Full wwPDB EM Validation Report ⓘ

Nov 10, 2024 – 02:59 pm GMT

PDB ID	:	8RRX
EMDB ID	:	EMD-19468
Title	:	Structure of RyR1 reconstituted into lipid nanodisc in primed state in complex with Ca2+, ATP, caffeine and Nb9657
Authors	:	Li, C.; Efremov, R.G.
Deposited on	:	2024-01-23
Resolution	:	3.10 Å(reported)

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

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

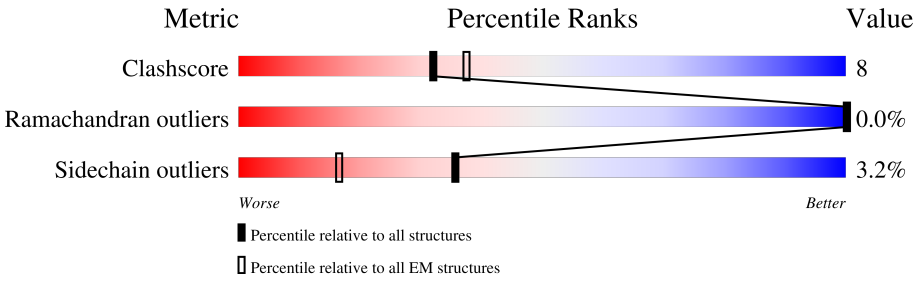
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	F	107	82% 16%
1	H	107	82% 16%
1	J	107	85% 14%
1	L	107	83% 15%
2	A	5027	5% 67% 18% 14%
2	D	5027	5% 67% 18% 14%
2	G	5027	5% 67% 18% 14%
2	I	5027	5% 67% 18% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	137	42% 63% 28% 8%
3	E	137	42% 64% 28% 8%
3	K	137	41% 61% 30% 8%
3	M	137	42% 64% 27% 8%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 144144 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	L	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	100	ASP	GLY	conflict	UNP Q8HYX6
L	100	ASP	GLY	conflict	UNP Q8HYX6
J	100	ASP	GLY	conflict	UNP Q8HYX6
F	100	ASP	GLY	conflict	UNP Q8HYX6

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	4319	Total	C	N	O	S	1	0
			34151	21750	5888	6285	228		
2	A	4319	Total	C	N	O	S	1	0
			34153	21752	5888	6285	228		
2	D	4319	Total	C	N	O	S	1	0
			34153	21752	5888	6285	228		
2	G	4319	Total	C	N	O	S	1	0
			34151	21750	5888	6285	228		

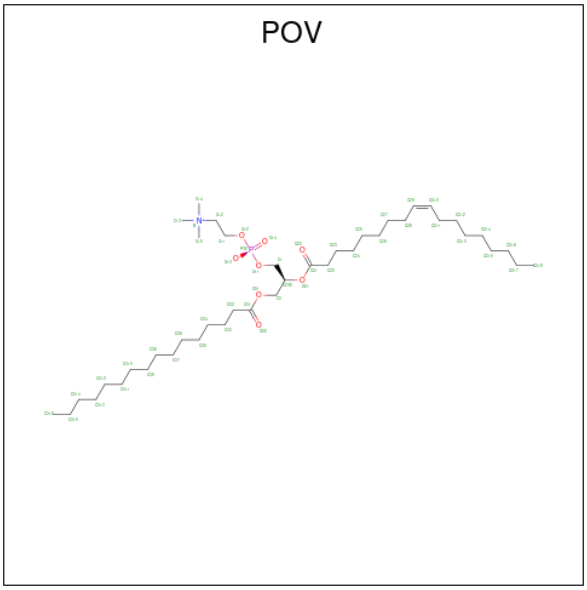
- Molecule 3 is a protein called Nanobody 9657.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	126	Total	C	N	O	S	0	0
			967	597	170	195	5		
3	C	126	Total	C	N	O	S	0	0
			967	597	170	195	5		
3	E	126	Total	C	N	O	S	0	0
			967	597	170	195	5		
3	M	126	Total	C	N	O	S	0	0
			967	597	170	195	5		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	I	1	Total	Zn	0
			1	1	
4	A	1	Total	Zn	0
			1	1	
4	D	1	Total	Zn	0
			1	1	
4	G	1	Total	Zn	0
			1	1	

- Molecule 5 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: $C_{42}H_{82}NO_8P$).



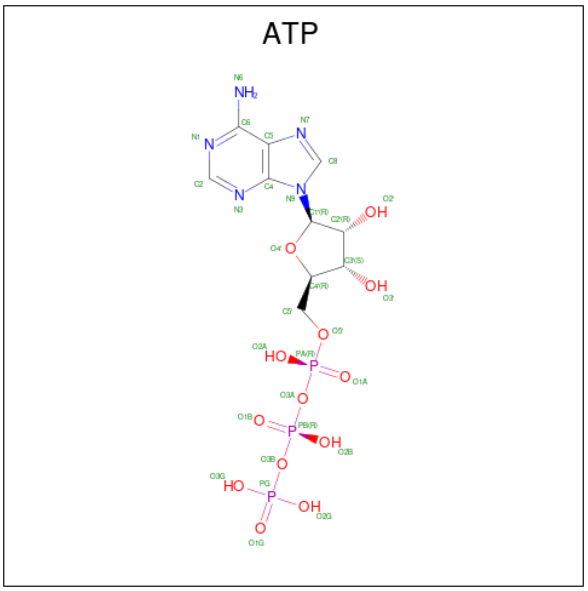
Mol	Chain	Residues	Atoms					AltConf
5	I	1	Total	C	N	O	P	0
			52	42	1	8	1	

Continued on next page...

Continued from previous page...

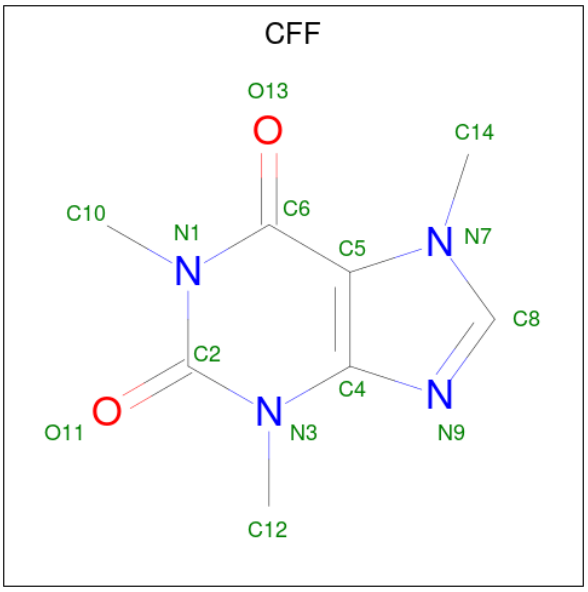
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	G	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	G	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 7 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
7	I	1	Total C N O 14 8 4 2	0
7	A	1	Total C N O 14 8 4 2	0
7	D	1	Total C N O 14 8 4 2	0
7	G	1	Total C N O 14 8 4 2	0

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

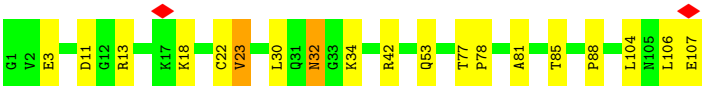
Mol	Chain	Residues	Atoms	AltConf
8	I	1	Total Ca 1 1	0
8	A	1	Total Ca 1 1	0
8	D	1	Total Ca 1 1	0
8	G	1	Total Ca 1 1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

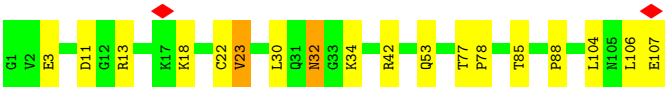
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



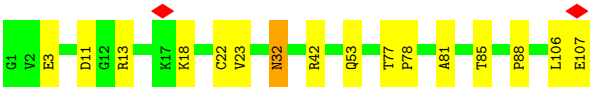
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain L:



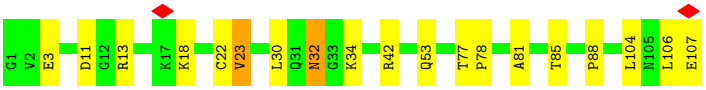
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J:



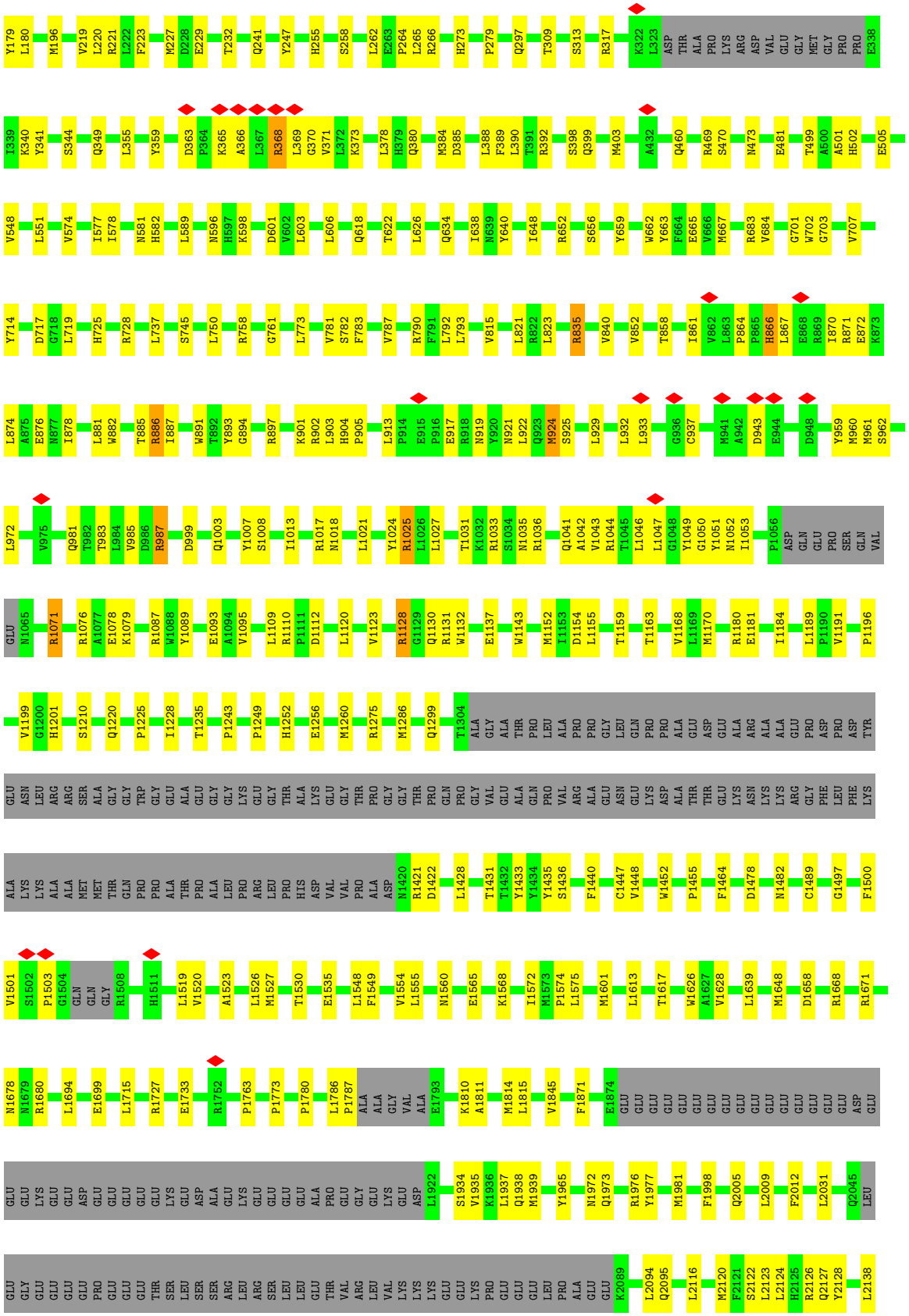
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

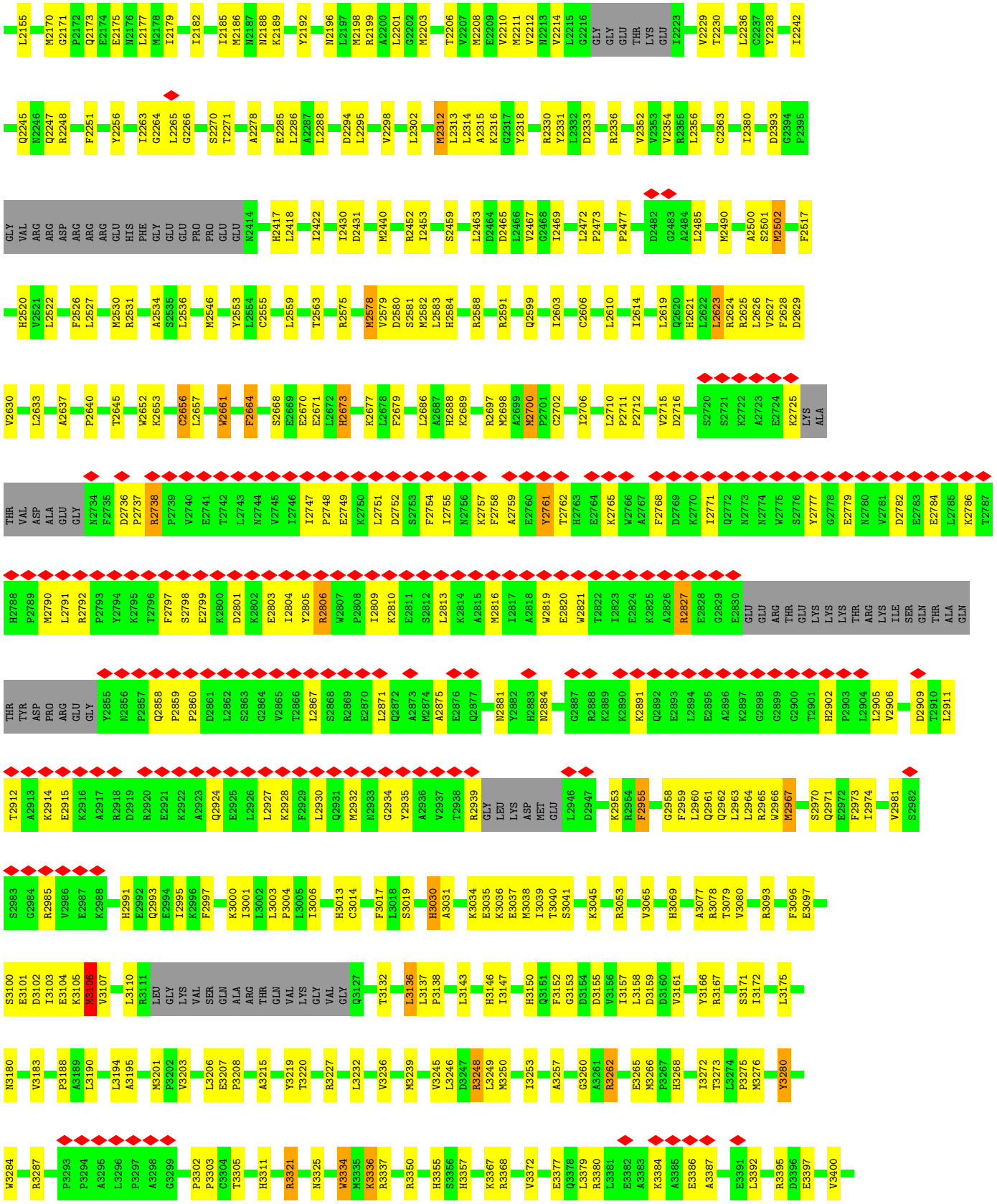
Chain F:

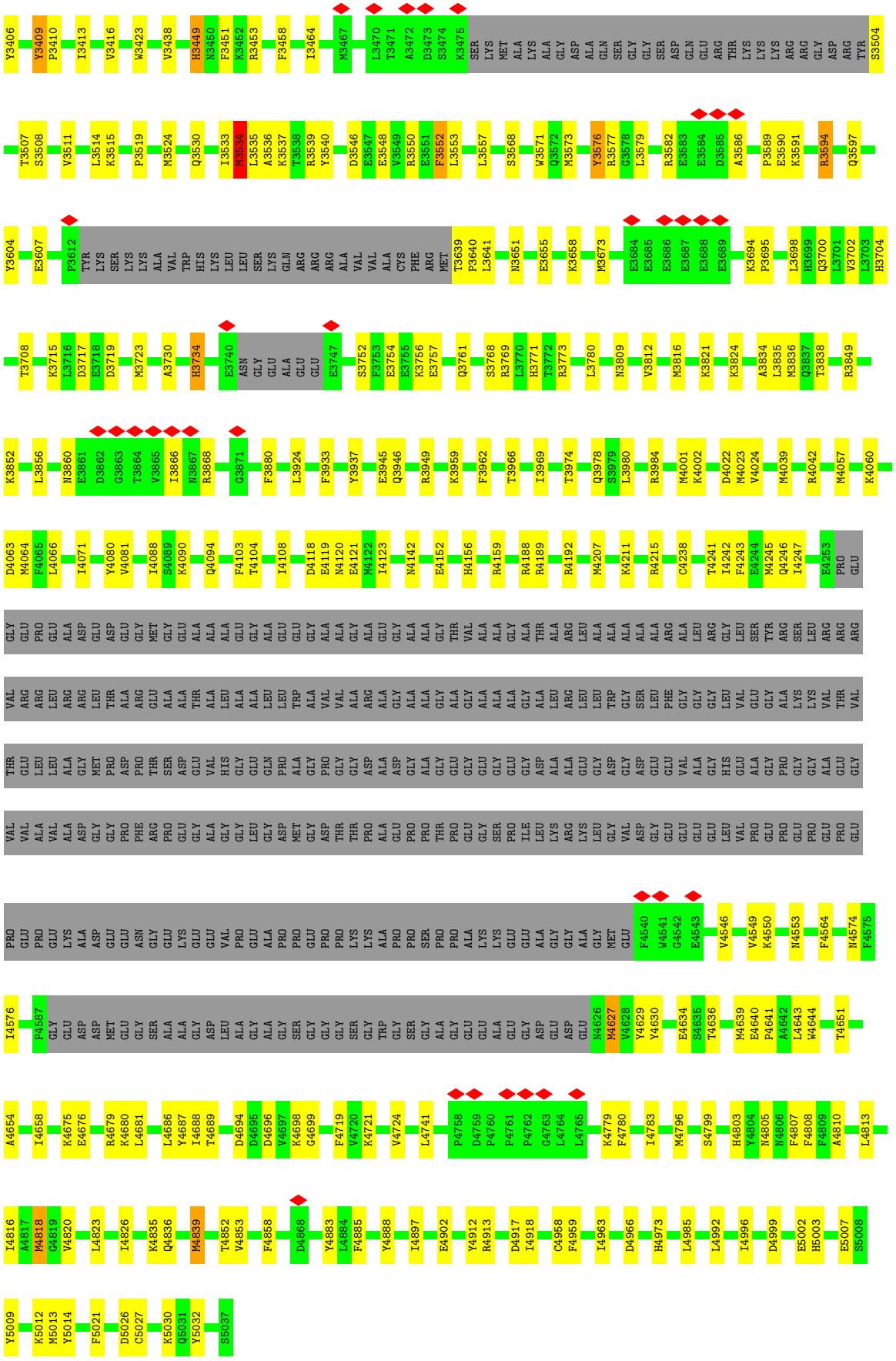


• Molecule 2: Ryanodine receptor 1

Chain I:

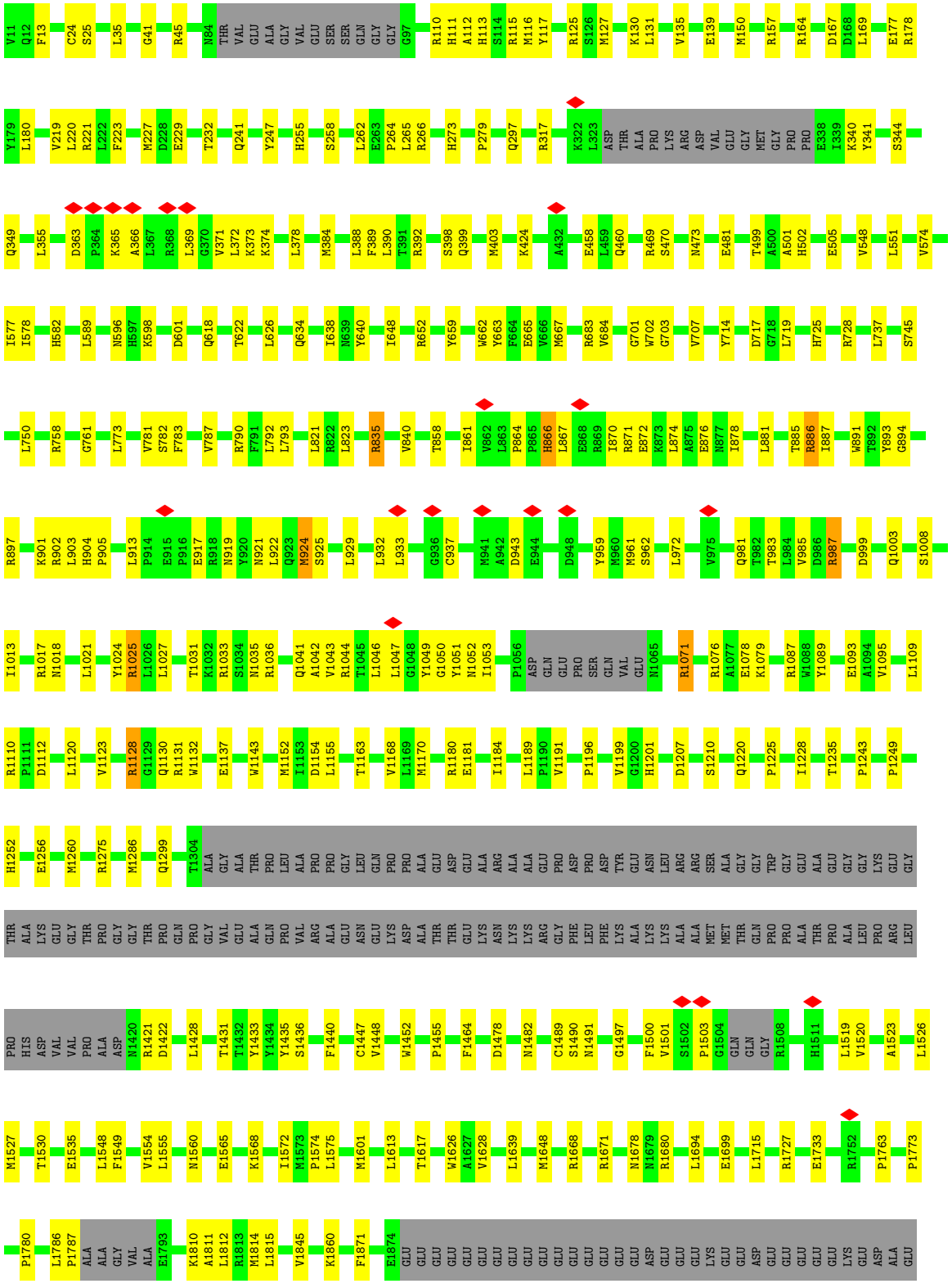


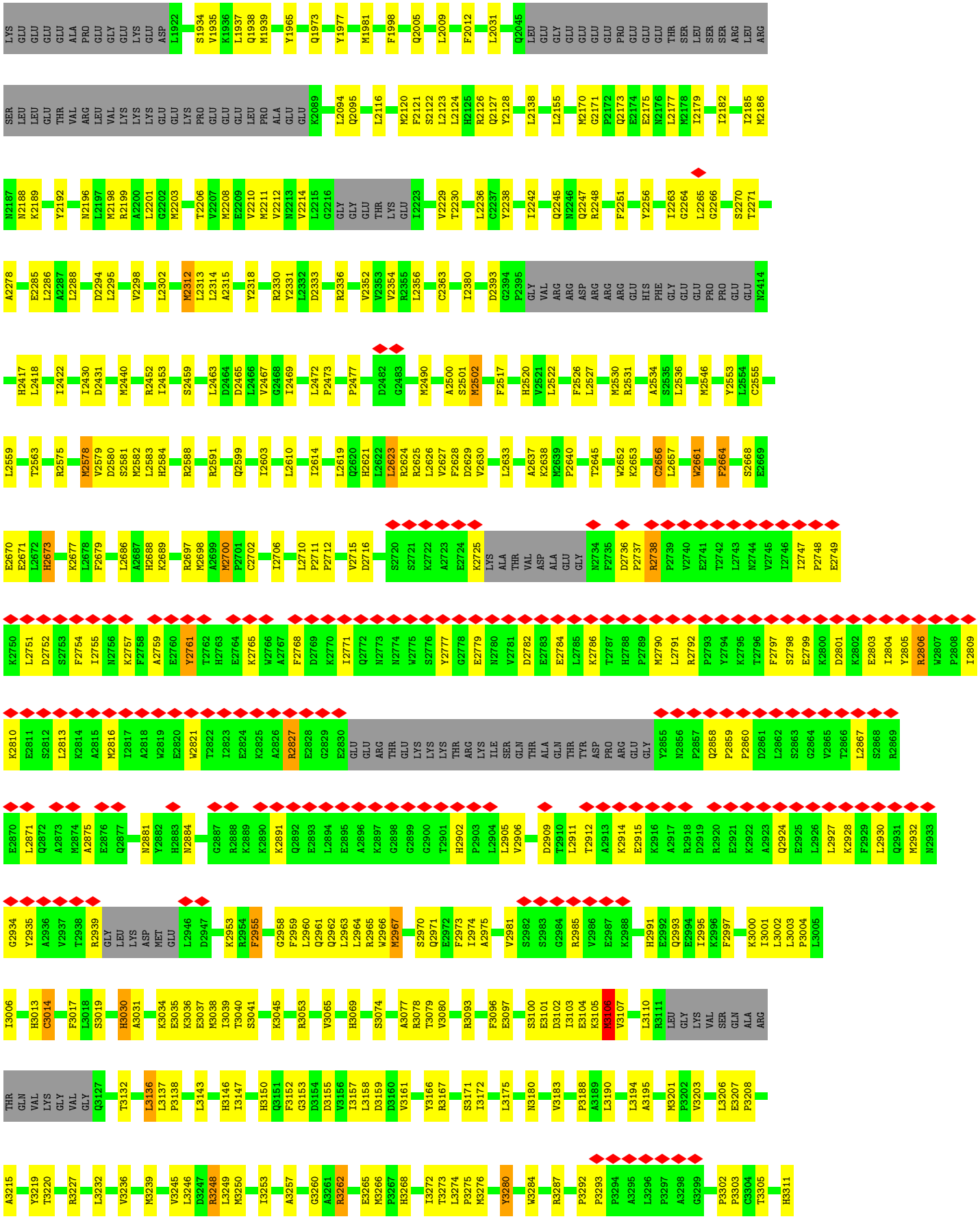


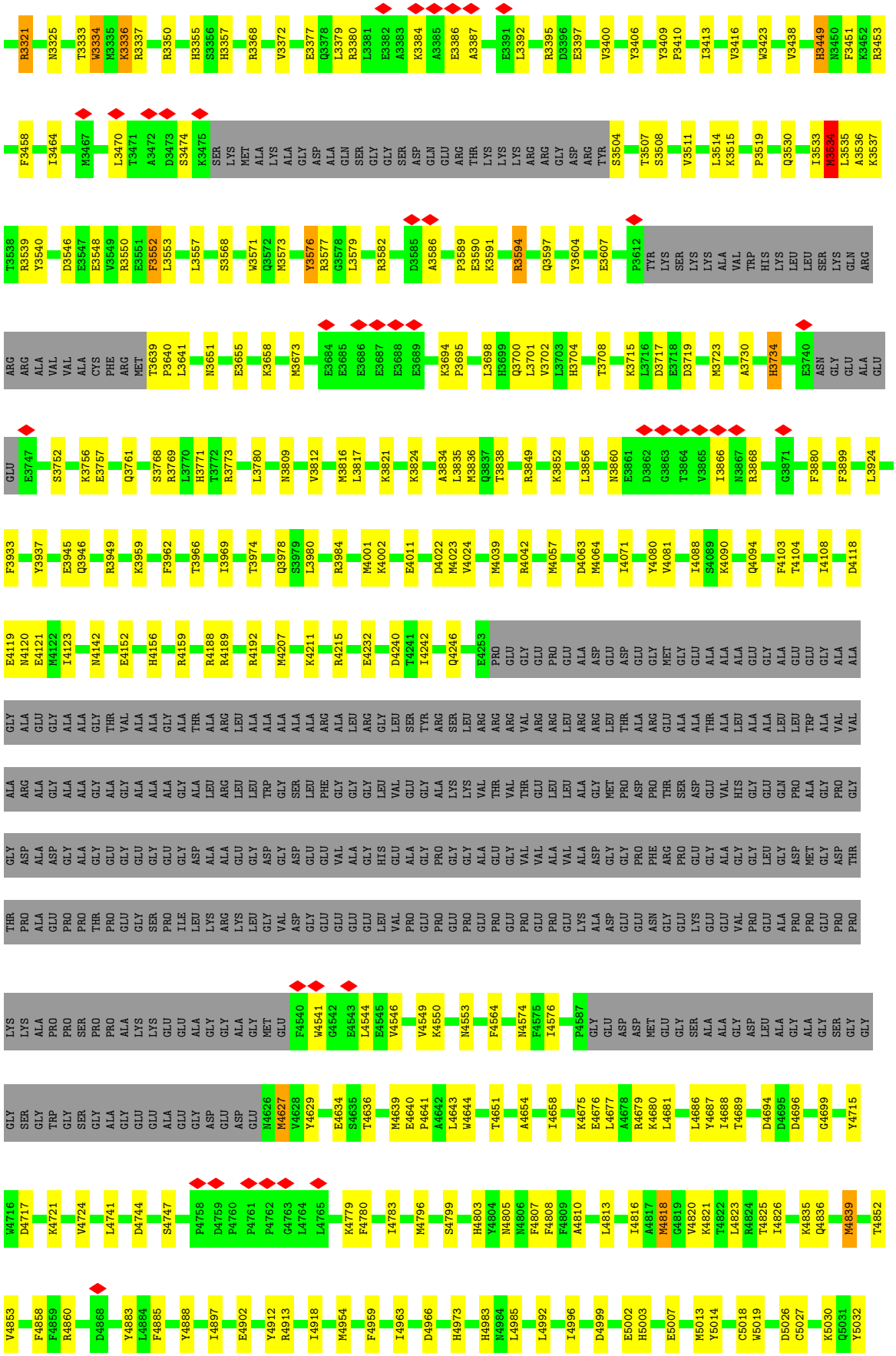

Y3406 Y3409 P3410 I3413 V3416 W3423 V3438 H3449 M3450 F3451 K3452 R3453 F3458 I3464 M3467 L3470 T3471 A3472 D3473 S3474 K3475 SER LYS MET ALA LYS ALA GLY ASP ALA GLN SER GLY GLY SER ASP GLN GLU ARG THR LYS LYS LYS ARG ARG GLY ASP ARG TYR S3504
T3507 S3508 V3511 L3514 K3515 P3519 M3524 Q3530 I3533 M3534 L3535 A3536 K3537 T3538 R3539 Y3540 D3546 E3547 E3548 V3549 A3550 E3551 F3562 L3553 L3557 S3568 W3571 Q3572 M3573 Y3576 R3577 G3578 L3579 R3582 E3583 E3584 D3585 A3586 P3589 E3590 K3591 R3594 Q3597
Y3604 E3607 P3612 TYR LYS SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG ARG ARG ALA VAL VAL ALA CYS PHE ARG MET T3639 P3640 L3641 N3651 E3655 K3658 M3673 E3684 E3685 E3686 E3687 E3688 E3689 K3694 P3695 L3698 H3699 Q3700 L3701 V3702 L3703 H3704
T3708 K3715 L3716 D3717 E3718 D3719 M3723 A3730 H3734 E3740 ASN GLY GLU ALA GLU GLU E3747 S3752 F3753 E3754 E3755 K3756 E3757 Q3761 S3768 R3769 L3770 H3771 T3772 R3773 L3780 N3809 V3812 M3816 K3821 K3824 A3834 L3835 M3836 Q3837 T3838 R3849
K3852 L3856 N3860 E3861 D3862 G3863 T3864 V3865 I3866 N3867 R3868 G3871 F3880 L3924 F3933 Y3937 E3945 Q3946 R3949 K3959 F3962 T3966 I3969 T3974 Q3978 S3979 L3980 R3984 M4001 K4002 D4022 M4023 V4024 M4039 R4042 M4057 K4060
D4063 M4064 F4065 L4066 I4071 Y4080 V4081 I4088 S4089 K4090 Q4094 F4103 T4104 I4108 D4118 E4119 N4120 E4121 M4122 I4123 N4142 E4152 H4156 R4159 R4188 R4189 R4192 M4207 K4211 R4215 C4238 T4241 I4242 F4243 E4244 M4245 Q4246 I4247 E4253 PRO GLU
GLY GLU PRO GLU ALA ASP GLU ASP GLU GLY MET GLY GLU ALA ALA ALA GLY ALA ALA GLY ALA ALA GLU GLY ALA ALA GLY THR VAL ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ARG ALA LEU ARG GLY LEU SER TYR ARG SER LEU ARG 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 ALA GLY ASP 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 GLY GLU GLU GLY ALA ALA ALA GLU GLY ASP GLY ASP GLU GLU VAL ALA GLY HIS GLU ALA GLY PRO GLY GLY GLY ALA GLU GLY
VAL VAL ALA VAL ALA ASP GLY GLY PRO PHE ARG PRO GLU GLY VAL ALA ASP GLY ASP PRO THR THR PRO ALA GLU PRO PRO THR PRO GLU GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLY 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 GLU VAL PRO GLU ALA PRO PRO PRO PRO PRO LYS LYS ALA PRO PRO SER PRO PRO PRO ALA LYS LYS SER GLU GLU ALA GLY GLY ALA GLY MET GLU F4540 W4541 G4542 E4543 V4546 V4549 K4550 N4553 F4564 N4574 F4575
I4576 P4587 GLY GLU ASP ASP MET GLU GLY SER ALA ALA GLY ASP LEU ALA GLY SER GLY GLY GLY SER GLY TRP GLY SER GLY ALA GLY GLU GLU GLU ASP GLU ASP N4626 M4627 V4628 Y4629 Y4630 E4634 S4635 T4636 M4639 E4640 P4641 A4642 L4643 W4644 T4651
A4654 I4658 K4675 E4676 R4679 K4680 L4681 L4686 Y4687 I4688 T4689 D4694 P4695 D4696 V4697 K4698 G4699 F4719 V4720 K4721 V4724 L4741 P4758 D4759 P4760 P4761 P4762 G4763 L4764 L4765 K4779 F4780 I4783 M4796 S4799 H4803 Y4804 N4805 N4806 F4807 F4808 F4809 A4810 L4813
I4816 A4817 M4818 G4819 Y4820 L4823 I4826 K4835 Q4836 M4839 T4852 V4853 F4858 D4868 Y4883 L4884 F4885 Y4888 I4897 E4902 Y4912 R4913 D4917 I4918 C4958 F4959 I4963 D4966 H4973 L4985 L4992 I4996 D4999 E5002 H5003 E5007 S5008
Y5009 K5012 M5013 Y5014 F5021 D5026 C5027 K5030 Q5031 Y5032 S5037

• Molecule 2: Ryanodine receptor 1

Chain A:

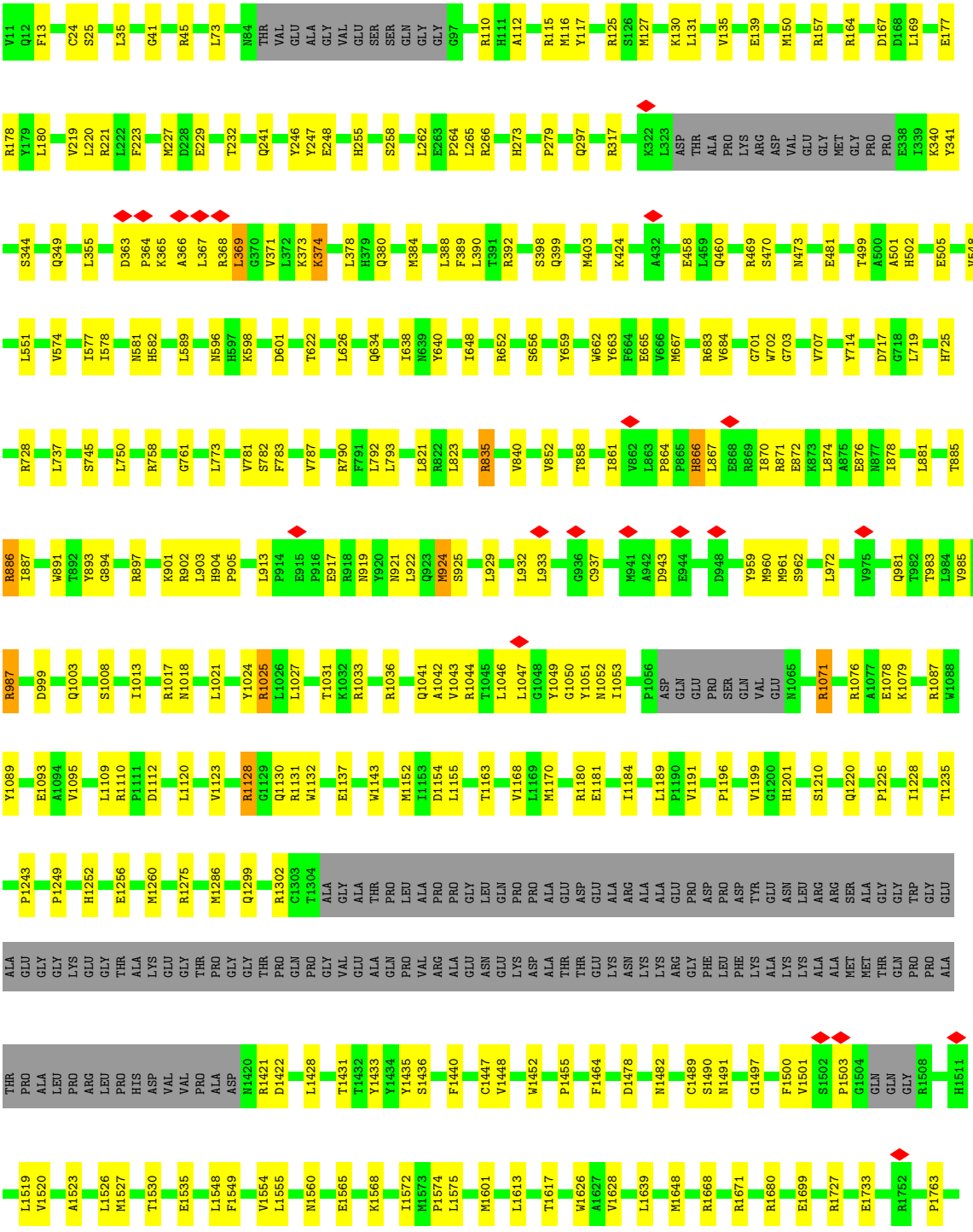


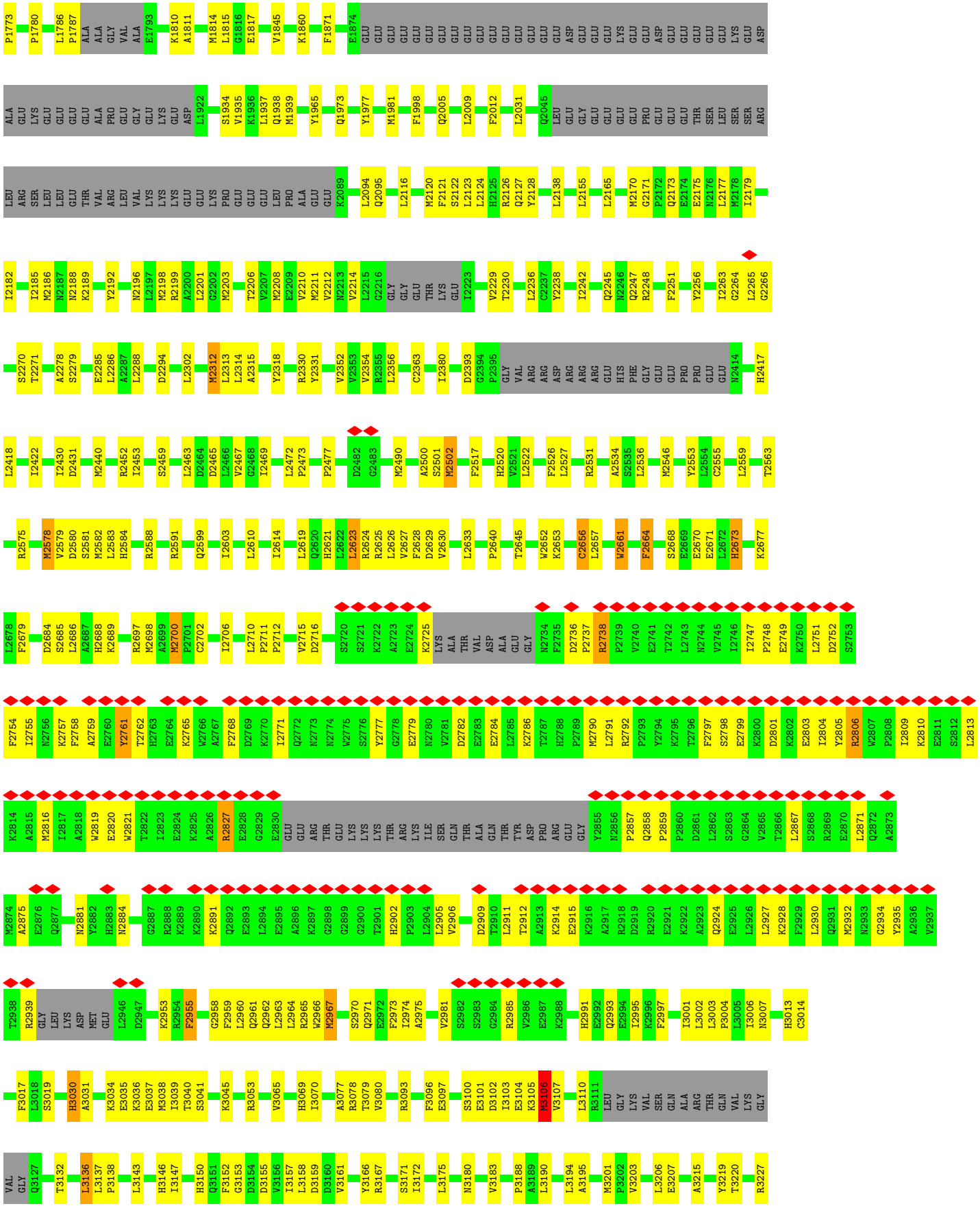


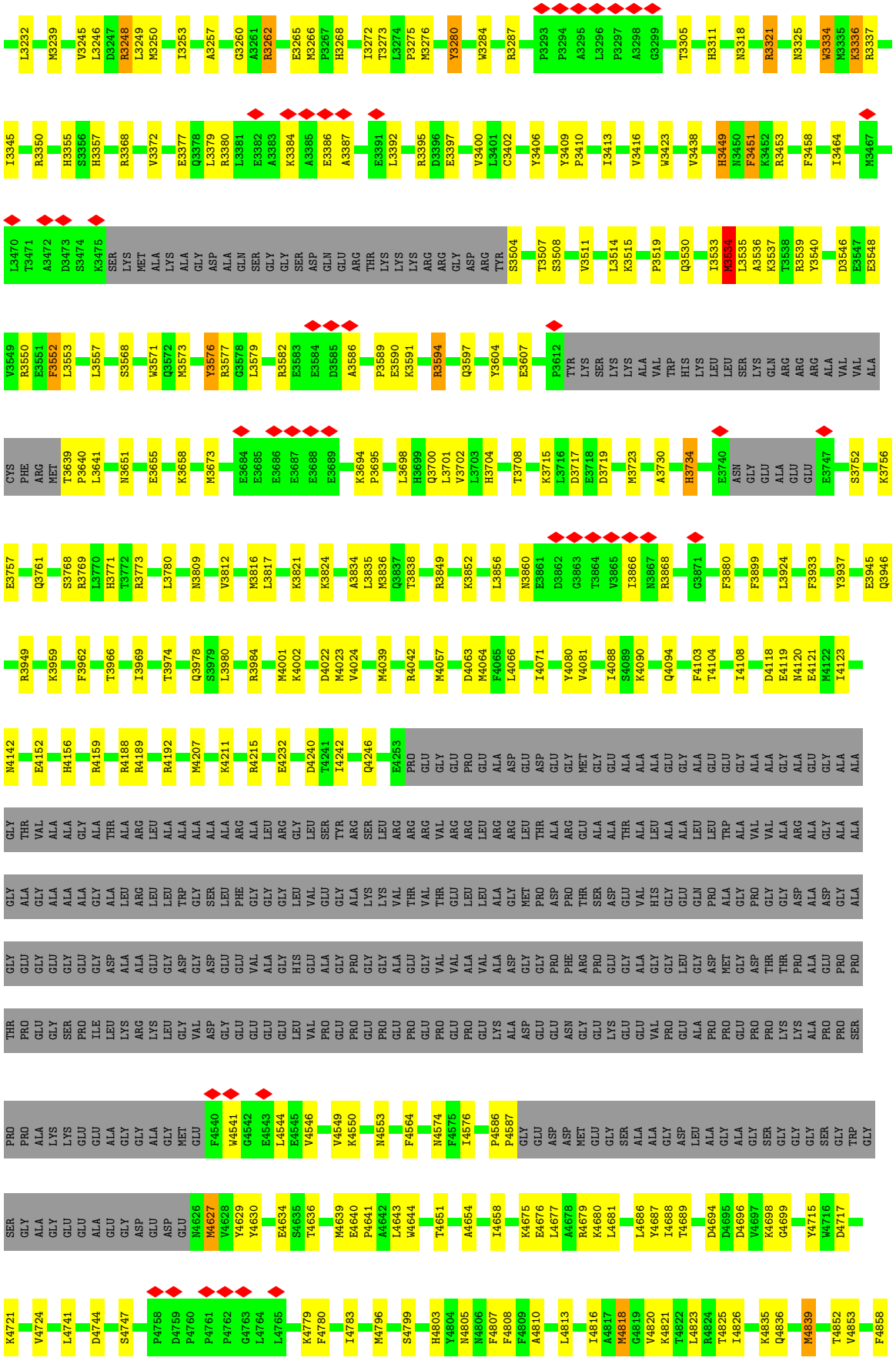


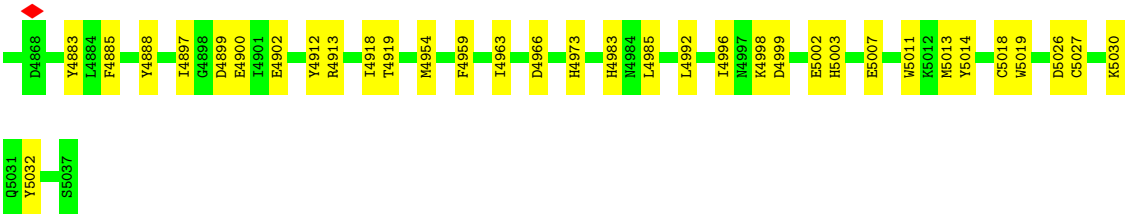
• Molecule 2: Ryanodine receptor 1

Chain D:

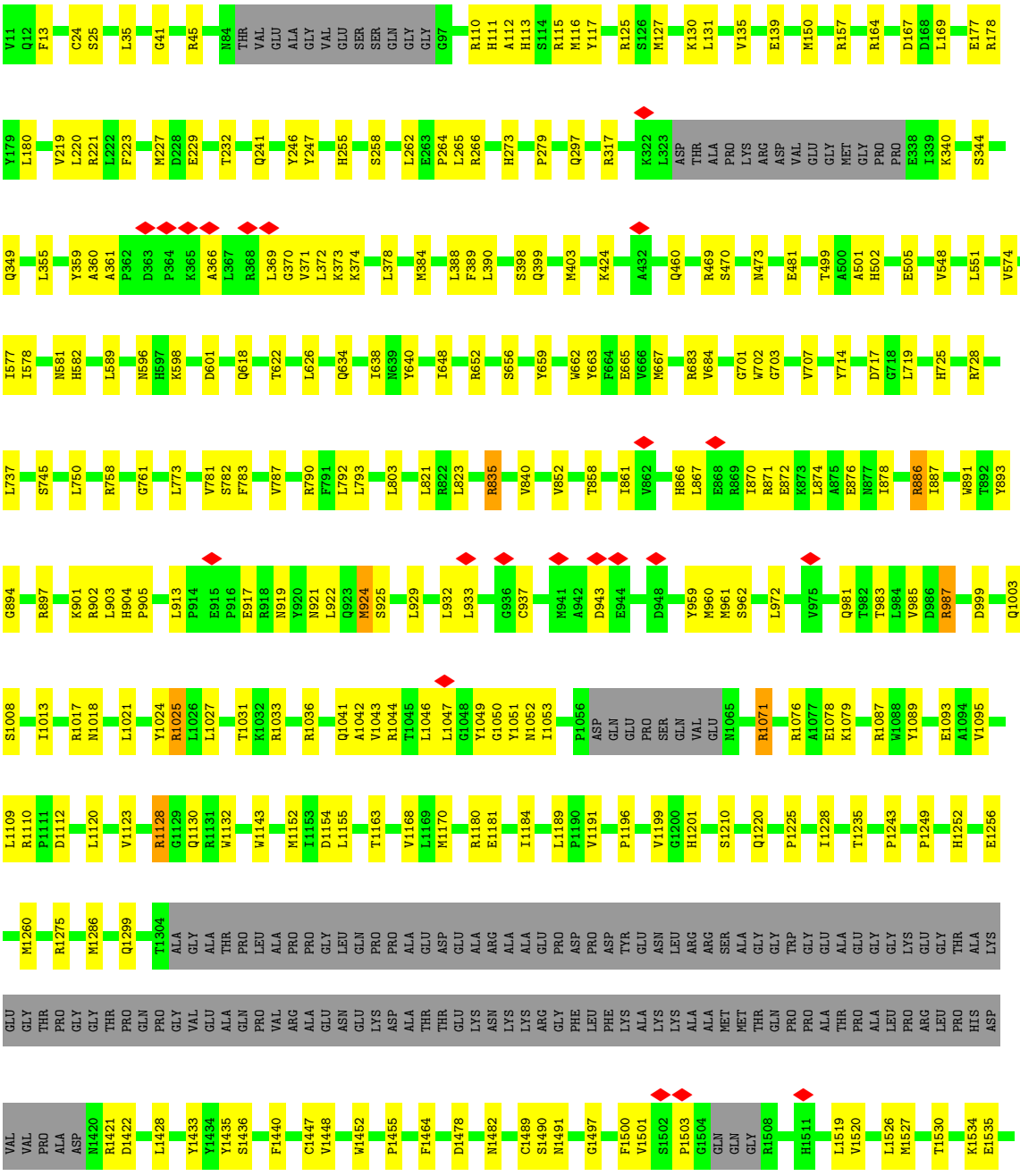


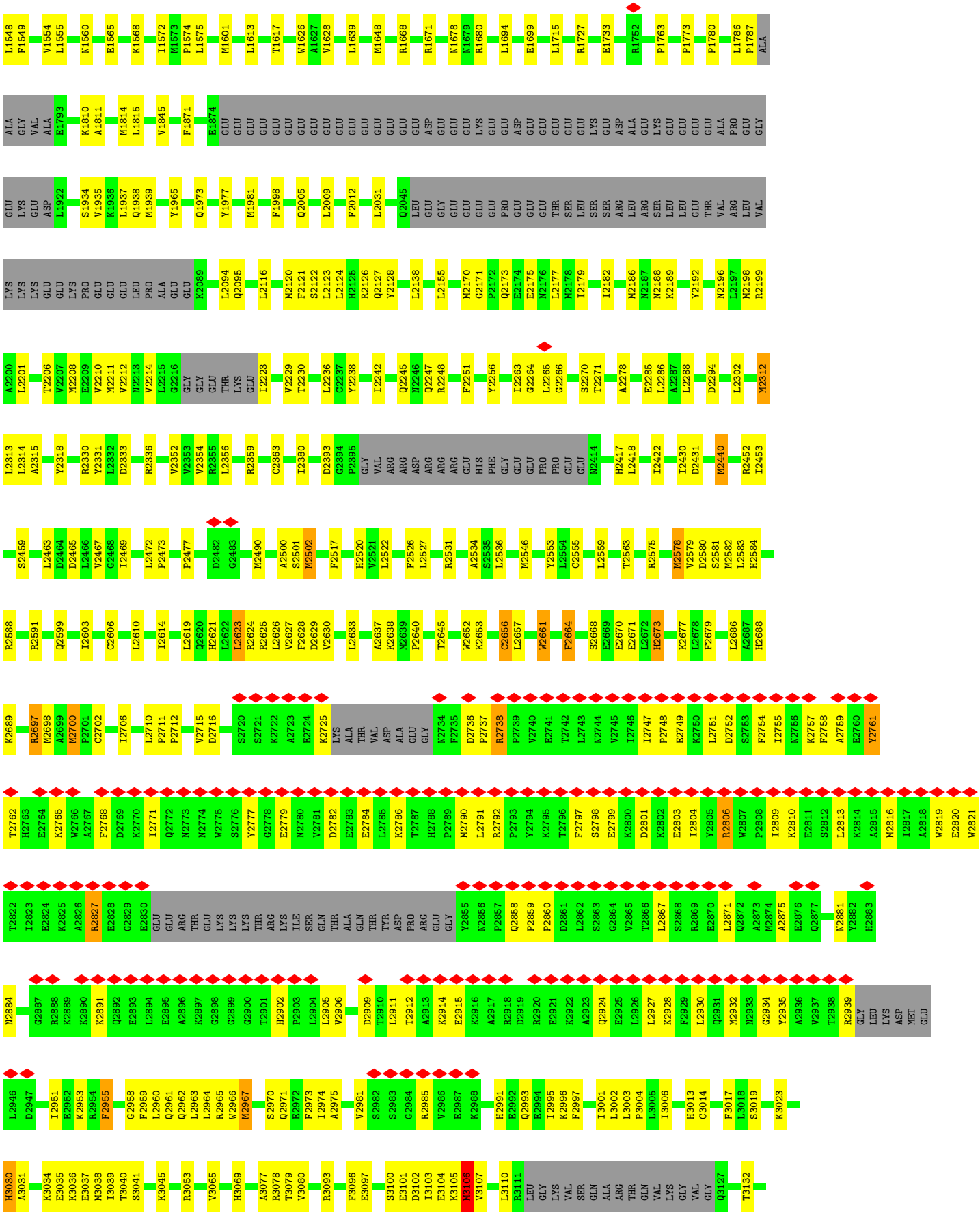


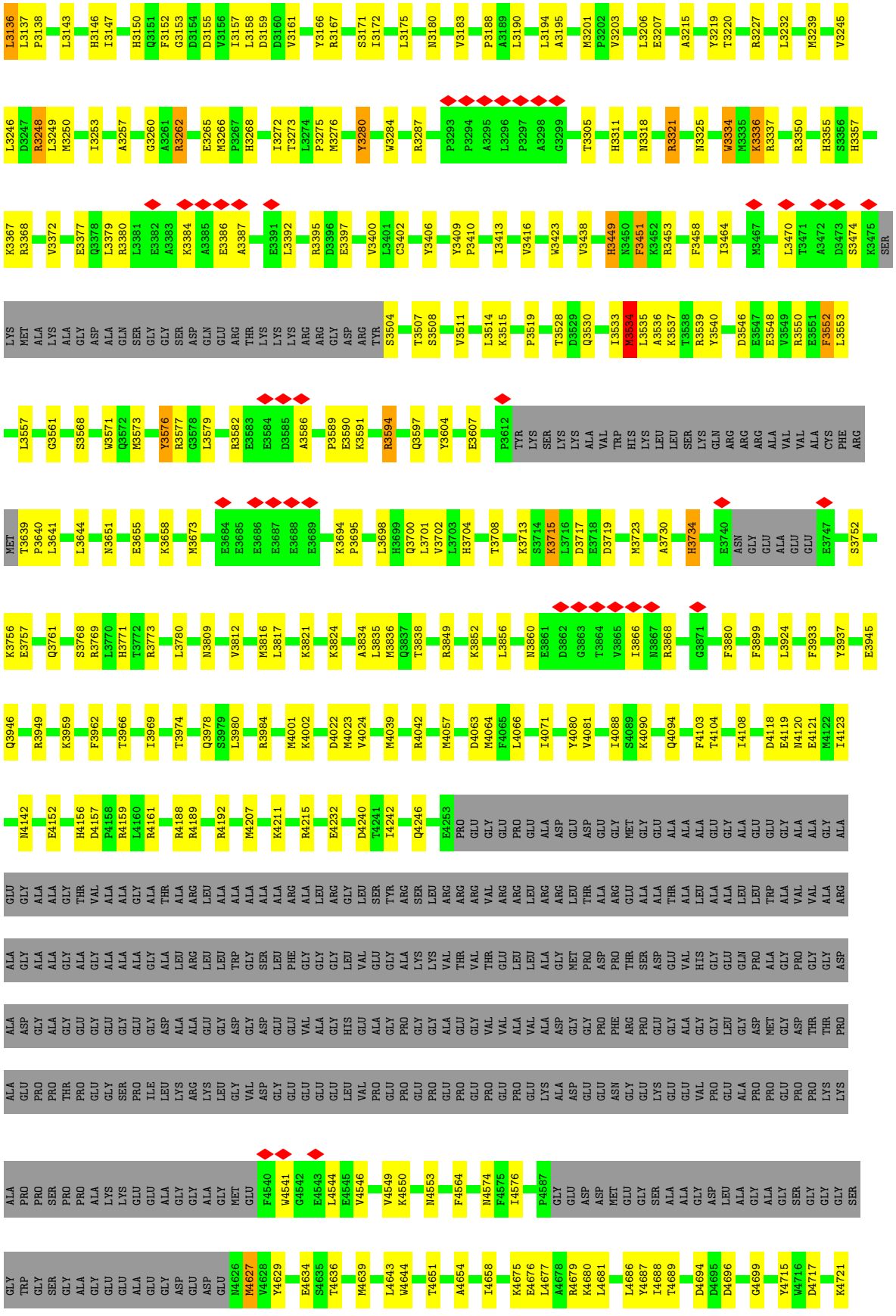




• Molecule 2: Ryanodine receptor 1

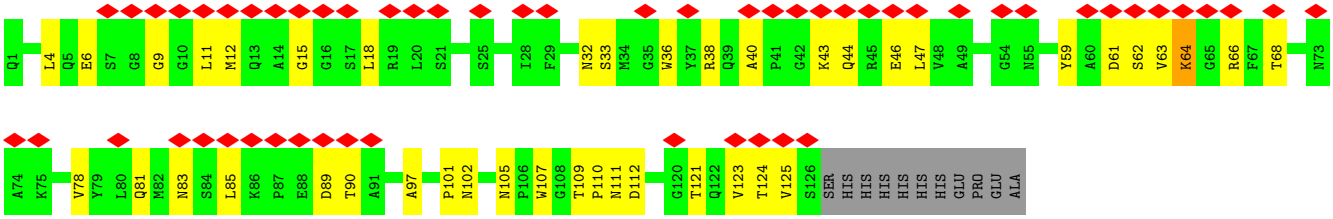






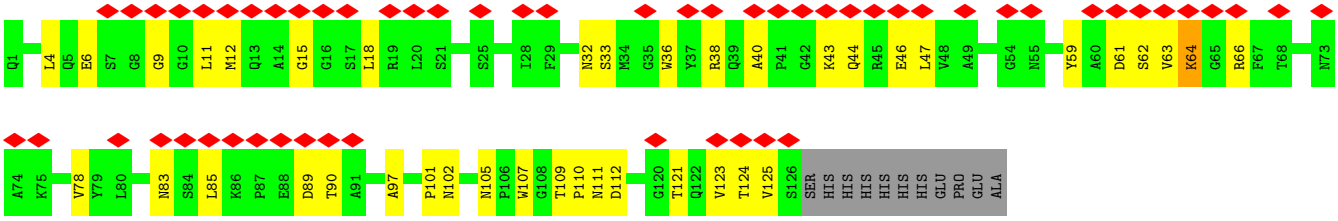
• Molecule 3: Nanobody 9657

Chain K:



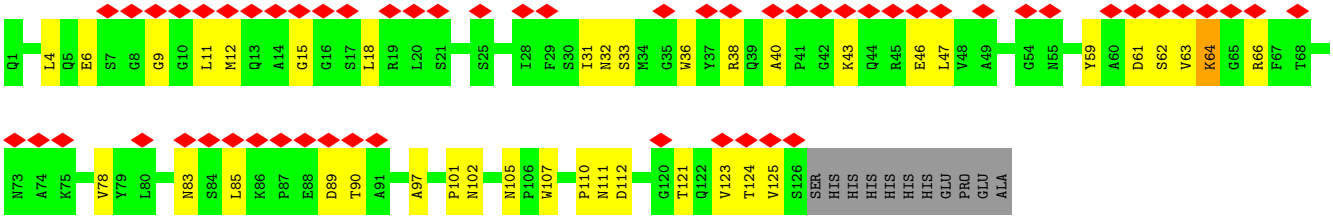
• Molecule 3: Nanobody 9657

Chain C:



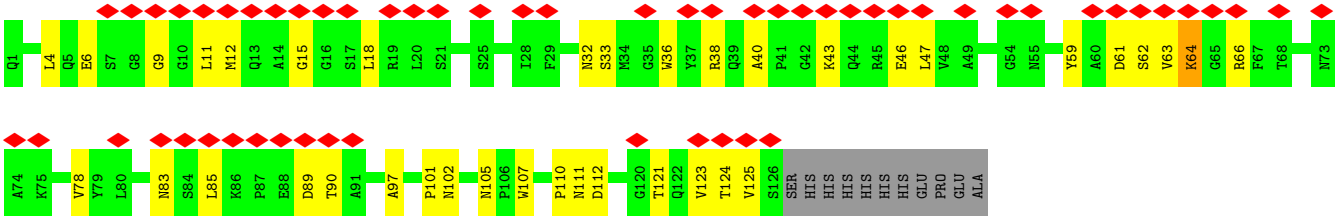
• Molecule 3: Nanobody 9657

Chain E:



• Molecule 3: Nanobody 9657

Chain M:


Q1 L4 Q5 E6 S7 G8 G9 G10 L11 M12 Q13 A14 G15 G16 S17 L18 R19 L20 S21 S25 I28 F29 N32 S33 M34 G35 W36 Y37 R38 Q39 A40 P41 G42 K43 Q44 R45 E46 L47 V48 A49 G54 N55 Y59 A60 D61 S62 V63 K64 G65 R66 F67 T68 N73
A74 K75 V78 Y79 L80 N83 S84 L85 K86 P87 E88 D89 T90 A91 A97 P101 N102 N105 P106 W107 P110 N111 D112 G120 T121 Q122 V123 T124 V125 S126 SER HIS HIS HIS HIS HIS HIS GLU PRO GLU ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	175535	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.601	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.034	Depositor
Map value standard deviation	0.067	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	511.65, 511.65, 511.65	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.137, 1.137, 1.137	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ZN, CFF, POV, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	F	0.27	0/834	0.56	0/1123
1	H	0.27	0/834	0.56	0/1123
1	J	0.27	0/834	0.56	0/1123
1	L	0.27	0/834	0.56	0/1123
2	A	0.25	0/34923	0.49	4/47330 (0.0%)
2	D	0.25	0/34923	0.49	4/47330 (0.0%)
2	G	0.25	0/34920	0.49	4/47325 (0.0%)
2	I	0.25	0/34920	0.49	4/47325 (0.0%)
3	C	0.25	0/987	0.52	0/1340
3	E	0.25	0/987	0.52	0/1340
3	K	0.25	0/987	0.52	0/1340
3	M	0.25	0/987	0.52	0/1340
All	All	0.25	0/146970	0.49	16/199162 (0.0%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1503	PRO	N-CA-CB	5.72	110.16	103.30
2	I	1503	PRO	N-CA-CB	5.71	110.16	103.30
2	D	1503	PRO	N-CA-CB	5.71	110.16	103.30
2	A	1503	PRO	N-CA-CB	5.68	110.12	103.30
2	D	3136	LEU	CA-CB-CG	5.66	128.32	115.30
2	I	3136	LEU	CA-CB-CG	5.64	128.28	115.30
2	A	3136	LEU	CA-CB-CG	5.64	128.28	115.30
2	G	3136	LEU	CA-CB-CG	5.64	128.28	115.30
2	D	3106	MET	CA-CB-CG	5.49	122.64	113.30
2	I	3106	MET	CA-CB-CG	5.47	122.59	113.30
2	A	3106	MET	CA-CB-CG	5.46	122.57	113.30
2	G	3106	MET	CA-CB-CG	5.45	122.56	113.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	3534	MET	CA-CB-CG	5.09	121.95	113.30
2	A	3534	MET	CA-CB-CG	5.08	121.94	113.30
2	G	3534	MET	CA-CB-CG	5.08	121.94	113.30
2	D	3534	MET	CA-CB-CG	5.06	121.90	113.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	818	0	824	14	0
1	H	818	0	824	13	0
1	J	818	0	824	11	0
1	L	818	0	824	12	0
2	A	34153	0	33544	573	0
2	D	34153	0	33544	576	0
2	G	34151	0	33538	575	0
2	I	34151	0	33538	580	0
3	C	967	0	916	25	0
3	E	967	0	916	25	0
3	K	967	0	916	28	0
3	M	967	0	916	23	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
5	A	52	0	82	1	0
5	D	52	0	82	3	0
5	G	52	0	82	3	0
5	I	52	0	82	1	0
6	A	31	0	12	3	0
6	D	31	0	12	3	0
6	G	31	0	12	3	0
6	I	31	0	12	2	0
7	A	14	0	10	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	14	0	10	2	0
7	G	14	0	10	2	0
7	I	14	0	10	1	0
8	A	1	0	0	0	0
8	D	1	0	0	0	0
8	G	1	0	0	0	0
8	I	1	0	0	0	0
All	All	144144	0	141540	2394	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 8.

All (2394) 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)
2:A:3132:THR:HA	2:A:3136:LEU:HB3	1.61	0.83
2:G:3132:THR:HA	2:G:3136:LEU:HB3	1.61	0.82
2:I:3132:THR:HA	2:I:3136:LEU:HB3	1.61	0.82
2:I:4823:LEU:HD13	2:G:4839:MET:HE2	1.61	0.81
2:I:4839:MET:HE2	2:A:4823:LEU:HD13	1.62	0.81
2:D:3132:THR:HA	2:D:3136:LEU:HB3	1.61	0.80
2:D:1520:VAL:HG23	2:D:1527:MET:HG2	1.64	0.79
2:G:1520:VAL:HG23	2:G:1527:MET:HG2	1.64	0.78
2:I:1520:VAL:HG23	2:I:1527:MET:HG2	1.64	0.78
2:D:2710:LEU:HD12	2:D:2711:PRO:HD2	1.65	0.78
2:I:913:LEU:HB3	2:I:917:GLU:HB2	1.65	0.77
2:D:913:LEU:HB3	2:D:917:GLU:HB2	1.65	0.77
2:A:1520:VAL:HG23	2:A:1527:MET:HG2	1.65	0.77
2:I:2710:LEU:HD12	2:I:2711:PRO:HD2	1.65	0.77
2:A:1973:GLN:HE22	2:A:3641:LEU:H	1.33	0.76
2:A:2710:LEU:HD12	2:A:2711:PRO:HD2	1.65	0.76
2:G:913:LEU:HB3	2:G:917:GLU:HB2	1.65	0.76
2:A:913:LEU:HB3	2:A:917:GLU:HB2	1.65	0.76
2:G:2710:LEU:HD12	2:G:2711:PRO:HD2	1.65	0.76
2:D:1973:GLN:HE22	2:D:3641:LEU:H	1.33	0.76
2:A:2626:LEU:HD22	2:A:2640:PRO:HB3	1.68	0.75
2:I:2626:LEU:HD22	2:I:2640:PRO:HB3	1.68	0.75
2:D:4839:MET:HE2	2:G:4823:LEU:HD13	1.70	0.74
2:G:1973:GLN:HE22	2:G:3641:LEU:H	1.32	0.74
2:G:2626:LEU:HD22	2:G:2640:PRO:HB3	1.68	0.74
2:I:1973:GLN:HE22	2:I:3641:LEU:H	1.33	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2626:LEU:HD22	2:D:2640:PRO:HB3	1.68	0.73
2:A:4839:MET:HE2	2:D:4823:LEU:HD13	1.71	0.73
2:D:897:ARG:HD3	2:D:905:PRO:HD3	1.70	0.73
2:A:665:GLU:HB3	2:A:792:LEU:HB2	1.71	0.73
2:D:1008:SER:HB2	2:D:1017:ARG:HE	1.54	0.72
2:I:665:GLU:HB3	2:I:792:LEU:HB2	1.71	0.72
2:I:3110:LEU:HD13	2:I:3183:VAL:HG12	1.71	0.72
2:A:897:ARG:HD3	2:A:905:PRO:HD3	1.70	0.72
2:I:972:LEU:HB2	2:I:1044:ARG:HE	1.55	0.72
2:A:1008:SER:HB2	2:A:1017:ARG:HE	1.55	0.72
2:D:665:GLU:HB3	2:D:792:LEU:HB2	1.71	0.72
2:G:665:GLU:HB3	2:G:792:LEU:HB2	1.71	0.72
2:I:220:LEU:HD12	2:I:390:LEU:HB3	1.70	0.72
2:I:2248:ARG:HE	2:I:3868:ARG:HD2	1.55	0.72
2:A:220:LEU:HD12	2:A:390:LEU:HB3	1.71	0.72
2:A:2248:ARG:HE	2:A:3868:ARG:HD2	1.55	0.72
2:G:1008:SER:HB2	2:G:1017:ARG:HE	1.55	0.72
2:D:972:LEU:HB2	2:D:1044:ARG:HE	1.55	0.71
2:D:220:LEU:HD12	2:D:390:LEU:HB3	1.71	0.71
2:I:1008:SER:HB2	2:I:1017:ARG:HE	1.55	0.71
2:A:972:LEU:HB2	2:A:1044:ARG:HE	1.55	0.71
2:G:972:LEU:HB2	2:G:1044:ARG:HE	1.55	0.71
2:G:897:ARG:HD3	2:G:905:PRO:HD3	1.70	0.71
2:G:3110:LEU:HD13	2:G:3183:VAL:HG12	1.71	0.71
2:I:2967:MET:HE2	2:I:3045:LYS:HB3	1.71	0.71
2:A:2967:MET:HE2	2:A:3045:LYS:HB3	1.71	0.71
3:M:66:ARG:HH11	3:M:83:ASN:HB3	1.56	0.71
2:I:897:ARG:HD3	2:I:905:PRO:HD3	1.71	0.71
3:E:66:ARG:HH11	3:E:83:ASN:HB3	1.56	0.70
2:A:3110:LEU:HD13	2:A:3183:VAL:HG12	1.71	0.70
2:G:220:LEU:HD12	2:G:390:LEU:HB3	1.71	0.70
2:D:130:LYS:NZ	2:G:2459:SER:O	2.24	0.70
2:D:2248:ARG:HE	2:D:3868:ARG:HD2	1.55	0.70
3:K:66:ARG:HH11	3:K:83:ASN:HB3	1.56	0.70
2:D:3110:LEU:HD13	2:D:3183:VAL:HG12	1.71	0.70
2:A:130:LYS:NZ	2:D:2459:SER:O	2.25	0.70
2:I:130:LYS:NZ	2:A:2459:SER:O	2.24	0.70
2:G:2248:ARG:HE	2:G:3868:ARG:HD2	1.55	0.70
3:C:66:ARG:HH11	3:C:83:ASN:HB3	1.56	0.70
2:A:2677:LYS:HE3	2:A:2909:ASP:HB2	1.74	0.69
2:I:2459:SER:O	2:G:130:LYS:NZ	2.24	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2677:LYS:HE3	2:G:2909:ASP:HB2	1.74	0.69
2:D:2967:MET:HE2	2:D:3045:LYS:HB3	1.73	0.69
2:I:4918:ILE:HD11	2:A:4888:TYR:HA	1.75	0.69
2:I:2677:LYS:HE3	2:I:2909:ASP:HB2	1.74	0.68
2:D:2677:LYS:HE3	2:D:2909:ASP:HB2	1.73	0.68
2:G:3534:MET:HA	2:G:3537:LYS:HB2	1.75	0.68
2:I:3107:VAL:HG21	2:I:3171:SER:HB2	1.76	0.68
2:I:3534:MET:HA	2:I:3537:LYS:HB2	1.75	0.68
2:A:2779:GLU:HG3	2:A:2792:ARG:HG2	1.76	0.68
2:A:3107:VAL:HG21	2:A:3171:SER:HB2	1.76	0.68
2:D:3534:MET:HA	2:D:3537:LYS:HB2	1.75	0.68
2:D:2960:LEU:HD13	2:D:3038:MET:HG3	1.76	0.68
2:D:4918:ILE:HD11	2:G:4888:TYR:HA	1.76	0.68
2:G:891:TRP:HA	2:G:902:ARG:HB3	1.76	0.68
2:A:2116:LEU:O	2:A:2120:MET:HG2	1.95	0.67
2:A:2960:LEU:HD13	2:A:3038:MET:HG3	1.76	0.67
2:D:2971:GLN:HA	2:D:2974:ILE:HG12	1.76	0.67
2:G:2967:MET:HE2	2:G:3045:LYS:HB3	1.75	0.67
3:K:38:ARG:HG3	3:K:46:GLU:HG3	1.76	0.67
2:A:3534:MET:HA	2:A:3537:LYS:HB2	1.75	0.67
3:E:38:ARG:HG3	3:E:46:GLU:HG3	1.76	0.67
2:I:2960:LEU:HD13	2:I:3038:MET:HG3	1.76	0.67
2:I:4888:TYR:HA	2:G:4918:ILE:HD11	1.76	0.67
2:I:2971:GLN:HA	2:I:2974:ILE:HG12	1.76	0.67
2:I:891:TRP:HA	2:I:902:ARG:HB3	1.76	0.67
2:I:2116:LEU:O	2:I:2120:MET:HG2	1.95	0.67
2:G:2960:LEU:HD13	2:G:3038:MET:HG3	1.76	0.67
2:D:891:TRP:HA	2:D:902:ARG:HB3	1.76	0.67
2:D:2116:LEU:O	2:D:2120:MET:HG2	1.94	0.67
2:G:220:LEU:HD21	2:G:262:LEU:HD23	1.76	0.67
2:G:2116:LEU:O	2:G:2120:MET:HG2	1.94	0.67
2:I:1180:ARG:HG3	2:I:1181:GLU:HG3	1.78	0.66
2:A:1180:ARG:HG3	2:A:1181:GLU:HG3	1.78	0.66
2:A:2431:ASP:HB2	2:A:2501:SER:HB2	1.78	0.66
2:A:2971:GLN:HA	2:A:2974:ILE:HG12	1.76	0.66
2:D:2431:ASP:HB2	2:D:2501:SER:HB2	1.78	0.66
2:G:2779:GLU:HG3	2:G:2792:ARG:HG2	1.76	0.66
2:I:2431:ASP:HB2	2:I:2501:SER:HB2	1.78	0.66
2:G:2431:ASP:HB2	2:G:2501:SER:HB2	1.78	0.66
2:G:2971:GLN:HA	2:G:2974:ILE:HG12	1.76	0.66
2:D:1180:ARG:HG3	2:D:1181:GLU:HG3	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1180:ARG:HG3	2:G:1181:GLU:HG3	1.78	0.66
2:I:220:LEU:HD21	2:I:262:LEU:HD23	1.76	0.66
2:A:399:GLN:O	2:A:403:MET:HG3	1.96	0.66
2:A:220:LEU:HD21	2:A:262:LEU:HD23	1.76	0.66
2:A:891:TRP:HA	2:A:902:ARG:HB3	1.76	0.66
2:A:4918:ILE:HD11	2:D:4888:TYR:HA	1.77	0.66
2:D:2779:GLU:HG3	2:D:2792:ARG:HG2	1.76	0.66
2:D:3107:VAL:HG21	2:D:3171:SER:HB2	1.76	0.66
2:G:2645:THR:HB	2:G:2702:CYS:HA	1.78	0.66
2:G:3107:VAL:HG21	2:G:3171:SER:HB2	1.76	0.66
2:I:2779:GLU:HG3	2:I:2792:ARG:HG2	1.76	0.66
2:A:1568:LYS:HE2	2:A:1574:PRO:HD3	1.78	0.66
3:C:38:ARG:HG3	3:C:46:GLU:HG3	1.76	0.66
2:D:220:LEU:HD21	2:D:262:LEU:HD23	1.76	0.66
2:D:758:ARG:HH11	2:D:761:GLY:HA2	1.61	0.65
2:I:399:GLN:O	2:I:403:MET:HG3	1.96	0.65
2:I:2645:THR:HB	2:I:2702:CYS:HA	1.78	0.65
2:D:1568:LYS:HE2	2:D:1574:PRO:HD3	1.78	0.65
2:D:3780:LEU:HD11	2:D:3816:MET:HB3	1.78	0.65
2:G:4818:MET:N	2:G:4818:MET:SD	2.70	0.65
2:A:4651:THR:HG22	2:A:4799:SER:HB3	1.78	0.65
2:D:4818:MET:N	2:D:4818:MET:SD	2.70	0.65
3:M:38:ARG:HG3	3:M:46:GLU:HG3	1.76	0.65
2:D:399:GLN:O	2:D:403:MET:HG3	1.96	0.65
2:A:758:ARG:HH11	2:A:761:GLY:HA2	1.61	0.65
2:D:4651:THR:HG22	2:D:4799:SER:HB3	1.78	0.65
2:G:3780:LEU:HD11	2:G:3816:MET:HB3	1.79	0.65
2:I:3780:LEU:HD11	2:I:3816:MET:HB3	1.78	0.65
2:G:399:GLN:O	2:G:403:MET:HG3	1.96	0.65
2:G:2624:ARG:NH2	2:G:2915:GLU:OE2	2.27	0.65
2:D:640:TYR:HB3	2:D:1613:LEU:HD11	1.79	0.65
2:G:4651:THR:HG22	2:G:4799:SER:HB3	1.78	0.65
2:I:4651:THR:HG22	2:I:4799:SER:HB3	1.78	0.65
2:D:2645:THR:HB	2:D:2702:CYS:HA	1.78	0.65
2:A:4818:MET:N	2:A:4818:MET:SD	2.70	0.64
2:I:2624:ARG:NH2	2:I:2915:GLU:OE2	2.27	0.64
2:A:3780:LEU:HD11	2:A:3816:MET:HB3	1.78	0.64
2:G:1568:LYS:HE2	2:G:1574:PRO:HD3	1.78	0.64
2:I:4818:MET:N	2:I:4818:MET:SD	2.70	0.64
2:D:363:ASP:HB3	2:D:366:ALA:HB3	1.79	0.64
2:G:640:TYR:HB3	2:G:1613:LEU:HD11	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:758:ARG:HH11	2:I:761:GLY:HA2	1.61	0.64
2:A:2645:THR:HB	2:A:2702:CYS:HA	1.78	0.64
2:G:601:ASP:OD1	2:G:1668:ARG:NH2	2.31	0.64
2:A:3132:THR:HG23	2:A:3136:LEU:HD12	1.80	0.64
2:I:3132:THR:HG23	2:I:3136:LEU:HD12	1.80	0.64
2:D:985:VAL:HG22	2:D:1043:VAL:HG21	1.80	0.64
2:D:4963:ILE:HG13	2:D:5030:LYS:HZ1	1.63	0.63
2:A:601:ASP:OD1	2:A:1668:ARG:NH2	2.31	0.63
2:D:601:ASP:OD1	2:D:1668:ARG:NH2	2.31	0.63
2:A:2624:ARG:NH2	2:A:2915:GLU:OE2	2.27	0.63
2:A:4963:ILE:HG13	2:A:5030:LYS:HZ1	1.63	0.63
2:G:3535:LEU:HB3	2:G:3539:ARG:HH21	1.64	0.63
2:I:1568:LYS:HE2	2:I:1574:PRO:HD3	1.78	0.63
2:G:758:ARG:HH11	2:G:761:GLY:HA2	1.61	0.63
2:G:985:VAL:HG22	2:G:1043:VAL:HG21	1.80	0.63
2:I:640:TYR:HB3	2:I:1613:LEU:HD11	1.79	0.63
2:I:1110:ARG:NH2	2:I:1112:ASP:OD2	2.32	0.63
2:A:3535:LEU:HB3	2:A:3539:ARG:HH21	1.64	0.63
2:D:1519:LEU:HD11	2:D:1572:ILE:HD13	1.80	0.63
2:G:663:TYR:HE1	2:G:745:SER:HB3	1.64	0.63
2:I:4963:ILE:HG13	2:I:5030:LYS:HZ1	1.64	0.63
2:D:3535:LEU:HB3	2:D:3539:ARG:HH21	1.64	0.63
2:I:601:ASP:OD1	2:I:1668:ARG:NH2	2.31	0.63
2:I:1519:LEU:HD11	2:I:1572:ILE:HD13	1.80	0.63
2:A:1110:ARG:NH2	2:A:1112:ASP:OD2	2.32	0.62
2:D:3157:ILE:HG23	2:D:3161:VAL:HG12	1.81	0.62
2:I:985:VAL:HG22	2:I:1043:VAL:HG21	1.80	0.62
2:A:929:LEU:HA	2:A:932:LEU:HD12	1.81	0.62
2:D:663:TYR:HE1	2:D:745:SER:HB3	1.64	0.62
2:G:3157:ILE:HG23	2:G:3161:VAL:HG12	1.81	0.62
2:G:4852:THR:HG21	2:G:4883:TYR:HA	1.81	0.62
2:A:663:TYR:HE1	2:A:745:SER:HB3	1.64	0.62
2:G:1519:LEU:HD11	2:G:1572:ILE:HD13	1.80	0.62
2:I:663:TYR:HE1	2:I:745:SER:HB3	1.64	0.62
2:I:3245:VAL:HG12	2:I:3248:ARG:HH12	1.65	0.62
2:I:3535:LEU:HB3	2:I:3539:ARG:HH21	1.64	0.62
2:A:640:TYR:HB3	2:A:1613:LEU:HD11	1.79	0.62
2:A:5027:CYS:SG	2:A:5030:LYS:NZ	2.66	0.62
2:G:1110:ARG:NH2	2:G:1112:ASP:OD2	2.32	0.62
2:G:2591:ARG:NH2	2:G:2629:ASP:OD2	2.32	0.62
2:I:929:LEU:HA	2:I:932:LEU:HD12	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1220:GLN:HG3	2:G:3519:PRO:HB3	1.82	0.62
2:D:5027:CYS:SG	2:D:5030:LYS:NZ	2.66	0.62
2:G:3132:THR:HG23	2:G:3136:LEU:HD12	1.80	0.62
2:I:4852:THR:HG21	2:I:4883:TYR:HA	1.81	0.62
2:D:1110:ARG:NH2	2:D:1112:ASP:OD2	2.32	0.62
2:D:4852:THR:HG21	2:D:4883:TYR:HA	1.81	0.62
2:I:2591:ARG:NH2	2:I:2629:ASP:OD2	2.33	0.62
2:D:3132:THR:HG23	2:D:3136:LEU:HD12	1.80	0.62
2:A:985:VAL:HG22	2:A:1043:VAL:HG21	1.80	0.61
2:A:3245:VAL:HG12	2:A:3248:ARG:HH12	1.65	0.61
2:D:2591:ARG:NH2	2:D:2629:ASP:OD2	2.33	0.61
2:A:1220:GLN:HG3	2:D:3519:PRO:HB3	1.81	0.61
2:A:1519:LEU:HD11	2:A:1572:ILE:HD13	1.80	0.61
2:I:3157:ILE:HG23	2:I:3161:VAL:HG12	1.81	0.61
2:A:2591:ARG:NH2	2:A:2629:ASP:OD2	2.33	0.61
2:D:929:LEU:HA	2:D:932:LEU:HD12	1.81	0.61
2:G:783:PHE:HB2	2:G:787:VAL:HG21	1.83	0.61
2:A:4852:THR:HG21	2:A:4883:TYR:HA	1.81	0.61
2:D:3557:LEU:HD21	2:D:3589:PRO:HB3	1.82	0.61
2:G:3245:VAL:HG12	2:G:3248:ARG:HH12	1.65	0.61
2:G:4963:ILE:HG13	2:G:5030:LYS:HZ1	1.66	0.61
2:A:3557:LEU:HD21	2:A:3589:PRO:HB3	1.82	0.61
2:D:783:PHE:HB2	2:D:787:VAL:HG21	1.82	0.61
2:G:929:LEU:HA	2:G:932:LEU:HD12	1.81	0.61
2:A:3157:ILE:HG23	2:A:3161:VAL:HG12	1.81	0.61
2:A:3590:GLU:O	2:A:3594:ARG:HG2	2.01	0.61
2:I:3557:LEU:HD21	2:I:3589:PRO:HB3	1.82	0.61
2:D:3937:TYR:O	2:D:4002:LYS:NZ	2.34	0.61
2:G:3557:LEU:HD21	2:G:3589:PRO:HB3	1.82	0.60
2:I:4576:ILE:HG21	2:I:4643:LEU:HB2	1.83	0.60
2:A:365:LYS:O	2:A:369:LEU:HG	2.02	0.60
2:A:4576:ILE:HG21	2:A:4643:LEU:HB2	1.83	0.60
2:D:3245:VAL:HG12	2:D:3248:ARG:HH12	1.64	0.60
2:I:232:THR:HG22	2:I:258:SER:HB3	1.84	0.60
2:A:265:LEU:HD12	2:A:279:PRO:HB2	1.83	0.60
2:D:1095:VAL:HB	2:D:1199:VAL:HG23	1.84	0.60
2:D:2393:ASP:OD1	2:D:2417:HIS:ND1	2.34	0.60
2:G:232:THR:HG22	2:G:258:SER:HB3	1.84	0.60
2:I:3519:PRO:HB3	2:G:1220:GLN:HG3	1.82	0.60
2:G:2534:ALA:HB1	2:G:2588:ARG:HE	1.67	0.60
2:G:3590:GLU:O	2:G:3594:ARG:HG2	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:983:THR:O	2:I:987:ARG:HD2	2.02	0.60
2:D:2534:ALA:HB1	2:D:2588:ARG:HE	1.67	0.60
2:D:897:ARG:NH1	3:E:102:ASN:O	2.35	0.60
2:D:4576:ILE:HG21	2:D:4643:LEU:HB2	1.83	0.60
2:G:3102:ASP:HA	2:G:3105:LYS:HE2	1.84	0.60
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.34	0.60
2:I:4241:THR:O	2:I:4245:MET:HG2	2.01	0.60
2:A:232:THR:HG22	2:A:258:SER:HB3	1.84	0.60
2:A:983:THR:O	2:A:987:ARG:HD2	2.02	0.60
2:I:1220:GLN:HG3	2:A:3519:PRO:HB3	1.83	0.60
2:A:3821:LYS:O	2:A:3824:LYS:NZ	2.35	0.60
2:A:3937:TYR:O	2:A:4002:LYS:NZ	2.34	0.60
2:D:1448:VAL:HG12	2:D:1554:VAL:HG23	1.84	0.60
2:D:3102:ASP:HA	2:D:3105:LYS:HE2	1.84	0.60
2:I:340:LYS:O	2:I:344:SER:OG	2.20	0.60
2:I:365:LYS:HD2	2:I:368:ARG:HD2	1.83	0.60
2:I:783:PHE:HB2	2:I:787:VAL:HG21	1.83	0.60
2:I:5014:TYR:HE2	7:I:5104:CFF:H101	1.66	0.60
2:A:4152:GLU:OE1	2:A:4192:ARG:NH1	2.35	0.60
2:G:983:THR:O	2:G:987:ARG:HD2	2.02	0.60
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.83	0.60
2:I:265:LEU:HD12	2:I:279:PRO:HB2	1.83	0.60
2:A:783:PHE:HB2	2:A:787:VAL:HG21	1.82	0.60
2:D:232:THR:HG22	2:D:258:SER:HB3	1.84	0.60
2:I:3590:GLU:O	2:I:3594:ARG:HG2	2.01	0.59
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.34	0.59
2:I:4090:LYS:HG2	2:I:4123:ILE:HD11	1.84	0.59
2:A:1095:VAL:HB	2:A:1199:VAL:HG23	1.84	0.59
2:G:4576:ILE:HG21	2:G:4643:LEU:HB2	1.83	0.59
2:I:551:LEU:HB3	2:I:589:LEU:HD21	1.85	0.59
2:I:897:ARG:NH1	3:K:102:ASN:O	2.34	0.59
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.84	0.59
2:A:2534:ALA:HB1	2:A:2588:ARG:HE	1.67	0.59
1:F:3:GLU:N	1:F:3:GLU:OE2	2.35	0.59
2:I:871:ARG:HG2	2:I:925:SER:HB2	1.84	0.59
2:I:5013:MET:HE1	2:I:5021:PHE:HB3	1.84	0.59
1:J:3:GLU:N	1:J:3:GLU:OE2	2.35	0.59
2:G:1448:VAL:HG12	2:G:1554:VAL:HG23	1.84	0.59
2:G:4090:LYS:HG2	2:G:4123:ILE:HD11	1.84	0.59
1:H:3:GLU:N	1:H:3:GLU:OE2	2.35	0.59
2:I:359:TYR:CE1	2:I:385:ASP:HB2	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:371:VAL:HG12	2:I:373:LYS:H	1.67	0.59
2:I:2534:ALA:HB1	2:I:2588:ARG:HE	1.67	0.59
2:A:4090:LYS:HG2	2:A:4123:ILE:HD11	1.84	0.59
2:D:3590:GLU:O	2:D:3594:ARG:HG2	2.01	0.59
2:I:2656:CYS:SG	2:I:2657:LEU:N	2.76	0.59
2:D:2777:TYR:HB3	2:D:2791:LEU:HD23	1.85	0.59
2:G:871:ARG:HG2	2:G:925:SER:HB2	1.84	0.59
2:G:4152:GLU:OE1	2:G:4192:ARG:NH1	2.35	0.59
2:I:2393:ASP:OD1	2:I:2417:HIS:ND1	2.34	0.59
2:I:2777:TYR:HB3	2:I:2791:LEU:HD23	1.85	0.59
2:I:3102:ASP:HA	2:I:3105:LYS:HE2	1.84	0.59
2:I:4152:GLU:OE1	2:I:4192:ARG:NH1	2.35	0.59
2:A:2777:TYR:HB3	2:A:2791:LEU:HD23	1.85	0.59
2:I:4836:GLN:O	2:I:4839:MET:HB3	2.03	0.59
3:K:105:ASN:ND2	3:K:112:ASP:OD1	2.36	0.59
2:A:551:LEU:HB3	2:A:589:LEU:HD21	1.85	0.59
2:A:2656:CYS:SG	2:A:2657:LEU:N	2.76	0.59
2:D:2624:ARG:NH2	2:D:2915:GLU:OE2	2.27	0.59
2:A:2472:LEU:HD23	2:A:2473:PRO:HD2	1.85	0.59
2:D:983:THR:O	2:D:987:ARG:HD2	2.01	0.59
2:D:4090:LYS:HG2	2:D:4123:ILE:HD11	1.84	0.59
2:I:3504:SER:O	2:I:3507:THR:OG1	2.21	0.59
1:L:3:GLU:N	1:L:3:GLU:OE2	2.35	0.59
2:A:1448:VAL:HG12	2:A:1554:VAL:HG23	1.84	0.59
2:A:2393:ASP:OD1	2:A:2417:HIS:ND1	2.34	0.59
2:D:4152:GLU:OE1	2:D:4192:ARG:NH1	2.35	0.59
2:G:265:LEU:HD12	2:G:279:PRO:HB2	1.83	0.59
2:G:897:ARG:NH1	3:M:102:ASN:O	2.36	0.59
2:G:2777:TYR:HB3	2:G:2791:LEU:HD23	1.84	0.59
2:I:3219:TYR:HE1	2:I:3232:LEU:HB3	1.68	0.59
2:D:265:LEU:HD12	2:D:279:PRO:HB2	1.83	0.59
3:M:105:ASN:ND2	3:M:112:ASP:OD1	2.36	0.59
2:A:3219:TYR:HE1	2:A:3232:LEU:HB3	1.68	0.58
2:D:551:LEU:HB3	2:D:589:LEU:HD21	1.85	0.58
2:D:3579:LEU:HD23	2:D:3582:ARG:HB2	1.85	0.58
2:G:41:GLY:O	2:G:45:ARG:NH1	2.37	0.58
2:G:551:LEU:HB3	2:G:589:LEU:HD21	1.85	0.58
2:G:2472:LEU:HD23	2:G:2473:PRO:HD2	1.85	0.58
2:I:1448:VAL:HG12	2:I:1554:VAL:HG23	1.84	0.58
2:G:2656:CYS:SG	2:G:2657:LEU:N	2.76	0.58
2:I:2875:ALA:HB2	2:I:2927:LEU:HD22	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3579:LEU:HD23	2:I:3582:ARG:HB2	1.85	0.58
2:A:41:GLY:O	2:A:45:ARG:NH1	2.37	0.58
2:A:3102:ASP:HA	2:A:3105:LYS:HE2	1.84	0.58
2:D:2875:ALA:HB2	2:D:2927:LEU:HD22	1.84	0.58
2:G:221:ARG:NH2	2:G:255:HIS:O	2.36	0.58
2:A:4836:GLN:O	2:A:4839:MET:HB3	2.03	0.58
2:D:219:VAL:HG21	2:D:398:SER:HB2	1.86	0.58
2:G:366:ALA:HB1	2:G:371:VAL:HG12	1.85	0.58
2:G:596:ASN:OD1	2:G:598:LYS:NZ	2.37	0.58
2:G:3821:LYS:O	2:G:3824:LYS:NZ	2.35	0.58
2:A:3504:SER:O	2:A:3507:THR:OG1	2.21	0.58
3:C:105:ASN:ND2	3:C:112:ASP:OD1	2.36	0.58
2:D:340:LYS:O	2:D:344:SER:OG	2.20	0.58
3:E:105:ASN:ND2	3:E:112:ASP:OD1	2.35	0.58
2:I:596:ASN:OD1	2:I:598:LYS:NZ	2.37	0.58
2:G:219:VAL:HG21	2:G:398:SER:HB2	1.86	0.58
2:I:2123:LEU:O	2:I:2127:GLN:HG2	2.03	0.58
2:A:871:ARG:HG2	2:A:925:SER:HB2	1.84	0.58
2:A:2624:ARG:HH12	2:A:2912:THR:HG22	1.69	0.58
2:D:2123:LEU:O	2:D:2127:GLN:HG2	2.03	0.58
2:D:2656:CYS:SG	2:D:2657:LEU:N	2.76	0.58
2:G:2123:LEU:O	2:G:2127:GLN:HG2	2.03	0.58
2:G:3504:SER:O	2:G:3507:THR:OG1	2.21	0.58
2:G:4836:GLN:O	2:G:4839:MET:HB3	2.03	0.58
2:I:3821:LYS:O	2:I:3824:LYS:NZ	2.35	0.57
2:A:340:LYS:O	2:A:344:SER:OG	2.20	0.57
2:A:2875:ALA:HB2	2:A:2927:LEU:HD22	1.84	0.57
2:A:3031:ALA:O	2:A:3036:LYS:NZ	2.29	0.57
3:C:32:ASN:OD1	3:C:33:SER:N	2.37	0.57
2:D:2472:LEU:HD23	2:D:2473:PRO:HD2	1.85	0.57
2:D:3219:TYR:HE1	2:D:3232:LEU:HB3	1.68	0.57
3:E:32:ASN:OD1	3:E:33:SER:N	2.37	0.57
2:I:41:GLY:O	2:I:45:ARG:NH1	2.37	0.57
3:K:32:ASN:OD1	3:K:33:SER:N	2.37	0.57
2:A:219:VAL:HG21	2:A:398:SER:HB2	1.86	0.57
2:G:340:LYS:O	2:G:344:SER:OG	2.20	0.57
2:G:2875:ALA:HB2	2:G:2927:LEU:HD22	1.84	0.57
2:G:3219:TYR:HE1	2:G:3232:LEU:HB3	1.68	0.57
2:I:2624:ARG:HH12	2:I:2912:THR:HG22	1.69	0.57
2:D:596:ASN:OD1	2:D:598:LYS:NZ	2.37	0.57
2:D:3100:SER:HB3	2:D:3167:ARG:HE	1.70	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2958:GLY:O	2:G:2962:GLN:HG2	2.04	0.57
2:A:469:ARG:O	2:A:473:ASN:ND2	2.37	0.57
2:D:41:GLY:O	2:D:45:ARG:NH1	2.37	0.57
2:D:871:ARG:HG2	2:D:925:SER:HB2	1.84	0.57
2:G:5014:TYR:HE2	7:G:5104:CFF:H101	1.69	0.57
2:I:219:VAL:HG21	2:I:398:SER:HB2	1.86	0.57
2:I:5027:CYS:SG	2:I:5030:LYS:NZ	2.66	0.57
2:A:2123:LEU:O	2:A:2127:GLN:HG2	2.04	0.57
2:D:2624:ARG:HH12	2:D:2912:THR:HG22	1.69	0.57
2:D:4836:GLN:O	2:D:4839:MET:HB3	2.03	0.57
2:G:2393:ASP:OD1	2:G:2417:HIS:ND1	2.34	0.57
2:G:3579:LEU:HD23	2:G:3582:ARG:HB2	1.85	0.57
2:I:2472:LEU:HD23	2:I:2473:PRO:HD2	1.85	0.57
2:A:3579:LEU:HD23	2:A:3582:ARG:HB2	1.85	0.57
2:D:5014:TYR:HE2	7:D:5104:CFF:H101	1.69	0.57
2:G:2624:ARG:HH12	2:G:2912:THR:HG22	1.69	0.57
3:M:32:ASN:OD1	3:M:33:SER:N	2.37	0.57
2:I:469:ARG:O	2:I:473:ASN:ND2	2.38	0.57
2:A:1089:TYR:HD1	2:A:1152:MET:HG3	1.70	0.57
2:I:999:ASP:O	2:I:1003:GLN:HG3	2.05	0.57
2:A:3100:SER:HB3	2:A:3167:ARG:HE	1.70	0.57
2:D:469:ARG:O	2:D:473:ASN:ND2	2.37	0.57
2:D:2958:GLY:O	2:D:2962:GLN:HG2	2.04	0.57
2:I:2958:GLY:O	2:I:2962:GLN:HG2	2.05	0.57
2:I:835:ARG:NH1	2:I:1210:SER:OG	2.38	0.56
3:K:6:GLU:HG3	3:K:121:THR:HG22	1.87	0.56
2:A:835:ARG:NH1	2:A:1210:SER:OG	2.38	0.56
2:A:897:ARG:NH1	3:C:102:ASN:O	2.38	0.56
2:A:2527:LEU:HG	2:A:2531:ARG:HH21	1.70	0.56
2:I:1286:MET:HE2	2:I:1464:PHE:HB3	1.87	0.56
2:A:596:ASN:OD1	2:A:598:LYS:NZ	2.37	0.56
2:A:999:ASP:O	2:A:1003:GLN:HG3	2.05	0.56
2:D:2229:VAL:HG11	2:D:2265:LEU:HD11	1.87	0.56
3:E:6:GLU:HG3	3:E:121:THR:HG22	1.87	0.56
2:G:999:ASP:O	2:G:1003:GLN:HG3	2.05	0.56
2:I:4242:ILE:O	2:I:4246:GLN:HG3	2.04	0.56
3:C:6:GLU:HG3	3:C:121:THR:HG22	1.87	0.56
2:D:24:CYS:SG	2:D:25:SER:N	2.78	0.56
2:D:221:ARG:NH2	2:D:255:HIS:O	2.36	0.56
2:D:835:ARG:NH1	2:D:1210:SER:OG	2.38	0.56
2:D:999:ASP:O	2:D:1003:GLN:HG3	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4983:HIS:O	6:D:5103:ATP:N6	2.38	0.56
2:G:371:VAL:HG22	2:G:373:LYS:H	1.69	0.56
2:G:469:ARG:O	2:G:473:ASN:ND2	2.37	0.56
2:G:835:ARG:NH1	2:G:1210:SER:OG	2.38	0.56
2:G:1286:MET:HE2	2:G:1464:PHE:HB3	1.87	0.56
2:G:2229:VAL:HG11	2:G:2265:LEU:HD11	1.87	0.56
2:G:5026:ASP:HA	2:G:5030:LYS:HE2	1.88	0.56
3:M:6:GLU:HG3	3:M:121:THR:HG22	1.87	0.56
2:I:2527:LEU:HG	2:I:2531:ARG:HH21	1.70	0.56
2:A:135:VAL:HG11	2:A:180:LEU:HD21	1.87	0.56
2:A:5026:ASP:HA	2:A:5030:LYS:HE2	1.88	0.56
2:D:3031:ALA:O	2:D:3036:LYS:NZ	2.29	0.56
2:G:3100:SER:HB3	2:G:3167:ARG:HE	1.69	0.56
2:I:2827:ARG:NH2	2:I:2935:TYR:OH	2.39	0.56
2:A:2958:GLY:O	2:A:2962:GLN:HG2	2.04	0.56
3:C:85:LEU:HD13	3:C:125:VAL:HG13	1.88	0.56
2:D:2527:LEU:HG	2:D:2531:ARG:HH21	1.70	0.56
2:I:177:GLU:OE2	2:A:2452:ARG:NH2	2.37	0.56
2:D:1815:LEU:HD22	2:D:1845:VAL:HG21	1.87	0.56
2:D:2881:ASN:HA	2:D:2884:ASN:ND2	2.21	0.56
2:A:1299:GLN:NE2	1:J:32:ASN:OD1	2.39	0.56
2:A:3410:PRO:HA	2:A:3413:ILE:HD12	1.88	0.56
2:D:110:ARG:NH2	2:D:117:TYR:OH	2.39	0.56
3:E:40:ALA:HB3	3:E:43:LYS:HB3	1.88	0.56
2:I:1089:TYR:HD1	2:I:1152:MET:HG3	1.70	0.56
2:I:5026:ASP:HA	2:I:5030:LYS:HE2	1.88	0.56
2:D:2827:ARG:NH2	2:D:2935:TYR:OH	2.39	0.56
2:D:3147:ILE:HD11	2:D:3153:GLY:HA2	1.87	0.56
2:D:3504:SER:O	2:D:3507:THR:OG1	2.21	0.56
2:I:135:VAL:HG11	2:I:180:LEU:HD21	1.87	0.56
2:I:894:GLY:HA3	2:I:903:LEU:HD13	1.88	0.56
2:I:2314:LEU:HD23	2:I:2314:LEU:H	1.71	0.56
2:A:2827:ARG:NH2	2:A:2935:TYR:OH	2.39	0.56
2:D:5026:ASP:HA	2:D:5030:LYS:HE2	1.88	0.56
2:G:110:ARG:NH2	2:G:117:TYR:OH	2.39	0.56
3:M:40:ALA:HB3	3:M:43:LYS:HB3	1.88	0.56
2:I:221:ARG:NH2	2:I:255:HIS:O	2.36	0.56
2:I:3100:SER:HB3	2:I:3167:ARG:HE	1.69	0.56
3:C:11:LEU:HG	3:C:124:THR:HB	1.88	0.56
2:D:3402:CYS:HG	2:D:3451:PHE:HE1	1.54	0.56
2:D:3410:PRO:HA	2:D:3413:ILE:HD12	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:11:LEU:HG	3:E:124:THR:HB	1.88	0.56
2:G:24:CYS:SG	2:G:25:SER:N	2.78	0.56
2:G:1089:TYR:HD1	2:G:1152:MET:HG3	1.70	0.56
2:G:5027:CYS:SG	2:G:5030:LYS:NZ	2.66	0.56
2:I:110:ARG:NH2	2:I:117:TYR:OH	2.39	0.55
2:I:2624:ARG:HH21	2:I:2906:VAL:HG21	1.71	0.55
2:A:24:CYS:SG	2:A:25:SER:N	2.78	0.55
2:G:135:VAL:HG11	2:G:180:LEU:HD21	1.87	0.55
2:G:157:ARG:NH1	2:G:167:ASP:OD2	2.39	0.55
2:G:894:GLY:HA3	2:G:903:LEU:HD13	1.88	0.55
2:G:2827:ARG:NH2	2:G:2935:TYR:OH	2.39	0.55
2:G:3034:LYS:O	2:G:3037:GLU:HG3	2.06	0.55
2:I:3036:LYS:HD2	2:I:3079:THR:HG21	1.88	0.55
2:A:3034:LYS:O	2:A:3037:GLU:HG3	2.07	0.55
2:D:1089:TYR:HD1	2:D:1152:MET:HG3	1.70	0.55
2:G:4983:HIS:O	6:G:5103:ATP:N6	2.38	0.55
2:I:24:CYS:SG	2:I:25:SER:N	2.78	0.55
2:I:157:ARG:NH1	2:I:167:ASP:OD2	2.39	0.55
2:A:1815:LEU:HD22	2:A:1845:VAL:HG21	1.88	0.55
2:D:2314:LEU:HD23	2:D:2314:LEU:H	1.72	0.55
2:G:2314:LEU:HD23	2:G:2314:LEU:H	1.72	0.55
2:G:3036:LYS:HD2	2:G:3079:THR:HG21	1.88	0.55
2:I:2229:VAL:HG11	2:I:2265:LEU:HD11	1.87	0.55
2:D:3530:GLN:O	2:D:3533:ILE:HB	2.07	0.55
2:I:247:TYR:HE2	2:I:359:TYR:HA	1.71	0.55
2:I:3034:LYS:O	2:I:3037:GLU:HG3	2.07	0.55
2:A:961:MET:HG3	2:A:962:SER:H	1.72	0.55
2:A:2314:LEU:HD23	2:A:2314:LEU:H	1.71	0.55
2:A:2624:ARG:HH21	2:A:2906:VAL:HG21	1.71	0.55
2:G:131:LEU:O	2:G:178:ARG:NH1	2.40	0.55
2:G:1815:LEU:HD22	2:G:1845:VAL:HG21	1.88	0.55
3:M:11:LEU:HG	3:M:124:THR:HB	1.88	0.55
2:I:870:ILE:HD11	2:I:1049:TYR:HB3	1.89	0.55
2:I:3147:ILE:HD11	2:I:3153:GLY:HA2	1.87	0.55
3:K:11:LEU:HG	3:K:124:THR:HB	1.88	0.55
2:A:3147:ILE:HD11	2:A:3153:GLY:HA2	1.88	0.55
2:D:3821:LYS:O	2:D:3824:LYS:NZ	2.35	0.55
2:G:3530:GLN:O	2:G:3533:ILE:HB	2.07	0.55
2:I:2881:ASN:HA	2:I:2884:ASN:ND2	2.21	0.55
2:A:110:ARG:NH2	2:A:117:TYR:OH	2.39	0.55
2:G:2527:LEU:HG	2:G:2531:ARG:HH21	1.70	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3147:ILE:HD11	2:G:3153:GLY:HA2	1.87	0.55
2:G:3410:PRO:HA	2:G:3413:ILE:HD12	1.88	0.55
2:I:359:TYR:HE1	2:I:385:ASP:HB2	1.72	0.55
2:I:3031:ALA:O	2:I:3036:LYS:NZ	2.29	0.55
2:A:221:ARG:NH2	2:A:255:HIS:O	2.36	0.55
2:A:2229:VAL:HG11	2:A:2265:LEU:HD11	1.87	0.55
3:C:40:ALA:HB3	3:C:43:LYS:HB3	1.88	0.55
2:G:2624:ARG:HH21	2:G:2906:VAL:HG21	1.71	0.55
3:M:85:LEU:HD13	3:M:125:VAL:HG13	1.88	0.55
2:I:131:LEU:O	2:I:178:ARG:NH1	2.40	0.55
2:I:3410:PRO:HA	2:I:3413:ILE:HD12	1.88	0.55
2:D:135:VAL:HG11	2:D:180:LEU:HD21	1.87	0.55
2:D:1286:MET:HE2	2:D:1464:PHE:HB3	1.89	0.55
2:D:1299:GLN:NE2	1:F:32:ASN:OD1	2.39	0.55
2:G:870:ILE:HD11	2:G:1049:TYR:HB3	1.89	0.55
2:G:2380:ILE:HG21	2:G:2469:ILE:HD11	1.89	0.55
2:I:622:THR:HG23	2:I:626:LEU:HD22	1.89	0.55
2:I:2867:LEU:HB2	2:I:2928:LYS:HZ3	1.72	0.55
3:K:40:ALA:HB3	3:K:43:LYS:HB3	1.88	0.55
2:A:177:GLU:OE2	2:D:2452:ARG:NH2	2.38	0.55
2:A:2881:ASN:HA	2:A:2884:ASN:ND2	2.21	0.55
3:E:85:LEU:HD13	3:E:125:VAL:HG13	1.88	0.55
2:G:3402:CYS:HG	2:G:3451:PHE:HE1	1.55	0.55
2:I:1815:LEU:HD22	2:I:1845:VAL:HG21	1.88	0.54
2:I:2623:LEU:O	2:I:2627:VAL:HG23	2.07	0.54
2:I:3768:SER:HA	2:I:3771:HIS:CD2	2.42	0.54
2:A:894:GLY:HA3	2:A:903:LEU:HD13	1.88	0.54
2:D:177:GLU:OE2	2:G:2452:ARG:NH2	2.38	0.54
2:D:3768:SER:HA	2:D:3771:HIS:CD2	2.42	0.54
2:A:131:LEU:O	2:A:178:ARG:NH1	2.40	0.54
2:A:317:ARG:NH1	2:A:349:GLN:OE1	2.40	0.54
2:D:317:ARG:NH1	2:D:349:GLN:OE1	2.41	0.54
2:G:2881:ASN:HA	2:G:2884:ASN:ND2	2.21	0.54
2:G:4242:ILE:O	2:G:4246:GLN:HG3	2.06	0.54
2:A:2380:ILE:HG21	2:A:2469:ILE:HD11	1.90	0.54
2:A:4242:ILE:O	2:A:4246:GLN:HG3	2.07	0.54
2:D:894:GLY:HA3	2:D:903:LEU:HD13	1.88	0.54
2:D:961:MET:HG3	2:D:962:SER:H	1.72	0.54
2:D:1033:ARG:HA	2:D:1033:ARG:NE	2.22	0.54
2:D:2624:ARG:HH21	2:D:2906:VAL:HG21	1.71	0.54
2:G:3768:SER:HA	2:G:3771:HIS:CD2	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:793:LEU:HD12	2:I:821:LEU:HD21	1.89	0.54
2:I:858:THR:HA	2:I:861:ILE:HD13	1.89	0.54
2:A:3036:LYS:HD2	2:A:3079:THR:HG21	1.89	0.54
2:A:3768:SER:HA	2:A:3771:HIS:CD2	2.42	0.54
2:D:870:ILE:HD11	2:D:1049:TYR:HB3	1.89	0.54
2:D:2623:LEU:O	2:D:2627:VAL:HG23	2.06	0.54
2:D:4242:ILE:O	2:D:4246:GLN:HG3	2.07	0.54
2:G:3194:LEU:HD21	2:G:3276:MET:SD	2.48	0.54
2:I:3194:LEU:HD21	2:I:3276:MET:SD	2.48	0.54
2:D:2380:ILE:HG21	2:D:2469:ILE:HD11	1.90	0.54
2:G:2623:LEU:O	2:G:2627:VAL:HG23	2.06	0.54
3:K:85:LEU:HD13	3:K:125:VAL:HG13	1.88	0.54
2:A:622:THR:HG23	2:A:626:LEU:HD22	1.89	0.54
2:A:2623:LEU:O	2:A:2627:VAL:HG23	2.06	0.54
2:D:131:LEU:O	2:D:178:ARG:NH1	2.40	0.54
2:D:3017:PHE:HD2	2:D:3039:ILE:HD12	1.73	0.54
2:D:3034:LYS:O	2:D:3037:GLU:HG3	2.06	0.54
2:D:3245:VAL:HG12	2:D:3248:ARG:NH1	2.23	0.54
2:G:793:LEU:HD12	2:G:821:LEU:HD21	1.89	0.54
2:I:2380:ILE:HG21	2:I:2469:ILE:HD11	1.89	0.54
2:I:2452:ARG:NH2	2:G:177:GLU:OE2	2.38	0.54
2:I:4826:ILE:HD12	2:G:4839:MET:SD	2.48	0.54
2:I:5009:TYR:HA	2:I:5012:LYS:HE3	1.89	0.54
2:A:365:LYS:HE2	2:A:369:LEU:HD21	1.90	0.54
2:A:858:THR:HA	2:A:861:ILE:HD13	1.89	0.54
2:A:1033:ARG:NE	2:A:1033:ARG:HA	2.22	0.54
2:A:2247:GLN:NE2	2:A:2278:ALA:O	2.41	0.54
2:A:4853:VAL:HG13	2:D:4807:PHE:HD2	1.72	0.54
2:G:2469:ILE:HD12	2:G:2472:LEU:HD12	1.89	0.54
2:G:2902:HIS:HB3	2:G:2905:LEU:HG	1.90	0.54
2:I:1299:GLN:NE2	1:L:32:ASN:OD1	2.39	0.54
2:A:683:ARG:HG2	2:A:717:ASP:HB3	1.89	0.54
2:G:317:ARG:NH1	2:G:349:GLN:OE1	2.40	0.54
2:A:3530:GLN:O	2:A:3533:ILE:HB	2.07	0.54
2:D:157:ARG:NH1	2:D:167:ASP:OD2	2.39	0.54
2:D:3036:LYS:HD2	2:D:3079:THR:HG21	1.89	0.54
2:G:683:ARG:HG2	2:G:717:ASP:HB3	1.89	0.54
2:G:2867:LEU:HB2	2:G:2928:LYS:HZ3	1.72	0.54
2:I:3530:GLN:O	2:I:3533:ILE:HB	2.07	0.54
2:D:858:THR:HA	2:D:861:ILE:HD13	1.89	0.54
2:D:4839:MET:SD	2:G:4826:ILE:HD12	2.48	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:107:TRP:HE1	3:M:110:PRO:HB2	1.73	0.54
2:I:683:ARG:HG2	2:I:717:ASP:HB3	1.89	0.53
2:I:2902:HIS:HB3	2:I:2905:LEU:HG	1.90	0.53
3:K:107:TRP:HE1	3:K:110:PRO:HB2	1.73	0.53
2:A:3194:LEU:HD21	2:A:3276:MET:SD	2.48	0.53
2:D:3143:LEU:O	2:D:3147:ILE:HG22	2.09	0.53
2:G:858:THR:HA	2:G:861:ILE:HD13	1.89	0.53
2:G:2247:GLN:NE2	2:G:2278:ALA:O	2.41	0.53
2:G:4681:LEU:HD12	2:G:4724:VAL:HG21	1.90	0.53
2:I:1033:ARG:NE	2:I:1033:ARG:HA	2.22	0.53
2:I:4807:PHE:HD2	2:G:4853:VAL:HG13	1.73	0.53
2:A:870:ILE:HD11	2:A:1049:TYR:HB3	1.89	0.53
2:D:622:THR:HG23	2:D:626:LEU:HD22	1.89	0.53
2:D:2599:GLN:O	2:D:2603:ILE:HG12	2.09	0.53
2:I:2599:GLN:O	2:I:2603:ILE:HG12	2.09	0.53
2:I:3017:PHE:HD2	2:I:3039:ILE:HD12	1.73	0.53
2:A:2902:HIS:HB3	2:A:2905:LEU:HG	1.90	0.53
2:A:3245:VAL:HG12	2:A:3248:ARG:NH1	2.23	0.53
2:D:4654:ALA:O	2:D:4658:ILE:HG12	2.09	0.53
2:G:652:ARG:HE	2:G:773:LEU:HD13	1.73	0.53
2:G:3017:PHE:HD2	2:G:3039:ILE:HD12	1.73	0.53
2:I:1699:GLU:HG3	2:I:1810:LYS:HE3	1.91	0.53
2:A:157:ARG:NH1	2:A:167:ASP:OD2	2.39	0.53
2:D:3194:LEU:HD21	2:D:3276:MET:SD	2.48	0.53
2:G:622:THR:HG23	2:G:626:LEU:HD22	1.89	0.53
2:G:1033:ARG:HA	2:G:1033:ARG:NE	2.22	0.53
2:G:2599:GLN:O	2:G:2603:ILE:HG12	2.09	0.53
2:G:3245:VAL:HG12	2:G:3248:ARG:NH1	2.23	0.53
2:I:365:LYS:HE2	2:I:368:ARG:NH1	2.24	0.53
2:I:2247:GLN:NE2	2:I:2278:ALA:O	2.41	0.53
2:I:2469:ILE:HD12	2:I:2472:LEU:HD12	1.89	0.53
2:D:3246:LEU:HA	2:D:3249:LEU:HD13	1.91	0.53
2:D:4681:LEU:HD12	2:D:4724:VAL:HG21	1.90	0.53
2:G:1478:ASP:OD1	2:G:1482:ASN:N	2.42	0.53
2:I:317:ARG:NH1	2:I:349:GLN:OE1	2.40	0.53
2:I:961:MET:HG3	2:I:962:SER:H	1.72	0.53
2:I:2230:THR:HG23	2:I:2270:SER:H	1.74	0.53
2:I:2418:LEU:HD23	2:I:2418:LEU:H	1.74	0.53
2:A:1041:GLN:OE1	2:A:1044:ARG:NH1	2.42	0.53
2:A:2469:ILE:HD12	2:A:2472:LEU:HD12	1.89	0.53
2:A:2599:GLN:O	2:A:2603:ILE:HG12	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:683:ARG:HG2	2:D:717:ASP:HB3	1.89	0.53
2:D:1041:GLN:OE1	2:D:1044:ARG:NH1	2.42	0.53
2:D:2469:ILE:HD12	2:D:2472:LEU:HD12	1.89	0.53
2:D:2867:LEU:HB2	2:D:2928:LYS:HZ3	1.73	0.53
2:D:2902:HIS:HB3	2:D:2905:LEU:HG	1.90	0.53
2:I:652:ARG:HE	2:I:773:LEU:HD13	1.73	0.53
2:I:3078:ARG:HH21	2:I:3152:PHE:HA	1.74	0.53
2:A:2418:LEU:HD23	2:A:2418:LEU:H	1.74	0.53
2:A:3078:ARG:HH21	2:A:3152:PHE:HA	1.74	0.53
2:A:4983:HIS:O	6:A:5103:ATP:N6	2.38	0.53
2:G:2621:HIS:O	2:G:2624:ARG:HG2	2.09	0.53
2:G:3093:ARG:O	2:G:3097:GLU:HG2	2.09	0.53
2:G:3246:LEU:HA	2:G:3249:LEU:HD13	1.90	0.53
2:I:1780:PRO:O	1:L:42:ARG:NH1	2.42	0.53
2:I:4839:MET:SD	2:A:4826:ILE:HD12	2.48	0.53
2:G:4654:ALA:O	2:G:4658:ILE:HG12	2.09	0.53
2:I:3284:TRP:HB3	2:I:3305:THR:HG21	1.91	0.53
2:A:470:SER:HA	2:A:473:ASN:HD21	1.74	0.53
2:A:3017:PHE:HD2	2:A:3039:ILE:HD12	1.73	0.53
2:G:3143:LEU:O	2:G:3147:ILE:HG22	2.09	0.53
2:G:3284:TRP:HB3	2:G:3305:THR:HG21	1.91	0.53
2:I:652:ARG:HD3	2:I:750:LEU:HB3	1.91	0.53
2:I:893:TYR:HA	2:I:904:HIS:H	1.74	0.53
2:I:2288:LEU:O	2:I:3849:ARG:NH1	2.41	0.53
2:I:3368:ARG:O	2:I:3372:VAL:HG23	2.09	0.53
2:A:652:ARG:HE	2:A:773:LEU:HD13	1.73	0.53
2:A:893:TYR:HA	2:A:904:HIS:H	1.74	0.53
2:D:652:ARG:HD3	2:D:750:LEU:HB3	1.91	0.53
2:D:2247:GLN:NE2	2:D:2278:ALA:O	2.41	0.53
2:G:1041:GLN:OE1	2:G:1044:ARG:NH1	2.42	0.53
2:G:1699:GLU:HG3	2:G:1810:LYS:HE3	1.91	0.53
2:G:3078:ARG:HH21	2:G:3152:PHE:HA	1.74	0.53
2:G:4090:LYS:HG3	2:G:4121:GLU:HB3	1.91	0.53
2:I:1478:ASP:OD1	2:I:1482:ASN:N	2.42	0.52
2:I:3093:ARG:O	2:I:3097:GLU:HG2	2.09	0.52
2:I:4853:VAL:HG13	2:A:4807:PHE:HD2	1.74	0.52
2:A:3143:LEU:O	2:A:3147:ILE:HG22	2.09	0.52
2:A:3284:TRP:HB3	2:A:3305:THR:HG21	1.91	0.52
2:A:4654:ALA:O	2:A:4658:ILE:HG12	2.09	0.52
2:G:2230:THR:HG23	2:G:2270:SER:H	1.74	0.52
2:G:3812:VAL:O	2:G:3816:MET:HG3	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4090:LYS:HG3	2:I:4121:GLU:HB3	1.91	0.52
2:A:4240:ASP:OD1	2:A:4675:LYS:NZ	2.36	0.52
2:D:652:ARG:HE	2:D:773:LEU:HD13	1.73	0.52
2:D:793:LEU:HD12	2:D:821:LEU:HD21	1.89	0.52
2:D:2736:ASP:OD1	2:D:2736:ASP:N	2.41	0.52
2:D:2997:PHE:CE2	2:D:3001:ILE:HD11	2.44	0.52
3:E:107:TRP:HE1	3:E:110:PRO:HB2	1.73	0.52
2:G:470:SER:HA	2:G:473:ASN:HD21	1.74	0.52
2:G:2418:LEU:HD23	2:G:2418:LEU:H	1.74	0.52
2:I:2302:LEU:HD23	2:I:2331:TYR:HB2	1.91	0.52
2:I:3143:LEU:O	2:I:3147:ILE:HG22	2.09	0.52
2:I:3245:VAL:HG12	2:I:3248:ARG:NH1	2.23	0.52
2:A:793:LEU:HD12	2:A:821:LEU:HD21	1.90	0.52
2:A:1478:ASP:OD1	2:A:1482:ASN:N	2.42	0.52
2:A:1699:GLU:HG3	2:A:1810:LYS:HE3	1.91	0.52
2:A:2621:HIS:O	2:A:2624:ARG:HG2	2.09	0.52
3:C:107:TRP:HE1	3:C:110:PRO:HB2	1.73	0.52
2:D:470:SER:HA	2:D:473:ASN:HD21	1.74	0.52
2:D:2716:ASP:OD1	2:D:2716:ASP:N	2.42	0.52
2:I:2621:HIS:O	2:I:2624:ARG:HG2	2.09	0.52
2:A:1780:PRO:O	1:J:42:ARG:NH1	2.43	0.52
2:A:2302:LEU:HD23	2:A:2331:TYR:HB2	1.91	0.52
2:D:2621:HIS:O	2:D:2624:ARG:HG2	2.09	0.52
2:D:3078:ARG:HH21	2:D:3152:PHE:HA	1.73	0.52
2:D:3093:ARG:O	2:D:3097:GLU:HG2	2.09	0.52
2:D:4627:MET:SD	2:D:4627:MET:N	2.81	0.52
2:G:652:ARG:HD3	2:G:750:LEU:HB3	1.91	0.52
2:G:893:TYR:HA	2:G:904:HIS:H	1.74	0.52
2:G:2736:ASP:OD1	2:G:2736:ASP:N	2.41	0.52
2:G:2997:PHE:CE2	2:G:3001:ILE:HD11	2.44	0.52
2:I:2012:PHE:CZ	2:I:2031:LEU:HD23	2.45	0.52
2:I:4681:LEU:HD12	2:I:4724:VAL:HG21	1.90	0.52
2:A:574:VAL:HA	2:A:577:ILE:HG12	1.92	0.52
2:A:2867:LEU:HB2	2:A:2928:LYS:HZ3	1.73	0.52
2:A:3093:ARG:O	2:A:3097:GLU:HG2	2.09	0.52
2:A:3368:ARG:O	2:A:3372:VAL:HG23	2.09	0.52
2:A:4681:LEU:HD12	2:A:4724:VAL:HG21	1.90	0.52
2:D:1780:PRO:O	1:F:42:ARG:NH1	2.42	0.52
2:D:2962:GLN:OE1	2:D:2965:ARG:NH1	2.42	0.52
2:D:3284:TRP:HB3	2:D:3305:THR:HG21	1.91	0.52
2:D:3368:ARG:O	2:D:3372:VAL:HG23	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:18:LYS:NZ	1:H:18:LYS:HB3	2.25	0.52
2:I:2997:PHE:CE2	2:I:3001:ILE:HD11	2.44	0.52
2:I:4634:GLU:HG2	2:I:4636:THR:H	1.75	0.52
2:A:2012:PHE:CZ	2:A:2031:LEU:HD23	2.45	0.52
2:A:2230:THR:HG23	2:A:2270:SER:H	1.74	0.52
2:D:1478:ASP:OD1	2:D:1482:ASN:N	2.42	0.52
2:D:1699:GLU:HG3	2:D:1810:LYS:HE3	1.91	0.52
2:G:2962:GLN:OE1	2:G:2965:ARG:NH1	2.42	0.52
1:H:32:ASN:OD1	2:G:1299:GLN:NE2	2.42	0.52
1:H:88:PRO:HB2	2:G:1680:ARG:HH12	1.74	0.52
2:I:1041:GLN:OE1	2:I:1044:ARG:NH1	2.42	0.52
2:I:2716:ASP:OD1	2:I:2716:ASP:N	2.42	0.52
2:A:3812:VAL:O	2:A:3816:MET:HG3	2.10	0.52
2:A:4627:MET:SD	2:A:4627:MET:N	2.81	0.52
2:A:4912:TYR:HD1	5:A:5101:POV:H28	1.75	0.52
2:D:2012:PHE:CZ	2:D:2031:LEU:HD23	2.45	0.52
2:D:2230:THR:HG23	2:D:2270:SER:H	1.74	0.52
2:D:2418:LEU:HD23	2:D:2418:LEU:H	1.74	0.52
2:G:264:PRO:HB2	2:G:266:ARG:HG2	1.92	0.52
2:G:1018:ASN:HB3	2:G:1021:LEU:HD23	1.92	0.52
2:I:264:PRO:HB2	2:I:266:ARG:HG2	1.92	0.52
2:I:3350:ARG:HG2	2:I:3350:ARG:HH11	1.75	0.52
2:D:574:VAL:HA	2:D:577:ILE:HG12	1.92	0.52
2:G:2970:SER:HA	2:G:2973:PHE:CE2	2.45	0.52
2:I:1680:ARG:HH12	1:L:88:PRO:HB2	1.75	0.52
2:I:4992:LEU:O	2:I:4996:ILE:HG13	2.10	0.52
2:A:2962:GLN:OE1	2:A:2965:ARG:NH1	2.42	0.52
2:A:2970:SER:HA	2:A:2973:PHE:CE2	2.45	0.52
2:D:246:TYR:CG	2:D:373:LYS:HE3	2.45	0.52
2:D:1680:ARG:HH12	1:F:88:PRO:HB2	1.75	0.52
2:D:2970:SER:HA	2:D:2973:PHE:CE2	2.45	0.52
2:D:3812:VAL:O	2:D:3816:MET:HG3	2.09	0.52
1:F:18:LYS:NZ	1:F:18:LYS:HB3	2.25	0.52
2:G:961:MET:HG3	2:G:962:SER:H	1.72	0.52
2:G:4680:LYS:HB3	2:G:4686:LEU:HD22	1.92	0.52
2:I:2670:GLU:O	2:I:2673:HIS:ND1	2.43	0.52
2:I:4654:ALA:O	2:I:4658:ILE:HG12	2.09	0.52
2:A:652:ARG:HD3	2:A:750:LEU:HB3	1.91	0.52
2:A:4634:GLU:HG2	2:A:4636:THR:H	1.75	0.52
2:A:4839:MET:CE	2:D:4823:LEU:HA	2.40	0.52
2:D:4240:ASP:OD1	2:D:4675:LYS:NZ	2.36	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2012:PHE:CZ	2:G:2031:LEU:HD23	2.45	0.52
2:G:4546:VAL:HG22	2:G:4550:LYS:HE3	1.92	0.52
2:I:5013:MET:HE3	2:I:5021:PHE:HD2	1.75	0.51
2:A:3246:LEU:HA	2:A:3249:LEU:HD13	1.90	0.51
2:A:4839:MET:SD	2:D:4826:ILE:HD12	2.50	0.51
2:D:4546:VAL:HG22	2:D:4550:LYS:HE3	1.92	0.51
2:D:4853:VAL:HG13	2:G:4807:PHE:HD2	1.74	0.51
2:D:4912:TYR:HD1	5:D:5102:POV:H28	1.75	0.51
2:G:246:TYR:CB	2:G:373:LYS:HD2	2.39	0.51
2:G:2670:GLU:O	2:G:2673:HIS:ND1	2.43	0.51
2:G:4634:GLU:HG2	2:G:4636:THR:H	1.75	0.51
2:I:548:VAL:HG11	2:I:582:HIS:HD2	1.75	0.51
2:I:3246:LEU:HA	2:I:3249:LEU:HD13	1.90	0.51
1:L:18:LYS:HB3	1:L:18:LYS:NZ	2.25	0.51
2:A:372:LEU:HB3	2:A:374:LYS:NZ	2.25	0.51
2:A:1025:ARG:NE	2:A:1025:ARG:HA	2.25	0.51
2:D:2670:GLU:O	2:D:2673:HIS:ND1	2.43	0.51
2:D:4090:LYS:HG3	2:D:4121:GLU:HB3	1.91	0.51
2:D:4839:MET:CE	2:G:4823:LEU:HA	2.41	0.51
2:I:470:SER:HA	2:I:473:ASN:HD21	1.74	0.51
2:I:2962:GLN:OE1	2:I:2965:ARG:NH1	2.42	0.51
2:I:3812:VAL:O	2:I:3816:MET:HG3	2.09	0.51
2:A:4680:LYS:HB3	2:A:4686:LEU:HD22	1.92	0.51
2:D:264:PRO:HB2	2:D:266:ARG:HG2	1.92	0.51
2:D:893:TYR:HA	2:D:904:HIS:H	1.74	0.51
2:D:4680:LYS:HB3	2:D:4686:LEU:HD22	1.92	0.51
2:G:574:VAL:HA	2:G:577:ILE:HG12	1.92	0.51
2:G:3368:ARG:O	2:G:3372:VAL:HG23	2.09	0.51
2:A:1786:LEU:HD12	2:A:1787:PRO:HD2	1.92	0.51
2:D:2930:LEU:O	2:D:2934:GLY:N	2.41	0.51
2:G:3350:ARG:HH11	2:G:3350:ARG:HG2	1.75	0.51
2:I:2095:GLN:HG3	2:I:2127:GLN:HB3	1.93	0.51
2:A:2670:GLU:O	2:A:2673:HIS:ND1	2.43	0.51
2:A:3194:LEU:HD13	2:A:3272:ILE:HG23	1.92	0.51
2:A:3350:ARG:HG2	2:A:3350:ARG:HH11	1.75	0.51
1:J:18:LYS:NZ	1:J:18:LYS:HB3	2.25	0.51
2:D:1786:LEU:HD12	2:D:1787:PRO:HD2	1.92	0.51
2:D:3194:LEU:HD13	2:D:3272:ILE:HG23	1.92	0.51
2:A:2122:SER:O	2:A:2126:ARG:HG3	2.11	0.51
2:A:2997:PHE:CE2	2:A:3001:ILE:HD11	2.44	0.51
2:A:3262:ARG:HB2	2:A:3265:GLU:HG2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2122:SER:O	2:D:2126:ARG:HG3	2.11	0.51
2:D:2288:LEU:O	2:D:3849:ARG:NH1	2.41	0.51
2:D:4634:GLU:HG2	2:D:4636:THR:H	1.75	0.51
2:A:4090:LYS:HG3	2:A:4121:GLU:HB3	1.91	0.51
2:A:4546:VAL:HG22	2:A:4550:LYS:HE3	1.92	0.51
2:D:2095:GLN:HG3	2:D:2127:GLN:HB3	1.93	0.51
2:I:1018:ASN:HB3	2:I:1021:LEU:HD23	1.92	0.51
2:I:1025:ARG:NE	2:I:1025:ARG:HA	2.25	0.51
2:I:2170:MET:SD	2:I:2171:GLY:N	2.84	0.51
2:I:4680:LYS:HB3	2:I:4686:LEU:HD22	1.92	0.51
2:A:2881:ASN:HA	2:A:2884:ASN:HD21	1.76	0.51
2:D:116:MET:HG2	2:D:139:GLU:HA	1.93	0.51
2:D:247:TYR:HD2	2:D:374:LYS:HB2	1.76	0.51
2:G:548:VAL:HG11	2:G:582:HIS:HD2	1.75	0.51
2:I:4912:TYR:HD1	5:I:5102:POV:H28	1.75	0.51
2:A:1286:MET:HE2	2:A:1464:PHE:HB3	1.93	0.51
2:G:2170:MET:SD	2:G:2171:GLY:N	2.84	0.51
1:H:42:ARG:NH1	2:G:1780:PRO:O	2.44	0.51
2:I:3321:ARG:HH11	2:I:3325:ASN:HD21	1.59	0.51
2:I:4823:LEU:HA	2:G:4839:MET:CE	2.40	0.51
2:A:3321:ARG:HH11	2:A:3325:ASN:HD21	1.59	0.51
2:D:1025:ARG:NE	2:D:1025:ARG:HA	2.25	0.51
2:D:3350:ARG:HG2	2:D:3350:ARG:HH11	1.75	0.51
2:G:2302:LEU:HD23	2:G:2331:TYR:HB2	1.91	0.51
2:I:574:VAL:HA	2:I:577:ILE:HG12	1.92	0.50
2:A:1018:ASN:HB3	2:A:1021:LEU:HD23	1.92	0.50
2:G:116:MET:HG2	2:G:139:GLU:HA	1.93	0.50
2:G:1025:ARG:NE	2:G:1025:ARG:HA	2.25	0.50
2:I:1786:LEU:HD12	2:I:1787:PRO:HD2	1.92	0.50
2:A:548:VAL:HG11	2:A:582:HIS:HD2	1.75	0.50
2:D:548:VAL:HG11	2:D:582:HIS:HD2	1.75	0.50
2:G:3262:ARG:HB2	2:G:3265:GLU:HG2	1.93	0.50
2:G:4912:TYR:HD1	5:G:5102:POV:H28	1.75	0.50
2:I:2736:ASP:OD1	2:I:2736:ASP:N	2.41	0.50
2:A:1680:ARG:HH12	1:J:88:PRO:HB2	1.76	0.50
2:A:3651:ASN:O	2:A:3655:GLU:HG2	2.11	0.50
2:D:2881:ASN:HA	2:D:2884:ASN:HD21	1.76	0.50
2:G:1786:LEU:HD12	2:G:1787:PRO:HD2	1.92	0.50
2:I:1811:ALA:HA	2:I:1814:MET:HE2	1.94	0.50
2:I:3717:ASP:OD1	2:I:3717:ASP:N	2.43	0.50
2:A:264:PRO:HB2	2:A:266:ARG:HG2	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2313:LEU:HG	2:D:2318:TYR:HB2	1.94	0.50
2:I:701:GLY:HA3	2:I:725:HIS:CE1	2.47	0.50
2:I:4546:VAL:HG22	2:I:4550:LYS:HE3	1.92	0.50
2:A:2173:GLN:O	2:A:2177:LEU:HD23	2.12	0.50
2:D:1018:ASN:HB3	2:D:1021:LEU:HD23	1.92	0.50
2:D:2302:LEU:HD23	2:D:2331:TYR:HB2	1.91	0.50
2:D:3065:VAL:O	2:D:3069:HIS:ND1	2.45	0.50
2:D:3262:ARG:HB2	2:D:3265:GLU:HG2	1.93	0.50
2:G:701:GLY:HA3	2:G:725:HIS:CE1	2.47	0.50
2:G:3194:LEU:HD13	2:G:3272:ILE:HG23	1.92	0.50
2:I:2970:SER:HA	2:I:2973:PHE:CE2	2.45	0.50
2:A:728:ARG:NH2	2:A:1489:CYS:SG	2.85	0.50
2:A:2170:MET:SD	2:A:2171:GLY:N	2.84	0.50
2:D:840:VAL:HG12	2:D:1199:VAL:HG12	1.94	0.50
2:D:2170:MET:SD	2:D:2171:GLY:N	2.84	0.50
2:D:3536:ALA:HB2	2:D:3553:LEU:HD11	1.94	0.50
2:D:3548:GLU:HG3	2:D:3552:PHE:CZ	2.47	0.50
2:G:1811:ALA:HA	2:G:1814:MET:HE2	1.94	0.50
2:G:2313:LEU:HG	2:G:2318:TYR:HB2	1.94	0.50
2:G:3536:ALA:HB2	2:G:3553:LEU:HD11	1.94	0.50
2:I:3550:ARG:HD3	2:I:3594:ARG:NH2	2.27	0.50
2:D:701:GLY:HA3	2:D:725:HIS:CE1	2.47	0.50
2:D:2173:GLN:O	2:D:2177:LEU:HD23	2.12	0.50
2:G:3065:VAL:O	2:G:3069:HIS:ND1	2.45	0.50
2:I:2122:SER:O	2:I:2126:ARG:HG3	2.11	0.50
2:I:3065:VAL:O	2:I:3069:HIS:ND1	2.45	0.50
2:I:3262:ARG:HB2	2:I:3265:GLU:HG2	1.93	0.50
2:I:4627:MET:SD	2:I:4627:MET:N	2.81	0.50
2:A:116:MET:HG2	2:A:139:GLU:HA	1.93	0.50
2:A:840:VAL:HG12	2:A:1199:VAL:HG12	1.94	0.50
2:A:3065:VAL:O	2:A:3069:HIS:ND1	2.45	0.50
2:D:3321:ARG:HH11	2:D:3325:ASN:HD21	1.59	0.50
1:F:53:GLN:N	1:F:53:GLN:OE1	2.45	0.50
2:G:2173:GLN:O	2:G:2177:LEU:HD23	2.12	0.50
2:I:840:VAL:HG12	2:I:1199:VAL:HG12	1.94	0.50
2:I:2175:GLU:O	2:I:2179:ILE:HG12	2.12	0.50
2:D:2924:GLN:O	2:D:2928:LYS:HG2	2.12	0.50
2:G:840:VAL:HG12	2:G:1199:VAL:HG12	1.94	0.50
2:G:2095:GLN:HG3	2:G:2127:GLN:HB3	1.93	0.50
2:G:3548:GLU:HG3	2:G:3552:PHE:CZ	2.47	0.50
2:G:3651:ASN:O	2:G:3655:GLU:HG2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4574:ASN:HD21	2:G:4810:ALA:HA	1.77	0.50
2:A:684:VAL:HG22	2:A:781:VAL:HG12	1.94	0.49
2:D:867:LEU:O	2:D:871:ARG:HB3	2.12	0.49
2:D:3651:ASN:O	2:D:3655:GLU:HG2	2.11	0.49
2:G:2175:GLU:O	2:G:2179:ILE:HG12	2.12	0.49
1:H:53:GLN:OE1	1:H:53:GLN:N	2.45	0.49
2:I:1977:TYR:HB2	2:I:1998:PHE:CE2	2.47	0.49
2:I:3835:LEU:HD22	2:I:3880:PHE:HZ	1.77	0.49
2:I:4574:ASN:HD21	2:I:4810:ALA:HA	1.77	0.49
2:A:2175:GLU:O	2:A:2179:ILE:HG12	2.12	0.49
2:A:2313:LEU:HG	2:A:2318:TYR:HB2	1.94	0.49
2:A:3550:ARG:HD3	2:A:3594:ARG:NH2	2.27	0.49
2:D:2175:GLU:O	2:D:2179:ILE:HG12	2.12	0.49
2:I:1668:ARG:HG3	2:I:1671:ARG:HH12	1.78	0.49
2:I:2313:LEU:HG	2:I:2318:TYR:HB2	1.94	0.49
2:I:4813:LEU:O	2:I:4816:ILE:HG12	2.13	0.49
1:L:53:GLN:OE1	1:L:53:GLN:N	2.45	0.49
2:A:1977:TYR:HB2	2:A:1998:PHE:CE2	2.47	0.49
2:A:3809:ASN:HB3	2:A:3812:VAL:HG22	1.94	0.49
2:D:728:ARG:NH2	2:D:1489:CYS:SG	2.85	0.49
2:G:2924:GLN:O	2:G:2928:LYS:HG2	2.12	0.49
3:M:15:GLY:H	3:M:85:LEU:HB2	1.78	0.49
2:I:2418:LEU:O	2:I:2422:ILE:HG12	2.13	0.49
2:I:3536:ALA:HB2	2:I:3553:LEU:HD11	1.94	0.49
2:I:3548:GLU:HG3	2:I:3552:PHE:CZ	2.47	0.49
2:I:3651:ASN:O	2:I:3655:GLU:HG2	2.11	0.49
2:A:1811:ALA:HA	2:A:1814:MET:HE2	1.94	0.49
2:A:3546:ASP:O	2:A:3550:ARG:HG3	2.12	0.49
2:A:3548:GLU:HG3	2:A:3552:PHE:CZ	2.47	0.49
2:D:684:VAL:HG22	2:D:781:VAL:HG12	1.94	0.49
2:D:3336:LYS:HD2	2:D:3464:ILE:HD11	1.95	0.49
2:D:3604:TYR:O	2:D:3607:GLU:HG3	2.12	0.49
3:E:15:GLY:H	3:E:85:LEU:HB2	1.77	0.49
2:G:638:ILE:HD12	2:G:703:GLY:HA2	1.95	0.49
2:G:1078:GLU:OE1	2:G:1235:THR:OG1	2.31	0.49
2:G:2288:LEU:O	2:G:3849:ARG:NH1	2.41	0.49
2:G:2930:LEU:O	2:G:2934:GLY:N	2.41	0.49
2:I:2173:GLN:O	2:I:2177:LEU:HD23	2.12	0.49
2:I:3194:LEU:HD13	2:I:3272:ILE:HG23	1.92	0.49
2:I:3695:PRO:HB2	2:I:3700:GLN:HG2	1.94	0.49
2:I:4839:MET:CE	2:A:4823:LEU:HA	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1052:ASN:OD1	2:A:1052:ASN:N	2.45	0.49
2:A:2095:GLN:HG3	2:A:2127:GLN:HB3	1.93	0.49
2:A:2418:LEU:O	2:A:2422:ILE:HG12	2.13	0.49
2:A:4813:LEU:O	2:A:4816:ILE:HG12	2.13	0.49
2:D:1078:GLU:OE1	2:D:1235:THR:OG1	2.31	0.49
2:D:3377:GLU:HA	2:D:3380:ARG:HG2	1.95	0.49
2:D:3550:ARG:HD3	2:D:3594:ARG:NH2	2.27	0.49
2:G:2628:PHE:HZ	2:G:2906:VAL:HA	1.78	0.49
2:G:2981:VAL:HA	2:G:2985:ARG:HD3	1.95	0.49
2:G:3604:TYR:O	2:G:3607:GLU:HG3	2.13	0.49
2:I:684:VAL:HG22	2:I:781:VAL:HG12	1.94	0.49
2:I:728:ARG:NH2	2:I:1489:CYS:SG	2.85	0.49
2:I:2500:ALA:HB2	2:I:2553:TYR:HD1	1.77	0.49
2:I:2871:LEU:HG	2:I:2927:LEU:HD21	1.95	0.49
2:A:1087:ARG:HG2	2:A:1154:ASP:HB3	1.95	0.49
2:A:3536:ALA:HB2	2:A:3553:LEU:HD11	1.94	0.49
2:D:1668:ARG:HG3	2:D:1671:ARG:HH12	1.78	0.49
2:D:2653:LYS:HB2	2:D:2661:TRP:CD1	2.48	0.49
2:D:2871:LEU:HG	2:D:2927:LEU:HD21	1.95	0.49
2:G:1668:ARG:HG3	2:G:1671:ARG:HH12	1.78	0.49
2:G:3321:ARG:HH11	2:G:3325:ASN:HD21	1.59	0.49
2:I:867:LEU:O	2:I:871:ARG:HB3	2.12	0.49
2:I:2930:LEU:O	2:I:2934:GLY:N	2.41	0.49
2:I:2981:VAL:HA	2:I:2985:ARG:HD3	1.95	0.49
2:I:3392:LEU:HA	2:I:3395:ARG:HD2	1.94	0.49
2:A:2500:ALA:HB2	2:A:2553:TYR:HD1	1.77	0.49
2:A:2981:VAL:HA	2:A:2985:ARG:HD3	1.95	0.49
2:A:3336:LYS:HD2	2:A:3464:ILE:HD11	1.95	0.49
2:A:5014:TYR:HE2	7:A:5104:CFF:H101	1.77	0.49
2:D:499:THR:HG23	2:D:502:HIS:H	1.78	0.49
2:D:2263:ILE:HA	2:D:2330:ARG:HH12	1.78	0.49
2:D:2500:ALA:HB2	2:D:2553:TYR:HD1	1.78	0.49
2:D:2981:VAL:HA	2:D:2985:ARG:HD3	1.95	0.49
2:D:3172:ILE:HD13	2:D:3194:LEU:HB2	1.95	0.49
2:G:2871:LEU:HG	2:G:2927:LEU:HD21	1.95	0.49
2:G:2881:ASN:HA	2:G:2884:ASN:HD21	1.76	0.49
2:G:4104:THR:O	2:G:4108:ILE:HG12	2.13	0.49
2:I:116:MET:HG2	2:I:139:GLU:HA	1.93	0.49
2:I:2238:TYR:O	2:I:2242:ILE:HG12	2.13	0.49
2:I:2881:ASN:HA	2:I:2884:ASN:HD21	1.76	0.49
2:I:2924:GLN:O	2:I:2928:LYS:HG2	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1087:ARG:HG2	2:D:1154:ASP:HB3	1.95	0.49
2:G:684:VAL:HG22	2:G:781:VAL:HG12	1.94	0.49
2:G:728:ARG:NH2	2:G:1489:CYS:SG	2.85	0.49
2:G:1013:ILE:H	2:G:1013:ILE:HD12	1.78	0.49
2:G:1087:ARG:HG2	2:G:1154:ASP:HB3	1.95	0.49
2:G:1977:TYR:HB2	2:G:1998:PHE:CE2	2.47	0.49
2:G:2500:ALA:HB2	2:G:2553:TYR:HD1	1.77	0.49
2:G:2653:LYS:HB2	2:G:2661:TRP:CD1	2.48	0.49
2:G:3172:ILE:HD13	2:G:3194:LEU:HB2	1.95	0.49
2:G:3546:ASP:O	2:G:3550:ARG:HG3	2.12	0.49
2:G:3550:ARG:HD3	2:G:3594:ARG:NH2	2.27	0.49
2:I:887:ILE:HD13	2:I:959:TYR:HB3	1.95	0.49
2:I:1078:GLU:OE1	2:I:1235:THR:OG1	2.31	0.49
2:I:3172:ILE:HD13	2:I:3194:LEU:HB2	1.95	0.49
3:K:15:GLY:H	3:K:85:LEU:HB2	1.77	0.49
2:A:701:GLY:HA3	2:A:725:HIS:CE1	2.47	0.49
2:A:3604:TYR:O	2:A:3607:GLU:HG3	2.12	0.49
2:D:638:ILE:HD12	2:D:703:GLY:HA2	1.95	0.49
2:D:1052:ASN:OD1	2:D:1052:ASN:N	2.45	0.49
2:D:1811:ALA:HA	2:D:1814:MET:HE2	1.94	0.49
2:D:2628:PHE:HZ	2:D:2906:VAL:HA	1.78	0.49
2:D:3188:PRO:HB3	2:D:3334:TRP:CZ2	2.48	0.49
2:G:3695:PRO:HB2	2:G:3700:GLN:HG2	1.94	0.49
2:G:3809:ASN:HB3	2:G:3812:VAL:HG22	1.94	0.49
2:G:4813:LEU:O	2:G:4816:ILE:HG12	2.13	0.49
1:H:77:THR:OG1	1:H:78:PRO:HD2	2.13	0.49
2:I:1497:GLY:HA2	2:I:1500:PHE:HD2	1.78	0.49
2:I:3546:ASP:O	2:I:3550:ARG:HG3	2.12	0.49
2:A:499:THR:HG23	2:A:502:HIS:H	1.78	0.49
2:A:3215:ALA:HA	2:A:3220:THR:HG21	1.95	0.49
2:A:3717:ASP:OD1	2:A:3717:ASP:N	2.43	0.49
1:J:53:GLN:OE1	1:J:53:GLN:N	2.45	0.49
2:D:246:TYR:CD2	2:D:373:LYS:HB3	2.48	0.49
2:D:1497:GLY:HA2	2:D:1500:PHE:HD2	1.78	0.49
2:D:3268:HIS:CE1	2:D:3272:ILE:HD12	2.48	0.49
2:D:4104:THR:O	2:D:4108:ILE:HG12	2.13	0.49
2:G:372:LEU:O	2:G:374:LYS:HG3	2.12	0.49
2:G:2122:SER:O	2:G:2126:ARG:HG3	2.11	0.49
2:G:3188:PRO:HB3	2:G:3334:TRP:CZ2	2.48	0.49
2:G:4242:ILE:HG22	2:G:4246:GLN:HE21	1.77	0.49
2:I:2768:PHE:O	2:I:2771:ILE:HG22	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:867:LEU:O	2:A:871:ARG:HB3	2.12	0.48
2:A:1076:ARG:HB3	2:A:1191:VAL:HG23	1.95	0.48
2:A:1078:GLU:OE1	2:A:1235:THR:OG1	2.31	0.48
2:A:2238:TYR:O	2:A:2242:ILE:HG12	2.13	0.48
2:A:2559:LEU:O	2:A:2563:THR:HG23	2.13	0.48
2:A:2653:LYS:HB2	2:A:2661:TRP:CD1	2.48	0.48
2:A:2792:ARG:NH2	2:A:2798:SER:OG	2.46	0.48
2:A:2924:GLN:O	2:A:2928:LYS:HG2	2.12	0.48
2:A:3172:ILE:HD13	2:A:3194:LEU:HB2	1.95	0.48
2:A:3188:PRO:HB3	2:A:3334:TRP:CZ2	2.48	0.48
2:A:3695:PRO:HB2	2:A:3700:GLN:HG2	1.94	0.48
2:D:1128:ARG:CZ	2:D:1130:GLN:HG3	2.44	0.48
2:D:2138:LEU:HB3	2:D:3658:LYS:HE2	1.95	0.48
2:D:2418:LEU:O	2:D:2422:ILE:HG12	2.13	0.48
2:D:3695:PRO:HB2	2:D:3700:GLN:HG2	1.94	0.48
2:G:1076:ARG:HB3	2:G:1191:VAL:HG23	1.95	0.48
2:G:2768:PHE:O	2:G:2771:ILE:HG22	2.13	0.48
2:I:2012:PHE:HZ	2:I:2031:LEU:HD23	1.78	0.48
2:I:3268:HIS:CE1	2:I:3272:ILE:HD12	2.48	0.48
2:A:887:ILE:HD13	2:A:959:TYR:HB3	1.95	0.48
2:A:2628:PHE:HZ	2:A:2906:VAL:HA	1.78	0.48
2:A:3103:ILE:O	2:A:3107:VAL:HG13	2.14	0.48
2:A:3835:LEU:HD22	2:A:3880:PHE:HZ	1.77	0.48
2:D:1076:ARG:HB3	2:D:1191:VAL:HG23	1.95	0.48
2:D:1977:TYR:HB2	2:D:1998:PHE:CE2	2.47	0.48
2:D:2559:LEU:O	2:D:2563:THR:HG23	2.13	0.48
2:D:3392:LEU:HA	2:D:3395:ARG:HD2	1.94	0.48
2:D:3546:ASP:O	2:D:3550:ARG:HG3	2.12	0.48
2:D:4813:LEU:O	2:D:4816:ILE:HG12	2.12	0.48
2:I:2759:ALA:HA	2:I:2809:ILE:HG12	1.95	0.48
2:I:3536:ALA:O	2:I:3540:TYR:N	2.46	0.48
2:A:638:ILE:HD12	2:A:703:GLY:HA2	1.95	0.48
2:A:2716:ASP:OD1	2:A:2716:ASP:N	2.42	0.48
2:A:2871:LEU:HG	2:A:2927:LEU:HD21	1.95	0.48
2:A:3195:ALA:HB2	2:A:3275:PRO:HB3	1.96	0.48
2:A:3268:HIS:CE1	2:A:3272:ILE:HD12	2.48	0.48
2:D:1422:ASP:OD1	2:D:1422:ASP:N	2.45	0.48
1:F:77:THR:OG1	1:F:78:PRO:HD2	2.13	0.48
2:G:499:THR:HG23	2:G:502:HIS:H	1.78	0.48
2:G:3268:HIS:CE1	2:G:3272:ILE:HD12	2.48	0.48
2:I:1087:ARG:HG2	2:I:1154:ASP:HB3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2792:ARG:NH2	2:I:2798:SER:OG	2.46	0.48
2:I:3147:ILE:HG13	2:I:3152:PHE:HB2	1.95	0.48
2:I:3377:GLU:HA	2:I:3380:ARG:HG2	1.95	0.48
2:I:3604:TYR:O	2:I:3607:GLU:HG3	2.13	0.48
2:A:1668:ARG:HG3	2:A:1671:ARG:HH12	1.78	0.48
2:A:2288:LEU:O	2:A:3849:ARG:NH1	2.41	0.48
2:A:3392:LEU:HA	2:A:3395:ARG:HD2	1.94	0.48
2:A:4104:THR:O	2:A:4108:ILE:HG12	2.13	0.48
2:D:1013:ILE:H	2:D:1013:ILE:HD12	1.78	0.48
2:D:3103:ILE:O	2:D:3107:VAL:HG13	2.14	0.48
2:G:2196:ASN:OD1	2:G:2199:ARG:NH2	2.46	0.48
2:G:3377:GLU:HA	2:G:3380:ARG:HG2	1.95	0.48
2:G:4954:MET:O	6:G:5103:ATP:O2'	2.27	0.48
2:I:1530:THR:HG22	2:I:1535:GLU:HA	1.95	0.48
2:I:2581:SER:O	2:I:2584:HIS:HB2	2.14	0.48
2:I:2653:LYS:HB2	2:I:2661:TRP:CD1	2.48	0.48
2:I:3215:ALA:HA	2:I:3220:THR:HG21	1.95	0.48
2:I:4104:THR:O	2:I:4108:ILE:HG12	2.13	0.48
1:J:77:THR:OG1	1:J:78:PRO:HD2	2.13	0.48
2:D:1530:THR:HG22	2:D:1535:GLU:HA	1.96	0.48
2:D:2238:TYR:O	2:D:2242:ILE:HG12	2.13	0.48
2:D:3809:ASN:HB3	2:D:3812:VAL:HG22	1.94	0.48
2:G:2138:LEU:HB3	2:G:3658:LYS:HE2	1.95	0.48
2:G:2238:TYR:O	2:G:2242:ILE:HG12	2.13	0.48
2:G:2418:LEU:O	2:G:2422:ILE:HG12	2.13	0.48
2:G:2581:SER:O	2:G:2584:HIS:HB2	2.14	0.48
2:G:3103:ILE:O	2:G:3107:VAL:HG13	2.14	0.48
2:G:3835:LEU:HD22	2:G:3880:PHE:HZ	1.77	0.48
2:I:3103:ILE:O	2:I:3107:VAL:HG13	2.14	0.48
2:A:904:HIS:ND1	2:A:905:PRO:HD2	2.29	0.48
2:A:1013:ILE:H	2:A:1013:ILE:HD12	1.78	0.48
2:A:1497:GLY:HA2	2:A:1500:PHE:HD2	1.78	0.48
2:D:3215:ALA:HA	2:D:3220:THR:HG21	1.95	0.48
2:D:4574:ASN:HD21	2:D:4810:ALA:HA	1.77	0.48
2:G:3536:ALA:O	2:G:3540:TYR:N	2.46	0.48
2:G:4992:LEU:O	2:G:4996:ILE:HG13	2.13	0.48
2:I:499:THR:HG23	2:I:502:HIS:H	1.78	0.48
2:I:861:ILE:HG23	2:I:933:LEU:HD22	1.96	0.48
2:I:2559:LEU:O	2:I:2563:THR:HG23	2.13	0.48
2:A:1530:THR:HG22	2:A:1535:GLU:HA	1.95	0.48
2:A:2768:PHE:O	2:A:2771:ILE:HG22	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:904:HIS:ND1	2:D:905:PRO:HD2	2.29	0.48
2:D:5003:HIS:HD2	2:D:5007:GLU:HB3	1.79	0.48
2:G:2963:LEU:HD13	2:G:3006:ILE:HD13	1.96	0.48
2:I:904:HIS:ND1	2:I:905:PRO:HD2	2.29	0.48
2:I:1076:ARG:HB3	2:I:1191:VAL:HG23	1.95	0.48
2:I:3188:PRO:HB3	2:I:3334:TRP:CZ2	2.48	0.48
2:I:3336:LYS:HD2	2:I:3464:ILE:HD11	1.95	0.48
2:I:3809:ASN:HB3	2:I:3812:VAL:HG22	1.94	0.48
2:A:5003:HIS:HD2	2:A:5007:GLU:HB3	1.79	0.48
2:D:2792:ARG:NH2	2:D:2798:SER:OG	2.46	0.48
2:D:3257:ALA:HB1	2:D:3321:ARG:HB3	1.96	0.48
2:G:904:HIS:ND1	2:G:905:PRO:HD2	2.29	0.48
2:G:2012:PHE:HZ	2:G:2031:LEU:HD23	1.79	0.48
2:G:2559:LEU:O	2:G:2563:THR:HG23	2.13	0.48
2:I:1013:ILE:H	2:I:1013:ILE:HD12	1.78	0.48
2:I:2628:PHE:HZ	2:I:2906:VAL:HA	1.78	0.48
2:A:861:ILE:HG23	2:A:933:LEU:HD22	1.96	0.48
2:A:2263:ILE:HA	2:A:2330:ARG:HH12	1.78	0.48
2:A:2759:ALA:HA	2:A:2809:ILE:HG12	1.95	0.48
2:D:364:PRO:HG2	2:D:365:LYS:HZ2	1.79	0.48
2:D:501:ALA:O	2:D:505:GLU:HG2	2.14	0.48
2:D:861:ILE:HG23	2:D:933:LEU:HD22	1.96	0.48
2:D:2768:PHE:O	2:D:2771:ILE:HG22	2.13	0.48
2:D:4721:LYS:HD2	2:D:4741:LEU:HB3	1.96	0.48
2:G:1256:GLU:HB2	2:G:1275:ARG:HE	1.79	0.48
2:G:2263:ILE:HA	2:G:2330:ARG:HH12	1.78	0.48
2:G:2792:ARG:NH2	2:G:2798:SER:OG	2.46	0.48
2:G:3717:ASP:OD1	2:G:3717:ASP:N	2.43	0.48
2:I:371:VAL:HG12	2:I:373:LYS:HG2	1.96	0.48
2:I:3257:ALA:HB1	2:I:3321:ARG:HB3	1.96	0.48
2:A:3257:ALA:HB1	2:A:3321:ARG:HB3	1.96	0.48
2:A:3377:GLU:HA	2:A:3380:ARG:HG2	1.95	0.48
2:A:3470:LEU:O	2:A:3474:SER:OG	2.28	0.48
2:G:861:ILE:HG23	2:G:933:LEU:HD22	1.96	0.48
2:G:4240:ASP:OD1	2:G:4675:LYS:NZ	2.36	0.48
2:I:2263:ILE:HA	2:I:2330:ARG:HH12	1.78	0.47
2:I:3195:ALA:HB2	2:I:3275:PRO:HB3	1.96	0.47
2:I:4243:PHE:CE2	2:I:4247:ILE:HD11	2.49	0.47
2:A:501:ALA:O	2:A:505:GLU:HG2	2.14	0.47
2:A:2138:LEU:HB3	2:A:3658:LYS:HE2	1.95	0.47
2:A:3147:ILE:HG13	2:A:3152:PHE:HB2	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:887:ILE:HD13	2:D:959:TYR:HB3	1.95	0.47
2:G:867:LEU:O	2:G:871:ARG:HB3	2.12	0.47
2:G:1128:ARG:CZ	2:G:1130:GLN:HG3	2.44	0.47
2:G:1497:GLY:HA2	2:G:1500:PHE:HD2	1.78	0.47
2:I:3416:VAL:HG23	2:I:3423:TRP:HZ3	1.79	0.47
2:A:2196:ASN:OD1	2:A:2199:ARG:NH2	2.46	0.47
2:A:2747:ILE:HD12	2:A:2748:PRO:HD2	1.95	0.47
2:D:1256:GLU:HB2	2:D:1275:ARG:HE	1.79	0.47
2:G:2430:ILE:HG21	2:G:2502:MET:HB2	1.96	0.47
2:G:3416:VAL:HG23	2:G:3423:TRP:HZ3	1.79	0.47
2:I:1128:ARG:CZ	2:I:1130:GLN:HG3	2.44	0.47
2:A:363:ASP:HB3	2:A:366:ALA:HB3	1.96	0.47
2:A:1128:ARG:CZ	2:A:1130:GLN:HG3	2.44	0.47
2:A:2012:PHE:HZ	2:A:2031:LEU:HD23	1.79	0.47
2:A:4574:ASN:HD21	2:A:4810:ALA:HA	1.77	0.47
1:J:106:LEU:HD22	1:J:107:GLU:H	1.79	0.47
2:D:2581:SER:O	2:D:2584:HIS:HB2	2.14	0.47
2:D:3835:LEU:HD22	2:D:3880:PHE:HZ	1.77	0.47
2:G:2212:VAL:HG22	2:G:2256:TYR:CZ	2.50	0.47
2:I:368:ARG:HD3	2:I:369:LEU:N	2.29	0.47
2:I:638:ILE:HD12	2:I:703:GLY:HA2	1.95	0.47
2:I:2138:LEU:HB3	2:I:3658:LYS:HE2	1.95	0.47
2:I:2430:ILE:HG21	2:I:2502:MET:HB2	1.96	0.47
2:I:2477:PRO:HG2	2:I:2536:LEU:HD11	1.96	0.47
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.30	0.47
2:A:4721:LYS:HD2	2:A:4741:LEU:HB3	1.96	0.47
2:A:4835:LYS:O	2:A:4839:MET:HB2	2.15	0.47
2:D:3195:ALA:HB2	2:D:3275:PRO:HB3	1.96	0.47
2:G:887:ILE:HD13	2:G:959:TYR:HB3	1.95	0.47
2:G:1046:LEU:HD22	2:G:1051:TYR:CZ	2.50	0.47
2:G:1422:ASP:OD1	2:G:1422:ASP:N	2.45	0.47
2:G:2477:PRO:HG2	2:G:2536:LEU:HD11	1.96	0.47
2:G:3257:ALA:HB1	2:G:3321:ARG:HB3	1.96	0.47
2:G:3336:LYS:HD2	2:G:3464:ILE:HD11	1.95	0.47
2:G:3392:LEU:HA	2:G:3395:ARG:HD2	1.94	0.47
2:I:815:VAL:O	2:I:1007:TYR:OH	2.28	0.47
2:I:1046:LEU:HD22	2:I:1051:TYR:CZ	2.50	0.47
2:I:2212:VAL:HG22	2:I:2256:TYR:CZ	2.50	0.47
2:I:4094:GLN:HG3	2:I:4108:ILE:HG21	1.96	0.47
2:I:5003:HIS:HD2	2:I:5007:GLU:HB3	1.79	0.47
2:A:2755:ILE:HD12	2:A:2813:LEU:HG	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2212:VAL:HG22	2:D:2256:TYR:CZ	2.50	0.47
2:D:2755:ILE:HD12	2:D:2813:LEU:HG	1.97	0.47
2:D:3147:ILE:HG13	2:D:3152:PHE:HB2	1.95	0.47
2:G:1733:GLU:HG2	2:G:2201:LEU:HD23	1.97	0.47
2:G:2285:GLU:OE2	2:G:3860:ASN:ND2	2.40	0.47
2:I:1763:PRO:HG3	2:I:2094:LEU:HD22	1.97	0.47
2:I:2747:ILE:HD12	2:I:2748:PRO:HD2	1.95	0.47
2:I:2963:LEU:HD13	2:I:3006:ILE:HD13	1.96	0.47
2:I:3103:ILE:HA	2:I:3106:MET:SD	2.55	0.47
1:L:77:THR:OG1	1:L:78:PRO:HD2	2.13	0.47
2:A:1727:ARG:NH2	2:A:1773:PRO:O	2.48	0.47
2:A:2212:VAL:HG22	2:A:2256:TYR:CZ	2.50	0.47
2:A:4242:ILE:HG22	2:A:4246:GLN:HE21	1.79	0.47
3:C:15:GLY:H	3:C:85:LEU:HB2	1.78	0.47
2:D:2579:VAL:O	2:D:2582:MET:HG3	2.15	0.47
3:E:90:THR:HG23	3:E:124:THR:HA	1.97	0.47
2:G:4721:LYS:HD2	2:G:4741:LEU:HB3	1.96	0.47
2:G:5003:HIS:HD2	2:G:5007:GLU:HB3	1.79	0.47
2:I:501:ALA:O	2:I:505:GLU:HG2	2.14	0.47
2:I:2196:ASN:OD1	2:I:2199:ARG:NH2	2.46	0.47
2:I:2799:GLU:O	2:I:2803:GLU:HG2	2.15	0.47
2:I:4835:LYS:O	2:I:4839:MET:HB2	2.14	0.47
2:I:4999:ASP:HB2	2:I:5002:GLU:HG2	1.97	0.47
1:L:106:LEU:HD22	1:L:107:GLU:H	1.79	0.47
2:A:355:LEU:HB3	2:A:378:LEU:HB3	1.97	0.47
2:A:2963:LEU:HD13	2:A:3006:ILE:HD13	1.96	0.47
2:A:3536:ALA:O	2:A:3540:TYR:N	2.47	0.47
2:A:4999:ASP:HB2	2:A:5002:GLU:HG2	1.97	0.47
2:D:943:ASP:HB3	2:D:1050:GLY:HA3	1.96	0.47
2:D:1763:PRO:HG3	2:D:2094:LEU:HD22	1.97	0.47
2:D:2430:ILE:HG21	2:D:2502:MET:HB2	1.96	0.47
2:D:3416:VAL:HG23	2:D:3423:TRP:HZ3	1.79	0.47
2:D:4992:LEU:O	2:D:4996:ILE:HG13	2.13	0.47
1:F:106:LEU:HD22	1:F:107:GLU:H	1.79	0.47
2:G:1052:ASN:OD1	2:G:1052:ASN:N	2.45	0.47
2:G:1530:THR:HG22	2:G:1535:GLU:HA	1.96	0.47
2:G:2747:ILE:HD12	2:G:2748:PRO:HD2	1.95	0.47
2:G:2799:GLU:O	2:G:2803:GLU:HG2	2.15	0.47
2:G:3215:ALA:HA	2:G:3220:THR:HG21	1.95	0.47
3:M:90:THR:HG23	3:M:124:THR:HA	1.97	0.47
2:A:1046:LEU:HD22	2:A:1051:TYR:CZ	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2581:SER:O	2:A:2584:HIS:HB2	2.14	0.47
2:A:3730:ALA:O	2:A:3734:HIS:HB2	2.15	0.47
2:D:2747:ILE:HD12	2:D:2748:PRO:HD2	1.95	0.47
2:D:2799:GLU:O	2:D:2803:GLU:HG2	2.15	0.47
2:D:4835:LYS:O	2:D:4839:MET:HB2	2.14	0.47
2:G:2579:VAL:O	2:G:2582:MET:HG3	2.15	0.47
2:G:3260:GLY:O	2:G:3262:ARG:NH1	2.48	0.47
2:G:4835:LYS:O	2:G:4839:MET:HB2	2.14	0.47
2:I:366:ALA:O	2:I:370:GLY:N	2.47	0.47
2:A:1256:GLU:HB2	2:A:1275:ARG:HE	1.79	0.47
2:A:3103:ILE:HA	2:A:3106:MET:SD	2.55	0.47
2:D:247:TYR:CD2	2:D:374:LYS:HB2	2.50	0.47
2:D:3536:ALA:O	2:D:3540:TYR:N	2.47	0.47
2:G:501:ALA:O	2:G:505:GLU:HG2	2.14	0.47
2:G:1763:PRO:HG3	2:G:2094:LEU:HD22	1.97	0.47
2:G:3103:ILE:HA	2:G:3106:MET:SD	2.55	0.47
2:I:2755:ILE:HD12	2:I:2813:LEU:HG	1.97	0.47
2:A:3031:ALA:HB1	2:A:3035:GLU:HB2	1.97	0.47
2:A:3416:VAL:HG23	2:A:3423:TRP:HZ3	1.79	0.47
2:A:3852:LYS:HE2	2:A:3852:LYS:HB2	1.78	0.47
2:D:872:GLU:O	2:D:876:GLU:HG2	2.15	0.47
2:D:4094:GLN:HG3	2:D:4108:ILE:HG21	1.96	0.47
2:G:355:LEU:HD23	2:G:378:LEU:HB3	1.97	0.47
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.48	0.47
2:G:3031:ALA:O	2:G:3036:LYS:NZ	2.29	0.47
2:G:3147:ILE:HG13	2:G:3152:PHE:HB2	1.95	0.47
2:G:4999:ASP:HB2	2:G:5002:GLU:HG2	1.97	0.47
2:I:3730:ALA:O	2:I:3734:HIS:HB2	2.15	0.46
2:A:872:GLU:O	2:A:876:GLU:HG2	2.15	0.46
2:A:2155:LEU:HB2	2:A:2188:ASN:HD22	1.80	0.46
2:D:4999:ASP:HB2	2:D:5002:GLU:HG2	1.97	0.46
2:G:355:LEU:HB3	2:G:378:LEU:HB3	1.97	0.46
2:G:1452:TRP:HB3	2:G:1548:LEU:HB3	1.98	0.46
2:G:1617:THR:HG22	2:G:1628:VAL:HG22	1.97	0.46
2:G:3195:ALA:HB2	2:G:3275:PRO:HB3	1.96	0.46
2:I:355:LEU:HD23	2:I:378:LEU:HB3	1.97	0.46
2:I:1256:GLU:HB2	2:I:1275:ARG:HE	1.79	0.46
2:I:1617:THR:HG22	2:I:1628:VAL:HG22	1.97	0.46
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.48	0.46
2:A:943:ASP:HB3	2:A:1050:GLY:HA3	1.96	0.46
2:A:1452:TRP:HB3	2:A:1548:LEU:HB3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1455:PRO:HG3	2:A:1549:PHE:HE1	1.81	0.46
2:A:1763:PRO:HG3	2:A:2094:LEU:HD22	1.97	0.46
2:A:2579:VAL:O	2:A:2582:MET:HG3	2.15	0.46
2:D:355:LEU:HD23	2:D:378:LEU:HB3	1.97	0.46
2:D:2155:LEU:HB2	2:D:2188:ASN:HD22	1.80	0.46
2:D:3260:GLY:O	2:D:3262:ARG:NH1	2.48	0.46
2:D:3336:LYS:HG2	2:D:3337:ARG:N	2.31	0.46
2:D:4242:ILE:HG22	2:D:4246:GLN:HE21	1.79	0.46
2:G:229:GLU:HG3	2:G:247:TYR:HB3	1.97	0.46
2:I:1155:LEU:HD13	2:I:1184:ILE:HG23	1.97	0.46
2:I:2575:ARG:HB3	2:I:2578:MET:HG2	1.97	0.46
2:I:3754:GLU:HG3	2:I:4719:PHE:CZ	2.49	0.46
2:I:4721:LYS:HD2	2:I:4741:LEU:HB3	1.96	0.46
2:A:870:ILE:O	2:A:874:LEU:HG	2.16	0.46
2:A:1733:GLU:HG2	2:A:2201:LEU:HD23	1.97	0.46
2:A:2430:ILE:HG21	2:A:2502:MET:HB2	1.96	0.46
2:A:2575:ARG:HB3	2:A:2578:MET:HG2	1.97	0.46
2:A:4992:LEU:O	2:A:4996:ILE:HG13	2.16	0.46
2:D:1455:PRO:HG3	2:D:1549:PHE:HE1	1.81	0.46
2:D:2477:PRO:HG2	2:D:2536:LEU:HD11	1.96	0.46
2:D:2759:ALA:HA	2:D:2809:ILE:HG12	1.96	0.46
2:G:3031:ALA:HB1	2:G:3035:GLU:HB2	1.97	0.46
2:G:3730:ALA:O	2:G:3734:HIS:HB2	2.15	0.46
3:M:89:ASP:HB2	3:M:125:VAL:HG21	1.97	0.46
2:I:229:GLU:HG3	2:I:247:TYR:HB3	1.97	0.46
2:I:355:LEU:HB3	2:I:378:LEU:HB3	1.97	0.46
2:I:1042:ALA:O	2:I:1046:LEU:HG	2.16	0.46
2:I:1452:TRP:HB3	2:I:1548:LEU:HB3	1.98	0.46
2:I:1733:GLU:HG2	2:I:2201:LEU:HD23	1.97	0.46
2:A:229:GLU:HG3	2:A:247:TYR:HB3	1.97	0.46
2:A:2736:ASP:OD1	2:A:2736:ASP:N	2.41	0.46
2:A:4546:VAL:HA	2:A:4549:VAL:HG22	1.98	0.46
2:D:1727:ARG:NH2	2:D:1773:PRO:O	2.48	0.46
2:D:2012:PHE:HZ	2:D:2031:LEU:HD23	1.79	0.46
2:D:2155:LEU:HB2	2:D:2188:ASN:ND2	2.30	0.46
2:D:2963:LEU:HD13	2:D:3006:ILE:HD13	1.96	0.46
2:D:3730:ALA:O	2:D:3734:HIS:HB2	2.15	0.46
2:G:247:TYR:HD2	2:G:374:LYS:HB2	1.80	0.46
2:G:981:GLN:HE21	2:G:1043:VAL:HG13	1.81	0.46
2:G:2700:MET:HB2	2:G:3001:ILE:HG22	1.98	0.46
2:I:870:ILE:O	2:I:874:LEU:HG	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1455:PRO:HG3	2:I:1549:PHE:HE1	1.81	0.46
2:A:1042:ALA:O	2:A:1046:LEU:HG	2.16	0.46
2:A:3962:PHE:O	2:A:3966:THR:HG23	2.16	0.46
2:A:4024:VAL:HG11	2:A:4142:ASN:HB3	1.97	0.46
3:C:90:THR:HG23	3:C:124:THR:HA	1.97	0.46
2:D:1046:LEU:HD22	2:D:1051:TYR:CZ	2.50	0.46
2:D:2575:ARG:HB3	2:D:2578:MET:HG2	1.97	0.46
2:D:2668:SER:HB3	2:D:2671:GLU:HG3	1.98	0.46
3:E:89:ASP:HB2	3:E:125:VAL:HG21	1.97	0.46
1:F:11:ASP:OD2	1:F:13:ARG:HG2	2.16	0.46
2:G:369:LEU:O	2:G:370:GLY:C	2.54	0.46
2:G:943:ASP:HB3	2:G:1050:GLY:HA3	1.96	0.46
2:G:2155:LEU:HB2	2:G:2188:ASN:ND2	2.30	0.46
2:G:2155:LEU:HB2	2:G:2188:ASN:HD22	1.81	0.46
2:G:2575:ARG:HB3	2:G:2578:MET:HG2	1.97	0.46
2:G:4094:GLN:HG3	2:G:4108:ILE:HG21	1.96	0.46
2:I:872:GLU:O	2:I:876:GLU:HG2	2.15	0.46
2:I:943:ASP:HB3	2:I:1050:GLY:HA3	1.96	0.46
2:I:2700:MET:HB2	2:I:3001:ILE:HG22	1.98	0.46
3:K:89:ASP:HB2	3:K:125:VAL:HG21	1.97	0.46
2:A:3260:GLY:O	2:A:3262:ARG:NH1	2.48	0.46
2:A:4094:GLN:HG3	2:A:4108:ILE:HG21	1.96	0.46
3:C:4:LEU:HD21	3:C:97:ALA:HB2	1.98	0.46
2:D:4024:VAL:HG11	2:D:4142:ASN:HB3	1.97	0.46
2:G:707:VAL:HG23	2:G:782:SER:OG	2.16	0.46
2:G:2755:ILE:HD12	2:G:2813:LEU:HG	1.97	0.46
2:G:2759:ALA:HA	2:G:2809:ILE:HG12	1.96	0.46
2:G:3379:LEU:HD12	2:G:3387:ALA:HA	1.98	0.46
1:H:11:ASP:OD2	1:H:13:ARG:HG2	2.16	0.46
2:I:2579:VAL:O	2:I:2582:MET:HG3	2.15	0.46
2:I:4024:VAL:HG11	2:I:4142:ASN:HB3	1.97	0.46
2:A:2155:LEU:HB2	2:A:2188:ASN:ND2	2.30	0.46
2:A:2867:LEU:HD21	2:A:2871:LEU:HB3	1.98	0.46
2:A:3280:TYR:CE2	2:A:3284:TRP:CD1	3.04	0.46
2:A:3379:LEU:HD12	2:A:3387:ALA:HA	1.98	0.46
2:D:150:MET:HB3	2:D:169:LEU:HD22	1.98	0.46
2:D:1452:TRP:HB3	2:D:1548:LEU:HB3	1.98	0.46
2:D:3103:ILE:HA	2:D:3106:MET:SD	2.55	0.46
2:D:4820:VAL:HB	2:D:4823:LEU:HD23	1.98	0.46
2:G:150:MET:HB3	2:G:169:LEU:HD22	1.98	0.46
2:G:872:GLU:O	2:G:876:GLU:HG2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2206:THR:O	2:G:2210:VAL:HG23	2.16	0.46
2:G:4675:LYS:O	2:G:4679:ARG:HG2	2.16	0.46
2:I:981:GLN:HE21	2:I:1043:VAL:HG13	1.81	0.46
2:I:2155:LEU:HB2	2:I:2188:ASN:ND2	2.30	0.46
2:I:3260:GLY:O	2:I:3262:ARG:NH1	2.48	0.46
2:I:3924:LEU:HD21	2:I:3984:ARG:HH21	1.81	0.46
2:A:1155:LEU:HD13	2:A:1184:ILE:HG23	1.97	0.46
2:A:2199:ARG:NH2	2:A:2245:GLN:OE1	2.49	0.46
2:A:2477:PRO:HG2	2:A:2536:LEU:HD11	1.96	0.46
2:A:2799:GLU:O	2:A:2803:GLU:HG2	2.15	0.46
2:A:3384:LYS:HG2	2:A:3386:GLU:H	1.81	0.46
2:D:355:LEU:HB3	2:D:378:LEU:HB3	1.97	0.46
2:D:823:LEU:HD11	2:D:1626:TRP:HB3	1.98	0.46
2:D:981:GLN:HE21	2:D:1043:VAL:HG13	1.81	0.46
2:D:1042:ALA:O	2:D:1046:LEU:HG	2.16	0.46
2:D:2196:ASN:OD1	2:D:2199:ARG:NH2	2.46	0.46
2:D:2199:ARG:NH2	2:D:2245:GLN:OE1	2.49	0.46
2:D:2206:THR:O	2:D:2210:VAL:HG23	2.16	0.46
2:D:3201:MET:HG3	2:D:3203:VAL:O	2.16	0.46
2:D:4675:LYS:O	2:D:4679:ARG:HG2	2.16	0.46
3:E:4:LEU:HD21	3:E:97:ALA:HB2	1.98	0.46
2:G:246:TYR:CG	2:G:373:LYS:HD2	2.51	0.46
2:G:2463:LEU:O	2:G:2467:VAL:HG22	2.16	0.46
2:G:3384:LYS:HG2	2:G:3386:GLU:H	1.81	0.46
2:I:2206:THR:O	2:I:2210:VAL:HG23	2.16	0.46
1:L:11:ASP:OD2	1:L:13:ARG:HG2	2.16	0.46
2:A:1027:LEU:HD13	2:A:1031:THR:HB	1.98	0.46
2:A:2782:ASP:N	2:A:2782:ASP:OD1	2.49	0.46
2:A:4675:LYS:O	2:A:4679:ARG:HG2	2.16	0.46
2:A:4820:VAL:HB	2:A:4823:LEU:HD23	1.98	0.46
2:A:4839:MET:CE	2:D:4823:LEU:HD13	2.44	0.46
2:D:707:VAL:HG23	2:D:782:SER:OG	2.16	0.46
2:G:2199:ARG:NH2	2:G:2245:GLN:OE1	2.49	0.46
2:G:2668:SER:HB3	2:G:2671:GLU:HG3	1.98	0.46
2:I:2463:LEU:O	2:I:2467:VAL:HG22	2.16	0.46
2:I:2867:LEU:HD21	2:I:2871:LEU:HB3	1.98	0.46
2:I:3379:LEU:HD12	2:I:3387:ALA:HA	1.98	0.46
2:I:3550:ARG:HE	2:I:3597:GLN:NE2	2.14	0.46
2:I:4066:LEU:HD23	2:I:4066:LEU:HA	1.85	0.46
2:A:707:VAL:HG23	2:A:782:SER:OG	2.16	0.46
2:A:1617:THR:HG22	2:A:1628:VAL:HG22	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2522:LEU:HA	2:A:2526:PHE:HB2	1.98	0.46
2:A:2930:LEU:O	2:A:2934:GLY:N	2.41	0.46
3:C:89:ASP:HB2	3:C:125:VAL:HG21	1.97	0.46
2:D:874:LEU:O	2:D:878:ILE:HG12	2.16	0.46
2:D:3511:VAL:HG23	2:D:3515:LYS:HD3	1.98	0.46
2:D:3550:ARG:HE	2:D:3597:GLN:NE2	2.14	0.46
2:G:870:ILE:O	2:G:874:LEU:HG	2.16	0.46
2:G:1027:LEU:HD23	2:G:1027:LEU:HA	1.83	0.46
2:G:1455:PRO:HG3	2:G:1549:PHE:HE1	1.81	0.46
2:G:2715:VAL:HG12	2:G:2953:LYS:HB3	1.98	0.46
2:G:2806:ARG:O	2:G:2810:LYS:HG2	2.16	0.46
2:G:3336:LYS:HG2	2:G:3337:ARG:N	2.31	0.46
2:G:3539:ARG:HH11	2:G:3552:PHE:HB2	1.81	0.46
2:I:2199:ARG:NH2	2:I:2245:GLN:OE1	2.49	0.45
2:I:3962:PHE:O	2:I:3966:THR:HG23	2.16	0.45
3:K:90:THR:HG23	3:K:124:THR:HA	1.97	0.45
2:A:2765:LYS:HA	2:A:2765:LYS:HD3	1.82	0.45
2:A:3336:LYS:HG2	2:A:3337:ARG:N	2.31	0.45
2:A:3924:LEU:HD21	2:A:3984:ARG:HH21	1.81	0.45
2:D:1155:LEU:HD13	2:D:1184:ILE:HG23	1.97	0.45
2:D:3379:LEU:HD12	2:D:3387:ALA:HA	1.98	0.45
2:D:4546:VAL:HA	2:D:4549:VAL:HG22	1.98	0.45
2:G:246:TYR:CD2	2:G:373:LYS:HB3	2.51	0.45
2:G:3550:ARG:HE	2:G:3597:GLN:NE2	2.14	0.45
2:G:4627:MET:SD	2:G:4627:MET:N	2.81	0.45
1:H:106:LEU:HD22	1:H:107:GLU:H	1.79	0.45
2:I:1027:LEU:HD13	2:I:1031:THR:HB	1.98	0.45
2:I:1052:ASN:OD1	2:I:1052:ASN:N	2.45	0.45
2:I:1934:SER:O	2:I:1938:GLN:HG2	2.17	0.45
2:I:2522:LEU:HA	2:I:2526:PHE:HB2	1.98	0.45
2:I:3101:GLU:O	2:I:3105:LYS:HG3	2.16	0.45
2:I:3511:VAL:HG23	2:I:3515:LYS:HD3	1.98	0.45
2:A:1497:GLY:O	2:A:1501:VAL:HG12	2.17	0.45
2:A:4694:ASP:OD1	2:A:4694:ASP:N	2.50	0.45
2:D:229:GLU:HG3	2:D:247:TYR:HB3	1.98	0.45
2:D:2700:MET:HB2	2:D:3001:ILE:HG22	1.98	0.45
2:D:2806:ARG:O	2:D:2810:LYS:HG2	2.16	0.45
2:D:3962:PHE:O	2:D:3966:THR:HG23	2.16	0.45
2:G:246:TYR:HB2	2:G:373:LYS:HD2	1.97	0.45
2:G:823:LEU:HD11	2:G:1626:TRP:HB3	1.98	0.45
2:G:1128:ARG:NH1	2:G:1130:GLN:HG3	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1934:SER:O	2:G:1938:GLN:HG2	2.17	0.45
2:G:1965:TYR:CZ	2:G:2031:LEU:HB2	2.52	0.45
2:I:1128:ARG:NH1	2:I:1130:GLN:HG3	2.32	0.45
2:I:3031:ALA:HB1	2:I:3035:GLU:HB2	1.97	0.45
2:I:3384:LYS:HG2	2:I:3386:GLU:H	1.81	0.45
2:A:355:LEU:HD23	2:A:378:LEU:HB3	1.97	0.45
2:A:2206:THR:O	2:A:2210:VAL:HG23	2.16	0.45
2:A:2668:SER:HB3	2:A:2671:GLU:HG3	1.98	0.45
2:A:2749:GLU:HG3	2:A:2752:ASP:HB2	1.99	0.45
2:A:3969:ILE:HD13	2:A:3980:LEU:HD12	1.99	0.45
2:D:870:ILE:O	2:D:874:LEU:HG	2.16	0.45
2:D:2463:LEU:O	2:D:2467:VAL:HG22	2.16	0.45
2:D:3031:ALA:HB1	2:D:3035:GLU:HB2	1.97	0.45
2:G:618:GLN:OE1	2:G:1678:ASN:ND2	2.46	0.45
2:G:3201:MET:HG3	2:G:3203:VAL:O	2.16	0.45
2:G:3470:LEU:O	2:G:3474:SER:OG	2.28	0.45
2:I:823:LEU:HD11	2:I:1626:TRP:HB3	1.98	0.45
2:I:2155:LEU:HB2	2:I:2188:ASN:HD22	1.80	0.45
2:I:2749:GLU:HG3	2:I:2752:ASP:HB2	1.99	0.45
2:I:2765:LYS:HZ2	2:I:2860:PRO:HA	1.81	0.45
2:I:3206:LEU:HD13	2:I:3246:LEU:HB3	1.98	0.45
2:I:4546:VAL:HA	2:I:4549:VAL:HG22	1.98	0.45
2:A:2661:TRP:HB3	2:A:2664:PHE:CD1	2.52	0.45
2:A:3511:VAL:HG23	2:A:3515:LYS:HD3	1.98	0.45
1:J:85:THR:O	1:J:85:THR:OG1	2.34	0.45
2:D:424:LYS:HE2	2:D:424:LYS:HB2	1.82	0.45
2:D:917:GLU:OE1	3:E:101:PRO:HB2	2.17	0.45
2:D:1617:THR:HG22	2:D:1628:VAL:HG22	1.97	0.45
2:D:1733:GLU:HG2	2:D:2201:LEU:HD23	1.97	0.45
2:D:3539:ARG:HH11	2:D:3552:PHE:HB2	1.81	0.45
2:I:150:MET:HB3	2:I:169:LEU:HD22	1.98	0.45
2:I:707:VAL:HG23	2:I:782:SER:OG	2.16	0.45
2:I:2627:VAL:HA	2:I:2630:VAL:HG12	1.99	0.45
2:I:4688:ILE:HG22	2:I:4689:THR:HG23	1.99	0.45
2:A:823:LEU:HD11	2:A:1626:TRP:HB3	1.98	0.45
2:A:886:ARG:HG2	2:A:891:TRP:CD1	2.51	0.45
2:A:1128:ARG:NH1	2:A:1130:GLN:HG3	2.31	0.45
2:A:3539:ARG:HH11	2:A:3552:PHE:HB2	1.81	0.45
2:D:886:ARG:HG2	2:D:891:TRP:CD1	2.51	0.45
2:D:2867:LEU:HD21	2:D:2871:LEU:HB3	1.98	0.45
2:D:3924:LEU:HD21	2:D:3984:ARG:HH21	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2627:VAL:HA	2:G:2630:VAL:HG12	1.99	0.45
2:G:3974:THR:O	2:G:3978:GLN:HG2	2.17	0.45
2:G:4546:VAL:HA	2:G:4549:VAL:HG22	1.98	0.45
3:M:59:TYR:HB3	3:M:63:VAL:HG21	1.99	0.45
2:I:2211:MET:HA	2:I:2214:VAL:HG12	1.99	0.45
2:I:2710:LEU:HD23	2:I:2955:PHE:CD1	2.52	0.45
2:I:2962:GLN:HA	2:I:2965:ARG:HH11	1.82	0.45
2:I:3207:GLU:H	2:I:3245:VAL:HG23	1.82	0.45
2:A:150:MET:HB3	2:A:169:LEU:HD22	1.98	0.45
2:A:1436:SER:OG	2:A:1565:GLU:HB2	2.17	0.45
2:A:2286:LEU:HD23	2:A:3868:ARG:HH22	1.81	0.45
2:A:2463:LEU:O	2:A:2467:VAL:HG22	2.16	0.45
2:A:3101:GLU:O	2:A:3105:LYS:HG3	2.16	0.45
2:D:1934:SER:O	2:D:1938:GLN:HG2	2.17	0.45
2:D:2302:LEU:HD12	2:D:2363:CYS:HB3	1.98	0.45
2:D:2661:TRP:HB3	2:D:2664:PHE:CD1	2.52	0.45
2:D:2715:VAL:HG12	2:D:2953:LYS:HB3	1.98	0.45
2:D:3280:TYR:CE2	2:D:3284:TRP:CD1	3.04	0.45
2:D:3384:LYS:HG2	2:D:3386:GLU:H	1.81	0.45
2:G:2286:LEU:HD23	2:G:3868:ARG:HH22	1.81	0.45
2:G:2710:LEU:HD23	2:G:2955:PHE:CD1	2.52	0.45
2:I:1422:ASP:N	2:I:1422:ASP:OD1	2.45	0.45
2:I:2302:LEU:HD12	2:I:2363:CYS:HB3	1.98	0.45
2:I:2668:SER:HB3	2:I:2671:GLU:HG3	1.98	0.45
2:I:3280:TYR:CE2	2:I:3284:TRP:CD1	3.04	0.45
2:I:4820:VAL:HB	2:I:4823:LEU:HD23	1.98	0.45
2:A:1965:TYR:CZ	2:A:2031:LEU:HB2	2.51	0.45
2:A:2211:MET:HA	2:A:2214:VAL:HG12	1.99	0.45
2:A:3206:LEU:HD13	2:A:3246:LEU:HB3	1.98	0.45
2:A:3207:GLU:H	2:A:3245:VAL:HG23	1.82	0.45
2:D:901:LYS:HB3	2:D:903:LEU:HG	1.99	0.45
2:D:1436:SER:OG	2:D:1565:GLU:HB2	2.17	0.45
2:D:1497:GLY:O	2:D:1501:VAL:HG12	2.17	0.45
2:G:874:LEU:O	2:G:878:ILE:HG12	2.16	0.45
2:G:1042:ALA:O	2:G:1046:LEU:HG	2.16	0.45
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.30	0.45
2:I:1436:SER:OG	2:I:1565:GLU:HB2	2.17	0.45
2:I:1447:CYS:HB3	2:I:1555:LEU:HB3	1.99	0.45
2:I:1658:ASP:OD1	2:I:1658:ASP:N	2.43	0.45
2:I:1965:TYR:CZ	2:I:2031:LEU:HB2	2.51	0.45
2:I:2263:ILE:HG13	2:I:2264:GLY:N	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2715:VAL:HG12	2:I:2953:LYS:HB3	1.98	0.45
2:I:3969:ILE:HD13	2:I:3980:LEU:HD12	1.99	0.45
2:A:2477:PRO:HD3	2:A:2546:MET:HG2	1.99	0.45
2:A:2627:VAL:HA	2:A:2630:VAL:HG12	1.99	0.45
2:A:3041:SER:O	2:A:3045:LYS:HG3	2.17	0.45
2:A:3201:MET:HG3	2:A:3203:VAL:O	2.16	0.45
2:A:3974:THR:O	2:A:3978:GLN:HG2	2.17	0.45
2:D:3104:GLU:HA	2:D:3107:VAL:HG22	1.99	0.45
2:D:3717:ASP:OD1	2:D:3717:ASP:N	2.43	0.45
2:D:3969:ILE:HD13	2:D:3980:LEU:HD12	1.99	0.45
2:G:1155:LEU:HD13	2:G:1184:ILE:HG23	1.97	0.45
2:G:2211:MET:HA	2:G:2214:VAL:HG12	1.99	0.45
2:G:2522:LEU:HA	2:G:2526:PHE:HB2	1.98	0.45
2:G:3206:LEU:HD13	2:G:3246:LEU:HB3	1.98	0.45
2:G:3962:PHE:O	2:G:3966:THR:HG23	2.16	0.45
2:I:921:ASN:HA	2:I:924:MET:HB2	1.99	0.45
3:K:59:TYR:HB3	3:K:63:VAL:HG21	1.99	0.45
2:A:901:LYS:HB3	2:A:903:LEU:HG	1.99	0.45
2:A:2806:ARG:O	2:A:2810:LYS:HG2	2.16	0.45
2:A:4687:TYR:OH	2:A:4699:GLY:O	2.30	0.45
2:D:1027:LEU:HD13	2:D:1031:THR:HB	1.98	0.45
2:D:2286:LEU:HD23	2:D:3868:ARG:HH22	1.81	0.45
2:D:2477:PRO:HD3	2:D:2546:MET:HG2	1.99	0.45
2:G:886:ARG:HG2	2:G:891:TRP:CD1	2.51	0.45
2:G:2263:ILE:HG13	2:G:2264:GLY:N	2.32	0.45
2:G:3511:VAL:HG23	2:G:3515:LYS:HD3	1.98	0.45
2:G:4024:VAL:HG11	2:G:4142:ASN:HB3	1.97	0.45
2:G:4688:ILE:HG22	2:G:4689:THR:HG23	1.99	0.45
3:M:4:LEU:HD21	3:M:97:ALA:HB2	1.98	0.45
2:I:886:ARG:HG2	2:I:891:TRP:CD1	2.52	0.45
2:I:1225:PRO:HG2	2:I:1228:ILE:HB	1.99	0.45
2:I:2286:LEU:HD23	2:I:3868:ARG:HH22	1.81	0.45
2:I:2751:LEU:O	2:I:2755:ILE:HG12	2.16	0.45
2:I:2906:VAL:HG23	2:I:2911:LEU:HD23	1.99	0.45
2:I:3449:HIS:ND1	2:I:3449:HIS:O	2.50	0.45
2:I:3974:THR:O	2:I:3978:GLN:HG2	2.17	0.45
3:K:4:LEU:HD21	3:K:97:ALA:HB2	1.98	0.45
2:A:1422:ASP:N	2:A:1422:ASP:OD1	2.45	0.45
2:A:1934:SER:O	2:A:1938:GLN:HG2	2.17	0.45
2:A:2263:ILE:HG13	2:A:2264:GLY:N	2.32	0.45
2:A:2302:LEU:HD12	2:A:2363:CYS:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2715:VAL:HG12	2:A:2953:LYS:HB3	1.98	0.45
2:A:2751:LEU:O	2:A:2755:ILE:HG12	2.17	0.45
2:A:3040:THR:HG21	2:A:3080:VAL:HG11	1.99	0.45
2:A:3104:GLU:HA	2:A:3107:VAL:HG22	1.99	0.45
2:D:369:LEU:O	2:D:371:VAL:HG23	2.17	0.45
2:D:1965:TYR:CZ	2:D:2031:LEU:HB2	2.51	0.45
2:D:2970:SER:O	2:D:2974:ILE:HG23	2.17	0.45
2:G:2749:GLU:HG3	2:G:2752:ASP:HB2	1.99	0.45
2:G:2867:LEU:HD21	2:G:2871:LEU:HB3	1.98	0.45
2:G:3280:TYR:CE2	2:G:3284:TRP:CD1	3.04	0.45
2:G:3540:TYR:HB3	2:G:3604:TYR:CD1	2.52	0.45
2:I:874:LEU:O	2:I:878:ILE:HG12	2.16	0.44
2:I:1123:VAL:HG12	2:I:1132:TRP:HB2	1.99	0.44
2:I:1497:GLY:O	2:I:1501:VAL:HG12	2.17	0.44
2:I:3041:SER:O	2:I:3045:LYS:HG3	2.17	0.44
2:I:3754:GLU:HG3	2:I:4719:PHE:HZ	1.81	0.44
2:I:4675:LYS:O	2:I:4679:ARG:HG2	2.16	0.44
2:A:981:GLN:HE21	2:A:1043:VAL:HG13	1.81	0.44
2:A:1937:LEU:HD13	2:A:2116:LEU:HA	1.99	0.44
2:A:2962:GLN:HA	2:A:2965:ARG:HH11	1.82	0.44
2:A:2970:SER:O	2:A:2974:ILE:HG23	2.17	0.44
2:A:3550:ARG:HE	2:A:3597:GLN:NE2	2.14	0.44
1:J:11:ASP:OD2	1:J:13:ARG:HG2	2.16	0.44
2:D:365:LYS:O	2:D:368:ARG:HG3	2.17	0.44
2:D:2266:GLY:HA2	2:D:2271:THR:HG21	1.99	0.44
2:D:3201:MET:SD	2:D:3203:VAL:HG12	2.58	0.44
2:D:3245:VAL:CG1	2:D:3248:ARG:HH12	2.30	0.44
2:D:4232:GLU:OE1	2:D:5019:TRP:NE1	2.31	0.44
2:G:1225:PRO:HG2	2:G:1228:ILE:HB	1.99	0.44
2:G:1243:PRO:HA	2:G:1601:MET:O	2.17	0.44
2:G:2302:LEU:HD12	2:G:2363:CYS:HB3	1.98	0.44
2:G:2661:TRP:HB3	2:G:2664:PHE:CD1	2.52	0.44
2:G:2716:ASP:OD1	2:G:2716:ASP:N	2.42	0.44
2:G:3101:GLU:O	2:G:3105:LYS:HG3	2.16	0.44
2:I:2625:ARG:NE	2:I:2625:ARG:HA	2.33	0.44
2:I:2970:SER:O	2:I:2974:ILE:HG23	2.17	0.44
2:I:3040:THR:HG21	2:I:3080:VAL:HG11	1.99	0.44
2:A:180:LEU:HD23	2:A:180:LEU:HA	1.88	0.44
2:A:921:ASN:HA	2:A:924:MET:HB2	1.99	0.44
2:A:1243:PRO:HA	2:A:1601:MET:O	2.17	0.44
2:A:1447:CYS:HB3	2:A:1555:LEU:HB3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3172:ILE:HD11	2:A:3190:LEU:HB3	1.99	0.44
2:A:4063:ASP:OD1	2:A:4064:MET:N	2.51	0.44
2:D:1128:ARG:NH1	2:D:1130:GLN:HG3	2.32	0.44
2:D:2522:LEU:HA	2:D:2526:PHE:HB2	1.99	0.44
2:D:2751:LEU:O	2:D:2755:ILE:HG12	2.16	0.44
2:D:2782:ASP:N	2:D:2782:ASP:OD1	2.50	0.44
2:D:3206:LEU:HD13	2:D:3246:LEU:HB3	1.98	0.44
2:D:4688:ILE:HG22	2:D:4689:THR:HG23	1.99	0.44
2:D:5013:MET:HG2	2:D:5018:CYS:HB3	2.00	0.44
5:D:5102:POV:H35A	5:D:5102:POV:H32	1.86	0.44
3:E:59:TYR:HB3	3:E:63:VAL:HG21	1.99	0.44
2:G:1497:GLY:O	2:G:1501:VAL:HG12	2.17	0.44
2:G:2765:LYS:HZ2	2:G:2860:PRO:HA	1.81	0.44
2:G:2782:ASP:HB2	2:G:2784:GLU:HG3	1.99	0.44
2:G:3023:LYS:HE2	2:G:3023:LYS:HB3	1.78	0.44
2:G:4063:ASP:OD1	2:G:4064:MET:N	2.51	0.44
2:G:4066:LEU:HD23	2:G:4066:LEU:HA	1.86	0.44
2:I:363:ASP:HB3	2:I:366:ALA:HB3	1.98	0.44
2:I:901:LYS:HB3	2:I:903:LEU:HG	1.99	0.44
2:I:2661:TRP:HB3	2:I:2664:PHE:CD1	2.52	0.44
2:I:3336:LYS:HG2	2:I:3337:ARG:N	2.31	0.44
2:A:874:LEU:O	2:A:878:ILE:HG12	2.16	0.44
2:A:1225:PRO:HG2	2:A:1228:ILE:HB	1.99	0.44
2:A:2266:GLY:HA2	2:A:2271:THR:HG21	2.00	0.44
2:A:2782:ASP:HB2	2:A:2784:GLU:HG3	1.99	0.44
2:A:3201:MET:SD	2:A:3203:VAL:HG12	2.58	0.44
2:A:3249:LEU:HD12	2:A:3249:LEU:H	1.83	0.44
2:A:3438:VAL:HG23	2:A:3514:LEU:HD13	2.00	0.44
2:A:3449:HIS:ND1	2:A:3449:HIS:O	2.50	0.44
2:A:4688:ILE:HG22	2:A:4689:THR:HG23	1.99	0.44
2:D:551:LEU:HD13	2:D:589:LEU:HD11	2.00	0.44
2:D:1123:VAL:HG12	2:D:1132:TRP:HB2	1.99	0.44
2:D:1225:PRO:HG2	2:D:1228:ILE:HB	1.99	0.44
2:D:1447:CYS:HB3	2:D:1555:LEU:HB3	1.99	0.44
2:D:3172:ILE:HD11	2:D:3190:LEU:HB3	1.99	0.44
2:G:901:LYS:HB3	2:G:903:LEU:HG	1.99	0.44
2:G:1027:LEU:HD13	2:G:1031:THR:HB	1.98	0.44
2:G:1109:LEU:HA	2:G:1120:LEU:HD13	2.00	0.44
2:G:2906:VAL:HG23	2:G:2911:LEU:HD23	1.99	0.44
2:G:3040:THR:HG21	2:G:3080:VAL:HG11	1.99	0.44
2:G:3146:HIS:CE1	2:G:3150:HIS:HD2	2.36	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3924:LEU:HD21	2:G:3984:ARG:HH21	1.81	0.44
2:I:2806:ARG:O	2:I:2810:LYS:HG2	2.16	0.44
2:I:2960:LEU:HA	2:I:2963:LEU:HD12	1.99	0.44
2:I:3201:MET:HG3	2:I:3203:VAL:O	2.16	0.44
2:I:4063:ASP:OD1	2:I:4064:MET:N	2.51	0.44
2:A:2700:MET:HB2	2:A:3001:ILE:HG22	1.97	0.44
2:D:574:VAL:O	2:D:578:ILE:HG12	2.18	0.44
2:D:2211:MET:HA	2:D:2214:VAL:HG12	1.99	0.44
2:D:2710:LEU:HD23	2:D:2955:PHE:CD1	2.52	0.44
2:D:3101:GLU:O	2:D:3105:LYS:HG3	2.16	0.44
2:G:4820:VAL:HB	2:G:4823:LEU:HD23	1.98	0.44
2:I:574:VAL:O	2:I:578:ILE:HG12	2.18	0.44
2:I:634:GLN:O	2:I:1639:LEU:HD12	2.18	0.44
2:I:1109:LEU:HA	2:I:1120:LEU:HD13	2.00	0.44
2:I:3539:ARG:HH11	2:I:3552:PHE:CB	2.31	0.44
2:I:4189:ARG:NH1	2:I:5032:TYR:OH	2.51	0.44
2:A:3003:LEU:HB2	2:A:3004:PRO:HD3	1.99	0.44
2:D:2263:ILE:HG13	2:D:2264:GLY:N	2.32	0.44
2:D:2725:LYS:HE2	2:D:2738:ARG:HH22	1.83	0.44
2:G:551:LEU:HD13	2:G:589:LEU:HD11	2.00	0.44
2:G:574:VAL:O	2:G:578:ILE:HG12	2.18	0.44
2:G:1123:VAL:HG12	2:G:1132:TRP:HB2	1.99	0.44
2:G:2970:SER:O	2:G:2974:ILE:HG23	2.17	0.44
2:G:3539:ARG:HH11	2:G:3552:PHE:CB	2.31	0.44
2:G:3969:ILE:HD13	2:G:3980:LEU:HD12	1.99	0.44
2:I:3172:ILE:HD11	2:I:3190:LEU:HB3	1.99	0.44
2:I:3249:LEU:HD12	2:I:3249:LEU:H	1.83	0.44
2:I:3719:ASP:O	2:I:3723:MET:HG3	2.18	0.44
2:A:574:VAL:O	2:A:578:ILE:HG12	2.17	0.44
2:A:2710:LEU:HD23	2:A:2955:PHE:CD1	2.52	0.44
2:A:2906:VAL:HG23	2:A:2911:LEU:HD23	1.99	0.44
2:D:355:LEU:HB3	2:D:378:LEU:HD22	2.00	0.44
2:D:2749:GLU:HG3	2:D:2752:ASP:HB2	1.98	0.44
2:D:3040:THR:HG21	2:D:3080:VAL:HG11	1.99	0.44
2:D:3438:VAL:HG23	2:D:3514:LEU:HD13	2.00	0.44
2:D:3449:HIS:ND1	2:D:3449:HIS:O	2.50	0.44
2:D:3539:ARG:HH11	2:D:3552:PHE:CB	2.31	0.44
2:D:3974:THR:O	2:D:3978:GLN:HG2	2.17	0.44
2:D:4211:LYS:O	2:D:4215:ARG:HG3	2.18	0.44
2:G:3104:GLU:HA	2:G:3107:VAL:HG22	1.99	0.44
2:G:3172:ILE:HD11	2:G:3190:LEU:HB3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3249:LEU:H	2:G:3249:LEU:HD12	1.83	0.44
2:G:3719:ASP:O	2:G:3723:MET:HG3	2.18	0.44
2:I:2263:ILE:HG13	2:I:2264:GLY:H	1.83	0.44
2:I:2477:PRO:HD3	2:I:2546:MET:HG2	1.99	0.44
2:A:458:GLU:H	2:A:458:GLU:HG3	1.67	0.44
2:A:3719:ASP:O	2:A:3723:MET:HG3	2.18	0.44
2:A:4651:THR:HG21	2:A:4803:HIS:CE1	2.53	0.44
3:C:59:TYR:HB3	3:C:63:VAL:HG21	1.99	0.44
2:D:2765:LYS:HZ3	2:D:2857:PRO:HB2	1.82	0.44
2:D:3146:HIS:CE1	2:D:3150:HIS:HD2	2.36	0.44
2:D:4081:VAL:HG12	2:D:4088:ILE:HD13	1.99	0.44
2:G:634:GLN:O	2:G:1639:LEU:HD12	2.18	0.44
2:G:2960:LEU:HA	2:G:2963:LEU:HD12	2.00	0.44
2:G:3449:HIS:ND1	2:G:3449:HIS:O	2.50	0.44
2:G:3834:ALA:O	2:G:3838:THR:HG23	2.18	0.44
2:I:130:LYS:O	2:I:130:LYS:HD3	2.18	0.44
2:I:1243:PRO:HA	2:I:1601:MET:O	2.17	0.44
2:I:1937:LEU:HD13	2:I:2116:LEU:HA	2.00	0.44
2:I:2689:LYS:O	2:I:2993:GLN:NE2	2.51	0.44
2:I:4211:LYS:O	2:I:4215:ARG:HG3	2.18	0.44
2:A:551:LEU:HD13	2:A:589:LEU:HD11	2.00	0.44
2:A:5013:MET:HG2	2:A:5018:CYS:HB3	2.00	0.44
2:D:1937:LEU:HD13	2:D:2116:LEU:HA	2.00	0.44
2:D:2759:ALA:HB2	2:D:2810:LYS:HZ1	1.83	0.44
2:D:3003:LEU:HB2	2:D:3004:PRO:HD3	1.99	0.44
2:D:3207:GLU:H	2:D:3245:VAL:HG23	1.82	0.44
2:D:3249:LEU:HD12	2:D:3249:LEU:H	1.83	0.44
2:D:4189:ARG:NH1	2:D:5032:TYR:OH	2.51	0.44
2:G:1041:GLN:HA	2:G:1044:ARG:HH11	1.83	0.44
2:G:2751:LEU:O	2:G:2755:ILE:HG12	2.16	0.44
2:G:3003:LEU:HB2	2:G:3004:PRO:HD3	1.99	0.44
2:G:3201:MET:SD	2:G:3203:VAL:HG12	2.58	0.44
2:G:3207:GLU:H	2:G:3245:VAL:HG23	1.82	0.44
2:G:3568:SER:O	2:G:3571:TRP:NE1	2.51	0.44
2:I:2266:GLY:HA2	2:I:2271:THR:HG21	2.00	0.44
2:I:3540:TYR:HB3	2:I:3604:TYR:CD1	2.52	0.44
2:I:3834:ALA:O	2:I:3838:THR:HG23	2.18	0.44
2:I:4215:ARG:HH21	6:I:5103:ATP:PG	2.41	0.44
2:A:2960:LEU:HA	2:A:2963:LEU:HD12	1.99	0.44
2:A:3245:VAL:CG1	2:A:3248:ARG:HH12	2.31	0.44
2:A:4081:VAL:HG12	2:A:4088:ILE:HD13	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1109:LEU:HA	2:D:1120:LEU:HD13	2.00	0.44
2:D:1860:LYS:HE3	2:D:1860:LYS:HB2	1.84	0.44
2:D:4063:ASP:OD1	2:D:4064:MET:N	2.51	0.44
2:G:2962:GLN:HA	2:G:2965:ARG:HH11	1.82	0.44
2:I:2725:LYS:HE2	2:I:2738:ARG:HH22	1.83	0.43
2:I:2960:LEU:HD22	2:I:3038:MET:HB2	2.00	0.43
2:I:3104:GLU:HA	2:I:3107:VAL:HG22	1.99	0.43
2:I:3273:THR:O	2:I:3276:MET:HB2	2.18	0.43
2:I:4885:PHE:CE2	2:I:4897:ILE:HD11	2.53	0.43
2:A:3586:ALA:HA	2:A:3591:LYS:HD2	2.01	0.43
2:D:921:ASN:HA	2:D:924:MET:HB2	1.99	0.43
2:D:1041:GLN:HA	2:D:1044:ARG:HH11	1.83	0.43
2:D:2627:VAL:HA	2:D:2630:VAL:HG12	1.99	0.43
2:G:1436:SER:OG	2:G:1565:GLU:HB2	2.17	0.43
2:G:2580:ASP:HA	2:G:2583:LEU:HD12	2.00	0.43
2:G:2960:LEU:HD22	2:G:3038:MET:HB2	2.00	0.43
2:G:3041:SER:O	2:G:3045:LYS:HG3	2.17	0.43
2:G:4211:LYS:O	2:G:4215:ARG:HG3	2.18	0.43
2:I:3003:LEU:HB2	2:I:3004:PRO:HD3	1.99	0.43
2:I:3438:VAL:HG23	2:I:3514:LEU:HD13	2.00	0.43
2:I:3539:ARG:HH11	2:I:3552:PHE:HB2	1.82	0.43
2:I:3568:SER:O	2:I:3571:TRP:NE1	2.51	0.43
2:A:1027:LEU:HA	2:A:1027:LEU:HD23	1.82	0.43
2:A:1860:LYS:HE3	2:A:1860:LYS:HB2	1.84	0.43
2:A:1935:VAL:O	2:A:1939:MET:HE2	2.18	0.43
2:A:2638:LYS:HE2	2:A:2638:LYS:HB3	1.87	0.43
2:A:3333:THR:O	2:A:3336:LYS:NZ	2.39	0.43
2:A:3540:TYR:HB3	2:A:3604:TYR:CD1	2.52	0.43
2:A:4189:ARG:NH1	2:A:5032:TYR:OH	2.51	0.43
2:D:2959:PHE:O	2:D:2963:LEU:HG	2.19	0.43
3:E:9:GLY:HA3	3:E:123:VAL:HG22	2.00	0.43
2:G:355:LEU:HB3	2:G:378:LEU:HD22	2.00	0.43
2:G:648:ILE:HD11	2:G:793:LEU:HD13	2.00	0.43
2:G:2440:MET:HE2	2:G:2440:MET:HA	1.98	0.43
2:G:4885:PHE:CE2	2:G:4897:ILE:HD11	2.53	0.43
2:G:5013:MET:HG2	2:G:5018:CYS:HB3	2.00	0.43
2:I:2754:PHE:HB2	2:I:2935:TYR:OH	2.18	0.43
2:A:3568:SER:O	2:A:3571:TRP:NE1	2.51	0.43
2:A:3694:LYS:HB2	2:A:3694:LYS:HE3	1.76	0.43
2:D:130:LYS:O	2:D:130:LYS:HD3	2.18	0.43
2:D:363:ASP:OD1	2:D:365:LYS:HG2	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3041:SER:O	2:D:3045:LYS:HG3	2.17	0.43
2:D:3698:LEU:O	2:D:3702:VAL:HG12	2.18	0.43
2:D:3946:GLN:OE1	2:D:3949:ARG:NH2	2.51	0.43
2:D:4885:PHE:CE2	2:D:4897:ILE:HD11	2.53	0.43
2:G:1447:CYS:HB3	2:G:1555:LEU:HB3	1.99	0.43
2:G:2477:PRO:HD3	2:G:2546:MET:HG2	1.99	0.43
2:G:2765:LYS:HA	2:G:2765:LYS:HD3	1.82	0.43
2:G:3946:GLN:OE1	2:G:3949:ARG:NH2	2.51	0.43
2:I:2759:ALA:HB2	2:I:2810:LYS:HZ1	1.83	0.43
2:I:3201:MET:SD	2:I:3203:VAL:HG12	2.58	0.43
2:I:3946:GLN:OE1	2:I:3949:ARG:NH2	2.51	0.43
2:A:1123:VAL:HG12	2:A:1132:TRP:HB2	1.99	0.43
2:A:2580:ASP:HA	2:A:2583:LEU:HD12	2.00	0.43
2:A:4779:LYS:HE3	2:A:4779:LYS:HB2	1.82	0.43
2:D:246:TYR:HB3	2:D:373:LYS:HA	2.00	0.43
2:D:634:GLN:O	2:D:1639:LEU:HD12	2.18	0.43
2:D:2679:PHE:HB2	2:D:2706:ILE:HG21	2.00	0.43
2:D:2689:LYS:O	2:D:2993:GLN:NE2	2.51	0.43
2:D:2782:ASP:HB2	2:D:2784:GLU:HG3	1.99	0.43
2:D:2906:VAL:HG23	2:D:2911:LEU:HD23	1.99	0.43
2:D:3540:TYR:HB3	2:D:3604:TYR:CD1	2.52	0.43
2:G:921:ASN:HA	2:G:924:MET:HB2	1.99	0.43
2:G:2266:GLY:HA2	2:G:2271:THR:HG21	1.99	0.43
2:G:3273:THR:O	2:G:3276:MET:HB2	2.18	0.43
2:G:3395:ARG:HG2	2:G:3453:ARG:NH1	2.33	0.43
2:I:648:ILE:HD11	2:I:793:LEU:HD13	2.00	0.43
2:I:1249:PRO:HG2	2:I:1252:HIS:HB2	2.01	0.43
2:I:2185:ILE:HD12	2:I:2203:MET:HE1	2.01	0.43
2:I:2782:ASP:HB2	2:I:2784:GLU:HG3	1.99	0.43
2:I:3000:LYS:HA	2:I:3000:LYS:HD3	1.86	0.43
2:I:3245:VAL:CG1	2:I:3248:ARG:HH12	2.31	0.43
2:I:3694:LYS:HB2	2:I:3694:LYS:HE3	1.77	0.43
2:I:4651:THR:HG21	2:I:4803:HIS:CE1	2.53	0.43
2:A:981:GLN:HG2	2:A:1047:LEU:HD11	2.01	0.43
2:A:2189:LYS:HA	2:A:2192:TYR:CE2	2.53	0.43
2:A:2679:PHE:HB2	2:A:2706:ILE:HG21	2.00	0.43
2:A:2725:LYS:HE2	2:A:2738:ARG:HH22	1.83	0.43
2:A:2754:PHE:HB2	2:A:2935:TYR:OH	2.18	0.43
2:A:2801:ASP:HA	2:A:2804:ILE:HG12	2.00	0.43
2:A:3539:ARG:HH11	2:A:3552:PHE:CB	2.31	0.43
2:A:3698:LEU:O	2:A:3702:VAL:HG12	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4211:LYS:O	2:A:4215:ARG:HG3	2.18	0.43
2:D:2580:ASP:HA	2:D:2583:LEU:HD12	2.00	0.43
2:D:2754:PHE:HB2	2:D:2935:TYR:OH	2.18	0.43
2:D:3568:SER:O	2:D:3571:TRP:NE1	2.51	0.43
2:D:3586:ALA:HA	2:D:3591:LYS:HD2	2.01	0.43
2:D:4694:ASP:OD1	2:D:4694:ASP:N	2.50	0.43
2:G:917:GLU:OE1	3:M:101:PRO:HB2	2.19	0.43
2:I:981:GLN:HG2	2:I:1047:LEU:HD11	2.01	0.43
2:I:2189:LYS:HA	2:I:2192:TYR:CE2	2.53	0.43
2:I:4694:ASP:OD1	2:I:4694:ASP:N	2.50	0.43
2:I:5013:MET:CE	2:I:5021:PHE:HB3	2.47	0.43
2:A:634:GLN:O	2:A:1639:LEU:HD12	2.18	0.43
2:A:2182:ILE:O	2:A:2186:MET:HG2	2.19	0.43
2:A:3639:THR:N	2:A:3640:PRO:HD2	2.34	0.43
2:A:4885:PHE:CE2	2:A:4897:ILE:HD11	2.53	0.43
2:D:1243:PRO:HA	2:D:1601:MET:O	2.17	0.43
2:G:1249:PRO:HG2	2:G:1252:HIS:HB2	2.01	0.43
2:G:2782:ASP:N	2:G:2782:ASP:OD1	2.49	0.43
2:I:551:LEU:HD13	2:I:589:LEU:HD11	2.00	0.43
2:I:919:ASN:HA	2:I:922:LEU:HB2	2.01	0.43
2:I:2124:LEU:HD11	2:I:2128:TYR:HE2	1.84	0.43
2:I:3107:VAL:HA	2:I:3175:LEU:HD21	2.01	0.43
2:I:3146:HIS:CE1	2:I:3150:HIS:HD2	2.36	0.43
2:A:223:PHE:O	2:A:388:LEU:HB2	2.19	0.43
2:A:648:ILE:HD11	2:A:793:LEU:HD13	2.00	0.43
2:A:1041:GLN:HA	2:A:1044:ARG:HH11	1.83	0.43
2:A:1109:LEU:HA	2:A:1120:LEU:HD13	2.00	0.43
2:A:2625:ARG:NE	2:A:2625:ARG:HA	2.33	0.43
2:D:648:ILE:HD11	2:D:793:LEU:HD13	2.00	0.43
2:I:659:TYR:O	2:I:662:TRP:NE1	2.51	0.43
2:I:3586:ALA:HA	2:I:3591:LYS:HD2	2.01	0.43
2:A:3946:GLN:OE1	2:A:3949:ARG:NH2	2.51	0.43
2:D:180:LEU:HD23	2:D:180:LEU:HA	1.88	0.43
2:D:2182:ILE:O	2:D:2186:MET:HG2	2.19	0.43
2:D:2625:ARG:NE	2:D:2625:ARG:HA	2.33	0.43
2:D:2960:LEU:HA	2:D:2963:LEU:HD12	2.00	0.43
2:D:3639:THR:N	2:D:3640:PRO:HD2	2.34	0.43
2:D:4651:THR:HG21	2:D:4803:HIS:CE1	2.53	0.43
2:G:223:PHE:O	2:G:388:LEU:HB2	2.19	0.43
2:G:919:ASN:HA	2:G:922:LEU:HB2	2.01	0.43
2:G:1871:PHE:HZ	2:G:2094:LEU:HD13	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1937:LEU:HD13	2:G:2116:LEU:HA	2.00	0.43
2:G:2182:ILE:O	2:G:2186:MET:HG2	2.19	0.43
2:G:2263:ILE:HG13	2:G:2264:GLY:H	1.83	0.43
2:G:2625:ARG:NE	2:G:2625:ARG:HA	2.32	0.43
2:G:3438:VAL:HG23	2:G:3514:LEU:HD13	2.00	0.43
2:G:4694:ASP:OD1	2:G:4694:ASP:N	2.50	0.43
2:G:5011:TRP:CH2	7:G:5104:CFF:H102	2.54	0.43
2:I:1041:GLN:HA	2:I:1044:ARG:HH11	1.83	0.43
2:I:3698:LEU:O	2:I:3702:VAL:HG12	2.18	0.43
2:I:4958:CYS:HA	6:I:5103:ATP:N7	2.34	0.43
2:A:130:LYS:O	2:A:130:LYS:HD3	2.18	0.43
2:A:355:LEU:HB3	2:A:378:LEU:HD22	2.00	0.43
2:A:1207:ASP:OD1	2:A:1207:ASP:N	2.50	0.43
2:A:2124:LEU:HD11	2:A:2128:TYR:HE2	1.84	0.43
2:A:3155:ASP:HA	2:A:3158:LEU:HD23	2.01	0.43
2:A:3273:THR:O	2:A:3276:MET:HB2	2.18	0.43
2:A:4780:PHE:HA	2:A:4783:ILE:HG22	2.01	0.43
2:A:4954:MET:O	6:A:5103:ATP:O2'	2.27	0.43
2:D:919:ASN:HA	2:D:922:LEU:HB2	2.01	0.43
2:D:2124:LEU:HD11	2:D:2128:TYR:HE2	1.84	0.43
2:D:2465:ASP:O	2:D:2469:ILE:HG22	2.19	0.43
2:D:2610:LEU:O	2:D:2614:ILE:HG12	2.19	0.43
2:D:3155:ASP:HA	2:D:3158:LEU:HD23	2.01	0.43
2:D:4071:ILE:HD12	2:D:4103:PHE:HE2	1.84	0.43
3:E:105:ASN:HD21	3:E:111:ASN:CB	2.32	0.43
2:G:981:GLN:HG2	2:G:1047:LEU:HD11	2.01	0.43
2:G:2754:PHE:HB2	2:G:2935:TYR:OH	2.18	0.43
2:G:2801:ASP:HA	2:G:2804:ILE:HG12	2.00	0.43
2:G:2996:LYS:HD3	2:G:2996:LYS:HA	1.87	0.43
2:G:3694:LYS:HB2	2:G:3694:LYS:HE3	1.76	0.43
2:G:3698:LEU:O	2:G:3702:VAL:HG12	2.18	0.43
2:G:4189:ARG:NH1	2:G:5032:TYR:OH	2.51	0.43
3:M:9:GLY:HA3	3:M:123:VAL:HG22	2.00	0.43
3:M:105:ASN:HD21	3:M:111:ASN:CB	2.32	0.43
2:I:737:LEU:HD12	2:I:737:LEU:HA	1.93	0.43
2:I:864:PRO:O	2:I:866:HIS:N	2.52	0.43
2:I:1871:PHE:HZ	2:I:2094:LEU:HD13	1.84	0.43
2:I:2580:ASP:HA	2:I:2583:LEU:HD12	2.00	0.43
2:I:2712:PRO:HD3	2:I:3013:HIS:CE1	2.54	0.43
2:I:2858:GLN:HB2	2:I:2859:PRO:HD3	2.01	0.43
2:I:3227:ARG:HB3	2:I:3232:LEU:HB2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3395:ARG:HG2	2:I:3453:ARG:NH1	2.33	0.43
3:K:68:THR:HG1	3:K:81:GLN:HB3	1.84	0.43
2:A:864:PRO:O	2:A:866:HIS:N	2.52	0.43
2:A:2821:TRP:HD1	2:A:2939:ARG:HA	1.84	0.43
2:A:3137:LEU:HB3	2:A:3138:PRO:HD3	2.01	0.43
3:C:9:GLY:HA3	3:C:123:VAL:HG22	2.00	0.43
2:D:223:PHE:O	2:D:388:LEU:HB2	2.19	0.43
2:D:365:LYS:HE3	2:D:365:LYS:HB3	1.90	0.43
2:D:2821:TRP:HD1	2:D:2939:ARG:HA	1.84	0.43
2:D:3395:ARG:HG2	2:D:3453:ARG:NH1	2.33	0.43
2:D:3834:ALA:O	2:D:3838:THR:HG23	2.18	0.43
2:G:2619:LEU:O	2:G:2623:LEU:HD23	2.19	0.43
2:I:3866:ILE:HG23	2:I:3868:ARG:H	1.84	0.42
2:I:4081:VAL:HG12	2:I:4088:ILE:HD13	1.99	0.42
3:K:47:LEU:O	3:K:62:SER:OG	2.37	0.42
2:A:2465:ASP:O	2:A:2469:ILE:HG22	2.19	0.42
2:A:2638:LYS:H	2:A:2638:LYS:HG2	1.71	0.42
2:A:2689:LYS:O	2:A:2993:GLN:NE2	2.51	0.42
2:A:2959:PHE:O	2:A:2963:LEU:HG	2.19	0.42
2:A:2960:LEU:HD22	2:A:3038:MET:HB2	2.00	0.42
2:A:2973:PHE:CD1	2:A:2995:ILE:HG12	2.54	0.42
2:A:3395:ARG:HG2	2:A:3453:ARG:NH1	2.33	0.42
2:D:2801:ASP:HA	2:D:2804:ILE:HG12	2.00	0.42
2:D:3273:THR:O	2:D:3276:MET:HB2	2.18	0.42
2:D:3694:LYS:HE3	2:D:3694:LYS:HB2	1.76	0.42
2:D:3719:ASP:O	2:D:3723:MET:HG3	2.18	0.42
2:D:4066:LEU:HD23	2:D:4066:LEU:HA	1.86	0.42
2:G:1935:VAL:O	2:G:1939:MET:HE2	2.19	0.42
2:G:2625:ARG:HA	2:G:2625:ARG:HE	1.84	0.42
2:G:2679:PHE:HB2	2:G:2706:ILE:HG21	2.00	0.42
2:G:2959:PHE:O	2:G:2963:LEU:HG	2.19	0.42
2:G:4998:LYS:HB2	2:G:4998:LYS:HE3	1.73	0.42
2:I:223:PHE:O	2:I:388:LEU:HB2	2.18	0.42
2:I:2465:ASP:O	2:I:2469:ILE:HG22	2.19	0.42
2:I:2610:LEU:O	2:I:2614:ILE:HG12	2.19	0.42
2:I:2625:ARG:HA	2:I:2625:ARG:HE	1.84	0.42
2:A:1079:LYS:HA	2:A:1189:LEU:HD11	2.00	0.42
2:A:2625:ARG:HA	2:A:2625:ARG:HE	1.84	0.42
2:A:4071:ILE:HD12	2:A:4103:PHE:HE2	1.84	0.42
2:A:4805:ASN:HB3	2:A:4808:PHE:CD2	2.55	0.42
2:D:248:GLU:HB2	2:D:373:LYS:NZ	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1871:PHE:HZ	2:D:2094:LEU:HD13	1.84	0.42
2:D:2189:LYS:HA	2:D:2192:TYR:CE2	2.53	0.42
2:D:2619:LEU:O	2:D:2623:LEU:HD23	2.19	0.42
2:D:2962:GLN:HA	2:D:2965:ARG:HH11	1.82	0.42
2:D:5011:TRP:CH2	7:D:5104:CFF:H102	2.54	0.42
2:G:2689:LYS:O	2:G:2993:GLN:NE2	2.51	0.42
2:G:3586:ALA:HA	2:G:3591:LYS:HD2	2.01	0.42
2:G:4081:VAL:HG12	2:G:4088:ILE:HD13	2.00	0.42
3:M:47:LEU:O	3:M:62:SER:OG	2.37	0.42
2:I:1079:LYS:HA	2:I:1189:LEU:HD11	2.01	0.42
2:I:2679:PHE:HB2	2:I:2706:ILE:HG21	2.00	0.42
2:I:2765:LYS:HA	2:I:2765:LYS:HD3	1.82	0.42
2:I:2801:ASP:HA	2:I:2804:ILE:HG12	2.00	0.42
2:I:2991:HIS:O	2:I:2995:ILE:HG13	2.20	0.42
2:I:3155:ASP:HA	2:I:3158:LEU:HD23	2.01	0.42
2:I:4780:PHE:HA	2:I:4783:ILE:HG22	2.01	0.42
2:I:5013:MET:HE3	2:I:5021:PHE:CD2	2.54	0.42
2:A:659:TYR:O	2:A:662:TRP:NE1	2.51	0.42
2:A:919:ASN:HA	2:A:922:LEU:HB2	2.01	0.42
2:A:3107:VAL:HA	2:A:3175:LEU:HD21	2.01	0.42
2:A:3146:HIS:CE1	2:A:3150:HIS:HD2	2.36	0.42
2:A:3227:ARG:HB3	2:A:3232:LEU:HB2	2.01	0.42
3:C:105:ASN:HD21	3:C:111:ASN:CB	2.32	0.42
2:D:112:ALA:O	2:D:115:ARG:NH1	2.53	0.42
2:D:2625:ARG:HA	2:D:2625:ARG:HE	1.84	0.42
2:D:2765:LYS:HD3	2:D:2765:LYS:HA	1.81	0.42
2:D:2858:GLN:HB2	2:D:2859:PRO:HD3	2.01	0.42
2:G:2189:LYS:HA	2:G:2192:TYR:CE2	2.53	0.42
2:G:2759:ALA:HB2	2:G:2810:LYS:HZ1	1.84	0.42
2:G:2991:HIS:O	2:G:2995:ILE:HG13	2.20	0.42
2:G:3137:LEU:HB3	2:G:3138:PRO:HD3	2.01	0.42
2:G:4651:THR:HG21	2:G:4803:HIS:CE1	2.53	0.42
2:I:355:LEU:HB3	2:I:378:LEU:HD22	2.00	0.42
2:I:1035:ASN:OD1	3:K:109:THR:OG1	2.37	0.42
2:I:2619:LEU:O	2:I:2623:LEU:HD23	2.19	0.42
2:I:2821:TRP:HD1	2:I:2939:ARG:HA	1.84	0.42
2:I:2959:PHE:O	2:I:2963:LEU:HG	2.19	0.42
2:I:3284:TRP:CE3	2:I:3287:ARG:HD3	2.55	0.42
2:I:4959:PHE:CD1	2:I:4985:LEU:HD11	2.55	0.42
2:A:2185:ILE:HD12	2:A:2203:MET:HE1	2.02	0.42
2:A:2759:ALA:HB2	2:A:2810:LYS:HZ1	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3158:LEU:HD12	2:A:3159:ASP:HB2	2.01	0.42
2:D:659:TYR:O	2:D:662:TRP:NE1	2.51	0.42
2:D:2263:ILE:HG13	2:D:2264:GLY:H	1.83	0.42
2:D:3284:TRP:CE3	2:D:3287:ARG:HD3	2.55	0.42
2:D:4959:PHE:CD1	2:D:4985:LEU:HD11	2.55	0.42
2:D:4998:LYS:HB2	2:D:4998:LYS:HE3	1.73	0.42
2:G:3158:LEU:HD12	2:G:3159:ASP:HB2	2.01	0.42
2:G:3752:SER:O	2:G:3756:LYS:HG3	2.20	0.42
2:G:4071:ILE:HD12	2:G:4103:PHE:HE2	1.84	0.42
2:I:1154:ASP:OD1	2:I:1159:THR:OG1	2.25	0.42
2:I:2312:MET:HA	2:I:2315:ALA:HB3	2.01	0.42
2:I:2973:PHE:CD1	2:I:2995:ILE:HG12	2.54	0.42
2:I:3639:THR:N	2:I:3640:PRO:HD2	2.34	0.42
2:A:2263:ILE:HG13	2:A:2264:GLY:H	1.84	0.42
2:A:2610:LEU:O	2:A:2614:ILE:HG12	2.19	0.42
2:A:2712:PRO:HD3	2:A:3013:HIS:CE1	2.54	0.42
2:A:2858:GLN:HB2	2:A:2859:PRO:HD3	2.02	0.42
2:D:981:GLN:HG2	2:D:1047:LEU:HD11	2.01	0.42
2:D:1163:THR:HG22	2:D:1168:VAL:HA	2.02	0.42
2:D:3107:VAL:HA	2:D:3175:LEU:HD21	2.01	0.42
2:D:3752:SER:O	2:D:3756:LYS:HG3	2.20	0.42
2:G:2465:ASP:O	2:G:2469:ILE:HG22	2.19	0.42
2:G:2712:PRO:HD3	2:G:3013:HIS:CE1	2.54	0.42
2:G:2725:LYS:HE2	2:G:2738:ARG:HH22	1.83	0.42
2:G:3250:MET:O	2:G:3253:ILE:HG22	2.20	0.42
2:G:4188:ARG:HG2	2:G:4188:ARG:HH11	1.85	0.42
2:A:2312:MET:HA	2:A:2315:ALA:HB3	2.01	0.42
2:A:4118:ASP:OD1	2:A:4119:GLU:N	2.53	0.42
2:A:4715:TYR:CE2	2:A:4717:ASP:HB3	2.55	0.42
2:D:2973:PHE:CD1	2:D:2995:ILE:HG12	2.54	0.42
2:D:4188:ARG:HG2	2:D:4188:ARG:HH11	1.85	0.42
2:D:4687:TYR:OH	2:D:4699:GLY:O	2.30	0.42
2:D:4698:LYS:HE3	2:D:4698:LYS:HB2	1.91	0.42
2:G:130:LYS:O	2:G:130:LYS:HD3	2.18	0.42
2:G:2638:LYS:HE2	2:G:2638:LYS:HB3	1.87	0.42
2:G:2686:LEU:HD23	2:G:3001:ILE:HD13	2.02	0.42
2:G:2821:TRP:HD1	2:G:2939:ARG:HA	1.84	0.42
2:G:3227:ARG:HB3	2:G:3232:LEU:HB2	2.01	0.42
2:G:3769:ARG:O	2:G:3773:ARG:NH1	2.53	0.42
3:M:85:LEU:HD23	3:M:85:LEU:HA	1.94	0.42
2:I:618:GLN:OE1	2:I:1678:ASN:ND2	2.46	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2182:ILE:O	2:I:2186:MET:HG2	2.19	0.42
2:I:3397:GLU:O	2:I:3400:VAL:HG12	2.20	0.42
2:I:4071:ILE:HD12	2:I:4103:PHE:HE2	1.84	0.42
2:I:4698:LYS:HE3	2:I:4698:LYS:HB2	1.91	0.42
3:K:9:GLY:HA3	3:K:123:VAL:HG22	2.00	0.42
1:L:85:THR:O	1:L:85:THR:OG1	2.34	0.42
2:A:112:ALA:O	2:A:115:ARG:NH1	2.53	0.42
2:A:3757:GLU:O	2:A:3761:GLN:HG2	2.20	0.42
2:D:2960:LEU:HD22	2:D:3038:MET:HB2	2.00	0.42
2:D:4779:LYS:HE3	2:D:4779:LYS:HB2	1.82	0.42
2:D:4780:PHE:HA	2:D:4783:ILE:HG22	2.01	0.42
2:D:4954:MET:O	6:D:5103:ATP:O2'	2.28	0.42
2:G:1079:LYS:HA	2:G:1189:LEU:HD11	2.00	0.42
2:G:2359:ARG:HD3	2:G:2359:ARG:HA	1.92	0.42
2:G:2858:GLN:HB2	2:G:2859:PRO:HD3	2.01	0.42
2:G:2973:PHE:CD1	2:G:2995:ILE:HG12	2.54	0.42
2:G:3107:VAL:HA	2:G:3175:LEU:HD21	2.01	0.42
2:G:3284:TRP:CE3	2:G:3287:ARG:HD3	2.55	0.42
2:G:3959:LYS:HG3	2:G:4022:ASP:OD2	2.20	0.42
2:G:4780:PHE:HA	2:G:4783:ILE:HG22	2.01	0.42
2:I:180:LEU:HD23	2:I:180:LEU:HA	1.88	0.42
2:I:937:CYS:HB3	2:I:1053:ILE:HB	2.01	0.42
2:I:2686:LEU:HD23	2:I:3001:ILE:HD13	2.02	0.42
2:I:2960:LEU:O	2:I:2964:LEU:HG	2.19	0.42
3:K:105:ASN:HD21	3:K:111:ASN:CB	2.32	0.42
2:A:2958:GLY:O	2:A:2961:GLN:HG2	2.20	0.42
2:A:2991:HIS:O	2:A:2995:ILE:HG13	2.20	0.42
2:A:3019:SER:HB3	2:A:3030:HIS:HB3	2.02	0.42
2:A:3250:MET:O	2:A:3253:ILE:HG22	2.20	0.42
2:A:3834:ALA:O	2:A:3838:THR:HG23	2.18	0.42
2:A:3866:ILE:HG23	2:A:3868:ARG:H	1.84	0.42
2:D:2958:GLY:O	2:D:2961:GLN:HG2	2.20	0.42
2:D:2991:HIS:O	2:D:2995:ILE:HG13	2.20	0.42
2:D:3137:LEU:HB3	2:D:3138:PRO:HD3	2.01	0.42
2:D:3227:ARG:HB3	2:D:3232:LEU:HB2	2.01	0.42
2:D:3250:MET:O	2:D:3253:ILE:HG22	2.20	0.42
2:D:3757:GLU:O	2:D:3761:GLN:HG2	2.20	0.42
2:G:667:MET:HG2	2:G:790:ARG:HB3	2.02	0.42
2:G:1440:PHE:CD2	2:G:1560:ASN:HB3	2.55	0.42
2:G:3397:GLU:O	2:G:3400:VAL:HG12	2.20	0.42
2:G:3852:LYS:O	2:G:3856:LEU:HG	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3866:ILE:HG23	2:G:3868:ARG:H	1.84	0.42
2:I:1071:ARG:HG3	2:I:1196:PRO:HG3	2.02	0.42
2:I:1935:VAL:O	2:I:1939:MET:HE2	2.20	0.42
2:I:2958:GLY:O	2:I:2961:GLN:HG2	2.20	0.42
2:I:3757:GLU:O	2:I:3761:GLN:HG2	2.20	0.42
2:A:1249:PRO:HG2	2:A:1252:HIS:HB2	2.01	0.42
2:A:3000:LYS:HA	2:A:3000:LYS:HD3	1.86	0.42
2:A:3100:SER:HB3	2:A:3167:ARG:NE	2.35	0.42
2:D:1302:ARG:H	2:D:1302:ARG:HG2	1.66	0.42
1:F:85:THR:O	1:F:85:THR:OG1	2.34	0.42
2:G:2974:ILE:HG13	2:G:2975:ALA:N	2.35	0.42
2:G:4959:PHE:CD1	2:G:4985:LEU:HD11	2.55	0.42
5:G:5102:POV:H35A	5:G:5102:POV:H32	1.86	0.42
3:M:18:LEU:HD11	3:M:85:LEU:HD11	2.01	0.42
2:I:3752:SER:O	2:I:3756:LYS:HG3	2.20	0.42
2:I:3852:LYS:O	2:I:3856:LEU:HG	2.20	0.42
2:I:3959:LYS:HG3	2:I:4022:ASP:OD2	2.20	0.42
3:K:18:LEU:HD11	3:K:85:LEU:HD11	2.01	0.42
2:A:372:LEU:HD22	2:A:372:LEU:N	2.35	0.42
2:A:937:CYS:HB3	2:A:1053:ILE:HB	2.01	0.42
2:A:1433:TYR:HB3	2:A:1575:LEU:HD23	2.02	0.42
2:D:380:GLN:OE1	2:D:380:GLN:N	2.53	0.42
2:D:1249:PRO:HG2	2:D:1252:HIS:HB2	2.01	0.42
2:D:3158:LEU:HD12	2:D:3159:ASP:HB2	2.01	0.42
2:G:2124:LEU:HD11	2:G:2128:TYR:HE2	1.84	0.42
2:G:3406:TYR:CZ	2:G:3508:SER:HB2	2.55	0.42
2:G:3757:GLU:O	2:G:3761:GLN:HG2	2.20	0.42
2:G:4188:ARG:HA	2:G:4188:ARG:NE	2.35	0.42
2:I:2463:LEU:HD11	2:I:2517:PHE:HE1	1.85	0.41
2:I:4188:ARG:NE	2:I:4188:ARG:HA	2.35	0.41
2:I:4805:ASN:HB3	2:I:4808:PHE:CD2	2.55	0.41
2:A:1035:ASN:OD1	3:C:109:THR:OG1	2.38	0.41
2:A:2765:LYS:HZ2	2:A:2860:PRO:HA	1.84	0.41
2:A:3284:TRP:CE3	2:A:3287:ARG:HD3	2.55	0.41
2:A:3406:TYR:CZ	2:A:3508:SER:HB2	2.55	0.41
2:A:3769:ARG:O	2:A:3773:ARG:NH1	2.53	0.41
2:D:1071:ARG:HG3	2:D:1196:PRO:HG3	2.02	0.41
2:D:1079:LYS:HA	2:D:1189:LEU:HD11	2.01	0.41
2:D:2285:GLU:OE2	2:D:3860:ASN:ND2	2.40	0.41
2:D:3866:ILE:HG23	2:D:3868:ARG:H	1.84	0.41
2:D:4744:ASP:HB3	2:D:4747:SER:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:656:SER:HA	2:G:852:VAL:HG12	2.02	0.41
2:G:4715:TYR:CE2	2:G:4717:ASP:HB3	2.55	0.41
2:I:112:ALA:O	2:I:115:ARG:NH1	2.53	0.41
2:I:2633:LEU:HB2	2:I:2689:LYS:HE2	2.01	0.41
2:I:2782:ASP:OD1	2:I:2782:ASP:N	2.49	0.41
2:I:3158:LEU:HD12	2:I:3159:ASP:HB2	2.01	0.41
2:A:1871:PHE:HZ	2:A:2094:LEU:HD13	1.84	0.41
2:A:2463:LEU:HD11	2:A:2517:PHE:HE1	1.85	0.41
2:A:2633:LEU:HB2	2:A:2689:LYS:HE2	2.01	0.41
2:A:4188:ARG:HG2	2:A:4188:ARG:HH11	1.85	0.41
2:A:4839:MET:HE2	2:D:4823:LEU:HD22	2.01	0.41
2:A:4959:PHE:CD1	2:A:4985:LEU:HD11	2.55	0.41
2:D:2960:LEU:O	2:D:2964:LEU:HG	2.20	0.41
2:D:3852:LYS:O	2:D:3856:LEU:HG	2.20	0.41
2:D:4715:TYR:CE2	2:D:4717:ASP:HB3	2.55	0.41
3:E:31:ILE:HD13	3:E:31:ILE:HA	1.87	0.41
2:G:2312:MET:HA	2:G:2315:ALA:HB3	2.01	0.41
2:G:2610:LEU:O	2:G:2614:ILE:HG12	2.19	0.41
2:G:2960:LEU:O	2:G:2964:LEU:HG	2.20	0.41
2:G:3155:ASP:HA	2:G:3158:LEU:HD23	2.01	0.41
2:G:3639:THR:N	2:G:3640:PRO:HD2	2.34	0.41
2:I:2485:LEU:HD23	2:I:2485:LEU:HA	1.89	0.41
2:I:3367:LYS:HE3	2:I:3367:LYS:HB3	1.87	0.41
2:I:3769:ARG:O	2:I:3773:ARG:NH1	2.53	0.41
2:I:5009:TYR:O	2:I:5012:LYS:HG2	2.20	0.41
2:I:5012:LYS:HG3	2:I:5013:MET:N	2.35	0.41
2:A:1008:SER:HB2	2:A:1017:ARG:NE	2.29	0.41
2:A:2285:GLU:OE2	2:A:3860:ASN:ND2	2.40	0.41
2:A:4744:ASP:HB3	2:A:4747:SER:HB3	2.02	0.41
2:D:937:CYS:HB3	2:D:1053:ILE:HB	2.01	0.41
2:D:1433:TYR:HB3	2:D:1575:LEU:HD23	2.02	0.41
2:D:2165:LEU:HD23	2:D:2165:LEU:HA	1.91	0.41
2:D:2208:MET:HG2	2:D:2236:LEU:HD11	2.03	0.41
2:D:2633:LEU:HB2	2:D:2689:LYS:HE2	2.01	0.41
2:D:2712:PRO:HD3	2:D:3013:HIS:CE1	2.54	0.41
2:D:3769:ARG:O	2:D:3773:ARG:NH1	2.53	0.41
2:D:4677:LEU:HG	2:D:4681:LEU:HD23	2.03	0.41
3:E:18:LEU:HD11	3:E:85:LEU:HD11	2.01	0.41
3:E:47:LEU:O	3:E:62:SER:OG	2.37	0.41
2:G:112:ALA:O	2:G:115:ARG:NH1	2.52	0.41
2:G:937:CYS:HB3	2:G:1053:ILE:HB	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2463:LEU:HD11	2:G:2517:PHE:HE1	1.85	0.41
2:G:3528:THR:OG1	2:G:3561:GLY:O	2.39	0.41
2:I:1027:LEU:HD23	2:I:1027:LEU:HA	1.82	0.41
2:I:1440:PHE:CD2	2:I:1560:ASN:HB3	2.55	0.41
2:I:4188:ARG:HG2	2:I:4188:ARG:HH11	1.84	0.41
2:A:1163:THR:HG22	2:A:1168:VAL:HA	2.02	0.41
2:A:2960:LEU:O	2:A:2964:LEU:HG	2.20	0.41
2:A:3077:ALA:HA	2:A:3080:VAL:HB	2.03	0.41
2:A:3752:SER:O	2:A:3756:LYS:HG3	2.20	0.41
3:C:36:TRP:HE1	3:C:78:VAL:HG11	1.86	0.41
3:C:61:ASP:O	3:C:64:LYS:HD2	2.21	0.41
2:D:2185:ILE:HD12	2:D:2203:MET:HE1	2.02	0.41
2:D:3077:ALA:HA	2:D:3080:VAL:HB	2.03	0.41
2:D:3406:TYR:CZ	2:D:3508:SER:HB2	2.55	0.41
2:D:3817:LEU:HB2	2:D:3899:PHE:CE1	2.56	0.41
2:D:4188:ARG:NE	2:D:4188:ARG:HA	2.35	0.41
2:G:737:LEU:HD12	2:G:737:LEU:HA	1.93	0.41
2:G:1163:THR:HG22	2:G:1168:VAL:HA	2.02	0.41
2:G:2223:ILE:HD12	2:G:2223:ILE:HA	1.95	0.41
2:G:3019:SER:HB3	2:G:3030:HIS:HB3	2.02	0.41
2:G:4805:ASN:HB3	2:G:4808:PHE:CD2	2.55	0.41
2:G:4899:ASP:OD1	2:G:4900:GLU:N	2.54	0.41
2:I:3137:LEU:HB3	2:I:3138:PRO:HD3	2.01	0.41
2:I:3576:TYR:CE1	2:I:3582:ARG:HG2	2.56	0.41
2:I:4238:CYS:O	2:I:4242:ILE:HG13	2.21	0.41
2:I:4917:ASP:HB2	2:A:4888:TYR:HE1	1.86	0.41
2:A:2208:MET:HG2	2:A:2236:LEU:HD11	2.03	0.41
2:A:2757:LYS:O	2:A:2761:TYR:HB2	2.21	0.41
2:A:3576:TYR:CE1	2:A:3582:ARG:HG2	2.56	0.41
2:A:3959:LYS:HG3	2:A:4022:ASP:OD2	2.20	0.41
2:A:4232:GLU:OE1	2:A:5019:TRP:NE1	2.31	0.41
3:C:47:LEU:O	3:C:62:SER:OG	2.37	0.41
2:D:367:LEU:O	2:D:368:ARG:C	2.59	0.41
2:D:719:LEU:HD12	2:D:737:LEU:HD13	2.03	0.41
2:D:2463:LEU:HD11	2:D:2517:PHE:HE1	1.85	0.41
2:D:3019:SER:HB3	2:D:3030:HIS:HB3	2.02	0.41
2:D:4118:ASP:OD1	2:D:4119:GLU:N	2.53	0.41
2:D:4805:ASN:HB3	2:D:4808:PHE:CD2	2.55	0.41
2:G:1093:GLU:HB3	2:G:1201:HIS:HB3	2.03	0.41
2:G:4902:GLU:O	2:G:4913:ARG:NH2	2.54	0.41
1:H:23:VAL:HG22	1:H:104:LEU:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:78:PRO:HA	1:H:81:ALA:HB3	2.02	0.41
2:I:667:MET:HG2	2:I:790:ARG:HB3	2.02	0.41
2:I:1093:GLU:HB3	2:I:1201:HIS:HB3	2.03	0.41
2:I:3406:TYR:CZ	2:I:3508:SER:HB2	2.55	0.41
2:A:1071:ARG:HG3	2:A:1196:PRO:HG3	2.02	0.41
2:A:1812:LEU:HD12	2:A:1812:LEU:HA	1.95	0.41
2:A:2251:PHE:CG	2:A:2286:LEU:HD22	2.56	0.41
2:A:2619:LEU:O	2:A:2623:LEU:HD23	2.19	0.41
2:A:3817:LEU:HB2	2:A:3899:PHE:CE1	2.56	0.41
2:A:4188:ARG:HA	2:A:4188:ARG:NE	2.35	0.41
3:C:18:LEU:HD11	3:C:85:LEU:HD11	2.01	0.41
1:J:78:PRO:HA	1:J:81:ALA:HB3	2.02	0.41
2:D:2005:GLN:O	2:D:2009:LEU:HG	2.21	0.41
2:D:3536:ALA:HA	2:D:3539:ARG:HB2	2.02	0.41
1:F:23:VAL:HG22	1:F:104:LEU:O	2.21	0.41
2:G:424:LYS:HE2	2:G:424:LYS:HB2	1.82	0.41
2:G:3180:ASN:ND2	2:G:3183:VAL:HG13	2.36	0.41
2:I:309:THR:O	2:I:313:SER:OG	2.32	0.41
2:I:369:LEU:HB3	2:I:371:VAL:HG23	2.01	0.41
2:I:1024:TYR:OH	2:I:1036:ARG:NH2	2.54	0.41
2:I:1431:THR:HG21	2:I:1523:ALA:HB2	2.03	0.41
2:I:2251:PHE:CG	2:I:2286:LEU:HD22	2.56	0.41
2:I:2757:LYS:O	2:I:2761:TYR:HB2	2.21	0.41
2:I:3253:ILE:HD12	2:I:3253:ILE:HA	1.86	0.41
2:I:3284:TRP:CE3	2:I:3287:ARG:HB2	2.56	0.41
3:K:85:LEU:HD23	3:K:85:LEU:HA	1.94	0.41
2:A:424:LYS:HB2	2:A:424:LYS:HE2	1.82	0.41
2:A:719:LEU:HD12	2:A:737:LEU:HD13	2.03	0.41
2:A:2686:LEU:HD23	2:A:3001:ILE:HD13	2.02	0.41
2:A:3180:ASN:ND2	2:A:3183:VAL:HG13	2.36	0.41
2:D:2757:LYS:O	2:D:2761:TYR:HB2	2.21	0.41
2:D:3180:ASN:ND2	2:D:3183:VAL:HG13	2.36	0.41
2:D:3959:LYS:HG3	2:D:4022:ASP:OD2	2.20	0.41
2:D:4919:THR:HG21	5:D:5102:POV:H31H	2.03	0.41
2:G:1024:TYR:OH	2:G:1036:ARG:NH2	2.54	0.41
2:G:1071:ARG:HG3	2:G:1196:PRO:HG3	2.02	0.41
2:G:2633:LEU:HB2	2:G:2689:LYS:HE2	2.01	0.41
2:G:2757:LYS:O	2:G:2761:TYR:HB2	2.21	0.41
2:G:2951:ILE:HG21	2:G:3034:LYS:HZ2	1.86	0.41
2:G:3100:SER:HB3	2:G:3167:ARG:NE	2.35	0.41
2:G:3576:TYR:CE1	2:G:3582:ARG:HG2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4118:ASP:OD1	2:G:4119:GLU:N	2.53	0.41
3:M:61:ASP:O	3:M:64:LYS:HD2	2.21	0.41
2:I:380:GLN:OE1	2:I:380:GLN:N	2.53	0.41
2:I:882:TRP:O	2:I:885:THR:OG1	2.33	0.41
2:I:1433:TYR:HB3	2:I:1575:LEU:HD23	2.02	0.41
2:I:2312:MET:SD	2:I:2313:LEU:N	2.94	0.41
2:I:2333:ASP:HA	2:I:2336:ARG:NE	2.36	0.41
2:I:2758:PHE:O	2:I:2762:THR:HG23	2.21	0.41
2:I:3077:ALA:HA	2:I:3080:VAL:HB	2.03	0.41
2:I:3180:ASN:ND2	2:I:3183:VAL:HG13	2.36	0.41
2:I:4060:LYS:HA	2:I:4060:LYS:HD3	1.87	0.41
2:I:4118:ASP:OD1	2:I:4119:GLU:N	2.53	0.41
2:A:13:PHE:HA	2:A:164:ARG:HA	2.03	0.41
2:A:1093:GLU:HB3	2:A:1201:HIS:HB3	2.03	0.41
2:A:1128:ARG:HH12	2:A:1132:TRP:HE1	1.68	0.41
2:A:1431:THR:HG21	2:A:1523:ALA:HB2	2.03	0.41
2:A:2312:MET:SD	2:A:2313:LEU:N	2.94	0.41
2:A:3397:GLU:O	2:A:3400:VAL:HG12	2.20	0.41
2:A:3536:ALA:HA	2:A:3539:ARG:HB2	2.03	0.41
2:A:3852:LYS:O	2:A:3856:LEU:HG	2.20	0.41
3:C:44:GLN:HE22	3:C:46:GLU:HG2	1.86	0.41
2:D:1431:THR:HG21	2:D:1523:ALA:HB2	2.03	0.41
2:D:1440:PHE:CD2	2:D:1560:ASN:HB3	2.55	0.41
2:D:2121:PHE:CZ	2:D:3701:LEU:HB2	2.56	0.41
2:D:2312:MET:HA	2:D:2315:ALA:HB3	2.01	0.41
2:D:3284:TRP:CE3	2:D:3287:ARG:HB2	2.56	0.41
2:D:4586:PRO:HA	2:D:4587:PRO:HD3	1.93	0.41
2:D:4715:TYR:HE2	2:D:4717:ASP:HB3	1.85	0.41
3:E:36:TRP:HE1	3:E:78:VAL:HG11	1.86	0.41
3:E:85:LEU:HD23	3:E:85:LEU:HA	1.95	0.41
1:F:18:LYS:HB3	1:F:18:LYS:HZ2	1.84	0.41
1:F:78:PRO:HA	1:F:81:ALA:HB3	2.02	0.41
2:G:803:LEU:HD23	2:G:803:LEU:HA	1.88	0.41
2:G:2121:PHE:CZ	2:G:3701:LEU:HB2	2.56	0.41
2:G:2251:PHE:CG	2:G:2286:LEU:HD22	2.56	0.41
2:G:3817:LEU:HB2	2:G:3899:PHE:CE1	2.56	0.41
2:G:3852:LYS:HE2	2:G:3852:LYS:HB2	1.79	0.41
2:G:4677:LEU:HG	2:G:4681:LEU:HD23	2.02	0.41
2:G:4715:TYR:HE2	2:G:4717:ASP:HB3	1.85	0.41
1:H:85:THR:O	1:H:85:THR:OG1	2.34	0.41
2:I:656:SER:HA	2:I:852:VAL:HG12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:719:LEU:HD12	2:I:737:LEU:HD13	2.03	0.41
2:I:1163:THR:HG22	2:I:1168:VAL:HA	2.02	0.41
2:I:1694:LEU:HB3	2:I:1715:LEU:HD12	2.03	0.41
2:I:2005:GLN:O	2:I:2009:LEU:HG	2.21	0.41
2:I:2285:GLU:OE2	2:I:3860:ASN:ND2	2.40	0.41
2:I:3250:MET:O	2:I:3253:ILE:HG22	2.20	0.41
2:I:3302:PRO:HA	2:I:3303:PRO:HD3	1.98	0.41
3:K:32:ASN:HD21	3:K:101:PRO:HB3	1.86	0.41
2:A:341:TYR:CE1	2:A:392:ARG:HB2	2.56	0.41
2:A:618:GLN:OE1	2:A:1678:ASN:ND2	2.46	0.41
2:A:667:MET:HG2	2:A:790:ARG:HB3	2.02	0.41
2:A:1131:ARG:NH2	2:A:1137:GLU:OE2	2.54	0.41
2:A:2005:GLN:O	2:A:2009:LEU:HG	2.21	0.41
2:A:2138:LEU:HD23	2:A:2138:LEU:HA	1.85	0.41
2:A:2295:LEU:HA	2:A:2298:VAL:HG12	2.03	0.41
2:A:2333:ASP:HA	2:A:2336:ARG:NE	2.36	0.41
2:A:2637:ALA:C	2:A:2640:PRO:HD2	2.41	0.41
2:A:2737:PRO:HD2	2:A:2891:LYS:HD3	2.03	0.41
2:A:2801:ASP:HB2	2:A:2805:TYR:CE2	2.56	0.41
2:A:3208:PRO:HB2	2:A:3236:VAL:HG13	2.02	0.41
2:A:3284:TRP:CE3	2:A:3287:ARG:HB2	2.56	0.41
2:A:3292:PRO:HA	2:A:3293:PRO:HD3	2.00	0.41
2:A:4011:GLU:H	2:A:4011:GLU:HG2	1.72	0.41
2:A:4640:GLU:HB3	2:A:4641:PRO:HD3	2.03	0.41
2:A:4836:GLN:HB3	2:D:4826:ILE:HD11	2.03	0.41
2:A:4839:MET:HE2	2:D:4823:LEU:HA	2.02	0.41
2:A:4902:GLU:O	2:A:4913:ARG:NH2	2.54	0.41
2:D:13:PHE:HA	2:D:164:ARG:HA	2.03	0.41
2:D:341:TYR:CE1	2:D:392:ARG:HB2	2.56	0.41
2:D:656:SER:HA	2:D:852:VAL:HG12	2.02	0.41
2:D:864:PRO:O	2:D:866:HIS:N	2.52	0.41
2:D:2686:LEU:HD23	2:D:3001:ILE:HD13	2.02	0.41
2:D:2758:PHE:O	2:D:2762:THR:HG23	2.21	0.41
2:D:3100:SER:HB3	2:D:3167:ARG:NE	2.35	0.41
2:D:3397:GLU:O	2:D:3400:VAL:HG12	2.20	0.41
2:D:3514:LEU:HD12	2:D:3514:LEU:HA	1.95	0.41
2:D:3704:HIS:O	2:D:3708:THR:HG23	2.21	0.41
2:D:4215:ARG:NH2	6:D:5103:ATP:O2G	2.54	0.41
2:D:4640:GLU:HB3	2:D:4641:PRO:HD3	2.03	0.41
2:D:4899:ASP:OD1	2:D:4900:GLU:N	2.54	0.41
2:D:4902:GLU:O	2:D:4913:ARG:NH2	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:360:ALA:O	2:G:361:ALA:C	2.59	0.41
2:G:2208:MET:HG2	2:G:2236:LEU:HD11	2.03	0.41
2:G:2352:VAL:O	2:G:2356:LEU:HG	2.21	0.41
2:G:2563:THR:HG22	2:G:2606:CYS:HA	2.03	0.41
2:G:2737:PRO:HD2	2:G:2891:LYS:HD3	2.03	0.41
2:G:2819:TRP:O	2:G:2820:GLU:HG3	2.21	0.41
2:G:2958:GLY:O	2:G:2961:GLN:HG2	2.20	0.41
2:G:3253:ILE:HG23	2:G:3318:ASN:HD22	1.86	0.41
2:G:3284:TRP:CE3	2:G:3287:ARG:HB2	2.56	0.41
2:G:3367:LYS:HE3	2:G:3367:LYS:HB3	1.87	0.41
2:G:3594:ARG:HA	2:G:3594:ARG:HE	1.86	0.41
3:M:36:TRP:HE1	3:M:78:VAL:HG11	1.85	0.41
2:I:2208:MET:HG2	2:I:2236:LEU:HD11	2.03	0.41
2:I:2295:LEU:HA	2:I:2298:VAL:HG12	2.03	0.41
2:I:3704:HIS:O	2:I:3708:THR:HG23	2.21	0.41
2:I:4630:TYR:OH	2:G:4860:ARG:NH2	2.54	0.41
2:I:4823:LEU:HA	2:G:4839:MET:HE3	2.02	0.41
3:K:44:GLN:HE22	3:K:46:GLU:HG2	1.86	0.41
3:K:61:ASP:O	3:K:64:LYS:HD2	2.21	0.41
2:A:371:VAL:CG1	2:A:373:LYS:HG2	2.51	0.41
2:A:1024:TYR:OH	2:A:1036:ARG:NH2	2.54	0.41
2:A:1440:PHE:CD2	2:A:1560:ASN:HB3	2.55	0.41
2:A:1490:SER:OG	2:A:1491:ASN:N	2.55	0.41
2:A:2121:PHE:CZ	2:A:3701:LEU:HB2	2.56	0.41
2:A:2354:VAL:HG11	2:A:2453:ILE:HD12	2.03	0.41
2:A:3274:LEU:HD23	2:A:3274:LEU:HA	1.90	0.41
2:A:4860:ARG:NH2	2:D:4630:TYR:OH	2.54	0.41
2:D:73:LEU:HD12	2:D:73:LEU:HA	1.96	0.41
2:D:1128:ARG:HH12	2:D:1132:TRP:HE1	1.69	0.41
2:D:2974:ILE:HG13	2:D:2975:ALA:N	2.35	0.41
2:D:3253:ILE:HG23	2:D:3318:ASN:HD22	1.86	0.41
2:D:4821:LYS:O	2:D:4825:THR:HG23	2.21	0.41
2:D:4839:MET:HE2	2:G:4823:LEU:HA	2.03	0.41
2:G:13:PHE:HA	2:G:164:ARG:HA	2.03	0.41
2:G:581:ASN:N	2:G:581:ASN:OD1	2.54	0.41
2:G:659:TYR:O	2:G:662:TRP:NE1	2.51	0.41
2:G:2354:VAL:HG11	2:G:2453:ILE:HD12	2.03	0.41
2:G:2637:ALA:C	2:G:2640:PRO:HD2	2.41	0.41
2:G:3077:ALA:HA	2:G:3080:VAL:HB	2.03	0.41
2:I:1131:ARG:NH2	2:I:1137:GLU:OE2	2.54	0.40
2:I:1972:ASN:O	2:I:1976:ARG:HG3	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2352:VAL:O	2:I:2356:LEU:HG	2.21	0.40
2:I:2354:VAL:HG11	2:I:2453:ILE:HD12	2.03	0.40
2:I:2526:PHE:O	2:I:2530:MET:HG3	2.21	0.40
2:I:3038:MET:H	2:I:3038:MET:HG2	1.77	0.40
2:I:3208:PRO:HB2	2:I:3236:VAL:HG13	2.02	0.40
2:I:4888:TYR:HE1	2:G:4917:ASP:HB2	1.86	0.40
2:I:4902:GLU:O	2:I:4913:ARG:NH2	2.54	0.40
1:L:30:LEU:HB2	1:L:34:LYS:HB2	2.03	0.40
2:A:3594:ARG:HA	2:A:3594:ARG:HE	1.86	0.40
2:D:581:ASN:N	2:D:581:ASN:OD1	2.54	0.40
2:D:667:MET:HG2	2:D:790:ARG:HB3	2.02	0.40
2:D:1131:ARG:NH2	2:D:1137:GLU:OE2	2.54	0.40
2:D:1935:VAL:O	2:D:1939:MET:HE2	2.22	0.40
2:D:2251:PHE:CG	2:D:2286:LEU:HD22	2.56	0.40
2:D:2737:PRO:HD2	2:D:2891:LYS:HD3	2.03	0.40
2:D:3001:ILE:HG13	2:D:3002:LEU:N	2.37	0.40
2:D:4541:TRP:CE3	2:D:4544:LEU:HD21	2.56	0.40
3:E:61:ASP:O	3:E:64:LYS:HD2	2.21	0.40
2:G:111:HIS:CE1	2:G:113:HIS:HB3	2.56	0.40
2:G:719:LEU:HD12	2:G:737:LEU:HD13	2.03	0.40
2:G:2333:ASP:HA	2:G:2336:ARG:NE	2.36	0.40
2:G:2638:LYS:H	2:G:2638:LYS:HG2	1.71	0.40
2:G:3713:LYS:NZ	2:G:3715:LYS:O	2.54	0.40
2:G:4232:GLU:OE1	2:G:5019:TRP:NE1	2.31	0.40
2:G:4919:THR:HG21	5:G:5102:POV:H31H	2.03	0.40
2:I:111:HIS:CE1	2:I:113:HIS:HB3	2.56	0.40
2:I:341:TYR:CE1	2:I:392:ARG:HB2	2.56	0.40
2:I:2737:PRO:HD2	2:I:2891:LYS:HD3	2.03	0.40
2:I:2801:ASP:HB2	2:I:2805:TYR:CE2	2.56	0.40
2:I:3524:MET:O	2:I:3576:TYR:OH	2.37	0.40
2:I:3536:ALA:HA	2:I:3539:ARG:HB2	2.03	0.40
2:A:3001:ILE:HG13	2:A:3002:LEU:N	2.36	0.40
2:A:3014:CYS:SG	2:A:3074:SER:HB3	2.62	0.40
2:A:4541:TRP:CE3	2:A:4544:LEU:HD21	2.57	0.40
2:A:4677:LEU:HG	2:A:4681:LEU:HD23	2.02	0.40
2:D:1093:GLU:HB3	2:D:1201:HIS:HB3	2.03	0.40
2:D:2352:VAL:O	2:D:2356:LEU:HG	2.21	0.40
2:D:2801:ASP:HB2	2:D:2805:TYR:CE2	2.56	0.40
2:D:3257:ALA:O	2:D:3325:ASN:ND2	2.54	0.40
1:F:30:LEU:HB2	1:F:34:LYS:HB2	2.03	0.40
2:G:1490:SER:OG	2:G:1491:ASN:N	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3034:LYS:O	2:G:3038:MET:HG2	2.21	0.40
2:I:581:ASN:OD1	2:I:581:ASN:N	2.54	0.40
2:I:2563:THR:HG22	2:I:2606:CYS:HA	2.03	0.40
2:I:3409:TYR:N	2:I:3410:PRO:HD2	2.37	0.40
2:I:4779:LYS:HB2	2:I:4779:LYS:HE3	1.82	0.40
3:K:109:THR:OG1	3:K:110:PRO:HD3	2.22	0.40
2:A:4215:ARG:NH2	6:A:5103:ATP:O2G	2.54	0.40
2:A:4715:TYR:HE2	2:A:4717:ASP:HB3	1.86	0.40
2:D:1043:VAL:O	2:D:1047:LEU:HG	2.22	0.40
2:D:2354:VAL:HG11	2:D:2453:ILE:HD12	2.03	0.40
2:D:2819:TRP:O	2:D:2820:GLU:HG3	2.21	0.40
3:E:32:ASN:HD21	3:E:101:PRO:HB3	1.86	0.40
2:G:180:LEU:HD23	2:G:180:LEU:HA	1.88	0.40
2:G:1128:ARG:HH12	2:G:1132:TRP:HE1	1.69	0.40
2:G:1433:TYR:HB3	2:G:1575:LEU:HD23	2.02	0.40
2:G:2138:LEU:HD23	2:G:2138:LEU:HA	1.85	0.40
2:G:2758:PHE:O	2:G:2762:THR:HG23	2.21	0.40
2:G:3704:HIS:O	2:G:3708:THR:HG23	2.21	0.40
2:G:4157:ASP:O	2:G:4161:ARG:HD3	2.22	0.40
2:G:4541:TRP:CE3	2:G:4544:LEU:HD21	2.57	0.40
2:G:4744:ASP:HB3	2:G:4747:SER:HB3	2.02	0.40
2:G:5000:GLU:HA	2:G:5003:HIS:ND1	2.37	0.40
1:H:30:LEU:HB2	1:H:34:LYS:HB2	2.04	0.40
2:I:13:PHE:HA	2:I:164:ARG:HA	2.03	0.40
2:I:179:TYR:HB2	2:I:196:MET:O	2.21	0.40
2:I:371:VAL:CG1	2:I:373:LYS:HG2	2.52	0.40
2:I:881:LEU:O	2:I:885:THR:HG23	2.21	0.40
2:I:2819:TRP:O	2:I:2820:GLU:HG3	2.21	0.40
2:I:3594:ARG:HE	2:I:3594:ARG:HA	1.86	0.40
3:K:36:TRP:HE1	3:K:78:VAL:HG11	1.86	0.40
1:L:23:VAL:HG22	1:L:104:LEU:O	2.21	0.40
2:A:1694:LEU:HB3	2:A:1715:LEU:HD12	2.03	0.40
2:A:2352:VAL:O	2:A:2356:LEU:HG	2.21	0.40
2:A:2526:PHE:O	2:A:2530:MET:HG3	2.22	0.40
2:A:3302:PRO:HA	2:A:3303:PRO:HD3	1.98	0.40
2:A:4813:LEU:HD23	2:A:4813:LEU:HA	1.92	0.40
3:C:32:ASN:HD21	3:C:101:PRO:HB3	1.86	0.40
2:D:458:GLU:H	2:D:458:GLU:HG3	1.67	0.40
2:D:1814:MET:O	2:D:1817:GLU:HG2	2.22	0.40
2:D:2247:GLN:HG3	2:D:2279:SER:HA	2.04	0.40
2:D:2684:ASP:OD1	2:D:2685:SER:N	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3345:ILE:HD12	2:D:3345:ILE:HA	1.95	0.40
2:D:3576:TYR:CE1	2:D:3582:ARG:HG2	2.56	0.40
2:G:1534:LYS:HE3	2:G:1534:LYS:HB2	1.93	0.40
2:G:1694:LEU:HB3	2:G:1715:LEU:HD12	2.03	0.40
2:G:2005:GLN:O	2:G:2009:LEU:HG	2.21	0.40
2:G:3644:LEU:HD23	2:G:3644:LEU:HA	1.92	0.40
2:G:4215:ARG:NH2	6:G:5103:ATP:O2G	2.54	0.40
2:G:4821:LYS:O	2:G:4825:THR:HG23	2.21	0.40
2:I:603:LEU:HD23	2:I:606:LEU:HD12	2.04	0.40
2:I:917:GLU:OE1	3:K:101:PRO:HB2	2.21	0.40
2:I:2138:LEU:HD23	2:I:2138:LEU:HA	1.85	0.40
2:I:2312:MET:O	2:I:2316:LYS:HG2	2.22	0.40
2:I:2637:ALA:C	2:I:2640:PRO:HD2	2.41	0.40
2:I:3019:SER:HB3	2:I:3030:HIS:HB3	2.02	0.40
2:I:3550:ARG:HH21	2:I:3597:GLN:HE22	1.70	0.40
2:I:4640:GLU:HB3	2:I:4641:PRO:HD3	2.03	0.40
2:A:111:HIS:CE1	2:A:113:HIS:HB3	2.56	0.40
2:A:363:ASP:HB3	2:A:366:ALA:CB	2.51	0.40
2:A:881:LEU:O	2:A:885:THR:HG23	2.22	0.40
2:A:2974:ILE:HG13	2:A:2975:ALA:N	2.35	0.40
2:A:3034:LYS:O	2:A:3038:MET:HG2	2.21	0.40
2:A:3704:HIS:O	2:A:3708:THR:HG23	2.21	0.40
2:A:4821:LYS:O	2:A:4825:THR:HG23	2.21	0.40
3:C:109:THR:OG1	3:C:110:PRO:HD3	2.22	0.40
2:D:881:LEU:O	2:D:885:THR:HG23	2.21	0.40
2:D:1024:TYR:OH	2:D:1036:ARG:NH2	2.54	0.40
2:D:1490:SER:OG	2:D:1491:ASN:N	2.55	0.40
2:D:3007:ASN:OD1	2:D:3070:ILE:HG13	2.22	0.40
2:G:2697:ARG:C	2:G:2697:ARG:HH11	2.25	0.40
2:G:3001:ILE:HG13	2:G:3002:LEU:N	2.36	0.40
2:G:3245:VAL:CG1	2:G:3248:ARG:HH12	2.31	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
1	H	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
1	J	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
1	L	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
2	A	4280/5027 (85%)	4203 (98%)	77 (2%)	0	100	100
2	D	4280/5027 (85%)	4201 (98%)	78 (2%)	1 (0%)	100	100
2	G	4280/5027 (85%)	4201 (98%)	79 (2%)	0	100	100
2	I	4280/5027 (85%)	4203 (98%)	77 (2%)	0	100	100
3	C	124/137 (90%)	118 (95%)	6 (5%)	0	100	100
3	E	124/137 (90%)	118 (95%)	6 (5%)	0	100	100
3	K	124/137 (90%)	118 (95%)	6 (5%)	0	100	100
3	M	124/137 (90%)	118 (95%)	6 (5%)	0	100	100
All	All	18036/21084 (86%)	17684 (98%)	351 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	374	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	88/88 (100%)	85 (97%)	3 (3%)	32	62
1	H	88/88 (100%)	85 (97%)	3 (3%)	32	62
1	J	88/88 (100%)	85 (97%)	3 (3%)	32	62
1	L	88/88 (100%)	85 (97%)	3 (3%)	32	62
2	A	3674/4270 (86%)	3555 (97%)	119 (3%)	34	63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	3674/4270 (86%)	3553 (97%)	121 (3%)	33 62
2	G	3673/4270 (86%)	3552 (97%)	121 (3%)	33 62
2	I	3673/4270 (86%)	3552 (97%)	121 (3%)	33 62
3	C	104/114 (91%)	102 (98%)	2 (2%)	52 75
3	E	104/114 (91%)	102 (98%)	2 (2%)	52 75
3	K	104/114 (91%)	102 (98%)	2 (2%)	52 75
3	M	104/114 (91%)	102 (98%)	2 (2%)	52 75
All	All	15462/17888 (86%)	14960 (97%)	502 (3%)	36 63

All (502) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	22	CYS
1	H	23	VAL
1	H	32	ASN
2	I	35	LEU
2	I	125	ARG
2	I	127	MET
2	I	227	MET
2	I	241	GLN
2	I	273	HIS
2	I	297	GLN
2	I	368	ARG
2	I	384	MET
2	I	389	PHE
2	I	460	GLN
2	I	481	GLU
2	I	702	TRP
2	I	714	TYR
2	I	835	ARG
2	I	866	HIS
2	I	886	ARG
2	I	924	MET
2	I	960	MET
2	I	987	ARG
2	I	1025	ARG
2	I	1071	ARG
2	I	1128	ARG
2	I	1143	TRP
2	I	1170	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	1260	MET
2	I	1421	ARG
2	I	1428	LEU
2	I	1435	TYR
2	I	1526	LEU
2	I	1648	MET
2	I	1981	MET
2	I	2198	MET
2	I	2294	ASP
2	I	2312	MET
2	I	2440	MET
2	I	2490	MET
2	I	2502	MET
2	I	2520	HIS
2	I	2555	CYS
2	I	2578	MET
2	I	2623	LEU
2	I	2652	TRP
2	I	2656	CYS
2	I	2661	TRP
2	I	2664	PHE
2	I	2673	HIS
2	I	2688	HIS
2	I	2697	ARG
2	I	2698	MET
2	I	2700	MET
2	I	2738	ARG
2	I	2761	TYR
2	I	2786	LYS
2	I	2790	MET
2	I	2797	PHE
2	I	2806	ARG
2	I	2816	MET
2	I	2827	ARG
2	I	2914	LYS
2	I	2932	MET
2	I	2955	PHE
2	I	2966	TRP
2	I	2967	MET
2	I	3014	CYS
2	I	3030	HIS
2	I	3053	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	3096	PHE
2	I	3106	MET
2	I	3166	TYR
2	I	3239	MET
2	I	3248	ARG
2	I	3262	ARG
2	I	3266	MET
2	I	3280	TYR
2	I	3311	HIS
2	I	3321	ARG
2	I	3334	TRP
2	I	3336	LYS
2	I	3355	HIS
2	I	3357	HIS
2	I	3409	TYR
2	I	3449	HIS
2	I	3451	PHE
2	I	3458	PHE
2	I	3534	MET
2	I	3552	PHE
2	I	3573	MET
2	I	3576	TYR
2	I	3577	ARG
2	I	3594	ARG
2	I	3673	MET
2	I	3715	LYS
2	I	3734	HIS
2	I	3836	MET
2	I	3933	PHE
2	I	3945	GLU
2	I	4001	MET
2	I	4023	MET
2	I	4039	MET
2	I	4042	ARG
2	I	4057	MET
2	I	4080	TYR
2	I	4120	ASN
2	I	4156	HIS
2	I	4159	ARG
2	I	4207	MET
2	I	4553	ASN
2	I	4564	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	4627	MET
2	I	4629	TYR
2	I	4639	MET
2	I	4644	TRP
2	I	4676	GLU
2	I	4696	ASP
2	I	4796	MET
2	I	4818	MET
2	I	4839	MET
2	I	4858	PHE
2	I	4966	ASP
2	I	4973	HIS
3	K	12	MET
3	K	64	LYS
1	L	22	CYS
1	L	23	VAL
1	L	32	ASN
2	A	35	LEU
2	A	125	ARG
2	A	127	MET
2	A	227	MET
2	A	241	GLN
2	A	273	HIS
2	A	297	GLN
2	A	384	MET
2	A	389	PHE
2	A	460	GLN
2	A	481	GLU
2	A	702	TRP
2	A	714	TYR
2	A	835	ARG
2	A	866	HIS
2	A	886	ARG
2	A	924	MET
2	A	987	ARG
2	A	1025	ARG
2	A	1071	ARG
2	A	1128	ARG
2	A	1143	TRP
2	A	1170	MET
2	A	1260	MET
2	A	1421	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	1428	LEU
2	A	1435	TYR
2	A	1526	LEU
2	A	1648	MET
2	A	1981	MET
2	A	2198	MET
2	A	2294	ASP
2	A	2312	MET
2	A	2440	MET
2	A	2490	MET
2	A	2502	MET
2	A	2520	HIS
2	A	2555	CYS
2	A	2578	MET
2	A	2623	LEU
2	A	2652	TRP
2	A	2656	CYS
2	A	2661	TRP
2	A	2664	PHE
2	A	2673	HIS
2	A	2688	HIS
2	A	2697	ARG
2	A	2698	MET
2	A	2700	MET
2	A	2738	ARG
2	A	2761	TYR
2	A	2786	LYS
2	A	2790	MET
2	A	2797	PHE
2	A	2806	ARG
2	A	2816	MET
2	A	2827	ARG
2	A	2914	LYS
2	A	2932	MET
2	A	2955	PHE
2	A	2966	TRP
2	A	2967	MET
2	A	3014	CYS
2	A	3030	HIS
2	A	3053	ARG
2	A	3096	PHE
2	A	3106	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	3166	TYR
2	A	3239	MET
2	A	3248	ARG
2	A	3262	ARG
2	A	3266	MET
2	A	3280	TYR
2	A	3311	HIS
2	A	3321	ARG
2	A	3334	TRP
2	A	3336	LYS
2	A	3355	HIS
2	A	3357	HIS
2	A	3409	TYR
2	A	3449	HIS
2	A	3451	PHE
2	A	3458	PHE
2	A	3534	MET
2	A	3552	PHE
2	A	3573	MET
2	A	3576	TYR
2	A	3577	ARG
2	A	3594	ARG
2	A	3673	MET
2	A	3715	LYS
2	A	3734	HIS
2	A	3836	MET
2	A	3933	PHE
2	A	3945	GLU
2	A	4001	MET
2	A	4023	MET
2	A	4039	MET
2	A	4042	ARG
2	A	4057	MET
2	A	4080	TYR
2	A	4120	ASN
2	A	4156	HIS
2	A	4159	ARG
2	A	4207	MET
2	A	4553	ASN
2	A	4564	PHE
2	A	4627	MET
2	A	4629	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	4639	MET
2	A	4644	TRP
2	A	4676	GLU
2	A	4696	ASP
2	A	4796	MET
2	A	4818	MET
2	A	4839	MET
2	A	4858	PHE
2	A	4966	ASP
2	A	4973	HIS
3	C	12	MET
3	C	64	LYS
1	J	22	CYS
1	J	23	VAL
1	J	32	ASN
2	D	35	LEU
2	D	125	ARG
2	D	127	MET
2	D	227	MET
2	D	241	GLN
2	D	273	HIS
2	D	297	GLN
2	D	369	LEU
2	D	384	MET
2	D	389	PHE
2	D	460	GLN
2	D	481	GLU
2	D	702	TRP
2	D	714	TYR
2	D	835	ARG
2	D	866	HIS
2	D	886	ARG
2	D	924	MET
2	D	960	MET
2	D	987	ARG
2	D	1025	ARG
2	D	1071	ARG
2	D	1128	ARG
2	D	1143	TRP
2	D	1170	MET
2	D	1260	MET
2	D	1421	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	1428	LEU
2	D	1435	TYR
2	D	1526	LEU
2	D	1648	MET
2	D	1981	MET
2	D	2198	MET
2	D	2294	ASP
2	D	2312	MET
2	D	2440	MET
2	D	2490	MET
2	D	2502	MET
2	D	2520	HIS
2	D	2555	CYS
2	D	2578	MET
2	D	2623	LEU
2	D	2652	TRP
2	D	2656	CYS
2	D	2661	TRP
2	D	2664	PHE
2	D	2673	HIS
2	D	2688	HIS
2	D	2697	ARG
2	D	2698	MET
2	D	2700	MET
2	D	2738	ARG
2	D	2761	TYR
2	D	2786	LYS
2	D	2790	MET
2	D	2797	PHE
2	D	2806	ARG
2	D	2816	MET
2	D	2827	ARG
2	D	2914	LYS
2	D	2932	MET
2	D	2955	PHE
2	D	2966	TRP
2	D	2967	MET
2	D	3014	CYS
2	D	3030	HIS
2	D	3053	ARG
2	D	3096	PHE
2	D	3106	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	3166	TYR
2	D	3239	MET
2	D	3248	ARG
2	D	3262	ARG
2	D	3266	MET
2	D	3280	TYR
2	D	3311	HIS
2	D	3321	ARG
2	D	3334	TRP
2	D	3336	LYS
2	D	3355	HIS
2	D	3357	HIS
2	D	3409	TYR
2	D	3449	HIS
2	D	3451	PHE
2	D	3458	PHE
2	D	3534	MET
2	D	3552	PHE
2	D	3573	MET
2	D	3576	TYR
2	D	3577	ARG
2	D	3594	ARG
2	D	3673	MET
2	D	3715	LYS
2	D	3734	HIS
2	D	3836	MET
2	D	3933	PHE
2	D	3945	GLU
2	D	4001	MET
2	D	4023	MET
2	D	4039	MET
2	D	4042	ARG
2	D	4057	MET
2	D	4080	TYR
2	D	4120	ASN
2	D	4156	HIS
2	D	4159	ARG
2	D	4207	MET
2	D	4553	ASN
2	D	4564	PHE
2	D	4627	MET
2	D	4629	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	4639	MET
2	D	4644	TRP
2	D	4676	GLU
2	D	4696	ASP
2	D	4796	MET
2	D	4818	MET
2	D	4839	MET
2	D	4858	PHE
2	D	4966	ASP
2	D	4973	HIS
3	E	12	MET
3	E	64	LYS
1	F	22	CYS
1	F	23	VAL
1	F	32	ASN
2	G	35	LEU
2	G	125	ARG
2	G	127	MET
2	G	227	MET
2	G	241	GLN
2	G	273	HIS
2	G	297	GLN
2	G	359	TYR
2	G	384	MET
2	G	389	PHE
2	G	460	GLN
2	G	481	GLU
2	G	702	TRP
2	G	714	TYR
2	G	835	ARG
2	G	866	HIS
2	G	886	ARG
2	G	924	MET
2	G	960	MET
2	G	987	ARG
2	G	1025	ARG
2	G	1071	ARG
2	G	1128	ARG
2	G	1143	TRP
2	G	1170	MET
2	G	1260	MET
2	G	1421	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	1428	LEU
2	G	1435	TYR
2	G	1526	LEU
2	G	1648	MET
2	G	1981	MET
2	G	2198	MET
2	G	2294	ASP
2	G	2312	MET
2	G	2440	MET
2	G	2490	MET
2	G	2502	MET
2	G	2520	HIS
2	G	2555	CYS
2	G	2578	MET
2	G	2623	LEU
2	G	2652	TRP
2	G	2656	CYS
2	G	2661	TRP
2	G	2664	PHE
2	G	2673	HIS
2	G	2688	HIS
2	G	2697	ARG
2	G	2698	MET
2	G	2700	MET
2	G	2738	ARG
2	G	2761	TYR
2	G	2786	LYS
2	G	2790	MET
2	G	2797	PHE
2	G	2806	ARG
2	G	2816	MET
2	G	2827	ARG
2	G	2914	LYS
2	G	2932	MET
2	G	2955	PHE
2	G	2966	TRP
2	G	2967	MET
2	G	3014	CYS
2	G	3030	HIS
2	G	3053	ARG
2	G	3096	PHE
2	G	3106	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	3166	TYR
2	G	3239	MET
2	G	3248	ARG
2	G	3262	ARG
2	G	3266	MET
2	G	3280	TYR
2	G	3311	HIS
2	G	3321	ARG
2	G	3334	TRP
2	G	3336	LYS
2	G	3355	HIS
2	G	3357	HIS
2	G	3409	TYR
2	G	3449	HIS
2	G	3451	PHE
2	G	3458	PHE
2	G	3534	MET
2	G	3552	PHE
2	G	3573	MET
2	G	3576	TYR
2	G	3577	ARG
2	G	3594	ARG
2	G	3673	MET
2	G	3715	LYS
2	G	3734	HIS
2	G	3836	MET
2	G	3933	PHE
2	G	3945	GLU
2	G	4001	MET
2	G	4023	MET
2	G	4039	MET
2	G	4042	ARG
2	G	4057	MET
2	G	4080	TYR
2	G	4120	ASN
2	G	4156	HIS
2	G	4159	ARG
2	G	4207	MET
2	G	4553	ASN
2	G	4564	PHE
2	G	4627	MET
2	G	4629	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	4639	MET
2	G	4644	TRP
2	G	4676	GLU
2	G	4696	ASP
2	G	4796	MET
2	G	4818	MET
2	G	4839	MET
2	G	4858	PHE
2	G	4966	ASP
2	G	4973	HIS
3	M	12	MET
3	M	64	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	32	ASN
2	I	473	ASN
2	I	981	GLN
2	I	1299	GLN
2	I	3146	HIS
2	I	3597	GLN
2	I	3806	ASN
2	I	4574	ASN
3	K	44	GLN
1	L	32	ASN
2	A	473	ASN
2	A	981	GLN
2	A	3146	HIS
2	A	3597	GLN
2	A	3806	ASN
2	A	4246	GLN
2	A	4574	ASN
3	C	44	GLN
2	D	473	ASN
2	D	981	GLN
2	D	1299	GLN
2	D	3146	HIS
2	D	3597	GLN
2	D	4246	GLN
2	D	4574	ASN
3	E	44	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	32	ASN
2	G	473	ASN
2	G	981	GLN
2	G	1299	GLN
2	G	3146	HIS
2	G	3597	GLN
2	G	4246	GLN
2	G	4574	ASN
3	M	44	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
5	POV	I	5102	-	51,51,51	0.49	0	57,59,59	0.45	0
7	CFF	A	5104	-	8,15,15	2.40	3 (37%)	8,23,23	1.20	1 (12%)
5	POV	D	5102	-	51,51,51	0.49	0	57,59,59	0.45	0
6	ATP	A	5103	-	26,33,33	0.59	0	31,52,52	0.85	3 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	ATP	I	5103	-	26,33,33	0.91	1 (3%)	31,52,52	1.59	5 (16%)
7	CFF	I	5104	-	8,15,15	2.40	3 (37%)	8,23,23	1.20	1 (12%)
7	CFF	G	5104	-	8,15,15	2.38	3 (37%)	8,23,23	1.18	1 (12%)
6	ATP	G	5103	-	26,33,33	0.58	0	31,52,52	0.84	3 (9%)
5	POV	G	5102	-	51,51,51	0.49	0	57,59,59	0.45	0
7	CFF	D	5104	-	8,15,15	2.41	3 (37%)	8,23,23	1.19	1 (12%)
6	ATP	D	5103	-	26,33,33	0.59	0	31,52,52	0.85	3 (9%)
5	POV	A	5101	-	51,51,51	0.49	0	57,59,59	0.45	0

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
5	POV	I	5102	-	-	17/55/55/55	-
7	CFF	A	5104	-	-	-	0/2/2/2
5	POV	D	5102	-	-	17/55/55/55	-
6	ATP	A	5103	-	-	5/18/38/38	0/3/3/3
6	ATP	I	5103	-	-	3/18/38/38	0/3/3/3
7	CFF	I	5104	-	-	-	0/2/2/2
7	CFF	G	5104	-	-	-	0/2/2/2
6	ATP	G	5103	-	-	5/18/38/38	0/3/3/3
5	POV	G	5102	-	-	17/55/55/55	-
7	CFF	D	5104	-	-	-	0/2/2/2
6	ATP	D	5103	-	-	5/18/38/38	0/3/3/3
5	POV	A	5101	-	-	17/55/55/55	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	5104	CFF	C5-C4	4.54	1.45	1.39
7	I	5104	CFF	C5-C4	4.53	1.45	1.39
7	D	5104	CFF	C5-C4	4.53	1.45	1.39
7	G	5104	CFF	C5-C4	4.52	1.45	1.39
7	D	5104	CFF	C5-C6	4.35	1.48	1.41
7	I	5104	CFF	C5-C6	4.34	1.48	1.41
7	A	5104	CFF	C5-C6	4.34	1.48	1.41
7	G	5104	CFF	C5-C6	4.28	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	5103	ATP	C5-C4	2.33	1.47	1.40
7	D	5104	CFF	C6-N1	2.23	1.41	1.38
7	A	5104	CFF	C6-N1	2.18	1.41	1.38
7	I	5104	CFF	C6-N1	2.17	1.41	1.38
7	G	5104	CFF	C6-N1	2.17	1.41	1.38

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	5103	ATP	PA-O3A-PB	-3.89	119.48	132.83
6	I	5103	ATP	PB-O3B-PG	-3.87	119.54	132.83
6	I	5103	ATP	N3-C2-N1	-3.20	123.67	128.68
6	I	5103	ATP	C3'-C2'-C1'	3.07	105.60	100.98
6	I	5103	ATP	C4-C5-N7	-2.42	106.87	109.40
7	A	5104	CFF	C5-C6-N1	-2.34	115.70	118.20
7	D	5104	CFF	C5-C6-N1	-2.34	115.71	118.20
7	I	5104	CFF	C5-C6-N1	-2.33	115.72	118.20
7	G	5104	CFF	C5-C6-N1	-2.33	115.72	118.20
6	D	5103	ATP	C5-C6-N6	2.29	123.83	120.35
6	A	5103	ATP	C5-C6-N6	2.26	123.79	120.35
6	G	5103	ATP	C5-C6-N6	2.26	123.78	120.35
6	A	5103	ATP	C3'-C2'-C1'	2.06	104.08	100.98
6	G	5103	ATP	C3'-C2'-C1'	2.05	104.07	100.98
6	D	5103	ATP	C3'-C2'-C1'	2.05	104.06	100.98
6	A	5103	ATP	PB-O3B-PG	2.01	139.72	132.83
6	D	5103	ATP	PB-O3B-PG	2.01	139.72	132.83
6	G	5103	ATP	PB-O3B-PG	2.01	139.71	132.83

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	5102	POV	C1-O11-P-O14
5	A	5101	POV	C1-O11-P-O14
5	D	5102	POV	C1-O11-P-O14
5	G	5102	POV	C1-O11-P-O14
6	I	5103	ATP	C5'-O5'-PA-O1A
6	I	5103	ATP	C5'-O5'-PA-O2A
6	A	5103	ATP	PB-O3B-PG-O2G
6	A	5103	ATP	C5'-O5'-PA-O2A
6	A	5103	ATP	C5'-O5'-PA-O3A
6	D	5103	ATP	PB-O3B-PG-O2G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	D	5103	ATP	C5'-O5'-PA-O2A
6	D	5103	ATP	C5'-O5'-PA-O3A
6	G	5103	ATP	PB-O3B-PG-O2G
6	G	5103	ATP	C5'-O5'-PA-O2A
6	G	5103	ATP	C5'-O5'-PA-O3A
5	I	5102	POV	C22-C21-O21-C2
5	A	5101	POV	C22-C21-O21-C2
5	D	5102	POV	C22-C21-O21-C2
5	G	5102	POV	C22-C21-O21-C2
5	I	5102	POV	C21-C22-C23-C24
5	A	5101	POV	C21-C22-C23-C24
5	D	5102	POV	C21-C22-C23-C24
5	G	5102	POV	C21-C22-C23-C24
5	I	5102	POV	C31-C32-C33-C34
5	A	5101	POV	C31-C32-C33-C34
5	D	5102	POV	C31-C32-C33-C34
5	G	5102	POV	C31-C32-C33-C34
5	I	5102	POV	O22-C21-O21-C2
5	A	5101	POV	O22-C21-O21-C2
5	D	5102	POV	O22-C21-O21-C2
5	G	5102	POV	O22-C21-O21-C2
5	G	5102	POV	C39-C310-C311-C312
5	I	5102	POV	C39-C310-C311-C312
5	A	5101	POV	C39-C310-C311-C312
5	D	5102	POV	C39-C310-C311-C312
5	D	5102	POV	C312-C313-C314-C315
5	I	5102	POV	C312-C313-C314-C315
5	A	5101	POV	C312-C313-C314-C315
5	G	5102	POV	C312-C313-C314-C315
5	I	5102	POV	C211-C212-C213-C214
5	A	5101	POV	C211-C212-C213-C214
5	D	5102	POV	C211-C212-C213-C214
5	G	5102	POV	C211-C212-C213-C214
5	I	5102	POV	O11-C1-C2-O21
5	A	5101	POV	O11-C1-C2-O21
5	D	5102	POV	O11-C1-C2-O21
5	G	5102	POV	O11-C1-C2-O21
5	I	5102	POV	C11-C12-N-C14
5	A	5101	POV	C11-C12-N-C14
5	D	5102	POV	C11-C12-N-C14
5	G	5102	POV	C11-C12-N-C14
6	I	5103	ATP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	I	5102	POV	C11-C12-N-C15
5	A	5101	POV	C11-C12-N-C15
5	D	5102	POV	C11-C12-N-C15
5	G	5102	POV	C11-C12-N-C15
5	I	5102	POV	O11-C1-C2-C3
5	A	5101	POV	O11-C1-C2-C3
5	D	5102	POV	O11-C1-C2-C3
5	G	5102	POV	O11-C1-C2-C3
5	I	5102	POV	C11-C12-N-C13
5	A	5101	POV	C11-C12-N-C13
5	D	5102	POV	C11-C12-N-C13
5	G	5102	POV	C11-C12-N-C13
5	I	5102	POV	C29-C210-C211-C212
5	A	5101	POV	C29-C210-C211-C212
5	D	5102	POV	C29-C210-C211-C212
5	G	5102	POV	C29-C210-C211-C212
5	I	5102	POV	C1-O11-P-O12
5	A	5101	POV	C1-O11-P-O12
5	D	5102	POV	C1-O11-P-O12
5	G	5102	POV	C1-O11-P-O12
5	A	5101	POV	C36-C37-C38-C39
5	I	5102	POV	C36-C37-C38-C39
5	D	5102	POV	C36-C37-C38-C39
5	G	5102	POV	C36-C37-C38-C39
6	A	5103	ATP	PB-O3B-PG-O1G
6	D	5103	ATP	PB-O3B-PG-O1G
6	G	5103	ATP	PB-O3B-PG-O1G
6	A	5103	ATP	PB-O3B-PG-O3G
6	D	5103	ATP	PB-O3B-PG-O3G
6	G	5103	ATP	PB-O3B-PG-O3G
5	I	5102	POV	O31-C31-C32-C33
5	A	5101	POV	O31-C31-C32-C33
5	D	5102	POV	O31-C31-C32-C33
5	G	5102	POV	O31-C31-C32-C33

There are no ring outliers.

12 monomers are involved in 25 short contacts:

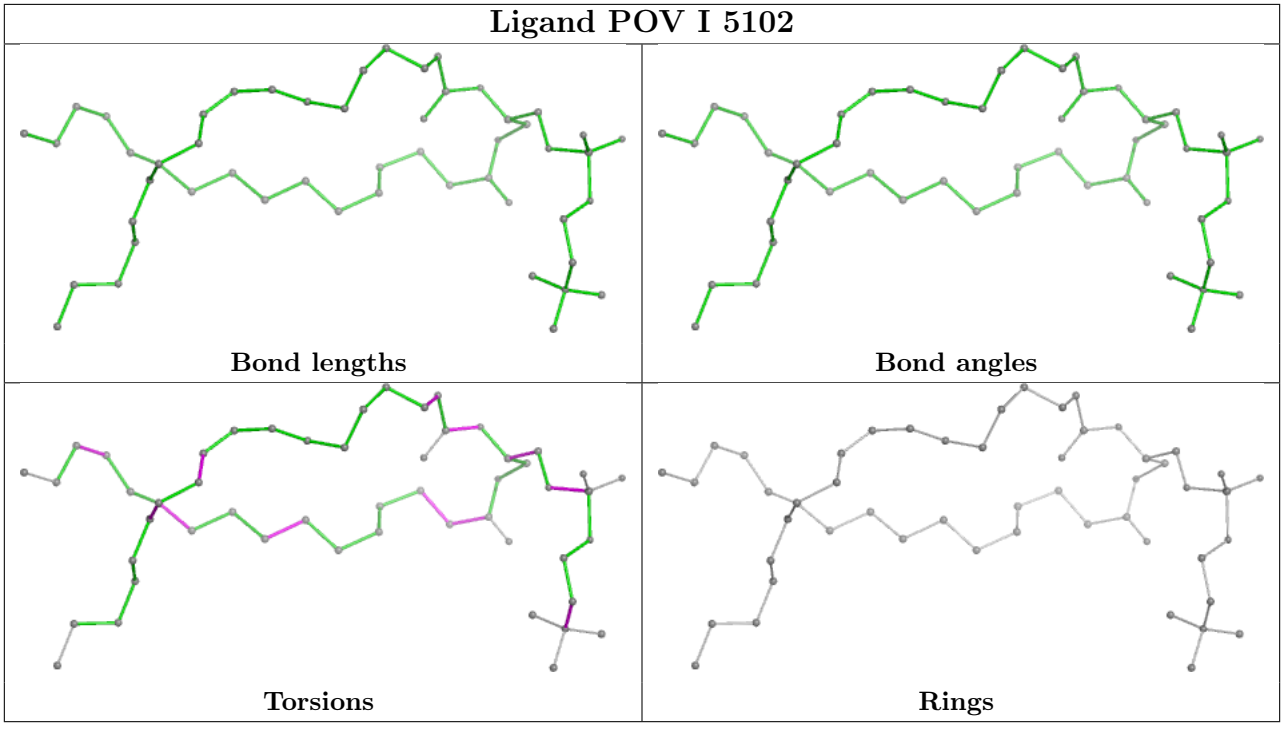
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	5102	POV	1	0
7	A	5104	CFF	1	0
5	D	5102	POV	3	0

Continued on next page...

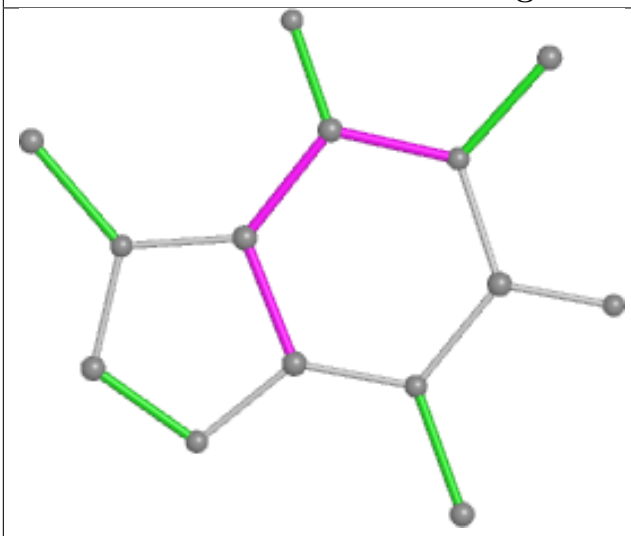
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	5103	ATP	3	0
6	I	5103	ATP	2	0
7	I	5104	CFF	1	0
7	G	5104	CFF	2	0
6	G	5103	ATP	3	0
5	G	5102	POV	3	0
7	D	5104	CFF	2	0
6	D	5103	ATP	3	0
5	A	5101	POV	1	0

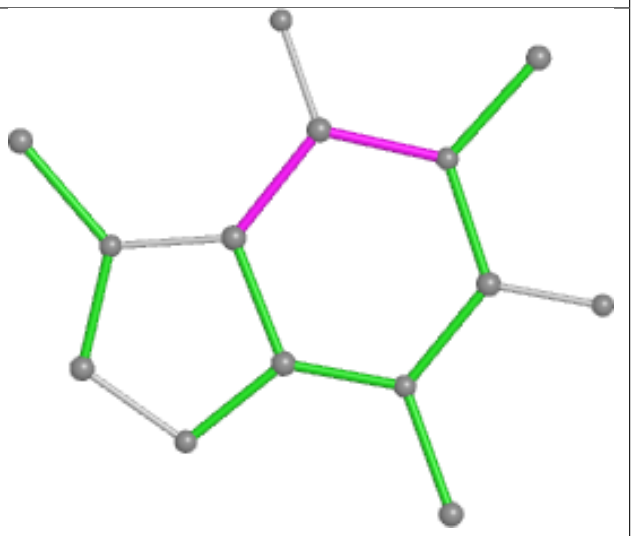
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



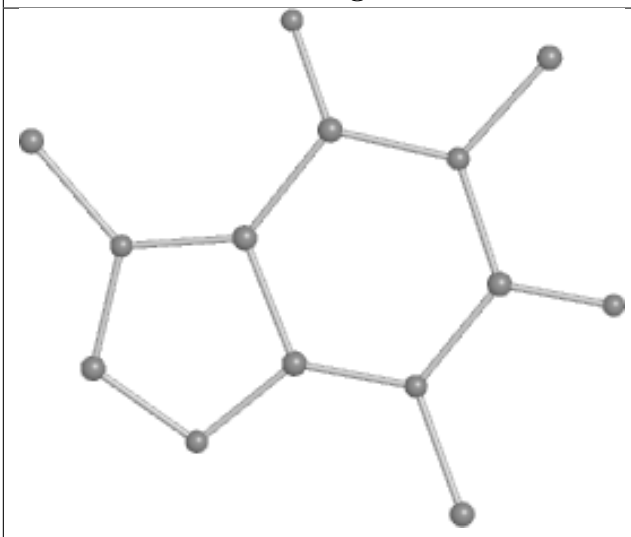
Ligand CFF A 5104



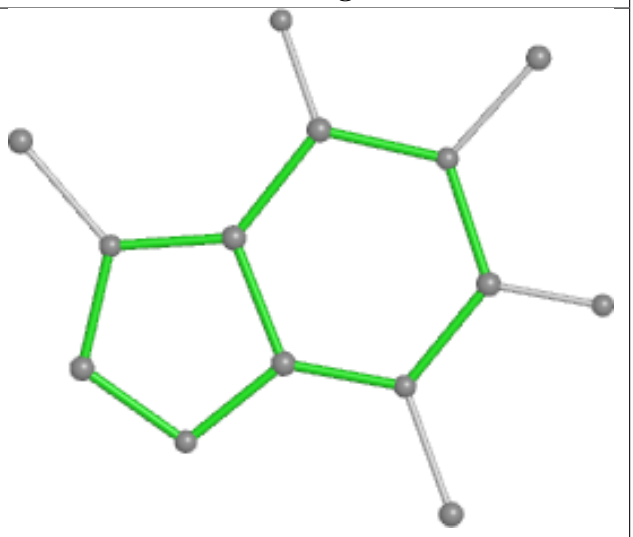
Bond lengths



Bond angles

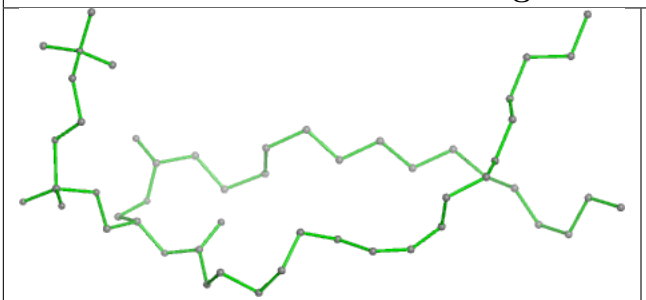


Torsions

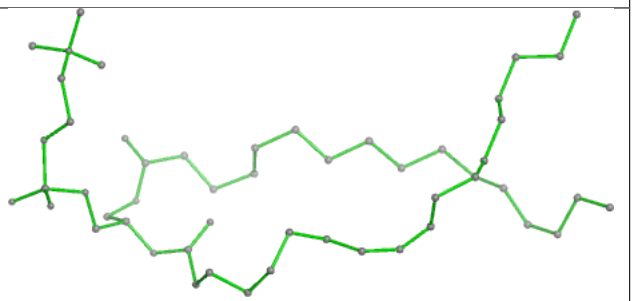


Rings

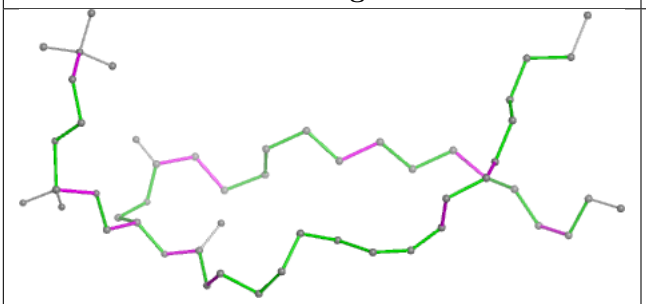
Ligand POV D 5102



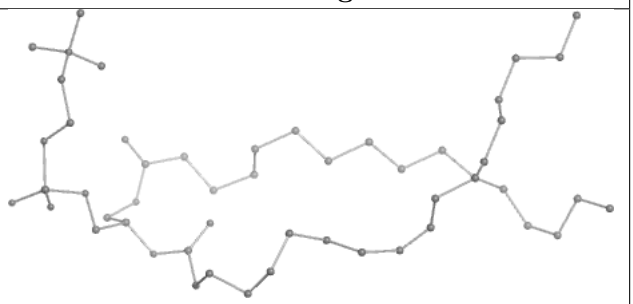
Bond lengths



Bond angles

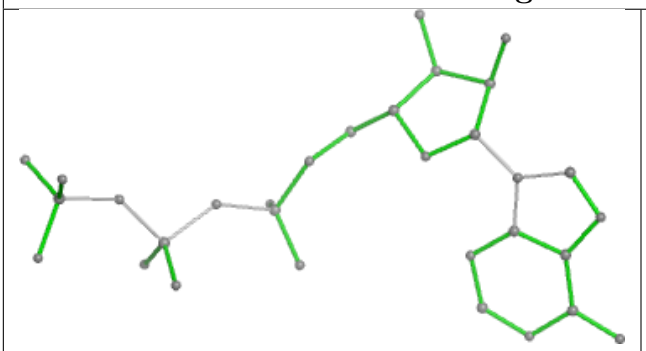


Torsions

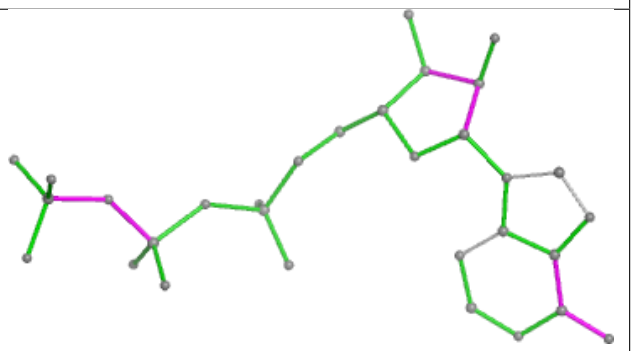


Rings

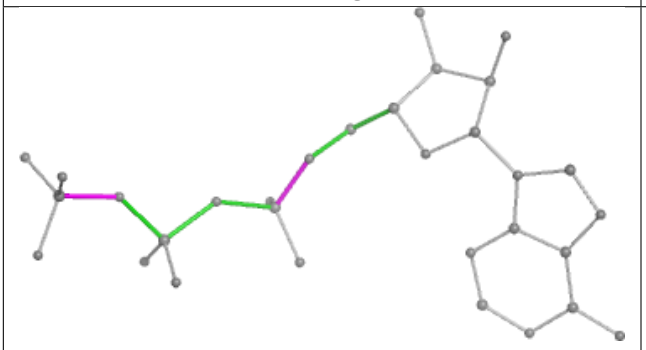
Ligand ATP A 5103



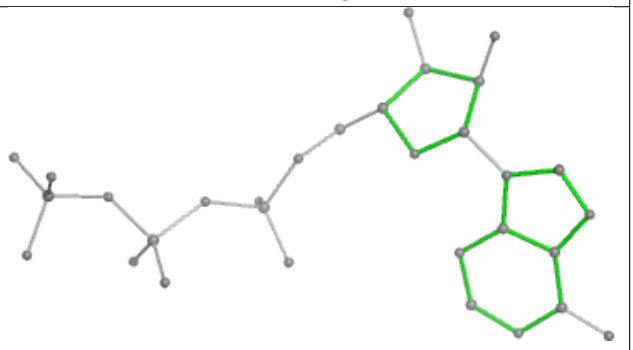
Bond lengths



Bond angles

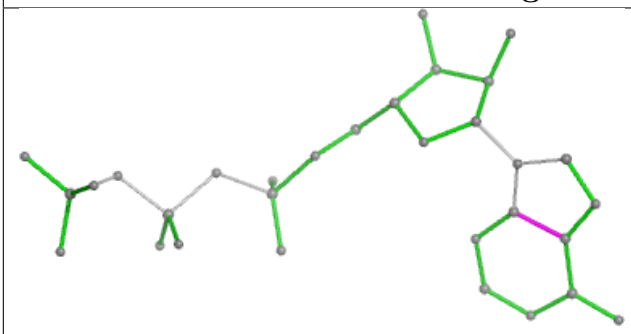


Torsions

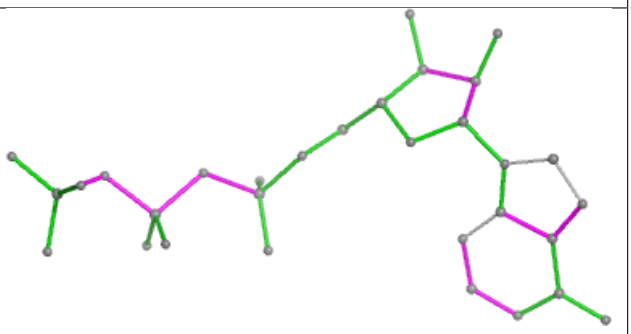


Rings

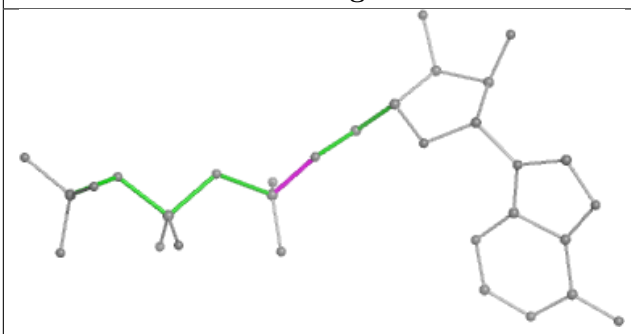
Ligand ATP I 5103



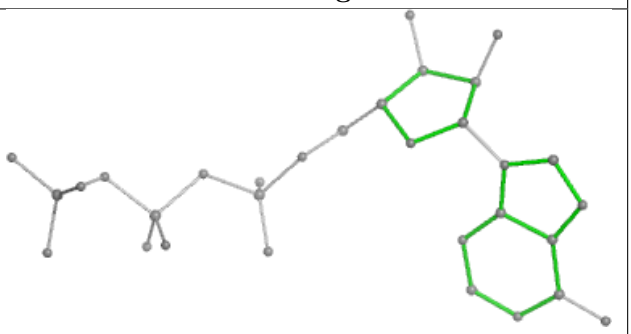
Bond lengths



Bond angles

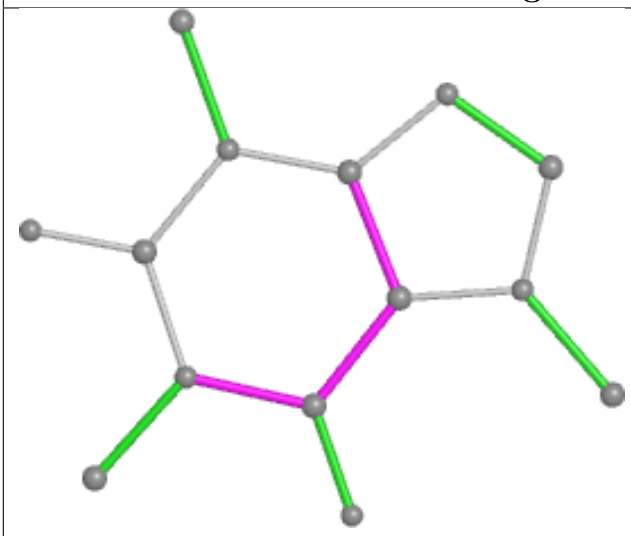


Torsions

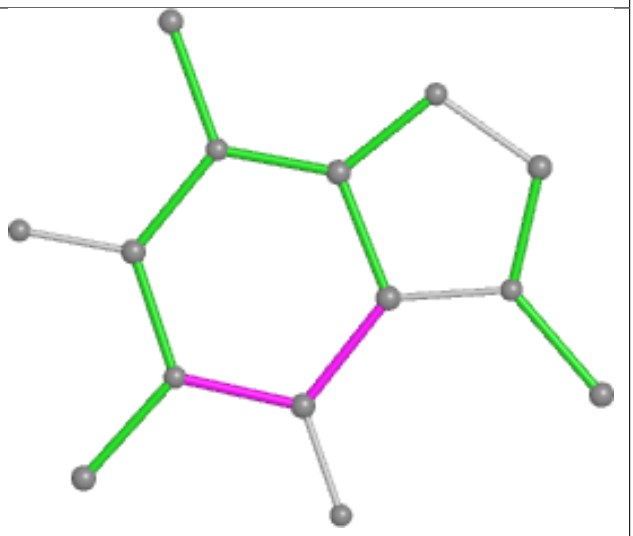


Rings

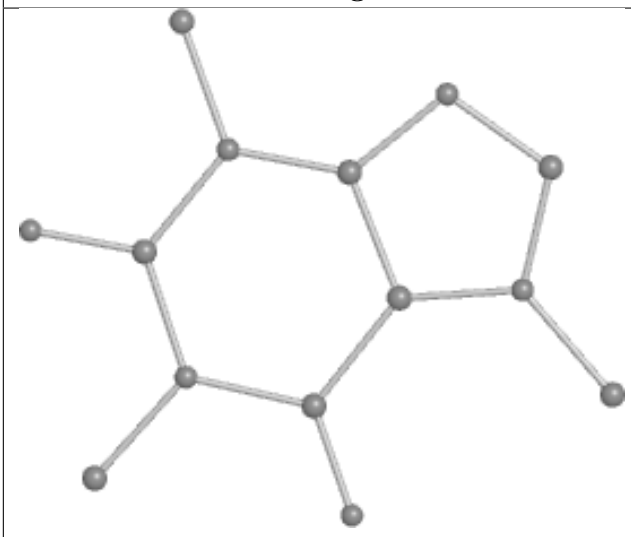
Ligand CFF I 5104



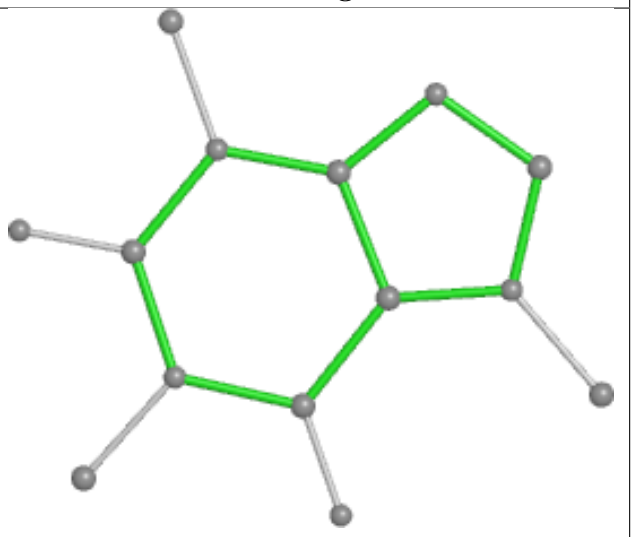
Bond lengths



Bond angles

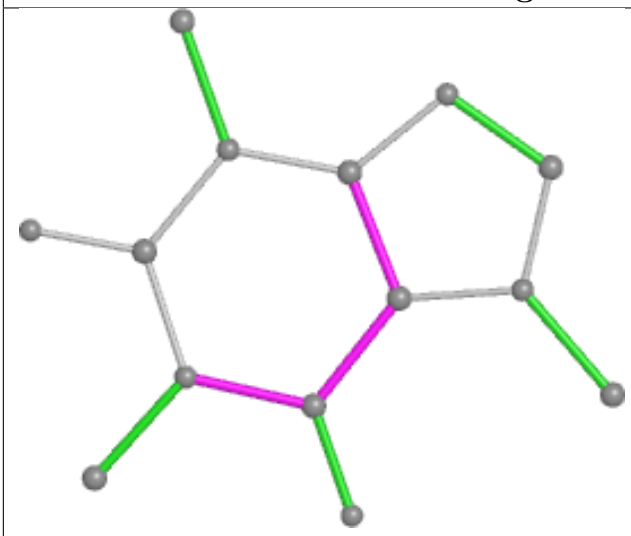


Torsions

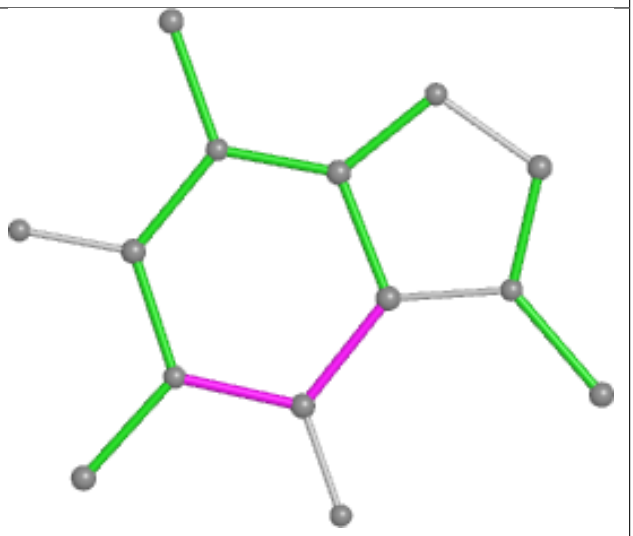


Rings

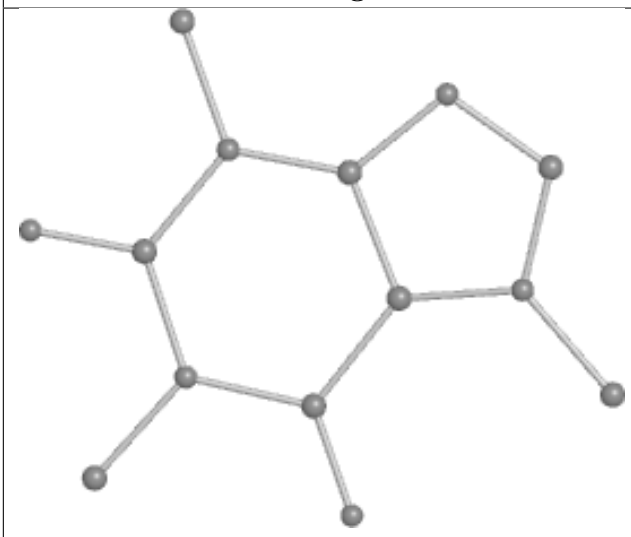
Ligand CFF G 5104



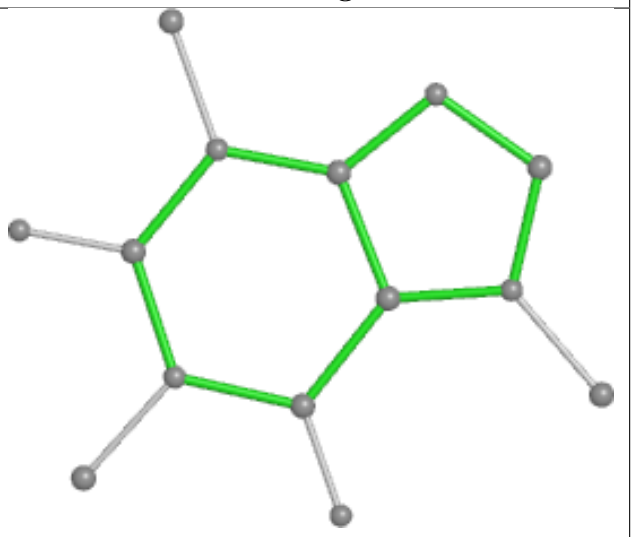
Bond lengths



Bond angles

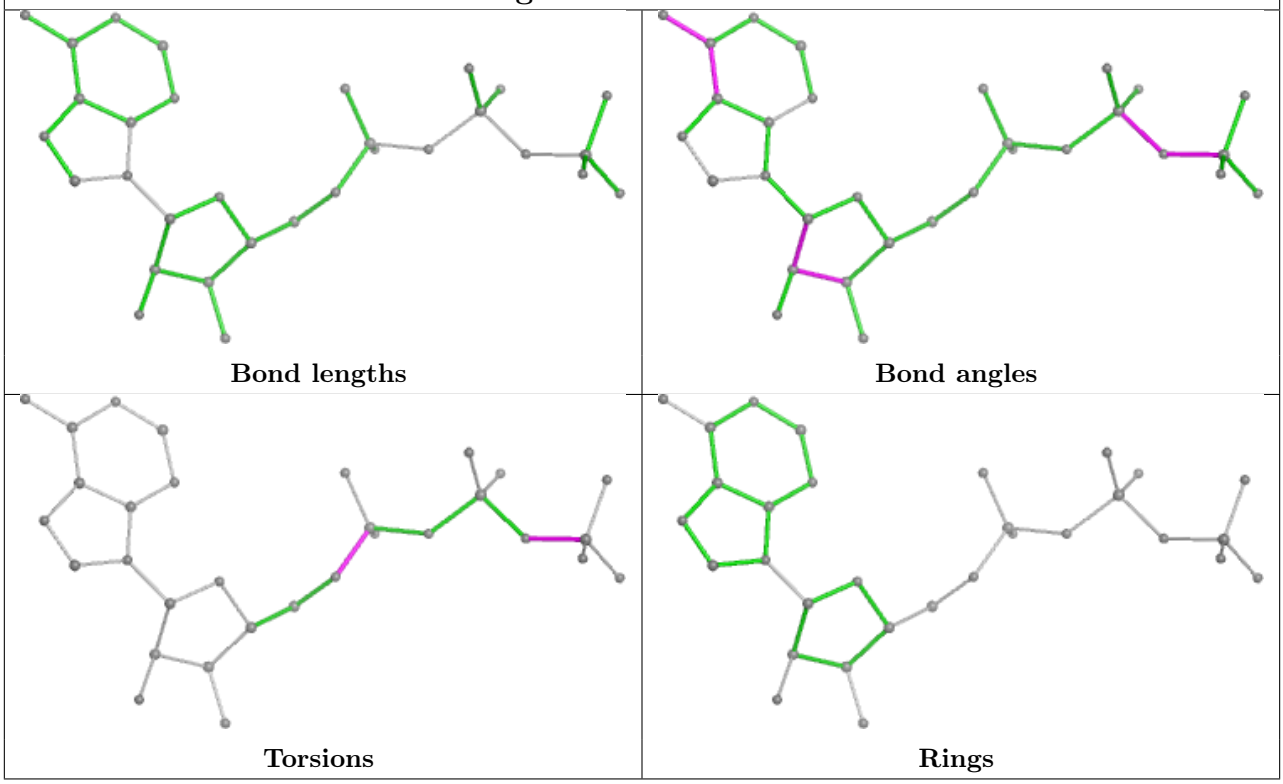


Torsions

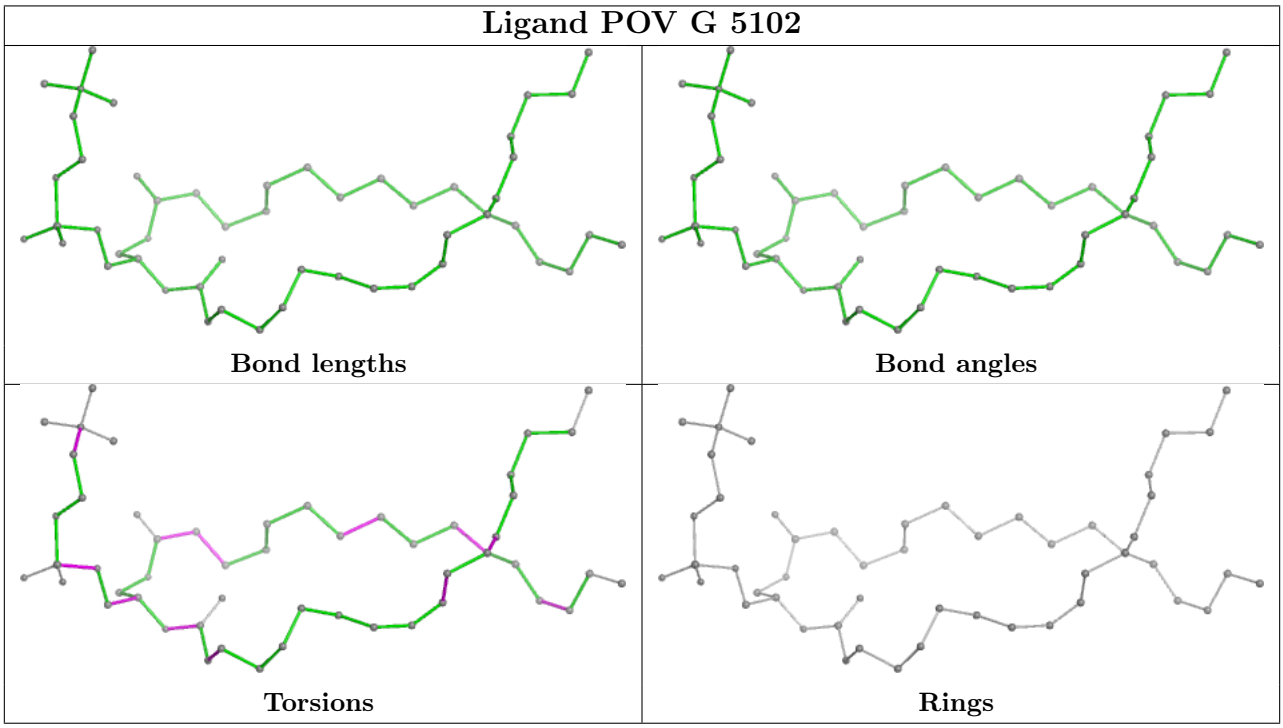


Rings

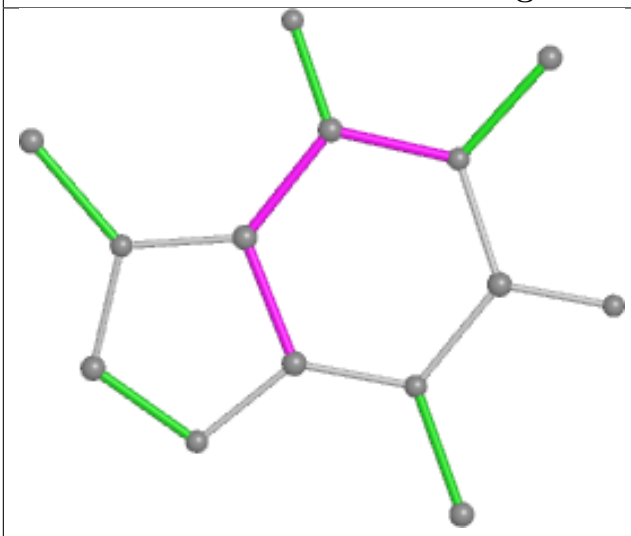
Ligand ATP G 5103



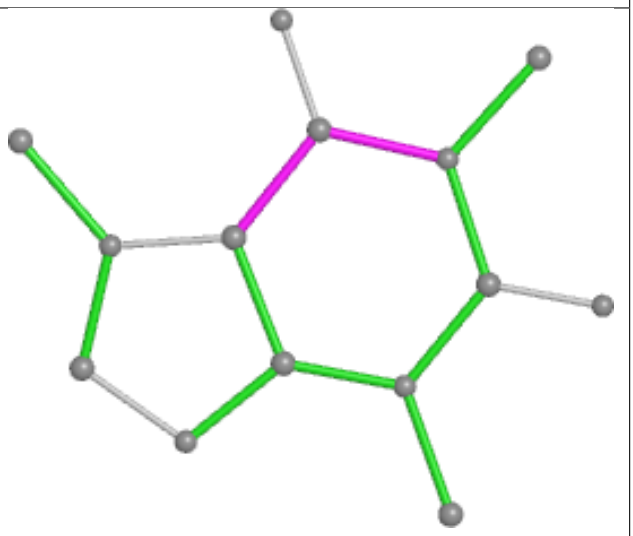
Ligand POV G 5102



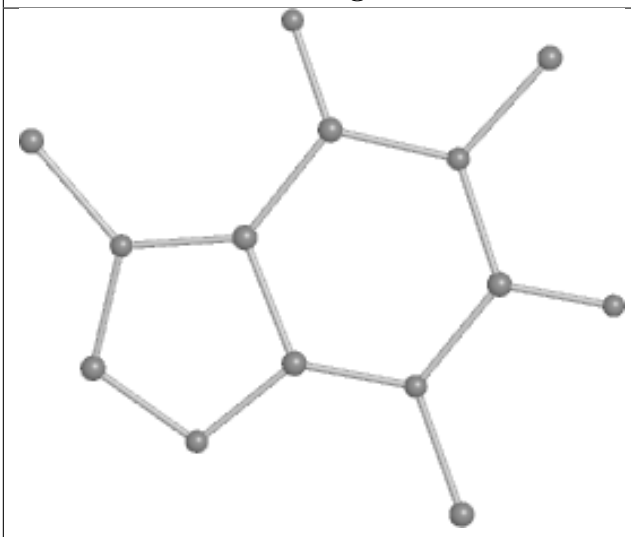
Ligand CFF D 5104



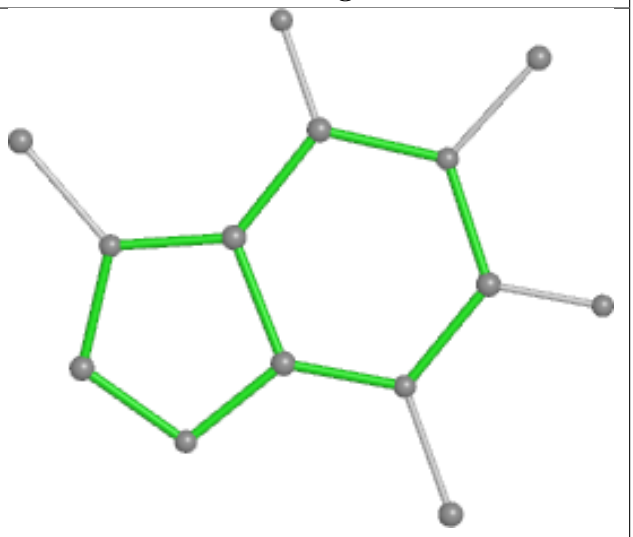
Bond lengths



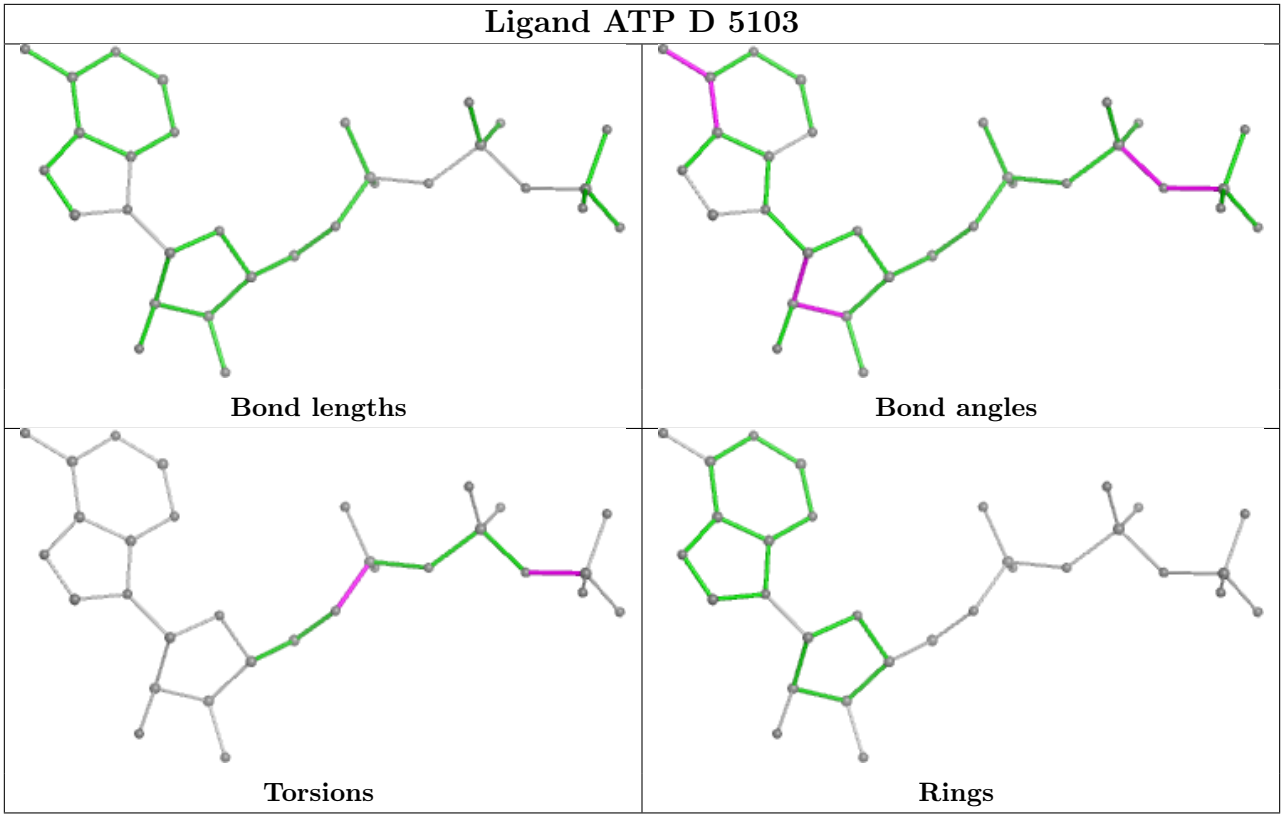
Bond angles

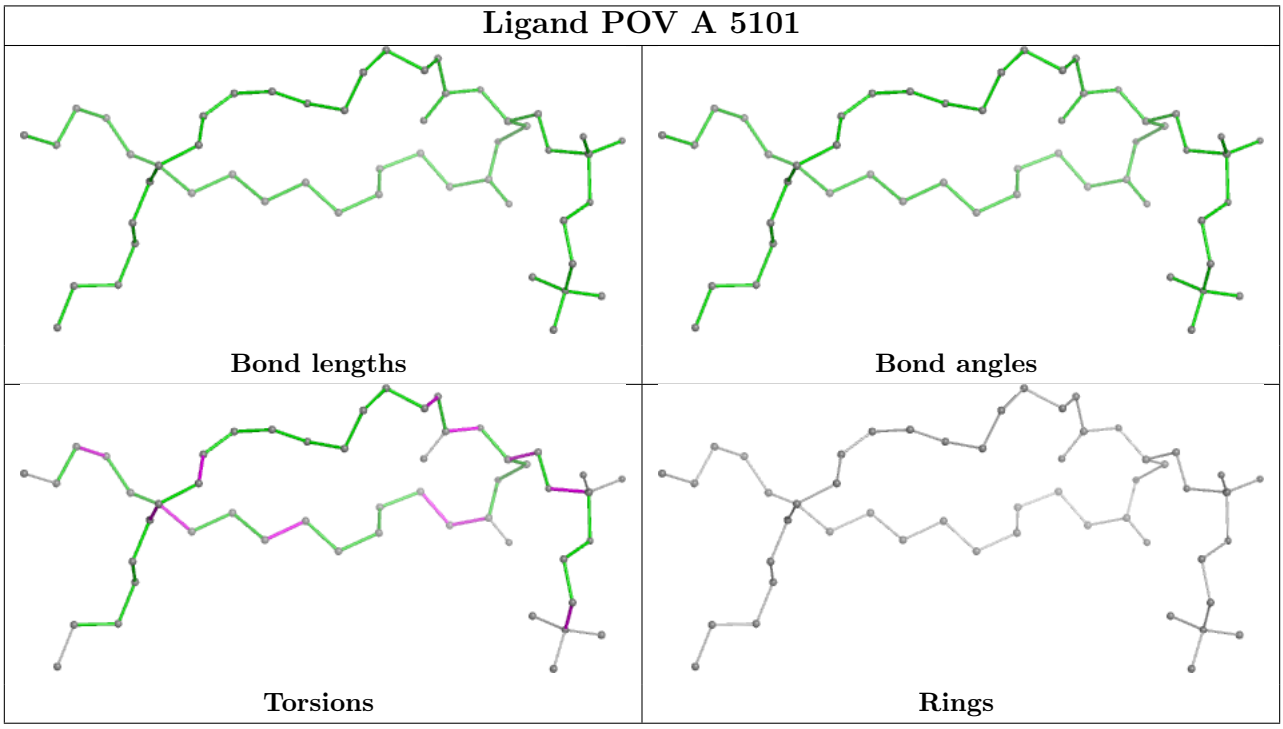


Torsions



Rings





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

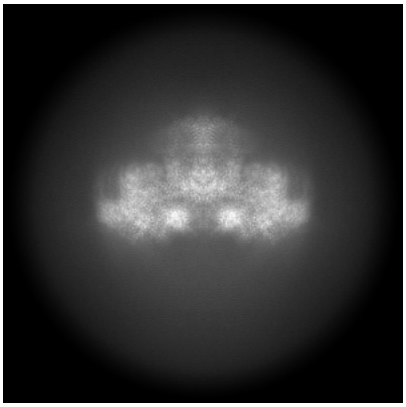
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19468. These allow visual inspection of the internal detail of the map and identification of artifacts.

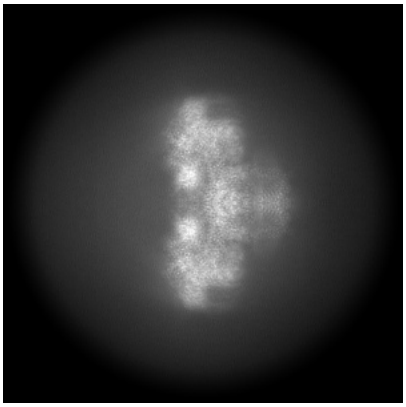
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

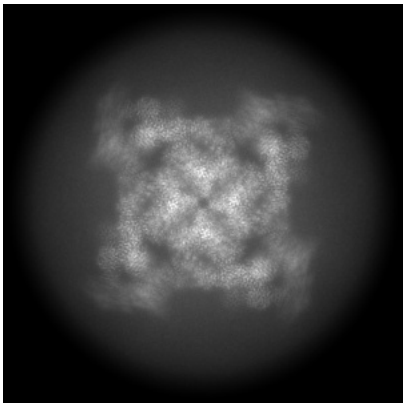
6.1.1 Primary map



X



Y

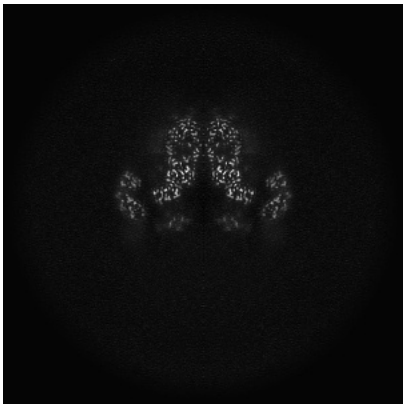


Z

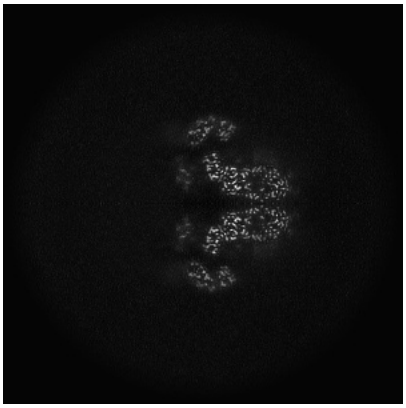
The images above show the map projected in three orthogonal directions.

6.2 Central slices

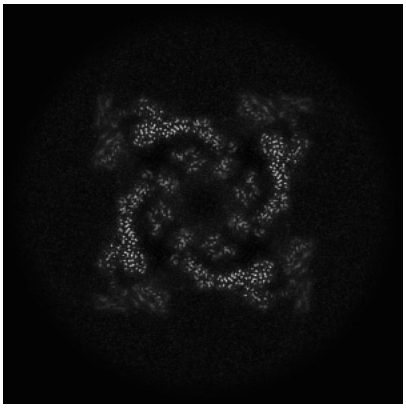
6.2.1 Primary map



X Index: 225



Y Index: 225

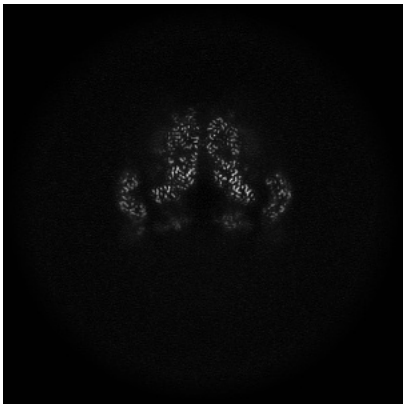


Z Index: 225

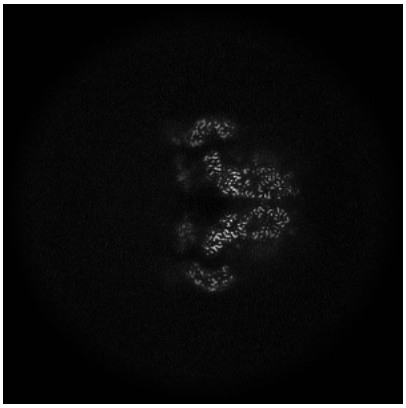
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

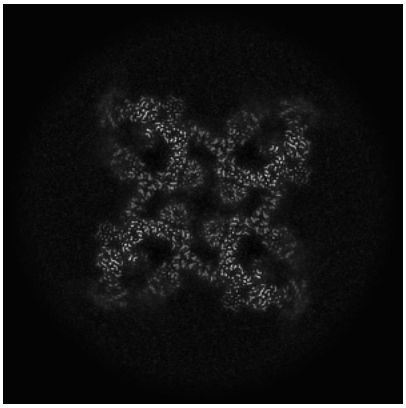
6.3.1 Primary map



X Index: 223



Y Index: 223

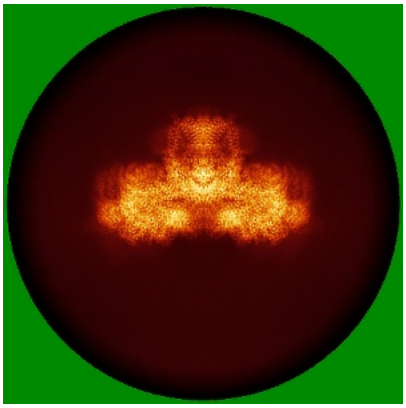


Z Index: 210

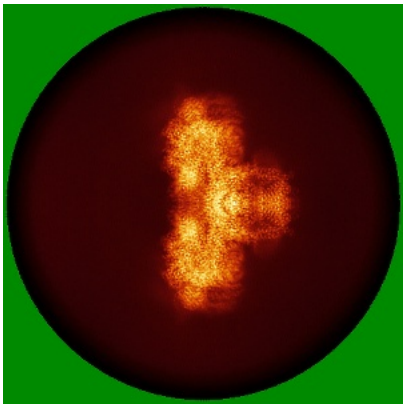
The images above show the largest variance slices of the map in three orthogonal directions.

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

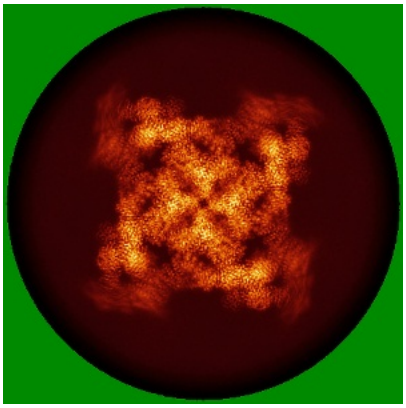
6.4.1 Primary map



X



Y

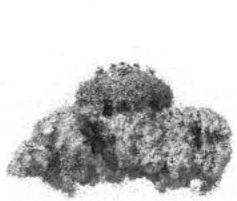


Z

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.

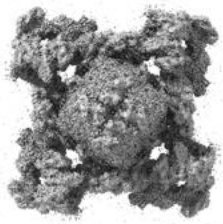
6.5 Orthogonal surface views (i)

6.5.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

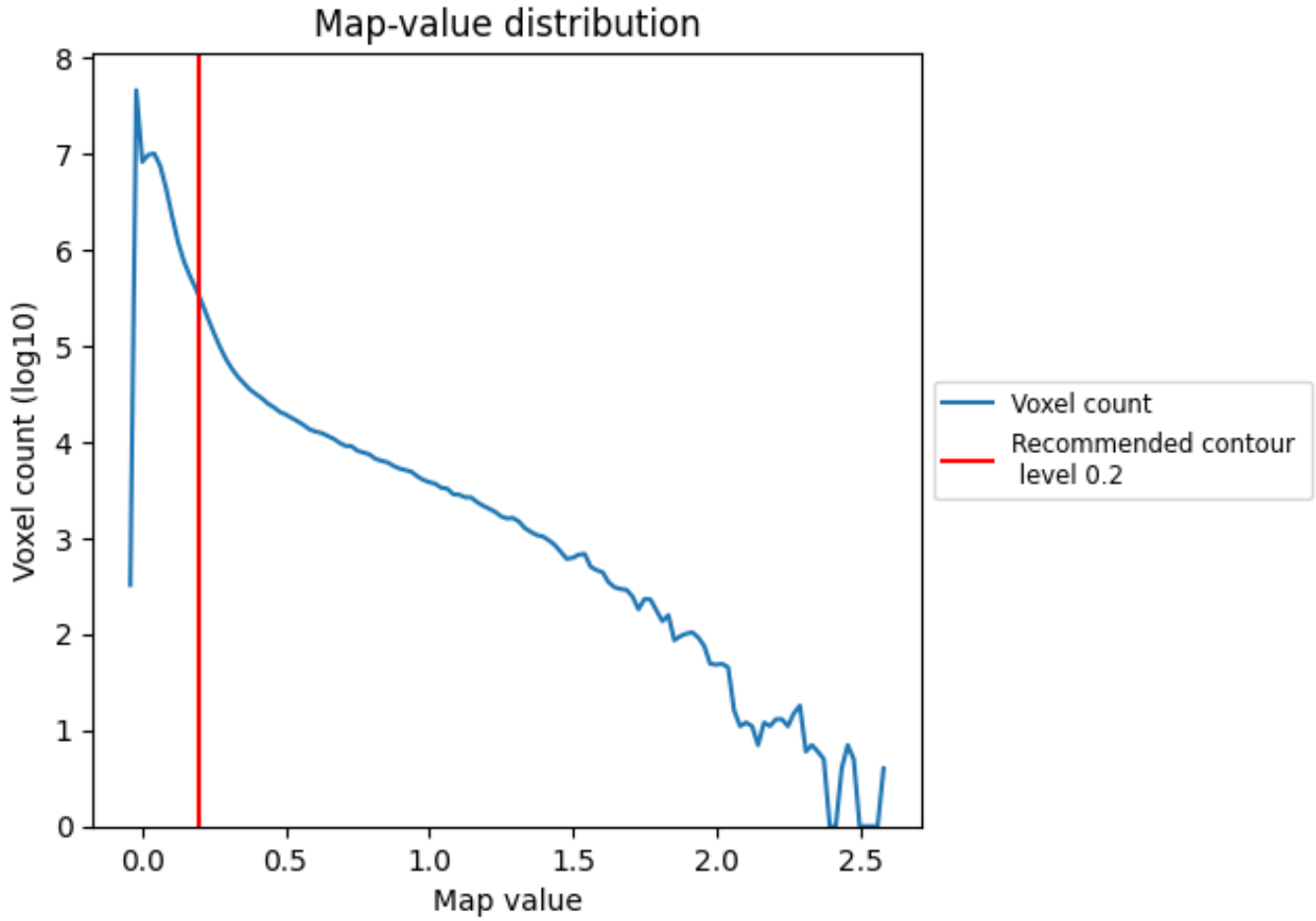
6.6 Mask visualisation (i)

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

7 Map analysis

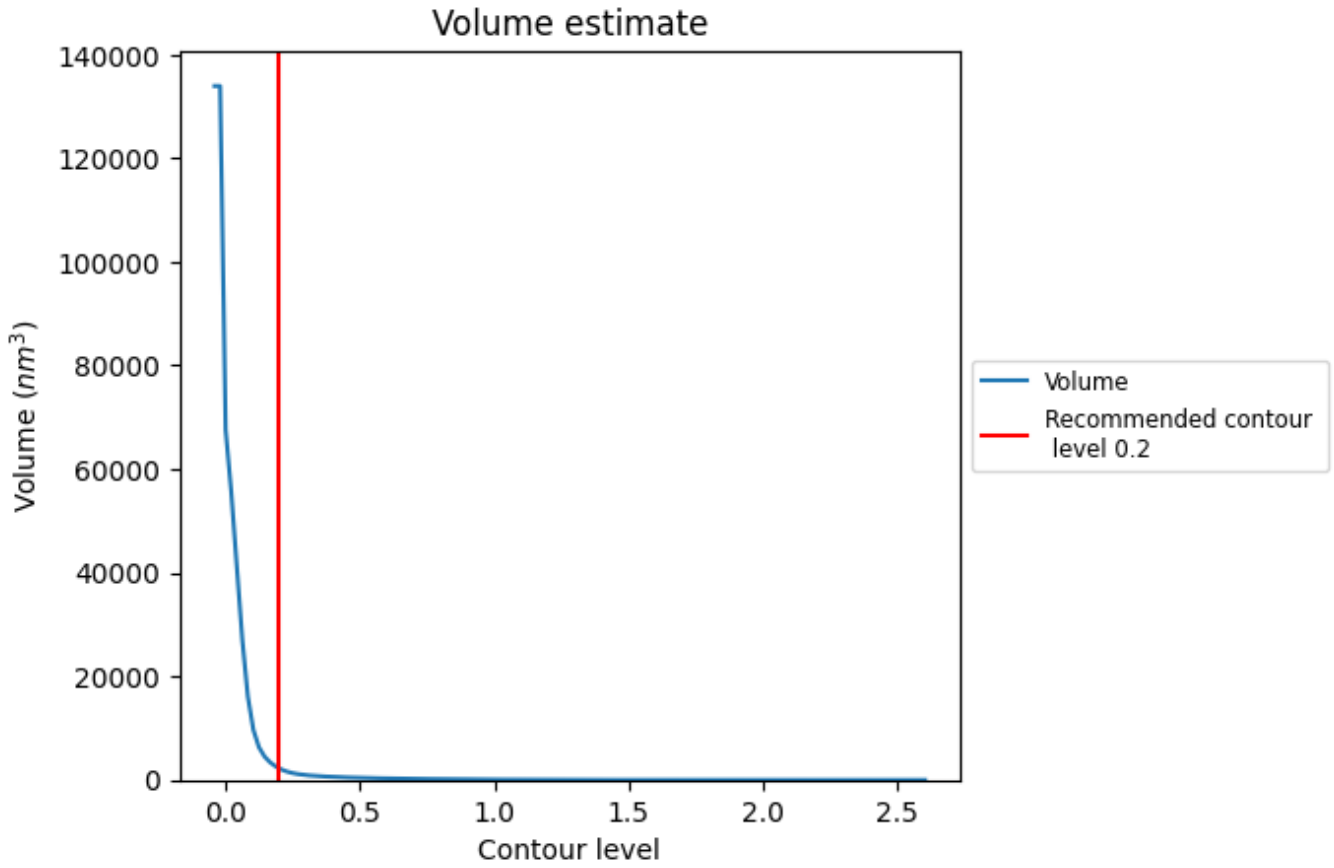
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

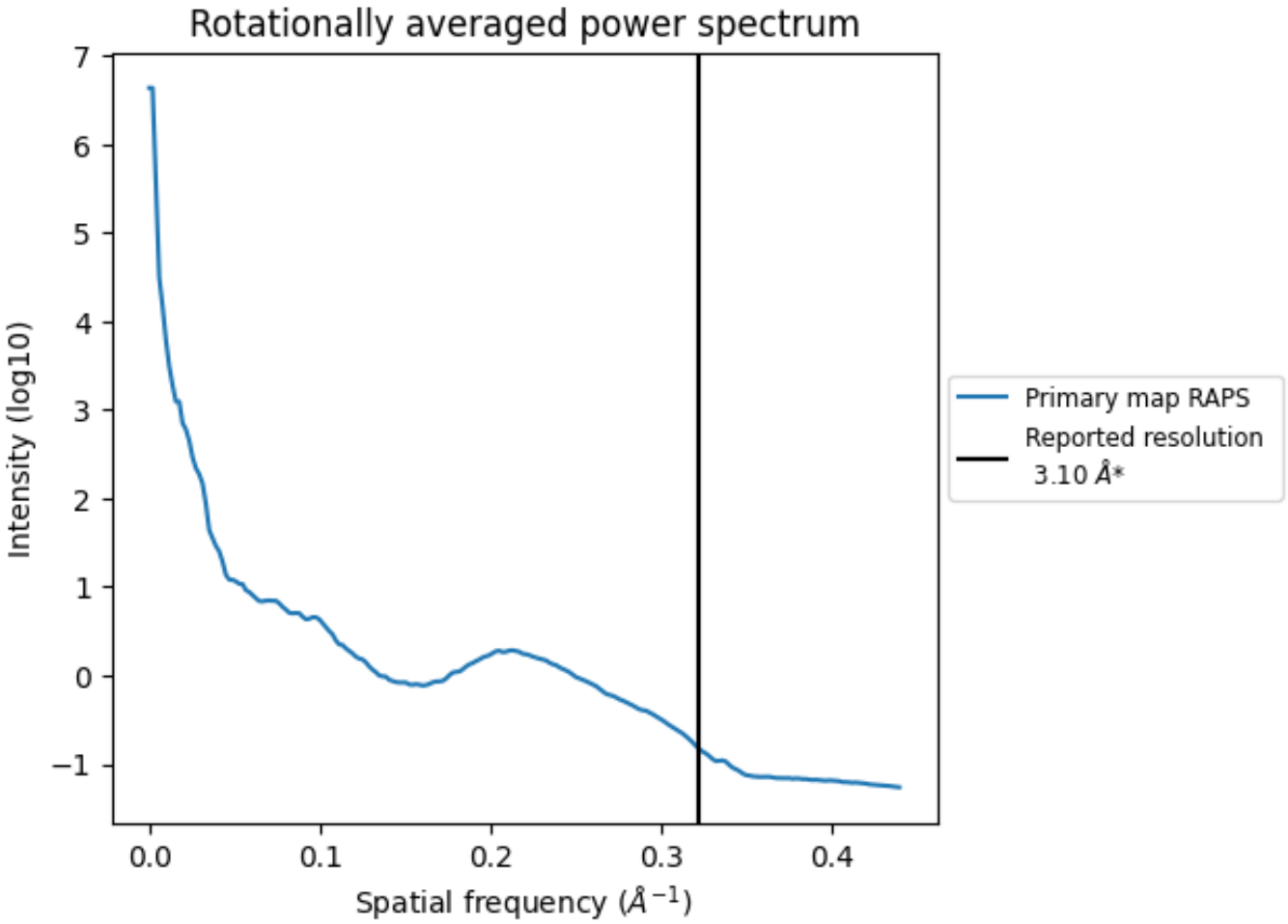
7.2 Volume estimate



The volume at the recommended contour level is 2259 nm^3; this corresponds to an approximate mass of 2041 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)

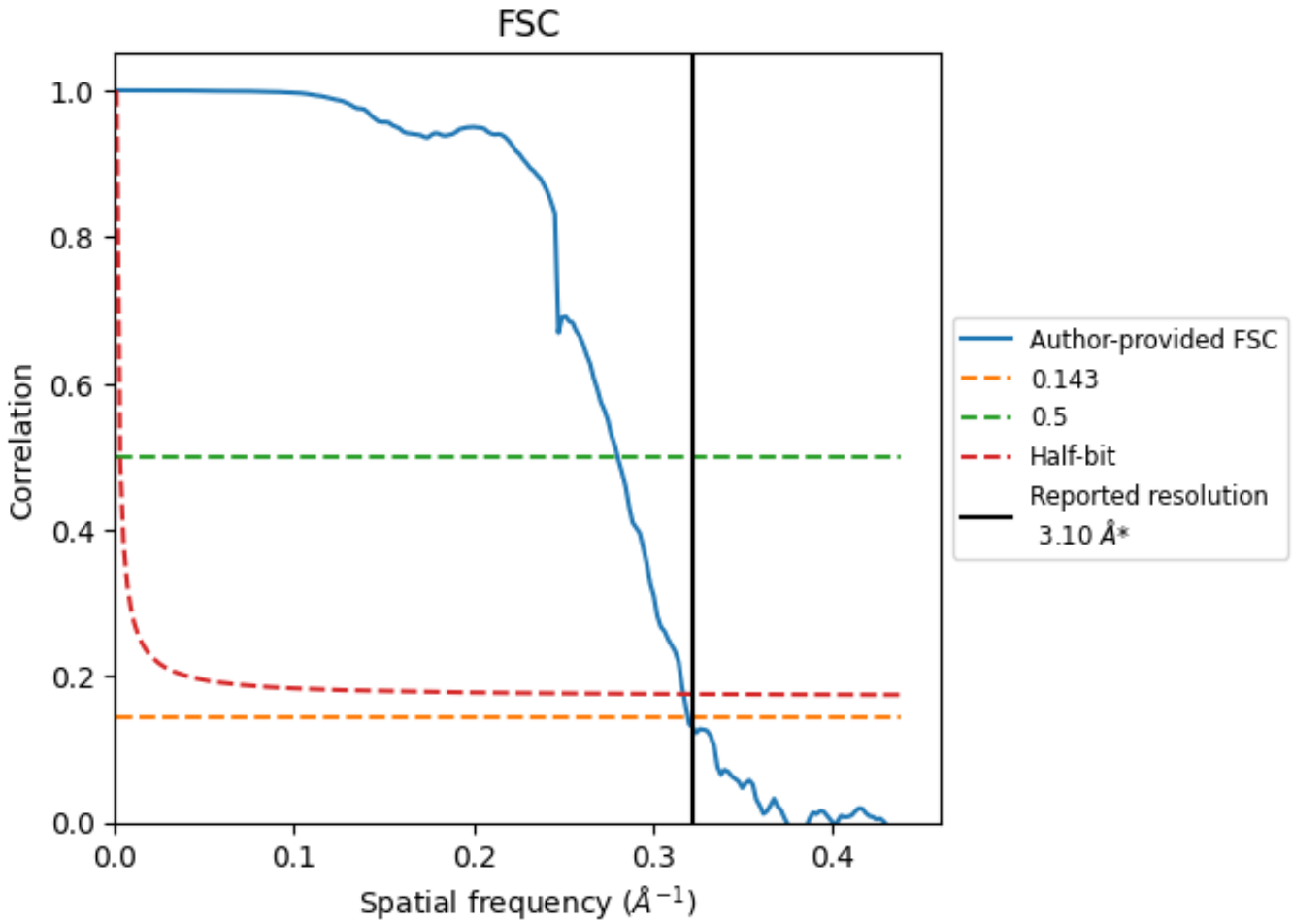


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

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 0.323 Å^{-1}

8.2 Resolution estimates (i)

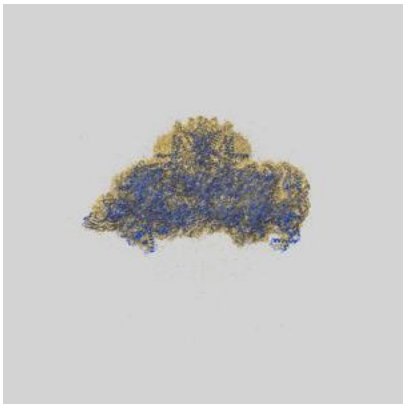
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.13	3.57	3.15
Unmasked-calculated*	-	-	-

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

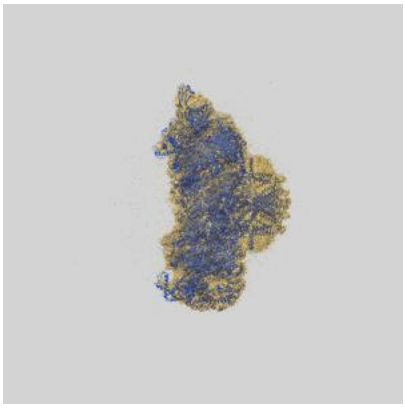
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19468 and PDB model 8RRX. Per-residue inclusion information can be found in section 3 on page 8.

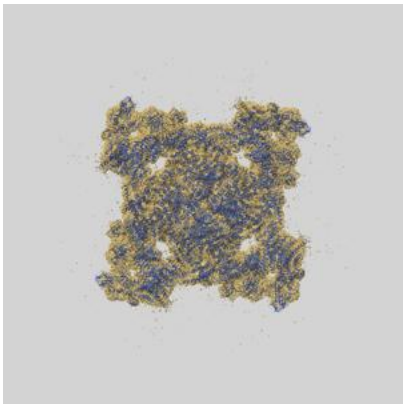
9.1 Map-model overlay



X



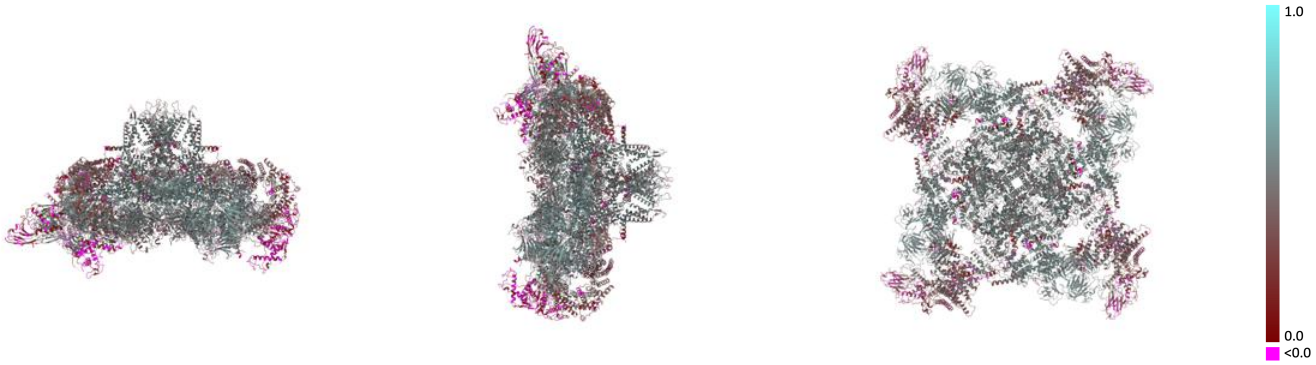
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

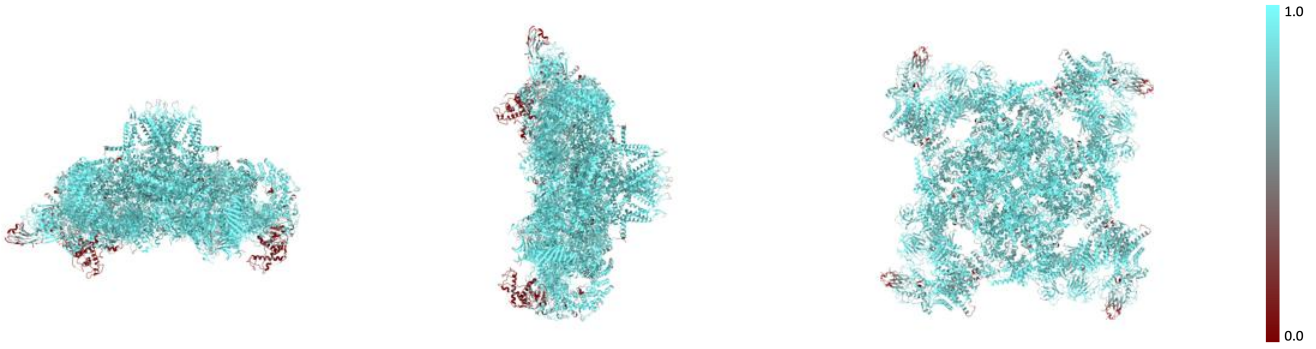
9.2 Q-score mapped to coordinate model (i)



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.

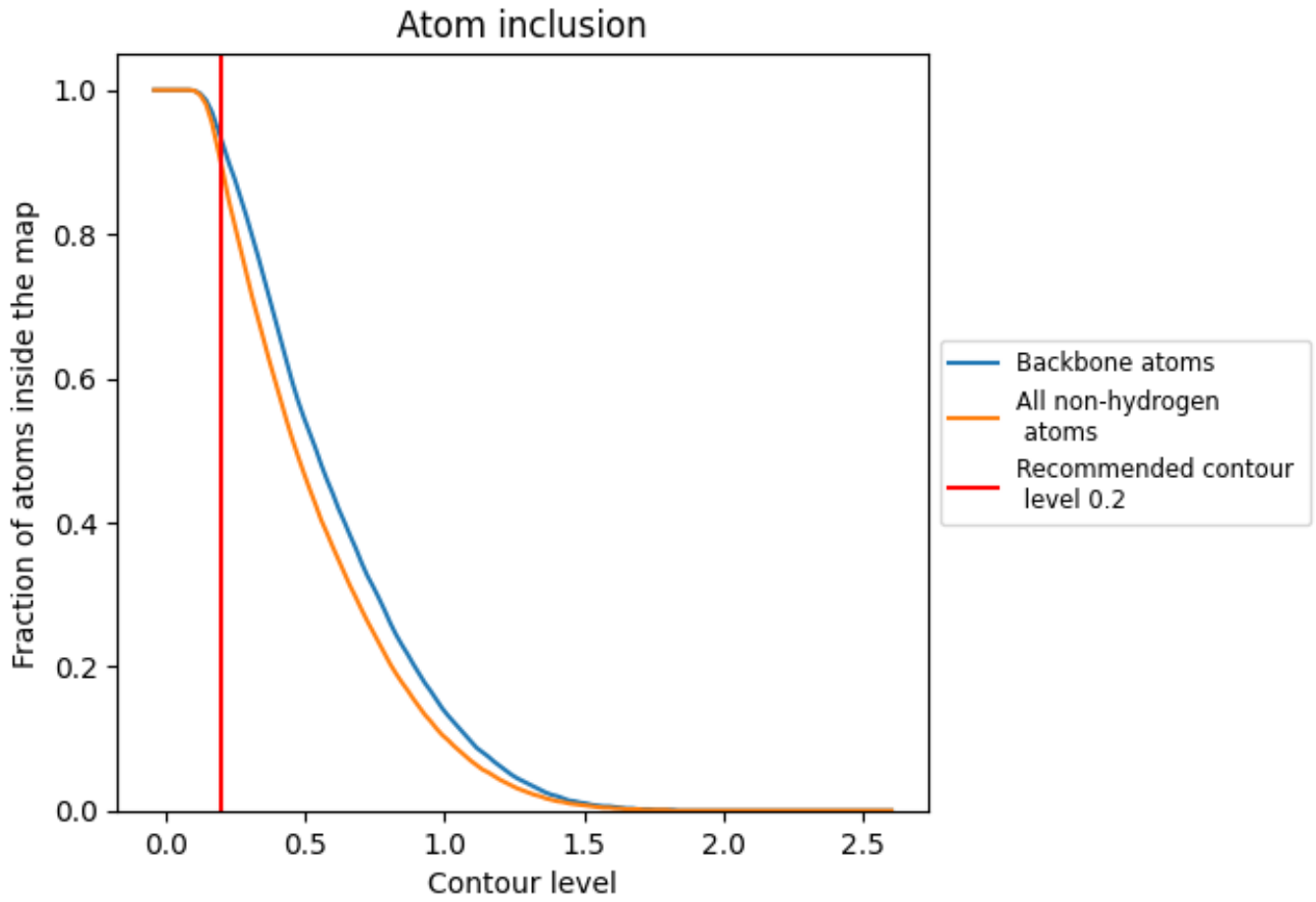
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 90% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8980	0.4240
A	0.9090	0.4300
C	0.4850	0.1360
D	0.9090	0.4300
E	0.4900	0.1350
F	0.9070	0.5000
G	0.9090	0.4300
H	0.9020	0.5020
I	0.9090	0.4300
J	0.9070	0.5040
K	0.4870	0.1370
L	0.9030	0.5030
M	0.4910	0.1370