wwPDB EM Map/Model Validation Report (i)

Oct 17, 2016 – 06:44 PM EDT

PDB ID	:	5TAN
EMDB ID:	:	EMD-8380
Title	:	Structure of rabbit RyR1 (Caffeine/ATP/Ca2+ dataset, class 3)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-10
Resolution	:	4.30 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

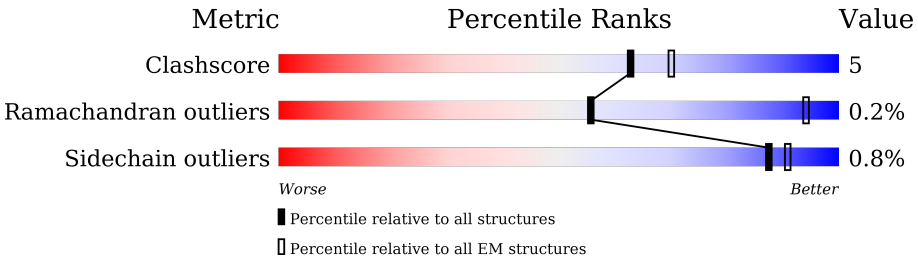
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 4.30 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	81% 19% .
1	F	108	81% 19% .
1	H	108	81% 19% .
1	J	108	81% 19% .
2	B	4416	84% 11% 5%
2	E	4416	83% 11% 5%
2	G	4416	83% 11% 5%
2	I	4416	84% 11% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 121456 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.

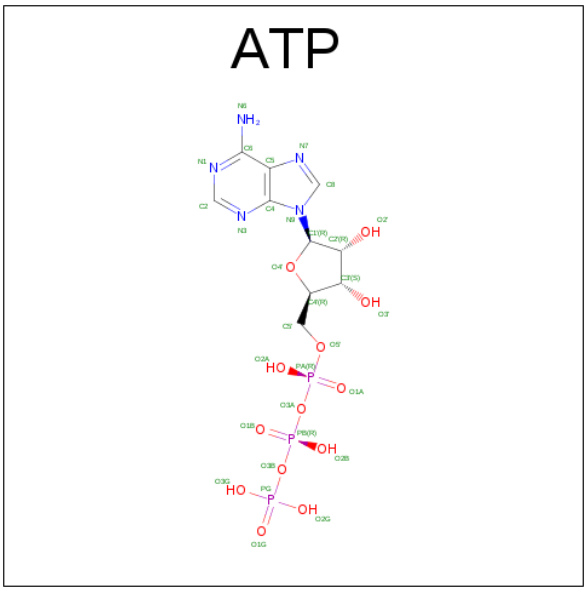
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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.

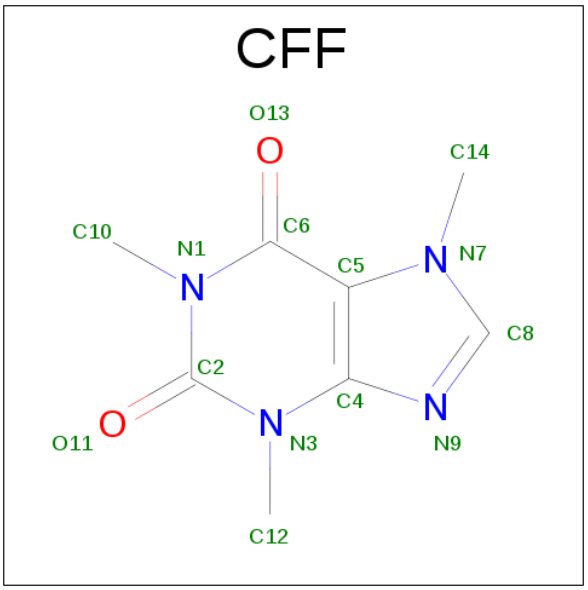
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	G	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$).



Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	4	2	
4	E	1	Total	C	N	O	0
			14	8	4	2	
4	I	1	Total	C	N	O	0
			14	8	4	2	
4	G	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

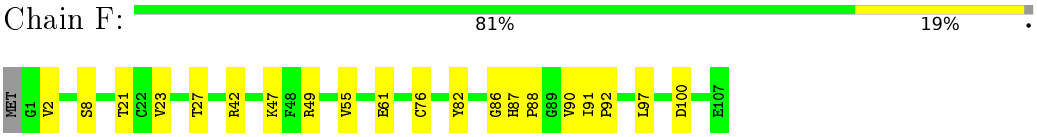
Mol	Chain	Residues	Atoms		AltConf
6	G	1	Total	Ca	0
			1	1	
6	B	1	Total	Ca	0
			1	1	
6	I	1	Total	Ca	0
			1	1	
6	E	1	Total	Ca	0
			1	1	

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:

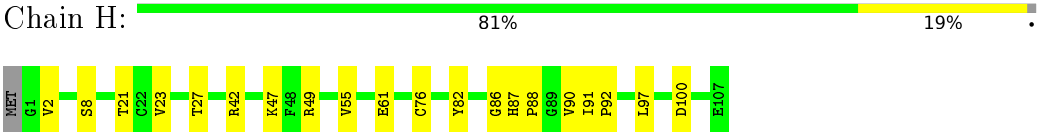


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:

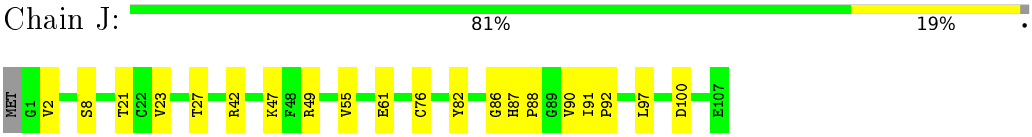
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



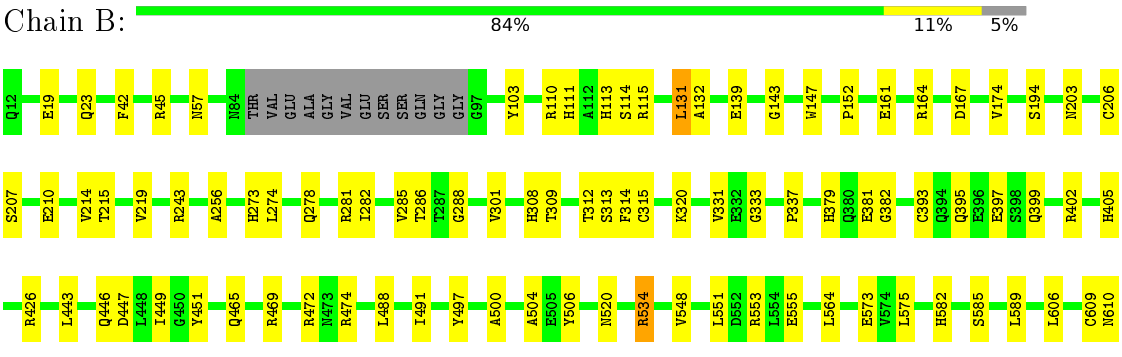
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J:



- Molecule 2: Ryanodine receptor 1

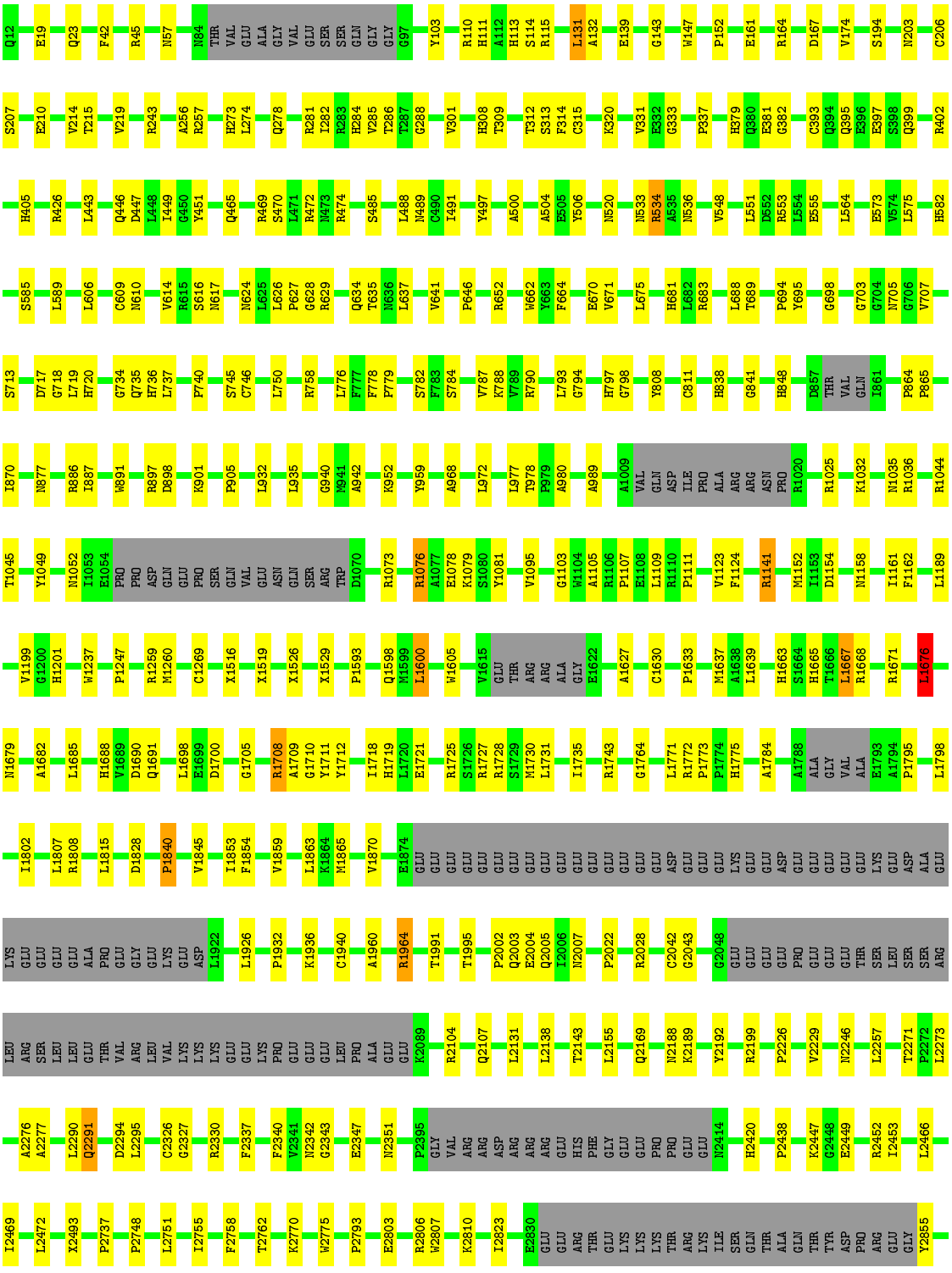
Chain B:

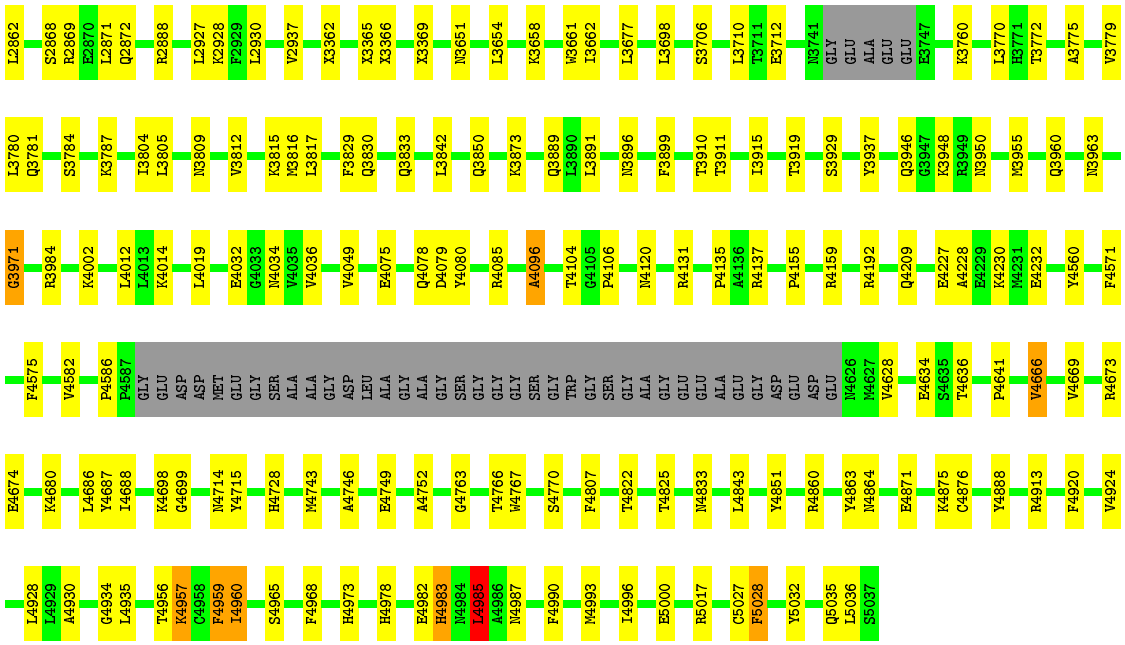


V614 R615 S616 N617 M624 L625 L626 P627 G628 T635 N636 L637 V641 P646 R652 F664 E670 V671 L675 H681 L682 R683 L688 T689 P694 Y695 G698 G703 G704 N705 G706 V707 S713 D717 G718 L719 H720 G734 Q735 H736 L737 P740
S745 C746 L750 R758 L776 F777 F778 P779 S782 F783 S784 V787 K788 V789 R790 L793 G794 H797 G798 Y808 H838 G841 H848 D857 THR VAL GLN I861 I870 N877 R886 I887 W891 R897 D898 K901 P905 L932
L935 G940 N941 A942 K952 Y959 A968 L972 L977 T978 P979 A980 A989 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO R1020 R1025 K1032 N1035 R1036 R1044 T1045 N1052 I1053 E1054 PRO PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER
ARG TRP D1070 R1073 R1076 A1077 E1078 K1079 S1080 Y1081 V1095 G1103 W1104 A1105 R1106 P1107 E1108 L1109 R1110 P1111 V1123 F1124 R1141 M1152 I1153 D1154 N1158 I1161 F1162 L1189 V1199 G1200 H1201 T1236 W1237 R1259 M1260 C1269 X1516 X1519 X1526 X1529
P1593 L1600 W1605 M1608 V1615 GLU THR ARG ARG ALA GLY E1622 A1627 C1630 P1633 M1637 A1638 L1639 H1663 S1664 H1665 T1666 L1667 R1668 R1671 L1676 N1679 L1685 H1688 V1689 D1690 Q1691 L1698 E1699 D1700 R1708 A1709 G1710 Y1711 Y1712 I1718 H1719
L1720 E1721 R1725 S1726 R1727 R1728 S1729 M1730 L1731 I1735 R1743 G1764 L1771 R1772 P1773 P1774 H1775 A1784 A1788 ALA GLY VAL ALA E1793 A1794 P1795 L1798 I1802 L1807 R1808 L1815 D1828 P1840 V1845 I1853 F1854 V1859 L1863 K1864 M1865 V1870
E1874 GLU GLU 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 GLU ASP ALA GLU LYS GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 L1926 P1932 K1936 C1940 A1960
R1964 Q1973 Y1977 T1991 T1995 P2002 Q2003 E2004 Q2005 I2006 N2007 P2022 R2028 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 L2131 L2138 T2143 L2155 Q2169 N2188 K2189 Y2192 R2199 P2226 V2229 N2246 L2257 T2271 P2272 L2273 A2276 A2277 L2290 Q2291 D2294 L2295 C2326 G2327 R2330 F2337 F2340 V2341 N2342 G2343
E2347 N2351 P2395 GLY VAL ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 H2420 P2438 K2447 G2448 E2449 R2452 I2453 L2466 I2469 L2472 S2868 R2869 E2870 L2871 Q2872 R2888 L2927 K2928 F2929 L2930 V2937 T2762 K2770 W2775
P2793 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 L2862 S2868 R2869 E2870 L2871 Q2872 R2888 L2927 K2928 F2929 L2930 V2937 X3362 X3365 X3366
X3369 N3651 L3654 K3658 Q3889 L3890 L3891 N3896 F3899 T3910 T3911 I3915 T3919 S3929 N3741 GLY GLU ALA GLU GLU E3747 K3760 L3770 H3771 T3772 A3775 V3779 L3780 Q3781 S3784 K3787 I3804 L3805 N3809 E4032 G4033 N4034 V4035 V4036 V4049 E4075 L3842
F3847 Q3850 K3873 Q3889 L3890 L3891 N3896 F3899 T3910 T3911 I3915 T3919 S3929 Y3937 Q3946 G3947 K3948 R3949 N3950 M3955 Q3960 N3963 G3971 R3984 K4002 L4012 L4013 K4014 L4019 E4032 G4033 N4034 V4035 V4036 V4049 E4075
Q4078 D4079 Y4080 R4085 A4096 T4104 G4105 P4106 N4120 R4131 P4135 A4136 R4137 P4155 R4159 R4192 Q4209 E4227 A4228 E4229 K4230 M4231 E4232 Y4560 F4571 F4575 V4582 P4586 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 GLU ALA GLU GLY ASP GLU ASP GLU N4626 M4627 V4628 E4634 S4635 T4636 P4641 V4666 V4669 R4673 E4674 K4680 L4686 Y4687 I4688 K4698 G4699 N4714 Y4715 H4728 R4736 M4743 A4746
E4749 A4752 G4763 T4766 W4767 S4770 F4807 T4822 T4825 N4833 L4843 Y4851 R4860 N4864 E4871 C4876 R4913 V4914 F4920 V4924 L4928 L4929 A4930 G4934 L4935 T4956 K4957 C4958 F4959 I4960 S4965 F4968 H4973 H4978 E4982

- Molecule 2: Ryanodine receptor 1

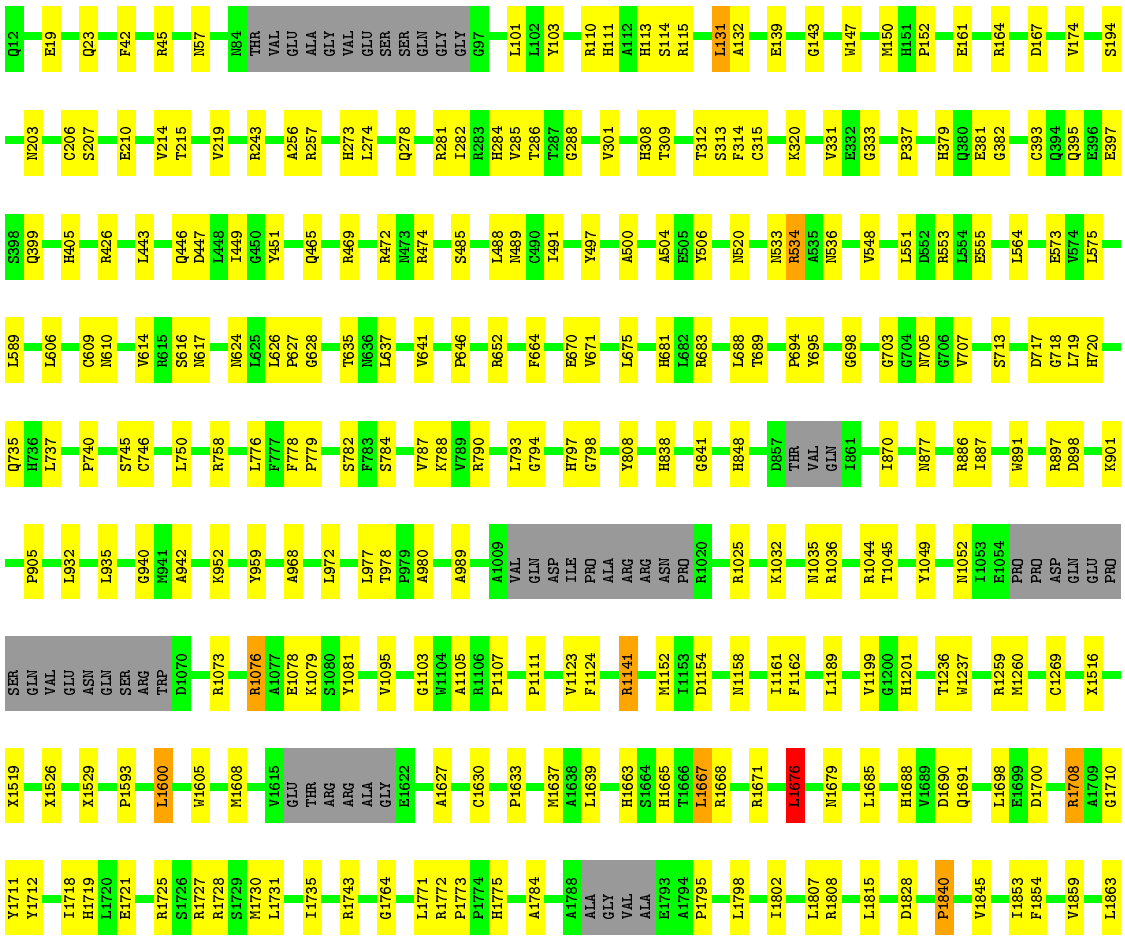
Chain E:

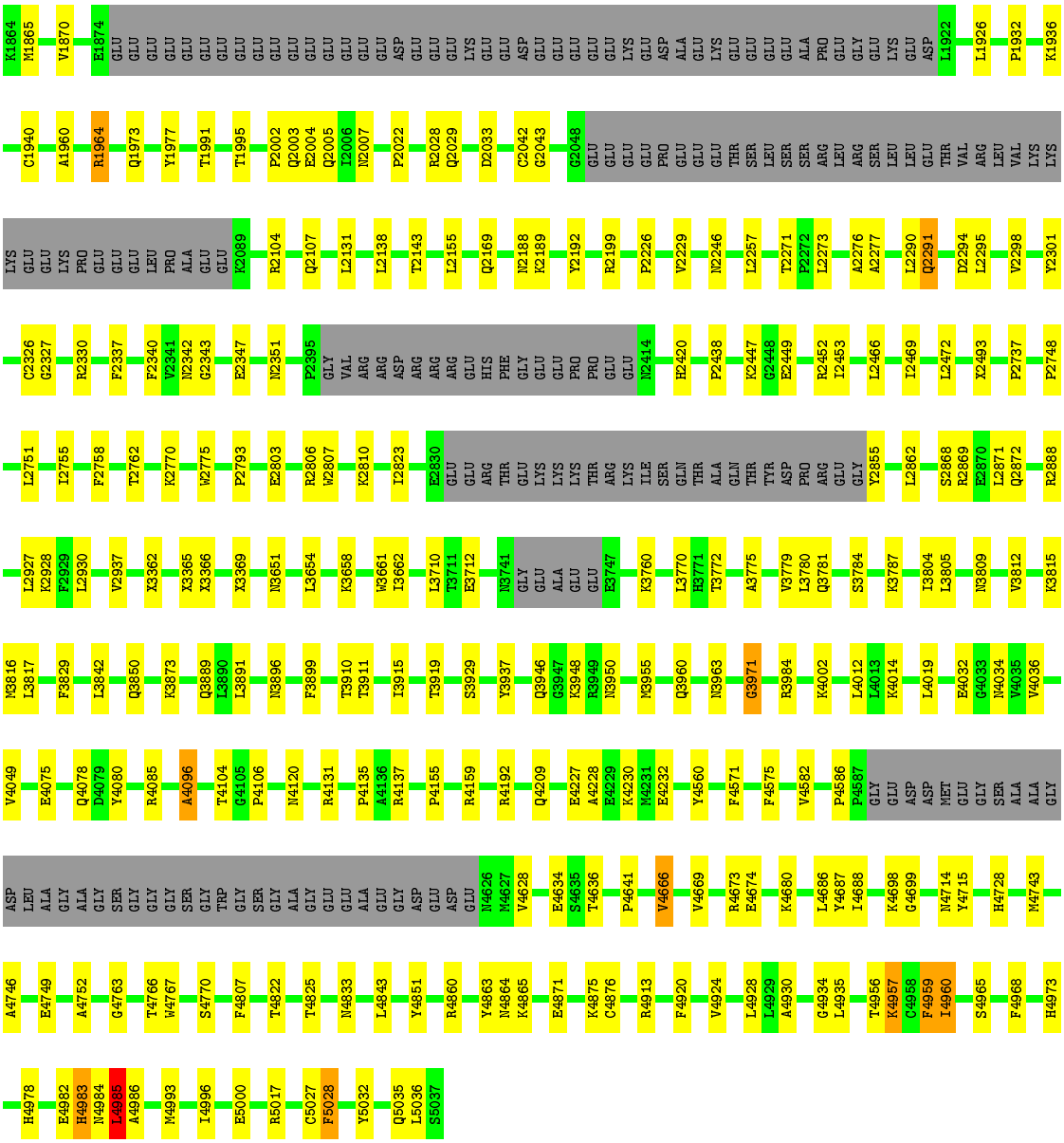




- Molecule 2: Ryanodine receptor 1

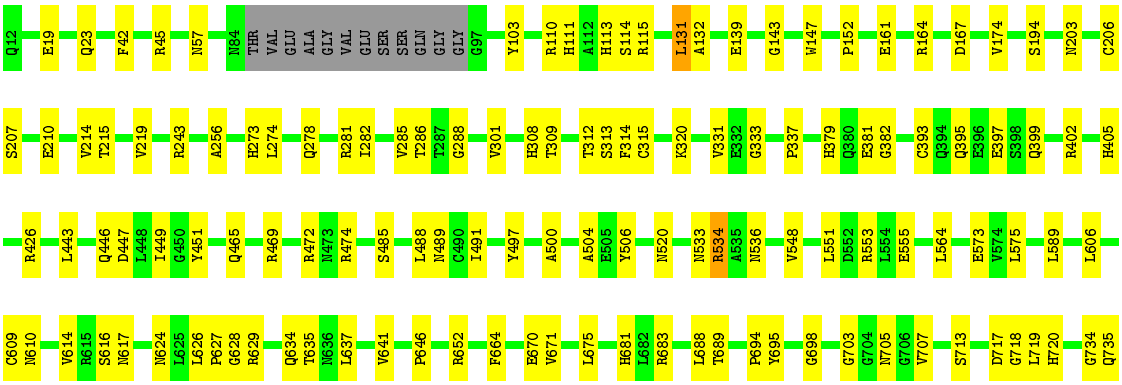
Chain I:

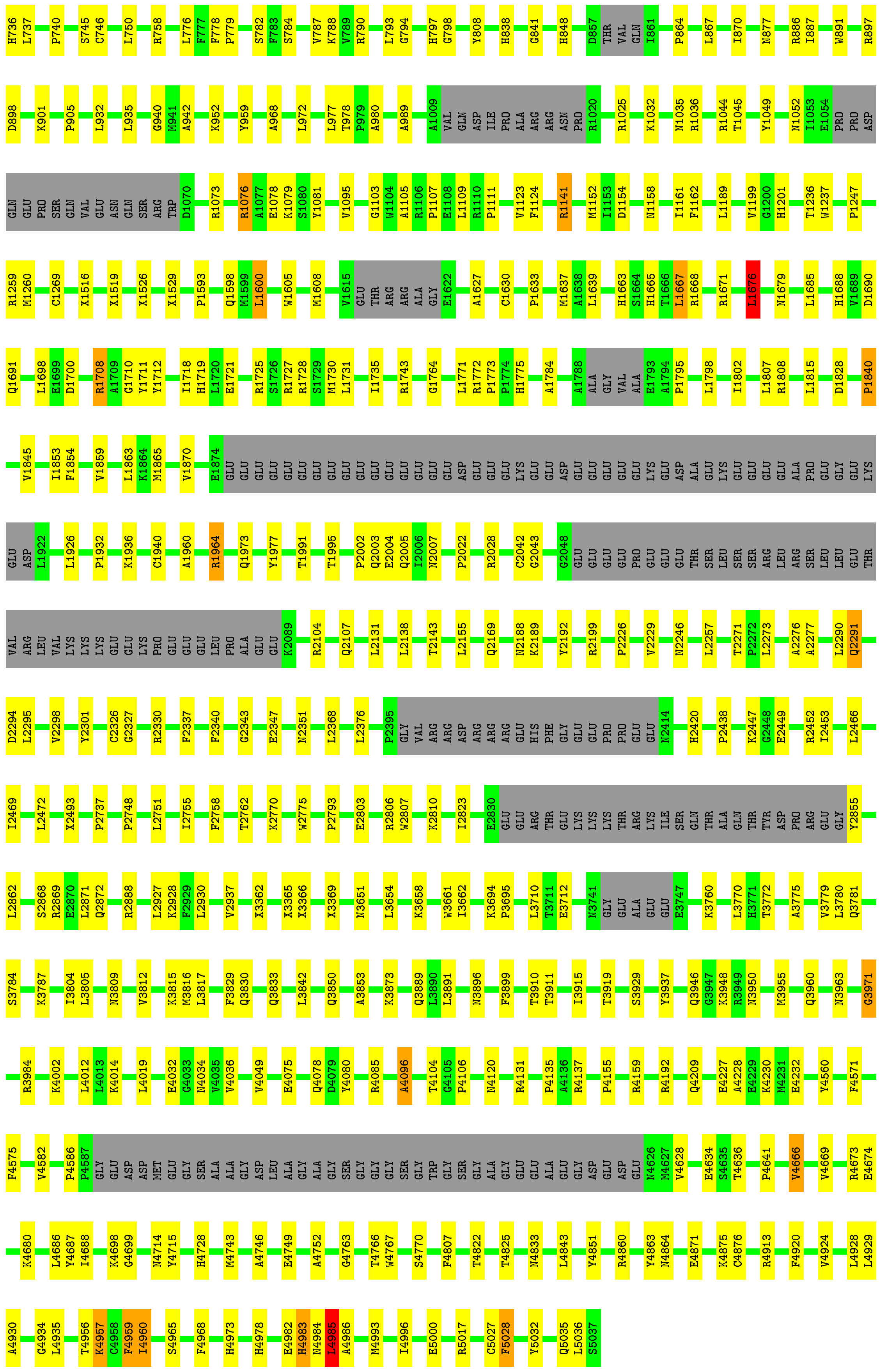




• Molecule 2: Ryanodine receptor 1

Chain G:




H736 L737 P740 S745 C746 L750 R758 L776 F777 F778 P779 S782 F783 S784 V787 K788 V789 R790 L793 G794 H797 G798 Y808 H838 G841 H848 D857 THR VAL GLN I861 P864 L867 I870 N877 R886 I887 W891 R897
D898 K901 P905 L932 L935 G940 M941 A942 K952 Y959 A968 L972 L977 T978 P979 A980 A989 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO R1020 R1025 K1032 N1035 R1036 R1044 T1045 Y1049 N1052 I1053 E1054 PRO PRO ASP
GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1073 R1076 A1077 E1078 K1079 S1080 Y1081 V1095 G1103 W1104 A1105 R1106 P1107 E1108 L1109 R1110 P1111 V1123 F1124 R1141 M1152 I1153 D1154 N1158 I1161 F1162 L1189 V1199 G1200 H1201 T1236 W1237 P1247
R1259 M1260 C1269 X1516 X1519 X1526 X1529 P1593 Q1598 M1599 L1600 W1605 M1608 V1615 GLU THR ARG ARG ALA GLY E1622 A1627 C1630 P1633 M1637 A1638 L1639 H1663 S1664 H1665 T1666 L1667 R1668 R1671 L1676 N1679 L1685 H1688 V1689 D1690
Q1691 L1698 E1699 D1700 R1708 A1709 G1710 Y1711 Y1712 I1718 H1719 L1720 E1721 R1725 S1726 R1727 R1728 S1729 M1730 L1731 I1735 R1743 G1764 L1771 R1772 P1773 P1774 H1775 A1784 A1788 ALA GLY VAL ALA E1793 A1794 P1795 L1798 I1802 L1807 R1808 L1815 D1828 P1840
V1845 I1853 F1854 V1859 L1863 K1864 M1865 V1870 E1874 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 P1932 K1936 C1940 A1960 R1964 Q1973 Y1977 T1991 T1995 P2002 Q2003 E2004 Q2005 I2006 N2007 P2022 R2028 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 GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU K2089 R2104 Q2107 L2131 L2138 T2143 L2155 Q2169 N2188 K2189 Y2192 R2199 P2226 V2229 N2246 L2257 T2271 P2272 L2273 A2276 A2277 L2290 Q2291
D2294 L2295 V2298 Y2301 C2326 G2327 R2330 F2337 F2340 G2343 E2347 N2351 L2368 L2376 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 H2420 P2438 K2447 G2448 E2449 R2452 I2453 L2466
I2469 L2472 X2493 P2737 P2748 L2751 I2755 F2758 T2762 K2770 W2775 P2793 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
L2862 S2868 R2869 E2870 L2871 Q2872 R2888 L2927 K2928 F2929 L2930 V2937 X3362 X3365 X3366 X3369 N3651 L3654 K3658 W3661 I3662 K3694 P3695 L3710 T3711 E3712 N3741 GLY GLU ALA GLU GLU E3747 K3760 L3770 H3771 T3772 A3775 V3779 L3780 Q3781
S3784 K3787 I3804 L3805 N3809 V3812 K3815 M3816 L3817 F3829 Q3830 Q3833 L3842 Q3850 A3853 K3873 Q3889 L3890 L3891 N3896 F3899 T3910 T3911 I3915 T3919 S3929 Y3937 Q3946 G3947 K3948 R3949 N3950 M3955 Q3960 N3963 G3971
R3984 K4002 L4012 L4013 K4014 L4019 E4032 G4033 N4034 V4035 V4036 V4049 E4075 Q4078 D4079 Y4080 R4085 A4096 T4104 G4105 P4106 N4120 R4131 P4135 A4136 R4137 P4155 R4159 R4192 Q4209 E4227 A4228 E4229 K4230 M4231 E4232 Y4560 F4571
F4575 V4582 P4586 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 V4628 E4634 S4635 T4636 P4641 V4666 V4669 R4673 E4674
K4680 L4686 Y4687 I4688 K4698 G4699 N4714 Y4715 H4728 M4743 A4746 E4749 A4752 G4763 T4766 W4767 S4770 F4807 T4822 T4825 N4833 L4843 Y4851 R4860 Y4863 N4864 E4871 K4875 C4876 R4913 F4920 V4924 L4928 L4929
A4930 G4934 L4935 T4956 K4957 C4958 F4959 I4960 S4965 F4968 H4973 H4978 E4982 H4983 N4984 L4985 A4986 M4993 I4996 E5000 R5017 C5027 F5028 Y5032 Q5035 L5036 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: CFF, ZN, CA, ATP

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	0.32	0/834	0.53	0/1123
1	F	0.32	0/834	0.53	0/1123
1	H	0.32	0/834	0.53	0/1123
1	J	0.32	0/834	0.53	0/1123
2	B	0.31	0/25428	0.55	8/34534 (0.0%)
2	E	0.31	0/25428	0.55	8/34534 (0.0%)
2	G	0.31	0/25428	0.55	8/34534 (0.0%)
2	I	0.31	0/25428	0.55	8/34534 (0.0%)
All	All	0.31	0/105048	0.55	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
1	A	0	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	18
2	E	0	18
2	G	0	18
2	I	0	18
All	All	0	76

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	131	LEU	CA-CB-CG	8.10	133.92	115.30
2	B	131	LEU	CA-CB-CG	8.09	133.90	115.30
2	E	131	LEU	CA-CB-CG	8.09	133.90	115.30
2	G	131	LEU	CA-CB-CG	8.09	133.90	115.30
2	I	4985	LEU	CA-CB-CG	6.89	131.16	115.30
2	B	1600	LEU	CA-CB-CG	6.89	131.15	115.30
2	G	1600	LEU	CA-CB-CG	6.88	131.14	115.30
2	E	1600	LEU	CA-CB-CG	6.88	131.12	115.30
2	G	4985	LEU	CA-CB-CG	6.88	131.12	115.30
2	B	4985	LEU	CA-CB-CG	6.88	131.11	115.30
2	I	1600	LEU	CA-CB-CG	6.87	131.11	115.30
2	E	4985	LEU	CA-CB-CG	6.86	131.08	115.30
2	B	1676	LEU	CA-CB-CG	6.77	130.87	115.30
2	I	1676	LEU	CA-CB-CG	6.77	130.87	115.30
2	E	1676	LEU	CA-CB-CG	6.76	130.85	115.30
2	G	1676	LEU	CA-CB-CG	6.76	130.85	115.30
2	G	977	LEU	CA-CB-CG	6.08	129.29	115.30
2	E	977	LEU	CA-CB-CG	6.07	129.27	115.30
2	B	977	LEU	CA-CB-CG	6.06	129.24	115.30
2	I	977	LEU	CA-CB-CG	6.06	129.24	115.30
2	E	2290	LEU	CA-CB-CG	5.73	128.48	115.30
2	G	2290	LEU	CA-CB-CG	5.72	128.47	115.30
2	B	2290	LEU	CA-CB-CG	5.72	128.46	115.30
2	I	2290	LEU	CA-CB-CG	5.71	128.44	115.30
2	I	688	LEU	CA-CB-CG	5.41	127.73	115.30
2	B	688	LEU	CA-CB-CG	5.40	127.71	115.30
2	E	688	LEU	CA-CB-CG	5.39	127.69	115.30
2	G	688	LEU	CA-CB-CG	5.38	127.68	115.30
2	B	1667	LEU	CA-CB-CG	5.20	127.25	115.30
2	E	1667	LEU	CA-CB-CG	5.20	127.26	115.30
2	G	1667	LEU	CA-CB-CG	5.20	127.25	115.30
2	I	1667	LEU	CA-CB-CG	5.18	127.21	115.30

There are no chirality outliers.

All (76) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1690	ASP	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide

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Mol	Chain	Res	Type	Group
2	B	1840	PRO	Peptide
2	B	2291	GLN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	312	THR	Peptide
2	B	3971	GLY	Peptide
2	B	4096	ALA	Peptide
2	B	4666	VAL	Peptide
2	B	4807	PHE	Peptide
2	B	624	ASN	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1690	ASP	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	1840	PRO	Peptide
2	E	2291	GLN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	312	THR	Peptide
2	E	3971	GLY	Peptide
2	E	4096	ALA	Peptide
2	E	4666	VAL	Peptide
2	E	4807	PHE	Peptide
2	E	624	ASN	Peptide
2	E	694	PRO	Peptide
2	E	808	TYR	Peptide
1	F	8	SER	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1690	ASP	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	1840	PRO	Peptide
2	G	2291	GLN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide

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Mol	Chain	Res	Type	Group
2	G	312	THR	Peptide
2	G	3971	GLY	Peptide
2	G	4096	ALA	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	624	ASN	Peptide
2	G	694	PRO	Peptide
2	G	808	TYR	Peptide
1	H	8	SER	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1690	ASP	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	1840	PRO	Peptide
2	I	2291	GLN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	312	THR	Peptide
2	I	3971	GLY	Peptide
2	I	4096	ALA	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	624	ASN	Peptide
2	I	694	PRO	Peptide
2	I	808	TYR	Peptide
1	J	8	SER	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	12	0
1	F	818	0	824	12	0
1	H	818	0	824	12	0
1	J	818	0	824	12	0
2	B	29499	0	24753	296	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	29499	0	24753	305	0
2	G	29499	0	24753	299	0
2	I	29499	0	24753	295	0
3	B	31	0	12	1	0
3	E	31	0	12	1	0
3	G	31	0	12	1	0
3	I	31	0	12	1	0
4	B	14	0	10	1	0
4	E	14	0	10	1	0
4	G	14	0	10	1	0
4	I	14	0	10	1	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
All	All	121456	0	102396	1213	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 (1213) 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:E:5028:PHE:CE1	2:E:5032:TYR:CD2	2.32	1.18
2:B:5028:PHE:CE1	2:B:5032:TYR:CD2	2.32	1.17
2:G:5028:PHE:CE1	2:G:5032:TYR:CD2	2.32	1.17
2:I:5028:PHE:CE1	2:I:5032:TYR:CD2	2.32	1.16
2:E:5028:PHE:HE1	2:E:5032:TYR:CE2	1.64	1.16
2:B:5028:PHE:HE1	2:B:5032:TYR:CE2	1.64	1.15
2:I:5028:PHE:HE1	2:I:5032:TYR:CE2	1.64	1.14
2:G:5028:PHE:HE1	2:G:5032:TYR:CE2	1.64	1.14
2:B:5028:PHE:HE1	2:B:5032:TYR:CD2	1.67	1.12
2:E:5028:PHE:HE1	2:E:5032:TYR:CD2	1.67	1.11
2:I:5028:PHE:HE1	2:I:5032:TYR:CD2	1.67	1.10
2:G:5028:PHE:HE1	2:G:5032:TYR:CD2	1.67	1.09
2:G:5028:PHE:CE1	2:G:5032:TYR:CE2	2.54	0.94
2:G:5028:PHE:CE1	2:G:5032:TYR:HD2	1.81	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:5028:PHE:CE1	2:I:5032:TYR:HD2	1.81	0.92
2:I:5028:PHE:CE1	2:I:5032:TYR:CE2	2.54	0.92
2:B:5028:PHE:CE1	2:B:5032:TYR:HD2	1.81	0.92
2:E:5028:PHE:CE1	2:E:5032:TYR:CE2	2.54	0.92
2:B:5028:PHE:CE1	2:B:5032:TYR:CE2	2.54	0.91
2:B:4230:LYS:HD2	2:B:4959:PHE:CD1	2.05	0.90
2:G:4230:LYS:HD2	2:G:4959:PHE:CD1	2.05	0.90
2:I:4230:LYS:HD2	2:I:4959:PHE:CD1	2.05	0.90
2:E:4230:LYS:HD2	2:E:4959:PHE:CD1	2.05	0.90
2:E:5028:PHE:CE1	2:E:5032:TYR:HD2	1.81	0.89
2:B:4230:LYS:HD2	2:B:4959:PHE:CE1	2.16	0.81
2:E:4230:LYS:HD2	2:E:4959:PHE:CE1	2.16	0.81
2:G:4230:LYS:HD2	2:G:4959:PHE:CE1	2.16	0.80
2:I:4230:LYS:HD2	2:I:4959:PHE:CE1	2.16	0.80
2:B:4230:LYS:CG	2:B:4959:PHE:HE1	1.96	0.78
2:E:4230:LYS:CG	2:E:4959:PHE:HE1	1.96	0.78
2:I:4230:LYS:CG	2:I:4959:PHE:HE1	1.96	0.78
2:G:4230:LYS:CG	2:G:4959:PHE:HE1	1.96	0.78
2:E:4192:ARG:HH11	2:E:5028:PHE:HD2	1.36	0.74
2:B:4192:ARG:HH11	2:B:5028:PHE:HD2	1.36	0.73
2:G:4192:ARG:HH11	2:G:5028:PHE:HD2	1.36	0.73
2:I:4192:ARG:HH11	2:I:5028:PHE:HD2	1.36	0.72
2:B:111:HIS:HD2	2:B:114:SER:H	1.41	0.69
2:G:111:HIS:HD2	2:G:114:SER:H	1.41	0.68
2:E:111:HIS:HD2	2:E:114:SER:H	1.41	0.68
2:G:379:HIS:HD2	2:G:382:GLY:H	1.42	0.68
2:E:4957:LYS:HB2	2:E:4957:LYS:NZ	2.08	0.68
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.58	0.68
2:G:4957:LYS:NZ	2:G:4957:LYS:HB2	2.08	0.68
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.58	0.68
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.58	0.68
2:B:379:HIS:HD2	2:B:382:GLY:H	1.42	0.68
2:I:111:HIS:HD2	2:I:114:SER:H	1.41	0.68
2:B:4957:LYS:NZ	2:B:4957:LYS:HB2	2.08	0.67
2:E:5028:PHE:HE1	2:E:5032:TYR:HE2	1.39	0.67
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.58	0.67
2:I:4957:LYS:HB2	2:I:4957:LYS:NZ	2.08	0.66
2:I:379:HIS:HD2	2:I:382:GLY:H	1.42	0.66
2:E:4230:LYS:HG2	2:E:4959:PHE:HE1	1.60	0.66
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.78	0.66
2:E:379:HIS:HD2	2:E:382:GLY:H	1.42	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.78	0.65
2:G:4983:HIS:H	2:G:4983:HIS:CD2	2.15	0.65
2:B:4230:LYS:HG2	2:B:4959:PHE:HE1	1.60	0.65
2:I:4230:LYS:HG2	2:I:4959:PHE:HE1	1.60	0.65
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.78	0.65
2:G:4230:LYS:HD2	2:G:4959:PHE:HD1	1.62	0.65
2:E:161:GLU:HA	2:G:3984:ARG:HH22	1.62	0.64
2:E:4983:HIS:H	2:E:4983:HIS:CD2	2.15	0.64
2:G:4230:LYS:HG2	2:G:4959:PHE:HE1	1.61	0.64
2:I:4230:LYS:CD	2:I:4959:PHE:CE1	2.81	0.64
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.31	0.64
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.80	0.64
2:B:3984:ARG:HH22	2:I:161:GLU:HA	1.63	0.64
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.31	0.64
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.78	0.63
2:B:4230:LYS:CD	2:B:4959:PHE:CE1	2.81	0.63
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.80	0.63
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.80	0.63
2:I:4230:LYS:HD2	2:I:4959:PHE:HD1	1.62	0.63
2:I:4983:HIS:H	2:I:4983:HIS:CD2	2.15	0.63
2:E:4230:LYS:CD	2:E:4959:PHE:CE1	2.81	0.63
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.81	0.63
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.80	0.63
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.80	0.63
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.80	0.63
2:G:4230:LYS:CD	2:G:4959:PHE:CE1	2.81	0.63
2:B:4983:HIS:H	2:B:4983:HIS:CD2	2.15	0.62
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.32	0.62
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.32	0.62
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.33	0.62
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.31	0.62
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.31	0.62
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.32	0.62
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.32	0.62
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.81	0.62
2:B:331:VAL:HG12	2:B:333:GLY:H	1.65	0.62
2:B:4228:ALA:HB2	2:E:4973:HIS:HE1	1.64	0.62
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.81	0.62
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.82	0.61
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.81	0.61
2:I:3984:ARG:HH22	2:G:161:GLU:HA	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.81	0.61
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.81	0.61
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.33	0.61
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.81	0.61
2:E:331:VAL:HG12	2:E:333:GLY:H	1.65	0.61
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.33	0.61
2:I:331:VAL:HG12	2:I:333:GLY:H	1.65	0.61
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.82	0.61
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.83	0.61
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.80	0.61
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.33	0.61
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.82	0.61
2:E:4230:LYS:CG	2:E:4959:PHE:CE1	2.82	0.61
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.82	0.61
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.83	0.61
2:B:5028:PHE:HE1	2:B:5032:TYR:HE2	1.39	0.61
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.82	0.61
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.81	0.61
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.83	0.61
2:G:5028:PHE:HE1	2:G:5032:TYR:HE2	1.39	0.61
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.34	0.61
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.33	0.61
2:G:4230:LYS:CG	2:G:4959:PHE:CE1	2.83	0.60
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.83	0.60
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.34	0.60
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.33	0.60
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.82	0.60
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.82	0.60
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.84	0.60
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.66	0.60
2:G:331:VAL:HG12	2:G:333:GLY:H	1.65	0.60
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.81	0.60
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.66	0.60
2:E:4968:PHE:CZ	2:E:4978:HIS:CE1	2.90	0.60
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.84	0.60
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.84	0.60
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.84	0.60
2:G:4674:GLU:HG3	2:G:4714:ASN:HB3	1.84	0.60
2:B:4674:GLU:HG3	2:B:4714:ASN:HB3	1.84	0.60
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.84	0.60
2:I:4674:GLU:HG3	2:I:4714:ASN:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:5028:PHE:HE1	2:I:5032:TYR:HE2	1.39	0.60
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.84	0.60
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.82	0.60
2:B:161:GLU:HA	2:E:3984:ARG:HH22	1.66	0.59
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.84	0.59
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.84	0.59
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.84	0.59
2:B:23:GLN:OE1	2:B:203:ASN:ND2	2.36	0.59
2:E:609:CYS:SG	2:E:610:ASN:N	2.75	0.59
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.84	0.59
2:B:609:CYS:SG	2:B:610:ASN:N	2.75	0.59
2:G:609:CYS:SG	2:G:610:ASN:N	2.75	0.59
2:I:4968:PHE:CZ	2:I:4978:HIS:CE1	2.90	0.59
2:B:4968:PHE:CZ	2:B:4978:HIS:CE1	2.90	0.59
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.85	0.59
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.84	0.59
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.66	0.59
2:B:4230:LYS:HD2	2:B:4959:PHE:HD1	1.62	0.59
2:E:4674:GLU:HG3	2:E:4714:ASN:HB3	1.84	0.59
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.66	0.59
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.85	0.59
2:B:4973:HIS:HE1	2:I:4228:ALA:HB2	1.67	0.59
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.37	0.58
2:I:609:CYS:SG	2:I:610:ASN:N	2.75	0.58
2:E:4228:ALA:HB2	2:G:4973:HIS:HE1	1.68	0.58
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.37	0.58
2:G:23:GLN:OE1	2:G:203:ASN:ND2	2.35	0.58
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.85	0.58
2:G:4968:PHE:CZ	2:G:4978:HIS:CE1	2.90	0.58
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.84	0.58
2:E:23:GLN:OE1	2:E:203:ASN:ND2	2.36	0.58
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.37	0.58
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.37	0.58
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.86	0.58
2:B:4230:LYS:CG	2:B:4959:PHE:CE1	2.83	0.58
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.85	0.58
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.37	0.58
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.69	0.58
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.86	0.58
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.85	0.58
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.77	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.36	0.58
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.36	0.58
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.86	0.58
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.85	0.58
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.77	0.57
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.86	0.57
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.69	0.57
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.37	0.57
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.87	0.57
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.86	0.57
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.77	0.57
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.86	0.57
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.86	0.57
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.87	0.57
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.86	0.57
2:I:4973:HIS:HE1	2:G:4228:ALA:HB2	1.68	0.57
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.68	0.57
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.87	0.57
2:I:4983:HIS:N	2:I:4983:HIS:CD2	2.73	0.57
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.86	0.57
2:B:614:VAL:HG22	2:B:616:SER:H	1.70	0.57
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.77	0.57
2:I:4230:LYS:CG	2:I:4959:PHE:CE1	2.82	0.57
2:B:4983:HIS:N	2:B:4983:HIS:CD2	2.73	0.57
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.70	0.57
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.86	0.56
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.87	0.56
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.87	0.56
2:E:614:VAL:HG22	2:E:616:SER:H	1.70	0.56
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.87	0.56
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.87	0.56
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.87	0.56
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.68	0.56
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.87	0.56
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.39	0.56
1:F:55:VAL:HA	2:E:1784:ALA:HA	1.87	0.56
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.87	0.56
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.87	0.56
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.70	0.56
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.86	0.56
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4983:HIS:N	2:G:4983:HIS:CD2	2.73	0.56
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.39	0.56
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.39	0.56
2:E:2420:HIS:ND1	2:E:2493:UNK:O	2.36	0.56
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.87	0.56
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.39	0.56
2:I:614:VAL:HG22	2:I:616:SER:H	1.70	0.56
2:E:4993:MET:HA	2:E:4996:ILE:HD12	1.89	0.55
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.87	0.55
2:B:3770:LEU:HD21	2:B:3775:ALA:HB3	1.88	0.55
2:E:4230:LYS:HD2	2:E:4959:PHE:HD1	1.62	0.55
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.70	0.55
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.87	0.55
2:I:4993:MET:HA	2:I:4996:ILE:HD12	1.89	0.55
2:I:683:ARG:NH1	2:I:707:VAL:O	2.39	0.55
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.88	0.55
2:G:626:LEU:HG	2:G:628:GLY:H	1.71	0.55
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.87	0.55
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.86	0.55
2:I:626:LEU:HG	2:I:628:GLY:H	1.72	0.55
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.40	0.55
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.40	0.55
2:B:626:LEU:HG	2:B:628:GLY:H	1.71	0.55
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.87	0.55
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.38	0.55
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.87	0.55
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.88	0.55
2:G:4993:MET:HA	2:G:4996:ILE:HD12	1.89	0.55
2:I:23:GLN:OE1	2:I:203:ASN:ND2	2.36	0.55
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.40	0.55
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.89	0.55
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.40	0.55
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.88	0.55
2:B:4993:MET:HA	2:B:4996:ILE:HD12	1.89	0.55
2:E:626:LEU:HG	2:E:628:GLY:H	1.72	0.55
2:G:3770:LEU:HD21	2:G:3775:ALA:HB3	1.88	0.54
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.88	0.54
2:I:3770:LEU:HD21	2:I:3775:ALA:HB3	1.88	0.54
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.41	0.54
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.90	0.54
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.81	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.81	0.54
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.90	0.54
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.40	0.54
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.72	0.54
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.73	0.54
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.40	0.54
2:G:4960:ILE:N	2:G:4960:ILE:HD13	2.23	0.54
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.41	0.54
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.90	0.54
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.40	0.54
2:E:4983:HIS:N	2:E:4983:HIS:CD2	2.73	0.54
2:B:1727:ARG:NH2	2:B:1773:PRO:O	2.38	0.54
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.88	0.54
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.90	0.54
2:G:614:VAL:HG22	2:G:616:SER:H	1.70	0.54
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.72	0.54
2:I:2189:LYS:HA	2:I:2192:TYR:HD2	1.73	0.54
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.89	0.54
2:E:520:ASN:ND2	2:E:555:GLU:OE2	2.41	0.54
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.81	0.54
2:B:309:THR:O	2:B:313:SER:OG	2.26	0.54
2:B:4230:LYS:CD	2:B:4959:PHE:HE1	2.20	0.54
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.73	0.54
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.90	0.54
2:B:683:ARG:NH1	2:B:707:VAL:O	2.39	0.54
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.41	0.54
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.41	0.54
2:I:4960:ILE:N	2:I:4960:ILE:HD13	2.23	0.54
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.73	0.54
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.73	0.54
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.90	0.54
2:G:520:ASN:ND2	2:G:555:GLU:OE2	2.41	0.54
2:G:683:ARG:NH1	2:G:707:VAL:O	2.39	0.54
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.90	0.54
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.41	0.54
2:B:2189:LYS:HA	2:B:2192:TYR:HD2	1.73	0.53
2:E:309:THR:O	2:E:313:SER:OG	2.26	0.53
2:E:3770:LEU:HD21	2:E:3775:ALA:HB3	1.88	0.53
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.81	0.53
2:E:5028:PHE:CD1	2:E:5032:TYR:CD2	2.96	0.53
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:309:THR:O	2:G:313:SER:OG	2.26	0.53
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.42	0.53
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.89	0.53
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	1.90	0.53
2:B:214:VAL:HG12	2:B:274:LEU:HD12	1.91	0.53
2:B:520:ASN:ND2	2:B:555:GLU:OE2	2.41	0.53
2:E:683:ARG:NH1	2:E:707:VAL:O	2.39	0.53
2:I:520:ASN:ND2	2:I:555:GLU:OE2	2.41	0.53
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.90	0.53
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	1.90	0.53
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.91	0.53
1:F:76:CYS:HB2	1:F:97:LEU:HB2	1.90	0.53
2:G:2189:LYS:HA	2:G:2192:TYR:HD2	1.73	0.53
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.90	0.53
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.41	0.53
2:E:2189:LYS:HA	2:E:2192:TYR:HD2	1.73	0.53
2:E:695:TYR:OH	2:E:1073:ARG:NH1	2.40	0.53
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.91	0.53
2:E:4960:ILE:HD13	2:E:4960:ILE:N	2.22	0.53
2:G:214:VAL:HG12	2:G:274:LEU:HD12	1.91	0.53
2:I:652:ARG:HD2	2:I:750:LEU:HB3	1.91	0.53
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.91	0.53
2:G:2347:GLU:O	2:G:2351:ASN:N	2.36	0.53
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.38	0.53
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.91	0.53
2:B:4924:VAL:HA	2:B:4928:LEU:HB2	1.91	0.53
2:E:4230:LYS:CD	2:E:4959:PHE:HE1	2.20	0.53
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.90	0.53
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.91	0.53
2:G:978:THR:HB	2:G:980:ALA:H	1.74	0.53
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.91	0.53
2:E:214:VAL:HG12	2:E:274:LEU:HD12	1.91	0.52
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.73	0.52
2:E:978:THR:HB	2:E:980:ALA:H	1.74	0.52
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.91	0.52
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.73	0.52
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	1.91	0.52
2:I:675:LEU:HD11	2:I:1633:PRO:HB3	1.91	0.52
2:B:4960:ILE:HD13	2:B:4960:ILE:N	2.23	0.52
1:A:76:CYS:HB2	1:A:97:LEU:HB2	1.90	0.52
2:B:2420:HIS:ND1	2:B:2493:UNK:O	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.40	0.52
2:E:675:LEU:HD11	2:E:1633:PRO:HB3	1.91	0.52
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.43	0.52
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.43	0.52
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.43	0.52
1:J:76:CYS:HB2	1:J:97:LEU:HB2	1.90	0.52
2:B:5028:PHE:CD1	2:B:5032:TYR:CD2	2.96	0.52
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.38	0.52
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.92	0.52
2:B:111:HIS:CD2	2:B:114:SER:H	2.26	0.52
2:B:652:ARG:HD2	2:B:750:LEU:HB3	1.91	0.52
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.91	0.52
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.92	0.52
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.91	0.52
2:I:309:THR:O	2:I:313:SER:OG	2.26	0.52
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.92	0.52
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.43	0.52
2:B:3760:LYS:NZ	2:B:5000:GLU:OE1	2.41	0.52
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.43	0.52
2:E:4924:VAL:HA	2:E:4928:LEU:HB2	1.91	0.52
2:G:652:ARG:HD2	2:G:750:LEU:HB3	1.91	0.52
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.92	0.52
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.43	0.52
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.43	0.52
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.91	0.52
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.43	0.52
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.91	0.52
1:H:55:VAL:HA	2:G:1784:ALA:HA	1.91	0.52
1:H:76:CYS:HB2	1:H:97:LEU:HB2	1.90	0.52
2:I:695:TYR:OH	2:I:1073:ARG:NH1	2.40	0.52
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.43	0.52
2:B:695:TYR:OH	2:B:1073:ARG:NH1	2.40	0.52
2:E:4960:ILE:HD11	2:E:4985:LEU:HD23	1.92	0.52
2:I:2420:HIS:ND1	2:I:2493:UNK:O	2.36	0.52
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.91	0.52
2:G:4960:ILE:HD11	2:G:4985:LEU:HD23	1.92	0.52
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.40	0.52
2:I:978:THR:HB	2:I:980:ALA:H	1.75	0.52
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.43	0.51
2:E:652:ARG:HD2	2:E:750:LEU:HB3	1.91	0.51
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:132:ALA:HA	2:I:194:SER:HB2	1.91	0.51
2:I:2257:LEU:HD11	2:I:2276:ALA:HB2	1.93	0.51
2:B:675:LEU:HD11	2:B:1633:PRO:HB3	1.91	0.51
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.92	0.51
2:E:3891:LEU:HB3	2:E:3899:PHE:HE2	1.76	0.51
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.91	0.51
2:G:3891:LEU:HB3	2:G:3899:PHE:HE2	1.76	0.51
2:G:4924:VAL:HA	2:G:4928:LEU:HB2	1.91	0.51
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.92	0.51
2:B:2257:LEU:HD11	2:B:2276:ALA:HB2	1.92	0.51
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.44	0.51
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.91	0.51
2:I:4924:VAL:HA	2:I:4928:LEU:HB2	1.91	0.51
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	1.92	0.51
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.92	0.51
2:G:5028:PHE:CD1	2:G:5032:TYR:CD2	2.95	0.51
2:B:683:ARG:HG2	2:B:717:ASP:HB3	1.93	0.51
2:B:978:THR:HB	2:B:980:ALA:H	1.74	0.51
2:G:675:LEU:HD11	2:G:1633:PRO:HB3	1.91	0.51
2:G:132:ALA:HA	2:G:194:SER:HB2	1.91	0.51
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	1.93	0.51
2:G:2420:HIS:ND1	2:G:2493:UNK:O	2.36	0.51
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.91	0.51
2:G:683:ARG:HG2	2:G:717:ASP:HB3	1.93	0.51
2:I:214:VAL:HG12	2:I:274:LEU:HD12	1.91	0.51
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.91	0.51
2:B:132:ALA:HA	2:B:194:SER:HB2	1.91	0.51
2:E:132:ALA:HA	2:E:194:SER:HB2	1.91	0.51
2:E:4985:LEU:HB2	3:E:5101:ATP:HN61	1.76	0.51
2:I:1637:MET:SD	2:I:1708:ARG:NH1	2.84	0.51
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.44	0.51
2:I:3891:LEU:HB3	2:I:3899:PHE:HE2	1.76	0.51
2:B:1516:UNK:N	2:B:1529:UNK:O	2.44	0.51
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.92	0.51
2:B:4985:LEU:HB2	3:B:5101:ATP:HN61	1.76	0.51
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.43	0.51
2:G:1516:UNK:N	2:G:1529:UNK:O	2.44	0.51
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.44	0.51
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.92	0.51
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.46	0.51
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.43	0.51
2:I:111:HIS:CD2	2:I:114:SER:H	2.26	0.51
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.77	0.51
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.77	0.50
2:E:395:GLN:HG3	2:E:397:GLU:H	1.77	0.50
2:G:111:HIS:CD2	2:G:114:SER:H	2.26	0.50
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.46	0.50
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.44	0.50
2:E:1516:UNK:N	2:E:1529:UNK:O	2.44	0.50
2:E:2868:SER:O	2:E:2872:GLN:N	2.44	0.50
2:E:683:ARG:HG2	2:E:717:ASP:HB3	1.93	0.50
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.92	0.50
2:G:2868:SER:O	2:G:2872:GLN:N	2.44	0.50
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.77	0.50
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.92	0.50
2:I:4985:LEU:HB2	3:I:5101:ATP:HN61	1.76	0.50
2:B:4960:ILE:HD11	2:B:4985:LEU:HD23	1.92	0.50
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.77	0.50
2:G:1637:MET:SD	2:G:1708:ARG:NH1	2.84	0.50
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.44	0.50
2:I:4960:ILE:HD11	2:I:4985:LEU:HD23	1.92	0.50
2:I:683:ARG:HG2	2:I:717:ASP:HB3	1.93	0.50
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.44	0.50
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.94	0.50
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.46	0.50
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.77	0.50
2:I:395:GLN:HG3	2:I:397:GLU:H	1.76	0.50
2:B:3891:LEU:HB3	2:B:3899:PHE:HE2	1.76	0.50
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.77	0.50
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.93	0.50
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.92	0.50
2:B:1637:MET:SD	2:B:1708:ARG:NH1	2.84	0.50
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.94	0.50
2:I:4956:THR:O	2:I:4965:SER:N	2.42	0.50
2:B:838:HIS:HA	2:B:1201:HIS:HB3	1.94	0.50
2:I:5028:PHE:CD1	2:I:5032:TYR:CD2	2.96	0.50
2:B:2155:LEU:HD13	2:B:2188:ASN:HD21	1.77	0.50
2:B:2868:SER:O	2:B:2872:GLN:N	2.44	0.50
2:E:2155:LEU:HD13	2:E:2188:ASN:HD21	1.77	0.50
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.44	0.50
2:G:695:TYR:OH	2:G:1073:ARG:NH1	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1516:UNK:N	2:I:1529:UNK:O	2.44	0.50
2:I:3780:LEU:HD11	2:I:3816:MET:HG3	1.94	0.50
2:G:395:GLN:HG3	2:G:397:GLU:H	1.76	0.49
2:G:4985:LEU:HB2	3:G:5101:ATP:HN61	1.76	0.49
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.45	0.49
2:I:2155:LEU:HD13	2:I:2188:ASN:HD21	1.77	0.49
2:E:838:HIS:HA	2:E:1201:HIS:HB3	1.94	0.49
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.46	0.49
2:B:1808:ARG:HD3	2:B:1853:ILE:HG22	1.95	0.49
2:B:2347:GLU:O	2:B:2351:ASN:N	2.36	0.49
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.93	0.49
2:E:3760:LYS:NZ	2:E:5000:GLU:OE1	2.41	0.49
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.93	0.49
2:G:3780:LEU:HD11	2:G:3816:MET:HG3	1.95	0.49
1:A:21:THR:HA	1:A:49:ARG:HA	1.95	0.49
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.94	0.49
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	1.94	0.49
2:E:1637:MET:SD	2:E:1708:ARG:NH1	2.84	0.49
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.93	0.49
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.45	0.49
2:B:320:LYS:NZ	2:B:381:GLU:O	2.42	0.49
2:B:395:GLN:HG3	2:B:397:GLU:H	1.76	0.49
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	1.94	0.49
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.94	0.49
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.84	0.49
2:E:4036:VAL:HG11	2:E:5035:GLN:HB3	1.95	0.49
2:E:548:VAL:HG12	2:E:564:LEU:HD22	1.95	0.49
2:G:838:HIS:HA	2:G:1201:HIS:HB3	1.94	0.49
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.78	0.49
2:B:794:GLY:H	2:B:798:GLY:HA3	1.78	0.49
1:F:21:THR:HA	1:F:49:ARG:HA	1.95	0.49
1:F:92:PRO:HD3	2:E:627:PRO:HB2	1.95	0.49
2:G:548:VAL:HG12	2:G:564:LEU:HD22	1.95	0.49
2:G:794:GLY:H	2:G:798:GLY:HA3	1.78	0.49
1:J:21:THR:HA	1:J:49:ARG:HA	1.95	0.49
2:B:3804:ILE:O	2:B:3809:ASN:ND2	2.46	0.49
2:E:794:GLY:H	2:E:798:GLY:HA3	1.78	0.49
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.95	0.49
2:B:1259:ARG:HH12	2:B:1593:PRO:HA	1.78	0.49
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.77	0.49
2:G:1259:ARG:HH12	2:G:1593:PRO:HA	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3760:LYS:NZ	2:I:5000:GLU:OE1	2.41	0.49
2:I:794:GLY:H	2:I:798:GLY:HA3	1.78	0.49
2:I:838:HIS:HA	2:I:1201:HIS:HB3	1.94	0.49
2:B:4036:VAL:HG11	2:B:5035:GLN:HB3	1.95	0.49
2:B:548:VAL:HG12	2:B:564:LEU:HD22	1.95	0.49
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.95	0.49
2:G:2155:LEU:HD13	2:G:2188:ASN:HD21	1.77	0.49
2:I:1808:ARG:HD3	2:I:1853:ILE:HG22	1.95	0.49
2:I:2347:GLU:O	2:I:2351:ASN:N	2.36	0.49
2:I:548:VAL:HG12	2:I:564:LEU:HD22	1.95	0.49
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.95	0.48
2:E:1259:ARG:HH12	2:E:1593:PRO:HA	1.78	0.48
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	1.95	0.48
2:G:4956:THR:O	2:G:4965:SER:N	2.42	0.48
1:H:21:THR:HA	1:H:49:ARG:HA	1.95	0.48
2:I:1259:ARG:HH12	2:I:1593:PRO:HA	1.78	0.48
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.78	0.48
2:E:45:ARG:HG2	2:E:443:LEU:HD21	1.95	0.48
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.95	0.48
2:G:1863:LEU:HB3	2:G:1870:VAL:HG21	1.96	0.48
1:H:92:PRO:HD3	2:G:627:PRO:HB2	1.94	0.48
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.77	0.48
2:I:256:ALA:HB1	2:I:286:THR:HG21	1.95	0.48
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.43	0.48
2:E:1808:ARG:HD3	2:E:1853:ILE:HG22	1.95	0.48
2:E:2143:THR:O	2:E:3651:ASN:ND2	2.39	0.48
2:E:3804:ILE:O	2:E:3809:ASN:ND2	2.46	0.48
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.95	0.48
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.95	0.48
2:B:256:ALA:HB1	2:B:286:THR:HG21	1.95	0.48
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.84	0.48
2:G:776:LEU:HG	2:G:848:HIS:HA	1.95	0.48
2:I:776:LEU:HG	2:I:848:HIS:HA	1.95	0.48
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.45	0.48
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.96	0.48
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.96	0.48
2:E:4957:LYS:CB	2:E:4957:LYS:NZ	2.77	0.48
2:G:164:ARG:N	2:G:167:ASP:OD2	2.46	0.48
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.95	0.48
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.45	0.48
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:256:ALA:HB1	2:G:286:THR:HG21	1.95	0.48
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.96	0.48
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	1.95	0.48
2:I:3804:ILE:O	2:I:3809:ASN:ND2	2.46	0.48
2:I:45:ARG:HG2	2:I:443:LEU:HD21	1.95	0.48
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.96	0.48
2:E:111:HIS:CD2	2:E:114:SER:H	2.26	0.48
2:E:164:ARG:N	2:E:167:ASP:OD2	2.46	0.48
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.79	0.48
2:G:3804:ILE:O	2:G:3809:ASN:ND2	2.46	0.48
2:I:2104:ARG:HA	2:I:2107:GLN:HB3	1.95	0.48
2:I:2758:PHE:O	2:I:2762:THR:N	2.46	0.48
2:B:776:LEU:HG	2:B:848:HIS:HA	1.95	0.48
2:E:2104:ARG:HA	2:E:2107:GLN:HB3	1.95	0.48
2:E:776:LEU:HG	2:E:848:HIS:HA	1.95	0.48
2:G:1808:ARG:HD2	2:G:1854:PHE:HA	1.96	0.48
2:B:1863:LEU:HB3	2:B:1870:VAL:HG21	1.96	0.48
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.32	0.48
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.96	0.48
2:G:1808:ARG:HD3	2:G:1853:ILE:HG22	1.95	0.48
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.79	0.48
2:G:4763:GLY:O	2:G:4766:THR:OG1	2.31	0.48
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.96	0.48
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.79	0.48
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.47	0.48
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.47	0.48
2:I:4571:PHE:O	2:I:4575:PHE:N	2.47	0.48
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.96	0.48
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.32	0.47
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.96	0.47
2:G:45:ARG:HG2	2:G:443:LEU:HD21	1.95	0.47
2:G:4571:PHE:O	2:G:4575:PHE:N	2.47	0.47
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.96	0.47
2:I:1863:LEU:HB3	2:I:1870:VAL:HG21	1.96	0.47
2:B:1808:ARG:HD2	2:B:1854:PHE:HA	1.96	0.47
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.96	0.47
2:E:256:ALA:HB1	2:E:286:THR:HG21	1.95	0.47
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.95	0.47
2:I:2868:SER:O	2:I:2872:GLN:N	2.44	0.47
2:I:4036:VAL:HG11	2:I:5035:GLN:HB3	1.95	0.47
2:I:4957:LYS:HZ1	2:I:4957:LYS:HB2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.95	0.47
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.32	0.47
2:B:2447:LYS:HG3	2:B:2449:GLU:H	1.80	0.47
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.78	0.47
2:E:1730:MET:O	2:E:1772:ARG:NH1	2.47	0.47
2:E:4763:GLY:O	2:E:4766:THR:OG1	2.31	0.47
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.96	0.47
2:G:4036:VAL:HG11	2:G:5035:GLN:HB3	1.95	0.47
2:I:2447:LYS:HG3	2:I:2449:GLU:H	1.79	0.47
2:I:4230:LYS:CD	2:I:4959:PHE:HE1	2.20	0.47
1:A:27:THR:HB	1:A:100:ASP:HB3	1.97	0.47
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.96	0.47
1:F:27:THR:HB	1:F:100:ASP:HB3	1.97	0.47
2:G:2758:PHE:O	2:G:2762:THR:N	2.46	0.47
2:G:4957:LYS:NZ	2:G:4957:LYS:CB	2.77	0.47
2:G:4230:LYS:CD	2:G:4959:PHE:HE1	2.20	0.47
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.95	0.47
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.96	0.47
2:B:2104:ARG:HA	2:B:2107:GLN:HB3	1.95	0.47
2:G:2104:ARG:HA	2:G:2107:GLN:HB3	1.95	0.47
2:G:2143:THR:O	2:G:3651:ASN:ND2	2.39	0.47
2:G:2447:LYS:HG3	2:G:2449:GLU:H	1.79	0.47
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.32	0.47
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.96	0.47
2:B:2143:THR:O	2:B:3651:ASN:ND2	2.39	0.47
2:B:45:ARG:HG2	2:B:443:LEU:HD21	1.95	0.47
2:E:1808:ARG:HD2	2:E:1854:PHE:HA	1.96	0.47
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	1.95	0.47
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.84	0.47
2:I:164:ARG:N	2:I:167:ASP:OD2	2.46	0.47
2:B:164:ARG:N	2:B:167:ASP:OD2	2.46	0.47
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.95	0.47
2:E:2447:LYS:HG3	2:E:2449:GLU:H	1.80	0.47
2:G:3760:LYS:NZ	2:G:5000:GLU:OE1	2.41	0.47
2:B:1730:MET:O	2:B:1772:ARG:NH1	2.47	0.47
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	1.95	0.47
2:G:320:LYS:NZ	2:G:381:GLU:O	2.42	0.47
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.96	0.47
2:E:243:ARG:NH1	2:E:301:VAL:O	2.43	0.47
2:I:2004:GLU:HA	2:I:2007:ASN:HD22	1.79	0.47
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.95	0.47
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.80	0.47
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.97	0.47
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.48	0.47
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.48	0.47
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.50	0.47
2:I:215:THR:HG22	2:I:273:HIS:HA	1.97	0.47
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.47	0.47
2:B:3915:ILE:O	2:B:3919:THR:N	2.47	0.47
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.47	0.47
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.96	0.47
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.50	0.47
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.95	0.47
2:I:320:LYS:NZ	2:I:381:GLU:O	2.42	0.47
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.80	0.47
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.38	0.46
2:I:1808:ARG:HD2	2:I:1854:PHE:HA	1.95	0.46
2:G:379:HIS:CD2	2:G:381:GLU:H	2.33	0.46
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.48	0.46
2:I:2327:GLY:HA2	2:I:2330:ARG:HD3	1.98	0.46
2:I:4833:ASN:HB3	2:I:4935:LEU:HD23	1.97	0.46
2:E:2327:GLY:HA2	2:E:2330:ARG:HD3	1.98	0.46
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.43	0.46
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.48	0.46
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.97	0.46
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.31	0.46
2:I:4822:THR:O	2:I:4825:THR:OG1	2.29	0.46
2:B:215:THR:HG22	2:B:273:HIS:HA	1.97	0.46
2:E:1735:ILE:HG23	2:E:1771:LEU:HD23	1.97	0.46
2:E:1863:LEU:HB3	2:E:1870:VAL:HG21	1.96	0.46
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.48	0.46
2:I:1730:MET:O	2:I:1772:ARG:NH1	2.47	0.46
2:I:379:HIS:CD2	2:I:381:GLU:H	2.33	0.46
2:I:485:SER:O	2:I:489:ASN:N	2.38	0.46
2:I:4957:LYS:NZ	2:I:4957:LYS:CB	2.77	0.46
2:B:2327:GLY:HA2	2:B:2330:ARG:HD3	1.98	0.46
2:E:215:THR:HG22	2:E:273:HIS:HA	1.97	0.46
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.98	0.46
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.48	0.46
2:E:4930:ALA:O	2:E:4934:GLY:N	2.49	0.46
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.84	0.46
1:A:55:VAL:HA	2:B:1784:ALA:HA	1.96	0.46
2:E:2758:PHE:O	2:E:2762:THR:N	2.46	0.46
2:G:215:THR:HG22	2:G:273:HIS:HA	1.97	0.46
1:J:27:THR:HB	1:J:100:ASP:HB3	1.97	0.46
2:B:243:ARG:NH1	2:B:301:VAL:O	2.43	0.46
2:B:4833:ASN:HB3	2:B:4935:LEU:HD23	1.97	0.46
1:A:92:PRO:HD3	2:B:627:PRO:HB2	1.98	0.46
2:E:1991:THR:O	2:E:1995:THR:OG1	2.34	0.46
2:G:2327:GLY:HA2	2:G:2330:ARG:HD3	1.98	0.46
2:G:4833:ASN:HB3	2:G:4935:LEU:HD23	1.97	0.46
2:G:4930:ALA:O	2:G:4934:GLY:N	2.49	0.46
2:G:940:GLY:O	2:G:1052:ASN:N	2.49	0.46
1:H:27:THR:HB	1:H:100:ASP:HB3	1.97	0.46
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	1.98	0.46
2:B:1735:ILE:HG23	2:B:1771:LEU:HD23	1.97	0.46
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.98	0.46
2:B:4957:LYS:CB	2:B:4957:LYS:NZ	2.77	0.46
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.96	0.46
2:E:1815:LEU:HD22	2:E:1845:VAL:HG21	1.98	0.46
2:I:4930:ALA:O	2:I:4934:GLY:N	2.49	0.46
2:B:841:GLY:HA2	2:B:1073:ARG:HD2	1.98	0.46
2:B:1815:LEU:HD22	2:B:1845:VAL:HG21	1.98	0.46
2:G:1991:THR:O	2:G:1995:THR:OG1	2.34	0.46
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.98	0.46
2:G:3915:ILE:O	2:G:3919:THR:N	2.47	0.46
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.98	0.46
1:H:87:HIS:H	1:H:91:ILE:HB	1.81	0.46
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.98	0.46
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.98	0.46
2:B:4822:THR:O	2:B:4825:THR:OG1	2.29	0.46
2:B:4930:ALA:O	2:B:4934:GLY:N	2.49	0.46
2:B:793:LEU:HB2	2:B:797:HIS:H	1.81	0.46
1:F:87:HIS:H	1:F:91:ILE:HB	1.81	0.46
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	1.98	0.46
2:G:1735:ILE:HG23	2:G:1771:LEU:HD23	1.97	0.46
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.97	0.46
2:G:243:ARG:NH1	2:G:301:VAL:O	2.43	0.46
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.98	0.46
2:I:940:GLY:O	2:I:1052:ASN:N	2.49	0.46
1:J:55:VAL:HA	2:I:1784:ALA:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:87:HIS:H	1:J:91:ILE:HB	1.81	0.46
2:B:3842:LEU:O	2:B:3929:SER:OG	2.33	0.45
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	1.98	0.45
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.97	0.45
2:E:451:TYR:O	2:E:474:ARG:NH1	2.47	0.45
2:I:1865:MET:HB3	2:I:1926:LEU:HB2	1.98	0.45
2:I:243:ARG:NH1	2:I:301:VAL:O	2.43	0.45
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.50	0.45
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.48	0.45
2:B:1936:LYS:O	2:B:1940:CYS:N	2.46	0.45
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.43	0.45
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.98	0.45
2:G:451:TYR:O	2:G:474:ARG:NH1	2.47	0.45
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	1.99	0.45
1:J:2:VAL:HG21	1:J:61:GLU:HB2	1.98	0.45
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.81	0.45
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.50	0.45
2:E:2347:GLU:O	2:E:2351:ASN:N	2.36	0.45
2:E:3842:LEU:O	2:E:3929:SER:OG	2.33	0.45
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.32	0.45
2:E:4822:THR:O	2:E:4825:THR:OG1	2.29	0.45
2:G:793:LEU:HB2	2:G:797:HIS:H	1.81	0.45
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.81	0.45
2:I:451:TYR:O	2:I:474:ARG:NH1	2.47	0.45
2:I:4209:GLN:HE22	2:I:4560:TYR:HE2	1.64	0.45
1:A:87:HIS:H	1:A:91:ILE:HB	1.81	0.45
2:B:1865:MET:HB3	2:B:1926:LEU:HB2	1.98	0.45
2:B:379:HIS:CD2	2:B:381:GLU:H	2.33	0.45
2:E:1865:MET:HB3	2:E:1926:LEU:HB2	1.98	0.45
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.98	0.45
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.98	0.45
2:E:4833:ASN:HB3	2:E:4935:LEU:HD23	1.97	0.45
2:G:1865:MET:HB3	2:G:1926:LEU:HB2	1.98	0.45
2:G:4978:HIS:CD2	2:G:4982:GLU:HB2	2.52	0.45
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.81	0.45
2:G:206:CYS:SG	2:G:207:SER:N	2.89	0.45
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.80	0.45
2:I:793:LEU:HB2	2:I:797:HIS:H	1.81	0.45
2:B:4763:GLY:O	2:B:4766:THR:OG1	2.31	0.45
2:E:3948:LYS:HG2	2:E:4012:LEU:HD22	1.99	0.45
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1815:LEU:HD22	2:G:1845:VAL:HG21	1.98	0.45
2:I:1735:ILE:HG23	2:I:1771:LEU:HD23	1.97	0.45
2:I:206:CYS:SG	2:I:207:SER:N	2.89	0.45
2:B:2758:PHE:O	2:B:2762:THR:N	2.46	0.45
2:B:3829:PHE:HD1	2:B:3915:ILE:HD11	1.82	0.45
2:B:940:GLY:O	2:B:1052:ASN:N	2.49	0.45
2:E:379:HIS:CD2	2:E:381:GLU:H	2.33	0.45
2:E:793:LEU:HB2	2:E:797:HIS:H	1.81	0.45
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.98	0.45
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.32	0.45
2:I:4978:HIS:CD2	2:I:4982:GLU:HB2	2.52	0.45
2:B:174:VAL:O	2:E:2452:ARG:NH1	2.50	0.45
2:B:4209:GLN:HE22	2:B:4560:TYR:HE2	1.64	0.45
2:B:4851:TYR:HD2	2:B:4920:PHE:HD1	1.65	0.45
1:F:2:VAL:HG21	1:F:61:GLU:HB2	1.98	0.45
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.81	0.45
2:I:1991:THR:O	2:I:1995:THR:OG1	2.34	0.45
2:I:3829:PHE:HD1	2:I:3915:ILE:HD11	1.82	0.45
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	1.99	0.45
2:B:1991:THR:O	2:B:1995:THR:OG1	2.34	0.45
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.82	0.45
2:B:3948:LYS:HG2	2:B:4012:LEU:HD22	1.99	0.45
2:E:206:CYS:SG	2:E:207:SER:N	2.89	0.45
2:E:4209:GLN:HE22	2:E:4560:TYR:HE2	1.64	0.45
2:G:3948:LYS:HG2	2:G:4012:LEU:HD22	1.99	0.45
2:I:1815:LEU:HD22	2:I:1845:VAL:HG21	1.98	0.45
2:B:451:TYR:O	2:B:474:ARG:NH1	2.47	0.45
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.98	0.45
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.99	0.45
2:G:485:SER:O	2:G:489:ASN:N	2.38	0.45
2:I:3842:LEU:O	2:I:3929:SER:OG	2.33	0.45
1:A:2:VAL:HG21	1:A:61:GLU:HB2	1.98	0.44
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.98	0.44
2:B:3971:GLY:N	2:B:4032:GLU:OE2	2.50	0.44
2:E:1105:ALA:N	2:E:1189:LEU:O	2.51	0.44
2:E:1731:LEU:HA	2:E:1772:ARG:HH12	1.82	0.44
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	1.99	0.44
2:E:3829:PHE:HD1	2:E:3915:ILE:HD11	1.82	0.44
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.82	0.44
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.98	0.44
2:I:4851:TYR:HD2	2:I:4920:PHE:HD1	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:5028:PHE:O	2:I:5028:PHE:CG	2.70	0.44
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.38	0.44
2:B:1731:LEU:HA	2:B:1772:ARG:HH12	1.82	0.44
2:B:379:HIS:NE2	2:B:381:GLU:OE1	2.50	0.44
2:E:940:GLY:O	2:E:1052:ASN:N	2.49	0.44
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	2.00	0.44
2:G:1730:MET:O	2:G:1772:ARG:NH1	2.47	0.44
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.82	0.44
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.32	0.44
2:E:257:ARG:O	2:E:284:HIS:NE2	2.48	0.44
2:E:4571:PHE:O	2:E:4575:PHE:N	2.47	0.44
2:G:4209:GLN:HE22	2:G:4560:TYR:HE2	1.64	0.44
2:I:1078:GLU:HB3	2:I:1081:TYR:HD2	1.82	0.44
2:I:2143:THR:O	2:I:3651:ASN:ND2	2.39	0.44
2:B:1105:ALA:N	2:B:1189:LEU:O	2.51	0.44
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	2.00	0.44
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	2.00	0.44
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	1.99	0.44
2:B:4978:HIS:CD2	2:B:4982:GLU:HB2	2.52	0.44
2:E:5028:PHE:CG	2:E:5028:PHE:O	2.70	0.44
2:G:1731:LEU:HA	2:G:1772:ARG:HH12	1.83	0.44
2:B:1663:HIS:O	2:B:1667:LEU:N	2.51	0.44
2:B:206:CYS:SG	2:B:207:SER:N	2.89	0.44
2:B:5028:PHE:CG	2:B:5028:PHE:O	2.70	0.44
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.99	0.44
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	1.99	0.44
2:G:3842:LEU:O	2:G:3929:SER:OG	2.33	0.44
1:H:2:VAL:HG21	1:H:61:GLU:HB2	1.98	0.44
2:I:3948:LYS:HG2	2:I:4012:LEU:HD22	1.99	0.44
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	1.99	0.44
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.98	0.44
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	2.00	0.44
2:E:379:HIS:NE2	2:E:381:GLU:OE1	2.50	0.44
2:G:379:HIS:NE2	2:G:381:GLU:OE1	2.50	0.44
2:B:2452:ARG:NH1	2:I:174:VAL:O	2.50	0.44
2:I:379:HIS:NE2	2:I:381:GLU:OE1	2.50	0.44
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	1.99	0.44
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	2.00	0.44
2:B:2793:PRO:HG3	2:B:2855:TYR:CZ	2.53	0.44
2:E:4843:LEU:HD22	2:E:4928:LEU:HD11	2.00	0.44
2:E:4851:TYR:HD2	2:E:4920:PHE:HD1	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1105:ALA:N	2:G:1189:LEU:O	2.51	0.44
2:G:143:GLY:HA3	2:G:147:TRP:HE1	1.83	0.44
2:G:898:ASP:HB3	2:G:901:LYS:HB2	2.00	0.44
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.98	0.44
2:I:897:ARG:HB2	2:I:905:PRO:HG3	2.00	0.44
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	2.00	0.44
2:B:1802:ILE:HG21	2:B:1807:LEU:HD22	2.00	0.44
2:B:282:ILE:HD12	2:B:314:PHE:HD2	1.83	0.44
2:B:4571:PHE:O	2:B:4575:PHE:N	2.47	0.44
2:E:1802:ILE:HG21	2:E:1807:LEU:HD22	2.00	0.44
2:E:2793:PRO:HG3	2:E:2855:TYR:CZ	2.53	0.44
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	2.00	0.44
2:G:4851:TYR:HD2	2:G:4920:PHE:HD1	1.65	0.44
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	1.99	0.43
2:B:897:ARG:HB2	2:B:905:PRO:HG3	2.00	0.43
2:E:143:GLY:HA3	2:E:147:TRP:HE1	1.83	0.43
2:E:4978:HIS:CD2	2:E:4982:GLU:HB2	2.52	0.43
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	2.00	0.43
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	2.00	0.43
2:G:4673:ARG:HH12	2:G:4698:LYS:HE3	1.83	0.43
2:G:4822:THR:O	2:G:4825:THR:OG1	2.29	0.43
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.83	0.43
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.99	0.43
2:I:4673:ARG:HH12	2:I:4698:LYS:HE3	1.83	0.43
1:A:82:TYR:O	1:A:86:GLY:N	2.51	0.43
2:B:1078:GLU:HB3	2:B:1081:TYR:HD2	1.82	0.43
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.42	0.43
2:B:4956:THR:O	2:B:4965:SER:N	2.42	0.43
2:E:4680:LYS:HD3	2:E:4686:LEU:HD22	2.00	0.43
1:F:87:HIS:HA	1:F:88:PRO:HD3	1.90	0.43
2:E:174:VAL:O	2:G:2452:ARG:NH1	2.51	0.43
2:G:4843:LEU:HD22	2:G:4928:LEU:HD11	2.00	0.43
2:G:606:LEU:O	2:G:617:ASN:ND2	2.51	0.43
2:G:897:ARG:HB2	2:G:905:PRO:HG3	2.00	0.43
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	2.00	0.43
2:I:1802:ILE:HG21	2:I:1807:LEU:HD22	2.00	0.43
2:I:606:LEU:O	2:I:617:ASN:ND2	2.51	0.43
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.99	0.43
2:B:4996:ILE:HG12	4:B:5102:CFF:H123	2.00	0.43
2:B:606:LEU:O	2:B:617:ASN:ND2	2.51	0.43
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1802:ILE:HG21	2:G:1807:LEU:HD22	2.00	0.43
2:G:282:ILE:HD12	2:G:314:PHE:HD2	1.83	0.43
2:G:3829:PHE:HD1	2:G:3915:ILE:HD11	1.82	0.43
2:G:5028:PHE:O	2:G:5028:PHE:CG	2.70	0.43
2:I:898:ASP:HB3	2:I:901:LYS:HB2	2.00	0.43
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.83	0.43
2:E:282:ILE:HD12	2:E:314:PHE:HD2	1.83	0.43
2:E:897:ARG:HB2	2:E:905:PRO:HG3	2.00	0.43
1:F:82:TYR:O	1:F:86:GLY:N	2.51	0.43
2:G:1663:HIS:O	2:G:1667:LEU:N	2.51	0.43
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	1.99	0.43
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	2.00	0.43
2:I:446:GLN:HA	2:I:449:ILE:HD12	2.01	0.43
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	2.00	0.43
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.49	0.43
2:E:606:LEU:O	2:E:617:ASN:ND2	2.51	0.43
2:E:898:ASP:HB3	2:E:901:LYS:HB2	2.00	0.43
2:G:1154:ASP:O	2:G:1158:ASN:N	2.52	0.43
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.52	0.43
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	1.99	0.43
2:I:1731:LEU:HA	2:I:1772:ARG:HH12	1.82	0.43
2:I:2793:PRO:HG3	2:I:2855:TYR:CZ	2.53	0.43
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	1.99	0.43
1:J:92:PRO:HD3	2:I:627:PRO:HB2	1.99	0.43
2:B:4843:LEU:HD22	2:B:4928:LEU:HD11	2.00	0.43
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.82	0.43
2:E:4673:ARG:HH12	2:E:4698:LYS:HE3	1.83	0.43
2:G:1078:GLU:HB3	2:G:1081:TYR:HD2	1.82	0.43
2:G:446:GLN:HA	2:G:449:ILE:HD12	2.01	0.43
2:I:1154:ASP:O	2:I:1158:ASN:N	2.52	0.43
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.52	0.43
2:I:4843:LEU:HD22	2:I:4928:LEU:HD11	2.00	0.43
2:I:534:ARG:NH2	2:I:573:GLU:OE2	2.52	0.43
2:B:4673:ARG:HH12	2:B:4698:LYS:HE3	1.83	0.43
2:E:485:SER:O	2:E:489:ASN:N	2.38	0.43
2:G:1936:LYS:O	2:G:1940:CYS:N	2.46	0.43
2:E:1078:GLU:HB3	2:E:1081:TYR:HD2	1.82	0.43
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	2.00	0.43
2:E:278:GLN:N	2:E:315:CYS:SG	2.92	0.43
2:E:446:GLN:HA	2:E:449:ILE:HD12	2.01	0.43
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:101:LEU:HB3	2:I:150:MET:HE1	2.01	0.43
2:I:2823:ILE:HG12	2:I:2937:VAL:HG22	2.01	0.43
2:E:1032:LYS:O	2:E:1036:ARG:N	2.47	0.43
2:E:2823:ILE:HG12	2:E:2937:VAL:HG22	2.01	0.43
2:E:4957:LYS:HB2	2:E:4957:LYS:HZ1	1.83	0.43
2:E:689:THR:H	2:E:778:PHE:HE2	1.67	0.43
2:I:3362:UNK:O	2:I:3366:UNK:N	2.52	0.43
2:I:3915:ILE:O	2:I:3919:THR:N	2.47	0.43
2:B:1973:GLN:O	2:B:1977:TYR:N	2.44	0.43
2:B:446:GLN:HA	2:B:449:ILE:HD12	2.01	0.43
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	2.00	0.43
2:E:2869:ARG:HA	2:E:2872:GLN:HB3	2.01	0.43
2:E:4996:ILE:HG12	4:E:5102:CFF:H123	2.00	0.43
2:B:1708:ARG:HG2	2:B:1711:TYR:CE2	2.54	0.42
2:E:1936:LYS:O	2:E:1940:CYS:N	2.46	0.42
2:E:2342:ASN:N	2:E:2342:ASN:OD1	2.53	0.42
2:E:3362:UNK:O	2:E:3366:UNK:N	2.52	0.42
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.49	0.42
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.83	0.42
2:G:1708:ARG:HG2	2:G:1711:TYR:CE2	2.54	0.42
2:G:2823:ILE:HG12	2:G:2937:VAL:HG22	2.01	0.42
2:G:2793:PRO:HG3	2:G:2855:TYR:CZ	2.53	0.42
2:I:4767:TRP:HE3	2:I:4770:SER:HB2	1.84	0.42
2:I:689:THR:H	2:I:778:PHE:HE2	1.66	0.42
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.84	0.42
2:B:898:ASP:HB3	2:B:901:LYS:HB2	2.00	0.42
2:E:1708:ARG:HG2	2:E:1711:TYR:CE2	2.54	0.42
2:G:534:ARG:NH2	2:G:573:GLU:OE2	2.52	0.42
2:G:734:GLY:O	2:G:736:HIS:ND1	2.52	0.42
2:I:143:GLY:HA3	2:I:147:TRP:HE1	1.83	0.42
2:I:1973:GLN:O	2:I:1977:TYR:N	2.44	0.42
2:B:143:GLY:HA3	2:B:147:TRP:HE1	1.83	0.42
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.52	0.42
2:B:2869:ARG:HA	2:B:2872:GLN:HB3	2.01	0.42
2:B:3889:GLN:HE22	2:B:3963:ASN:HB3	1.85	0.42
2:G:2869:ARG:HA	2:G:2872:GLN:HB3	2.01	0.42
2:G:3362:UNK:O	2:G:3366:UNK:N	2.52	0.42
2:I:1105:ALA:N	2:I:1189:LEU:O	2.51	0.42
2:I:2138:LEU:HD11	2:I:3654:LEU:HD11	2.01	0.42
2:I:4996:ILE:HG12	4:I:5102:CFF:H123	2.00	0.42
1:J:82:TYR:O	1:J:86:GLY:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:HIS:O	2:B:399:GLN:NE2	2.53	0.42
2:B:3362:UNK:O	2:B:3366:UNK:N	2.52	0.42
2:B:465:GLN:HG3	2:B:3710:LEU:HB3	2.02	0.42
2:B:3809:ASN:HB3	2:B:3812:VAL:HG22	2.01	0.42
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.52	0.42
2:E:2138:LEU:HD11	2:E:3654:LEU:HD11	2.01	0.42
2:E:4634:GLU:HG3	2:E:4636:THR:H	1.84	0.42
2:G:4996:ILE:HG12	4:G:5102:CFF:H123	2.00	0.42
1:H:87:HIS:HA	1:H:88:PRO:HD3	1.90	0.42
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	2.00	0.42
2:B:2823:ILE:HG12	2:B:2937:VAL:HG22	2.01	0.42
2:E:113:HIS:O	2:E:399:GLN:NE2	2.53	0.42
2:E:3365:UNK:O	2:E:3369:UNK:N	2.53	0.42
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.40	0.42
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.84	0.42
1:H:82:TYR:O	1:H:86:GLY:N	2.51	0.42
2:I:1663:HIS:O	2:I:1667:LEU:N	2.51	0.42
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	2.01	0.42
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	2.02	0.42
2:I:3365:UNK:O	2:I:3369:UNK:N	2.53	0.42
2:I:681:HIS:HB3	2:I:784:SER:HB3	2.02	0.42
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	2.01	0.42
2:B:4688:ILE:HG21	2:B:4728:HIS:HB3	2.01	0.42
2:B:4984:ASN:C	2:B:4986:ALA:H	2.23	0.42
2:E:1154:ASP:O	2:E:1158:ASN:N	2.52	0.42
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.85	0.42
2:E:932:LEU:HA	2:E:935:LEU:HD12	2.02	0.42
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.53	0.42
2:I:1236:THR:OG1	2:I:1608:MET:SD	2.77	0.42
2:I:1936:LYS:O	2:I:1940:CYS:N	2.46	0.42
2:I:3809:ASN:HB3	2:I:3812:VAL:HG22	2.01	0.42
2:B:1154:ASP:O	2:B:1158:ASN:N	2.52	0.42
2:B:3365:UNK:O	2:B:3369:UNK:N	2.53	0.42
2:B:500:ALA:HB1	2:B:504:ALA:HB2	2.02	0.42
2:E:1124:PHE:HB2	2:E:1162:PHE:CE2	2.55	0.42
2:B:4736:ARG:NH1	2:E:4079:ASP:OD1	2.53	0.42
2:E:670:GLU:HG3	2:E:787:VAL:HG13	2.01	0.42
2:G:932:LEU:HA	2:G:935:LEU:HD12	2.02	0.42
2:I:282:ILE:HD12	2:I:314:PHE:HD2	1.83	0.42
2:B:2138:LEU:HD11	2:B:3654:LEU:HD11	2.01	0.42
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3677:LEU:O	2:B:3698:LEU:N	2.52	0.42
2:G:3365:UNK:O	2:G:3369:UNK:N	2.53	0.42
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.53	0.42
2:I:1124:PHE:HB2	2:I:1162:PHE:CE2	2.55	0.42
2:I:2466:LEU:HA	2:I:2469:ILE:HD12	2.01	0.42
2:I:465:GLN:HG3	2:I:3710:LEU:HB3	2.02	0.42
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.53	0.42
2:I:4075:GLU:HA	2:I:4078:GLN:HB2	2.02	0.42
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.32	0.42
2:B:2342:ASN:N	2:B:2342:ASN:OD1	2.53	0.42
2:B:4767:TRP:HE3	2:B:4770:SER:HB2	1.84	0.42
2:B:689:THR:H	2:B:778:PHE:HE2	1.67	0.42
2:B:681:HIS:HB3	2:B:784:SER:HB3	2.02	0.42
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.83	0.42
2:E:500:ALA:HB1	2:E:504:ALA:HB2	2.02	0.42
2:G:1236:THR:OG1	2:G:1608:MET:SD	2.77	0.42
2:G:278:GLN:N	2:G:315:CYS:SG	2.92	0.42
2:G:4075:GLU:HA	2:G:4078:GLN:HB2	2.02	0.42
2:G:4767:TRP:HE3	2:G:4770:SER:HB2	1.84	0.42
2:I:3971:GLY:N	2:I:4032:GLU:OE2	2.50	0.42
2:I:4688:ILE:HG21	2:I:4728:HIS:HB3	2.01	0.42
2:I:4749:GLU:HA	2:I:4752:ALA:HB3	2.02	0.42
1:A:87:HIS:HA	1:A:88:PRO:HD3	1.90	0.42
2:B:1124:PHE:HB2	2:B:1162:PHE:CE2	2.55	0.42
2:B:551:LEU:HD21	2:B:589:LEU:HB2	2.02	0.42
2:E:3889:GLN:HE22	2:E:3963:ASN:HB3	1.85	0.42
2:G:1124:PHE:HB2	2:G:1162:PHE:CE2	2.55	0.42
2:G:614:VAL:HA	2:G:2169:GLN:HB3	2.02	0.42
2:G:3809:ASN:HB3	2:G:3812:VAL:HG22	2.01	0.42
2:G:3971:GLY:N	2:G:4032:GLU:OE2	2.50	0.42
2:I:1032:LYS:O	2:I:1036:ARG:N	2.47	0.42
2:B:4749:GLU:HA	2:B:4752:ALA:HB3	2.02	0.41
2:B:670:GLU:HG3	2:B:787:VAL:HG13	2.01	0.41
2:E:3809:ASN:HB3	2:E:3812:VAL:HG22	2.01	0.41
2:E:3915:ILE:O	2:E:3919:THR:N	2.47	0.41
2:E:4228:ALA:O	2:E:4232:GLU:N	2.52	0.41
2:E:465:GLN:HG3	2:E:3710:LEU:HB3	2.02	0.41
2:E:681:HIS:HB3	2:E:784:SER:HB3	2.02	0.41
2:G:2466:LEU:HA	2:G:2469:ILE:HD12	2.01	0.41
2:G:3889:GLN:HE22	2:G:3963:ASN:HB3	1.85	0.41
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2452:ARG:NH1	2:G:174:VAL:O	2.53	0.41
2:B:278:GLN:N	2:B:315:CYS:SG	2.92	0.41
2:B:4634:GLU:HG3	2:B:4636:THR:H	1.84	0.41
2:E:790:ARG:HG2	2:E:1627:ALA:HA	2.01	0.41
2:E:614:VAL:HA	2:E:2169:GLN:HB3	2.02	0.41
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	2.01	0.41
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	2.02	0.41
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	2.01	0.41
2:G:2138:LEU:HD11	2:G:3654:LEU:HD11	2.01	0.41
2:G:4080:TYR:CZ	2:G:4096:ALA:HB3	2.55	0.41
2:I:4634:GLU:HG3	2:I:4636:THR:H	1.84	0.41
2:B:1141:ARG:H	2:B:1141:ARG:HD2	1.85	0.41
2:B:790:ARG:HG2	2:B:1627:ALA:HA	2.01	0.41
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	2.01	0.41
2:B:614:VAL:HA	2:B:2169:GLN:HB3	2.02	0.41
2:B:2466:LEU:HA	2:B:2469:ILE:HD12	2.01	0.41
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.53	0.41
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	2.01	0.41
2:E:2466:LEU:HA	2:E:2469:ILE:HD12	2.01	0.41
2:E:4075:GLU:HA	2:E:4078:GLN:HB2	2.01	0.41
2:E:4688:ILE:HG21	2:E:4728:HIS:HB3	2.01	0.41
2:G:113:HIS:O	2:G:399:GLN:NE2	2.53	0.41
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.86	0.41
2:G:288:GLY:HA3	2:G:405:HIS:CE1	2.56	0.41
2:I:1025:ARG:O	2:I:1032:LYS:NZ	2.38	0.41
2:I:3889:GLN:HE22	2:I:3963:ASN:HB3	1.85	0.41
2:I:870:ILE:HD12	2:I:870:ILE:HA	1.92	0.41
2:B:1236:THR:OG1	2:B:1608:MET:SD	2.77	0.41
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.86	0.41
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.86	0.41
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.53	0.41
2:E:3971:GLY:N	2:E:4032:GLU:OE2	2.50	0.41
2:E:4586:PRO:HA	2:E:4628:VAL:HG11	2.02	0.41
2:G:1728:ARG:HA	2:G:1731:LEU:HB2	2.03	0.41
2:G:4749:GLU:HA	2:G:4752:ALA:HB3	2.02	0.41
2:G:4984:ASN:C	2:G:4986:ALA:H	2.23	0.41
2:G:681:HIS:HB3	2:G:784:SER:HB3	2.02	0.41
2:G:689:THR:H	2:G:778:PHE:HE2	1.66	0.41
2:I:1708:ARG:HG2	2:I:1711:TYR:CE2	2.54	0.41
2:I:614:VAL:HA	2:I:2169:GLN:HB3	2.02	0.41
2:I:2869:ARG:HA	2:I:2872:GLN:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.86	0.41
2:I:4865:LYS:HG3	2:I:4875:LYS:HZ3	1.84	0.41
2:G:1032:LYS:O	2:G:1036:ARG:N	2.47	0.41
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.52	0.41
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.53	0.41
2:I:4863:TYR:HD2	2:I:4875:LYS:HB2	1.86	0.41
2:I:4984:ASN:C	2:I:4986:ALA:H	2.23	0.41
2:I:5027:CYS:O	2:I:5027:CYS:SG	2.79	0.41
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.40	0.41
2:B:1032:LYS:O	2:B:1036:ARG:N	2.47	0.41
2:B:1728:ARG:HA	2:B:1731:LEU:HB2	2.03	0.41
2:E:288:GLY:HA3	2:E:405:HIS:CE1	2.56	0.41
2:E:320:LYS:NZ	2:E:381:GLU:O	2.42	0.41
2:E:4749:GLU:HA	2:E:4752:ALA:HB3	2.02	0.41
2:E:734:GLY:O	2:E:736:HIS:ND1	2.52	0.41
2:G:3694:LYS:HA	2:G:3695:PRO:HD3	1.95	0.41
2:G:4688:ILE:HG21	2:G:4728:HIS:HB3	2.01	0.41
2:G:5027:CYS:SG	2:G:5027:CYS:O	2.79	0.41
2:I:113:HIS:O	2:I:399:GLN:NE2	2.53	0.41
2:I:4014:LYS:HE2	2:I:4135:PRO:HG3	2.03	0.41
2:I:670:GLU:HG3	2:I:787:VAL:HG13	2.02	0.41
2:I:790:ARG:HG2	2:I:1627:ALA:HA	2.01	0.41
1:J:87:HIS:HA	1:J:88:PRO:HD3	1.90	0.41
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.53	0.41
2:B:4075:GLU:HA	2:B:4078:GLN:HB2	2.02	0.41
2:E:1728:ARG:HA	2:E:1731:LEU:HB2	2.03	0.41
2:E:2871:LEU:HD22	2:E:2927:LEU:HD22	2.02	0.41
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.53	0.41
2:E:4080:TYR:CZ	2:E:4096:ALA:HB3	2.55	0.41
2:E:4014:LYS:HE2	2:E:4135:PRO:HG3	2.03	0.41
2:E:698:GLY:HA2	2:E:703:GLY:HA2	2.03	0.41
2:G:1247:PRO:HA	2:G:1598:GLN:HA	2.03	0.41
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	2.01	0.41
2:G:465:GLN:HG3	2:G:3710:LEU:HB3	2.02	0.41
2:G:500:ALA:HB1	2:G:504:ALA:HB2	2.02	0.41
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.86	0.41
2:E:1663:HIS:O	2:E:1667:LEU:N	2.51	0.41
2:E:3706:SER:OG	2:E:3781:GLN:NE2	2.54	0.41
2:B:4914:VAL:HG23	2:E:4888:TYR:CD1	2.56	0.41
2:G:790:ARG:HG2	2:G:1627:ALA:HA	2.01	0.41
2:G:4863:TYR:HD2	2:G:4875:LYS:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.85	0.41
2:I:2871:LEU:HD22	2:I:2927:LEU:HD22	2.02	0.41
2:I:500:ALA:HB1	2:I:504:ALA:HB2	2.02	0.41
2:I:932:LEU:HA	2:I:935:LEU:HD12	2.02	0.41
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.49	0.41
2:B:698:GLY:HA2	2:B:703:GLY:HA2	2.03	0.41
2:E:1141:ARG:HD2	2:E:1141:ARG:H	1.85	0.41
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	2.02	0.41
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.86	0.41
2:E:4767:TRP:HE3	2:E:4770:SER:HB2	1.84	0.41
2:E:534:ARG:NH2	2:E:573:GLU:OE2	2.52	0.41
2:G:4586:PRO:HA	2:G:4628:VAL:HG11	2.02	0.41
2:G:670:GLU:HG3	2:G:787:VAL:HG13	2.02	0.41
2:I:4586:PRO:HA	2:I:4628:VAL:HG11	2.02	0.41
2:B:4014:LYS:HE2	2:B:4135:PRO:HG3	2.03	0.41
2:G:1141:ARG:HD2	2:G:1141:ARG:H	1.85	0.41
2:I:1728:ARG:HA	2:I:1731:LEU:HB2	2.03	0.41
2:I:257:ARG:O	2:I:284:HIS:NE2	2.48	0.41
2:B:2871:LEU:HD22	2:B:2927:LEU:HD22	2.02	0.41
2:B:288:GLY:HA3	2:B:405:HIS:CE1	2.56	0.41
2:E:470:SER:O	2:E:474:ARG:NE	2.50	0.41
2:E:4956:THR:O	2:E:4965:SER:N	2.42	0.41
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	2.03	0.41
2:G:113:HIS:CE1	2:G:402:ARG:HB3	2.56	0.41
2:G:42:PHE:HD1	2:G:447:ASP:HB3	1.86	0.41
2:G:551:LEU:HD21	2:G:589:LEU:HB2	2.02	0.41
2:I:288:GLY:HA3	2:I:405:HIS:CE1	2.56	0.41
2:I:4080:TYR:CZ	2:I:4096:ALA:HB3	2.55	0.41
2:B:4957:LYS:HZ1	2:B:4957:LYS:HB2	1.82	0.40
2:E:113:HIS:CE1	2:E:402:ARG:HB3	2.56	0.40
2:E:551:LEU:HD21	2:E:589:LEU:HB2	2.02	0.40
2:E:582:HIS:O	2:E:585:SER:OG	2.30	0.40
2:E:870:ILE:HD11	2:E:1049:TYR:CG	2.56	0.40
2:G:1973:GLN:O	2:G:1977:TYR:N	2.44	0.40
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	2.02	0.40
2:G:2871:LEU:HD22	2:G:2927:LEU:HD22	2.02	0.40
2:G:4929:LEU:HA	2:G:4929:LEU:HD13	1.92	0.40
2:I:870:ILE:HD11	2:I:1049:TYR:CG	2.56	0.40
2:I:551:LEU:HD21	2:I:589:LEU:HB2	2.02	0.40
2:B:3706:SER:OG	2:B:3781:GLN:NE2	2.54	0.40
2:B:113:HIS:CE1	2:B:402:ARG:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4080:TYR:CZ	2:B:4096:ALA:HB3	2.55	0.40
2:B:42:PHE:HD1	2:B:447:ASP:HB3	1.86	0.40
2:B:582:HIS:O	2:B:585:SER:OG	2.30	0.40
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.87	0.40
2:B:932:LEU:HA	2:B:935:LEU:HD12	2.02	0.40
2:E:877:ASN:HD22	2:E:1045:THR:HG23	1.87	0.40
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.87	0.40
2:G:4634:GLU:HG3	2:G:4636:THR:H	1.84	0.40
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	2.02	0.40
2:B:3847:PHE:HE1	2:B:3950:ASN:HD22	1.70	0.40
2:B:5027:CYS:O	2:B:5027:CYS:SG	2.79	0.40
2:B:5028:PHE:CD1	2:B:5028:PHE:O	2.75	0.40
2:B:734:GLY:O	2:B:736:HIS:ND1	2.52	0.40
2:E:1247:PRO:HA	2:E:1598:GLN:HA	2.03	0.40
2:E:1679:ASN:HA	2:E:1682:ALA:HB3	2.03	0.40
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	2.04	0.40
2:E:42:PHE:HD1	2:E:447:ASP:HB3	1.86	0.40
2:E:4987:ASN:HA	2:E:4990:PHE:HD2	1.87	0.40
2:E:5028:PHE:O	2:E:5028:PHE:CD1	2.75	0.40
2:E:662:TRP:HZ3	2:E:811:CYS:HA	1.87	0.40
2:G:3891:LEU:HB3	2:G:3899:PHE:CE2	2.55	0.40
2:G:864:PRO:HD2	2:G:867:LEU:HD12	2.03	0.40
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.87	0.40
2:B:4586:PRO:HA	2:B:4628:VAL:HG11	2.02	0.40
2:B:870:ILE:HA	2:B:870:ILE:HD12	1.92	0.40
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	2.02	0.40
2:E:1705:GLY:HA2	2:E:1709:ALA:HB3	2.04	0.40
2:E:3677:LEU:O	2:E:3698:LEU:N	2.52	0.40
2:E:5027:CYS:O	2:E:5027:CYS:SG	2.79	0.40
2:E:629:ARG:HD3	2:E:634:GLN:HG2	2.04	0.40
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	2.04	0.40
2:G:4014:LYS:HE2	2:G:4135:PRO:HG3	2.03	0.40
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.49	0.40
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	2.01	0.40
2:I:2029:GLN:O	2:I:2033:ASP:N	2.48	0.40
2:I:2298:VAL:HA	2:I:2301:TYR:HB2	2.03	0.40
2:I:3805:LEU:HG	2:I:3805:LEU:H	1.77	0.40
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.86	0.40
2:B:3891:LEU:HB3	2:B:3899:PHE:CE2	2.55	0.40
2:B:534:ARG:NH2	2:B:573:GLU:OE2	2.52	0.40
2:E:4863:TYR:HD2	2:E:4875:LYS:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:864:PRO:HA	2:E:865:PRO:HD3	1.93	0.40
2:G:2298:VAL:HA	2:G:2301:TYR:HB2	2.03	0.40
2:G:2368:LEU:HD13	2:G:2376:LEU:HD23	2.04	0.40
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.86	0.40
2:G:629:ARG:HD3	2:G:634:GLN:HG2	2.04	0.40
2:G:698:GLY:HA2	2:G:703:GLY:HA2	2.03	0.40
2:G:870:ILE:HD11	2:G:1049:TYR:CG	2.56	0.40
2:I:278:GLN:N	2:I:315:CYS:SG	2.92	0.40
2:I:42:PHE:HD1	2:I:447:ASP:HB3	1.86	0.40
2:I:698:GLY:HA2	2:I:703:GLY:HA2	2.03	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%)	94 (90%)	11 (10%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	B	3235/4416 (73%)	2890 (89%)	339 (10%)	6 (0%)	52	86
2	E	3235/4416 (73%)	2894 (90%)	335 (10%)	6 (0%)	52	86
2	G	3235/4416 (73%)	2890 (89%)	339 (10%)	6 (0%)	52	86
2	I	3235/4416 (73%)	2891 (89%)	338 (10%)	6 (0%)	52	86
All	All	13360/18096 (74%)	11941 (89%)	1395 (10%)	24 (0%)	56	86

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5028	PHE
2	E	5028	PHE
2	I	5028	PHE
2	G	5028	PHE
2	B	1708	ARG
2	E	1708	ARG
2	I	1708	ARG
2	G	1708	ARG
2	B	1932	PRO
2	B	4641	PRO
2	B	4985	LEU
2	E	1932	PRO
2	E	4641	PRO
2	E	4985	LEU
2	I	1932	PRO
2	I	4641	PRO
2	I	4985	LEU
2	G	1932	PRO
2	G	4641	PRO
2	G	4985	LEU
2	B	1840	PRO
2	E	1840	PRO
2	I	1840	PRO
2	G	1840	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	2493/3022 (82%)	2473 (99%)	20 (1%)	86 93
2	E	2493/3022 (82%)	2473 (99%)	20 (1%)	86 93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	G	2493/3022 (82%)	2473 (99%)	20 (1%)	86 93
2	I	2493/3022 (82%)	2473 (99%)	20 (1%)	86 93
All	All	10324/12444 (83%)	10244 (99%)	80 (1%)	87 93

All (80) 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	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	4137	ARG
2	B	4913	ARG
2	B	4957	LYS
2	B	4959	PHE
2	B	4960	ILE
2	B	4983	HIS
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
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

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Mol	Chain	Res	Type
2	E	4137	ARG
2	E	4913	ARG
2	E	4957	LYS
2	E	4959	PHE
2	E	4960	ILE
2	E	4983	HIS
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
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	4137	ARG
2	I	4913	ARG
2	I	4957	LYS
2	I	4959	PHE
2	I	4960	ILE
2	I	4983	HIS
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
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	4137	ARG
2	G	4913	ARG

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Mol	Chain	Res	Type
2	G	4957	LYS
2	G	4959	PHE
2	G	4960	ILE
2	G	4983	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (149) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	25	HIS
1	F	87	HIS
1	A	25	HIS
1	A	87	HIS
1	H	25	HIS
1	H	87	HIS
1	J	25	HIS
1	J	87	HIS
2	B	57	ASN
2	B	111	HIS
2	B	113	HIS
2	B	273	HIS
2	B	379	HIS
2	B	383	HIS
2	B	395	GLN
2	B	405	HIS
2	B	413	GLN
2	B	520	ASN
2	B	797	HIS
2	B	838	HIS
2	B	1598	GLN
2	B	1679	ASN
2	B	1691	GLN
2	B	1693	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	2005	GLN
2	B	2007	ASN
2	B	2127	GLN
2	B	2291	GLN
2	B	3809	ASN
2	B	3889	GLN
2	B	3896	ASN
2	B	3946	GLN

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Mol	Chain	Res	Type
2	B	3950	ASN
2	B	3960	GLN
2	B	3976	ASN
2	B	4034	ASN
2	B	4054	ASN
2	B	4120	ASN
2	B	4142	ASN
2	B	4209	GLN
2	B	4806	ASN
2	B	4933	GLN
2	E	57	ASN
2	E	111	HIS
2	E	113	HIS
2	E	273	HIS
2	E	379	HIS
2	E	383	HIS
2	E	395	GLN
2	E	405	HIS
2	E	413	GLN
2	E	520	ASN
2	E	797	HIS
2	E	838	HIS
2	E	1598	GLN
2	E	1679	ASN
2	E	1691	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	2005	GLN
2	E	2127	GLN
2	E	2291	GLN
2	E	3809	ASN
2	E	3889	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	3976	ASN
2	E	4034	ASN
2	E	4054	ASN
2	E	4120	ASN
2	E	4142	ASN
2	E	4201	ASN

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Mol	Chain	Res	Type
2	E	4209	GLN
2	E	4806	ASN
2	E	4933	GLN
2	I	57	ASN
2	I	111	HIS
2	I	113	HIS
2	I	273	HIS
2	I	379	HIS
2	I	383	HIS
2	I	395	GLN
2	I	405	HIS
2	I	413	GLN
2	I	520	ASN
2	I	797	HIS
2	I	838	HIS
2	I	1598	GLN
2	I	1679	ASN
2	I	1691	GLN
2	I	1693	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	2127	GLN
2	I	2291	GLN
2	I	3809	ASN
2	I	3889	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	3976	ASN
2	I	4034	ASN
2	I	4054	ASN
2	I	4120	ASN
2	I	4142	ASN
2	I	4201	ASN
2	I	4209	GLN
2	I	4806	ASN
2	I	4933	GLN
2	G	57	ASN
2	G	111	HIS
2	G	113	HIS
2	G	273	HIS

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Mol	Chain	Res	Type
2	G	379	HIS
2	G	383	HIS
2	G	395	GLN
2	G	405	HIS
2	G	413	GLN
2	G	520	ASN
2	G	797	HIS
2	G	838	HIS
2	G	1598	GLN
2	G	1679	ASN
2	G	1691	GLN
2	G	1693	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	2127	GLN
2	G	2291	GLN
2	G	3809	ASN
2	G	3889	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	3976	ASN
2	G	4034	ASN
2	G	4054	ASN
2	G	4120	ASN
2	G	4142	ASN
2	G	4201	ASN
2	G	4209	GLN
2	G	4806	ASN
2	G	4933	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
3	ATP	B	5101	-	26,33,33	0.88	1 (3%)	26,52,52	1.77	1 (3%)
4	CFF	B	5102	-	8,15,15	2.49	3 (37%)	8,23,23	1.16	1 (12%)
3	ATP	E	5101	-	26,33,33	0.88	1 (3%)	26,52,52	1.77	1 (3%)
4	CFF	E	5102	-	8,15,15	2.47	3 (37%)	8,23,23	1.15	1 (12%)
3	ATP	G	5101	-	26,33,33	0.88	1 (3%)	26,52,52	1.77	1 (3%)
4	CFF	G	5102	-	8,15,15	2.47	3 (37%)	8,23,23	1.16	1 (12%)
3	ATP	I	5101	-	26,33,33	0.87	1 (3%)	26,52,52	1.77	1 (3%)
4	CFF	I	5102	-	8,15,15	2.49	3 (37%)	8,23,23	1.15	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	B	5102	-	-	0/0/0/0	0/2/2/2
3	ATP	E	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	E	5102	-	-	0/0/0/0	0/2/2/2
3	ATP	G	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	G	5102	-	-	0/0/0/0	0/2/2/2
3	ATP	I	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	I	5102	-	-	0/0/0/0	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	5102	CFF	C4-N3	-4.93	1.33	1.39
4	B	5102	CFF	C4-N3	-4.88	1.33	1.39
4	E	5102	CFF	C4-N3	-4.82	1.33	1.39
4	G	5102	CFF	C4-N3	-4.81	1.33	1.39
4	E	5102	CFF	C6-N1	-3.88	1.32	1.38
4	B	5102	CFF	C6-N1	-3.87	1.32	1.38
4	G	5102	CFF	C6-N1	-3.85	1.32	1.38
4	I	5102	CFF	C6-N1	-3.81	1.32	1.38
4	E	5102	CFF	O13-C6	-2.32	1.18	1.24
4	I	5102	CFF	O13-C6	-2.32	1.18	1.24
4	G	5102	CFF	O13-C6	-2.32	1.18	1.24
4	B	5102	CFF	O13-C6	-2.32	1.18	1.24
3	I	5101	ATP	C5-C4	2.70	1.46	1.40
3	B	5101	ATP	C5-C4	2.72	1.46	1.40
3	G	5101	ATP	C5-C4	2.72	1.46	1.40
3	E	5101	ATP	C5-C4	2.74	1.46	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	5101	ATP	N3-C2-N1	-7.16	123.24	128.87
3	I	5101	ATP	N3-C2-N1	-7.14	123.26	128.87
3	B	5101	ATP	N3-C2-N1	-7.14	123.26	128.87
3	E	5101	ATP	N3-C2-N1	-7.14	123.26	128.87
4	E	5102	CFF	C14-N7-C8	-2.58	111.86	125.31
4	B	5102	CFF	C14-N7-C8	-2.57	111.88	125.31
4	I	5102	CFF	C14-N7-C8	-2.57	111.91	125.31
4	G	5102	CFF	C14-N7-C8	-2.57	111.91	125.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	ATP	1	0
4	B	5102	CFF	1	0
3	E	5101	ATP	1	0
4	E	5102	CFF	1	0
3	G	5101	ATP	1	0
4	G	5102	CFF	1	0
3	I	5101	ATP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	5102	CFF	1	0

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	14
2	B	14
2	I	14
2	E	14

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	72.44
1	E	4345:UNK	C	4540:PHE	N	72.44
1	I	4345:UNK	C	4540:PHE	N	72.44
1	G	4345:UNK	C	4540:PHE	N	72.44
1	B	3613:UNK	C	3639:THR	N	42.93
1	E	3613:UNK	C	3639:THR	N	42.93
1	I	3613:UNK	C	3639:THR	N	42.93
1	G	3613:UNK	C	3639:THR	N	42.93
1	B	4253:GLU	C	4320:UNK	N	27.35
1	E	4253:GLU	C	4320:UNK	N	27.35
1	I	4253:GLU	C	4320:UNK	N	27.35
1	G	4253:GLU	C	4320:UNK	N	27.35
1	B	3163:UNK	C	3170:UNK	N	16.17
1	E	3163:UNK	C	3170:UNK	N	16.17
1	I	3163:UNK	C	3170:UNK	N	16.17
1	G	3163:UNK	C	3170:UNK	N	16.17
1	B	3063:UNK	C	3134:UNK	N	14.81
1	E	3063:UNK	C	3134:UNK	N	14.81
1	I	3063:UNK	C	3134:UNK	N	14.81
1	G	3063:UNK	C	3134:UNK	N	14.81
1	B	2703:UNK	C	2734:ASN	N	14.74
1	E	2703:UNK	C	2734:ASN	N	14.74

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	2703:UNK	C	2734:ASN	N	14.74
1	G	2703:UNK	C	2734:ASN	N	14.74
1	B	3468:UNK	C	3511:UNK	N	14.16
1	E	3468:UNK	C	3511:UNK	N	14.16
1	I	3468:UNK	C	3511:UNK	N	14.16
1	G	3468:UNK	C	3511:UNK	N	14.16
1	B	3236:UNK	C	3241:UNK	N	13.24
1	E	3236:UNK	C	3241:UNK	N	13.24
1	I	3236:UNK	C	3241:UNK	N	13.24
1	G	3236:UNK	C	3241:UNK	N	13.24
1	B	2976:UNK	C	2995:UNK	N	12.70
1	E	2976:UNK	C	2995:UNK	N	12.70
1	I	2976:UNK	C	2995:UNK	N	12.70
1	G	2976:UNK	C	2995:UNK	N	12.70
1	B	1564:UNK	C	1573:MET	N	12.34
1	E	1564:UNK	C	1573:MET	N	12.34
1	I	1564:UNK	C	1573:MET	N	12.34
1	G	1564:UNK	C	1573:MET	N	12.34
1	B	3254:UNK	C	3261:UNK	N	8.53
1	E	3254:UNK	C	3261:UNK	N	8.53
1	I	3254:UNK	C	3261:UNK	N	8.53
1	G	3254:UNK	C	3261:UNK	N	8.53
1	B	1297:UNK	C	1430:UNK	N	6.12
1	E	1297:UNK	C	1430:UNK	N	6.12
1	I	1297:UNK	C	1430:UNK	N	6.12
1	G	1297:UNK	C	1430:UNK	N	6.12
1	B	2479:LEU	C	2487:UNK	N	3.24
1	E	2479:LEU	C	2487:UNK	N	3.24
1	I	2479:LEU	C	2487:UNK	N	3.24
1	G	2479:LEU	C	2487:UNK	N	3.24
1	B	2939:ARG	C	2942:UNK	N	3.23
1	E	2939:ARG	C	2942:UNK	N	3.23
1	G	2939:ARG	C	2942:UNK	N	3.23
1	I	2939:ARG	C	2942:UNK	N	3.22