3946:GLN:NE2	2.47	0.47
1:D:4892:ARG:HH22	1:C:4897:ILE:N	2.12	0.47
1:D:4929:LEU:N	1:D:4929:LEU:CD2	2.77	0.47
1:C:449:ILE:HG13	1:C:525:LEU:HD12	1.95	0.47
1:C:455:PRO:HG3	1:C:467:LYS:HB3	1.96	0.47
1:C:3763:LEU:O	1:C:3767:GLN:OE1	2.31	0.47
1:C:4555:LEU:HD22	1:C:4656:LEU:HD11	1.95	0.47
1:A:1707:LEU:O	1:A:1709:ALA:N	2.47	0.47
1:A:2113:SER:O	1:A:2113:SER:OG	2.30	0.47
1:B:1703:LEU:HB2	1:B:1707:LEU:HB3	1.97	0.47
1:D:2930:LEU:HD13	1:D:2937:VAL:HG21	1.96	0.47
1:D:3889:GLN:NE2	1:D:3963:ASN:OD1	2.47	0.47
1:D:4582:VAL:HG11	1:C:4860:ARG:HH11	1.80	0.47
1:C:3924:LEU:HD22	1:C:3984:ARG:HD2	1.95	0.47
1:C:4671:PHE:HE1	1:C:4716:TRP:HB2	1.78	0.47
1:A:2742:THR:HG21	1:A:2814:LYS:HD3	1.96	0.47
1:A:3962:PHE:O	1:A:3966:THR:HG23	2.14	0.47
1:D:1077:ALA:HB3	1:D:1189:LEU:HD11	1.96	0.47
1:C:3729:MET:O	1:C:3732:SER:OG	2.30	0.47
1:A:219:VAL:HG12	1:A:261:ARG:HB2	1.96	0.47
1:A:313:SER:HB2	1:A:350:HIS:CE1	2.50	0.47
1:A:2299:VAL:HG11	1:A:2356:LEU:HB3	1.95	0.47
1:A:4865:LYS:HA	1:A:4865:LYS:CE	2.42	0.47
1:A:4921:PHE:HD2	1:B:4892:ARG:HD2	1.79	0.47
1:B:1707:LEU:O	1:B:1709:ALA:N	2.48	0.47
1:D:219:VAL:HG12	1:D:261:ARG:HB2	1.97	0.47
1:C:1707:LEU:O	1:C:1709:ALA:N	2.47	0.47
1:A:670:GLU:HG3	1:A:787:VAL:HA	1.95	0.47
1:A:1026:LEU:HA	1:A:1032:LYS:HE2	1.96	0.47
1:A:1840:PRO:HB3	1:A:1843:LYS:HD3	1.97	0.47
1:B:1580:PHE:HE2	1:B:1592:PRO:HG2	1.78	0.47
1:B:2474:LEU:HD23	1:B:2474:LEU:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2257:LEU:HD11	1:D:2276:ALA:HB2	1.94	0.47
1:C:2192:TYR:HD1	1:C:2242:ILE:HD13	1.79	0.47
1:C:2809:ILE:HD11	1:C:2926:LEU:HD13	1.96	0.47
1:A:192:ASP:OD1	1:A:192:ASP:N	2.46	0.47
1:A:646:PRO:HD2	1:A:779:PRO:HB2	1.97	0.47
1:A:3236:UNK:N	1:A:3240:UNK:N	2.61	0.47
1:A:4158:PRO:HA	1:A:4161:ARG:HD3	1.96	0.47
1:B:2181:SER:O	1:B:2185:ILE:HG23	2.14	0.47
1:B:4690:GLU:HG2	1:B:4691:GLN:H	1.78	0.47
1:B:4946:GLN:O	1:B:4949:GLN:N	2.47	0.47
1:D:723:THR:H	1:D:726:VAL:HG12	1.79	0.47
1:D:1026:LEU:HA	1:D:1032:LYS:HE2	1.96	0.47
1:D:1839:VAL:HG13	1:D:1841:VAL:HG22	1.97	0.47
1:D:2192:TYR:HD1	1:D:2242:ILE:HD13	1.80	0.47
1:D:2474:LEU:HD23	1:D:2474:LEU:H	1.80	0.47
1:D:4866:SER:OG	1:D:4867:GLU:N	2.45	0.47
1:C:4011:GLU:HG2	1:C:4012:LEU:HD12	1.97	0.47
1:C:4869:GLU:HB3	1:C:4870:ASP:H	1.36	0.47
1:A:2287:ALA:O	1:A:2349:ASN:ND2	2.43	0.47
1:A:3957:VAL:O	1:A:3961:VAL:HG23	2.15	0.47
1:A:4690:GLU:HG2	1:A:4691:GLN:H	1.78	0.47
1:B:154:SER:OG	1:B:155:LYS:N	2.47	0.47
1:B:1857:GLU:HA	1:B:1860:LYS:HE2	1.97	0.47
1:B:3906:GLN:HE22	1:B:3913:ILE:HB	1.80	0.47
1:D:213:TYR:CD1	1:D:337:PRO:HB2	2.50	0.47
1:D:661:LYS:HB3	1:D:808:TYR:CD2	2.50	0.47
1:D:3937:TYR:OH	1:D:3944:GLU:OE2	2.32	0.47
1:C:978:THR:HG22	1:C:981:GLN:H	1.80	0.47
1:C:1747:LEU:HB3	1:C:1760:HIS:HB3	1.96	0.47
1:C:4716:TRP:HZ2	1:C:4996:ILE:HG21	1.79	0.47
1:A:138:GLN:HG2	1:A:139:GLU:H	1.79	0.47
1:A:1124:PHE:HE1	1:A:1139:PHE:HB3	1.79	0.47
1:D:1194:LEU:HB3	1:D:1198:GLN:HB2	1.96	0.47
1:D:4629:TYR:HE1	1:C:4860:ARG:HH12	1.62	0.47
1:C:2335:LEU:HD22	1:C:2353:VAL:HG21	1.96	0.47
1:C:3758:MET:C	1:C:3758:MET:SD	2.93	0.47
1:A:1204:LEU:HD23	1:A:1227:ALA:HB2	1.97	0.47
1:A:4917:ASP:OD2	1:B:4892:ARG:NH1	2.48	0.47
1:B:4865:LYS:HG3	1:B:4875:LYS:HG2	1.95	0.47
1:D:45:ARG:HD2	1:D:137:LEU:O	2.15	0.47
1:D:2449:GLU:OE2	1:D:2452:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4019:LEU:O	1:D:4023:MET:HG2	2.15	0.47
1:C:1740:PRO:HA	1:C:1743:ARG:HG2	1.97	0.47
1:C:2474:LEU:HD23	1:C:2474:LEU:H	1.80	0.47
1:A:3887:PHE:O	1:A:3891:LEU:HG	2.15	0.46
1:D:669:ASP:N	1:D:669:ASP:OD1	2.48	0.46
1:D:4978:HIS:HE1	1:D:5027:CYS:HB2	1.80	0.46
1:C:1119:GLU:HA	1:C:1133:HIS:CD2	2.49	0.46
1:C:1960:ALA:O	1:C:1963:GLU:HG3	2.14	0.46
1:C:2736:ASP:OD1	1:C:2736:ASP:N	2.46	0.46
1:A:102:LEU:HD13	1:A:160:GLY:HA2	1.96	0.46
1:A:1727:ARG:HH21	1:A:1772:ARG:HG3	1.79	0.46
1:B:106:ALA:HA	1:B:149:THR:HA	1.97	0.46
1:B:707:VAL:HG12	1:B:713:SER:HB2	1.97	0.46
1:B:4031:LEU:HD23	1:B:4031:LEU:H	1.81	0.46
1:B:4832:HIS:NE2	1:B:4942:GLU:OE1	2.48	0.46
1:A:4017:LEU:HD12	1:A:4139:ILE:HG13	1.98	0.46
1:B:224:HIS:N	1:B:229:GLU:O	2.39	0.46
1:B:1026:LEU:HA	1:B:1032:LYS:HE2	1.96	0.46
1:B:4022:ASP:O	1:B:4025:VAL:HG12	2.15	0.46
1:B:4654:ALA:CB	1:B:4795:TYR:CE1	2.98	0.46
1:D:4689:THR:HA	1:D:4732:PHE:HE2	1.81	0.46
1:C:1026:LEU:HA	1:C:1032:LYS:HE2	1.96	0.46
1:C:1667:LEU:HD21	1:C:1710:GLY:HA3	1.97	0.46
1:C:4219:PHE:CE1	1:C:4946:GLN:OE1	2.69	0.46
1:C:4662:ASN:HA	1:C:4666:VAL:HG23	1.97	0.46
1:A:1867:GLU:O	1:A:1871:PHE:N	2.38	0.46
1:A:2674:UNK:HA	1:A:2679:UNK:CB	2.45	0.46
1:B:358:THR:HG1	1:B:383:HIS:HD1	1.64	0.46
1:B:1667:LEU:HD21	1:B:1710:GLY:HA3	1.97	0.46
1:B:4864:ASN:HA	1:B:4874:MET:SD	2.55	0.46
1:B:4865:LYS:CG	1:B:4875:LYS:HG2	2.45	0.46
1:D:2348:GLU:HG2	1:D:3849:ARG:HE	1.81	0.46
1:D:3889:GLN:HG3	1:D:3964:SER:HA	1.96	0.46
1:A:669:ASP:N	1:A:669:ASP:OD1	2.48	0.46
1:A:2271:THR:HG22	1:A:2273:LEU:H	1.80	0.46
1:B:414:PHE:HE1	1:B:436:LEU:HD12	1.80	0.46
1:B:1851:MET:HB2	1:B:1853:ILE:HG12	1.97	0.46
1:B:2159:LEU:HD13	1:B:2201:LEU:HD23	1.97	0.46
1:B:4818:MET:C	1:B:4818:MET:SD	2.94	0.46
1:C:5000:GLU:HA	1:C:5003:HIS:ND1	2.31	0.46
1:A:560:ILE:HA	1:A:563:VAL:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2095:GLN:HE21	1:A:2128:TYR:HD1	1.63	0.46
1:A:3491:UNK:O	1:A:3495:UNK:CB	2.64	0.46
1:B:197:GLN:NE2	1:B:198:THR:O	2.48	0.46
1:B:1194:LEU:HB3	1:B:1198:GLN:HB2	1.97	0.46
1:B:5000:GLU:HA	1:B:5003:HIS:ND1	2.31	0.46
1:D:1850:VAL:HA	1:D:1945:TYR:CE1	2.51	0.46
1:C:1194:LEU:HB3	1:C:1198:GLN:HB2	1.97	0.46
1:C:1240:LYS:HZ1	1:C:1242:LEU:HB3	1.80	0.46
1:C:1712:TYR:O	1:C:1716:ILE:HG12	2.15	0.46
1:C:3906:GLN:HE22	1:C:3913:ILE:HB	1.81	0.46
1:C:4223:ASN:ND2	1:C:4946:GLN:NE2	2.63	0.46
1:C:4844:LEU:HD12	1:C:4928:LEU:HG	1.96	0.46
1:A:108:LEU:HD13	1:A:147:TRP:NE1	2.31	0.46
1:A:795:GLY:H	1:A:811:CYS:HB2	1.80	0.46
1:A:1077:ALA:HB3	1:A:1189:LEU:HD11	1.97	0.46
1:A:2337:PHE:HA	1:A:2340:PHE:HB2	1.98	0.46
2:A:5101:ACP:O2G	2:A:5101:ACP:O2B	2.33	0.46
1:B:758:ARG:HG2	1:B:759:ILE:O	2.16	0.46
1:B:4654:ALA:CB	1:B:4795:TYR:HE1	2.29	0.46
1:D:4184:MET:HB2	1:D:4190:ILE:HG22	1.97	0.46
1:C:257:ARG:O	1:C:284:HIS:NE2	2.44	0.46
1:C:1685:LEU:HD23	1:C:1718:ILE:HD12	1.97	0.46
1:C:3771:HIS:O	1:C:3775:ALA:N	2.49	0.46
1:A:710:ASP:OD1	1:A:713:SER:OG	2.31	0.46
1:A:1228:ILE:HD11	1:B:3573:UNK:HA	1.97	0.46
1:A:3941:ASP:OD1	1:A:3941:ASP:N	2.47	0.46
1:B:592:LYS:O	1:B:1594:ARG:HB2	2.16	0.46
1:D:149:THR:HG23	1:D:151:HIS:CE1	2.50	0.46
1:D:4895:GLY:HA2	1:D:4921:PHE:HE1	1.81	0.46
1:C:1141:ARG:NH2	1:C:1144:GLN:OE1	2.49	0.46
1:A:700:GLU:HA	1:A:1646:ARG:HA	1.98	0.46
1:A:1101:ARG:HH21	1:A:1115:LEU:HG	1.79	0.46
1:A:3944:GLU:HG2	1:A:3947:GLY:H	1.81	0.46
1:B:669:ASP:N	1:B:669:ASP:OD1	2.49	0.46
1:B:978:THR:HG22	1:B:981:GLN:H	1.80	0.46
1:B:1712:TYR:O	1:B:1716:ILE:HG12	2.15	0.46
1:B:4816:ILE:HD12	1:B:4816:ILE:HA	1.65	0.46
1:B:4818:MET:HA	1:B:4823:LEU:CG	2.41	0.46
1:D:661:LYS:HE3	1:D:750:LEU:HB3	1.98	0.46
1:D:978:THR:HG22	1:D:981:GLN:H	1.80	0.46
1:D:1072:VAL:HG22	1:D:1195:GLY:HA2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1203:ASN:ND2	1:D:1210:SER:O	2.43	0.46
1:D:1639:LEU:N	1:D:1648:MET:O	2.46	0.46
1:D:2182:ILE:O	1:D:2185:ILE:HG12	2.15	0.46
1:C:3733:CYS:SG	1:C:3803:SER:OG	2.52	0.46
1:A:213:TYR:CD2	1:A:337:PRO:HB2	2.51	0.46
1:A:3888:LEU:HD13	1:A:3891:LEU:HD12	1.97	0.46
1:B:1934:SER:O	1:B:1937:LEU:HG	2.16	0.46
1:D:358:THR:HG1	1:D:383:HIS:HD1	1.64	0.46
1:D:700:GLU:HA	1:D:1646:ARG:HA	1.98	0.46
1:D:4180:ARG:HG2	1:D:4194:TYR:CE1	2.51	0.46
1:D:4235:VAL:HG21	1:D:5019:TRP:CH2	2.51	0.46
1:D:4828:SER:HA	1:D:4831:THR:HG22	1.98	0.46
1:D:4904:PRO:HG3	1:D:4913:ARG:HE	1.81	0.46
1:C:3759:GLU:O	1:C:3762:ARG:N	2.49	0.46
1:A:4914:VAL:HG23	1:B:4888:TYR:HD2	1.80	0.45
1:B:313:SER:HB2	1:B:350:HIS:CE1	2.51	0.45
1:B:4638:TYR:O	1:B:4641:PRO:HD2	2.16	0.45
1:D:2012:PHE:HB3	1:D:2021:CYS:HA	1.98	0.45
1:D:4017:LEU:HA	1:D:4020:GLN:OE1	2.16	0.45
1:C:3996:PHE:HA	1:C:3999:MET:SD	2.56	0.45
1:C:4666:VAL:N	1:C:4667:PRO:HD2	2.31	0.45
1:C:4985:LEU:O	1:C:4989:MET:HG2	2.17	0.45
1:A:1720:LEU:HB2	1:A:1724:CYS:SG	2.57	0.45
1:A:4654:ALA:O	1:A:4658:ILE:HG12	2.16	0.45
1:D:138:GLN:HG2	1:D:139:GLU:N	2.31	0.45
1:D:330:ASP:OD1	1:D:330:ASP:N	2.49	0.45
1:D:652:ARG:HD3	1:D:773:LEU:HD12	1.98	0.45
1:D:1119:GLU:HA	1:D:1133:HIS:CD2	2.51	0.45
1:D:2736:ASP:OD1	1:D:2736:ASP:N	2.46	0.45
1:D:4865:LYS:HZ3	1:D:4865:LYS:CB	2.27	0.45
1:C:1676:LEU:HD22	1:C:2167:ILE:HG22	1.97	0.45
1:C:2012:PHE:HB3	1:C:2021:CYS:HA	1.99	0.45
1:A:162:LYS:O	1:A:164:ARG:NH1	2.49	0.45
1:A:1580:PHE:CE2	1:A:1592:PRO:HG2	2.51	0.45
1:A:3804:ILE:HG22	1:A:3805:LEU:HD12	1.97	0.45
1:A:4716:TRP:HZ2	1:A:4996:ILE:HG21	1.81	0.45
1:B:1101:ARG:HH21	1:B:1115:LEU:HG	1.80	0.45
1:B:2272:PRO:HA	1:B:2275:VAL:HG12	1.98	0.45
1:B:3676:ASP:OD1	1:B:3677:LEU:N	2.50	0.45
1:B:3832:ILE:O	1:B:3836:MET:HG2	2.16	0.45
1:D:759:ILE:HG13	1:D:760:ASN:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:TYR:CD1	1:C:337:PRO:HB2	2.51	0.45
1:A:543:ASN:O	1:A:547:VAL:HG23	2.17	0.45
1:A:1931:LEU:HD22	1:A:1935:VAL:HG11	1.99	0.45
1:B:3840:SER:OG	1:B:3877:ASP:OD2	2.32	0.45
1:B:4573:ILE:HD13	1:B:4809:PHE:CD2	2.45	0.45
1:B:4821:LYS:HA	1:B:4824:ARG:NH2	2.31	0.45
1:C:214:VAL:HG21	1:C:390:LEU:HD12	1.98	0.45
1:C:4063:ASP:OD2	1:C:4067:LYS:NZ	2.46	0.45
1:A:1857:GLU:HA	1:A:1860:LYS:HE2	1.98	0.45
1:A:2474:LEU:HD23	1:A:2474:LEU:H	1.80	0.45
1:A:3963:ASN:O	1:A:3966:THR:OG1	2.30	0.45
1:A:4221:VAL:HG22	1:A:4233:LEU:HD11	1.98	0.45
1:A:4901:ILE:CB	1:A:4913:ARG:HH21	2.27	0.45
1:A:5017:ARG:HH21	1:A:5019:TRP:HE1	1.63	0.45
1:B:2812:SER:HB2	1:B:2926:LEU:HD22	1.98	0.45
1:B:3845:ASN:O	1:B:3849:ARG:HG2	2.17	0.45
1:B:4024:VAL:HG23	1:B:4142:ASN:ND2	2.32	0.45
1:D:294:THR:HG23	1:D:295:GLU:N	2.32	0.45
1:D:313:SER:HB2	1:D:350:HIS:CE1	2.52	0.45
1:D:3769:ARG:O	1:D:3771:HIS:CE1	2.70	0.45
1:C:293:LEU:HD13	1:C:298:GLY:N	2.31	0.45
1:C:647:ASN:HB3	1:C:822:ARG:NH1	2.31	0.45
1:C:2348:GLU:HG3	1:C:3849:ARG:HH21	1.80	0.45
1:C:4869:GLU:C	1:C:4870:ASP:O	2.55	0.45
1:C:4904:PRO:HB3	1:C:4913:ARG:HD3	1.98	0.45
1:A:119:SER:OG	1:A:120:CYS:N	2.49	0.45
1:B:144:GLU:HG2	1:B:145:ALA:N	2.32	0.45
1:B:1677:GLY:HA2	1:B:1721:GLU:HG2	1.99	0.45
1:B:1866:ILE:HG22	1:B:1870:VAL:HG23	1.99	0.45
1:C:719:LEU:O	1:C:719:LEU:HD12	2.17	0.45
1:C:1677:GLY:HA2	1:C:1721:GLU:HG2	1.99	0.45
1:C:2182:ILE:O	1:C:2185:ILE:HG12	2.16	0.45
1:A:693:SER:N	1:A:694:PRO:HD2	2.31	0.45
1:A:758:ARG:HG2	1:A:759:ILE:O	2.17	0.45
1:A:3763:LEU:C	1:A:3763:LEU:CD1	2.85	0.45
1:D:257:ARG:O	1:D:284:HIS:NE2	2.50	0.45
1:D:1098:GLY:HA3	1:D:1198:GLN:HE22	1.80	0.45
1:C:119:SER:OG	1:C:120:CYS:N	2.50	0.45
1:A:505:GLU:HA	1:A:511:ALA:HB3	1.98	0.45
1:A:1194:LEU:HB3	1:A:1198:GLN:HB2	1.98	0.45
1:A:4937:ILE:CD1	1:D:4934:GLY:HA2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1240:LYS:NZ	1:B:1244:GLN:OE1	2.49	0.45
1:D:2272:PRO:HA	1:D:2275:VAL:HG12	1.98	0.45
1:C:700:GLU:HA	1:C:1646:ARG:HA	1.98	0.45
1:A:22:LEU:HD11	1:A:200:TRP:HB3	1.99	0.45
1:A:131:LEU:HD21	1:B:2456:ILE:HA	1.99	0.45
1:A:1839:VAL:HG13	1:A:1841:VAL:HG22	1.98	0.45
1:A:2367:ALA:HB3	1:A:2379:ALA:HB2	1.98	0.45
1:B:330:ASP:OD1	1:B:330:ASP:N	2.49	0.45
1:B:1143:TRP:CD1	1:B:1164:LEU:HD13	2.52	0.45
1:B:4865:LYS:C	1:B:4865:LYS:CD	2.85	0.45
1:D:24:CYS:SG	1:D:35:LEU:HB2	2.57	0.45
1:D:272:SER:HB2	1:D:334:MET:HA	1.98	0.45
1:D:416:LYS:HA	1:D:416:LYS:HD3	1.77	0.45
1:C:795:GLY:H	1:C:811:CYS:HB2	1.82	0.45
1:C:1101:ARG:HH21	1:C:1115:LEU:HG	1.81	0.45
1:C:1730:MET:SD	1:C:1772:ARG:NH1	2.90	0.45
1:C:3801:GLY:HA2	1:C:3804:ILE:HG22	1.99	0.45
1:C:3842:LEU:HD21	1:C:3954:ALA:HB2	1.99	0.45
1:A:723:THR:H	1:A:726:VAL:HG12	1.82	0.45
1:A:2012:PHE:HB3	1:A:2021:CYS:HA	1.99	0.45
1:A:3937:TYR:O	1:A:4002:LYS:NZ	2.50	0.45
1:A:4926:VAL:HG12	1:A:4927:ILE:CD1	2.47	0.45
1:B:1000:ARG:O	1:B:1005:TRP:N	2.50	0.45
1:B:2734:ASN:HB3	1:B:2735:PHE:H	1.59	0.45
1:B:2781:VAL:HG22	1:B:2789:PRO:HD2	1.99	0.45
1:D:1857:GLU:HA	1:D:1860:LYS:HE2	1.98	0.45
1:D:2794:TYR:HA	1:D:2797:PHE:HD2	1.82	0.45
1:D:4024:VAL:HG13	1:D:4142:ASN:ND2	2.32	0.45
1:D:4101:LYS:HG3	1:C:4731:ILE:HA	1.98	0.45
1:D:4705:VAL:HG22	1:D:4711:PHE:HD1	1.82	0.45
1:C:213:TYR:CG	1:C:337:PRO:HB2	2.51	0.45
1:C:3779:VAL:HG23	1:C:3797:THR:HG22	1.99	0.45
1:C:3845:ASN:O	1:C:3849:ARG:HG2	2.17	0.45
1:C:4922:PHE:CD2	1:C:4922:PHE:O	2.70	0.45
1:A:179:TYR:HB3	1:A:197:GLN:HB2	1.99	0.44
1:A:3808:GLY:HA2	1:A:3893:GLU:OE2	2.17	0.44
1:B:495:ASN:HD21	1:B:550:LYS:HB3	1.82	0.44
1:B:1119:GLU:HB3	1:B:1134:LEU:HD11	2.00	0.44
1:B:1935:VAL:O	1:B:1939:MET:HG2	2.17	0.44
1:B:4183:ILE:HD13	1:B:5010:VAL:HG21	1.99	0.44
1:D:134:ASP:N	1:D:134:ASP:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:592:LYS:O	1:D:1594:ARG:HB2	2.16	0.44
1:D:1622:GLU:HA	1:D:1626:TRP:CD2	2.52	0.44
1:D:1867:GLU:O	1:D:1871:PHE:N	2.37	0.44
1:D:2191:PHE:HZ	1:D:2239:PHE:HA	1.82	0.44
1:D:2781:VAL:HG22	1:D:2789:PRO:HD2	1.99	0.44
1:C:313:SER:HB2	1:C:350:HIS:CE1	2.52	0.44
1:C:614:VAL:O	1:C:618:GLN:NE2	2.50	0.44
1:C:1840:PRO:HB3	1:C:1843:LYS:HD3	1.98	0.44
1:C:4812:HIS:O	1:C:4816:ILE:HG12	2.17	0.44
1:A:78:LEU:HD11	1:A:147:TRP:CG	2.52	0.44
1:A:1237:TRP:HH2	1:A:1652:GLU:HA	1.81	0.44
1:A:1661:ARG:HA	1:A:1661:ARG:HD2	1.85	0.44
1:A:3729:MET:HG3	1:A:3770:LEU:CD1	2.42	0.44
1:B:213:TYR:CD1	1:B:337:PRO:HB2	2.52	0.44
1:B:3765:TYR:CE1	1:B:4750:ILE:HG22	2.41	0.44
1:B:4869:GLU:CD	1:B:4869:GLU:N	2.71	0.44
1:B:4958:CYS:SG	1:B:4978:HIS:HD2	2.37	0.44
1:D:615:ARG:NH2	1:D:1677:GLY:O	2.48	0.44
1:D:2165:LEU:HD13	1:D:2178:MET:HB3	1.97	0.44
1:D:4868:ASP:HB3	1:D:4869:GLU:H	1.66	0.44
1:C:543:ASN:O	1:C:547:VAL:HG23	2.17	0.44
1:C:4550:LYS:HA	1:C:4553:ASN:HD21	1.81	0.44
1:A:35:LEU:HD23	1:A:49:LEU:HD22	2.00	0.44
1:A:1738:LEU:HD11	1:A:1963:GLU:HG3	1.99	0.44
1:A:4865:LYS:CE	1:A:4865:LYS:CA	2.96	0.44
1:B:35:LEU:HD23	1:B:49:LEU:HD22	1.99	0.44
1:B:119:SER:OG	1:B:120:CYS:N	2.50	0.44
1:B:294:THR:HG23	1:B:295:GLU:N	2.32	0.44
1:B:693:SER:N	1:B:694:PRO:HD2	2.33	0.44
1:B:1736:VAL:HG21	1:B:1956:GLU:HG3	1.99	0.44
1:B:4158:PRO:HA	1:B:4161:ARG:HD3	1.98	0.44
1:D:4205:TRP:O	1:D:4205:TRP:CG	2.70	0.44
1:D:4865:LYS:HD3	1:D:4866:SER:N	2.32	0.44
1:C:150:MET:HE1	1:C:163:VAL:HG11	1.98	0.44
1:C:751:SER:OG	1:C:752:VAL:N	2.50	0.44
1:C:758:ARG:HG2	1:C:759:ILE:O	2.18	0.44
1:C:1851:MET:HB2	1:C:1853:ILE:HG12	1.98	0.44
1:C:2794:TYR:HA	1:C:2797:PHE:HD2	1.82	0.44
1:C:3763:LEU:C	1:C:3763:LEU:CD1	2.85	0.44
1:A:3670:GLU:OE1	1:A:3670:GLU:N	2.44	0.44
1:A:3767:GLN:HG3	1:A:3809:ASN:ND2	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:VAL:HG12	1:B:261:ARG:HB2	2.00	0.44
1:B:795:GLY:H	1:B:811:CYS:HB2	1.83	0.44
1:B:4142:ASN:HA	1:B:4145:VAL:HG12	1.99	0.44
1:B:4654:ALA:O	1:B:4658:ILE:HG12	2.17	0.44
1:D:1931:LEU:HD22	1:D:1935:VAL:HG11	1.99	0.44
1:C:629:ARG:HD2	1:C:634:GLN:HG2	1.98	0.44
1:C:1736:VAL:HG21	1:C:1956:GLU:HG3	2.00	0.44
1:C:2348:GLU:HG2	1:C:3849:ARG:HE	1.81	0.44
1:C:4219:PHE:CZ	1:C:4946:GLN:OE1	2.70	0.44
1:B:1158:ASN:HB3	1:B:1182:ILE:HG13	1.99	0.44
1:B:4631:PHE:HE2	1:B:4640:GLU:HA	1.83	0.44
1:B:4895:GLY:O	1:C:4892:ARG:CG	2.65	0.44
1:D:181:HIS:N	1:D:192:ASP:O	2.49	0.44
1:D:2236:LEU:HB3	1:D:2275:VAL:HG21	2.00	0.44
1:C:312:THR:OG1	1:C:313:SER:N	2.51	0.44
1:C:723:THR:H	1:C:726:VAL:HG12	1.82	0.44
1:A:1000:ARG:O	1:A:1005:TRP:N	2.50	0.44
1:A:3772:THR:HG23	1:A:3773:ARG:N	2.32	0.44
1:A:4850:LEU:CD1	1:B:4814:LEU:HD22	2.48	0.44
1:B:668:VAL:O	1:B:741:GLU:N	2.50	0.44
1:D:299:LEU:HG	1:D:378:LEU:HG	1.99	0.44
1:D:426:ARG:NE	1:D:505:GLU:O	2.45	0.44
1:D:4662:ASN:O	1:D:4666:VAL:HB	2.18	0.44
1:C:138:GLN:HG2	1:C:139:GLU:N	2.33	0.44
1:C:219:VAL:HG12	1:C:261:ARG:HB2	1.99	0.44
1:C:675:LEU:HD12	1:C:675:LEU:HA	1.89	0.44
1:C:1961:PHE:HA	1:C:1964:ARG:HG2	2.00	0.44
1:C:2159:LEU:HD22	1:C:2201:LEU:HD23	2.00	0.44
1:C:4095:LYS:HB3	1:C:4095:LYS:HE2	1.68	0.44
1:A:1225:PRO:HG2	1:A:1228:ILE:HB	1.99	0.44
1:A:2115:GLU:H	1:A:2115:GLU:CD	2.20	0.44
1:A:3775:ALA:O	1:A:3778:MET:HG3	2.17	0.44
1:B:312:THR:OG1	1:B:313:SER:N	2.51	0.44
1:B:455:PRO:HG3	1:B:467:LYS:HB3	1.99	0.44
1:B:723:THR:H	1:B:726:VAL:HG12	1.82	0.44
1:D:4666:VAL:N	1:D:4667:PRO:HD2	2.30	0.44
1:D:4818:MET:HE3	1:D:4818:MET:C	2.38	0.44
1:C:1077:ALA:HB3	1:C:1189:LEU:HD11	1.98	0.44
1:C:1239:SER:OG	1:C:1240:LYS:N	2.51	0.44
1:C:4702:ASP:HA	1:C:4778:TRP:HE1	1.83	0.44
1:C:4866:SER:O	1:C:4867:GLU:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:LYS:HD3	1:A:416:LYS:HA	1.78	0.44
1:A:1737:PRO:HD3	1:A:1771:LEU:HD21	2.00	0.44
1:A:4828:SER:HA	1:A:4831:THR:HG22	2.00	0.44
1:A:4928:LEU:HD22	1:A:4928:LEU:HA	1.78	0.44
1:B:214:VAL:HG22	1:B:341:TYR:HE1	1.83	0.44
1:B:2005:GLN:HE22	1:B:3641:LEU:HD22	1.83	0.44
1:B:2012:PHE:HB3	1:B:2021:CYS:HA	2.00	0.44
1:A:184:THR:HA	1:A:189:LEU:HG	2.00	0.44
1:A:1639:LEU:N	1:A:1648:MET:O	2.45	0.44
1:A:2781:VAL:HG22	1:A:2789:PRO:HD2	2.00	0.44
1:A:3773:ARG:HA	1:A:3815:LYS:HE3	1.97	0.44
1:B:109:LEU:HD23	1:B:148:TRP:HD1	1.82	0.44
1:B:3895:HIS:HE1	1:B:3970:GLN:HB3	1.82	0.44
1:B:4011:GLU:HG2	1:B:4012:LEU:HD12	1.99	0.44
1:B:4821:LYS:HG3	1:B:4822:THR:N	2.33	0.44
1:D:421:PHE:HE1	1:D:436:LEU:HD21	1.83	0.44
1:D:3720:TYR:HA	1:D:3723:MET:HB2	2.00	0.44
1:D:3903:LEU:HD12	1:D:3903:LEU:HA	1.88	0.44
1:D:4180:ARG:NH1	1:D:4981:GLU:HB3	2.33	0.44
1:D:4820:VAL:CG1	1:D:4823:LEU:H	2.31	0.44
1:C:273:HIS:CD2	1:C:337:PRO:HB3	2.53	0.44
1:C:693:SER:N	1:C:694:PRO:HD2	2.33	0.44
1:A:3845:ASN:O	1:A:3849:ARG:HG2	2.16	0.43
1:B:1961:PHE:HA	1:B:1964:ARG:HG2	2.00	0.43
1:D:20:VAL:HG11	1:D:202:MET:HB3	2.00	0.43
1:D:312:THR:OG1	1:D:313:SER:N	2.51	0.43
1:D:1689:VAL:HG13	1:D:1690:ASP:H	1.82	0.43
1:D:4011:GLU:HG2	1:D:4012:LEU:HD12	1.99	0.43
1:C:1839:VAL:HG13	1:C:1841:VAL:HG22	2.00	0.43
1:C:2734:ASN:HB3	1:C:2735:PHE:H	1.57	0.43
1:A:1119:GLU:HA	1:A:1133:HIS:CD2	2.53	0.43
1:A:2003:GLN:O	1:A:2007:ASN:ND2	2.51	0.43
1:B:670:GLU:H	1:B:740:PRO:HB3	1.83	0.43
1:B:1661:ARG:HD2	1:B:1661:ARG:HA	1.85	0.43
1:D:1158:ASN:HB3	1:D:1182:ILE:HG13	1.99	0.43
1:D:4037:ASN:HB2	1:D:5035:GLN:NE2	2.33	0.43
1:D:4960:ILE:HG12	1:D:4985:LEU:CD2	2.49	0.43
1:D:5000:GLU:HA	1:D:5003:HIS:ND1	2.34	0.43
1:C:294:THR:HG23	1:C:295:GLU:N	2.33	0.43
1:C:299:LEU:HG	1:C:378:LEU:HG	1.99	0.43
1:C:2766:TRP:HA	1:C:2769:ASP:OD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5017:ARG:HH21	1:C:5019:TRP:HE1	1.64	0.43
1:A:4642:ALA:HB1	1:A:4645:CYS:SG	2.59	0.43
1:B:233:ILE:HG22	1:B:257:ARG:HB3	2.00	0.43
1:B:615:ARG:NH2	1:B:1677:GLY:O	2.50	0.43
1:B:3663:LEU:N	1:B:3663:LEU:HD12	2.33	0.43
1:B:3765:TYR:HE2	1:B:3769:ARG:HH22	1.66	0.43
1:B:4654:ALA:HB2	1:B:4795:TYR:HE1	1.82	0.43
1:D:747:CYS:SG	1:D:756:SER:HB2	2.58	0.43
1:D:1118:ASP:OD1	1:D:1118:ASP:N	2.52	0.43
1:D:1961:PHE:HA	1:D:1964:ARG:HG2	2.01	0.43
1:D:4866:SER:HB3	1:D:4871:GLU:CD	2.38	0.43
1:C:252:VAL:HA	1:C:255:HIS:ND1	2.33	0.43
1:C:617:ASN:OD1	1:C:618:GLN:HG3	2.18	0.43
1:A:294:THR:HG23	1:A:295:GLU:N	2.32	0.43
1:A:664:PHE:HB2	1:A:746:CYS:HB2	2.01	0.43
1:A:721:LEU:HD12	1:A:721:LEU:HA	1.89	0.43
1:A:1119:GLU:HB3	1:A:1134:LEU:HD11	1.99	0.43
1:A:4235:VAL:HG21	1:A:5019:TRP:CH2	2.53	0.43
1:A:4687:TYR:OH	1:A:4699:GLY:O	2.30	0.43
1:B:1119:GLU:HA	1:B:1133:HIS:CD2	2.53	0.43
1:D:137:LEU:O	1:D:137:LEU:HD12	2.18	0.43
1:D:2348:GLU:HG3	1:D:3849:ARG:HH21	1.84	0.43
1:D:2874:MET:N	1:D:2874:MET:SD	2.92	0.43
1:D:4158:PRO:HA	1:D:4161:ARG:HD3	2.00	0.43
1:D:4177:TYR:HE2	1:D:4199:GLU:HB2	1.84	0.43
1:D:4572:ALA:O	1:D:4576:ILE:HG12	2.18	0.43
1:C:707:VAL:HG12	1:C:713:SER:HB2	2.00	0.43
1:C:1118:ASP:N	1:C:1118:ASP:OD1	2.51	0.43
1:C:3670:GLU:OE1	1:C:3670:GLU:N	2.44	0.43
1:C:3765:TYR:HH	1:C:4750:ILE:HG22	1.82	0.43
1:C:3887:PHE:O	1:C:3891:LEU:HG	2.18	0.43
1:A:181:HIS:CD2	1:A:196:MET:HB3	2.54	0.43
1:A:2248:ARG:HG3	1:A:2286:LEU:HD21	2.00	0.43
1:A:3821:LYS:O	1:A:3824:LYS:NZ	2.37	0.43
1:A:4865:LYS:O	1:A:4867:GLU:N	2.51	0.43
1:B:76:ARG:HB2	1:B:79:GLN:NE2	2.33	0.43
1:D:649:PHE:HB3	1:D:776:LEU:HD22	2.01	0.43
1:D:1000:ARG:O	1:D:1005:TRP:N	2.50	0.43
1:D:4020:GLN:HA	1:D:4023:MET:HE3	2.01	0.43
1:C:1000:ARG:O	1:C:1005:TRP:N	2.51	0.43
1:C:1580:PHE:CE2	1:C:1592:PRO:HG2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3965:LEU:HA	1:C:3968:TYR:CD1	2.53	0.43
1:B:719:LEU:HD22	1:B:735:GLN:HG2	2.01	0.43
1:B:1124:PHE:HE1	1:B:1139:PHE:HB3	1.84	0.43
1:B:3944:GLU:HG2	1:B:3947:GLY:H	1.83	0.43
1:D:614:VAL:O	1:D:618:GLN:NE2	2.51	0.43
1:D:3674:ILE:CD1	1:D:3769:ARG:HD2	2.43	0.43
1:D:4794:TRP:HA	1:D:4797:VAL:HG12	1.99	0.43
1:A:4671:PHE:HE1	1:A:4716:TRP:HB2	1.84	0.43
1:A:4904:PRO:HG3	1:A:4913:ARG:HH12	1.72	0.43
1:B:3957:VAL:O	1:B:3961:VAL:HG23	2.19	0.43
1:B:4586:PRO:HB3	1:B:4628:VAL:HG21	1.99	0.43
1:B:4935:LEU:HD23	1:B:4935:LEU:HA	1.72	0.43
1:D:119:SER:OG	1:D:120:CYS:N	2.50	0.43
1:D:664:PHE:CD2	1:D:746:CYS:HB2	2.53	0.43
1:D:693:SER:N	1:D:694:PRO:HD2	2.33	0.43
1:C:1720:LEU:HB2	1:C:1724:CYS:SG	2.58	0.43
1:C:4838:VAL:HA	1:C:4841:VAL:HG12	2.01	0.43
1:A:138:GLN:HG2	1:A:139:GLU:N	2.34	0.43
1:A:426:ARG:NE	1:A:505:GLU:O	2.42	0.43
1:A:2158:CYS:O	1:A:2162:ILE:HG12	2.19	0.43
1:A:4929:LEU:HD22	1:A:4929:LEU:HA	1.79	0.43
1:B:1580:PHE:CE2	1:B:1592:PRO:HG2	2.54	0.43
1:B:2766:TRP:HA	1:B:2769:ASP:OD2	2.18	0.43
1:D:2105:TRP:HB3	1:D:2120:MET:HE1	2.01	0.43
1:C:110:ARG:HA	1:C:117:TYR:HA	2.00	0.43
1:C:330:ASP:N	1:C:330:ASP:OD1	2.49	0.43
1:C:2005:GLN:HE22	1:C:3641:LEU:HD22	1.84	0.43
1:C:4716:TRP:CZ2	1:C:4996:ILE:HG21	2.54	0.43
1:A:213:TYR:CG	1:A:337:PRO:HB2	2.53	0.43
1:A:617:ASN:OD1	1:A:618:GLN:HG3	2.19	0.43
1:A:4716:TRP:CZ2	1:A:4996:ILE:HG12	2.54	0.43
1:B:138:GLN:HG2	1:B:139:GLU:N	2.33	0.43
1:B:670:GLU:OE2	1:B:788:LYS:HB2	2.18	0.43
1:B:1719:HIS:NE2	1:B:1802:ILE:HD11	2.34	0.43
1:B:2113:SER:O	1:B:2113:SER:OG	2.31	0.43
1:D:1580:PHE:CE2	1:D:1592:PRO:HG2	2.54	0.43
1:D:2030:ASP:N	1:D:2030:ASP:OD1	2.52	0.43
1:D:2766:TRP:HA	1:D:2769:ASP:OD2	2.19	0.43
1:C:142:THR:OG1	1:C:144:GLU:OE1	2.29	0.43
1:C:635:THR:HB	1:C:1639:LEU:HD23	2.00	0.43
1:C:2030:ASP:N	1:C:2030:ASP:OD1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2781:VAL:HG22	1:C:2789:PRO:HD2	2.00	0.43
1:C:4013:LEU:O	1:C:4017:LEU:HD23	2.18	0.43
1:C:4065:PHE:CZ	1:C:4132:PHE:HB2	2.53	0.43
1:C:4158:PRO:HA	1:C:4161:ARG:HD3	2.00	0.43
1:C:4705:VAL:HG22	1:C:4711:PHE:HD1	1.83	0.43
1:C:4922:PHE:O	1:C:4922:PHE:CG	2.70	0.43
1:A:580:GLU:HG2	1:A:583:ILE:HD11	2.00	0.43
1:A:1736:VAL:HG21	1:A:1956:GLU:HG3	2.00	0.43
1:A:1961:PHE:HA	1:A:1964:ARG:HG2	2.00	0.43
1:A:3760:LYS:HZ2	1:A:3760:LYS:CA	2.20	0.43
1:A:3927:GLN:HA	1:A:3930:ILE:HG22	2.00	0.43
1:B:293:LEU:HD13	1:B:298:GLY:N	2.33	0.43
1:B:527:ALA:HA	1:B:563:VAL:HG23	2.01	0.43
1:B:5036:LEU:HD12	1:B:5036:LEU:HA	1.91	0.43
1:D:3804:ILE:HG22	1:D:3805:LEU:HD12	2.00	0.43
1:A:719:LEU:N	1:A:719:LEU:HD23	2.33	0.42
1:A:2030:ASP:N	1:A:2030:ASP:OD1	2.51	0.42
1:B:181:HIS:NE2	1:B:183:SER:HB2	2.34	0.42
1:B:675:LEU:HD12	1:B:675:LEU:HA	1.89	0.42
1:B:1237:TRP:HH2	1:B:1652:GLU:HA	1.84	0.42
1:B:2030:ASP:OD1	1:B:2030:ASP:N	2.52	0.42
1:B:2291:GLN:HG3	1:B:2295:LEU:HG	2.00	0.42
1:B:2794:TYR:HA	1:B:2797:PHE:HD2	1.84	0.42
1:B:4921:PHE:CD1	1:B:4925:ILE:HG21	2.53	0.42
1:D:839:LEU:HD13	1:D:1075:PHE:CZ	2.54	0.42
1:C:695:TYR:O	1:C:697:GLY:N	2.49	0.42
1:C:1072:VAL:HG22	1:C:1195:GLY:HA2	1.99	0.42
1:A:2766:TRP:HA	1:A:2769:ASP:OD2	2.19	0.42
1:A:4060:LYS:NZ	1:A:4064:MET:HB3	2.34	0.42
1:B:1288:UNK:O	1:B:1598:GLN:N	2.45	0.42
1:B:3655:GLU:O	1:B:3658:LYS:HG2	2.19	0.42
1:B:4584:ASP:HA	1:B:4627:MET:HA	1.99	0.42
1:B:4865:LYS:CG	1:B:4875:LYS:HG3	2.48	0.42
1:D:299:LEU:HD23	1:D:299:LEU:HA	1.92	0.42
1:D:2335:LEU:HD22	1:D:2353:VAL:HG21	2.01	0.42
1:D:3767:GLN:NE2	1:D:3804:ILE:HA	2.18	0.42
1:D:3845:ASN:O	1:D:3849:ARG:HG2	2.18	0.42
1:D:4017:LEU:HD12	1:D:4139:ILE:HG13	2.02	0.42
1:C:2738:ARG:HD2	1:C:2819:TRP:HZ2	1.84	0.42
1:C:3964:SER:O	1:C:3968:TYR:CD1	2.72	0.42
1:C:4921:PHE:O	1:C:4925:ILE:HG22	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LEU:O	1:A:194:SER:OG	2.25	0.42
1:A:2794:TYR:HA	1:A:2797:PHE:HD2	1.85	0.42
1:A:3754:GLU:OE1	1:A:3754:GLU:CA	2.67	0.42
1:A:3906:GLN:HE22	1:A:3913:ILE:HB	1.83	0.42
1:A:5000:GLU:HA	1:A:5003:HIS:ND1	2.34	0.42
1:B:614:VAL:O	1:B:618:GLN:NE2	2.52	0.42
1:B:4889:VAL:HG12	1:B:4897:ILE:HG22	2.01	0.42
1:D:2773:ASN:OD1	1:D:2775:TRP:NE1	2.50	0.42
1:D:4998:LYS:HB3	1:D:5003:HIS:NE2	2.34	0.42
1:C:560:ILE:HA	1:C:563:VAL:HG12	2.01	0.42
1:C:1158:ASN:HB3	1:C:1182:ILE:HG13	2.00	0.42
1:C:2367:ALA:HB3	1:C:2379:ALA:HB2	2.00	0.42
1:C:4184:MET:HB2	1:C:4190:ILE:HG22	2.00	0.42
1:A:3965:LEU:HA	1:A:3968:TYR:CD1	2.55	0.42
1:A:4674:GLU:HG2	1:A:4715:TYR:HB2	2.02	0.42
1:B:252:VAL:HA	1:B:255:HIS:CG	2.54	0.42
1:B:1087:ARG:HB3	1:B:1223:PHE:CG	2.54	0.42
1:B:2890:LYS:HA	1:B:2890:LYS:HD2	1.81	0.42
1:B:3842:LEU:HD21	1:B:3954:ALA:HB2	2.00	0.42
1:B:4017:LEU:HA	1:B:4020:GLN:HE21	1.85	0.42
1:B:4235:VAL:HG21	1:B:5019:TRP:CH2	2.55	0.42
1:D:15:ARG:HG3	1:D:18:ASP:OD2	2.20	0.42
1:D:3992:PHE:HD2	1:D:3996:PHE:CE2	2.37	0.42
1:D:4222:VAL:HG11	1:D:4950:VAL:HG23	2.00	0.42
1:C:293:LEU:HD13	1:C:298:GLY:H	1.82	0.42
1:C:2737:PRO:HG3	1:C:2891:LYS:HD3	2.00	0.42
1:A:1992:ALA:O	1:A:1996:ARG:HG2	2.20	0.42
1:B:195:PHE:HE2	1:C:2361:PRO:HB3	1.84	0.42
1:B:650:VAL:HB	1:B:777:PHE:CD2	2.54	0.42
1:B:2215:LEU:HD23	1:B:2215:LEU:HA	1.89	0.42
1:B:2243:SER:OG	1:B:2244:ARG:N	2.52	0.42
1:B:4654:ALA:HB2	1:B:4795:TYR:CE1	2.54	0.42
1:C:839:LEU:HD13	1:C:1075:PHE:CZ	2.53	0.42
1:C:1661:ARG:HA	1:C:1661:ARG:HD2	1.85	0.42
1:C:3830:GLN:O	1:C:3833:GLN:HG2	2.19	0.42
1:C:3941:ASP:OD1	1:C:3941:ASP:N	2.49	0.42
1:A:580:GLU:HG3	1:A:620:LEU:HD22	2.02	0.42
1:A:1624:LEU:HD12	1:A:1624:LEU:HA	1.91	0.42
1:A:2737:PRO:HG3	1:A:2891:LYS:HD3	2.01	0.42
1:A:2810:LYS:HG2	1:A:2814:LYS:HE2	2.02	0.42
1:A:4040:ILE:O	1:A:4044:MET:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3809:ASN:O	1:B:3812:VAL:HG12	2.20	0.42
1:B:4552:LEU:HD12	1:B:4552:LEU:HA	1.90	0.42
1:B:4705:VAL:HG22	1:B:4711:PHE:HD1	1.84	0.42
1:D:719:LEU:O	1:D:720:HIS:CG	2.73	0.42
1:D:3988:ALA:O	1:D:3992:PHE:HD1	2.02	0.42
1:D:4679:ARG:NH1	1:D:5017:ARG:HD3	2.34	0.42
1:C:110:ARG:HH21	1:C:115:ARG:HB3	1.85	0.42
1:C:517:GLU:O	1:C:521:LEU:HD23	2.19	0.42
1:C:3888:LEU:HD13	1:C:3891:LEU:HD12	2.01	0.42
1:C:3901:ASN:OD1	1:C:3904:ARG:NH1	2.47	0.42
1:A:1622:GLU:HA	1:A:1626:TRP:CD2	2.54	0.42
1:A:1719:HIS:NE2	1:A:1802:ILE:HD11	2.34	0.42
1:A:2747:ILE:HD13	1:A:2814:LYS:HA	2.01	0.42
1:A:3835:LEU:HD21	1:A:3880:PHE:CZ	2.55	0.42
1:A:4705:VAL:HG22	1:A:4711:PHE:HD1	1.85	0.42
1:B:3771:HIS:O	1:B:3775:ALA:N	2.52	0.42
1:D:162:LYS:O	1:D:164:ARG:NH1	2.52	0.42
1:D:721:LEU:HB3	1:D:728:ARG:HB2	2.01	0.42
1:D:1649:ASP:OD1	1:D:1652:GLU:HB2	2.20	0.42
1:D:3771:HIS:HB3	1:D:3773:ARG:NH1	2.35	0.42
1:D:3989:VAL:HA	1:D:3992:PHE:HB2	2.00	0.42
1:D:4689:THR:HA	1:D:4732:PHE:CE2	2.55	0.42
1:C:2158:CYS:O	1:C:2162:ILE:HG12	2.20	0.42
1:C:4027:LEU:HA	1:C:4030:LEU:HG	2.02	0.42
1:A:614:VAL:O	1:A:618:GLN:NE2	2.53	0.42
1:A:1667:LEU:HD21	1:A:1710:GLY:HA3	2.00	0.42
1:A:1939:MET:N	1:A:1939:MET:SD	2.92	0.42
1:A:4180:ARG:HH21	1:A:4192:ARG:HD3	1.84	0.42
1:A:4960:ILE:HB	1:A:4983:HIS:CD2	2.55	0.42
1:B:416:LYS:HA	1:B:416:LYS:HD3	1.78	0.42
1:B:1720:LEU:HB2	1:B:1724:CYS:SG	2.60	0.42
1:B:2880:GLU:O	1:B:2884:ASN:ND2	2.53	0.42
1:B:4818:MET:SD	1:B:4818:MET:O	2.78	0.42
1:B:4925:ILE:O	1:B:4925:ILE:HD12	2.20	0.42
1:B:4940:PHE:O	1:B:4944:ARG:HB2	2.20	0.42
1:D:213:TYR:CG	1:D:337:PRO:HB2	2.54	0.42
1:D:1939:MET:N	1:D:1939:MET:SD	2.92	0.42
1:D:2142:TYR:CE2	1:D:2197:LEU:HB2	2.55	0.42
1:D:3655:GLU:O	1:D:3658:LYS:HG2	2.19	0.42
1:D:3965:LEU:HA	1:D:3968:TYR:CD1	2.54	0.42
1:D:4093:PHE:O	1:D:4097:MET:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2121:PHE:O	1:C:3725:TYR:OH	2.34	0.42
1:C:2126:ARG:HE	1:C:2126:ARG:HB3	1.73	0.42
1:A:293:LEU:HD13	1:A:298:GLY:N	2.34	0.42
1:A:719:LEU:HD22	1:A:736:HIS:C	2.40	0.42
1:A:1098:GLY:HA3	1:A:1198:GLN:HE22	1.85	0.42
1:A:3793:MET:O	1:A:3797:THR:OG1	2.26	0.42
1:B:277:GLY:HA2	1:B:315:CYS:SG	2.60	0.42
1:B:1098:GLY:HA3	1:B:1198:GLN:HE22	1.85	0.42
1:B:1225:PRO:HG2	1:B:1228:ILE:HB	2.00	0.42
1:B:1622:GLU:HA	1:B:1626:TRP:CD2	2.55	0.42
1:B:1867:GLU:O	1:B:1871:PHE:N	2.37	0.42
1:B:2292:GLU:H	1:B:2295:LEU:HG	1.85	0.42
1:B:2792:ARG:HD2	1:B:2796:THR:HG21	2.01	0.42
1:B:3535:UNK:O	1:B:3537:UNK:N	2.53	0.42
1:B:3804:ILE:HA	1:B:3804:ILE:HD13	1.93	0.42
1:B:3893:GLU:HG3	1:B:3894:GLY:N	2.34	0.42
1:D:1624:LEU:HD12	1:D:1624:LEU:HA	1.92	0.42
1:C:1095:VAL:HB	1:C:1199:VAL:HG13	2.02	0.42
1:C:2880:GLU:O	1:C:2884:ASN:ND2	2.52	0.42
1:C:3662:ILE:O	1:C:3664:THR:N	2.52	0.42
1:C:4978:HIS:O	1:C:4982:GLU:HB2	2.20	0.42
1:A:214:VAL:HG22	1:A:341:TYR:HE1	1.84	0.42
1:A:2175:GLU:O	1:A:2179:ILE:HG12	2.20	0.42
1:A:2182:ILE:O	1:A:2185:ILE:HG12	2.19	0.42
1:A:2881:ASN:HA	1:A:2884:ASN:ND2	2.35	0.42
1:A:3719:ASP:HB3	1:A:3722:TYR:HB3	2.01	0.42
1:B:20:VAL:HG11	1:B:202:MET:HB3	2.02	0.42
1:B:491:ILE:O	1:B:495:ASN:HB2	2.20	0.42
1:B:595:ARG:HH21	1:B:633:LEU:HD21	1.85	0.42
1:B:617:ASN:OD1	1:B:618:GLN:HG3	2.20	0.42
1:B:1143:TRP:HD1	1:B:1164:LEU:HD13	1.84	0.42
1:B:2158:CYS:O	1:B:2162:ILE:HG12	2.20	0.42
1:B:3965:LEU:HA	1:B:3968:TYR:CD1	2.55	0.42
1:B:4218:ILE:HD11	1:B:4985:LEU:HD11	2.01	0.42
1:D:664:PHE:CZ	1:D:779:PRO:HB3	2.55	0.42
1:D:695:TYR:O	1:D:697:GLY:N	2.48	0.42
1:D:1720:LEU:HB2	1:D:1724:CYS:SG	2.60	0.42
1:D:2871:LEU:HA	1:D:2874:MET:HG2	2.02	0.42
1:D:3662:ILE:O	1:D:3664:THR:N	2.52	0.42
1:D:3721:LEU:HD12	1:D:3722:TYR:N	2.35	0.42
1:D:3842:LEU:HD21	1:D:3954:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4892:ARG:NH1	1:C:4896:GLY:HA3	2.34	0.42
1:C:926:GLY:O	1:C:929:LEU:HG	2.20	0.42
1:C:3535:UNK:O	1:C:3537:UNK:N	2.53	0.42
1:C:3986:TRP:HA	1:C:3989:VAL:HG22	2.01	0.42
1:C:4549:VAL:O	1:C:4553:ASN:ND2	2.53	0.42
1:A:262:LEU:HB3	1:A:280:LEU:HD23	2.02	0.41
1:A:357:LEU:HD11	1:A:388:LEU:HD11	2.02	0.41
1:A:717:ASP:OD1	1:A:720:HIS:HB2	2.20	0.41
1:A:719:LEU:O	1:A:720:HIS:CG	2.73	0.41
1:A:2099:SER:O	1:A:2103:VAL:HG23	2.20	0.41
1:A:2330:ARG:HA	1:A:2330:ARG:HD2	1.81	0.41
1:A:2368:LEU:HD13	1:A:2376:LEU:HG	2.02	0.41
1:A:4095:LYS:HB3	1:A:4095:LYS:HE2	1.69	0.41
1:A:4184:MET:HB2	1:A:4190:ILE:HG22	2.01	0.41
1:B:482:GLY:O	1:B:484:LEU:HD12	2.18	0.41
1:B:647:ASN:HB3	1:B:822:ARG:NH1	2.35	0.41
1:B:717:ASP:OD1	1:B:720:HIS:HB2	2.20	0.41
1:B:1730:MET:SD	1:B:1772:ARG:NH1	2.93	0.41
1:B:2191:PHE:HZ	1:B:2239:PHE:HA	1.85	0.41
1:B:4572:ALA:O	1:B:4576:ILE:HG12	2.20	0.41
1:B:4936:ILE:HD12	1:B:4936:ILE:HA	1.79	0.41
1:D:138:GLN:HG2	1:D:139:GLU:H	1.85	0.41
1:D:1228:ILE:HG23	1:D:1229:ASN:N	2.34	0.41
1:D:1685:LEU:HD23	1:D:1718:ILE:HD12	2.02	0.41
1:D:2005:GLN:HE22	1:D:3641:LEU:HD22	1.85	0.41
1:D:3890:LEU:HA	1:D:3893:GLU:HB3	2.02	0.41
1:C:197:GLN:NE2	1:C:198:THR:O	2.53	0.41
1:C:322:LYS:HD2	1:C:322:LYS:HA	1.88	0.41
1:C:421:PHE:HE1	1:C:436:LEU:HD21	1.84	0.41
1:C:523:TYR:O	1:C:526:LEU:HG	2.20	0.41
1:C:1225:PRO:HG2	1:C:1228:ILE:HB	2.02	0.41
1:C:1622:GLU:HA	1:C:1626:TRP:CD2	2.55	0.41
1:C:1624:LEU:HD12	1:C:1624:LEU:HA	1.91	0.41
1:C:4093:PHE:O	1:C:4097:MET:HG2	2.19	0.41
1:C:4572:ALA:O	1:C:4576:ILE:HG12	2.20	0.41
1:C:4959:PHE:HE2	1:C:4985:LEU:HD21	1.84	0.41
1:C:4998:LYS:HB3	1:C:5003:HIS:NE2	2.35	0.41
1:A:20:VAL:HG11	1:A:202:MET:HB3	2.02	0.41
1:A:1186:ASP:OD1	1:A:1186:ASP:N	2.50	0.41
1:A:1689:VAL:HG13	1:A:1690:ASP:H	1.84	0.41
1:B:4040:ILE:O	1:B:4044:MET:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4063:ASP:OD2	1:B:4067:LYS:NZ	2.47	0.41
1:B:4878:ASP:O	1:B:4881:THR:OG1	2.29	0.41
1:B:4957:LYS:HA	1:B:4957:LYS:HD2	1.87	0.41
1:B:4993:MET:SD	1:B:4997:ASN:ND2	2.93	0.41
1:D:229:GLU:HG2	1:D:247:TYR:HB3	2.02	0.41
1:D:1288:UNK:O	1:D:1598:GLN:N	2.44	0.41
1:D:2737:PRO:HG3	1:D:2891:LYS:HD3	2.02	0.41
1:C:40:GLU:OE2	1:C:44:ASN:N	2.48	0.41
1:C:104:GLY:H	1:C:150:MET:HB3	1.85	0.41
1:C:181:HIS:CD2	1:C:196:MET:HB2	2.55	0.41
1:C:221:ARG:HB3	1:C:391:THR:HG22	2.02	0.41
1:C:688:LEU:HD21	1:C:777:PHE:HE1	1.83	0.41
1:C:1078:GLU:HG3	1:C:1237:TRP:HE1	1.85	0.41
1:C:2881:ASN:HA	1:C:2884:ASN:ND2	2.36	0.41
1:C:4010:ILE:HG13	1:C:4011:GLU:N	2.35	0.41
1:C:4031:LEU:HD23	1:C:4031:LEU:H	1.85	0.41
1:C:4946:GLN:O	1:C:4949:GLN:N	2.53	0.41
1:A:1574:PRO:HD2	1:A:1577:ALA:HB2	2.01	0.41
1:A:4577:LEU:HD11	1:A:4807:PHE:HD1	1.86	0.41
1:A:4794:TRP:HA	1:A:4797:VAL:HG12	2.02	0.41
1:A:4867:GLU:CG	1:A:4867:GLU:O	2.68	0.41
1:B:24:CYS:SG	1:B:35:LEU:HB2	2.60	0.41
1:B:1240:LYS:NZ	1:B:1242:LEU:HB3	2.35	0.41
1:B:4794:TRP:HA	1:B:4797:VAL:HG12	2.02	0.41
1:D:260:TRP:CZ3	1:D:284:HIS:HD2	2.38	0.41
1:D:3723:MET:HE1	1:D:3793:MET:HA	2.02	0.41
1:D:3927:GLN:O	1:D:3930:ILE:HG22	2.20	0.41
1:C:564:LEU:HA	1:C:567:VAL:HG12	2.02	0.41
1:C:670:GLU:H	1:C:740:PRO:HB3	1.85	0.41
1:C:710:ASP:OD1	1:C:713:SER:OG	2.31	0.41
1:C:750:LEU:HD21	1:C:777:PHE:HE2	1.85	0.41
1:C:3655:GLU:O	1:C:3658:LYS:HG2	2.20	0.41
1:A:1847:THR:O	1:A:1850:VAL:HG12	2.19	0.41
1:B:70:GLU:HG2	1:B:108:LEU:HD23	2.03	0.41
1:B:505:GLU:HA	1:B:511:ALA:HB3	2.01	0.41
1:B:4207:MET:HE1	1:B:4209:GLN:HB3	2.03	0.41
1:B:4577:LEU:HD11	1:B:4807:PHE:CD1	2.55	0.41
1:B:4966:ASP:N	1:B:4966:ASP:OD1	2.53	0.41
1:D:76:ARG:H	1:D:76:ARG:HD3	1.86	0.41
1:D:1719:HIS:NE2	1:D:1802:ILE:HD11	2.35	0.41
1:D:3996:PHE:HA	1:D:3999:MET:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1749:PRO:HA	1:C:1750:PRO:HD3	1.96	0.41
1:C:1931:LEU:HD22	1:C:1935:VAL:HG11	2.03	0.41
1:C:1992:ALA:O	1:C:1996:ARG:HG2	2.19	0.41
1:C:4863:TYR:CE2	1:C:4876:CYS:SG	3.13	0.41
1:C:4966:ASP:OD1	1:C:4966:ASP:N	2.54	0.41
1:A:299:LEU:HG	1:A:378:LEU:HG	2.02	0.41
1:A:4037:ASN:HB2	1:A:5035:GLN:NE2	2.35	0.41
1:A:4550:LYS:HA	1:A:4553:ASN:HD21	1.86	0.41
1:A:4679:ARG:NH1	1:A:5017:ARG:HD3	2.35	0.41
1:A:4869:GLU:O	1:A:4870:ASP:O	2.38	0.41
1:B:2099:SER:O	1:B:2103:VAL:HG23	2.21	0.41
1:B:2182:ILE:O	1:B:2185:ILE:HG12	2.19	0.41
1:B:2287:ALA:HA	1:B:2290:LEU:HG	2.01	0.41
1:B:2775:TRP:CE2	1:B:2786:LYS:HE3	2.56	0.41
1:B:3406:UNK:O	1:B:3410:UNK:N	2.54	0.41
1:D:926:GLY:O	1:D:929:LEU:HG	2.20	0.41
1:D:2099:SER:O	1:D:2103:VAL:HG23	2.21	0.41
1:D:4674:GLU:HG2	1:D:4715:TYR:HB2	2.02	0.41
1:C:221:ARG:NH1	1:C:253:CYS:O	2.46	0.41
1:C:686:TRP:CZ3	1:C:777:PHE:HB3	2.54	0.41
1:C:4223:ASN:ND2	1:C:4946:GLN:CD	2.74	0.41
1:A:2252:ASP:N	1:A:2252:ASP:OD1	2.53	0.41
1:A:2606:UNK:O	1:A:2608:UNK:N	2.53	0.41
1:B:149:THR:CG2	1:B:151:HIS:HE1	2.33	0.41
1:B:515:TRP:HA	1:B:518:ILE:HG22	2.03	0.41
1:B:517:GLU:O	1:B:521:LEU:HD23	2.20	0.41
1:B:1083:VAL:HG21	1:B:1088:TRP:NE1	2.35	0.41
1:B:1574:PRO:HD2	1:B:1577:ALA:HB2	2.01	0.41
1:B:1649:ASP:OD1	1:B:1652:GLU:HB2	2.20	0.41
1:B:2881:ASN:HA	1:B:2884:ASN:ND2	2.35	0.41
1:B:3644:LEU:HG	1:B:3645:PRO:HD2	2.03	0.41
1:B:4553:ASN:HA	1:B:4556:SER:HB3	2.02	0.41
1:B:4821:LYS:CG	1:B:4822:THR:N	2.83	0.41
1:B:4872:PRO:CD	1:B:4873:ASP:H	2.34	0.41
1:D:1667:LEU:HD12	1:D:1714:LEU:HD12	2.02	0.41
1:D:1854:PHE:HD1	1:D:1858:ASP:HB3	1.85	0.41
1:D:4181:ILE:HG12	1:D:4195:PHE:CE1	2.55	0.41
1:C:705:ASN:ND2	1:C:709:ASP:OD2	2.53	0.41
1:C:873:LYS:HA	1:C:873:LYS:HD3	1.93	0.41
1:C:3644:LEU:HG	1:C:3645:PRO:HD2	2.02	0.41
1:A:4093:PHE:O	1:A:4097:MET:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4572:ALA:O	1:A:4576:ILE:HG12	2.20	0.41
1:B:926:GLY:O	1:B:929:LEU:HG	2.20	0.41
1:B:4068:LEU:O	1:B:4071:ILE:HG22	2.20	0.41
1:D:648:ILE:HD13	1:D:779:PRO:HG2	2.02	0.41
1:D:2880:GLU:O	1:D:2884:ASN:ND2	2.53	0.41
1:D:3406:UNK:O	1:D:3410:UNK:N	2.54	0.41
1:D:4091:LYS:HD3	1:D:4091:LYS:HA	1.91	0.41
1:C:2890:LYS:HA	1:C:2890:LYS:HD2	1.80	0.41
1:C:3843:ASP:HB3	1:C:3846:ALA:HB3	2.03	0.41
1:A:517:GLU:O	1:A:521:LEU:HD23	2.20	0.41
1:A:1087:ARG:HB3	1:A:1223:PHE:CG	2.56	0.41
1:A:4207:MET:HE1	1:A:4209:GLN:HB3	2.03	0.41
1:D:1101:ARG:HH21	1:D:1115:LEU:HG	1.85	0.41
1:D:1658:ASP:OD1	1:D:1658:ASP:N	2.54	0.41
1:D:2368:LEU:HD13	1:D:2376:LEU:HD21	2.03	0.41
1:D:3941:ASP:OD1	1:D:3941:ASP:N	2.46	0.41
1:D:4207:MET:HE1	1:D:4210:VAL:HG23	2.02	0.41
1:C:24:CYS:SG	1:C:35:LEU:HB2	2.60	0.41
1:C:1087:ARG:HD3	1:C:1223:PHE:CE1	2.56	0.41
1:C:3668:SER:O	1:C:3672:ARG:NH2	2.46	0.41
1:C:3903:LEU:HD12	1:C:3903:LEU:HA	1.91	0.41
1:C:4798:MET:HB3	1:C:4812:HIS:NE2	2.35	0.41
1:C:4863:TYR:CD2	1:C:4876:CYS:SG	3.14	0.41
1:A:926:GLY:O	1:A:929:LEU:HG	2.20	0.41
1:A:1072:VAL:HG22	1:A:1195:GLY:HA2	2.02	0.41
1:A:2348:GLU:OE1	1:A:3849:ARG:NE	2.54	0.41
1:A:3406:UNK:O	1:A:3410:UNK:N	2.54	0.41
1:A:3535:UNK:O	1:A:3537:UNK:N	2.53	0.41
1:A:3760:LYS:HZ3	1:A:3760:LYS:CB	2.28	0.41
1:A:3761:GLN:OE1	1:A:3764:LEU:HG	2.21	0.41
1:A:4691:GLN:NE2	1:A:4692:PRO:HD2	2.36	0.41
1:A:4860:ARG:HD2	1:A:4861:LYS:N	2.36	0.41
1:B:77:ALA:HA	1:B:80:GLU:CD	2.40	0.41
1:B:1072:VAL:HG22	1:B:1195:GLY:HA2	2.02	0.41
1:B:1866:ILE:HG22	1:B:1866:ILE:O	2.21	0.41
1:B:2310:CYS:O	1:B:2314:LEU:HG	2.21	0.41
1:B:3889:GLN:HB2	1:B:3964:SER:HA	2.03	0.41
1:B:4020:GLN:O	1:B:4024:VAL:HG22	2.21	0.41
1:B:4691:GLN:NE2	1:B:4692:PRO:HD2	2.36	0.41
1:B:4918:ILE:HD13	1:B:4918:ILE:HA	1.89	0.41
1:B:4985:LEU:CB	2:B:5101:ACP:N1	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:617:ASN:OD1	1:D:618:GLN:HG3	2.20	0.41
1:D:1866:ILE:O	1:D:1866:ILE:HG22	2.21	0.41
1:D:2881:ASN:HA	1:D:2884:ASN:ND2	2.35	0.41
1:D:3535:UNK:O	1:D:3537:UNK:N	2.53	0.41
1:D:3809:ASN:O	1:D:3812:VAL:HG12	2.21	0.41
1:D:4031:LEU:HD23	1:D:4031:LEU:H	1.85	0.41
1:D:4065:PHE:CZ	1:D:4132:PHE:HB2	2.56	0.41
1:D:4937:ILE:HD11	1:C:4934:GLY:HA2	1.97	0.41
1:C:621:ILE:HD13	1:C:621:ILE:HA	1.92	0.41
1:C:649:PHE:HD1	1:C:776:LEU:HD13	1.86	0.41
1:C:956:PRO:HB2	1:C:958:THR:HG22	2.03	0.41
1:C:1039:LEU:HD23	1:C:1039:LEU:HA	1.85	0.41
1:C:2191:PHE:HZ	1:C:2239:PHE:HB2	1.86	0.41
1:C:2606:UNK:O	1:C:2608:UNK:N	2.54	0.41
1:C:3896:ASN:O	1:C:3896:ASN:ND2	2.51	0.41
1:C:4700:GLN:HE21	1:C:4703:ARG:HE	1.68	0.41
1:C:4859:PHE:HZ	1:C:4912:TYR:HD1	1.69	0.41
1:C:4929:LEU:O	1:C:4933:GLN:HB2	2.21	0.41
1:A:523:TYR:O	1:A:526:LEU:HG	2.21	0.41
1:A:695:TYR:O	1:A:697:GLY:N	2.48	0.41
1:A:705:ASN:ND2	1:A:709:ASP:OD2	2.53	0.41
1:A:1608:MET:HA	1:A:1609:PRO:HD3	1.97	0.41
1:A:3913:ILE:HD13	1:A:3913:ILE:HA	1.91	0.41
1:A:4049:VAL:HA	1:A:4163:PHE:HZ	1.86	0.41
1:B:19:GLU:HB2	1:B:206:CYS:HB3	2.02	0.41
1:B:4700:GLN:HE21	1:B:4703:ARG:HE	1.69	0.41
1:D:108:LEU:HD13	1:D:147:TRP:NE1	2.36	0.41
1:D:372:LEU:HD11	1:D:374:LYS:HZ2	1.85	0.41
1:D:551:LEU:HD21	1:D:589:LEU:HD22	2.03	0.41
1:D:2355:ARG:O	1:D:2358:ILE:HG22	2.21	0.41
1:C:464:LYS:HE3	1:C:464:LYS:HB2	1.96	0.41
1:C:1166:GLY:HA3	1:C:1216:ILE:HD13	2.03	0.41
1:C:3677:LEU:HD22	1:C:3697:PRO:HB2	2.02	0.41
1:C:3751:VAL:HG23	1:C:3755:GLU:HB3	2.03	0.41
1:A:1866:ILE:HG22	1:A:1866:ILE:O	2.21	0.40
1:A:2310:CYS:O	1:A:2314:LEU:HG	2.21	0.40
1:A:2880:GLU:O	1:A:2884:ASN:ND2	2.55	0.40
1:A:3986:TRP:HA	1:A:3989:VAL:HG22	2.02	0.40
1:B:614:VAL:HG12	1:B:2169:GLN:HG2	2.03	0.40
1:B:1118:ASP:OD1	1:B:1118:ASP:N	2.53	0.40
1:B:4027:LEU:HA	1:B:4030:LEU:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4674:GLU:HG2	1:B:4715:TYR:HB2	2.04	0.40
1:D:1225:PRO:HG2	1:D:1228:ILE:HB	2.03	0.40
1:D:1749:PRO:HA	1:D:1750:PRO:HD3	1.96	0.40
1:D:4160:LEU:HA	1:D:4163:PHE:HD1	1.86	0.40
1:D:4582:VAL:HG21	1:C:4860:ARG:NH1	2.35	0.40
1:D:4838:VAL:HA	1:D:4841:VAL:HG12	2.04	0.40
1:C:3406:UNK:O	1:C:3410:UNK:N	2.54	0.40
1:C:3712:GLU:O	1:C:3712:GLU:HG2	2.21	0.40
1:C:4662:ASN:O	1:C:4666:VAL:HB	2.21	0.40
1:A:661:LYS:HG2	1:A:749:ASP:HA	2.01	0.40
1:A:1676:LEU:HA	1:A:1725:ARG:HH22	1.86	0.40
1:A:3492:UNK:O	1:A:3495:UNK:O	2.40	0.40
1:A:4702:ASP:HA	1:A:4778:TRP:HE1	1.86	0.40
1:B:1929:MET:SD	1:B:1929:MET:N	2.94	0.40
1:B:2447:LYS:HD2	1:B:2447:LYS:HA	1.80	0.40
1:B:4068:LEU:HD12	1:B:4111:LEU:HD11	2.03	0.40
1:B:4865:LYS:HA	1:B:4865:LYS:CE	2.23	0.40
1:D:14:LEU:HD23	1:D:14:LEU:HA	1.86	0.40
1:D:573:GLU:O	1:D:577:ILE:HG12	2.20	0.40
1:D:595:ARG:HH21	1:D:633:LEU:HD21	1.87	0.40
1:D:635:THR:HB	1:D:1639:LEU:HD23	2.03	0.40
1:D:2878:LEU:HD13	1:D:2926:LEU:HD23	2.03	0.40
1:C:717:ASP:OD1	1:C:720:HIS:HB2	2.21	0.40
1:C:2175:GLU:O	1:C:2179:ILE:HG12	2.21	0.40
1:C:4011:GLU:HG2	1:C:4012:LEU:N	2.37	0.40
1:C:4055:VAL:HG22	1:C:4059:LEU:HG	2.02	0.40
1:A:82:LEU:HD21	1:A:143:GLY:C	2.41	0.40
1:A:1220:GLN:NE2	1:B:3527:UNK:O	2.47	0.40
1:A:1224:GLU:HG3	1:A:1225:PRO:HD2	2.04	0.40
1:A:3754:GLU:OE1	1:A:3754:GLU:HA	2.21	0.40
1:A:3887:PHE:CZ	1:A:3891:LEU:HD21	2.57	0.40
1:A:3935:TRP:HD1	1:D:76:ARG:NH1	2.14	0.40
1:B:584:LYS:HE3	1:B:584:LYS:HB2	1.88	0.40
1:B:2192:TYR:CD1	1:B:2242:ILE:HD13	2.56	0.40
1:B:4095:LYS:HB3	1:B:4095:LYS:HE2	1.69	0.40
1:B:4838:VAL:HA	1:B:4841:VAL:HG12	2.04	0.40
1:B:4859:PHE:HZ	1:B:4912:TYR:HD1	1.70	0.40
1:D:2158:CYS:O	1:D:2162:ILE:HG12	2.21	0.40
1:D:2386:ILE:HD13	1:D:2386:ILE:HA	1.92	0.40
1:D:2606:UNK:O	1:D:2608:UNK:N	2.54	0.40
1:D:3771:HIS:O	1:D:3775:ALA:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3835:LEU:HD21	1:D:3880:PHE:CZ	2.57	0.40
1:D:4920:PHE:CZ	1:D:4924:VAL:HG11	2.55	0.40
1:D:4937:ILE:CD1	1:C:4934:GLY:CA	2.95	0.40
1:C:28:VAL:HG11	1:C:189:LEU:HD21	2.03	0.40
1:C:1676:LEU:HA	1:C:1725:ARG:HH22	1.86	0.40
1:C:1731:LEU:HA	1:C:1772:ARG:HH12	1.86	0.40
1:C:4022:ASP:O	1:C:4025:VAL:HG12	2.20	0.40
1:C:4104:THR:OG1	1:C:4107:GLU:OE1	2.37	0.40
1:A:4869:GLU:HB3	1:A:4870:ASP:H	1.35	0.40
1:B:221:ARG:NH2	1:B:253:CYS:HA	2.33	0.40
1:B:2296:GLU:HA	1:B:2299:VAL:HG12	2.02	0.40
1:B:2606:UNK:O	1:B:2608:UNK:N	2.54	0.40
1:B:3887:PHE:O	1:B:3891:LEU:HG	2.22	0.40
1:D:523:TYR:O	1:D:526:LEU:HG	2.21	0.40
1:D:649:PHE:HD1	1:D:776:LEU:HD13	1.86	0.40
1:D:664:PHE:HD2	1:D:746:CYS:HB2	1.87	0.40
1:D:3887:PHE:CZ	1:D:3891:LEU:HD21	2.57	0.40
1:C:1128:ARG:HG3	1:C:1130:GLN:HG2	2.03	0.40
1:A:661:LYS:HB3	1:A:808:TYR:CD2	2.57	0.40
1:A:2191:PHE:HZ	1:A:2239:PHE:HB2	1.86	0.40
1:A:3804:ILE:HD13	1:A:3804:ILE:HA	1.92	0.40
1:A:4838:VAL:O	1:A:4841:VAL:HG12	2.21	0.40
1:A:4933:GLN:HE21	1:D:4930:ALA:HA	1.86	0.40
1:B:299:LEU:HD23	1:B:299:LEU:HA	1.91	0.40
1:B:652:ARG:HH11	1:B:773:LEU:HD12	1.87	0.40
1:B:695:TYR:O	1:B:697:GLY:N	2.51	0.40
1:B:1252:HIS:HE1	1:B:1254:HIS:CE1	2.40	0.40
1:B:2348:GLU:OE1	1:B:3849:ARG:NE	2.53	0.40
1:B:3771:HIS:HB3	1:B:3773:ARG:NH1	2.36	0.40
1:B:3778:MET:HA	1:B:3781:GLN:HG2	2.03	0.40
1:B:4716:TRP:CH2	1:B:4996:ILE:HG12	2.56	0.40
1:B:4936:ILE:HG22	1:B:4937:ILE:HD13	2.03	0.40
1:B:4998:LYS:HB3	1:B:5003:HIS:NE2	2.37	0.40
1:D:80:GLU:OE2	1:D:80:GLU:N	2.54	0.40
1:D:479:GLN:HE21	1:D:539:LEU:HD22	1.87	0.40
1:D:744:VAL:HG13	1:D:757:PHE:HE1	1.86	0.40
1:D:1139:PHE:HZ	1:D:1177:THR:HG22	1.87	0.40
1:D:2126:ARG:HE	1:D:2126:ARG:HB3	1.73	0.40
1:D:4142:ASN:HA	1:D:4145:VAL:HG12	2.04	0.40
1:D:4183:ILE:HG23	1:D:5021:PHE:HB2	2.04	0.40
1:D:4838:VAL:O	1:D:4841:VAL:HG12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:GLY:HA2	1:C:315:CYS:SG	2.62	0.40
1:C:3830:GLN:HA	1:C:3833:GLN:HG2	2.04	0.40
1:C:5031:GLN:HE21	1:C:5031:GLN:HB3	1.74	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	3191/5037 (63%)	2943 (92%)	243 (8%)	5 (0%)	47	81
1	B	3191/5037 (63%)	2934 (92%)	247 (8%)	10 (0%)	41	76
1	C	3191/5037 (63%)	2929 (92%)	254 (8%)	8 (0%)	41	76
1	D	3191/5037 (63%)	2932 (92%)	253 (8%)	6 (0%)	47	81
All	All	12764/20148 (63%)	11738 (92%)	997 (8%)	29 (0%)	50	81

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4866	SER
1	A	4870	ASP
1	B	3662	ILE
1	B	3666	ASP
1	B	4867	GLU
1	D	2292	GLU
1	D	3751	VAL
1	D	4867	GLU
1	C	2292	GLU
1	C	4870	ASP
1	C	4875	LYS
1	A	1708	ARG

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Mol	Chain	Res	Type
1	B	1708	ARG
1	B	3668	SER
1	B	4869	GLU
1	D	1708	ARG
1	C	1708	ARG
1	C	3685	GLU
1	C	4867	GLU
1	B	4868	ASP
1	B	3751	VAL
1	B	4866	SER
1	D	1840	PRO
1	B	1840	PRO
1	A	1840	PRO
1	C	1840	PRO
1	A	3774	GLY
1	D	4666	VAL
1	C	4666	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	2452/3264 (75%)	2421 (99%)	31 (1%)	69	82
1	B	2452/3264 (75%)	2419 (99%)	33 (1%)	69	82
1	C	2455/3264 (75%)	2425 (99%)	30 (1%)	71	84
1	D	2458/3264 (75%)	2431 (99%)	27 (1%)	73	85
All	All	9817/13056 (75%)	9696 (99%)	121 (1%)	72	84

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	275	ARG
1	A	719	LEU
1	A	822	ARG
1	A	830	ARG

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Mol	Chain	Res	Type
1	A	2773	ASN
1	A	3752	SER
1	A	3758	MET
1	A	3759	GLU
1	A	3760	LYS
1	A	3766	GLN
1	A	3769	ARG
1	A	3770	LEU
1	A	3771	HIS
1	A	4668	LEU
1	A	4859	PHE
1	A	4860	ARG
1	A	4861	LYS
1	A	4865	LYS
1	A	4867	GLU
1	A	4868	ASP
1	A	4921	PHE
1	A	4924	VAL
1	A	4925	ILE
1	A	4927	ILE
1	A	4928	LEU
1	A	4929	LEU
1	A	4931	ILE
1	A	4932	ILE
1	A	4933	GLN
1	A	4938	ASP
1	A	5031	GLN
1	B	76	ARG
1	B	151	HIS
1	B	275	ARG
1	B	822	ARG
1	B	3663	LEU
1	B	3664	THR
1	B	3666	ASP
1	B	3751	VAL
1	B	3758	MET
1	B	3760	LYS
1	B	3769	ARG
1	B	3773	ARG
1	B	3928	GLU
1	B	4000	MET
1	B	4180	ARG

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Mol	Chain	Res	Type
1	B	4795	TYR
1	B	4808	PHE
1	B	4809	PHE
1	B	4816	ILE
1	B	4861	LYS
1	B	4865	LYS
1	B	4867	GLU
1	B	4869	GLU
1	B	4923	PHE
1	B	4925	ILE
1	B	4935	LEU
1	B	4936	ILE
1	B	4937	ILE
1	B	4938	ASP
1	B	4943	LEU
1	B	4944	ARG
1	B	4957	LYS
1	B	5031	GLN
1	D	76	ARG
1	D	275	ARG
1	D	822	ARG
1	D	830	ARG
1	D	2355	ARG
1	D	3675	ASP
1	D	3676	ASP
1	D	3759	GLU
1	D	3773	ARG
1	D	4085	ARG
1	D	4820	VAL
1	D	4821	LYS
1	D	4861	LYS
1	D	4865	LYS
1	D	4867	GLU
1	D	4869	GLU
1	D	4871	GLU
1	D	4918	ILE
1	D	4928	LEU
1	D	4929	LEU
1	D	4931	ILE
1	D	4932	ILE
1	D	4933	GLN
1	D	4935	LEU

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Mol	Chain	Res	Type
1	D	4936	ILE
1	D	4985	LEU
1	D	5031	GLN
1	C	163	VAL
1	C	275	ARG
1	C	822	ARG
1	C	830	ARG
1	C	3755	GLU
1	C	3759	GLU
1	C	3760	LYS
1	C	3761	GLN
1	C	3773	ARG
1	C	3896	ASN
1	C	3928	GLU
1	C	3965	LEU
1	C	4180	ARG
1	C	4574	ASN
1	C	4719	PHE
1	C	4861	LYS
1	C	4863	TYR
1	C	4865	LYS
1	C	4868	ASP
1	C	4875	LYS
1	C	4923	PHE
1	C	4931	ILE
1	C	4932	ILE
1	C	4933	GLN
1	C	4936	ILE
1	C	4937	ILE
1	C	4938	ASP
1	C	4944	ARG
1	C	4946	GLN
1	C	5031	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	536	ASN
1	A	634	GLN
1	A	735	GLN
1	A	2095	GLN
1	A	4223	ASN

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Mol	Chain	Res	Type
1	A	4933	GLN
1	A	4946	GLN
1	B	536	ASN
1	B	634	GLN
1	B	3809	ASN
1	B	3927	GLN
1	B	4020	GLN
1	B	4574	ASN
1	B	5035	GLN
1	D	151	HIS
1	D	536	ASN
1	D	2180	GLN
1	D	3761	GLN
1	D	3767	GLN
1	D	3927	GLN
1	D	4574	ASN
1	C	536	ASN
1	C	2107	GLN
1	C	3761	GLN
1	C	4223	ASN
1	C	4574	ASN
1	C	4933	GLN
1	C	4946	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 9 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ACP	A	5101	4	27,33,33	1.35	5 (18%)	32,52,52	1.51	5 (15%)
2	ACP	B	5101	4	27,33,33	0.89	1 (3%)	32,52,52	0.84	2 (6%)
2	ACP	D	5101	4	27,33,33	1.37	5 (18%)	32,52,52	1.46	4 (12%)
2	ACP	C	5101	4	27,33,33	1.33	5 (18%)	32,52,52	1.50	4 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACP	A	5101	4	-	5/15/38/38	0/3/3/3
2	ACP	B	5101	4	-	8/15/38/38	0/3/3/3
2	ACP	D	5101	4	-	9/15/38/38	0/3/3/3
2	ACP	C	5101	4	-	7/15/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5101	ACP	PG-O3G	2.87	1.61	1.54
2	C	5101	ACP	PG-O3G	2.86	1.61	1.54
2	C	5101	ACP	PG-O2G	2.85	1.61	1.54
2	D	5101	ACP	PG-O3G	2.83	1.61	1.54
2	D	5101	ACP	PG-O2G	2.83	1.61	1.54
2	A	5101	ACP	PG-O2G	2.83	1.61	1.54
2	D	5101	ACP	PB-O3A	2.75	1.61	1.58
2	A	5101	ACP	PB-O3A	2.61	1.61	1.58
2	D	5101	ACP	C5-C4	2.49	1.47	1.40
2	B	5101	ACP	PB-O2B	-2.40	1.50	1.56
2	C	5101	ACP	PB-O3A	2.39	1.61	1.58
2	A	5101	ACP	C5-C4	2.31	1.47	1.40
2	C	5101	ACP	C5-C4	2.26	1.46	1.40
2	D	5101	ACP	PB-O2B	2.15	1.61	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5101	ACP	PB-O2B	2.14	1.61	1.56
2	C	5101	ACP	PB-O2B	2.12	1.61	1.56

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	5101	ACP	PB-O3A-PA	-4.14	119.42	132.56
2	A	5101	ACP	PB-O3A-PA	-4.07	119.65	132.56
2	D	5101	ACP	PB-O3A-PA	-3.87	120.27	132.56
2	A	5101	ACP	N3-C2-N1	-3.70	122.90	128.68
2	C	5101	ACP	N3-C2-N1	-3.65	122.98	128.68
2	D	5101	ACP	C3'-C2'-C1'	3.43	106.14	100.98
2	C	5101	ACP	C3'-C2'-C1'	3.33	105.99	100.98
2	A	5101	ACP	C3'-C2'-C1'	3.31	105.97	100.98
2	D	5101	ACP	N3-C2-N1	-3.20	123.68	128.68
2	D	5101	ACP	C4-C5-N7	-2.72	106.57	109.40
2	A	5101	ACP	C4-C5-N7	-2.52	106.77	109.40
2	C	5101	ACP	C4-C5-N7	-2.51	106.78	109.40
2	B	5101	ACP	O1G-PG-C3B	-2.28	106.32	111.24
2	B	5101	ACP	C5-C6-N6	2.26	123.79	120.35
2	A	5101	ACP	C2-N1-C6	2.05	122.25	118.75

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5101	ACP	C5'-O5'-PA-O1A
2	A	5101	ACP	C5'-O5'-PA-O3A
2	B	5101	ACP	PG-C3B-PB-O1B
2	B	5101	ACP	PG-C3B-PB-O3A
2	B	5101	ACP	C5'-O5'-PA-O2A
2	B	5101	ACP	C5'-O5'-PA-O3A
2	B	5101	ACP	C4'-C5'-O5'-PA
2	D	5101	ACP	PG-C3B-PB-O1B
2	D	5101	ACP	PG-C3B-PB-O3A
2	D	5101	ACP	C5'-O5'-PA-O1A
2	D	5101	ACP	C5'-O5'-PA-O2A
2	D	5101	ACP	C5'-O5'-PA-O3A
2	D	5101	ACP	C4'-C5'-O5'-PA
2	C	5101	ACP	PB-C3B-PG-O1G
2	C	5101	ACP	PB-C3B-PG-O2G
2	C	5101	ACP	PB-C3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
2	C	5101	ACP	PG-C3B-PB-O1B
2	C	5101	ACP	PG-C3B-PB-O2B
2	C	5101	ACP	PG-C3B-PB-O3A
2	B	5101	ACP	O4'-C4'-C5'-O5'
2	B	5101	ACP	C3'-C4'-C5'-O5'
2	C	5101	ACP	O4'-C4'-C5'-O5'
2	B	5101	ACP	PG-C3B-PB-O2B
2	D	5101	ACP	PG-C3B-PB-O2B
2	D	5101	ACP	C3'-C4'-C5'-O5'
2	A	5101	ACP	C4'-C5'-O5'-PA
2	A	5101	ACP	PG-C3B-PB-O1B
2	D	5101	ACP	O4'-C4'-C5'-O5'
2	A	5101	ACP	C3'-C4'-C5'-O5'

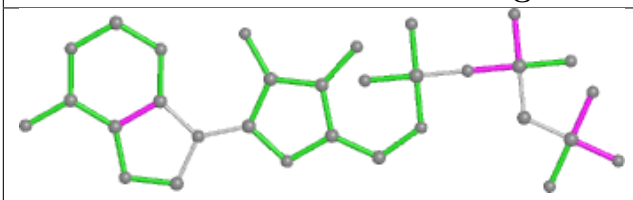
There are no ring outliers.

4 monomers are involved in 22 short contacts:

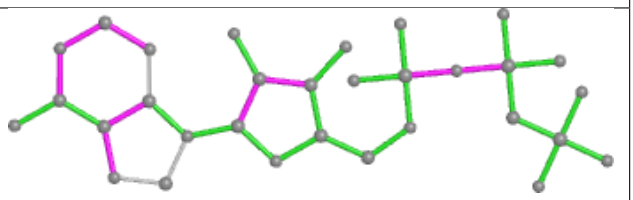
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5101	ACP	7	0
2	B	5101	ACP	4	0
2	D	5101	ACP	8	0
2	C	5101	ACP	3	0

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

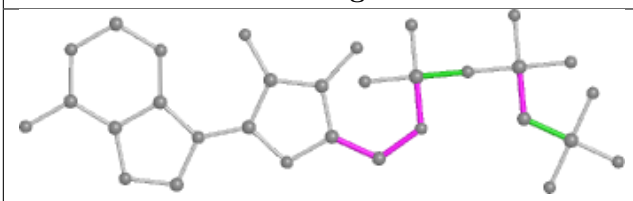
Ligand ACP A 5101



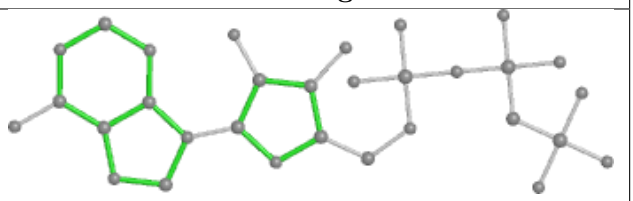
Bond lengths



Bond angles

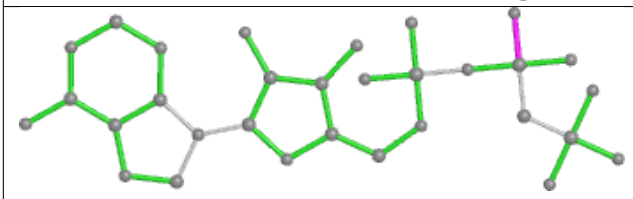


Torsions

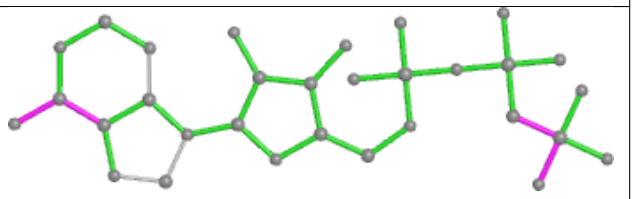


Rings

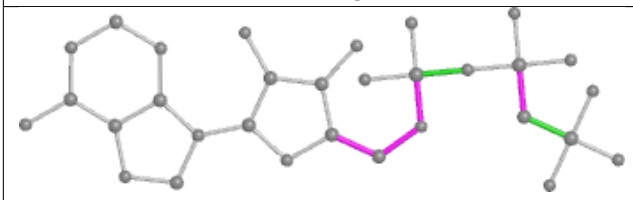
Ligand ACP B 5101



Bond lengths



Bond angles



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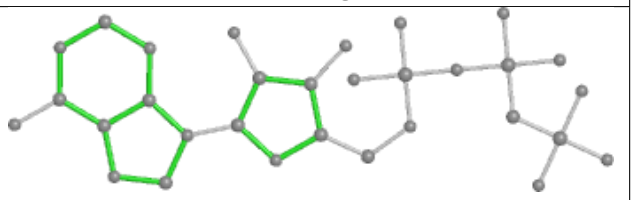
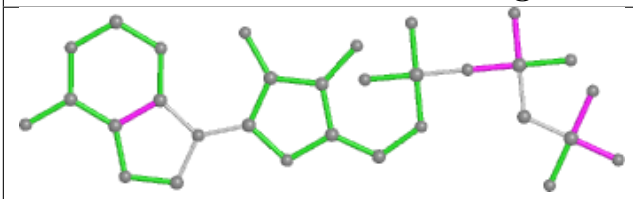
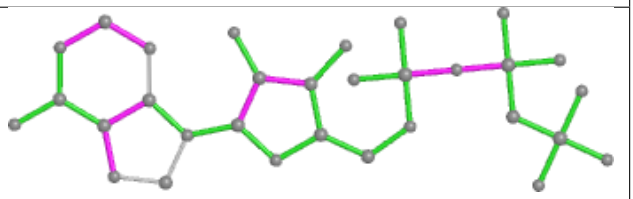


Rings

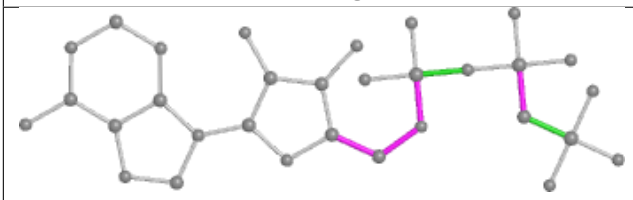
Ligand ACP D 5101



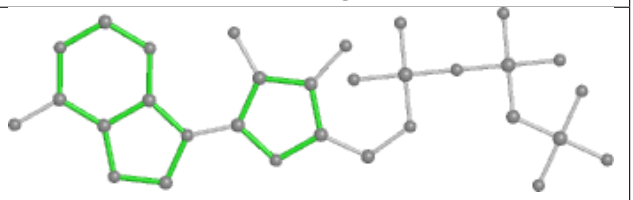
Bond lengths



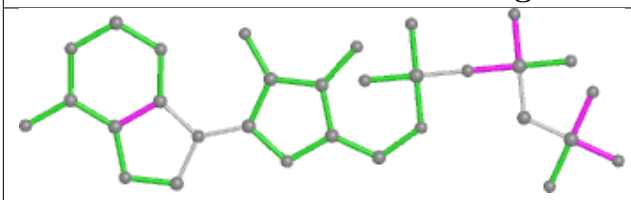
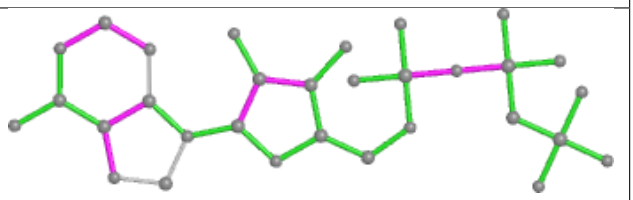
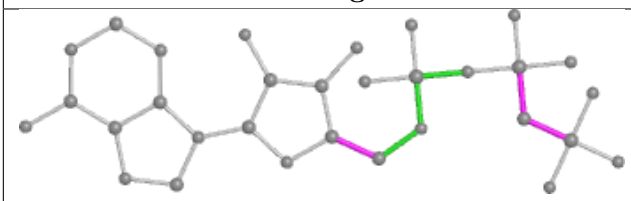
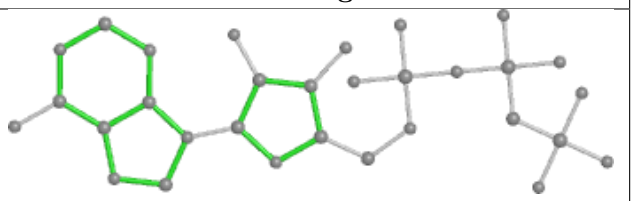
Bond angles



Torsions



Rings

Ligand ACP C 5101	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	6
1	B	6
1	C	6
1	A	6

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	3302:UNK	C	3303:UNK	N	17.16
1	B	3302:UNK	C	3303:UNK	N	17.15
1	C	3302:UNK	C	3303:UNK	N	17.10
1	A	3302:UNK	C	3303:UNK	N	17.01
1	A	3510:UNK	C	3511:UNK	N	16.97
1	C	3510:UNK	C	3511:UNK	N	16.95
1	B	3510:UNK	C	3511:UNK	N	16.94
1	D	3510:UNK	C	3511:UNK	N	16.94
1	A	3136:UNK	C	3137:UNK	N	13.76
1	C	3136:UNK	C	3137:UNK	N	13.74
1	B	3136:UNK	C	3137:UNK	N	13.71
1	D	3136:UNK	C	3137:UNK	N	13.71
1	A	3235:UNK	C	3236:UNK	N	12.12

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	3235:UNK	C	3236:UNK	N	11.05
1	D	3235:UNK	C	3236:UNK	N	11.02
1	B	3235:UNK	C	3236:UNK	N	11.01
1	B	3205:UNK	C	3206:UNK	N	5.74
1	D	3205:UNK	C	3206:UNK	N	5.73
1	C	3205:UNK	C	3206:UNK	N	5.67
1	A	3205:UNK	C	3206:UNK	N	5.65
1	C	1297:UNK	C	1298:UNK	N	5.21
1	A	1297:UNK	C	1298:UNK	N	5.20
1	B	1297:UNK	C	1298:UNK	N	5.20
1	D	1297:UNK	C	1298:UNK	N	5.19

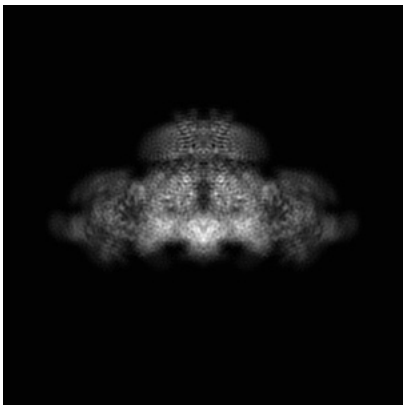
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22615. These allow visual inspection of the internal detail of the map and identification of artifacts.

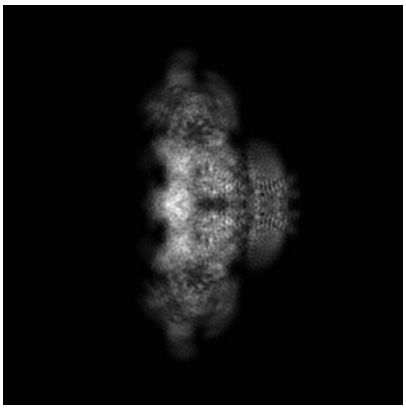
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

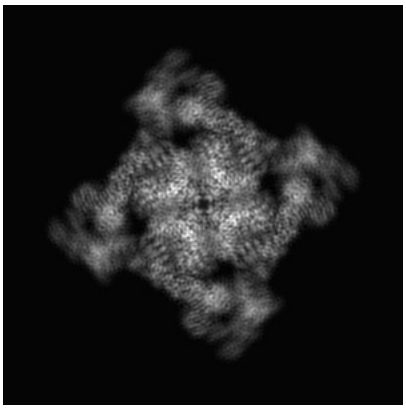
6.1.1 Primary map



X

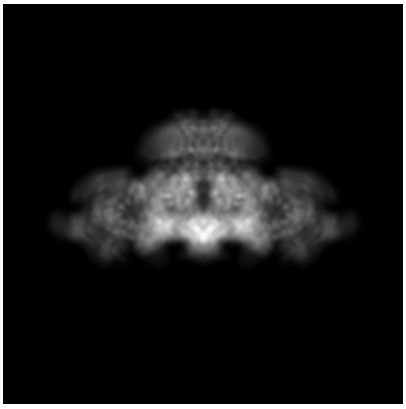


Y

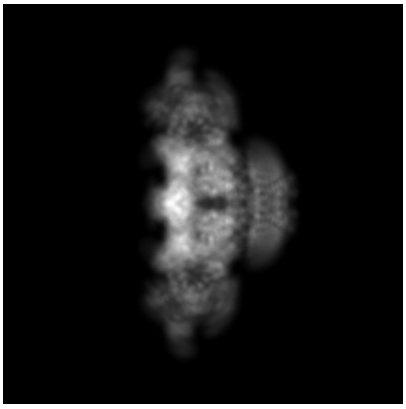


Z

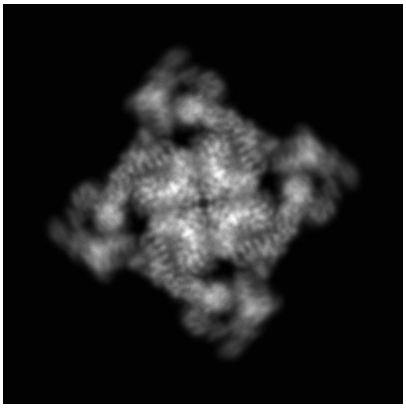
6.1.2 Raw map



X



Y

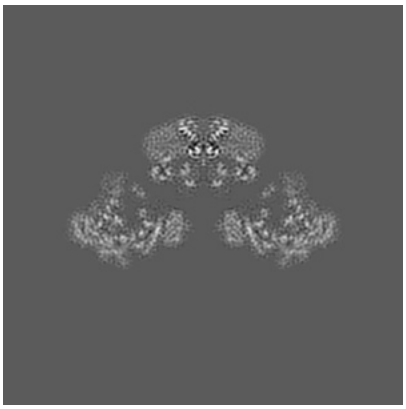


Z

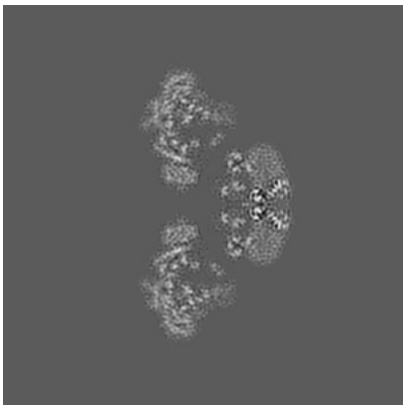
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



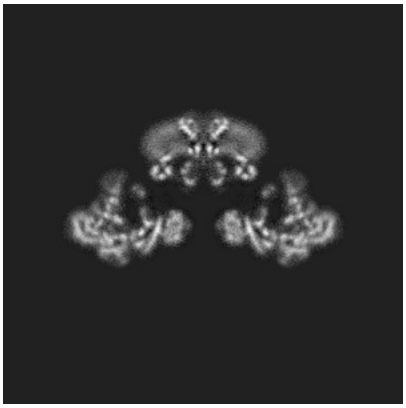
X Index: 176



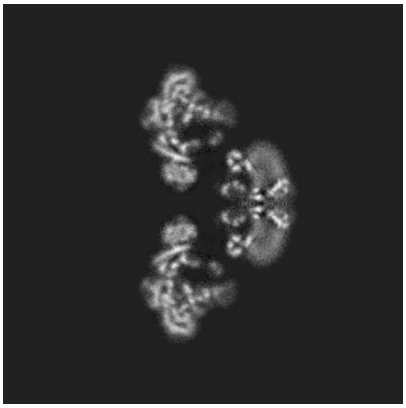
Y Index: 176

Z Index: 176

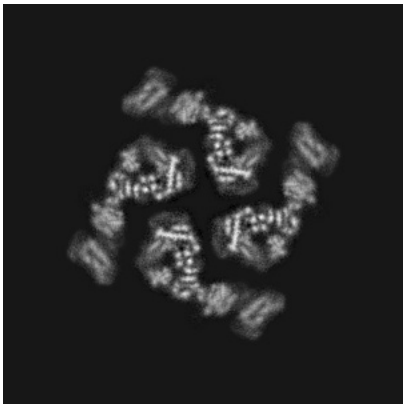
6.2.2 Raw map



X Index: 176



Y Index: 176

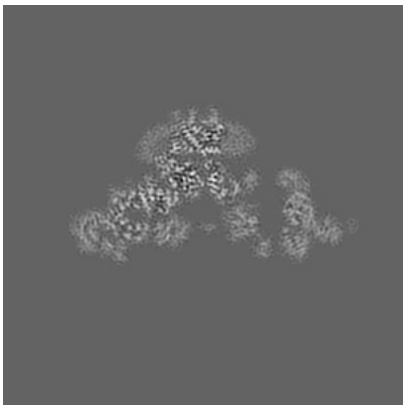


Z Index: 176

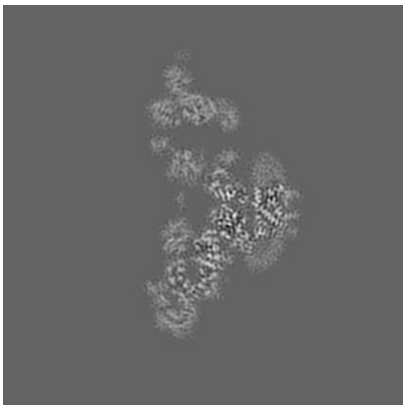
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

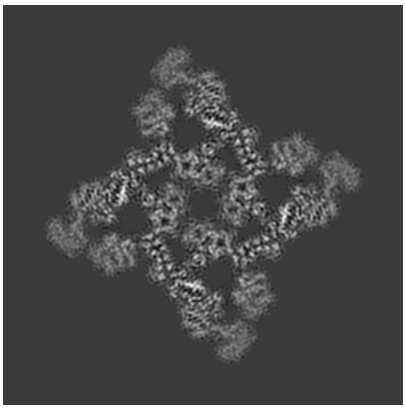
6.3.1 Primary map



X Index: 165

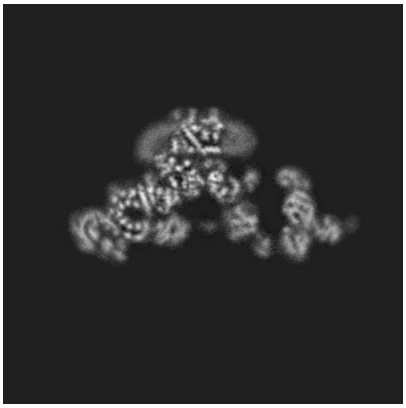


Y Index: 187

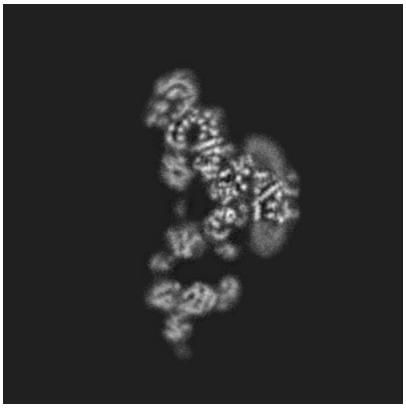


Z Index: 160

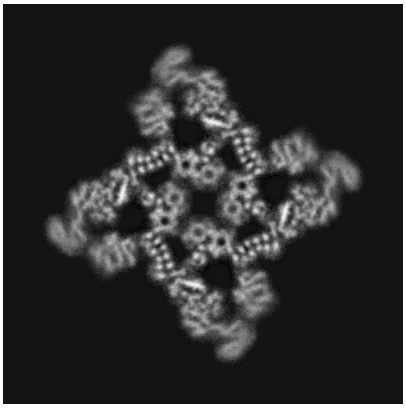
6.3.2 Raw map



X Index: 165



Y Index: 165

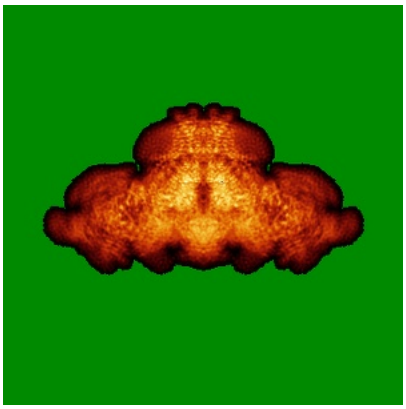


Z Index: 160

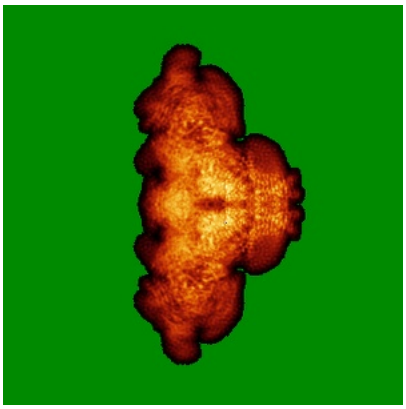
The images above show the largest variance slices of the map in three orthogonal directions.

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

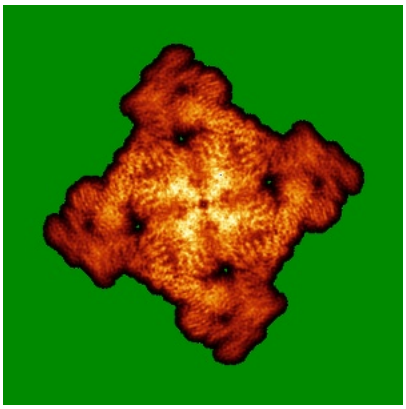
6.4.1 Primary map



X

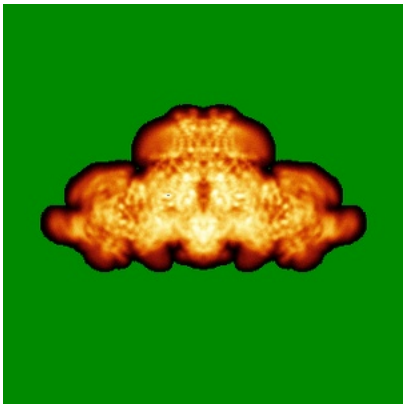


Y

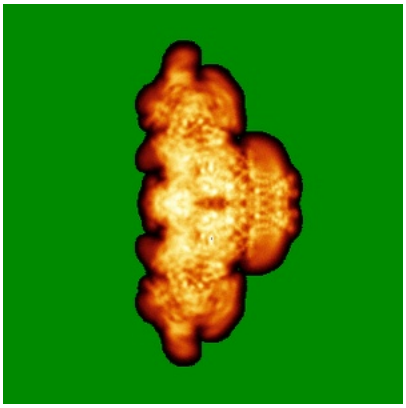


Z

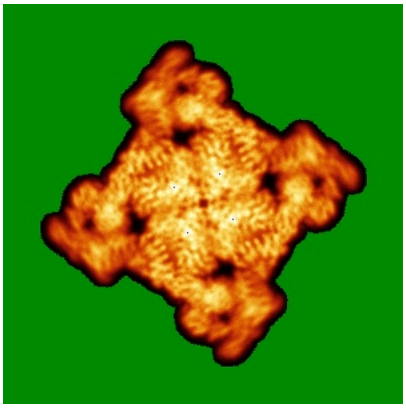
6.4.2 Raw map



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 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

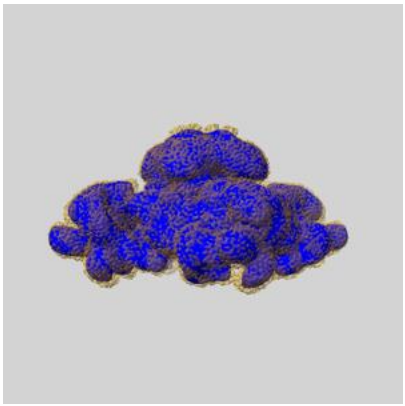
6.6 Mask visualisation

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

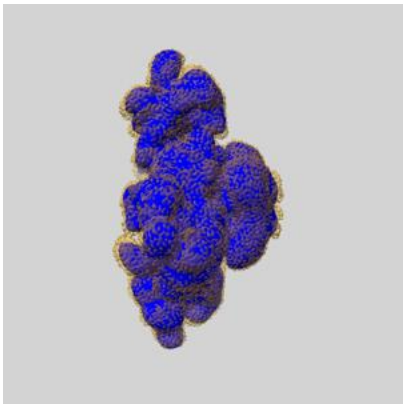
A mask typically either:

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

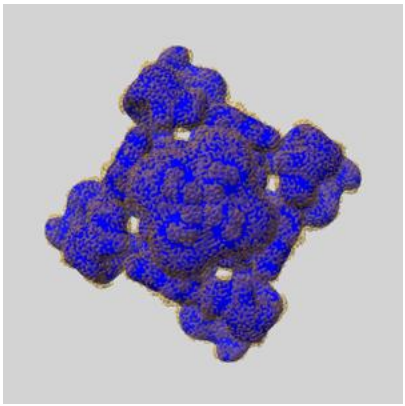
6.6.1 emd_22615_msk_1.map



X



Y

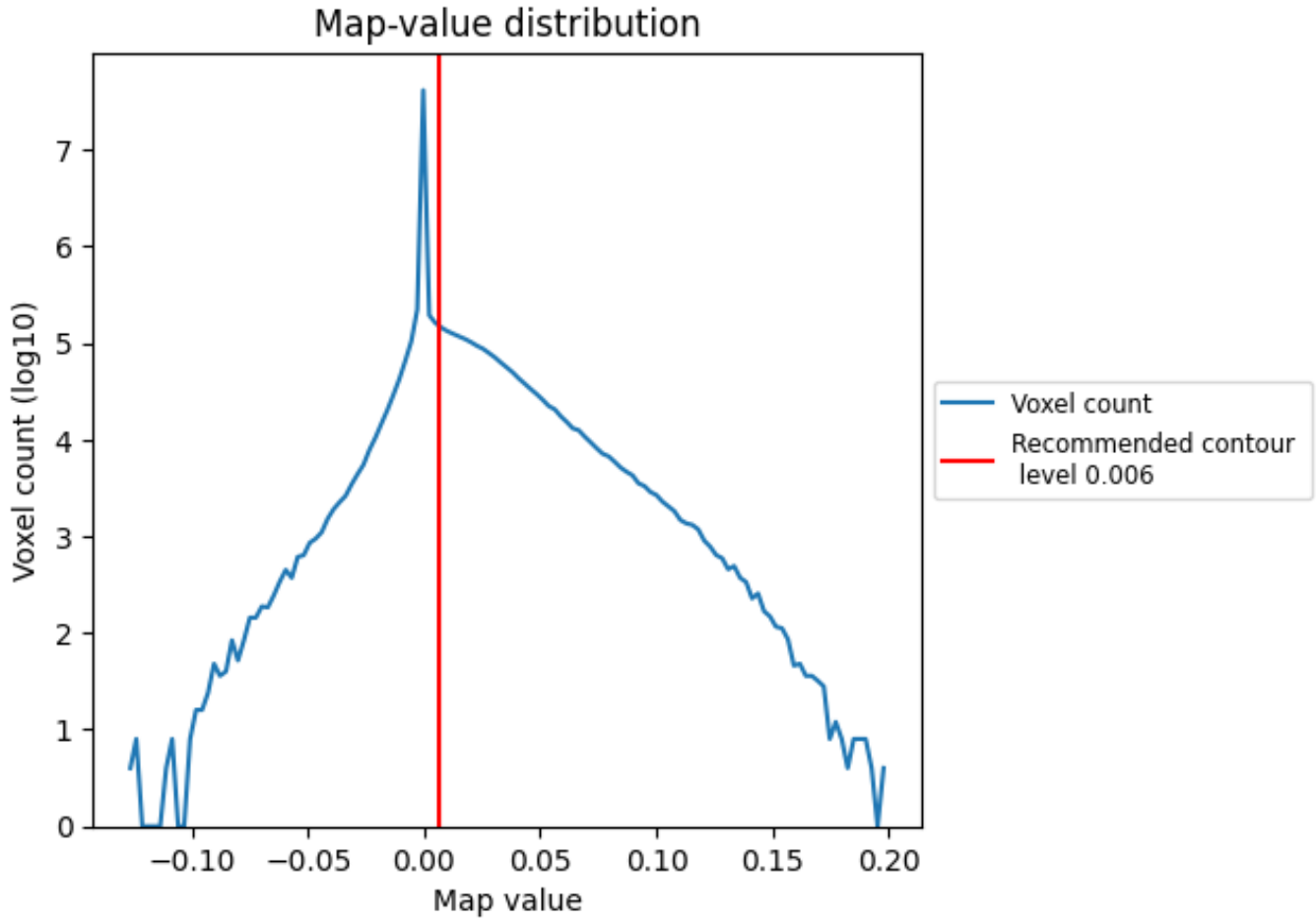


Z

7 Map analysis

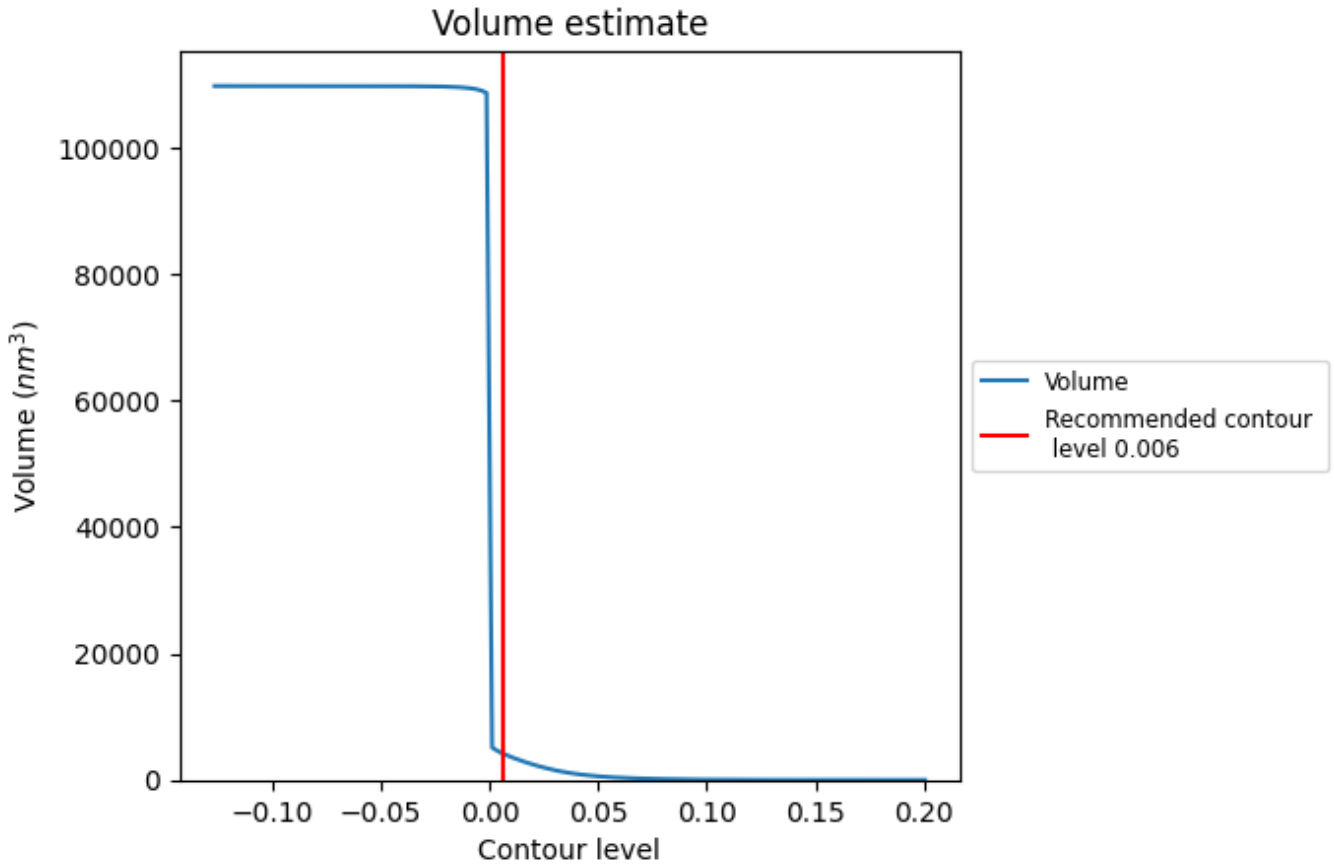
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

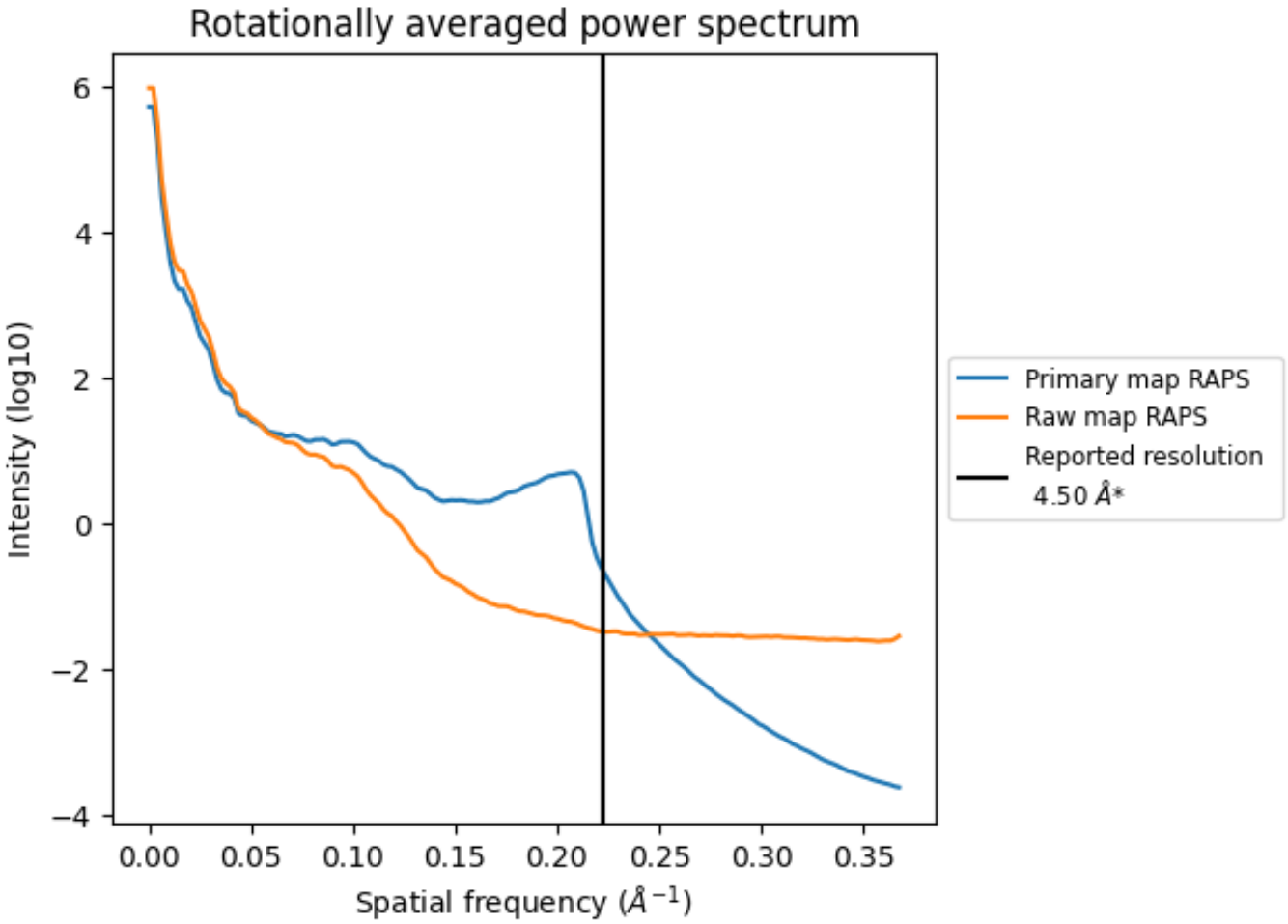
7.2 Volume estimate



The volume at the recommended contour level is 4210 nm^3; this corresponds to an approximate mass of 3803 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)

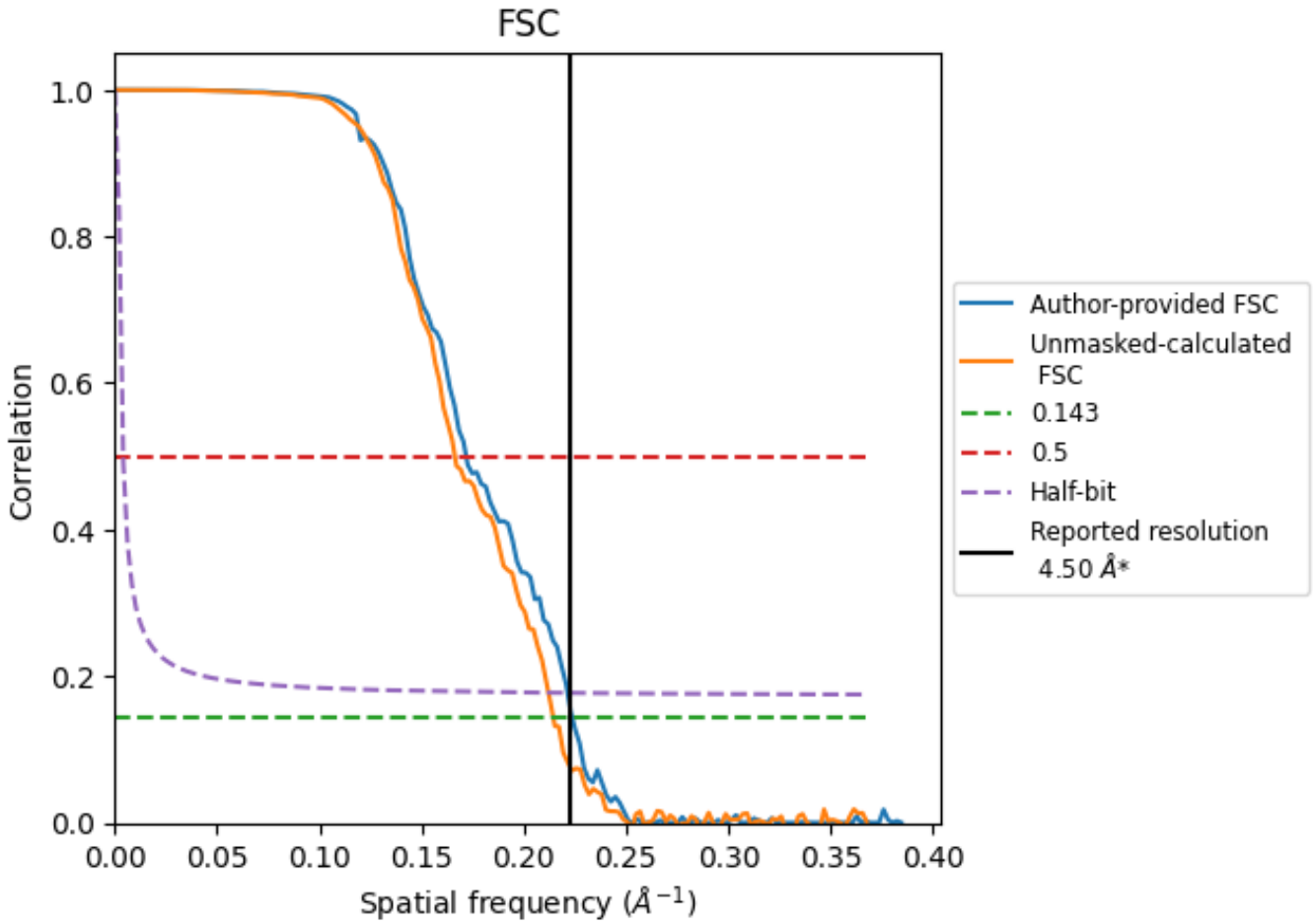


*Reported resolution corresponds to spatial frequency of 0.222 Å^{-1}

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 0.222 Å^{-1}

8.2 Resolution estimates (i)

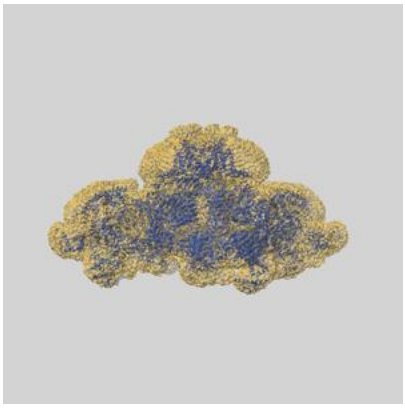
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.47	5.82	4.52
Unmasked-calculated*	4.66	6.01	4.71

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

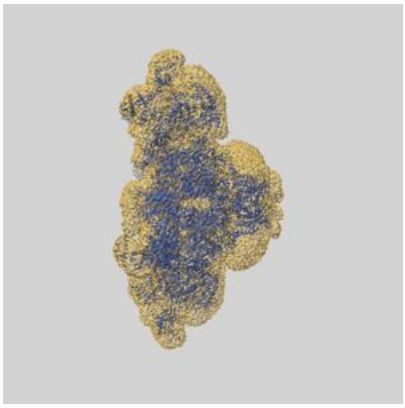
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22615 and PDB model 7K0S. Per-residue inclusion information can be found in section 3 on page 5.

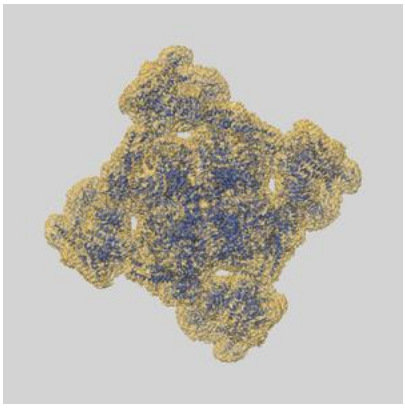
9.1 Map-model overlay



X



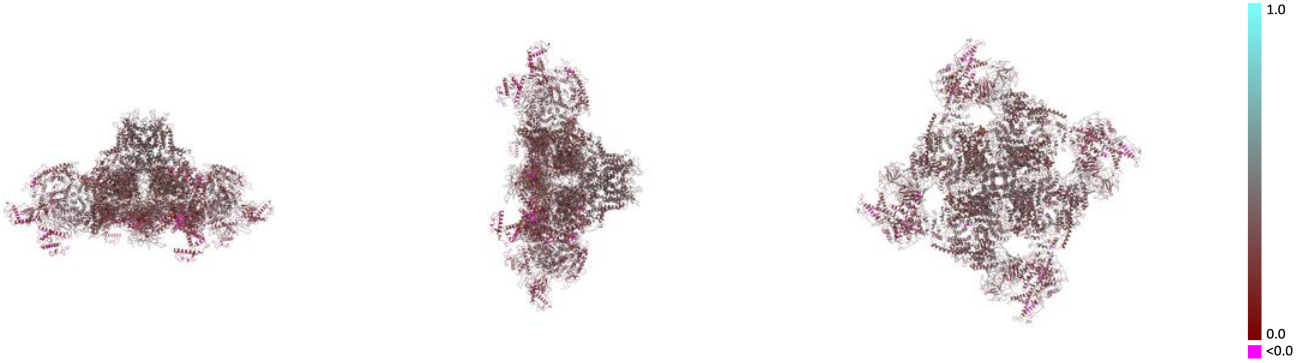
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

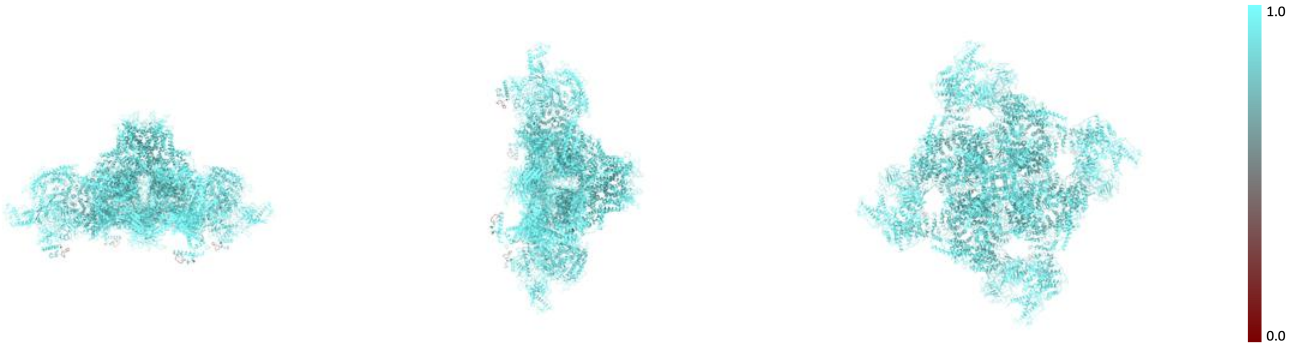
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

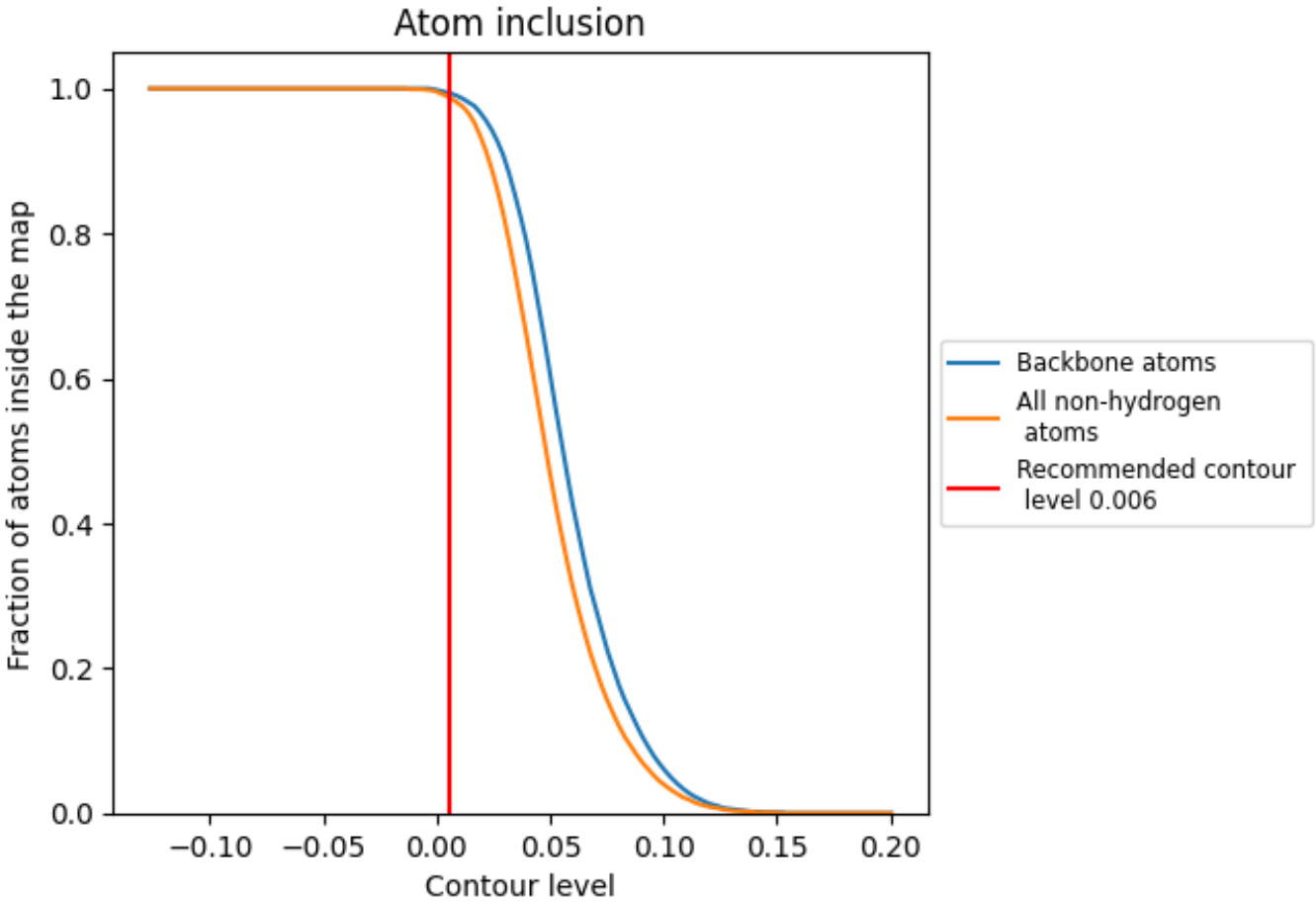
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.006).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9870	0.3120
A	0.9870	0.3110
B	0.9870	0.3120
C	0.9870	0.3120
D	0.9870	0.3110