wwPDB EM Map/Model Validation Report (i)

Oct 17, 2016 – 04:38 PM EDT

PDB ID	:	5T9R
EMDB ID:	:	EMD-8374
Title	:	Structure of rabbit RyR1 (Ca2+-only dataset, class 3)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-09
Resolution	:	5.80 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

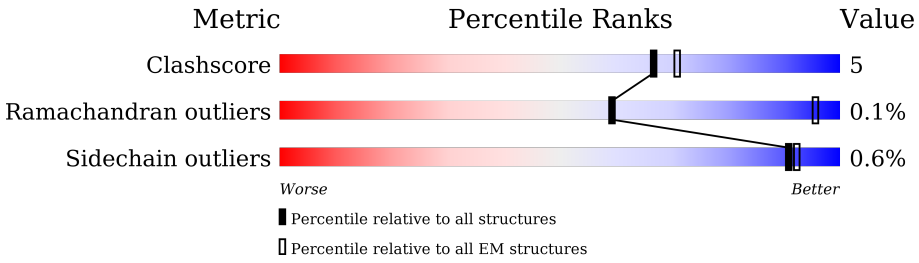
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 5.80 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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%

Mol	Chain	Length	Quality of chain
1	A	108	80% 19% .
1	F	108	80% 19% .
1	H	108	81% 18% .
1	J	108	81% 18% .
2	B	4676	79% 10% 11%
2	E	4676	79% 10% 11%
2	G	4676	79% 10% 11%
2	I	4676	78% 10% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 120756 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	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	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		

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	E	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	I	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	G	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		

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

Mol	Chain	Residues	Atoms		AltConf
3	G	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

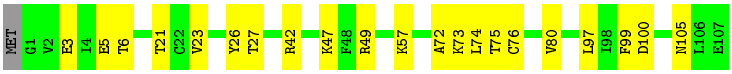
Mol	Chain	Residues	Atoms	AltConf
4	G	1	Total Ca 1 1	0
4	B	1	Total Ca 1 1	0
4	I	1	Total Ca 1 1	0
4	E	1	Total Ca 1 1	0

3 Residue-property plots (i)

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

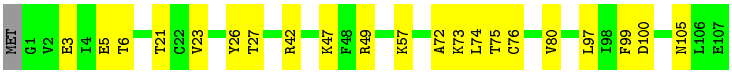
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



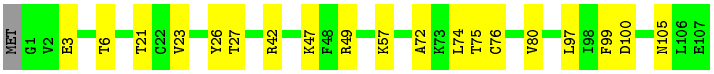
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



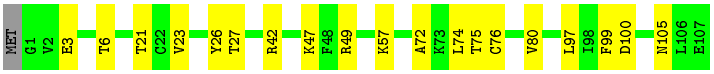
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



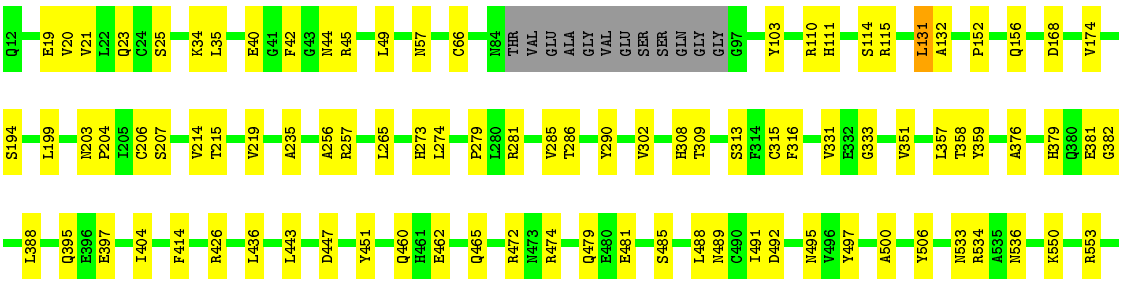
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

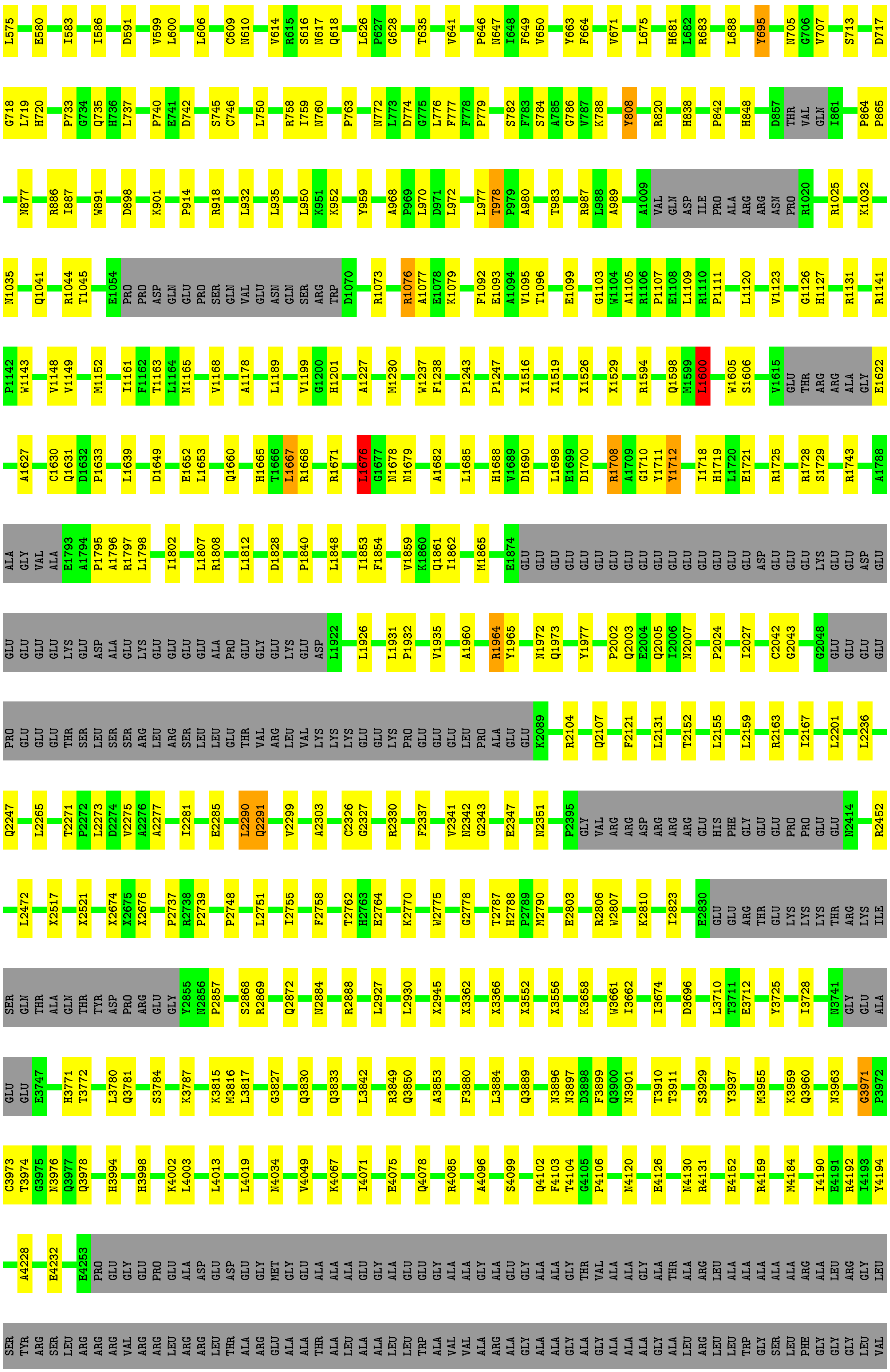
Chain J:

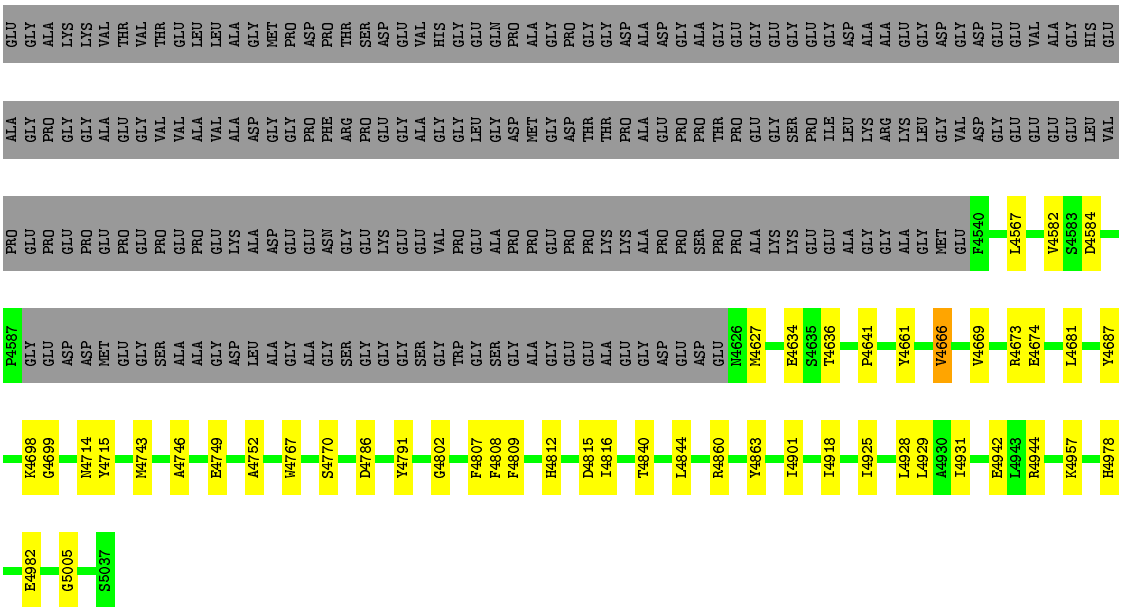


- Molecule 2: Ryanodine receptor 1

Chain B:

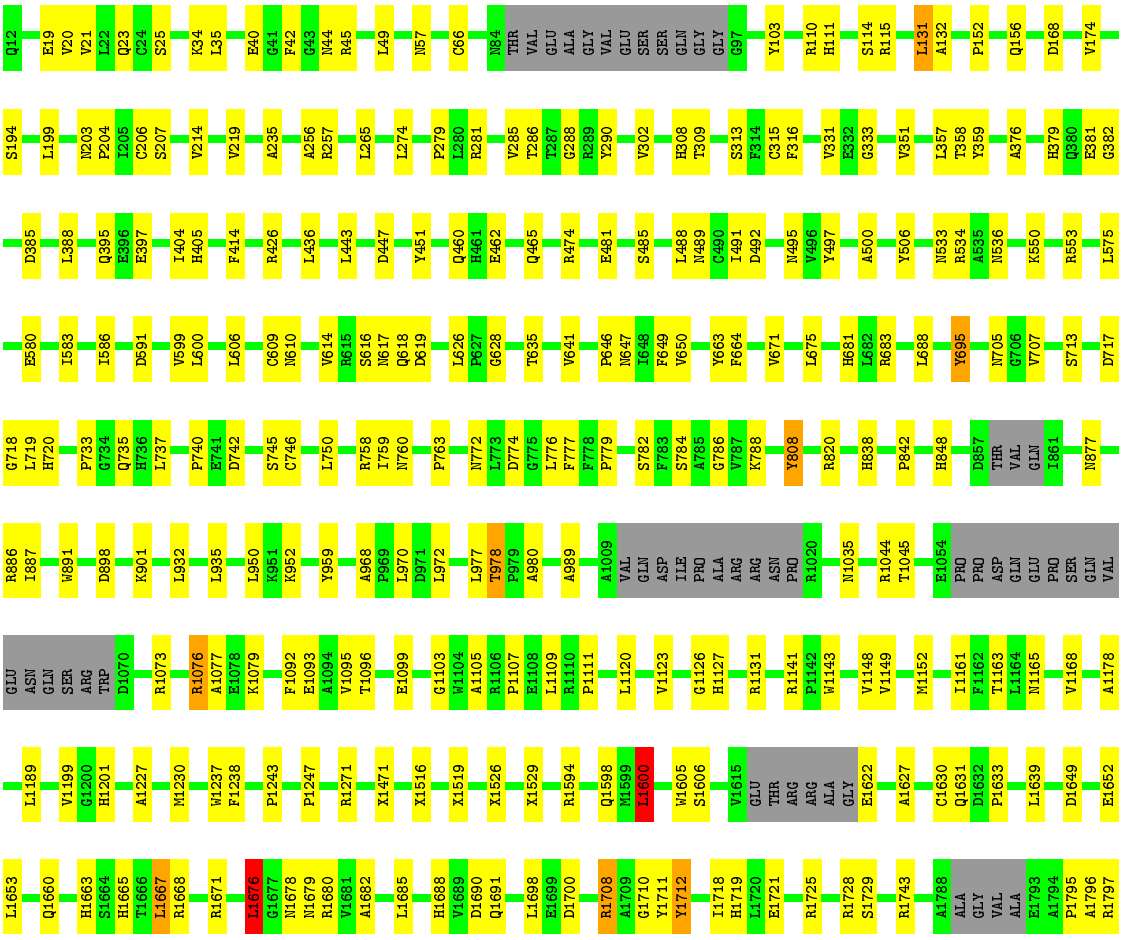


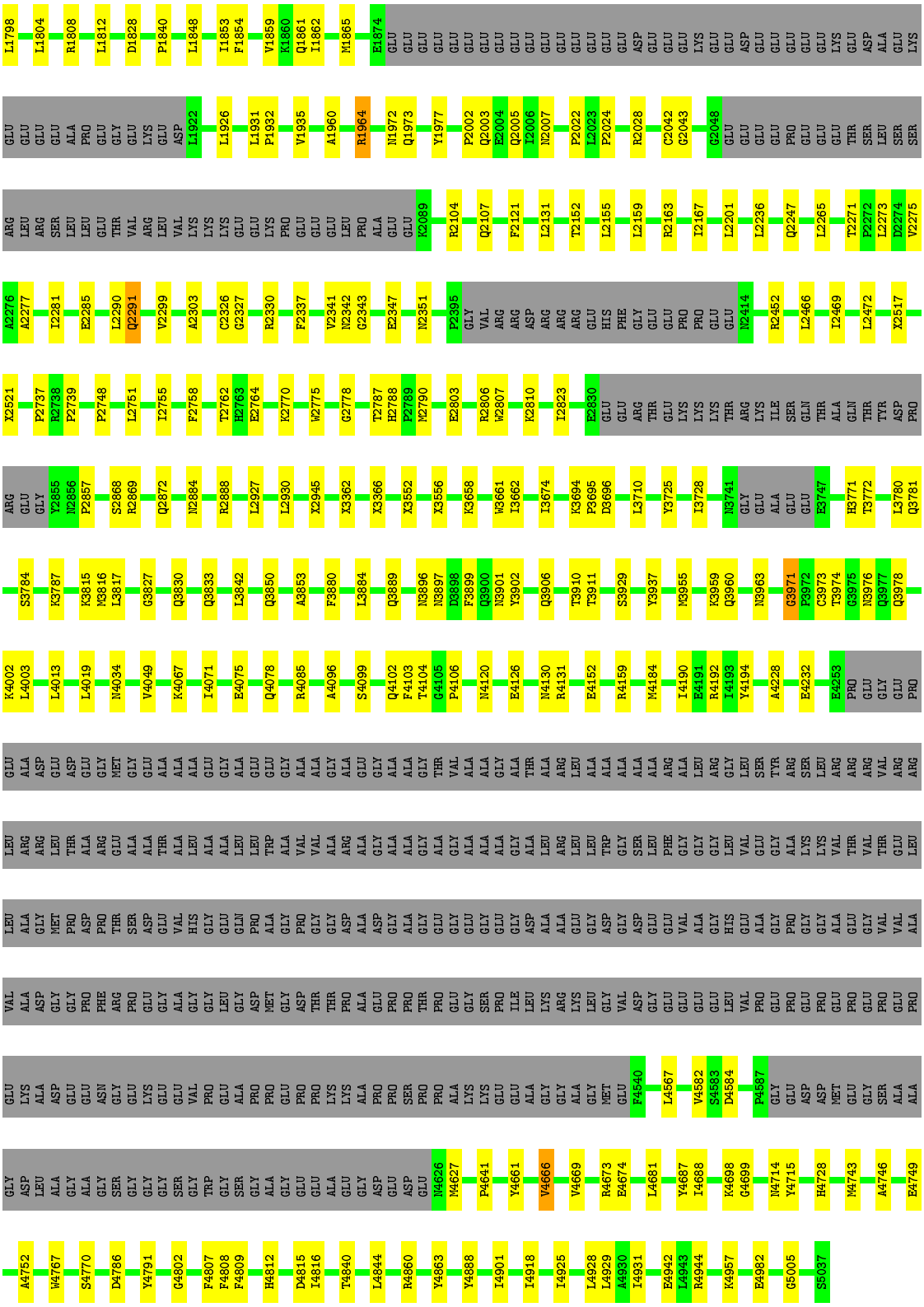

L575 E580 I583 I586 D591 V599 L600 L606 C609 N610 V614 R615 S616 N617 Q618 L626 P627 G628 T635 V641 P646 N647 I648 F649 V650 Y663 F664 V671 L675 H681 L682 R683 L688 Y695 N705 G706 V707 S713 D717
G718 L719 H720 P733 G734 Q735 H736 L737 P740 E741 D742 S745 C746 L750 R758 I759 N760 P763 N772 L773 D774 G775 L776 F777 F778 P779 S782 F783 S784 A785 G786 V787 K788 Y808 R820 H838 P842 H848 D857 THR VAL GLN I861 P864 P865
N877 R886 I887 W891 D898 K901 P914 R918 L932 L935 L950 K951 K952 Y959 A968 P969 L970 D971 L972 L977 T978 P979 A980 T983 R987 L988 A989 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO R1020 R1025 K1032
N1035 Q1041 R1044 T1045 E1054 PRO PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1073 R1076 A1077 E1078 K1079 F1092 E1093 A1094 V1095 T1096 E1099 G1103 W1104 A1105 R1106 P1107 E1108 L1109 R1110 P1111 L1120 V1123 G1126 H1127 R1131 R1141
P1142 W1143 V1148 V1149 M1152 I1161 F1162 T1163 L1164 N1165 V1168 A1178 L1189 V1199 G1200 H1201 A1227 M1230 W1237 F1238 P1243 P1247 X1516 X1519 X1526 X1529 R1594 Q1598 M1599 L1600 W1605 S1606 V1615 GLU THR ARG ARG ALA GLY E1622
A1627 C1630 Q1631 D1632 P1633 L1639 D1649 E1652 L1653 Q1660 H1665 T1666 L1667 R1668 R1671 L1676 G1677 N1678 N1679 A1682 L1685 H1688 V1689 D1690 L1698 E1699 D1700 R1708 A1709 G1710 Y1711 Y1712 I1718 H1719 L1720 E1721 R1725 R1728 S1729 R1743 A1788
ALA GLY VAL ALA E1793 A1794 P1795 A1796 R1797 L1798 I1802 L1807 R1808 L1812 D1828 P1840 L1848 I1853 F1854 V1859 K1860 Q1861 I1862 M1865 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU
GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 L1926 L1931 P1932 V1935 A1960 R1964 Y1965 N1972 Q1973 Y1977 P2002 Q2003 E2004 Q2005 I2006 N2007 P2024 I2027 C2042 G2043 G2048 GLU GLU GLU GLU
PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU LEU PRO ALA GLU GLU K2089 R2104 Q2107 F2121 L2131 T2152 L2155 L2159 R2163 I2167 L2201 L2236
Q2247 L2265 T2271 P2272 L2273 D2274 V2275 A2276 A2277 I2281 E2285 L2290 Q2291 V2299 A2303 C2326 G2327 R2330 F2337 V2341 N2342 G2343 E2347 N2351 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 R2452
L2472 X2517 X2521 X2674 X2675 X2676 P2737 R2738 P2739 P2748 L2751 I2755 F2758 T2762 H2763 E2764 K2770 W2775 G2778 T2787 H2788 P2789 M2790 E2803 R2806 W2807 K2810 I2823 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE
SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2855 N2856 P2857 S2868 R2869 Q2872 N2884 R2888 L2927 L2930 X2945 X3362 X3366 X3552 X3556 K3658 W3661 I3662 I3674 D3696 L3710 T3711 E3712 Y3725 I3728 N3741 GLY GLU ALA
GLU GLU E3747 H3771 T3772 L3780 Q3781 S3784 K3787 K3815 M3816 L3817 G3827 Q3830 Q3833 L3842 R3849 Q3850 A3853 F3880 L3884 Q3889 N3896 N3897 D3898 F3899 Q3900 N3901 T3910 T3911 S3929 Y3937 M3955 K3959 Q3960 N3963 G3971 P3972
C3973 T3974 G3975 N3976 Q3977 Q3978 H3994 H3998 K4002 L4003 L4013 L4019 N4034 V4049 K4067 I4071 E4075 Q4078 R4085 A4096 S4099 Q4102 F4103 T4104 G4105 P4106 N4120 E4126 N4130 R4131 E4152 R4159 M4184 I4190 E4191 R4192 I4193 Y4194
A4228 E4232 E4253 PRO GLU GLY GLU PRO GLU ALA ASP GLU ASP GLU GLY MET GLY GLU ALA ALA ALA GLU GLY ALA GLU GLU GLY ALA ALA GLY ALA GLU GLY ALA ALA GLY THR VAL ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ALA ARG ALA LEU ARG GLY LEU
SER TYR ARG SER LEU ARG ARG VAL ARG ARG LEU ARG ARG LEU THR ALA ARG GLU ALA ALA THR ALA LEU ALA ALA LEU LEU TRP ALA VAL VAL ALA ARG ALA GLY ALA ALA GLY ALA GLY ALA ALA ALA GLY ALA LEU ARG LEU LEU TRP GLY SER LEU PHE GLY GLY GLY LEU VAL



• Molecule 2: Ryanodine receptor 1

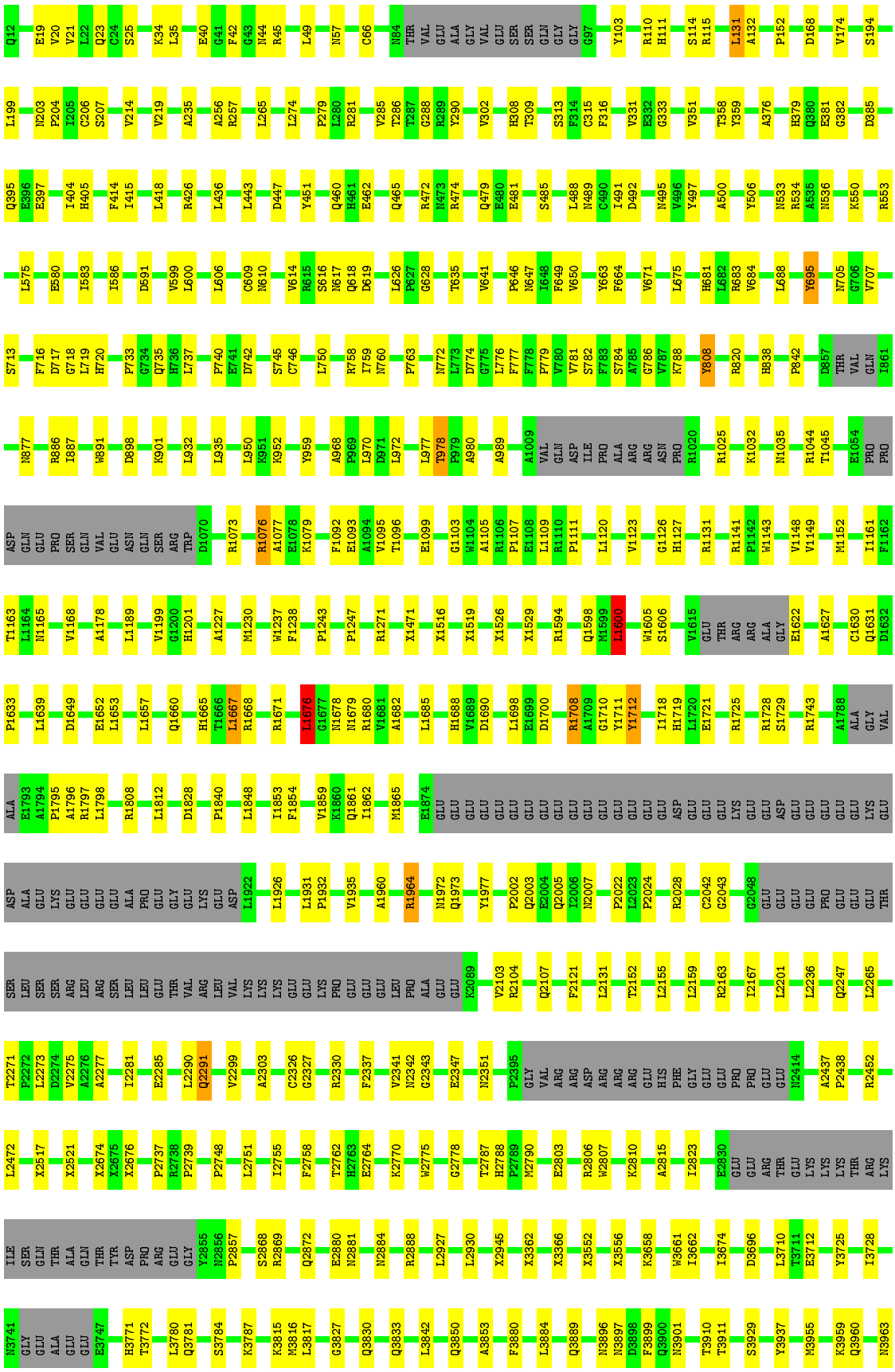
Chain E:

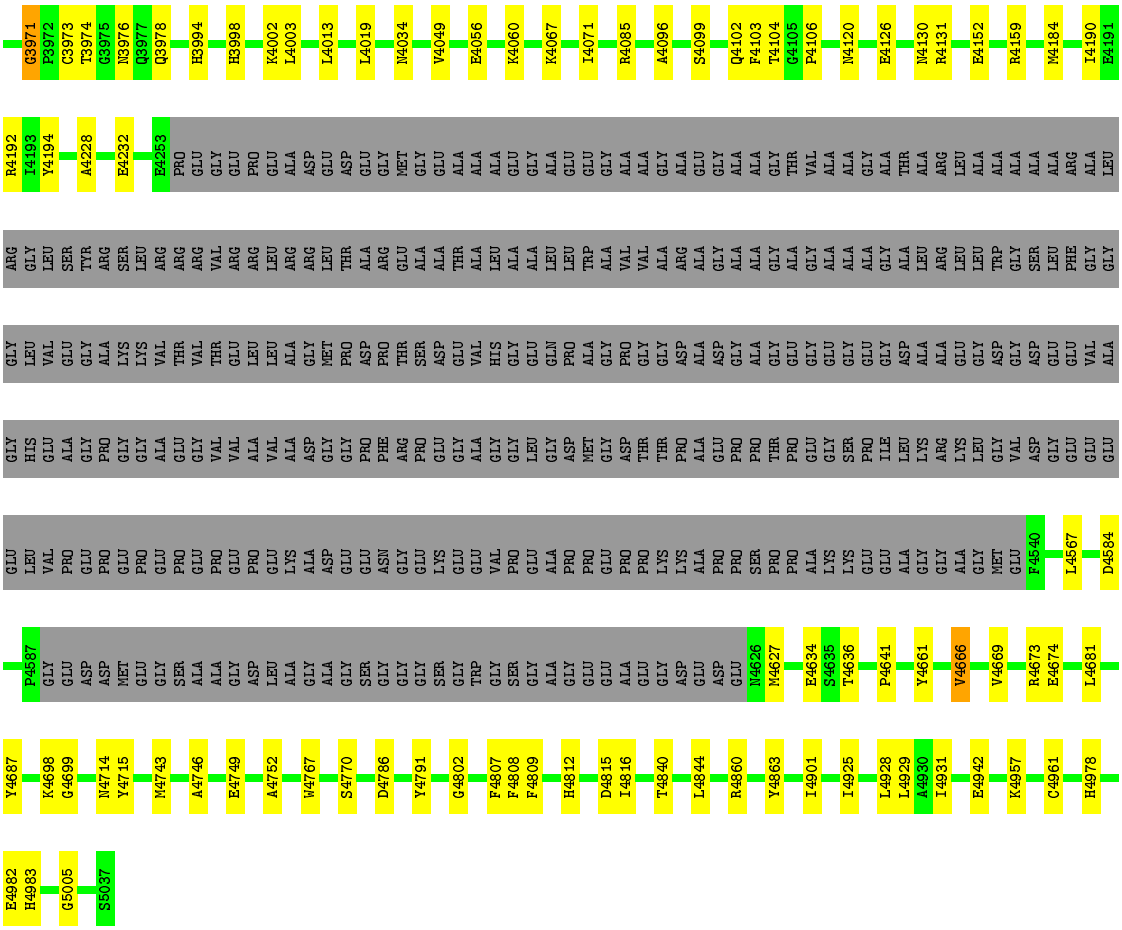




- Molecule 2: Ryanodine receptor 1

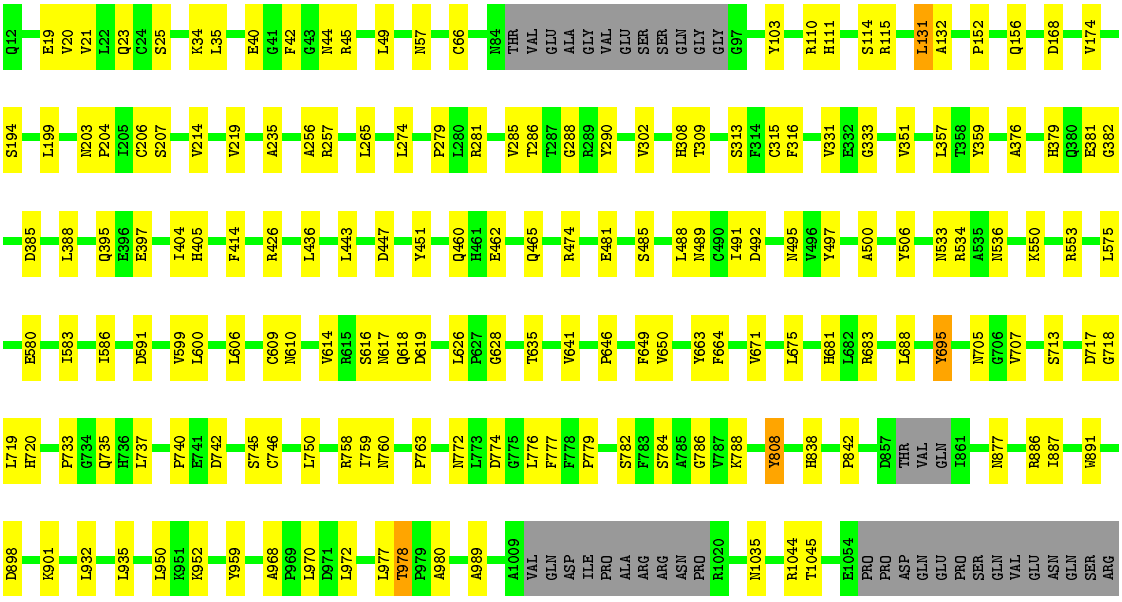
Chain I:

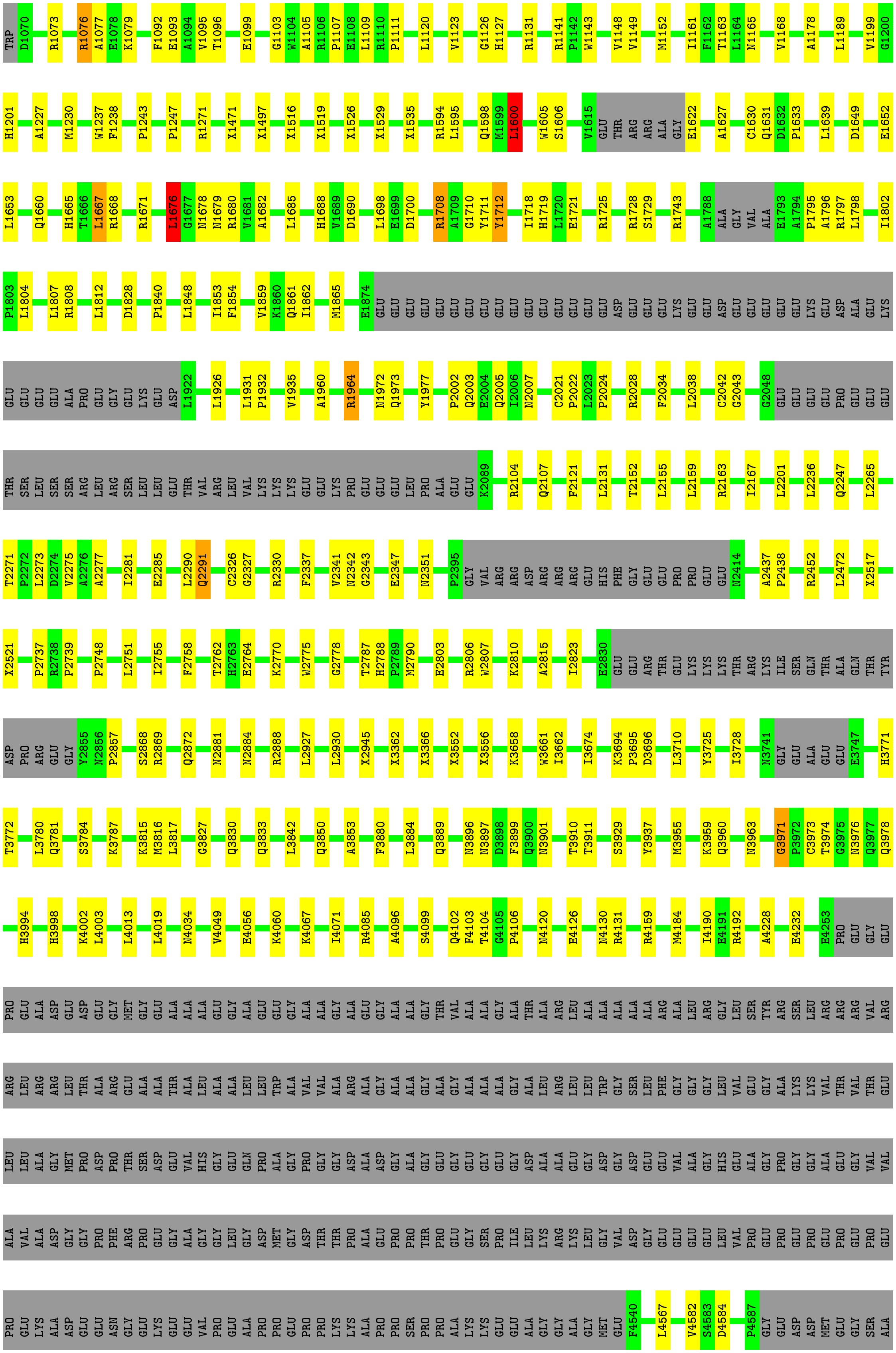


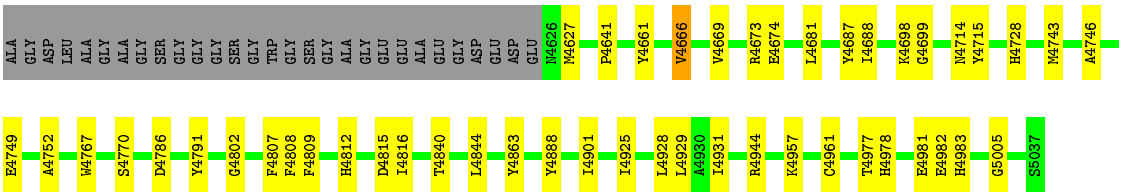


• Molecule 2: Ryanodine receptor 1

Chain G:




TRP D1070 R1073 R1076 A1077 E1078 K1079 F1092 E1093 A1094 V1095 T1096 E1099 G1103 W1104 A1105 R1106 P1107 E1108 L1109 R1110 P1111 L1120 V1123 G1126 H1127 R1131 R1141 P1142 W1143 V1148 V1149 M1152 I1161 F1162 T1163 L1164 N1165 V1168 A1178 L1189 V1199 G1200
H1201 A1227 M1230 W1237 F1238 P1243 P1247 R1271 X1471 X1497 X1516 X1519 X1526 X1529 X1535 R1594 L1595 Q1598 M1599 L1600 W1605 S1606 V1615 GLU THR ARG ARG ALA GLY E1622 A1627 C1630 Q1631 D1632 P1633 L1639 D1649 E1652
L1653 Q1660 H1665 T1666 L1667 R1668 R1671 L1676 G1677 N1678 N1679 R1680 V1681 A1682 L1685 H1688 V1689 D1690 L1698 E1699 D1700 R1708 A1709 G1710 Y1711 Y1712 I1718 H1719 L1720 E1721 R1725 R1728 S1729 R1743 A1788 ALA GLY VAL ALA E1793 A1794 P1795 A1796 R1797 L1798 I1802
P1803 L1804 L1807 R1808 L1812 D1828 P1840 L1848 I1853 F1854 V1859 K1860 Q1861 I1862 M1865 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS
GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 L1926 L1931 P1932 V1935 A1960 R1964 N1972 Q1973 Y1977 P2002 Q2003 E2004 Q2005 I2006 N2007 C2021 P2022 L2023 P2024 R2028 F2034 L2038 C2042 G2043 G2048 GLU GLU GLU GLU PRO GLU GLU GLU
THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU K2089 R2104 Q2107 F2121 L2131 T2152 L2155 L2159 R2163 I2167 L2201 L2236 Q2247 L2265
T2271 P2272 L2273 D2274 V2275 A2276 A2277 I2281 E2285 L2290 Q2291 C2326 G2327 R2330 F2337 V2341 N2342 G2343 E2347 N2351 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 A2437 P2438 R2452 L2472 X2517
X2521 P2737 R2738 P2739 P2748 L2751 I2755 F2758 T2762 H2763 E2764 K2770 W2775 G2778 T2787 H2788 P2789 M2790 E2803 R2806 W2807 K2810 A2815 I2823 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR
ASP PRO ARG GLU GLY Y2855 N2856 P2857 S2868 R2869 Q2872 N2881 N2884 R2888 L2927 L2930 X2945 X3362 X3366 X3552 X3556 K3658 W3661 I3662 I3674 K3694 P3695 D3696 L3710 Y3725 I3728 N3741 GLY GLU ALA GLU GLU E3747 H3771
T3772 L3780 Q3781 S3784 K3787 K3815 M3816 L3817 G3827 Q3830 Q3833 L3842 Q3850 A3853 F3880 L3884 Q3889 N3896 N3897 D3898 F3899 Q3900 N3901 T3910 T3911 S3929 Y3937 M3955 K3959 Q3960 N3963 G3971 P3972 C3973 T3974 G3975 N3976 Q3977 Q3978
H3994 H3998 K4002 L4003 L4013 L4019 N4034 V4049 E4056 K4060 K4067 I4071 R4085 A4096 S4099 Q4102 F4103 T4104 G4105 P4106 N4120 E4126 N4130 R4131 R4159 M4184 I4190 E4191 R4192 A4228 E4232 E4253 PRO GLU GLY GLU
PRO GLU ALA ASP GLU ASP GLU GLY MET GLY GLU ALA ALA GLU GLY ALA GLU GLU GLY ALA ALA GLY ALA GLU GLY ALA ALA GLY THR VAL ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ALA ALA ARG ALA LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG VAL ARG
ARG LEU ARG ARG LEU THR ALA ARG GLU ALA ALA THR ALA LEU ALA ALA LEU LEU TRP ALA VAL VAL ALA ARG ALA GLY ALA ALA GLY ALA GLY ALA ALA ALA GLY ALA LEU ARG LEU LEU TRP GLY SER LEU PHE GLY GLY LEU VAL GLU GLY ALA LYS LYS VAL THR VAL THR GLU
LEU LEU ALA GLY MET PRO ASP PRO THR SER ASP GLU VAL HIS GLY GLU GLN PRO ALA GLY PRO GLY GLY ASP ALA ASP GLY ALA GLY GLU GLY GLU GLY GLU GLY ASP ALA ALA GLU GLY ASP GLY ASP GLU GLU VAL ALA GLY HIS GLU ALA GLY PRO GLY GLY ALA GLU GLY VAL VAL
ALA VAL ALA ASP GLY GLY PRO PHE ARG PRO GLU GLY ALA GLY GLY LEU GLU ASP MET GLY ASP THR THR PRO ALA GLU PRO PRO THR PRO GLU GLY SER PRO ILE LEU LYS ARG LYS ALA GLY VAL ASP GLY GLU GLU GLU GLU LEU VAL PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU
PRO GLU LYS ALA ASP GLU GLU ASN GLY GLU LYS GLU GLU VAL PRO GLU ALA PRO PRO GLU PRO PRO LYS LYS ALA PRO PRO SER PRO PRO ALA LYS LYS GLU GLU ALA GLY GLY ALA GLY MET GLU F4540 L4567 V4582 S4583 D4584 P4587 GLY GLU ASP ASP MET GLU GLY SER ALA


ALA GLY ASP LEU ALA GLY ALA GLY SER GLY GLY GLY SER GLY TRP GLY SER GLY ALA GLY GLU GLU ALA GLU GLY ASP GLU ASP GLU
N4626 M4627 P4641 Y4661 V4666 V4669 R4673 E4674 L4681 Y4687 I4688 K4698 G4699 N4714 Y4715 H4728 M4743 A4746
E4749 A4752 W4767 S4770 D4786 Y4791 G4802 F4807 F4808 F4809 H4812 D4815 I4816 T4840 L4844 Y4863 Y4888 I4901 I4925 L4928 L4929 A4930 I4931 R4944 K4957 C4961 T4977 H4978 E4981 E4982 H4983 G5005 S5037

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	#$\|Z\|$ >2	RMSZ	#$\|Z\|$ >2
1	A	0.29	0/834	0.52	0/1123
1	F	0.29	0/834	0.52	0/1123
1	H	0.29	0/834	0.52	0/1123
1	J	0.29	0/834	0.52	0/1123
2	B	0.30	1/25428 (0.0%)	0.54	8/34534 (0.0%)
2	E	0.29	1/25428 (0.0%)	0.54	8/34534 (0.0%)
2	G	0.30	1/25428 (0.0%)	0.54	8/34534 (0.0%)
2	I	0.30	1/25428 (0.0%)	0.54	8/34534 (0.0%)
All	All	0.29	4/105048 (0.0%)	0.54	32/142628 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	14
2	E	0	14
2	G	0	14
2	I	0	14
All	All	0	56

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	695	TYR	C-N	13.13	1.59	1.34
2	I	695	TYR	C-N	13.12	1.59	1.34
2	B	695	TYR	C-N	13.12	1.59	1.34
2	E	695	TYR	C-N	13.12	1.59	1.34

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	131	LEU	CA-CB-CG	8.21	134.19	115.30
2	I	131	LEU	CA-CB-CG	8.21	134.18	115.30
2	G	131	LEU	CA-CB-CG	8.21	134.17	115.30
2	E	131	LEU	CA-CB-CG	8.20	134.16	115.30
2	E	1600	LEU	CA-CB-CG	7.39	132.30	115.30
2	I	1600	LEU	CA-CB-CG	7.38	132.27	115.30
2	B	1600	LEU	CA-CB-CG	7.37	132.26	115.30
2	G	1600	LEU	CA-CB-CG	7.37	132.26	115.30
2	B	1676	LEU	CA-CB-CG	6.41	130.04	115.30
2	G	1676	LEU	CA-CB-CG	6.40	130.03	115.30
2	E	1676	LEU	CA-CB-CG	6.40	130.03	115.30
2	I	1676	LEU	CA-CB-CG	6.39	130.01	115.30
2	B	2290	LEU	CA-CB-CG	6.08	129.28	115.30
2	E	2290	LEU	CA-CB-CG	6.08	129.27	115.30
2	G	2290	LEU	CA-CB-CG	6.06	129.25	115.30
2	I	2290	LEU	CA-CB-CG	6.06	129.24	115.30
2	I	1667	LEU	CA-CB-CG	5.89	128.84	115.30
2	G	1667	LEU	CA-CB-CG	5.86	128.78	115.30
2	B	1667	LEU	CA-CB-CG	5.85	128.76	115.30
2	E	1667	LEU	CA-CB-CG	5.84	128.74	115.30
2	E	977	LEU	CA-CB-CG	5.77	128.58	115.30
2	I	977	LEU	CA-CB-CG	5.77	128.58	115.30
2	G	977	LEU	CA-CB-CG	5.77	128.58	115.30
2	B	977	LEU	CA-CB-CG	5.75	128.53	115.30
2	G	688	LEU	CA-CB-CG	5.43	127.78	115.30
2	I	688	LEU	CA-CB-CG	5.42	127.76	115.30
2	B	688	LEU	CA-CB-CG	5.41	127.75	115.30
2	E	688	LEU	CA-CB-CG	5.41	127.74	115.30
2	B	2291	GLN	C-N-CA	5.04	134.30	121.70
2	E	2291	GLN	C-N-CA	5.04	134.30	121.70
2	G	2291	GLN	C-N-CA	5.04	134.29	121.70
2	I	2291	GLN	C-N-CA	5.03	134.28	121.70

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1676	LEU	Peptide
2	B	1690	ASP	Peptide
2	B	1712	TYR	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	2291	GLN	Peptide

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Mol	Chain	Res	Type	Group
2	B	2342	ASN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	3971	GLY	Peptide
2	B	4666	VAL	Peptide
2	B	4807	PHE	Peptide
2	B	808	TYR	Peptide
2	E	1676	LEU	Peptide
2	E	1690	ASP	Peptide
2	E	1712	TYR	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	2291	GLN	Peptide
2	E	2342	ASN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	3971	GLY	Peptide
2	E	4666	VAL	Peptide
2	E	4807	PHE	Peptide
2	E	808	TYR	Peptide
2	G	1676	LEU	Peptide
2	G	1690	ASP	Peptide
2	G	1712	TYR	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	2291	GLN	Peptide
2	G	2342	ASN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	3971	GLY	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	808	TYR	Peptide
2	I	1676	LEU	Peptide
2	I	1690	ASP	Peptide
2	I	1712	TYR	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	2291	GLN	Peptide

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Mol	Chain	Res	Type	Group
2	I	2342	ASN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	3971	GLY	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	808	TYR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	11	0
1	F	818	0	824	12	0
1	H	818	0	824	10	0
1	J	818	0	824	10	0
2	B	29369	0	24721	266	0
2	E	29369	0	24720	263	0
2	G	29369	0	24720	262	0
2	I	29369	0	24720	265	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	120756	0	102177	1083	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 5.

All (1083) 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:G:788:LYS:HG2	2:G:1630:CYS:H	1.52	0.74
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.53	0.72
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.53	0.72
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.53	0.72
2:I:379:HIS:HD2	2:I:382:GLY:H	1.41	0.68
2:B:379:HIS:HD2	2:B:382:GLY:H	1.41	0.68
2:I:2452:ARG:NH1	2:G:174:VAL:O	2.28	0.67
2:E:379:HIS:HD2	2:E:382:GLY:H	1.41	0.66
2:E:256:ALA:HB1	2:E:286:THR:HG21	1.79	0.65
2:G:379:HIS:HD2	2:G:382:GLY:H	1.41	0.65
2:B:256:ALA:HB1	2:B:286:THR:HG21	1.78	0.65
2:I:4674:GLU:HG3	2:I:4714:ASN:HB3	1.79	0.65
2:G:256:ALA:HB1	2:G:286:THR:HG21	1.78	0.64
2:E:4674:GLU:HG3	2:E:4714:ASN:HB3	1.79	0.64
2:I:256:ALA:HB1	2:I:286:THR:HG21	1.79	0.64
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.63	0.64
2:B:4674:GLU:HG3	2:B:4714:ASN:HB3	1.79	0.64
2:G:4674:GLU:HG3	2:G:4714:ASN:HB3	1.79	0.63
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.63	0.63
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.81	0.63
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.80	0.63
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.81	0.62
2:E:465:GLN:HG3	2:E:3710:LEU:HB3	1.81	0.62
2:G:465:GLN:HG3	2:G:3710:LEU:HB3	1.81	0.62
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.81	0.62
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.63	0.62
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.63	0.62
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.81	0.62
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.81	0.61
2:I:465:GLN:HG3	2:I:3710:LEU:HB3	1.81	0.61
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.82	0.61
2:B:465:GLN:HG3	2:B:3710:LEU:HB3	1.81	0.61
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.83	0.61
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.81	0.61
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.82	0.61
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.32	0.61
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.81	0.61
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.83	0.61
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.83	0.61
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.83	0.60
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.83	0.60
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.84	0.60
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.83	0.60
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.84	0.60
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.83	0.60
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.84	0.60
2:I:111:HIS:HD2	2:I:114:SER:H	1.49	0.60
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.82	0.60
1:A:27:THR:HB	1:A:100:ASP:HB3	1.84	0.60
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.82	0.60
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.84	0.60
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.83	0.60
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.82	0.60
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.84	0.60
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.82	0.59
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.83	0.59
1:F:27:THR:HB	1:F:100:ASP:HB3	1.84	0.59
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.83	0.59
2:B:111:HIS:HD2	2:B:114:SER:H	1.49	0.59
2:B:4584:ASP:HA	2:B:4627:MET:HA	1.84	0.59
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.84	0.59
1:J:27:THR:HB	1:J:100:ASP:HB3	1.84	0.59
2:B:1077:ALA:HB3	2:B:1189:LEU:HD11	1.85	0.59
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.36	0.59
2:E:650:VAL:HB	2:E:777:PHE:HB2	1.85	0.59
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.68	0.59
2:G:111:HIS:HD2	2:G:114:SER:H	1.49	0.59
2:G:4584:ASP:HA	2:G:4627:MET:HA	1.84	0.59
2:E:111:HIS:HD2	2:E:114:SER:H	1.49	0.59
2:I:650:VAL:HB	2:I:777:PHE:HB2	1.85	0.59
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.83	0.59
2:E:1077:ALA:HB3	2:E:1189:LEU:HD11	1.85	0.59
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.68	0.59
2:G:650:VAL:HB	2:G:777:PHE:HB2	1.85	0.59
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.84	0.59
2:I:4584:ASP:HA	2:I:4627:MET:HA	1.84	0.59
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.36	0.58
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.36	0.58
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.37	0.58
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.86	0.58
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.37	0.58
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.36	0.58
2:B:609:CYS:SG	2:B:610:ASN:N	2.77	0.58
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.84	0.58
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.84	0.58
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.85	0.58
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.86	0.58
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.86	0.58
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.86	0.58
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.68	0.58
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.86	0.58
1:H:27:THR:HB	1:H:100:ASP:HB3	1.84	0.58
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.86	0.58
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.37	0.58
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.36	0.58
2:B:650:VAL:HB	2:B:777:PHE:HB2	1.85	0.58
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.36	0.58
2:G:1077:ALA:HB3	2:G:1189:LEU:HD11	1.85	0.58
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.84	0.58
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.36	0.58
2:I:1077:ALA:HB3	2:I:1189:LEU:HD11	1.85	0.58
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.36	0.58
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.36	0.58
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.84	0.57
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.36	0.57
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.68	0.57
2:E:609:CYS:SG	2:E:610:ASN:N	2.77	0.57
2:I:45:ARG:HG2	2:I:443:LEU:HD21	1.86	0.57
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.36	0.57
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.37	0.57
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.36	0.57
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.37	0.57
2:G:3973:CYS:SG	2:G:3976:ASN:ND2	2.78	0.57
2:I:609:CYS:SG	2:I:610:ASN:N	2.77	0.57
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.37	0.57
2:B:4567:LEU:HD12	2:B:4816:ILE:HD12	1.87	0.57
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.86	0.57
2:E:4584:ASP:HA	2:E:4627:MET:HA	1.84	0.57
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.37	0.57
2:G:45:ARG:HG2	2:G:443:LEU:HD21	1.87	0.57
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.86	0.57
2:G:23:GLN:OE1	2:G:203:ASN:ND2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:23:GLN:OE1	2:I:203:ASN:ND2	2.37	0.57
2:B:3973:CYS:SG	2:B:3976:ASN:ND2	2.78	0.57
1:F:3:GLU:HB2	1:F:75:THR:HB	1.86	0.57
2:G:609:CYS:SG	2:G:610:ASN:N	2.77	0.57
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.38	0.57
2:I:3973:CYS:SG	2:I:3976:ASN:ND2	2.78	0.57
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.32	0.57
2:E:3973:CYS:SG	2:E:3976:ASN:ND2	2.78	0.57
2:E:45:ARG:HG2	2:E:443:LEU:HD21	1.86	0.57
2:E:23:GLN:OE1	2:E:203:ASN:ND2	2.37	0.56
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.78	0.56
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.86	0.56
2:B:23:GLN:OE1	2:B:203:ASN:ND2	2.37	0.56
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.39	0.56
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.87	0.56
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.87	0.56
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.38	0.56
2:E:4567:LEU:HD12	2:E:4816:ILE:HD12	1.86	0.56
2:I:359:TYR:HA	2:I:376:ALA:HA	1.88	0.56
2:B:842:PRO:HD3	2:B:1073:ARG:HG3	1.88	0.56
2:B:359:TYR:HA	2:B:376:ALA:HA	1.88	0.56
2:B:4067:LYS:NZ	2:B:4102:GLN:O	2.39	0.56
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.88	0.56
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.88	0.56
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.86	0.56
1:A:3:GLU:HB2	1:A:75:THR:HB	1.86	0.56
2:B:132:ALA:HA	2:B:194:SER:HB2	1.87	0.56
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.39	0.56
2:E:132:ALA:HA	2:E:194:SER:HB2	1.87	0.56
2:G:1243:PRO:HB2	2:G:1600:LEU:HD22	1.88	0.56
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.39	0.56
2:I:4067:LYS:NZ	2:I:4102:GLN:O	2.39	0.56
2:B:4928:LEU:HD23	2:B:4931:ILE:HD12	1.87	0.56
2:E:1243:PRO:HB2	2:E:1600:LEU:HD22	1.88	0.56
2:G:4928:LEU:HD23	2:G:4931:ILE:HD12	1.87	0.56
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.39	0.56
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.79	0.56
2:I:4567:LEU:HD12	2:I:4816:ILE:HD12	1.87	0.56
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.88	0.56
2:G:842:PRO:HD3	2:G:1073:ARG:HG3	1.88	0.56
2:I:1243:PRO:HB2	2:I:1600:LEU:HD22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:132:ALA:HA	2:G:194:SER:HB2	1.87	0.56
2:G:4567:LEU:HD12	2:G:4816:ILE:HD12	1.87	0.56
2:I:842:PRO:HD3	2:I:1073:ARG:HG3	1.88	0.56
2:I:132:ALA:HA	2:I:194:SER:HB2	1.87	0.56
2:B:1243:PRO:HB2	2:B:1600:LEU:HD22	1.88	0.55
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.39	0.55
2:B:45:ARG:HG2	2:B:443:LEU:HD21	1.86	0.55
2:E:842:PRO:HD3	2:E:1073:ARG:HG3	1.88	0.55
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.87	0.55
2:E:4067:LYS:NZ	2:E:4102:GLN:O	2.39	0.55
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.88	0.55
1:H:3:GLU:HB2	1:H:75:THR:HB	1.86	0.55
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.88	0.55
1:F:26:TYR:OH	1:F:42:ARG:NH2	2.40	0.55
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.88	0.55
1:J:3:GLU:HB2	1:J:75:THR:HB	1.86	0.55
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.31	0.55
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	1.88	0.55
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.89	0.55
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.86	0.55
2:I:385:ASP:HB2	2:G:156:GLN:HE21	1.71	0.55
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.88	0.55
2:E:4928:LEU:HD23	2:E:4931:ILE:HD12	1.87	0.55
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.88	0.55
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.39	0.55
2:G:359:TYR:HA	2:G:376:ALA:HA	1.88	0.55
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.87	0.55
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.89	0.55
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.89	0.55
2:E:359:TYR:HA	2:E:376:ALA:HA	1.88	0.55
1:H:26:TYR:OH	1:H:42:ARG:NH2	2.40	0.55
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	1.88	0.55
2:B:614:VAL:HG22	2:B:616:SER:H	1.72	0.55
2:E:614:VAL:HG22	2:E:616:SER:H	1.72	0.55
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.88	0.55
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.78	0.55
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.89	0.55
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.88	0.55
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.88	0.55
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.40	0.55
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.38	0.55
2:G:4067:LYS:NZ	2:G:4102:GLN:O	2.39	0.55
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.89	0.55
1:J:26:TYR:OH	1:J:42:ARG:NH2	2.40	0.55
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	1.88	0.55
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.40	0.55
2:I:614:VAL:HG22	2:I:616:SER:H	1.72	0.55
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.88	0.54
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.89	0.54
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.89	0.54
2:E:695:TYR:OH	2:E:1073:ARG:NH1	2.41	0.54
2:G:614:VAL:HG22	2:G:616:SER:H	1.72	0.54
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.88	0.54
1:A:26:TYR:OH	1:A:42:ARG:NH2	2.40	0.54
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.89	0.54
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	1.88	0.54
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.89	0.54
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.39	0.54
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.89	0.54
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.31	0.54
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.40	0.54
2:E:618:GLN:OE1	2:E:1678:ASN:ND2	2.41	0.54
2:G:331:VAL:HG12	2:G:333:GLY:H	1.72	0.54
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.89	0.54
2:B:1865:MET:HB3	2:B:1926:LEU:HB2	1.90	0.54
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.79	0.54
2:I:1808:ARG:NH1	2:I:1853:ILE:O	2.40	0.54
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.89	0.54
2:E:2758:PHE:O	2:E:2762:THR:N	2.41	0.54
2:I:618:GLN:OE1	2:I:1678:ASN:ND2	2.41	0.54
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.73	0.54
2:B:2758:PHE:O	2:B:2762:THR:N	2.41	0.54
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.73	0.54
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.90	0.54
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.40	0.54
2:B:2452:ARG:NH1	2:I:174:VAL:O	2.41	0.54
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.90	0.54
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.89	0.54
2:B:618:GLN:OE1	2:B:1678:ASN:ND2	2.41	0.54
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.90	0.54
2:G:1865:MET:HB3	2:G:1926:LEU:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4928:LEU:HD23	2:I:4931:ILE:HD12	1.87	0.54
2:E:1865:MET:HB3	2:E:1926:LEU:HB2	1.90	0.54
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.73	0.54
2:I:331:VAL:HG12	2:I:333:GLY:H	1.72	0.54
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.39	0.54
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.89	0.53
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.42	0.53
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.74	0.53
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.88	0.53
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.89	0.53
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.89	0.53
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.91	0.53
2:I:695:TYR:OH	2:I:1073:ARG:NH1	2.41	0.53
2:B:591:ASP:O	2:B:1594:ARG:NH2	2.42	0.53
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.89	0.53
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.42	0.53
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.90	0.53
2:B:1973:GLN:O	2:B:1977:TYR:N	2.42	0.53
2:B:331:VAL:HG12	2:B:333:GLY:H	1.72	0.53
2:G:591:ASP:O	2:G:1594:ARG:NH2	2.42	0.53
2:I:1865:MET:HB3	2:I:1926:LEU:HB2	1.90	0.53
2:I:591:ASP:O	2:I:1594:ARG:NH2	2.42	0.53
2:B:485:SER:O	2:B:489:ASN:N	2.39	0.53
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.90	0.53
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.42	0.53
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.91	0.53
2:E:591:ASP:O	2:E:1594:ARG:NH2	2.42	0.53
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.91	0.53
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.90	0.53
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.90	0.53
2:I:4925:ILE:HA	2:I:4929:LEU:HD13	1.91	0.53
2:B:4925:ILE:HA	2:B:4929:LEU:HD13	1.91	0.53
2:G:675:LEU:HD11	2:G:1633:PRO:HB3	1.91	0.53
2:G:1808:ARG:HD3	2:G:1853:ILE:HG22	1.91	0.53
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.42	0.53
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.90	0.53
2:B:1808:ARG:NH1	2:B:1853:ILE:O	2.41	0.53
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	1.91	0.53
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.91	0.53
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.90	0.53
2:E:331:VAL:HG12	2:E:333:GLY:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1622:GLU:N	2:G:1627:ALA:O	2.42	0.53
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.74	0.53
2:G:4925:ILE:HA	2:G:4929:LEU:HD13	1.91	0.53
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.90	0.53
2:G:618:GLN:OE1	2:G:1678:ASN:ND2	2.41	0.53
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.42	0.53
2:B:695:TYR:OH	2:B:1073:ARG:NH1	2.41	0.53
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.42	0.53
2:E:4925:ILE:HA	2:E:4929:LEU:HD13	1.91	0.53
2:E:675:LEU:HD11	2:E:1633:PRO:HB3	1.91	0.53
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.38	0.53
2:I:2868:SER:O	2:I:2872:GLN:N	2.42	0.53
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.42	0.53
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.90	0.52
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.90	0.52
2:B:1622:GLU:N	2:B:1627:ALA:O	2.42	0.52
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.74	0.52
2:E:1973:GLN:O	2:E:1977:TYR:N	2.42	0.52
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	1.91	0.52
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.91	0.52
2:B:675:LEU:HD11	2:B:1633:PRO:HB3	1.91	0.52
2:E:1808:ARG:HD3	2:E:1853:ILE:HG22	1.91	0.52
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.73	0.52
2:G:168:ASP:HB3	2:G:199:LEU:HD22	1.91	0.52
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.38	0.52
2:E:1622:GLU:N	2:E:1627:ALA:O	2.42	0.52
2:E:168:ASP:HB3	2:E:199:LEU:HD22	1.91	0.52
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	1.91	0.52
2:B:168:ASP:HB3	2:B:199:LEU:HD22	1.91	0.52
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.91	0.52
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.91	0.52
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.91	0.52
2:E:683:ARG:NH1	2:E:707:VAL:O	2.40	0.52
1:H:6:THR:HA	1:H:72:ALA:HA	1.91	0.52
2:I:675:LEU:HD11	2:I:1633:PRO:HB3	1.91	0.52
2:B:1808:ARG:HD3	2:B:1853:ILE:HG22	1.91	0.52
2:G:1808:ARG:NH1	2:G:1853:ILE:O	2.40	0.52
2:B:156:GLN:HE21	2:E:385:ASP:HB2	1.74	0.52
2:G:695:TYR:OH	2:G:1073:ARG:NH1	2.41	0.52
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.74	0.52
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1622:GLU:N	2:I:1627:ALA:O	2.42	0.52
1:A:6:THR:HA	1:A:72:ALA:HA	1.91	0.52
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.42	0.52
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.42	0.52
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.75	0.52
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.42	0.52
2:I:2758:PHE:O	2:I:2762:THR:N	2.41	0.52
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.75	0.51
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.38	0.51
2:I:168:ASP:HB3	2:I:199:LEU:HD22	1.91	0.51
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.42	0.51
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	1.91	0.51
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.75	0.51
2:G:2758:PHE:O	2:G:2762:THR:N	2.41	0.51
2:I:1808:ARG:HD3	2:I:1853:ILE:HG22	1.91	0.51
2:I:1973:GLN:O	2:I:1977:TYR:N	2.42	0.51
2:B:2764:GLU:HG3	2:B:2857:PRO:HB2	1.93	0.51
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.93	0.51
2:E:2764:GLU:HG3	2:E:2857:PRO:HB2	1.93	0.51
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.92	0.51
2:G:4749:GLU:HA	2:G:4752:ALA:HB3	1.93	0.51
2:I:315:CYS:SG	2:I:316:PHE:N	2.84	0.51
2:I:898:ASP:HB3	2:I:901:LYS:HB2	1.93	0.51
1:F:6:THR:HA	1:F:72:ALA:HA	1.91	0.51
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.75	0.51
2:I:4749:GLU:HA	2:I:4752:ALA:HB3	1.93	0.51
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.93	0.51
2:B:898:ASP:HB3	2:B:901:LYS:HB2	1.93	0.51
2:E:451:TYR:O	2:E:474:ARG:NH1	2.44	0.51
2:G:2868:SER:O	2:G:2872:GLN:N	2.42	0.51
2:G:315:CYS:SG	2:G:316:PHE:N	2.84	0.51
2:G:40:GLU:HB3	2:G:44:ASN:HB3	1.93	0.51
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.44	0.51
2:B:4749:GLU:HA	2:B:4752:ALA:HB3	1.93	0.51
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.44	0.51
2:E:40:GLU:HB3	2:E:44:ASN:HB3	1.93	0.51
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.93	0.51
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.29	0.51
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.75	0.51
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.29	0.51
2:B:1653:LEU:HB3	2:B:1660:GLN:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.44	0.51
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.29	0.51
2:G:1973:GLN:O	2:G:1977:TYR:N	2.42	0.51
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.92	0.51
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.44	0.51
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.75	0.51
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.75	0.51
2:E:1653:LEU:HB3	2:E:1660:GLN:HB2	1.92	0.51
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.29	0.51
2:B:315:CYS:SG	2:B:316:PHE:N	2.84	0.50
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.42	0.50
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.44	0.50
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.93	0.50
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.76	0.50
2:E:4942:GLU:HG3	2:G:4944:ARG:HH11	1.77	0.50
2:G:683:ARG:NH1	2:G:707:VAL:O	2.40	0.50
2:I:40:GLU:HB3	2:I:44:ASN:HB3	1.93	0.50
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.94	0.50
2:E:898:ASP:HB3	2:E:901:LYS:HB2	1.93	0.50
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.94	0.50
1:J:6:THR:HA	1:J:72:ALA:HA	1.91	0.50
2:E:1808:ARG:NH1	2:E:1853:ILE:O	2.40	0.50
2:E:2868:SER:O	2:E:2872:GLN:N	2.42	0.50
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.94	0.50
2:I:2347:GLU:O	2:I:2351:ASN:N	2.45	0.50
2:I:451:TYR:O	2:I:474:ARG:NH1	2.44	0.50
2:B:683:ARG:NH1	2:B:707:VAL:O	2.40	0.50
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.92	0.50
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.76	0.50
2:E:2347:GLU:O	2:E:2351:ASN:N	2.45	0.50
2:E:4749:GLU:HA	2:E:4752:ALA:HB3	1.93	0.50
2:G:1653:LEU:HB3	2:G:1660:GLN:HB2	1.92	0.50
2:G:2347:GLU:O	2:G:2351:ASN:N	2.45	0.50
2:G:451:TYR:O	2:G:474:ARG:NH1	2.44	0.50
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.76	0.50
2:B:40:GLU:HB3	2:B:44:ASN:HB3	1.93	0.50
2:E:315:CYS:SG	2:E:316:PHE:N	2.84	0.50
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.76	0.50
2:I:20:VAL:HG12	2:I:204:PRO:HA	1.93	0.50
2:I:2778:GLY:HA3	2:I:2787:THR:HB	1.94	0.50
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.94	0.50
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.94	0.50
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.93	0.50
2:I:1099:GLU:OE2	2:I:1127:HIS:ND1	2.38	0.50
2:I:2764:GLU:HG3	2:I:2857:PRO:HB2	1.93	0.50
2:B:2868:SER:O	2:B:2872:GLN:N	2.42	0.50
2:G:898:ASP:HB3	2:G:901:LYS:HB2	1.93	0.50
2:I:1729:SER:HB3	2:I:2163:ARG:HH11	1.77	0.50
2:I:488:LEU:O	2:I:492:ASP:N	2.43	0.50
2:B:1729:SER:HB3	2:B:2163:ARG:HH11	1.77	0.49
2:B:3974:THR:O	2:B:3978:GLN:N	2.40	0.49
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.94	0.49
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.94	0.49
2:G:649:PHE:HB3	2:G:776:LEU:HD13	1.94	0.49
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.44	0.49
2:B:20:VAL:HG12	2:B:204:PRO:HA	1.93	0.49
2:B:2347:GLU:O	2:B:2351:ASN:N	2.45	0.49
2:I:1653:LEU:HB3	2:I:1660:GLN:HB2	1.92	0.49
2:I:649:PHE:HB3	2:I:776:LEU:HD13	1.94	0.49
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.44	0.49
2:G:1247:PRO:HA	2:G:1598:GLN:HA	1.95	0.49
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.94	0.49
2:B:3827:GLY:HA2	2:B:3830:GLN:HE21	1.78	0.49
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.44	0.49
2:G:2764:GLU:HG3	2:G:2857:PRO:HB2	1.93	0.49
2:I:1025:ARG:O	2:I:1032:LYS:NZ	2.44	0.49
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.94	0.49
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.92	0.49
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.93	0.49
2:E:1247:PRO:HA	2:E:1598:GLN:HA	1.95	0.49
2:E:1729:SER:HB3	2:E:2163:ARG:HH11	1.77	0.49
2:E:156:GLN:HE21	2:G:385:ASP:HB2	1.78	0.49
2:I:3780:LEU:HD11	2:I:3816:MET:HG3	1.95	0.49
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.93	0.49
2:B:451:TYR:O	2:B:474:ARG:NH1	2.44	0.49
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.94	0.49
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.94	0.49
1:F:76:CYS:HB2	1:F:97:LEU:HB2	1.95	0.49
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.95	0.49
2:G:1729:SER:HB3	2:G:2163:ARG:HH11	1.77	0.49
2:G:20:VAL:HG12	2:G:204:PRO:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3780:LEU:HD11	2:G:3816:MET:HG3	1.95	0.49
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.95	0.49
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	1.95	0.49
2:B:649:PHE:HB3	2:B:776:LEU:HD13	1.94	0.49
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.46	0.49
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.94	0.49
2:I:1247:PRO:HA	2:I:1598:GLN:HA	1.95	0.49
2:I:485:SER:O	2:I:489:ASN:N	2.39	0.49
2:E:20:VAL:HG12	2:E:204:PRO:HA	1.93	0.49
2:E:2778:GLY:HA3	2:E:2787:THR:HB	1.94	0.49
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.95	0.49
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.94	0.49
2:I:3897:ASN:O	2:I:3901:ASN:ND2	2.46	0.49
2:B:1099:GLU:OE2	2:B:1127:HIS:ND1	2.38	0.48
2:B:3897:ASN:O	2:B:3901:ASN:ND2	2.46	0.48
2:E:1516:UNK:N	2:E:1529:UNK:O	2.46	0.48
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	1.95	0.48
2:E:3897:ASN:O	2:E:3901:ASN:ND2	2.46	0.48
2:G:1093:GLU:OE1	2:G:1201:HIS:NE2	2.44	0.48
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.94	0.48
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.95	0.48
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.95	0.48
2:G:2778:GLY:HA3	2:G:2787:THR:HB	1.94	0.48
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.95	0.48
1:A:76:CYS:HB2	1:A:97:LEU:HB2	1.95	0.48
2:B:1516:UNK:N	2:B:1529:UNK:O	2.46	0.48
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	1.95	0.48
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.46	0.48
2:E:580:GLU:HG2	2:E:583:ILE:HD11	1.96	0.48
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.95	0.48
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	1.95	0.48
2:G:3827:GLY:HA2	2:G:3830:GLN:HE21	1.78	0.48
2:I:111:HIS:CD2	2:I:114:SER:H	2.31	0.48
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.94	0.48
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.46	0.48
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.96	0.48
2:G:3974:THR:O	2:G:3978:GLN:N	2.40	0.48
2:G:4184:MET:HB3	2:G:4190:ILE:HD13	1.96	0.48
2:G:580:GLU:HG2	2:G:583:ILE:HD11	1.95	0.48
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.94	0.48
2:B:1247:PRO:HA	2:B:1598:GLN:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2778:GLY:HA3	2:B:2787:THR:HB	1.94	0.48
2:B:580:GLU:HG2	2:B:583:ILE:HD11	1.96	0.48
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	1.95	0.48
2:E:4184:MET:HB3	2:E:4190:ILE:HD13	1.96	0.48
2:E:649:PHE:HB3	2:E:776:LEU:HD13	1.94	0.48
2:G:1516:UNK:N	2:G:1529:UNK:O	2.46	0.48
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.46	0.48
2:G:485:SER:O	2:G:489:ASN:N	2.39	0.48
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.46	0.48
2:I:21:VAL:HG12	2:I:66:CYS:HA	1.96	0.48
2:I:395:GLN:HG3	2:I:397:GLU:H	1.79	0.48
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.95	0.48
2:E:3827:GLY:HA2	2:E:3830:GLN:HE21	1.78	0.48
2:I:3974:THR:O	2:I:3978:GLN:N	2.40	0.48
2:I:580:GLU:HG2	2:I:583:ILE:HD11	1.96	0.48
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.46	0.48
2:B:395:GLN:HG3	2:B:397:GLU:H	1.79	0.48
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.96	0.48
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	1.95	0.48
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.38	0.48
2:I:3827:GLY:HA2	2:I:3830:GLN:HE21	1.78	0.48
2:B:1848:LEU:HD22	2:B:1853:ILE:HG13	1.95	0.48
2:G:111:HIS:CD2	2:G:114:SER:H	2.31	0.48
2:I:1676:LEU:HD23	2:I:2167:ILE:HG23	1.96	0.48
2:E:1848:LEU:HD22	2:E:1853:ILE:HG13	1.96	0.48
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.38	0.48
2:E:606:LEU:O	2:E:617:ASN:ND2	2.47	0.48
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.96	0.48
2:G:206:CYS:SG	2:G:207:SER:N	2.87	0.48
2:G:395:GLN:HG3	2:G:397:GLU:H	1.79	0.48
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.46	0.48
2:I:4184:MET:HB3	2:I:4190:ILE:HD13	1.96	0.48
1:J:76:CYS:HB2	1:J:97:LEU:HB2	1.95	0.48
2:G:21:VAL:HG12	2:G:66:CYS:HA	1.96	0.48
2:G:3897:ASN:O	2:G:3901:ASN:ND2	2.46	0.48
2:B:1093:GLU:OE1	2:B:1201:HIS:NE2	2.44	0.47
2:E:772:ASN:ND2	2:E:774:ASP:OD2	2.47	0.47
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.46	0.47
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.46	0.47
2:B:206:CYS:SG	2:B:207:SER:N	2.87	0.47
2:B:4944:ARG:HH11	2:I:4942:GLU:HG3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4192:ARG:HH12	2:B:4982:GLU:HG2	1.80	0.47
2:B:606:LEU:O	2:B:617:ASN:ND2	2.47	0.47
2:E:1093:GLU:OE1	2:E:1201:HIS:NE2	2.44	0.47
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.95	0.47
2:E:1972:ASN:HD21	2:E:2024:PRO:HB3	1.79	0.47
2:E:395:GLN:HG3	2:E:397:GLU:H	1.79	0.47
2:G:606:LEU:O	2:G:617:ASN:ND2	2.47	0.47
2:I:1972:ASN:HD21	2:I:2024:PRO:HB3	1.79	0.47
2:I:206:CYS:SG	2:I:207:SER:N	2.87	0.47
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.42	0.47
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.95	0.47
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.95	0.47
2:E:1676:LEU:HD23	2:E:2167:ILE:HG23	1.96	0.47
2:G:1848:LEU:HD22	2:G:1853:ILE:HG13	1.96	0.47
2:G:1972:ASN:HD21	2:G:2024:PRO:HB3	1.79	0.47
2:I:1093:GLU:OE1	2:I:1201:HIS:NE2	2.44	0.47
2:I:1516:UNK:N	2:I:1529:UNK:O	2.47	0.47
2:I:606:LEU:O	2:I:617:ASN:ND2	2.47	0.47
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.95	0.47
2:B:1965:TYR:OH	2:B:2027:ILE:O	2.28	0.47
2:E:2265:LEU:HD22	2:E:2330:ARG:HB3	1.97	0.47
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.96	0.47
2:E:4767:TRP:HE3	2:E:4770:SER:HB2	1.79	0.47
2:E:488:LEU:O	2:E:492:ASP:N	2.43	0.47
2:G:265:LEU:HD12	2:G:279:PRO:HB2	1.97	0.47
2:I:1848:LEU:HD22	2:I:1853:ILE:HG13	1.95	0.47
2:I:772:ASN:ND2	2:I:774:ASP:OD2	2.47	0.47
2:B:1676:LEU:HD23	2:B:2167:ILE:HG23	1.96	0.47
2:B:4184:MET:HB3	2:B:4190:ILE:HD13	1.96	0.47
2:E:206:CYS:SG	2:E:207:SER:N	2.87	0.47
2:E:265:LEU:HD12	2:E:279:PRO:HB2	1.97	0.47
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.96	0.47
2:G:2265:LEU:HD22	2:G:2330:ARG:HB3	1.97	0.47
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.96	0.47
2:I:2327:GLY:HA2	2:I:2330:ARG:HD3	1.96	0.47
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.96	0.47
2:G:4192:ARG:HH12	2:G:4982:GLU:HG2	1.80	0.47
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.96	0.47
2:G:978:THR:HB	2:G:980:ALA:H	1.80	0.47
1:H:76:CYS:HB2	1:H:97:LEU:HB2	1.95	0.47
2:B:3842:LEU:O	2:B:3929:SER:OG	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.96	0.47
2:G:2327:GLY:HA2	2:G:2330:ARG:HD3	1.96	0.47
2:I:1238:PHE:O	2:I:1606:SER:N	2.48	0.47
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.50	0.47
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.50	0.47
2:E:4192:ARG:HH12	2:E:4982:GLU:HG2	1.80	0.47
2:I:1131:ARG:NH1	2:I:1178:ALA:O	2.48	0.47
2:B:21:VAL:HG12	2:B:66:CYS:HA	1.96	0.47
2:E:647:ASN:ND2	2:E:820:ARG:O	2.39	0.47
2:G:1131:ARG:NH1	2:G:1178:ALA:O	2.48	0.47
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.96	0.47
2:I:2265:LEU:HD22	2:I:2330:ARG:HB3	1.97	0.47
2:I:4192:ARG:HH12	2:I:4982:GLU:HG2	1.80	0.47
2:B:174:VAL:O	2:E:2452:ARG:NH1	2.48	0.47
2:B:1972:ASN:HD21	2:B:2024:PRO:HB3	1.79	0.47
2:B:2265:LEU:HD22	2:B:2330:ARG:HB3	1.97	0.47
2:E:21:VAL:HG12	2:E:66:CYS:HA	1.96	0.47
2:G:733:PRO:HD2	2:G:763:PRO:HD2	1.97	0.47
2:G:772:ASN:ND2	2:G:774:ASP:OD2	2.47	0.47
2:E:733:PRO:HD2	2:E:763:PRO:HD2	1.97	0.47
2:E:978:THR:HB	2:E:980:ALA:H	1.80	0.47
2:G:1676:LEU:HD23	2:G:2167:ILE:HG23	1.96	0.47
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.50	0.47
2:I:3842:LEU:O	2:I:3929:SER:OG	2.33	0.47
2:B:309:THR:O	2:B:313:SER:OG	2.33	0.46
2:E:309:THR:O	2:E:313:SER:OG	2.33	0.46
2:E:3842:LEU:O	2:E:3929:SER:OG	2.33	0.46
2:G:1099:GLU:OE2	2:G:1127:HIS:ND1	2.38	0.46
2:G:3889:GLN:HE22	2:G:3963:ASN:HB3	1.81	0.46
2:G:488:LEU:O	2:G:492:ASP:N	2.43	0.46
2:I:265:LEU:HD12	2:I:279:PRO:HB2	1.97	0.46
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.96	0.46
2:B:772:ASN:ND2	2:B:774:ASP:OD2	2.47	0.46
2:E:485:SER:O	2:E:489:ASN:N	2.39	0.46
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.46	0.46
2:G:309:THR:O	2:G:313:SER:OG	2.33	0.46
2:G:4767:TRP:HE3	2:G:4770:SER:HB2	1.79	0.46
2:I:4767:TRP:HE3	2:I:4770:SER:HB2	1.79	0.46
2:I:733:PRO:HD2	2:I:763:PRO:HD2	1.97	0.46
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.96	0.46
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	1.97	0.46
2:E:1131:ARG:NH1	2:E:1178:ALA:O	2.48	0.46
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.81	0.46
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.96	0.46
2:B:265:LEU:HD12	2:B:279:PRO:HB2	1.97	0.46
2:B:4661:TYR:OH	2:B:4786:ASP:OD2	2.34	0.46
2:E:2327:GLY:HA2	2:E:2330:ARG:HD3	1.96	0.46
2:E:3889:GLN:HE22	2:E:3963:ASN:HB3	1.81	0.46
2:E:4096:ALA:HA	2:E:4099:SER:HB2	1.98	0.46
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.80	0.46
2:G:4661:TYR:OH	2:G:4786:ASP:OD2	2.34	0.46
2:B:4681:LEU:HD21	2:B:4687:TYR:HD2	1.80	0.46
2:I:1163:THR:HA	2:I:1168:VAL:HA	1.97	0.46
2:I:4228:ALA:O	2:I:4232:GLU:N	2.48	0.46
2:B:111:HIS:CD2	2:B:114:SER:H	2.31	0.46
2:B:733:PRO:HD2	2:B:763:PRO:HD2	1.97	0.46
2:E:1163:THR:HA	2:E:1168:VAL:HA	1.97	0.46
2:E:877:ASN:HD22	2:E:1045:THR:HG23	1.80	0.46
2:G:4681:LEU:HD21	2:G:4687:TYR:HD2	1.80	0.46
2:I:309:THR:O	2:I:313:SER:OG	2.33	0.46
2:I:4096:ALA:HA	2:I:4099:SER:HB2	1.98	0.46
2:I:4681:LEU:HD21	2:I:4687:TYR:HD2	1.80	0.46
2:B:2327:GLY:HA2	2:B:2330:ARG:HD3	1.96	0.46
2:B:4228:ALA:O	2:B:4232:GLU:N	2.48	0.46
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.81	0.46
2:G:4096:ALA:HA	2:G:4099:SER:HB2	1.98	0.46
2:G:495:ASN:HD21	2:G:550:LYS:HG3	1.81	0.46
2:B:1131:ARG:NH1	2:B:1178:ALA:O	2.48	0.46
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	1.97	0.46
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.96	0.46
2:B:4767:TRP:HE3	2:B:4770:SER:HB2	1.79	0.46
2:B:488:LEU:O	2:B:492:ASP:N	2.43	0.46
2:E:174:VAL:O	2:G:2452:ARG:NH1	2.49	0.46
2:G:2869:ARG:HH12	2:G:2945:UNK:C	2.29	0.46
2:G:3842:LEU:O	2:G:3929:SER:OG	2.33	0.46
2:I:4978:HIS:ND1	2:I:4982:GLU:OE1	2.44	0.46
2:I:495:ASN:HD21	2:I:550:LYS:HG3	1.81	0.46
2:B:3889:GLN:HE22	2:B:3963:ASN:HB3	1.81	0.46
2:B:4096:ALA:HA	2:B:4099:SER:HB2	1.98	0.46
2:I:683:ARG:NH1	2:I:707:VAL:O	2.40	0.46
2:I:3889:GLN:HE22	2:I:3963:ASN:HB3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4661:TYR:OH	2:I:4786:ASP:OD2	2.34	0.46
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.80	0.46
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.51	0.45
2:G:1796:ALA:HB1	2:G:1797:ARG:HH21	1.81	0.45
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.80	0.45
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.46	0.45
2:E:4661:TYR:OH	2:E:4786:ASP:OD2	2.34	0.45
2:G:2152:THR:HA	2:G:2155:LEU:HB2	1.99	0.45
2:I:379:HIS:CD2	2:I:381:GLU:H	2.35	0.45
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.47	0.45
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.51	0.45
2:E:111:HIS:CD2	2:E:114:SER:H	2.31	0.45
2:E:4228:ALA:O	2:E:4232:GLU:N	2.48	0.45
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	1.97	0.45
2:B:1163:THR:HA	2:B:1168:VAL:HA	1.97	0.45
2:B:647:ASN:ND2	2:B:820:ARG:O	2.39	0.45
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.51	0.45
2:I:978:THR:HB	2:I:980:ALA:H	1.80	0.45
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.99	0.45
2:E:4681:LEU:HD21	2:E:4687:TYR:HD2	1.80	0.45
2:G:379:HIS:CD2	2:G:381:GLU:H	2.35	0.45
2:G:4228:ALA:O	2:G:4232:GLU:N	2.48	0.45
2:I:4071:ILE:HG13	2:I:4103:PHE:HZ	1.81	0.45
2:E:4071:ILE:HG13	2:E:4103:PHE:HZ	1.81	0.45
2:E:495:ASN:HD21	2:E:550:LYS:HG3	1.81	0.45
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.98	0.45
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.99	0.45
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.81	0.45
2:E:1808:ARG:HD2	2:E:1854:PHE:HA	1.99	0.45
2:E:3974:THR:O	2:E:3978:GLN:N	2.40	0.45
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.99	0.45
2:G:4071:ILE:HG13	2:G:4103:PHE:HZ	1.81	0.45
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.98	0.45
2:B:495:ASN:HD21	2:B:550:LYS:HG3	1.81	0.45
2:B:978:THR:HB	2:B:980:ALA:H	1.80	0.45
2:E:3971:GLY:H	2:E:5005:GLY:HA3	1.82	0.45
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.99	0.45
2:B:2869:ARG:HH12	2:B:2945:UNK:C	2.29	0.45
2:B:4863:TYR:HA	2:B:4901:ILE:HG23	1.98	0.45
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.99	0.45
2:E:379:HIS:CD2	2:E:381:GLU:H	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	1.97	0.45
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.51	0.45
2:G:3880:PHE:O	2:G:3884:LEU:N	2.50	0.45
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.98	0.45
2:I:2152:THR:HA	2:I:2155:LEU:HB2	1.99	0.45
2:B:1096:THR:HG23	2:B:1199:VAL:HG22	1.99	0.45
2:B:379:HIS:CD2	2:B:381:GLU:H	2.35	0.45
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.98	0.45
2:G:1163:THR:HA	2:G:1168:VAL:HA	1.97	0.45
2:G:1808:ARG:HD2	2:G:1854:PHE:HA	1.99	0.45
2:I:1808:ARG:HD2	2:I:1854:PHE:HA	1.99	0.45
2:I:4863:TYR:HA	2:I:4901:ILE:HG23	1.98	0.45
2:B:1796:ALA:HB1	2:B:1797:ARG:HH21	1.82	0.44
2:B:3880:PHE:O	2:B:3884:LEU:N	2.50	0.44
2:B:4071:ILE:HG13	2:B:4103:PHE:HZ	1.81	0.44
2:B:4978:HIS:ND1	2:B:4982:GLU:OE1	2.44	0.44
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.99	0.44
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.98	0.44
2:B:2152:THR:HA	2:B:2155:LEU:HB2	1.99	0.44
2:E:3880:PHE:O	2:E:3884:LEU:N	2.50	0.44
2:I:1708:ARG:HG2	2:I:1711:TYR:CE2	2.53	0.44
2:I:750:LEU:HD21	2:I:777:PHE:HE2	1.82	0.44
2:B:1708:ARG:HG2	2:B:1711:TYR:CE2	2.52	0.44
2:B:313:SER:HB3	2:B:351:VAL:HB	1.99	0.44
2:B:742:ASP:HA	2:B:760:ASN:HD21	1.83	0.44
2:E:404:ILE:HG21	2:E:481:GLU:HG3	2.00	0.44
2:G:1096:THR:HG23	2:G:1199:VAL:HG22	2.00	0.44
2:I:1096:THR:HG23	2:I:1199:VAL:HG22	1.99	0.44
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.81	0.44
2:I:742:ASP:HA	2:I:760:ASN:HD21	1.82	0.44
2:I:647:ASN:ND2	2:I:820:ARG:O	2.39	0.44
2:E:1096:THR:HG23	2:E:1199:VAL:HG22	2.00	0.44
2:E:742:ASP:HA	2:E:760:ASN:HD21	1.82	0.44
2:G:1238:PHE:O	2:G:1606:SER:N	2.48	0.44
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.99	0.44
2:G:404:ILE:HG21	2:G:481:GLU:HG3	2.00	0.44
2:I:1865:MET:SD	2:I:1865:MET:N	2.91	0.44
2:B:1865:MET:SD	2:B:1865:MET:N	2.91	0.44
2:E:1238:PHE:O	2:E:1606:SER:N	2.48	0.44
2:E:1796:ALA:HB1	2:E:1797:ARG:HH21	1.81	0.44
2:E:750:LEU:HD21	2:E:777:PHE:HE2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1708:ARG:HG2	2:G:1711:TYR:CE2	2.53	0.44
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	2.00	0.44
2:B:1808:ARG:HD2	2:B:1854:PHE:HA	1.99	0.44
2:B:4791:TYR:OH	2:B:4815:ASP:O	2.36	0.44
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.47	0.44
2:E:1708:ARG:HG2	2:E:1711:TYR:CE2	2.53	0.44
2:E:1848:LEU:HB3	2:E:1853:ILE:HB	2.00	0.44
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	2.00	0.44
2:E:313:SER:HB3	2:E:351:VAL:HB	1.99	0.44
2:E:4863:TYR:HA	2:E:4901:ILE:HG23	1.98	0.44
2:G:742:ASP:HA	2:G:760:ASN:HD21	1.82	0.44
2:I:3880:PHE:O	2:I:3884:LEU:N	2.50	0.44
2:I:1796:ALA:HB1	2:I:1797:ARG:HH21	1.81	0.44
2:I:4791:TYR:OH	2:I:4815:ASP:O	2.36	0.44
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	2.00	0.44
2:G:3971:GLY:H	2:G:5005:GLY:HA3	1.82	0.44
2:G:750:LEU:HD21	2:G:777:PHE:HE2	1.82	0.44
2:I:1848:LEU:HB3	2:I:1853:ILE:HB	1.99	0.44
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.44	0.44
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	2.00	0.44
2:G:1865:MET:N	2:G:1865:MET:SD	2.91	0.44
2:G:290:TYR:O	2:G:302:VAL:N	2.51	0.44
2:G:4863:TYR:HA	2:G:4901:ILE:HG23	1.98	0.44
2:I:1639:LEU:HD12	2:I:1653:LEU:HD21	2.00	0.44
2:I:313:SER:HB3	2:I:351:VAL:HB	1.99	0.44
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	2.00	0.44
2:I:460:GLN:HG2	2:I:462:GLU:H	1.83	0.44
2:B:3971:GLY:H	2:B:5005:GLY:HA3	1.82	0.43
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	2.00	0.43
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	2.00	0.43
2:E:2152:THR:HA	2:E:2155:LEU:HB2	1.99	0.43
2:G:619:ASP:OD1	2:G:1680:ARG:NH1	2.42	0.43
2:I:3674:ILE:HD11	2:I:3728:ILE:HG22	2.00	0.43
2:E:1679:ASN:HA	2:E:1682:ALA:HB3	2.01	0.43
2:E:290:TYR:O	2:E:302:VAL:N	2.51	0.43
2:I:1271:ARG:HA	2:I:1471:UNK:HA	2.00	0.43
2:I:404:ILE:HG21	2:I:481:GLU:HG3	2.00	0.43
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	2.00	0.43
2:G:1679:ASN:HA	2:G:1682:ALA:HB3	2.01	0.43
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.99	0.43
2:B:404:ILE:HG21	2:B:481:GLU:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1865:MET:SD	2:E:1865:MET:N	2.91	0.43
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.99	0.43
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	2.00	0.43
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	2.00	0.43
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	2.00	0.43
2:E:460:GLN:HG2	2:E:462:GLU:H	1.83	0.43
2:G:2281:ILE:HG23	2:G:2341:VAL:HG11	2.00	0.43
2:I:2247:GLN:NE2	2:I:2285:GLU:OE2	2.52	0.43
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.99	0.43
2:B:1848:LEU:HB3	2:B:1853:ILE:HB	1.99	0.43
2:B:3696:ASP:OD2	2:B:3771:HIS:NE2	2.52	0.43
2:B:4003:LEU:HB2	2:B:4013:LEU:HD13	2.01	0.43
2:B:750:LEU:HD21	2:B:777:PHE:HE2	1.82	0.43
2:E:2281:ILE:HG23	2:E:2341:VAL:HG11	2.00	0.43
2:E:4791:TYR:OH	2:E:4815:ASP:O	2.36	0.43
2:G:1639:LEU:HD12	2:G:1653:LEU:HD21	2.00	0.43
2:I:290:TYR:O	2:I:302:VAL:N	2.51	0.43
2:I:35:LEU:HD13	2:I:49:LEU:HD13	2.01	0.43
2:E:2299:VAL:O	2:E:2303:ALA:N	2.52	0.43
2:G:1848:LEU:HB3	2:G:1853:ILE:HB	1.99	0.43
2:G:35:LEU:HD13	2:G:49:LEU:HD13	2.01	0.43
2:I:2121:PHE:O	2:I:3725:TYR:OH	2.37	0.43
2:I:235:ALA:HA	2:I:257:ARG:HD3	2.01	0.43
2:I:3696:ASP:OD2	2:I:3771:HIS:NE2	2.52	0.43
2:I:3971:GLY:H	2:I:5005:GLY:HA3	1.82	0.43
2:I:786:GLY:HA2	2:I:1631:GLN:HA	2.01	0.43
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.99	0.43
2:E:35:LEU:HD13	2:E:49:LEU:HD13	2.01	0.43
2:E:2121:PHE:O	2:E:3725:TYR:OH	2.37	0.43
2:E:3696:ASP:OD2	2:E:3771:HIS:NE2	2.52	0.43
2:E:4003:LEU:HB2	2:E:4013:LEU:HD13	2.01	0.43
2:G:3696:ASP:OD2	2:G:3771:HIS:NE2	2.52	0.43
2:G:4673:ARG:HH12	2:G:4698:LYS:HE3	1.83	0.43
1:J:23:VAL:HB	1:J:105:ASN:HA	2.01	0.43
2:B:2247:GLN:NE2	2:B:2285:GLU:OE2	2.52	0.43
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.92	0.43
2:B:2281:ILE:HG23	2:B:2341:VAL:HG11	2.00	0.43
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.46	0.43
2:B:4673:ARG:HH12	2:B:4698:LYS:HE3	1.83	0.43
2:E:3959:LYS:O	2:E:3963:ASN:ND2	2.52	0.43
2:G:838:HIS:HA	2:G:1201:HIS:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.92	0.43
2:G:485:SER:HA	2:G:488:LEU:HB2	2.01	0.43
2:I:2281:ILE:HG23	2:I:2341:VAL:HG11	2.00	0.43
2:I:4673:ARG:HH12	2:I:4698:LYS:HE3	1.83	0.43
2:B:786:GLY:HA2	2:B:1631:GLN:HA	2.01	0.43
2:B:1679:ASN:HA	2:B:1682:ALA:HB3	2.00	0.43
2:B:235:ALA:HA	2:B:257:ARG:HD3	2.01	0.43
2:E:619:ASP:OD1	2:E:1680:ARG:NH1	2.42	0.43
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	2.00	0.43
2:G:2247:GLN:NE2	2:G:2285:GLU:OE2	2.52	0.43
2:G:2437:ALA:HA	2:G:2438:PRO:HD3	1.92	0.43
2:G:4003:LEU:HB2	2:G:4013:LEU:HD13	2.01	0.43
2:G:4791:TYR:OH	2:G:4815:ASP:O	2.36	0.43
2:G:626:LEU:HG	2:G:628:GLY:H	1.84	0.43
2:I:2788:HIS:CE1	2:I:2790:MET:HB2	2.54	0.43
2:B:35:LEU:HD13	2:B:49:LEU:HD13	2.01	0.42
2:E:2104:ARG:HA	2:E:2107:GLN:HB3	2.01	0.42
2:E:2247:GLN:NE2	2:E:2285:GLU:OE2	2.52	0.42
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.92	0.42
2:E:3674:ILE:HD11	2:E:3728:ILE:HG22	2.00	0.42
2:E:485:SER:HA	2:E:488:LEU:HB2	2.01	0.42
2:G:1859:VAL:HA	2:G:1862:ILE:HG12	2.01	0.42
2:G:2104:ARG:HA	2:G:2107:GLN:HB3	2.01	0.42
2:G:2121:PHE:O	2:G:3725:TYR:OH	2.37	0.42
2:G:214:VAL:HG12	2:G:274:LEU:HD12	2.01	0.42
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	2.00	0.42
1:H:23:VAL:HB	1:H:105:ASN:HA	2.01	0.42
2:I:1679:ASN:HA	2:I:1682:ALA:HB3	2.00	0.42
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.92	0.42
2:B:2104:ARG:HA	2:B:2107:GLN:HB3	2.01	0.42
2:E:1126:GLY:HA3	2:E:1143:TRP:CE2	2.54	0.42
2:G:2236:LEU:HD23	2:G:2275:VAL:HG11	2.01	0.42
2:G:4840:THR:O	2:G:4844:LEU:N	2.47	0.42
2:I:2104:ARG:HA	2:I:2107:GLN:HB3	2.01	0.42
2:I:3959:LYS:O	2:I:3963:ASN:ND2	2.52	0.42
2:B:1859:VAL:HA	2:B:1862:ILE:HG12	2.01	0.42
2:B:2299:VAL:O	2:B:2303:ALA:N	2.52	0.42
2:B:2517:UNK:O	2:B:2521:UNK:N	2.53	0.42
2:B:3674:ILE:HD11	2:B:3728:ILE:HG22	2.00	0.42
2:B:3959:LYS:O	2:B:3963:ASN:ND2	2.52	0.42
2:E:1804:LEU:O	2:E:1808:ARG:N	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1859:VAL:HA	2:E:1862:ILE:HG12	2.01	0.42
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	2.00	0.42
2:E:4918:ILE:HD11	2:G:4888:TYR:HA	2.02	0.42
2:G:313:SER:HB3	2:G:351:VAL:HB	1.99	0.42
2:G:414:PHE:HE1	2:G:436:LEU:HB3	1.84	0.42
2:G:460:GLN:HG2	2:G:462:GLU:H	1.83	0.42
2:I:3362:UNK:O	2:I:3366:UNK:N	2.53	0.42
2:I:4056:GLU:O	2:I:4060:LYS:N	2.52	0.42
2:I:485:SER:HA	2:I:488:LEU:HB2	2.01	0.42
2:I:626:LEU:HG	2:I:628:GLY:H	1.85	0.42
2:B:1639:LEU:HD12	2:B:1653:LEU:HD21	2.00	0.42
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	2.00	0.42
2:B:2121:PHE:O	2:B:3725:TYR:OH	2.37	0.42
2:B:2788:HIS:CE1	2:B:2790:MET:HB2	2.54	0.42
2:B:460:GLN:HG2	2:B:462:GLU:H	1.83	0.42
2:E:1639:LEU:HD12	2:E:1653:LEU:HD21	2.00	0.42
2:E:3362:UNK:O	2:E:3366:UNK:N	2.53	0.42
2:E:950:LEU:HB3	2:E:970:LEU:HD22	2.02	0.42
2:G:2788:HIS:CE1	2:G:2790:MET:HB2	2.54	0.42
2:G:3362:UNK:O	2:G:3366:UNK:N	2.53	0.42
2:G:3674:ILE:HD11	2:G:3728:ILE:HG22	2.00	0.42
2:G:3959:LYS:O	2:G:3963:ASN:ND2	2.52	0.42
2:G:681:HIS:HB3	2:G:784:SER:HB3	2.02	0.42
1:H:21:THR:HA	1:H:49:ARG:HA	2.01	0.42
2:B:23:GLN:HE21	2:B:34:LYS:HB3	1.85	0.42
2:B:914:PRO:O	2:B:918:ARG:N	2.51	0.42
2:E:2236:LEU:HD23	2:E:2275:VAL:HG11	2.01	0.42
2:E:214:VAL:HG12	2:E:274:LEU:HD12	2.01	0.42
2:E:2788:HIS:CE1	2:E:2790:MET:HB2	2.54	0.42
2:E:932:LEU:HA	2:E:935:LEU:HD12	2.01	0.42
2:G:2517:UNK:O	2:G:2521:UNK:N	2.53	0.42
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	2.00	0.42
2:I:2517:UNK:O	2:I:2521:UNK:N	2.52	0.42
2:I:25:SER:HA	2:I:34:LYS:HA	2.02	0.42
2:I:414:PHE:HE1	2:I:436:LEU:HB3	1.84	0.42
2:I:838:HIS:HA	2:I:1201:HIS:HB3	2.01	0.42
2:B:25:SER:HA	2:B:34:LYS:HA	2.02	0.42
2:E:1227:ALA:HB1	2:E:1230:MET:HG3	2.02	0.42
2:E:2517:UNK:O	2:E:2521:UNK:N	2.53	0.42
2:E:2869:ARG:HH12	2:E:2945:UNK:C	2.32	0.42
1:F:21:THR:HA	1:F:49:ARG:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1126:GLY:HA3	2:G:1143:TRP:CE2	2.54	0.42
2:E:4673:ARG:HH12	2:E:4698:LYS:HE3	1.83	0.42
2:G:1227:ALA:HB1	2:G:1230:MET:HG3	2.02	0.42
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.47	0.42
2:I:1859:VAL:HA	2:I:1862:ILE:HG12	2.02	0.42
2:I:4003:LEU:HB2	2:I:4013:LEU:HD13	2.01	0.42
2:B:1238:PHE:O	2:B:1606:SER:N	2.48	0.42
2:B:932:LEU:HA	2:B:935:LEU:HD12	2.01	0.42
2:E:414:PHE:HE1	2:E:436:LEU:HB3	1.84	0.42
2:E:626:LEU:HG	2:E:628:GLY:H	1.84	0.42
2:G:25:SER:HA	2:G:34:LYS:HA	2.02	0.42
2:G:932:LEU:HA	2:G:935:LEU:HD12	2.01	0.42
2:G:950:LEU:HB3	2:G:970:LEU:HD22	2.02	0.42
2:I:1126:GLY:HA3	2:I:1143:TRP:CE2	2.54	0.42
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	2.02	0.42
2:I:42:PHE:HD1	2:I:447:ASP:HB3	1.85	0.42
1:A:23:VAL:HB	1:A:105:ASN:HA	2.01	0.42
2:B:4942:GLU:HG3	2:E:4944:ARG:HH11	1.84	0.42
2:B:626:LEU:HG	2:B:628:GLY:H	1.84	0.42
2:B:950:LEU:HB3	2:B:970:LEU:HD22	2.02	0.42
2:B:983:THR:O	2:B:987:ARG:N	2.51	0.42
2:E:235:ALA:HA	2:E:257:ARG:HD3	2.01	0.42
2:G:235:ALA:HA	2:G:257:ARG:HD3	2.01	0.42
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	2.02	0.42
2:I:2236:LEU:HD23	2:I:2275:VAL:HG11	2.01	0.42
2:I:214:VAL:HG12	2:I:274:LEU:HD12	2.01	0.42
2:I:663:TYR:HB2	2:I:808:TYR:HB3	2.02	0.42
2:B:485:SER:HA	2:B:488:LEU:HB2	2.01	0.42
2:E:23:GLN:HE21	2:E:34:LYS:HB3	1.85	0.42
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.47	0.42
2:E:838:HIS:HA	2:E:1201:HIS:HB3	2.01	0.42
2:I:3994:HIS:O	2:I:3998:HIS:ND1	2.39	0.42
2:B:214:VAL:HG12	2:B:274:LEU:HD12	2.01	0.41
2:B:3362:UNK:O	2:B:3366:UNK:N	2.53	0.41
2:B:414:PHE:HE1	2:B:436:LEU:HB3	1.84	0.41
2:B:681:HIS:HB3	2:B:784:SER:HB3	2.02	0.41
2:G:42:PHE:HD1	2:G:447:ASP:HB3	1.85	0.41
2:I:1148:VAL:N	2:I:1165:ASN:OD1	2.53	0.41
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.53	0.41
2:I:2299:VAL:O	2:I:2303:ALA:N	2.52	0.41
2:I:3850:GLN:HA	2:I:3853:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:932:LEU:HA	2:I:935:LEU:HD12	2.01	0.41
1:J:21:THR:HA	1:J:49:ARG:HA	2.01	0.41
2:B:1148:VAL:N	2:B:1165:ASN:OD1	2.54	0.41
2:B:759:ILE:HG22	2:B:760:ASN:H	1.86	0.41
2:E:25:SER:HA	2:E:34:LYS:HA	2.02	0.41
2:G:4802:GLY:HA2	2:G:4808:PHE:HB2	2.02	0.41
2:B:1126:GLY:HA3	2:B:1143:TRP:CE2	2.54	0.41
2:B:663:TYR:HB2	2:B:808:TYR:HB3	2.02	0.41
2:E:1271:ARG:HA	2:E:1471:UNK:HA	2.02	0.41
2:E:357:LEU:HD12	2:E:388:LEU:HD11	2.03	0.41
2:E:42:PHE:HD1	2:E:447:ASP:HB3	1.85	0.41
1:F:23:VAL:HB	1:F:105:ASN:HA	2.01	0.41
2:G:4056:GLU:O	2:G:4060:LYS:N	2.52	0.41
2:G:599:VAL:HG23	2:G:600:LEU:HD12	2.02	0.41
2:I:23:GLN:HE21	2:I:34:LYS:HB3	1.85	0.41
2:I:2880:GLU:O	2:I:2884:ASN:N	2.48	0.41
2:I:4802:GLY:HA2	2:I:4808:PHE:HB2	2.02	0.41
2:I:583:ILE:HA	2:I:586:ILE:HD12	2.03	0.41
2:I:759:ILE:HG22	2:I:760:ASN:H	1.86	0.41
2:B:3994:HIS:O	2:B:3998:HIS:ND1	2.39	0.41
2:B:42:PHE:HD1	2:B:447:ASP:HB3	1.85	0.41
2:E:4840:THR:O	2:E:4844:LEU:N	2.47	0.41
2:E:583:ILE:HA	2:E:586:ILE:HD12	2.03	0.41
2:E:681:HIS:HB3	2:E:784:SER:HB3	2.02	0.41
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	2.02	0.41
1:H:57:LYS:HB2	1:H:80:VAL:HB	2.03	0.41
2:I:2437:ALA:HA	2:I:2438:PRO:HD3	1.92	0.41
2:I:479:GLN:HE21	2:I:536:ASN:ND2	2.19	0.41
2:I:599:VAL:HG23	2:I:600:LEU:HD12	2.02	0.41
2:B:1041:GLN:O	2:B:1045:THR:OG1	2.30	0.41
2:B:2159:LEU:HD22	2:B:2201:LEU:HD23	2.03	0.41
2:B:4918:ILE:HD11	2:E:4888:TYR:HA	2.03	0.41
2:B:838:HIS:HA	2:B:1201:HIS:HB3	2.01	0.41
2:E:759:ILE:HG22	2:E:760:ASN:H	1.86	0.41
2:G:4978:HIS:ND1	2:G:4982:GLU:OE1	2.44	0.41
2:G:759:ILE:HG22	2:G:760:ASN:H	1.86	0.41
2:G:786:GLY:HA2	2:G:1631:GLN:HA	2.01	0.41
2:I:681:HIS:HB3	2:I:784:SER:HB3	2.02	0.41
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	2.02	0.41
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.38	0.41
2:B:4802:GLY:HA2	2:B:4808:PHE:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4840:THR:O	2:B:4844:LEU:N	2.47	0.41
2:B:599:VAL:HG23	2:B:600:LEU:HD12	2.02	0.41
2:E:663:TYR:HB2	2:E:808:TYR:HB3	2.02	0.41
2:I:950:LEU:HB3	2:I:970:LEU:HD22	2.02	0.41
1:A:21:THR:HA	1:A:49:ARG:HA	2.02	0.41
2:B:290:TYR:O	2:B:302:VAL:N	2.50	0.41
2:E:786:GLY:HA2	2:E:1631:GLN:HA	2.01	0.41
2:G:3694:LYS:HA	2:G:3695:PRO:HD3	1.95	0.41
2:G:2159:LEU:HD22	2:G:2201:LEU:HD23	2.03	0.41
2:G:23:GLN:HE21	2:G:34:LYS:HB3	1.85	0.41
2:G:3552:UNK:O	2:G:3556:UNK:N	2.54	0.41
2:I:4840:THR:O	2:I:4844:LEU:N	2.47	0.41
2:B:2236:LEU:HD23	2:B:2275:VAL:HG11	2.01	0.41
2:B:2674:UNK:O	2:B:2676:UNK:N	2.54	0.41
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	2.02	0.41
2:E:3694:LYS:HA	2:E:3695:PRO:HD3	1.95	0.41
2:G:1804:LEU:O	2:G:1808:ARG:N	2.45	0.41
2:G:357:LEU:HD12	2:G:388:LEU:HD11	2.03	0.41
2:G:288:GLY:HA3	2:G:405:HIS:CE1	2.56	0.41
2:G:4977:THR:O	2:G:4981:GLU:N	2.41	0.41
2:I:2103:VAL:O	2:I:2107:GLN:N	2.48	0.41
2:B:479:GLN:HE21	2:B:536:ASN:ND2	2.19	0.41
2:B:776:LEU:HG	2:B:848:HIS:HA	2.03	0.41
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	2.03	0.41
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.53	0.41
2:E:776:LEU:HG	2:E:848:HIS:HA	2.03	0.41
2:G:1148:VAL:N	2:G:1165:ASN:OD1	2.53	0.41
2:G:2021:CYS:HA	2:G:2022:PRO:HD3	1.94	0.41
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.53	0.41
2:G:3994:HIS:O	2:G:3998:HIS:ND1	2.39	0.41
2:I:1227:ALA:HB1	2:I:1230:MET:HG3	2.02	0.41
2:I:2159:LEU:HD22	2:I:2201:LEU:HD23	2.03	0.41
1:A:57:LYS:HB2	1:A:80:VAL:HB	2.03	0.41
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.54	0.41
2:B:583:ILE:HA	2:B:586:ILE:HD12	2.03	0.41
2:E:1099:GLU:OE2	2:E:1127:HIS:ND1	2.38	0.41
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.38	0.41
2:E:599:VAL:HG23	2:E:600:LEU:HD12	2.02	0.41
2:I:2869:ARG:HH12	2:I:2945:UNK:C	2.34	0.41
2:I:3552:UNK:O	2:I:3556:UNK:N	2.54	0.41
2:B:1227:ALA:HB1	2:B:1230:MET:HG3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:215:THR:HG22	2:B:273:HIS:HA	2.03	0.40
2:B:3552:UNK:O	2:B:3556:UNK:N	2.54	0.40
2:B:357:LEU:HD12	2:B:388:LEU:HD11	2.03	0.40
2:E:1663:HIS:O	2:E:1667:LEU:N	2.53	0.40
2:E:2466:LEU:HD23	2:E:2469:ILE:HD12	2.03	0.40
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	2.02	0.40
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	2.02	0.40
2:E:4688:ILE:HG21	2:E:4728:HIS:HB3	2.04	0.40
1:F:57:LYS:HB2	1:F:80:VAL:HB	2.03	0.40
2:G:1271:ARG:HA	2:G:1471:UNK:HA	2.04	0.40
2:G:1595:LEU:HD23	2:G:1595:LEU:HA	1.96	0.40
2:G:2815:ALA:HB3	2:G:2881:ASN:HD21	1.87	0.40
2:G:4961:CYS:HB3	2:G:4983:HIS:CE1	2.56	0.40
2:G:663:TYR:HB2	2:G:808:TYR:HB3	2.02	0.40
2:I:1729:SER:O	2:I:2163:ARG:NH1	2.54	0.40
2:I:4961:CYS:HB3	2:I:4983:HIS:CE1	2.56	0.40
2:B:1729:SER:O	2:B:2163:ARG:NH1	2.54	0.40
2:B:4809:PHE:HA	2:B:4812:HIS:HD1	1.85	0.40
2:B:864:PRO:HA	2:B:865:PRO:HD3	1.96	0.40
2:E:3552:UNK:O	2:E:3556:UNK:N	2.54	0.40
2:G:1497:UNK:HA	2:G:1535:UNK:HA	2.03	0.40
2:I:1657:LEU:HA	2:I:1657:LEU:HD13	1.97	0.40
2:I:684:VAL:HA	2:I:781:VAL:HA	2.03	0.40
2:B:358:THR:HG21	2:B:382:GLY:HA2	2.04	0.40
2:B:4075:GLU:HA	2:B:4078:GLN:HB2	2.04	0.40
2:B:4634:GLU:HG3	2:B:4636:THR:H	1.86	0.40
2:E:1729:SER:O	2:E:2163:ARG:NH1	2.54	0.40
2:E:288:GLY:HA3	2:E:405:HIS:CE1	2.56	0.40
2:E:4075:GLU:HA	2:E:4078:GLN:HB2	2.03	0.40
2:E:4809:PHE:HA	2:E:4812:HIS:HD1	1.85	0.40
1:F:5:GLU:HB2	1:F:73:LYS:HB3	2.04	0.40
2:G:4688:ILE:HG21	2:G:4728:HIS:HB3	2.04	0.40
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.38	0.40
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.54	0.40
2:I:4809:PHE:HA	2:I:4812:HIS:HD1	1.85	0.40
1:J:57:LYS:HB2	1:J:80:VAL:HB	2.03	0.40
1:A:5:GLU:HB2	1:A:73:LYS:HB3	2.04	0.40
2:E:1148:VAL:N	2:E:1165:ASN:OD1	2.54	0.40
2:E:2159:LEU:HD22	2:E:2201:LEU:HD23	2.03	0.40
2:E:358:THR:HG21	2:E:382:GLY:HA2	2.04	0.40
2:G:1802:ILE:HG21	2:G:1807:LEU:HD22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4634:GLU:HG3	2:I:4636:THR:H	1.86	0.40
2:I:716:PHE:HE2	2:I:759:ILE:HD11	1.87	0.40
2:B:1802:ILE:HG21	2:B:1807:LEU:HD22	2.04	0.40
2:B:3662:ILE:H	2:B:3662:ILE:HG13	1.77	0.40
2:B:2290:LEU:HB3	2:B:3849:ARG:NH1	2.37	0.40
2:E:3902:TYR:O	2:E:3906:GLN:NE2	2.55	0.40
2:E:4802:GLY:HA2	2:E:4808:PHE:HB2	2.02	0.40
2:G:2034:PHE:O	2:G:2038:LEU:N	2.55	0.40
2:G:1729:SER:O	2:G:2163:ARG:NH1	2.54	0.40
2:G:4809:PHE:HA	2:G:4812:HIS:HD1	1.85	0.40
2:G:583:ILE:HA	2:G:586:ILE:HD12	2.02	0.40
2:I:2674:UNK:O	2:I:2676:UNK:N	2.54	0.40
2:I:2815:ALA:HB3	2:I:2881:ASN:HD21	1.86	0.40
2:I:358:THR:HG21	2:I:382:GLY:HA2	2.04	0.40
2:I:288:GLY:HA3	2:I:405:HIS:CE1	2.56	0.40
2:I:415:ILE:HA	2:I:418:LEU:HD13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	F	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	H	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	J	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
2	B	3235/4676 (69%)	2923 (90%)	308 (10%)	4 (0%)	56	90
2	E	3235/4676 (69%)	2922 (90%)	309 (10%)	4 (0%)	56	90
2	G	3235/4676 (69%)	2922 (90%)	309 (10%)	4 (0%)	56	90

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	I	3235/4676 (69%)	2924 (90%)	307 (10%)	4 (0%)	56 90
All	All	13360/19136 (70%)	12064 (90%)	1280 (10%)	16 (0%)	59 90

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	E	1708	ARG
2	I	1708	ARG
2	G	1708	ARG
2	B	1840	PRO
2	B	1932	PRO
2	E	1840	PRO
2	E	1932	PRO
2	I	1840	PRO
2	I	1932	PRO
2	G	1840	PRO
2	G	1932	PRO
2	B	4641	PRO
2	E	4641	PRO
2	I	4641	PRO
2	G	4641	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	88/89 (99%)	88 (100%)	0	100 100
1	F	88/89 (99%)	88 (100%)	0	100 100
1	H	88/89 (99%)	88 (100%)	0	100 100
1	J	88/89 (99%)	88 (100%)	0	100 100
2	B	2493/3202 (78%)	2477 (99%)	16 (1%)	90 95
2	E	2493/3202 (78%)	2477 (99%)	16 (1%)	90 95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	G	2493/3202 (78%)	2477 (99%)	16 (1%)	90 95
2	I	2493/3202 (78%)	2477 (99%)	16 (1%)	90 95
All	All	10324/13164 (78%)	10260 (99%)	64 (1%)	91 95

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	534	ARG
2	B	553	ARG
2	B	978	THR
2	B	1076	ARG
2	B	1141	ARG
2	B	1600	LEU
2	B	1676	LEU
2	B	1964	ARG
2	B	3787	LYS
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4131	ARG
2	B	4957	LYS
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
2	E	978	THR
2	E	1076	ARG
2	E	1141	ARG
2	E	1600	LEU
2	E	1676	LEU
2	E	1964	ARG
2	E	3787	LYS
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4131	ARG
2	E	4957	LYS
2	I	131	LEU
2	I	534	ARG

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Mol	Chain	Res	Type
2	I	553	ARG
2	I	978	THR
2	I	1076	ARG
2	I	1141	ARG
2	I	1600	LEU
2	I	1676	LEU
2	I	1964	ARG
2	I	3787	LYS
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4131	ARG
2	I	4957	LYS
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	978	THR
2	G	1076	ARG
2	G	1141	ARG
2	G	1600	LEU
2	G	1676	LEU
2	G	1964	ARG
2	G	3787	LYS
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4131	ARG
2	G	4957	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (168) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	87	HIS
1	A	87	HIS
1	H	87	HIS
1	J	87	HIS
2	B	57	ASN
2	B	105	HIS
2	B	111	HIS
2	B	113	HIS

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Mol	Chain	Res	Type
2	B	156	GLN
2	B	273	HIS
2	B	379	HIS
2	B	395	GLN
2	B	405	HIS
2	B	413	GLN
2	B	479	GLN
2	B	495	ASN
2	B	582	HIS
2	B	797	HIS
2	B	838	HIS
2	B	877	ASN
2	B	949	ASN
2	B	1598	GLN
2	B	1679	ASN
2	B	1693	GLN
2	B	1719	HIS
2	B	1972	ASN
2	B	2005	GLN
2	B	2127	GLN
2	B	2788	HIS
2	B	3830	GLN
2	B	3889	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN
2	B	3963	ASN
2	B	3976	ASN
2	B	4034	ASN
2	B	4054	ASN
2	B	4120	ASN
2	B	4130	ASN
2	B	4142	ASN
2	B	4728	HIS
2	B	4832	HIS
2	E	57	ASN
2	E	105	HIS
2	E	111	HIS
2	E	113	HIS
2	E	156	GLN
2	E	273	HIS

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Mol	Chain	Res	Type
2	E	379	HIS
2	E	395	GLN
2	E	405	HIS
2	E	413	GLN
2	E	479	GLN
2	E	495	ASN
2	E	582	HIS
2	E	797	HIS
2	E	838	HIS
2	E	877	ASN
2	E	949	ASN
2	E	1598	GLN
2	E	1679	ASN
2	E	1693	GLN
2	E	1719	HIS
2	E	1972	ASN
2	E	2005	GLN
2	E	2127	GLN
2	E	2788	HIS
2	E	3830	GLN
2	E	3889	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	3963	ASN
2	E	3976	ASN
2	E	4034	ASN
2	E	4054	ASN
2	E	4120	ASN
2	E	4130	ASN
2	E	4142	ASN
2	E	4728	HIS
2	E	4832	HIS
2	I	23	GLN
2	I	57	ASN
2	I	105	HIS
2	I	111	HIS
2	I	113	HIS
2	I	156	GLN
2	I	203	ASN
2	I	273	HIS

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Mol	Chain	Res	Type
2	I	379	HIS
2	I	395	GLN
2	I	405	HIS
2	I	413	GLN
2	I	479	GLN
2	I	495	ASN
2	I	582	HIS
2	I	797	HIS
2	I	838	HIS
2	I	877	ASN
2	I	949	ASN
2	I	1598	GLN
2	I	1679	ASN
2	I	1693	GLN
2	I	1719	HIS
2	I	1972	ASN
2	I	2005	GLN
2	I	2127	GLN
2	I	2788	HIS
2	I	3830	GLN
2	I	3889	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	3963	ASN
2	I	3976	ASN
2	I	4034	ASN
2	I	4054	ASN
2	I	4120	ASN
2	I	4130	ASN
2	I	4142	ASN
2	I	4728	HIS
2	I	4832	HIS
2	G	23	GLN
2	G	57	ASN
2	G	105	HIS
2	G	111	HIS
2	G	113	HIS
2	G	156	GLN
2	G	203	ASN
2	G	273	HIS

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Mol	Chain	Res	Type
2	G	379	HIS
2	G	395	GLN
2	G	405	HIS
2	G	413	GLN
2	G	479	GLN
2	G	495	ASN
2	G	582	HIS
2	G	797	HIS
2	G	838	HIS
2	G	877	ASN
2	G	949	ASN
2	G	1598	GLN
2	G	1679	ASN
2	G	1693	GLN
2	G	1719	HIS
2	G	1972	ASN
2	G	2005	GLN
2	G	2127	GLN
2	G	2788	HIS
2	G	3830	GLN
2	G	3889	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	3963	ASN
2	G	3976	ASN
2	G	4034	ASN
2	G	4054	ASN
2	G	4120	ASN
2	G	4130	ASN
2	G	4142	ASN
2	G	4728	HIS
2	G	4832	HIS

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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	G	12
2	B	12
2	I	12
2	E	12

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3613:UNK	C	3639:THR	N	43.37
1	G	3613:UNK	C	3639:THR	N	43.37
1	E	3613:UNK	C	3639:THR	N	43.34
1	I	3613:UNK	C	3639:THR	N	43.32
1	B	3163:UNK	C	3170:UNK	N	16.45
1	E	3163:UNK	C	3170:UNK	N	16.45
1	I	3163:UNK	C	3170:UNK	N	16.45
1	G	3163:UNK	C	3170:UNK	N	16.45
1	B	3468:UNK	C	3511:UNK	N	15.10

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	3468:UNK	C	3511:UNK	N	15.10
1	I	3468:UNK	C	3511:UNK	N	15.10
1	G	3468:UNK	C	3511:UNK	N	15.10
1	I	3063:UNK	C	3134:UNK	N	14.88
1	B	3063:UNK	C	3134:UNK	N	14.87
1	E	3063:UNK	C	3134:UNK	N	14.87
1	G	3063:UNK	C	3134:UNK	N	14.86
1	I	2703:UNK	C	2734:ASN	N	14.34
1	E	2703:UNK	C	2734:ASN	N	14.33
1	B	2703:UNK	C	2734:ASN	N	14.32
1	G	2703:UNK	C	2734:ASN	N	14.32
1	B	3236:UNK	C	3241:UNK	N	13.55
1	E	3236:UNK	C	3241:UNK	N	13.55
1	I	3236:UNK	C	3241:UNK	N	13.55
1	G	3236:UNK	C	3241:UNK	N	13.55
1	I	1564:UNK	C	1573:MET	N	12.87
1	E	1564:UNK	C	1573:MET	N	12.85
1	G	1564:UNK	C	1573:MET	N	12.85
1	B	1564:UNK	C	1573:MET	N	12.84
1	B	2976:UNK	C	2995:UNK	N	12.50
1	E	2976:UNK	C	2995:UNK	N	12.50
1	I	2976:UNK	C	2995:UNK	N	12.50
1	G	2976:UNK	C	2995:UNK	N	12.50
1	B	3254:UNK	C	3261:UNK	N	8.64
1	E	3254:UNK	C	3261:UNK	N	8.64
1	I	3254:UNK	C	3261:UNK	N	8.64
1	G	3254:UNK	C	3261:UNK	N	8.64
1	I	1297:UNK	C	1430:UNK	N	5.73
1	B	1297:UNK	C	1430:UNK	N	5.72
1	E	1297:UNK	C	1430:UNK	N	5.72
1	G	1297:UNK	C	1430:UNK	N	5.72
1	B	2939:ARG	C	2942:UNK	N	3.71
1	E	2939:ARG	C	2942:UNK	N	3.71
1	I	2939:ARG	C	2942:UNK	N	3.71
1	G	2939:ARG	C	2942:UNK	N	3.71
1	G	2479:LEU	C	2487:UNK	N	3.27
1	B	2479:LEU	C	2487:UNK	N	3.26
1	E	2479:LEU	C	2487:UNK	N	3.26
1	I	2479:LEU	C	2487:UNK	N	3.25