wwPDB EM Map/Model Validation Report (i)

Oct 17, 2016 – 09:22 PM EDT

PDB ID	:	5TA3
EMDB ID:	:	EMD-8377
Title	:	Structure of rabbit RyR1 (Caffeine/ATP/Ca2+ dataset, class 2)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-09
Resolution	:	4.40 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

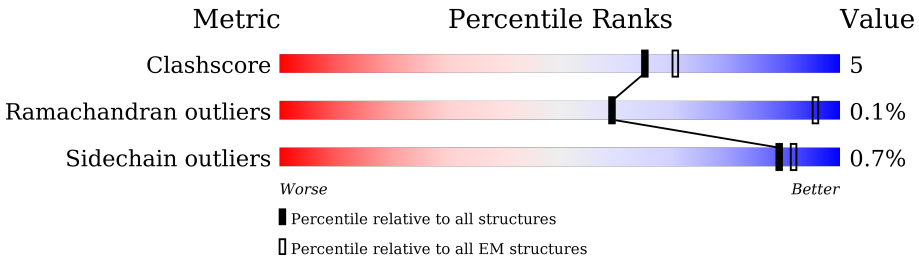
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 4.40 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	76% 23% .
1	F	108	72% 27% .
1	H	108	73% 26% .
1	J	108	71% 28% .
2	B	4416	84% 11% 5%
2	E	4416	84% 11% 5%
2	G	4416	84% 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.

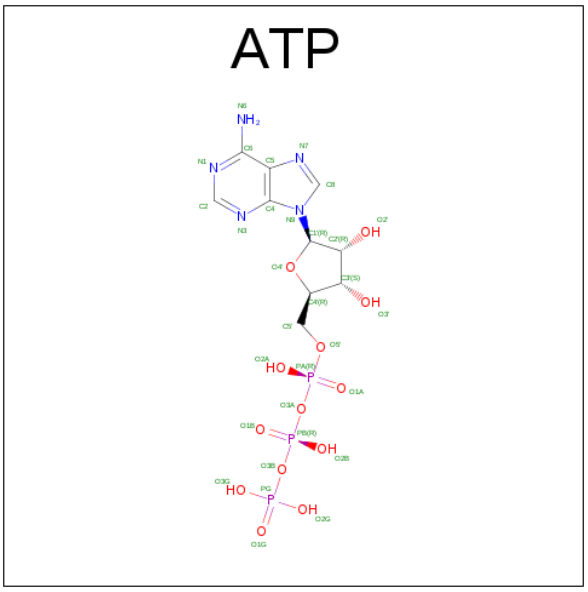
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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.

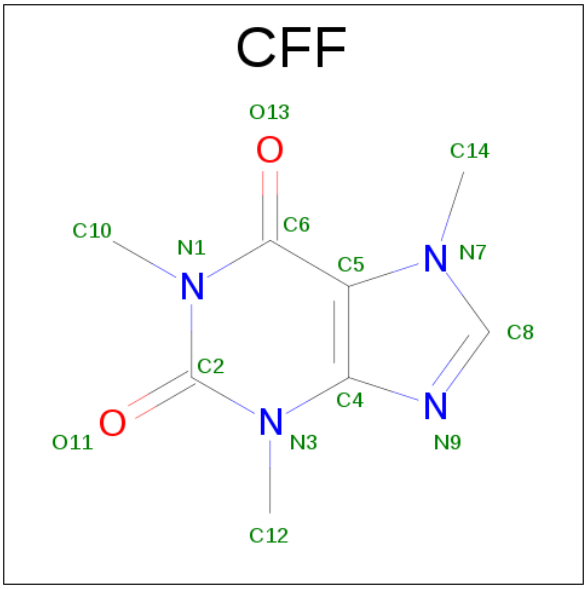
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- 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	G	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	E	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	G	1	Total	C	N	O	0
			14	8	4	2	
4	I	1	Total	C	N	O	0
			14	8	4	2	
4	E	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).

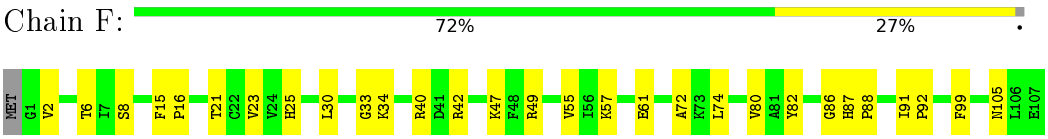
Mol	Chain	Residues	Atoms		AltConf
6	G	1	Total	Ca	0
			1	1	
6	B	1	Total	Ca	0
			1	1	
6	I	1	Total	Ca	0
			1	1	
6	E	1	Total	Ca	0
			1	1	

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.

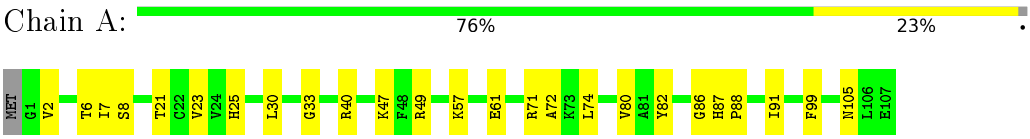
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



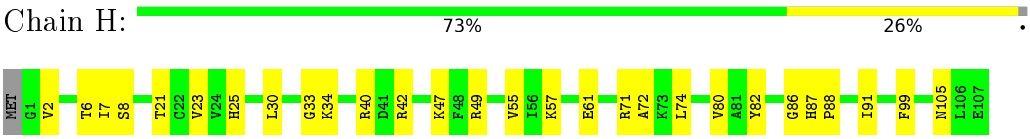
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



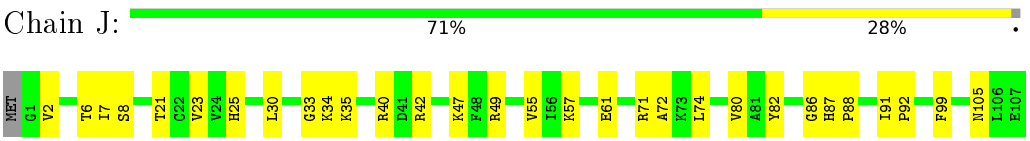
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



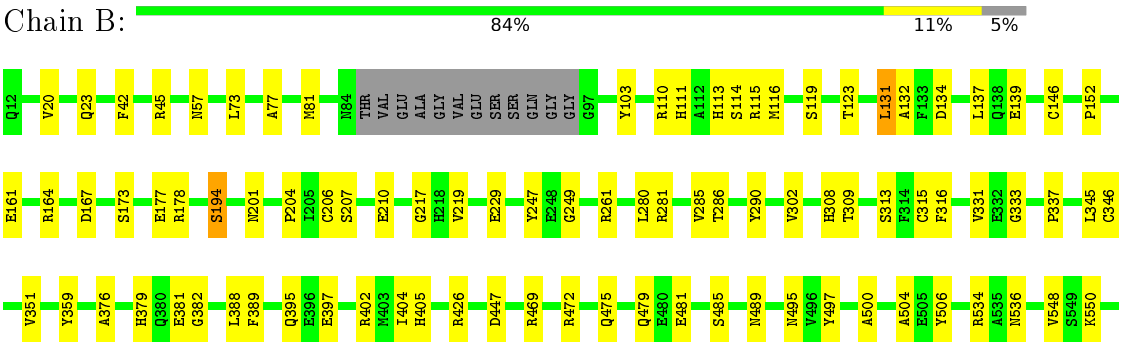
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

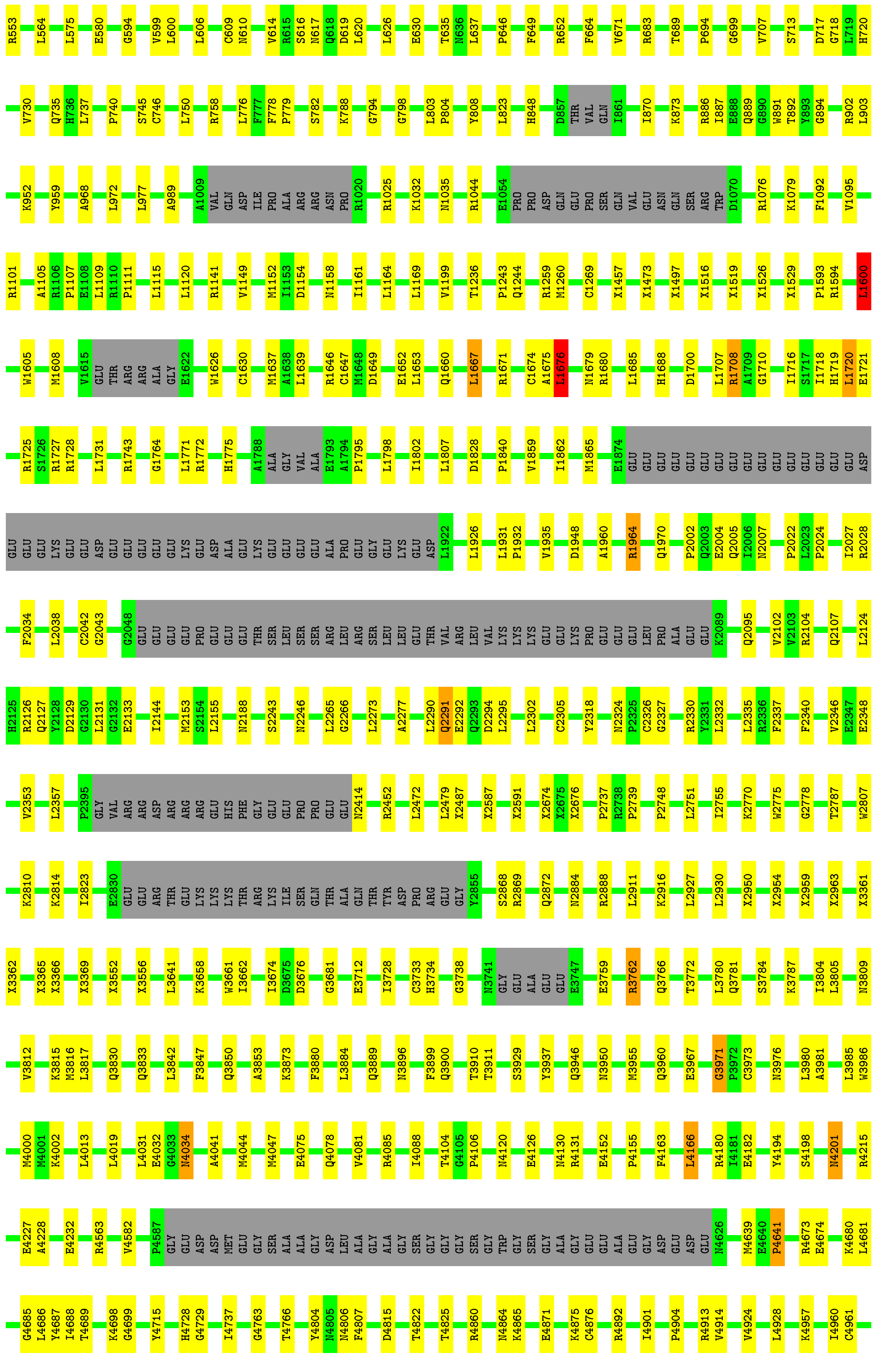
Chain J:



- Molecule 2: Ryanodine receptor 1

Chain B:




R553 L564 L575 E580 G594 V599 L600 L606 C609 N610 V614 R615 S616 N617 Q618 D619 L620 L626 E630 T635 N636 L637 P646 F649 R652 F664 V671 R683 T689 P694 G699 V707 S713 D717 G718 L719 H720
V730 Q735 H736 L737 P740 S745 C746 L750 R758 L776 F777 F778 P779 S782 K788 G794 G798 L803 P804 Y808 L823 H848 D857 THR VAL GLN I861 I870 K873 R886 I887 E888 Q889 G890 W891 T892 Y893 G894 R902 L903
K952 Y959 A968 L972 L977 A989 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO R1020 R1025 K1032 N1035 R1044 E1054 PRO PRO ASP GLN GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1076 K1079 F1092 V1095
R1101 A1105 R1106 P1107 E1108 L1109 R1110 P1111 L1115 L1120 R1141 V1149 M1152 I1153 D1154 N1158 I1161 L1164 L1169 V1199 T1236 P1243 Q1244 R1259 M1260 C1269 X1457 X1473 X1497 X1516 X1519 X1526 X1529 P1593 R1594 L1600
W1605 M1608 V1615 GLU THR ARG ARG ALA GLY E1622 W1626 C1630 M1637 A1638 L1639 R1646 C1647 M1648 D1649 E1652 L1653 Q1660 L1667 R1671 C1674 A1675 L1676 N1679 R1680 L1685 H1688 D1700 L1707 R1708 A1709 G1710 I1716 S1717 I1718 H1719 L1720 E1721
R1725 S1726 R1727 R1728 L1731 R1743 G1764 L1771 R1772 H1775 A1788 ALA GLY VAL ALA E1793 A1794 P1795 L1798 I1802 L1807 D1828 P1840 V1859 I1862 M1865 E1874 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 ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 L1926 L1931 P1932 V1935 D1948 A1960 R1964 Q1970 P2002 Q2003 E2004 Q2005 I2006 N2007 P2022 L2023 P2024 I2027 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 Q2095 V2102 V2103 R2104 Q2107 L2124
H2125 R2126 Q2127 Y2128 D2129 G2130 L2131 G2132 E2133 I2144 M2153 S2154 L2155 N2188 S2243 N2246 L2265 G2266 L2273 A2277 L2290 Q2291 E2292 Q2293 D2294 L2295 L2302 C2305 Y2318 N2324 P2325 C2326 G2327 R2330 Y2331 L2332 L2335 R2336 F2337 F2340 V2346 E2347 E2348
V2353 L2357 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 R2452 L2472 L2479 X2487 X2587 X2591 X2674 X2675 X2676 P2737 R2738 P2739 P2748 L2751 I2755 K2770 W2775 G2778 T2787 W2807
K2810 K2814 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 S2868 R2869 Q2872 N2884 R2888 L2911 K2916 L2927 L2930 X2950 X2954 X2959 X2963 X3361
X3362 X3365 X3366 X3369 X3552 X3556 L3641 K3658 W3661 I3662 I3674 D3675 D3676 G3681 E3712 I3728 C3733 H3734 G3738 N3741 GLY GLU ALA GLU GLU E3747 E3759 R3762 Q3766 T3772 L3780 Q3781 S3784 K3787 I3804 L3805 N3809
V3812 K3815 M3816 L3817 Q3830 Q3833 L3842 F3847 Q3850 A3853 K3873 F3880 L3884 Q3889 N3896 F3899 Q3900 T3910 T3911 S3929 Y3937 Q3946 N3950 M3955 Q3960 E3967 G3971 P3972 C3973 N3976 L3980 A3981 L3985 W3986
M4000 M4001 K4002 L4013 L4019 L4031 E4032 G4033 N4034 A4041 M4044 M4047 E4075 Q4078 V4081 R4085 I4088 T4104 G4105 P4106 N4120 E4126 N4130 R4131 E4152 P4155 F4163 L4166 R4180 I4181 E4182 Y4194 S4198 N4201 R4215
E4227 A4228 E4232 R4563 V4582 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 M4639 E4640 P4641 R4673 E4674 K4680 L4681
G4685 L4686 Y4687 I4688 T4689 K4698 G4699 Y4715 H4728 G4729 I4737 G4763 T4766 Y4804 N4805 N4806 F4807 D4815 T4822 T4825 R4860 N4864 K4865 E4871 K4875 C4876 R4892 I4901 P4904 R4913 V4914 V4924 L4928 K4957 I4960 C4961

G4964 E4981 E4982 H4983 N4984 L4985 M4993 I4996 G5005 R5017 L5036 S5037

- Molecule 2: Ryanodine receptor 1

Chain G: 84% 11% 5%

Q12 V20 Q23 F42 R45 N57 L73 A77 M81 N84 THR VAL GLU ALA GLY VAL GLU SER SER GLN GLY GLY G97 Y103 R110 H111 A112 H113 S114 R115 M116 S119 T123 L131 A132 F133 D134 L137 Q138 E139 C146 P152

R164 D167 S173 R178 S194 N201 P204 I205 C206 S207 E210 G217 H218 V219 E229 G249 R261 L280 R281 V285 T286 Y290 V302 H308 T309 S313 F314 C315 F316 V331 E332 G333 P337 L345 V351 Y359 A376

H379 Q380 E381 G382 F389 Q395 E396 E397 R402 M403 I404 H405 R426 D447 R469 Q479 E480 E481 S485 N489 N495 V496 Y497 A500 A504 E505 Y506 R534 A535 N536 V548 S549 K550 R553 L564 L575 E580 G594 V599

L600 L606 C609 N610 V614 R615 S616 N617 Q618 D619 L620 L626 R629 E630 Q634 T635 N636 L637 P646 F649 R652 F664 V671 H681 L682 R683 T689 P694 G699 V707 S713 D717 G718 L719 H720 V730 Q735 H736 L737

P740 S745 C746 L750 R758 L776 F777 F778 P779 S782 F783 S784 K788 G794 G798 Y808 L823 H848 D857 THR VAL GLN I861 I870 K873 R886 I887 E888 Q889 G890 W891 T892 Y893 G894 R902 L903 L913 R918 K952 Y959

A968 L972 L977 T983 R987 L988 A989 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO R1020 N1035 R1044 E1054 PRO PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1076 K1079 F1092 V1095 R1101 P1107 E1108

L1109 R1110 P1111 L1115 L1120 R1141 V1149 M1152 I1153 D1154 N1158 I1161 L1164 L1169 V1199 T1236 P1243 Q1244 R1259 M1260 C1269 X1457 X1473 X1497 X1516 X1519 X1526 X1529 P1593 R1594 L1600 W1605 M1608 V1615

GLU THR ARG ARG ALA GLY E1622 W1626 C1630 M1637 A1638 L1639 R1646 C1647 M1648 D1649 E1652 L1653 Q1660 L1667 R1671 C1674 A1675 L1676 G1677 N1678 N1679 R1680 L1685 H1688 Q1691 D1700 L1707 R1708 A1709 G1710 I1716 S1717 I1718 H1719 L1720 E1721 R1725 S1726

R1727 R1728 L1731 R1743 G1764 R1772 H1775 A1784 A1788 ALA GLY VAL ALA E1793 A1794 P1795 L1798 I1802 L1807 D1828 P1840 V1859 I1862 M1865 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU

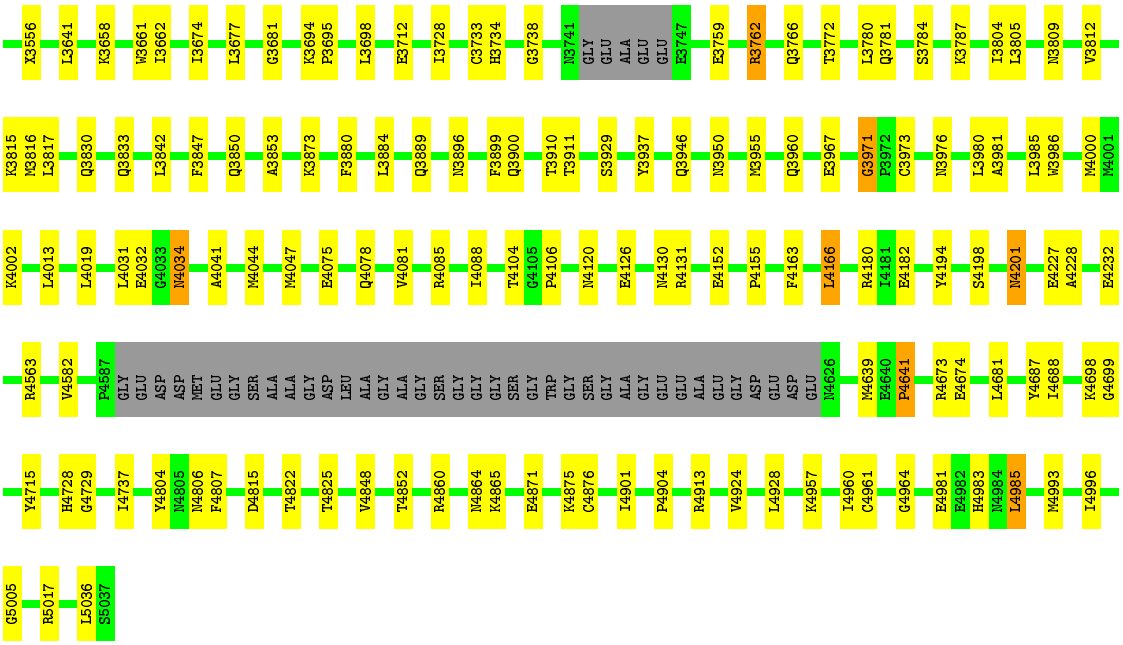
GLU LYS GLU GLU ASP GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 L1926 L1931 P1932 V1935 D1948 A1960 R1964 Q1970 P2002 Q2003 E2004 Q2005 I2006 N2007 P2022 L2023 P2024 I2027 R2028 F2034

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 Q2095 V2102 V2103 R2104 Q2107 L2124 H2125 R2126

Q2127 Y2128 D2129 G2130 L2131 G2132 E2133 L2155 N2188 S2243 N2246 L2265 G2266 L2273 A2277 L2290 Q2291 E2292 Q2293 D2294 L2295 C2305 Y2318 N2324 P2325 C2326 G2327 R2330 Y2331 L2332 L2335 R2336 F2337 F2340 V2346 E2347 E2348 V2353 L2357 P2395 GLY VAL

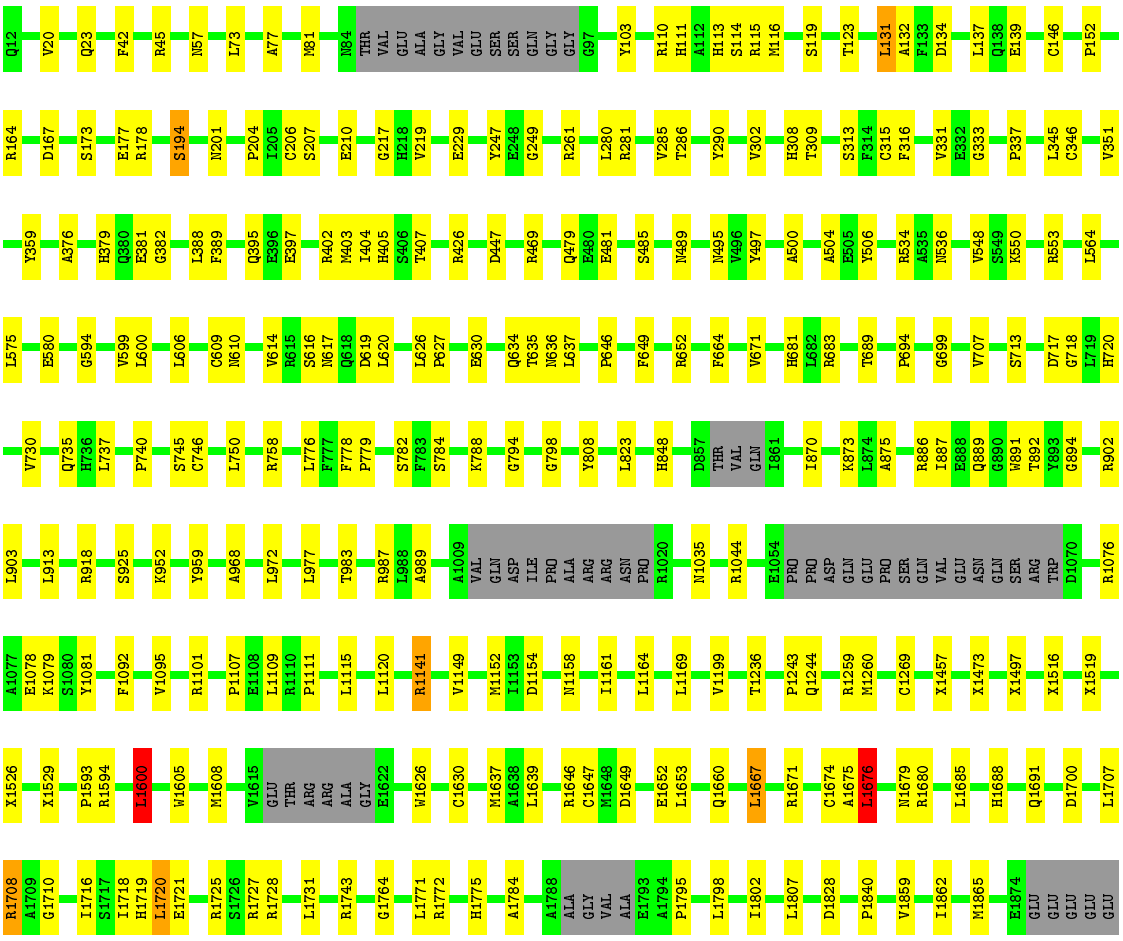
ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 I2430 R2452 L2472 L2479 X2487 X2502 P2737 R2738 P2739 P2748 L2751 I2755 K2770 W2775 G2778 T2787 W2807 K2810 K2814 I2823 E2830 GLU GLU ARG THR

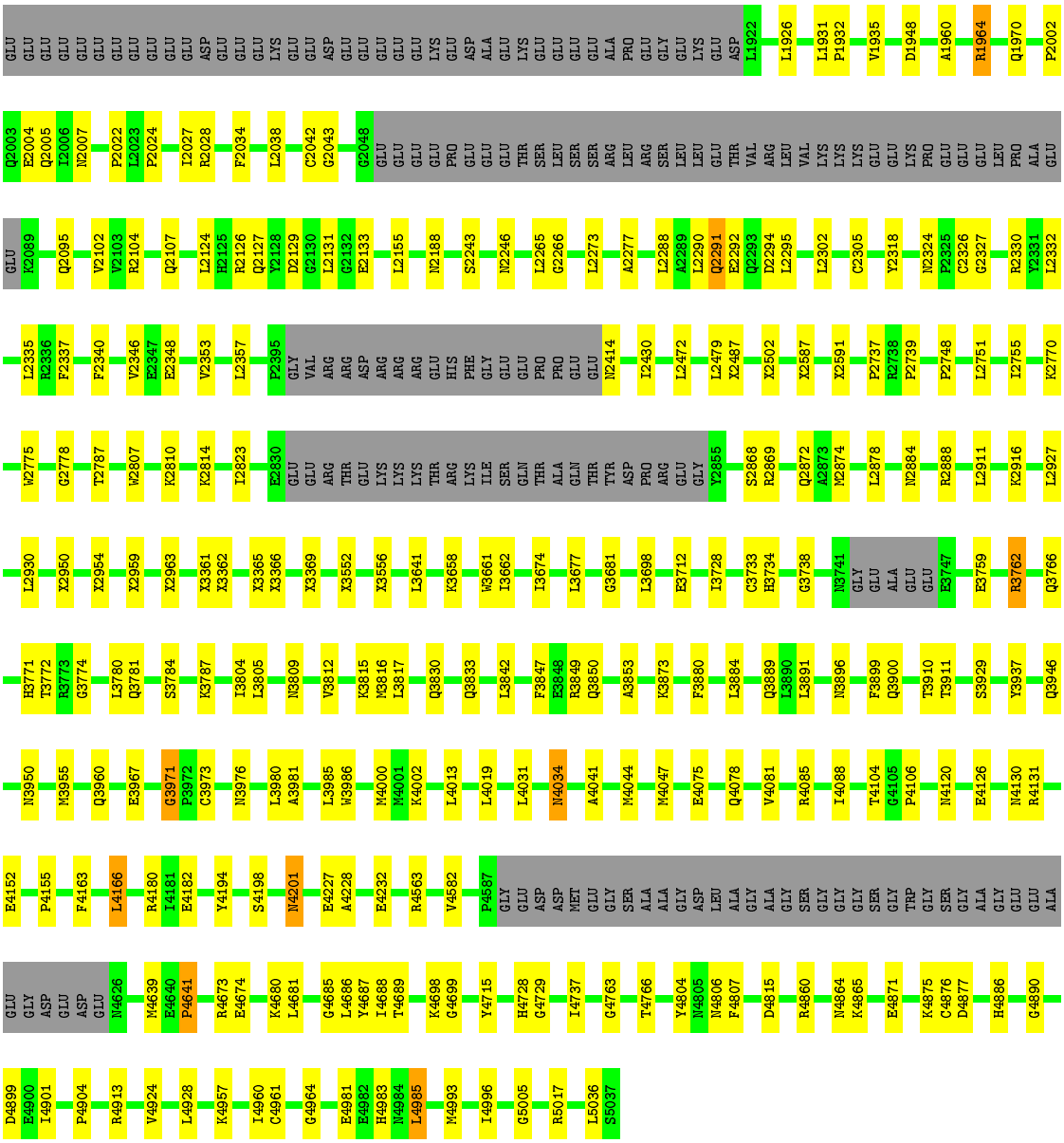
GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2855 S2868 R2869 Q2872 A2873 M2874 L2878 N2884 R2888 L2911 K2916 L2927 L2930 X2950 X2954 X2959 X2963 X3361 X3362 X3365 X3366 X3369 X3552



• Molecule 2: Ryanodine receptor 1

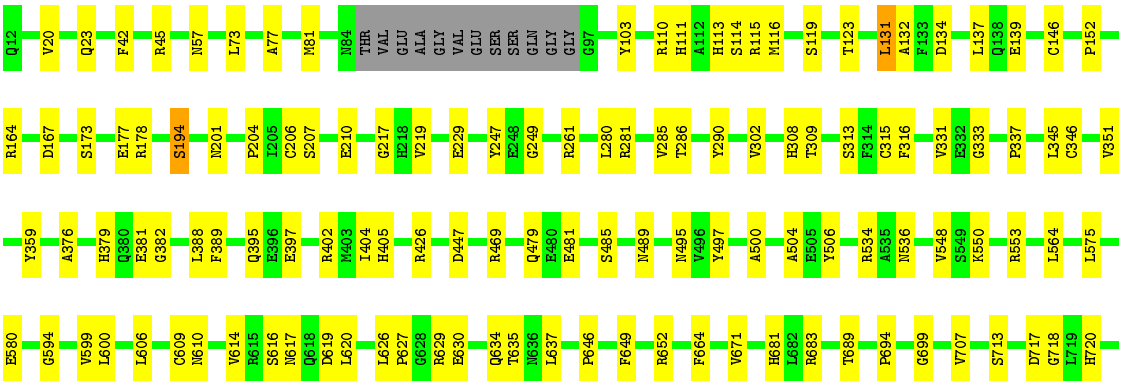
Chain I:

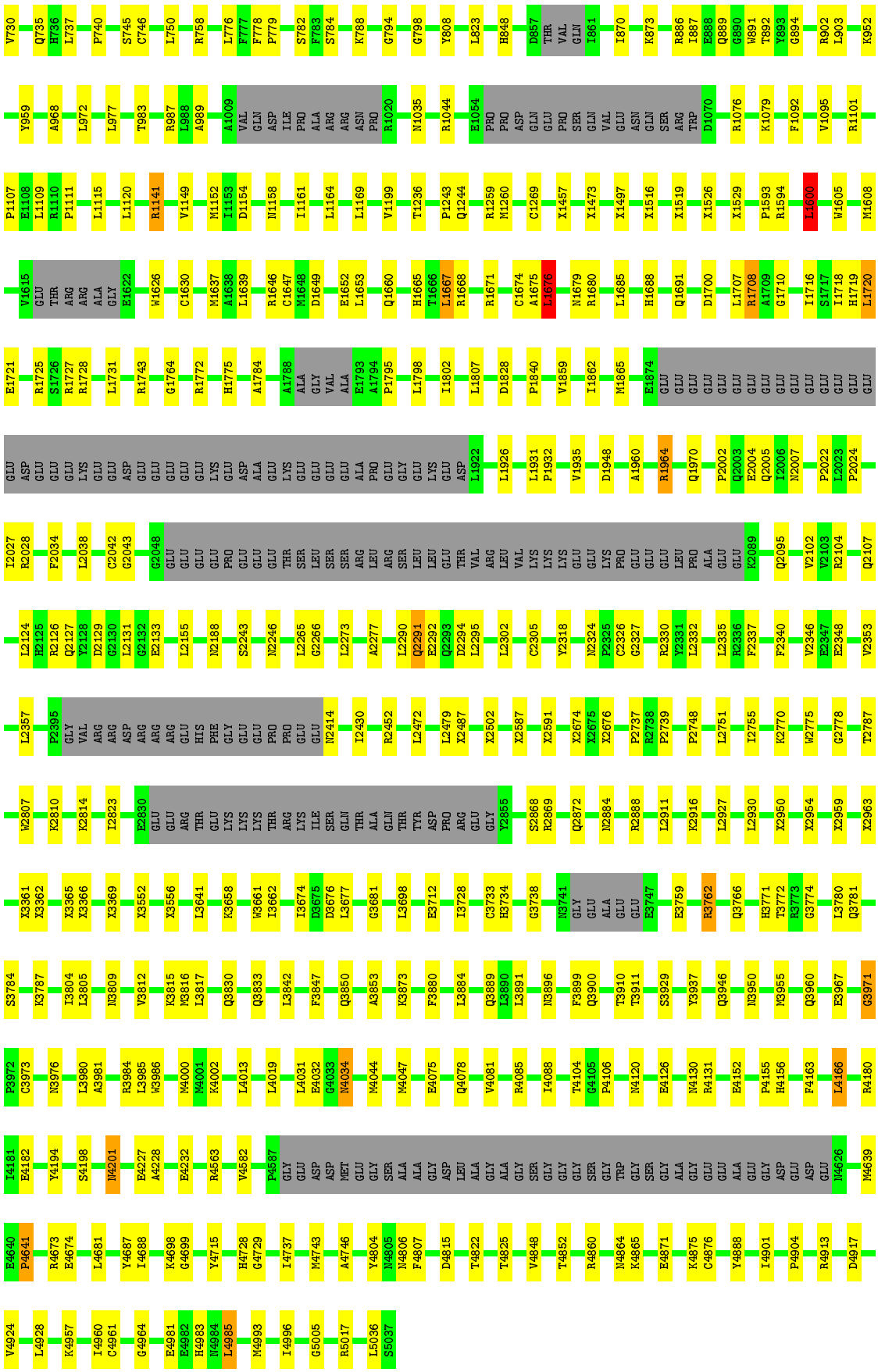




• Molecule 2: Ryanodine receptor 1

Chain E:





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	0.30	0/834	0.52	0/1123
1	F	0.30	0/834	0.52	0/1123
1	H	0.30	0/834	0.52	0/1123
1	J	0.30	0/834	0.52	0/1123
2	B	0.30	0/25428	0.54	9/34534 (0.0%)
2	E	0.30	0/25428	0.54	9/34534 (0.0%)
2	G	0.30	0/25428	0.54	9/34534 (0.0%)
2	I	0.30	0/25428	0.54	9/34534 (0.0%)
All	All	0.30	0/105048	0.54	36/142628 (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	14
2	E	0	14
2	G	0	14
2	I	0	14
All	All	0	60

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	131	LEU	CA-CB-CG	7.43	132.38	115.30
2	G	131	LEU	CA-CB-CG	7.42	132.36	115.30
2	I	131	LEU	CA-CB-CG	7.42	132.36	115.30
2	E	131	LEU	CA-CB-CG	7.41	132.34	115.30
2	G	4985	LEU	CA-CB-CG	6.93	131.25	115.30
2	E	4985	LEU	CA-CB-CG	6.93	131.24	115.30
2	B	4985	LEU	CA-CB-CG	6.92	131.22	115.30
2	I	4985	LEU	CA-CB-CG	6.92	131.21	115.30
2	B	1676	LEU	CA-CB-CG	6.56	130.40	115.30
2	G	1676	LEU	CA-CB-CG	6.56	130.39	115.30
2	E	1676	LEU	CA-CB-CG	6.56	130.38	115.30
2	I	1676	LEU	CA-CB-CG	6.54	130.34	115.30
2	I	1600	LEU	CA-CB-CG	6.10	129.34	115.30
2	B	1600	LEU	CA-CB-CG	6.10	129.32	115.30
2	E	1600	LEU	CA-CB-CG	6.09	129.31	115.30
2	G	1600	LEU	CA-CB-CG	6.09	129.30	115.30
2	B	2290	LEU	CA-CB-CG	5.55	128.07	115.30
2	G	2290	LEU	CA-CB-CG	5.55	128.08	115.30
2	E	2290	LEU	CA-CB-CG	5.55	128.06	115.30
2	I	2290	LEU	CA-CB-CG	5.53	128.02	115.30
2	I	977	LEU	CA-CB-CG	5.42	127.77	115.30
2	E	977	LEU	CA-CB-CG	5.42	127.76	115.30
2	B	977	LEU	CA-CB-CG	5.40	127.73	115.30
2	G	977	LEU	CA-CB-CG	5.40	127.72	115.30
2	G	4639	MET	C-N-CA	5.35	135.07	121.70
2	B	4639	MET	C-N-CA	5.34	135.04	121.70
2	E	4639	MET	C-N-CA	5.33	135.02	121.70
2	I	4639	MET	C-N-CA	5.32	135.01	121.70
2	G	1667	LEU	CA-CB-CG	5.27	127.43	115.30
2	I	1667	LEU	CA-CB-CG	5.27	127.42	115.30
2	B	1667	LEU	CA-CB-CG	5.26	127.40	115.30
2	E	1667	LEU	CA-CB-CG	5.26	127.39	115.30
2	G	4901	ILE	CG1-CB-CG2	-5.05	100.30	111.40
2	E	4901	ILE	CG1-CB-CG2	-5.03	100.34	111.40
2	B	4901	ILE	CG1-CB-CG2	-5.02	100.36	111.40
2	I	4901	ILE	CG1-CB-CG2	-5.02	100.36	111.40

There are no chirality outliers.

All (60) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	B	1676	LEU	Peptide
2	B	1720	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	194	SER	Peptide
2	B	2291	GLN	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	3971	GLY	Peptide
2	B	4641	PRO	Peptide
2	B	4807	PHE	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1720	LEU	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	194	SER	Peptide
2	E	2291	GLN	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	3971	GLY	Peptide
2	E	4641	PRO	Peptide
2	E	4807	PHE	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	1720	LEU	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	194	SER	Peptide
2	G	2291	GLN	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	3971	GLY	Peptide
2	G	4641	PRO	Peptide
2	G	4807	PHE	Peptide
2	G	694	PRO	Peptide
2	G	808	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	H	8	SER	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1720	LEU	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	194	SER	Peptide
2	I	2291	GLN	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	3971	GLY	Peptide
2	I	4641	PRO	Peptide
2	I	4807	PHE	Peptide
2	I	694	PRO	Peptide
2	I	808	TYR	Peptide
1	J	8	SER	Peptide

5.2 Too-close contacts

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	13	0
1	F	818	0	824	18	0
1	H	818	0	824	17	0
1	J	818	0	824	19	0
2	B	29499	0	24746	271	0
2	E	29499	0	24745	276	0
2	G	29499	0	24745	266	0
2	I	29499	0	24745	278	0
3	B	31	0	12	2	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	102365	1132	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 (1132) 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:I:4985:LEU:HB2	3:I:5101:ATP:HN61	1.52	0.74
2:B:4985:LEU:HB2	3:B:5101:ATP:HN61	1.51	0.74
2:E:4985:LEU:HB2	3:E:5101:ATP:HN61	1.51	0.73
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.71	0.73
2:G:4985:LEU:HB2	3:G:5101:ATP:HN61	1.52	0.73
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.56	0.71
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.56	0.70
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.56	0.69
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.56	0.68
2:I:2318:TYR:HH	2:I:2414:ASN:N	1.92	0.68
2:G:173:SER:HB3	2:G:178:ARG:H	1.60	0.67
2:B:2452:ARG:HH12	2:I:177:GLU:HG3	1.59	0.67
2:E:173:SER:HB3	2:E:178:ARG:H	1.60	0.67
2:E:2318:TYR:HH	2:E:2414:ASN:N	1.92	0.67
2:B:173:SER:HB3	2:B:178:ARG:H	1.60	0.66
2:B:2318:TYR:HH	2:B:2414:ASN:N	1.93	0.66
2:I:173:SER:HB3	2:I:178:ARG:H	1.60	0.66
2:G:2318:TYR:HH	2:G:2414:ASN:N	1.92	0.66
2:E:3762:ARG:O	2:E:3766:GLN:NE2	2.29	0.66
2:B:379:HIS:HD2	2:B:382:GLY:H	1.44	0.66
2:B:3762:ARG:O	2:B:3766:GLN:NE2	2.29	0.65
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.61	0.65
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.62	0.65
2:G:3762:ARG:O	2:G:3766:GLN:NE2	2.29	0.65
2:E:1259:ARG:HH12	2:E:1593:PRO:HA	1.62	0.65
2:I:3762:ARG:O	2:I:3766:GLN:NE2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:379:HIS:HD2	2:G:382:GLY:H	1.44	0.65
2:I:379:HIS:HD2	2:I:382:GLY:H	1.44	0.64
2:E:379:HIS:HD2	2:E:382:GLY:H	1.44	0.64
2:I:1259:ARG:HH12	2:I:1593:PRO:HA	1.62	0.64
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.61	0.64
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.31	0.64
2:G:4904:PRO:HB3	2:G:4913:ARG:HD3	1.80	0.64
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.62	0.64
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.61	0.63
2:I:4904:PRO:HB3	2:I:4913:ARG:HD3	1.80	0.63
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.63	0.63
2:E:4904:PRO:HB3	2:E:4913:ARG:HD3	1.80	0.63
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.62	0.63
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.31	0.63
2:B:4904:PRO:HB3	2:B:4913:ARG:HD3	1.80	0.63
2:G:1259:ARG:HH12	2:G:1593:PRO:HA	1.62	0.63
2:B:1259:ARG:HH12	2:B:1593:PRO:HA	1.62	0.63
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.63	0.63
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.64	0.63
2:B:132:ALA:HA	2:B:194:SER:HB2	1.81	0.63
2:E:132:ALA:HA	2:E:194:SER:HB2	1.81	0.62
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.32	0.62
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.64	0.62
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.64	0.62
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.31	0.62
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.82	0.62
2:I:111:HIS:HD2	2:I:114:SER:H	1.47	0.62
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.64	0.62
2:I:132:ALA:HA	2:I:194:SER:HB2	1.81	0.62
2:I:3981:ALA:HA	2:I:3986:TRP:HE1	1.65	0.62
2:B:3981:ALA:HA	2:B:3986:TRP:HE1	1.65	0.62
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.32	0.62
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.32	0.62
2:B:111:HIS:HD2	2:B:114:SER:H	1.47	0.62
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.33	0.62
2:G:132:ALA:HA	2:G:194:SER:HB2	1.81	0.62
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.82	0.62
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.32	0.62
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.33	0.62
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.64	0.62
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.82	0.62
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.64	0.61
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.82	0.61
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.82	0.61
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.82	0.61
2:G:111:HIS:HD2	2:G:114:SER:H	1.47	0.61
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.33	0.61
2:G:3981:ALA:HA	2:G:3986:TRP:HE1	1.65	0.61
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.33	0.61
2:E:3981:ALA:HA	2:E:3986:TRP:HE1	1.65	0.61
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.64	0.61
1:H:34:LYS:HD3	2:G:629:ARG:HD2	1.83	0.61
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.64	0.61
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.31	0.61
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.33	0.61
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.82	0.61
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.82	0.61
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.33	0.61
2:E:111:HIS:HD2	2:E:114:SER:H	1.47	0.60
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.82	0.60
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.82	0.60
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.83	0.60
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.33	0.60
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.84	0.60
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.84	0.60
2:I:4865:LYS:HG3	2:I:4875:LYS:HZ3	1.67	0.60
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.82	0.60
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.84	0.60
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.84	0.59
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.84	0.59
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.84	0.59
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.85	0.59
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.85	0.59
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.84	0.59
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.85	0.59
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.85	0.59
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.36	0.58
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.36	0.58
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.85	0.58
2:G:4860:ARG:HD2	2:I:4582:VAL:HG11	1.85	0.58
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.85	0.58
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.85	0.58
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.36	0.58
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.85	0.58
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.84	0.58
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.85	0.58
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.85	0.58
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.86	0.58
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.36	0.58
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.85	0.58
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.86	0.58
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.37	0.58
2:I:2107:GLN:HG3	2:I:3681:GLY:HA2	1.86	0.58
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.37	0.58
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.85	0.58
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.84	0.58
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.86	0.58
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.86	0.58
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.86	0.58
2:G:4865:LYS:HG3	2:G:4875:LYS:HZ3	1.68	0.58
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.69	0.58
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.85	0.58
2:E:2107:GLN:HG3	2:E:3681:GLY:HA2	1.86	0.58
2:G:2107:GLN:HG3	2:G:3681:GLY:HA2	1.86	0.58
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.86	0.58
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.69	0.57
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.86	0.57
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.86	0.57
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.85	0.57
2:E:4865:LYS:HG3	2:E:4875:LYS:HZ3	1.68	0.57
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.86	0.57
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.86	0.57
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.36	0.57
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.86	0.57
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.86	0.57
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.86	0.57
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.86	0.57
2:B:2107:GLN:HG3	2:B:3681:GLY:HA2	1.86	0.57
2:B:609:CYS:SG	2:B:610:ASN:N	2.78	0.57
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.87	0.57
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.87	0.56
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.87	0.56
1:J:55:VAL:HA	2:I:1784:ALA:HA	1.86	0.56
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.31	0.56
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.86	0.56
2:E:606:LEU:O	2:E:617:ASN:ND2	2.39	0.56
2:G:313:SER:HB3	2:G:351:VAL:HB	1.87	0.56
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.31	0.56
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.86	0.56
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.87	0.56
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.69	0.56
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.69	0.56
2:I:606:LEU:O	2:I:617:ASN:ND2	2.39	0.56
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.88	0.56
2:I:609:CYS:SG	2:I:610:ASN:N	2.78	0.56
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.87	0.56
2:E:609:CYS:SG	2:E:610:ASN:N	2.78	0.56
2:G:606:LEU:O	2:G:617:ASN:ND2	2.39	0.56
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.37	0.56
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.88	0.56
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.88	0.56
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.86	0.56
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.88	0.56
2:E:45:ARG:NH2	2:E:447:ASP:OD1	2.39	0.56
2:I:1731:LEU:HA	2:I:1772:ARG:HH12	1.71	0.56
2:I:4924:VAL:HA	2:I:4928:LEU:HB2	1.87	0.56
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.40	0.55
2:E:4924:VAL:HA	2:E:4928:LEU:HB2	1.87	0.55
2:E:652:ARG:HB2	2:E:750:LEU:HD13	1.88	0.55
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.40	0.55
2:B:217:GLY:O	2:B:261:ARG:NH1	2.40	0.55
2:E:1637:MET:SD	2:E:1708:ARG:NH1	2.80	0.55
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.86	0.55
2:G:609:CYS:SG	2:G:610:ASN:N	2.78	0.55
2:I:1637:MET:SD	2:I:1708:ARG:NH1	2.80	0.55
2:B:606:LEU:O	2:B:617:ASN:ND2	2.39	0.55
2:G:1731:LEU:HA	2:G:1772:ARG:HH12	1.71	0.55
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.39	0.55
2:I:652:ARG:HB2	2:I:750:LEU:HD13	1.88	0.55
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.39	0.55
2:B:2911:LEU:HB2	2:B:2916:LYS:HE3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:626:LEU:HD23	2:B:630:GLU:H	1.72	0.55
2:G:2911:LEU:HB2	2:G:2916:LYS:HE3	1.89	0.55
2:G:4924:VAL:HA	2:G:4928:LEU:HB2	1.87	0.55
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.39	0.55
2:B:313:SER:HB3	2:B:351:VAL:HB	1.87	0.55
2:B:3733:CYS:HA	2:B:3766:GLN:HG2	1.89	0.55
2:B:4924:VAL:HA	2:B:4928:LEU:HB2	1.87	0.55
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.40	0.55
2:E:313:SER:HB3	2:E:351:VAL:HB	1.88	0.55
2:I:217:GLY:O	2:I:261:ARG:NH1	2.39	0.55
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.89	0.55
2:E:217:GLY:O	2:E:261:ARG:NH1	2.39	0.55
2:E:2911:LEU:HB2	2:E:2916:LYS:HE3	1.89	0.55
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.39	0.55
2:I:2911:LEU:HB2	2:I:2916:LYS:HE3	1.89	0.55
2:E:626:LEU:HD23	2:E:630:GLU:H	1.71	0.55
2:G:3733:CYS:HA	2:G:3766:GLN:HG2	1.89	0.55
2:I:626:LEU:HD23	2:I:630:GLU:H	1.71	0.55
2:B:1731:LEU:HA	2:B:1772:ARG:HH12	1.71	0.55
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.39	0.55
2:G:217:GLY:O	2:G:261:ARG:NH1	2.39	0.55
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.31	0.55
2:G:626:LEU:HD23	2:G:630:GLU:H	1.72	0.55
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.89	0.55
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.89	0.54
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.89	0.54
2:G:1637:MET:SD	2:G:1708:ARG:NH1	2.80	0.54
2:G:315:CYS:SG	2:G:316:PHE:N	2.81	0.54
2:G:4993:MET:HA	2:G:4996:ILE:HD12	1.89	0.54
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.89	0.54
2:E:111:HIS:CD2	2:E:114:SER:H	2.25	0.54
2:G:652:ARG:HB2	2:G:750:LEU:HD13	1.88	0.54
2:B:1637:MET:SD	2:B:1708:ARG:NH1	2.80	0.54
2:B:4673:ARG:HH12	2:B:4698:LYS:HE3	1.73	0.54
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.89	0.54
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.90	0.54
2:I:3733:CYS:HA	2:I:3766:GLN:HG2	1.89	0.54
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.89	0.54
2:B:614:VAL:HG22	2:B:616:SER:H	1.72	0.54
2:E:614:VAL:HG22	2:E:616:SER:H	1.72	0.54
2:I:315:CYS:SG	2:I:316:PHE:N	2.81	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:313:SER:HB3	2:I:351:VAL:HB	1.88	0.54
2:B:111:HIS:CD2	2:B:114:SER:H	2.25	0.54
2:B:2479:LEU:O	2:B:2487:UNK:N	2.41	0.54
2:B:4993:MET:HA	2:B:4996:ILE:HD12	1.89	0.54
1:F:87:HIS:H	1:F:91:ILE:HB	1.73	0.54
1:H:87:HIS:H	1:H:91:ILE:HB	1.73	0.54
2:E:1948:ASP:OD1	2:E:2126:ARG:NH2	2.39	0.54
2:E:3733:CYS:HA	2:E:3766:GLN:HG2	1.89	0.54
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.73	0.54
2:G:614:VAL:HG22	2:G:616:SER:H	1.72	0.54
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.73	0.54
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.89	0.54
2:B:4198:SER:HB3	2:B:4201:ASN:HB2	1.90	0.54
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.73	0.54
2:B:4865:LYS:HG3	2:B:4875:LYS:HZ3	1.72	0.54
2:B:652:ARG:HB2	2:B:750:LEU:HD13	1.88	0.54
2:B:45:ARG:NH2	2:B:447:ASP:OD1	2.39	0.54
2:E:4673:ARG:HH12	2:E:4698:LYS:HE3	1.73	0.54
2:I:4993:MET:HA	2:I:4996:ILE:HD12	1.89	0.54
1:J:87:HIS:H	1:J:91:ILE:HB	1.73	0.54
1:A:87:HIS:H	1:A:91:ILE:HB	1.73	0.53
2:G:4681:LEU:HD21	2:G:4687:TYR:HD2	1.73	0.53
2:B:315:CYS:SG	2:B:316:PHE:N	2.81	0.53
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.73	0.53
2:E:1731:LEU:HA	2:E:1772:ARG:HH12	1.71	0.53
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.73	0.53
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.89	0.53
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.81	0.53
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.89	0.53
2:G:4198:SER:HB3	2:G:4201:ASN:HB2	1.90	0.53
2:I:1164:LEU:HB3	2:I:1169:LEU:HD21	1.90	0.53
2:E:315:CYS:SG	2:E:316:PHE:N	2.81	0.53
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.90	0.53
2:G:4673:ARG:HH12	2:G:4698:LYS:HE3	1.73	0.53
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.73	0.53
2:I:111:HIS:CD2	2:I:114:SER:H	2.25	0.53
2:E:4993:MET:HA	2:E:4996:ILE:HD12	1.89	0.53
2:E:730:VAL:O	2:E:735:GLN:NE2	2.42	0.53
2:G:1164:LEU:HB3	2:G:1169:LEU:HD21	1.90	0.53
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	1.91	0.53
2:I:2265:LEU:O	2:I:2330:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.91	0.53
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	1.91	0.53
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.89	0.53
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.81	0.53
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.73	0.53
2:I:4075:GLU:HA	2:I:4078:GLN:HB2	1.91	0.53
2:I:4673:ARG:HH12	2:I:4698:LYS:HE3	1.73	0.53
2:I:730:VAL:O	2:I:735:GLN:NE2	2.42	0.53
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	1.91	0.53
2:E:4681:LEU:HD21	2:E:4687:TYR:HD2	1.73	0.53
2:G:20:VAL:HG12	2:G:204:PRO:HA	1.91	0.53
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.91	0.53
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.42	0.53
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.73	0.53
2:E:20:VAL:HG12	2:E:204:PRO:HA	1.91	0.53
2:G:730:VAL:O	2:G:735:GLN:NE2	2.42	0.53
2:I:614:VAL:HG22	2:I:616:SER:H	1.72	0.53
2:B:1164:LEU:HB3	2:B:1169:LEU:HD21	1.90	0.53
2:B:2265:LEU:O	2:B:2330:ARG:NH1	2.42	0.53
2:G:2265:LEU:O	2:G:2330:ARG:NH1	2.42	0.53
2:I:2479:LEU:O	2:I:2487:UNK:N	2.42	0.53
2:B:4075:GLU:HA	2:B:4078:GLN:HB2	1.91	0.53
2:E:1164:LEU:HB3	2:E:1169:LEU:HD21	1.90	0.53
2:E:4075:GLU:HA	2:E:4078:GLN:HB2	1.91	0.53
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.91	0.53
2:G:4075:GLU:HA	2:G:4078:GLN:HB2	1.91	0.53
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.42	0.53
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	1.91	0.53
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.91	0.52
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.91	0.52
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.42	0.52
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.31	0.52
2:G:331:VAL:HG12	2:G:333:GLY:H	1.74	0.52
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.43	0.52
2:E:331:VAL:HG12	2:E:333:GLY:H	1.74	0.52
2:G:111:HIS:CD2	2:G:114:SER:H	2.25	0.52
2:I:683:ARG:NH1	2:I:707:VAL:O	2.40	0.52
2:B:730:VAL:O	2:B:735:GLN:NE2	2.42	0.52
2:E:4198:SER:HB3	2:E:4201:ASN:HB2	1.90	0.52
2:G:116:MET:HB2	2:G:137:LEU:HD12	1.92	0.52
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.81	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4681:LEU:HD21	2:I:4687:TYR:HD2	1.73	0.52
2:G:2479:LEU:O	2:G:2487:UNK:N	2.42	0.52
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.42	0.52
2:E:2265:LEU:O	2:E:2330:ARG:NH1	2.42	0.52
1:F:34:LYS:HD3	2:E:629:ARG:HD2	1.91	0.52
2:G:4961:CYS:HB3	2:G:4983:HIS:HE1	1.74	0.52
2:B:20:VAL:HG12	2:B:204:PRO:HA	1.91	0.52
2:B:331:VAL:HG12	2:B:333:GLY:H	1.74	0.52
2:B:116:MET:HB2	2:B:137:LEU:HD12	1.92	0.52
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.43	0.52
2:E:4961:CYS:HB3	2:E:4983:HIS:HE1	1.75	0.52
2:I:4198:SER:HB3	2:I:4201:ASN:HB2	1.90	0.52
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.91	0.52
2:G:1653:LEU:HB3	2:G:1660:GLN:HB2	1.92	0.52
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.43	0.52
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.92	0.52
2:B:4681:LEU:HD21	2:B:4687:TYR:HD2	1.73	0.52
2:G:2266:GLY:O	2:G:2330:ARG:NH2	2.43	0.52
2:G:4996:ILE:HD13	4:G:5102:CFF:H123	1.92	0.52
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.92	0.52
2:G:683:ARG:NH1	2:G:707:VAL:O	2.40	0.52
2:I:20:VAL:HG12	2:I:204:PRO:HA	1.91	0.52
2:E:2479:LEU:O	2:E:2487:UNK:N	2.42	0.51
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.92	0.51
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.91	0.51
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.92	0.51
2:I:45:ARG:NH2	2:I:447:ASP:OD1	2.39	0.51
2:E:309:THR:O	2:E:313:SER:OG	2.29	0.51
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.91	0.51
2:I:1653:LEU:HB3	2:I:1660:GLN:HB2	1.92	0.51
2:B:485:SER:O	2:B:489:ASN:N	2.38	0.51
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.93	0.51
2:E:1653:LEU:HB3	2:E:1660:GLN:HB2	1.92	0.51
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.92	0.51
2:G:3971:GLY:H	2:G:5005:GLY:HA3	1.76	0.51
2:I:4961:CYS:HB3	2:I:4983:HIS:HE1	1.74	0.51
2:B:4914:VAL:HG23	2:E:4888:TYR:HD1	1.75	0.51
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.44	0.51
2:G:309:THR:O	2:G:313:SER:OG	2.29	0.51
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.43	0.51
2:I:331:VAL:HG12	2:I:333:GLY:H	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.44	0.51
2:G:4182:GLU:OE2	2:G:4983:HIS:NE2	2.43	0.51
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.93	0.51
2:I:1948:ASP:OD1	2:I:2126:ARG:NH2	2.39	0.51
2:B:1457:UNK:N	2:B:1497:UNK:O	2.44	0.51
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.75	0.51
2:E:2266:GLY:O	2:E:2330:ARG:NH2	2.43	0.51
2:E:4044:MET:HA	2:E:4047:MET:HG2	1.92	0.51
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.75	0.51
2:I:1457:UNK:N	2:I:1497:UNK:O	2.44	0.51
2:I:2266:GLY:O	2:I:2330:ARG:NH2	2.43	0.51
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.44	0.51
2:B:1653:LEU:HB3	2:B:1660:GLN:HB2	1.92	0.51
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.76	0.51
2:G:1948:ASP:OD1	2:G:2126:ARG:NH2	2.39	0.51
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	1.92	0.51
2:I:4996:ILE:HD13	4:I:5102:CFF:H123	1.92	0.51
2:B:309:THR:O	2:B:313:SER:OG	2.29	0.51
2:B:4961:CYS:HB3	2:B:4983:HIS:HE1	1.75	0.51
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.44	0.51
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.76	0.51
2:G:45:ARG:NH2	2:G:447:ASP:OD1	2.39	0.51
2:I:116:MET:HB2	2:I:137:LEU:HD12	1.92	0.51
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.76	0.51
2:G:2868:SER:O	2:G:2872:GLN:N	2.44	0.51
2:G:4044:MET:HA	2:G:4047:MET:HG2	1.92	0.51
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	1.92	0.51
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.93	0.51
2:G:652:ARG:HD2	2:G:750:LEU:HB3	1.92	0.51
2:I:309:THR:O	2:I:313:SER:OG	2.29	0.51
2:B:161:GLU:HA	2:E:3984:ARG:HH22	1.76	0.50
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.75	0.50
2:E:3971:GLY:H	2:E:5005:GLY:HA3	1.76	0.50
2:E:4996:ILE:HD13	4:E:5102:CFF:H123	1.93	0.50
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.44	0.50
2:I:2104:ARG:HA	2:I:2107:GLN:HB3	1.93	0.50
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.43	0.50
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.93	0.50
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.44	0.50
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.93	0.50
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.93	0.50
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.44	0.50
2:I:652:ARG:HD2	2:I:750:LEU:HB3	1.93	0.50
2:B:1516:UNK:N	2:B:1529:UNK:O	2.45	0.50
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.81	0.50
2:B:2266:GLY:O	2:B:2330:ARG:NH2	2.43	0.50
2:E:2868:SER:O	2:E:2872:GLN:N	2.44	0.50
2:I:594:GLY:H	2:I:1594:ARG:HD3	1.76	0.50
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.93	0.50
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.44	0.50
2:I:3971:GLY:H	2:I:5005:GLY:HA3	1.76	0.50
2:B:1948:ASP:OD1	2:B:2126:ARG:NH2	2.39	0.50
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.93	0.50
2:E:1457:UNK:N	2:E:1497:UNK:O	2.44	0.50
2:G:1516:UNK:N	2:G:1529:UNK:O	2.45	0.50
2:B:4044:MET:HA	2:B:4047:MET:HG2	1.92	0.50
2:B:652:ARG:HD2	2:B:750:LEU:HB3	1.92	0.50
2:E:116:MET:HB2	2:E:137:LEU:HD12	1.92	0.50
2:E:1516:UNK:N	2:E:1529:UNK:O	2.45	0.50
2:G:3973:CYS:SG	2:G:3976:ASN:ND2	2.85	0.50
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.75	0.50
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.42	0.50
2:I:4044:MET:HA	2:I:4047:MET:HG2	1.92	0.50
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.94	0.50
2:B:3759:GLU:HA	2:B:3762:ARG:HE	1.77	0.50
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	1.92	0.50
2:B:594:GLY:H	2:B:1594:ARG:HD3	1.76	0.50
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.93	0.50
2:G:2104:ARG:HA	2:G:2107:GLN:HB3	1.94	0.50
2:G:4582:VAL:HG11	2:E:4860:ARG:HD2	1.94	0.50
2:B:4996:ILE:HD13	4:B:5102:CFF:H123	1.93	0.50
2:B:683:ARG:NH1	2:B:707:VAL:O	2.40	0.50
2:G:594:GLY:H	2:G:1594:ARG:HD3	1.76	0.50
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.76	0.49
2:B:3973:CYS:SG	2:B:3976:ASN:ND2	2.85	0.49
2:E:594:GLY:H	2:E:1594:ARG:HD3	1.76	0.49
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.94	0.49
2:I:2868:SER:O	2:I:2872:GLN:N	2.44	0.49
2:B:4892:ARG:NH2	2:I:4899:ASP:OD1	2.45	0.49
2:E:652:ARG:HD2	2:E:750:LEU:HB3	1.92	0.49
2:G:1457:UNK:N	2:G:1497:UNK:O	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.29	0.49
2:I:1516:UNK:N	2:I:1529:UNK:O	2.45	0.49
2:I:3973:CYS:SG	2:I:3976:ASN:ND2	2.85	0.49
2:B:3971:GLY:H	2:B:5005:GLY:HA3	1.76	0.49
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.94	0.49
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.94	0.49
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.94	0.49
2:E:3973:CYS:SG	2:E:3976:ASN:ND2	2.85	0.49
2:E:683:ARG:NH1	2:E:707:VAL:O	2.40	0.49
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	1.92	0.49
2:E:4182:GLU:OE2	2:E:4983:HIS:NE2	2.43	0.49
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.93	0.49
2:G:3759:GLU:HA	2:G:3762:ARG:HE	1.77	0.49
2:B:2868:SER:O	2:B:2872:GLN:N	2.44	0.49
2:E:2104:ARG:HA	2:E:2107:GLN:HB3	1.93	0.49
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.94	0.49
1:H:55:VAL:HA	2:G:1784:ALA:HA	1.95	0.49
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.94	0.49
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.94	0.49
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	1.95	0.49
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.94	0.49
1:H:21:THR:HA	1:H:49:ARG:HA	1.95	0.49
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.93	0.49
1:J:25:HIS:HB3	1:J:40:ARG:HD3	1.95	0.49
1:A:25:HIS:HB3	1:A:40:ARG:HD3	1.95	0.49
2:B:1243:PRO:HB2	2:B:1600:LEU:HD22	1.95	0.49
2:B:2104:ARG:HA	2:B:2107:GLN:HB3	1.94	0.49
2:I:485:SER:O	2:I:489:ASN:N	2.38	0.49
2:I:4182:GLU:OE2	2:I:4983:HIS:NE2	2.43	0.49
1:J:21:THR:HA	1:J:49:ARG:HA	1.95	0.49
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.95	0.48
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	1.95	0.48
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.94	0.48
2:B:2024:PRO:HB2	2:B:2027:ILE:HG12	1.95	0.48
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.96	0.48
1:H:25:HIS:HB3	1:H:40:ARG:HD3	1.95	0.48
2:I:2024:PRO:HB2	2:I:2027:ILE:HG12	1.95	0.48
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.49	0.48
2:I:3759:GLU:HA	2:I:3762:ARG:HE	1.77	0.48
1:J:35:LYS:HD3	2:I:636:ASN:HD21	1.77	0.48
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.49	0.48
2:E:2024:PRO:HB2	2:E:2027:ILE:HG12	1.95	0.48
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.49	0.48
2:G:2024:PRO:HB2	2:G:2027:ILE:HG12	1.95	0.48
2:B:3734:HIS:O	2:B:3738:GLY:N	2.40	0.48
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.29	0.48
2:E:73:LEU:HB3	2:E:77:ALA:HB3	1.96	0.48
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	1.95	0.48
2:G:485:SER:O	2:G:489:ASN:N	2.38	0.48
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.79	0.48
2:E:3759:GLU:HA	2:E:3762:ARG:HE	1.77	0.48
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.95	0.48
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.94	0.48
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	1.96	0.48
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	1.95	0.48
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.29	0.48
2:G:2004:GLU:HA	2:G:2007:ASN:HB2	1.96	0.48
2:G:395:GLN:HG3	2:G:397:GLU:H	1.79	0.48
2:I:1243:PRO:HB2	2:I:1600:LEU:HD22	1.95	0.48
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.96	0.48
2:B:164:ARG:N	2:B:167:ASP:OD2	2.45	0.48
2:B:395:GLN:HG3	2:B:397:GLU:H	1.79	0.48
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.79	0.48
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.96	0.48
2:I:73:LEU:HB3	2:I:77:ALA:HB3	1.96	0.48
1:A:21:THR:HA	1:A:49:ARG:HA	1.95	0.48
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	1.96	0.48
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.96	0.48
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.96	0.48
2:E:4563:ARG:NH1	2:E:4815:ASP:OD1	2.47	0.48
1:F:21:THR:HA	1:F:49:ARG:HA	1.95	0.48
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.79	0.48
2:I:4563:ARG:NH1	2:I:4815:ASP:OD1	2.47	0.48
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.96	0.47
1:F:25:HIS:HB3	1:F:40:ARG:HD3	1.95	0.47
2:G:123:THR:OG1	2:G:134:ASP:OD1	2.32	0.47
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.79	0.47
2:G:4563:ARG:NH1	2:G:4815:ASP:OD1	2.47	0.47
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.29	0.47
2:E:1243:PRO:HB2	2:E:1600:LEU:HD22	1.95	0.47
2:E:1802:ILE:HG21	2:E:1807:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.96	0.47
2:B:823:LEU:HD23	2:B:1626:TRP:HB3	1.96	0.47
2:G:823:LEU:HD23	2:G:1626:TRP:HB3	1.96	0.47
2:G:3980:LEU:HD22	2:G:3985:LEU:HD22	1.96	0.47
2:I:395:GLN:HG3	2:I:397:GLU:H	1.79	0.47
1:J:34:LYS:HE3	2:I:634:GLN:HB3	1.96	0.47
2:E:2004:GLU:HA	2:E:2007:ASN:HB2	1.96	0.47
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.48	0.47
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.96	0.47
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.48	0.47
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	1.96	0.47
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.96	0.47
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.96	0.47
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.96	0.47
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.96	0.47
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.95	0.47
2:G:73:LEU:HB3	2:G:77:ALA:HB3	1.96	0.47
2:I:123:THR:OG1	2:I:134:ASP:OD1	2.32	0.47
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.97	0.47
2:I:3980:LEU:HD22	2:I:3985:LEU:HD22	1.96	0.47
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.97	0.47
2:E:2346:VAL:HG22	2:E:2348:GLU:H	1.80	0.47
2:G:1243:PRO:HB2	2:G:1600:LEU:HD22	1.95	0.47
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.95	0.47
2:B:4182:GLU:OE2	2:B:4983:HIS:NE2	2.43	0.47
2:E:3980:LEU:HD22	2:E:3985:LEU:HD22	1.96	0.47
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.97	0.47
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.80	0.47
1:A:57:LYS:HB2	1:A:80:VAL:HB	1.97	0.47
2:B:1802:ILE:HG21	2:B:1807:LEU:HD22	1.97	0.47
2:B:2004:GLU:HA	2:B:2007:ASN:HB2	1.96	0.47
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.97	0.47
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.80	0.47
2:E:823:LEU:HD23	2:E:1626:TRP:HB3	1.96	0.47
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.49	0.47
2:I:823:LEU:HD23	2:I:1626:TRP:HB3	1.96	0.47
1:J:92:PRO:HD3	2:I:627:PRO:HB2	1.97	0.47
2:E:123:THR:OG1	2:E:134:ASP:OD1	2.32	0.47
2:E:1970:GLN:HB3	2:E:3641:LEU:HG	1.97	0.47
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.80	0.47
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.48	0.47
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.80	0.47
2:I:2353:VAL:O	2:I:2357:LEU:N	2.48	0.47
1:A:7:ILE:N	1:A:71:ARG:O	2.45	0.47
2:B:206:CYS:SG	2:B:207:SER:N	2.88	0.47
2:B:4563:ARG:NH1	2:B:4815:ASP:OD1	2.47	0.47
2:E:395:GLN:HG3	2:E:397:GLU:H	1.79	0.47
2:G:164:ARG:N	2:G:167:ASP:OD2	2.45	0.47
2:G:3847:PHE:HD1	2:G:3850:GLN:HE21	1.63	0.47
1:J:57:LYS:HB2	1:J:80:VAL:HB	1.97	0.47
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.48	0.47
2:B:1970:GLN:HB3	2:B:3641:LEU:HG	1.97	0.47
2:B:649:PHE:HB3	2:B:776:LEU:HD13	1.97	0.47
2:B:73:LEU:HB3	2:B:77:ALA:HB3	1.96	0.47
2:E:164:ARG:N	2:E:167:ASP:OD2	2.45	0.47
2:E:2129:ASP:O	2:E:2133:GLU:N	2.44	0.47
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	1.96	0.47
2:E:649:PHE:HB3	2:E:776:LEU:HD13	1.97	0.47
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.97	0.47
2:B:2346:VAL:HG22	2:B:2348:GLU:H	1.80	0.46
2:B:3980:LEU:HD22	2:B:3985:LEU:HD22	1.96	0.46
2:G:2353:VAL:O	2:G:2357:LEU:N	2.48	0.46
2:E:206:CYS:SG	2:E:207:SER:N	2.88	0.46
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.97	0.46
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.96	0.46
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.48	0.46
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.43	0.46
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.96	0.46
2:G:649:PHE:HB3	2:G:776:LEU:HD13	1.97	0.46
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.96	0.46
2:I:206:CYS:SG	2:I:207:SER:N	2.88	0.46
2:I:649:PHE:HB3	2:I:776:LEU:HD13	1.97	0.46
2:B:123:THR:OG1	2:B:134:ASP:OD1	2.32	0.46
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.96	0.46
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.97	0.46
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.96	0.46
2:G:2346:VAL:HG22	2:G:2348:GLU:H	1.80	0.46
2:I:699:GLY:H	2:I:1647:CYS:HB3	1.81	0.46
2:I:1802:ILE:HG21	2:I:1807:LEU:HD22	1.97	0.46
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.97	0.46
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.97	0.46
2:I:1970:GLN:HB3	2:I:3641:LEU:HG	1.97	0.46
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.97	0.46
2:B:2129:ASP:O	2:B:2133:GLU:N	2.45	0.46
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.81	0.46
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.97	0.46
2:E:619:ASP:OD1	2:E:1680:ARG:NH1	2.49	0.46
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.97	0.46
2:I:2004:GLU:HA	2:I:2007:ASN:HB2	1.96	0.46
2:I:3734:HIS:O	2:I:3738:GLY:N	2.40	0.46
2:I:776:LEU:HG	2:I:848:HIS:HA	1.98	0.46
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.48	0.46
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	1.97	0.46
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.97	0.46
2:B:280:LEU:HD21	2:B:316:PHE:HE2	1.81	0.46
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.48	0.46
2:B:619:ASP:OD1	2:B:1680:ARG:NH1	2.49	0.46
2:E:280:LEU:HD21	2:E:316:PHE:HE2	1.81	0.46
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.48	0.46
2:E:485:SER:O	2:E:489:ASN:N	2.38	0.46
2:I:2346:VAL:HG22	2:I:2348:GLU:H	1.80	0.46
2:G:206:CYS:SG	2:G:207:SER:N	2.88	0.46
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.81	0.46
2:I:164:ARG:N	2:I:167:ASP:OD2	2.45	0.46
2:I:2129:ASP:O	2:I:2133:GLU:N	2.44	0.46
2:I:280:LEU:HD21	2:I:316:PHE:HE2	1.81	0.46
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.49	0.46
2:B:2353:VAL:O	2:B:2357:LEU:N	2.48	0.46
1:F:55:VAL:HA	2:E:1784:ALA:HA	1.98	0.46
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.49	0.46
2:I:3847:PHE:HD1	2:I:3850:GLN:HE21	1.63	0.46
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	1.97	0.46
2:E:699:GLY:H	2:E:1647:CYS:HB3	1.81	0.46
2:G:359:TYR:HA	2:G:376:ALA:HA	1.98	0.46
2:G:776:LEU:HG	2:G:848:HIS:HA	1.98	0.46
1:H:57:LYS:HB2	1:H:80:VAL:HB	1.97	0.46
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.38	0.45
2:B:2318:TYR:OH	2:B:2414:ASN:N	2.50	0.45
2:E:2332:LEU:HD13	2:E:2335:LEU:HD12	1.98	0.45
2:E:2318:TYR:OH	2:E:2414:ASN:N	2.50	0.45
2:E:359:TYR:HA	2:E:376:ALA:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1970:GLN:HB3	2:G:3641:LEU:HG	1.97	0.45
2:G:4000:MET:HG3	2:G:4013:LEU:HD11	1.99	0.45
2:I:77:ALA:O	2:I:81:MET:N	2.49	0.45
2:B:1101:ARG:HH21	2:B:1115:LEU:HB3	1.82	0.45
2:B:2034:PHE:O	2:B:2038:LEU:N	2.50	0.45
2:G:699:GLY:H	2:G:1647:CYS:HB3	1.81	0.45
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.47	0.45
2:B:1269:CYS:HA	2:B:1473:UNK:HA	1.98	0.45
2:B:699:GLY:H	2:B:1647:CYS:HB3	1.81	0.45
2:B:379:HIS:CD2	2:B:381:GLU:H	2.35	0.45
2:E:2353:VAL:O	2:E:2357:LEU:N	2.48	0.45
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.97	0.45
2:E:776:LEU:HG	2:E:848:HIS:HA	1.97	0.45
2:E:892:THR:N	2:E:902:ARG:O	2.49	0.45
2:G:1101:ARG:HH21	2:G:1115:LEU:HB3	1.82	0.45
2:G:379:HIS:CD2	2:G:381:GLU:H	2.35	0.45
2:G:4081:VAL:HB	2:G:4088:ILE:HD12	1.99	0.45
2:I:379:HIS:CD2	2:I:381:GLU:H	2.35	0.45
2:E:4960:ILE:HD11	2:E:4985:LEU:HD23	1.98	0.45
2:G:2034:PHE:O	2:G:2038:LEU:N	2.50	0.45
2:G:870:ILE:HD12	2:G:873:LYS:HB2	1.99	0.45
2:B:889:GLN:O	2:B:902:ARG:NH1	2.50	0.45
2:E:1236:THR:OG1	2:E:1608:MET:SD	2.75	0.45
2:E:1859:VAL:HA	2:E:1862:ILE:HG12	1.99	0.45
2:E:2950:UNK:O	2:E:2954:UNK:N	2.50	0.45
2:E:3847:PHE:HD1	2:E:3850:GLN:HE21	1.63	0.45
1:F:57:LYS:HB2	1:F:80:VAL:HB	1.97	0.45
2:G:134:ASP:OD1	2:G:134:ASP:N	2.50	0.45
2:G:2874:MET:O	2:G:2878:LEU:N	2.45	0.45
2:G:280:LEU:HD21	2:G:316:PHE:HE2	1.81	0.45
1:H:2:VAL:HG21	1:H:61:GLU:HB2	1.98	0.45
2:I:4000:MET:HG3	2:I:4013:LEU:HD11	1.99	0.45
2:B:870:ILE:HD12	2:B:873:LYS:HB2	1.99	0.45
2:E:379:HIS:CD2	2:E:381:GLU:H	2.35	0.45
2:E:889:GLN:O	2:E:902:ARG:NH1	2.50	0.45
2:G:1802:ILE:HG21	2:G:1807:LEU:HD22	1.97	0.45
2:I:1101:ARG:HH21	2:I:1115:LEU:HB3	1.82	0.45
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	1.97	0.45
2:I:2243:SER:HB3	2:I:2246:ASN:H	1.82	0.45
2:I:4960:ILE:HD11	2:I:4985:LEU:HD23	1.98	0.45
2:I:870:ILE:HD12	2:I:873:LYS:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2778:GLY:HA3	2:B:2787:THR:HB	1.98	0.45
2:E:4000:MET:HG3	2:E:4013:LEU:HD11	1.99	0.45
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.49	0.45
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	1.97	0.45
2:G:1859:VAL:HA	2:G:1862:ILE:HG12	1.99	0.45
2:I:2950:UNK:O	2:I:2954:UNK:N	2.50	0.45
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.81	0.45
2:B:3847:PHE:HD1	2:B:3850:GLN:HE21	1.63	0.45
2:B:77:ALA:O	2:B:81:MET:N	2.49	0.45
2:E:4961:CYS:HB3	2:E:4983:HIS:CE1	2.52	0.45
2:E:548:VAL:HG12	2:E:564:LEU:HD22	1.99	0.45
2:E:870:ILE:HD12	2:E:873:LYS:HB2	1.99	0.45
2:E:894:GLY:HA3	2:E:903:LEU:HD22	1.99	0.45
2:G:1707:LEU:O	2:G:1710:GLY:N	2.35	0.45
2:G:2243:SER:HB3	2:G:2246:ASN:H	1.82	0.45
2:G:2318:TYR:OH	2:G:2414:ASN:N	2.50	0.45
2:G:548:VAL:HG12	2:G:564:LEU:HD22	1.99	0.45
2:I:134:ASP:OD1	2:I:134:ASP:N	2.50	0.45
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.33	0.45
2:B:1236:THR:OG1	2:B:1608:MET:SD	2.75	0.45
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.49	0.45
2:B:776:LEU:HG	2:B:848:HIS:HA	1.98	0.45
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.99	0.45
2:E:1269:CYS:HA	2:E:1473:UNK:HA	1.98	0.45
2:E:2778:GLY:HA3	2:E:2787:THR:HB	1.98	0.45
2:E:3361:UNK:O	2:E:3365:UNK:N	2.50	0.45
2:E:4957:LYS:HA	2:E:4964:GLY:HA2	1.99	0.45
1:F:2:VAL:HG21	1:F:61:GLU:HB2	1.98	0.45
2:I:359:TYR:HA	2:I:376:ALA:HA	1.98	0.45
2:B:4960:ILE:HD11	2:B:4985:LEU:HD23	1.98	0.45
2:E:134:ASP:OD1	2:E:134:ASP:N	2.50	0.45
2:G:983:THR:O	2:G:987:ARG:N	2.48	0.45
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.99	0.44
2:B:1859:VAL:HA	2:B:1862:ILE:HG12	1.99	0.44
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.82	0.44
2:G:2332:LEU:HD13	2:G:2335:LEU:HD12	1.98	0.44
2:G:4822:THR:O	2:G:4825:THR:OG1	2.29	0.44
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.99	0.44
2:I:4729:GLY:HA2	2:I:4737:ILE:HG13	1.99	0.44
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.99	0.44
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.81	0.44
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.83	0.44
2:G:4957:LYS:HA	2:G:4964:GLY:HA2	1.99	0.44
2:G:4960:ILE:HD11	2:G:4985:LEU:HD23	1.98	0.44
2:G:894:GLY:HA3	2:G:903:LEU:HD22	1.99	0.44
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.99	0.44
2:I:1236:THR:OG1	2:I:1608:MET:SD	2.75	0.44
2:I:2332:LEU:HD13	2:I:2335:LEU:HD12	1.98	0.44
2:B:3674:ILE:HD11	2:B:3728:ILE:HG22	1.99	0.44
2:B:4957:LYS:HA	2:B:4964:GLY:HA2	1.99	0.44
2:E:4729:GLY:HA2	2:E:4737:ILE:HG13	1.99	0.44
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.99	0.44
2:I:3674:ILE:HD11	2:I:3728:ILE:HG22	1.99	0.44
2:I:983:THR:O	2:I:987:ARG:N	2.48	0.44
1:A:2:VAL:HG21	1:A:61:GLU:HB2	1.98	0.44
2:E:2430:ILE:HG21	2:E:2502:UNK:HA	1.98	0.44
2:G:2950:UNK:O	2:G:2954:UNK:N	2.50	0.44
2:G:3361:UNK:O	2:G:3365:UNK:N	2.50	0.44
2:I:2778:GLY:HA3	2:I:2787:THR:HB	1.98	0.44
2:I:3552:UNK:O	2:I:3556:UNK:N	2.51	0.44
2:I:889:GLN:O	2:I:902:ARG:NH1	2.50	0.44
2:B:2332:LEU:HD13	2:B:2335:LEU:HD12	1.98	0.44
2:B:3361:UNK:O	2:B:3365:UNK:N	2.50	0.44
2:B:359:TYR:HA	2:B:376:ALA:HA	1.98	0.44
2:B:4000:MET:HG3	2:B:4013:LEU:HD11	1.99	0.44
2:E:1101:ARG:HH21	2:E:1115:LEU:HB3	1.82	0.44
2:G:1236:THR:OG1	2:G:1608:MET:SD	2.75	0.44
2:G:619:ASP:OD1	2:G:1680:ARG:NH1	2.49	0.44
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.83	0.44
2:I:4961:CYS:HB3	2:I:4983:HIS:CE1	2.52	0.44
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.49	0.44
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.99	0.44
2:B:2950:UNK:O	2:B:2954:UNK:N	2.51	0.44
2:B:4081:VAL:HB	2:B:4088:ILE:HD12	1.99	0.44
2:B:42:PHE:HD1	2:B:447:ASP:HB3	1.83	0.44
2:B:548:VAL:HG12	2:B:564:LEU:HD22	1.99	0.44
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.99	0.44
2:G:2778:GLY:HA3	2:G:2787:THR:HB	1.98	0.44
2:G:3674:ILE:HD11	2:G:3728:ILE:HG22	1.99	0.44
2:G:4031:LEU:HB3	2:G:4034:ASN:HB2	1.99	0.44
2:G:4961:CYS:HB3	2:G:4983:HIS:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:892:THR:N	2:G:902:ARG:O	2.49	0.44
2:I:1859:VAL:HA	2:I:1862:ILE:HG12	1.99	0.44
2:I:548:VAL:HG12	2:I:564:LEU:HD22	1.99	0.44
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.99	0.44
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.99	0.44
2:E:2243:SER:HB3	2:E:2246:ASN:H	1.82	0.44
2:G:77:ALA:O	2:G:81:MET:N	2.49	0.44
2:G:889:GLN:O	2:G:902:ARG:NH1	2.50	0.44
2:I:794:GLY:H	2:I:798:GLY:HA3	1.83	0.44
2:B:2022:PRO:HB2	2:B:2024:PRO:HD2	2.00	0.44
2:E:2022:PRO:HB2	2:E:2024:PRO:HD2	2.00	0.44
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.99	0.44
2:E:42:PHE:HD1	2:E:447:ASP:HB3	1.83	0.44
2:E:983:THR:O	2:E:987:ARG:N	2.48	0.44
2:G:3900:GLN:NE2	2:G:3967:GLU:O	2.51	0.44
2:G:42:PHE:HD1	2:G:447:ASP:HB3	1.83	0.44
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.99	0.44
2:I:1716:ILE:HG23	2:I:1720:LEU:HD13	2.00	0.44
2:I:3361:UNK:O	2:I:3365:UNK:N	2.50	0.44
2:B:1716:ILE:HG23	2:B:1720:LEU:HD13	2.00	0.44
2:B:4928:LEU:HA	2:B:4928:LEU:HD13	1.84	0.44
2:E:3552:UNK:O	2:E:3556:UNK:N	2.51	0.44
2:G:4729:GLY:HA2	2:G:4737:ILE:HG13	1.99	0.44
2:I:4031:LEU:HB3	2:I:4034:ASN:HB2	1.99	0.44
2:B:1865:MET:SD	2:B:1865:MET:N	2.91	0.43
2:B:2243:SER:HB3	2:B:2246:ASN:H	1.82	0.43
2:B:3552:UNK:O	2:B:3556:UNK:N	2.52	0.43
2:B:3900:GLN:NE2	2:B:3967:GLU:O	2.51	0.43
2:B:894:GLY:HA3	2:B:903:LEU:HD22	1.99	0.43
2:E:1707:LEU:O	2:E:1710:GLY:N	2.35	0.43
2:E:3804:ILE:HG22	2:E:3812:VAL:HG21	2.00	0.43
2:E:3900:GLN:NE2	2:E:3967:GLU:O	2.51	0.43
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.99	0.43
2:I:4081:VAL:HB	2:I:4088:ILE:HD12	1.99	0.43
2:I:4957:LYS:HA	2:I:4964:GLY:HA2	1.99	0.43
1:J:2:VAL:HG21	1:J:61:GLU:HB2	1.99	0.43
2:B:1707:LEU:O	2:B:1710:GLY:N	2.36	0.43
2:B:23:GLN:HB3	2:B:201:ASN:HB2	2.00	0.43
2:B:4961:CYS:HB3	2:B:4983:HIS:CE1	2.52	0.43
2:G:23:GLN:HB3	2:G:201:ASN:HB2	2.00	0.43
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:23:GLN:HB3	2:I:201:ASN:HB2	2.00	0.43
2:I:2318:TYR:OH	2:I:2414:ASN:N	2.50	0.43
2:I:3850:GLN:HA	2:I:3853:ALA:HB3	2.00	0.43
2:B:286:THR:HA	2:B:405:HIS:HB2	2.01	0.43
2:B:4763:GLY:O	2:B:4766:THR:OG1	2.33	0.43
2:E:1865:MET:SD	2:E:1865:MET:N	2.92	0.43
2:E:495:ASN:HD21	2:E:550:LYS:HG3	1.84	0.43
2:I:2022:PRO:HB2	2:I:2024:PRO:HD2	2.00	0.43
2:I:286:THR:HA	2:I:405:HIS:HB2	2.01	0.43
2:I:894:GLY:HA3	2:I:903:LEU:HD22	1.99	0.43
2:B:4031:LEU:HB3	2:B:4034:ASN:HB2	1.99	0.43
2:B:4729:GLY:HA2	2:B:4737:ILE:HG13	1.99	0.43
2:B:892:THR:N	2:B:902:ARG:O	2.49	0.43
2:E:23:GLN:HB3	2:E:201:ASN:HB2	2.00	0.43
2:E:3734:HIS:O	2:E:3738:GLY:N	2.40	0.43
2:E:4081:VAL:HB	2:E:4088:ILE:HD12	1.99	0.43
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	2.01	0.43
2:G:479:GLN:HE21	2:G:536:ASN:ND2	2.17	0.43
1:J:82:TYR:HB3	1:J:86:GLY:HA2	2.01	0.43
2:B:2095:GLN:NE2	2:B:2127:GLN:O	2.51	0.43
2:B:3804:ILE:HG22	2:B:3812:VAL:HG21	2.00	0.43
2:B:794:GLY:H	2:B:798:GLY:HA3	1.83	0.43
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	2.00	0.43
2:G:794:GLY:H	2:G:798:GLY:HA3	1.83	0.43
2:I:1269:CYS:HA	2:I:1473:UNK:HA	1.99	0.43
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	2.01	0.43
2:E:4688:ILE:HG21	2:E:4728:HIS:HB3	2.01	0.43
1:F:30:LEU:HD23	1:F:33:GLY:HA3	2.01	0.43
2:G:3552:UNK:O	2:G:3556:UNK:N	2.51	0.43
2:I:42:PHE:HD1	2:I:447:ASP:HB3	1.83	0.43
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.99	0.43
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	2.01	0.43
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	2.01	0.43
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.92	0.43
2:E:3674:ILE:HD11	2:E:3728:ILE:HG22	1.99	0.43
2:E:404:ILE:HG21	2:E:481:GLU:HG3	2.01	0.43
2:E:794:GLY:H	2:E:798:GLY:HA3	1.83	0.43
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.99	0.43
2:G:1154:ASP:O	2:G:1158:ASN:N	2.52	0.43
2:G:1269:CYS:HA	2:G:1473:UNK:HA	2.00	0.43
2:G:1675:ALA:HB1	2:G:1676:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4688:ILE:HG21	2:G:4728:HIS:HB3	2.01	0.43
2:I:1771:LEU:HA	2:I:1771:LEU:HD13	1.93	0.43
2:B:4822:THR:O	2:B:4825:THR:OG1	2.29	0.43
2:E:4031:LEU:HB3	2:E:4034:ASN:HB2	1.99	0.43
2:G:2022:PRO:HB2	2:G:2024:PRO:HD2	2.00	0.43
2:G:404:ILE:HG21	2:G:481:GLU:HG3	2.01	0.43
1:H:30:LEU:HD23	1:H:33:GLY:HA3	2.01	0.43
1:H:82:TYR:HB3	1:H:86:GLY:HA2	2.01	0.43
2:I:1154:ASP:O	2:I:1158:ASN:N	2.52	0.43
2:I:1865:MET:SD	2:I:1865:MET:N	2.92	0.43
2:I:2095:GLN:NE2	2:I:2127:GLN:O	2.51	0.43
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.47	0.43
2:B:1865:MET:HB3	2:B:1926:LEU:HB2	2.01	0.43
2:E:113:HIS:CE1	2:E:402:ARG:HB3	2.54	0.43
2:E:479:GLN:HE21	2:E:536:ASN:ND2	2.17	0.43
2:G:1716:ILE:HG23	2:G:1720:LEU:HD13	2.00	0.43
2:G:2095:GLN:NE2	2:G:2127:GLN:O	2.51	0.43
2:G:2129:ASP:O	2:G:2133:GLU:N	2.45	0.43
2:G:286:THR:HA	2:G:405:HIS:HB2	2.01	0.43
2:G:4848:VAL:O	2:G:4852:THR:OG1	2.29	0.43
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.92	0.43
2:I:2959:UNK:O	2:I:2963:UNK:N	2.52	0.43
2:I:3900:GLN:NE2	2:I:3967:GLU:O	2.51	0.43
1:J:7:ILE:N	1:J:71:ARG:O	2.45	0.43
2:B:2305:CYS:HA	2:B:2324:ASN:HD22	1.84	0.43
2:B:495:ASN:HD21	2:B:550:LYS:HG3	1.84	0.43
2:E:1716:ILE:HG23	2:E:1720:LEU:HD13	2.00	0.43
2:E:2305:CYS:HA	2:E:2324:ASN:HD22	1.84	0.43
2:E:286:THR:HA	2:E:405:HIS:HB2	2.01	0.43
2:G:2265:LEU:HD21	2:G:2273:LEU:HD13	2.01	0.43
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.99	0.43
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	2.01	0.43
2:I:2305:CYS:HA	2:I:2324:ASN:HD22	1.84	0.43
2:B:119:SER:HA	2:B:146:CYS:HA	2.01	0.42
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.92	0.42
2:E:1675:ALA:HB1	2:E:1676:LEU:HD13	2.01	0.42
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.47	0.42
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.92	0.42
2:I:2034:PHE:O	2:I:2038:LEU:N	2.50	0.42
1:J:30:LEU:HD23	1:J:33:GLY:HA3	2.01	0.42
2:G:1865:MET:SD	2:G:1865:MET:N	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:345:LEU:HD23	2:G:389:PHE:HB3	2.01	0.42
1:H:34:LYS:HE3	2:G:634:GLN:HB3	2.00	0.42
2:I:495:ASN:HD21	2:I:550:LYS:HG3	1.83	0.42
2:I:599:VAL:HG23	2:I:600:LEU:HD12	2.01	0.42
2:B:3842:LEU:O	2:B:3929:SER:OG	2.37	0.42
2:E:1154:ASP:O	2:E:1158:ASN:N	2.52	0.42
2:E:2034:PHE:O	2:E:2038:LEU:N	2.50	0.42
2:E:345:LEU:HD23	2:E:389:PHE:HB3	2.01	0.42
2:G:1865:MET:HB3	2:G:1926:LEU:HB2	2.01	0.42
2:G:290:TYR:O	2:G:302:VAL:N	2.52	0.42
2:I:1675:ALA:HB1	2:I:1676:LEU:HD13	2.01	0.42
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.47	0.42
2:I:3804:ILE:HG22	2:I:3812:VAL:HG21	2.00	0.42
2:I:404:ILE:HG21	2:I:481:GLU:HG3	2.01	0.42
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	2.02	0.42
2:B:290:TYR:O	2:B:302:VAL:N	2.52	0.42
2:B:404:ILE:HG21	2:B:481:GLU:HG3	2.01	0.42
2:E:1865:MET:HB3	2:E:1926:LEU:HB2	2.01	0.42
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	2.01	0.42
2:G:119:SER:HA	2:G:146:CYS:HA	2.01	0.42
2:G:2959:UNK:O	2:G:2963:UNK:N	2.53	0.42
2:G:3804:ILE:HG22	2:G:3812:VAL:HG21	2.00	0.42
1:A:30:LEU:HD23	1:A:33:GLY:HA3	2.01	0.42
2:B:2265:LEU:HD21	2:B:2273:LEU:HD13	2.01	0.42
2:E:2095:GLN:NE2	2:E:2127:GLN:O	2.51	0.42
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	2.02	0.42
2:E:4848:VAL:O	2:E:4852:THR:OG1	2.29	0.42
2:G:3365:UNK:O	2:G:3369:UNK:N	2.53	0.42
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	2.02	0.42
2:G:495:ASN:HD21	2:G:550:LYS:HG3	1.84	0.42
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	2.01	0.42
2:B:3365:UNK:O	2:B:3369:UNK:N	2.52	0.42
2:E:2265:LEU:HD21	2:E:2273:LEU:HD13	2.01	0.42
2:E:3771:HIS:O	2:E:3774:GLY:N	2.48	0.42
2:E:500:ALA:HB1	2:E:504:ALA:HB2	2.01	0.42
1:F:82:TYR:HB3	1:F:86:GLY:HA2	2.01	0.42
2:G:2452:ARG:HH12	2:E:177:GLU:HG3	1.84	0.42
2:G:3677:LEU:O	2:G:3698:LEU:N	2.52	0.42
2:G:113:HIS:CE1	2:G:402:ARG:HB3	2.54	0.42
2:I:1707:LEU:O	2:I:1710:GLY:N	2.35	0.42
2:B:2102:VAL:HB	2:B:2124:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:87:HIS:HA	1:F:88:PRO:HD3	1.91	0.42
2:G:3734:HIS:O	2:G:3738:GLY:N	2.40	0.42
2:G:599:VAL:HG23	2:G:600:LEU:HD12	2.01	0.42
2:I:1865:MET:HB3	2:I:1926:LEU:HB2	2.01	0.42
2:I:4688:ILE:HG21	2:I:4728:HIS:HB3	2.01	0.42
2:I:479:GLN:HE21	2:I:536:ASN:ND2	2.17	0.42
2:B:113:HIS:CE1	2:B:402:ARG:HB3	2.54	0.42
2:B:2155:LEU:HD13	2:B:2188:ASN:HD21	1.85	0.42
2:B:346:CYS:N	2:B:388:LEU:O	2.52	0.42
2:B:3971:GLY:N	2:B:4032:GLU:OE2	2.52	0.42
2:E:290:TYR:O	2:E:302:VAL:N	2.52	0.42
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	2.02	0.42
2:E:3842:LEU:O	2:E:3929:SER:OG	2.37	0.42
2:I:113:HIS:CE1	2:I:402:ARG:HB3	2.54	0.42
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	2.02	0.42
2:I:2155:LEU:HD13	2:I:2188:ASN:HD21	1.85	0.42
2:I:2430:ILE:HG21	2:I:2502:UNK:HA	2.02	0.42
2:I:2874:MET:O	2:I:2878:LEU:N	2.45	0.42
2:I:3365:UNK:O	2:I:3369:UNK:N	2.53	0.42
2:I:892:THR:N	2:I:902:ARG:O	2.49	0.42
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	2.01	0.42
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	2.02	0.42
2:B:4582:VAL:HG12	2:I:4877:ASP:HA	2.02	0.42
2:B:500:ALA:HB1	2:B:504:ALA:HB2	2.01	0.42
2:E:2959:UNK:O	2:E:2963:UNK:N	2.52	0.42
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.51	0.42
2:G:3842:LEU:O	2:G:3929:SER:OG	2.37	0.42
2:I:2265:LEU:HD21	2:I:2273:LEU:HD13	2.01	0.42
2:I:290:TYR:O	2:I:302:VAL:N	2.52	0.42
1:A:6:THR:HA	1:A:72:ALA:HA	2.02	0.42
1:A:82:TYR:HB3	1:A:86:GLY:HA2	2.01	0.42
2:B:1154:ASP:O	2:B:1158:ASN:N	2.52	0.42
2:B:134:ASP:OD1	2:B:134:ASP:N	2.50	0.42
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.51	0.42
2:B:689:THR:H	2:B:778:PHE:HE2	1.67	0.42
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	2.01	0.42
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.55	0.42
2:E:3365:UNK:O	2:E:3369:UNK:N	2.53	0.42
2:E:580:GLU:HG3	2:E:620:LEU:HD22	2.02	0.42
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.38	0.42
2:I:2869:ARG:HA	2:I:2872:GLN:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3362:UNK:O	2:I:3366:UNK:N	2.53	0.42
2:I:345:LEU:HD23	2:I:389:PHE:HB3	2.01	0.42
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.55	0.41
2:B:2869:ARG:HA	2:B:2872:GLN:HB3	2.02	0.41
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.38	0.41
2:B:4688:ILE:HG21	2:B:4728:HIS:HB3	2.01	0.41
2:B:4804:TYR:HB3	2:B:4806:ASN:HD22	1.86	0.41
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.51	0.41
2:E:3676:ASP:N	2:E:3676:ASP:OD1	2.53	0.41
1:F:6:THR:HA	1:F:72:ALA:HA	2.02	0.41
2:I:3771:HIS:O	2:I:3774:GLY:N	2.48	0.41
2:I:4928:LEU:HD13	2:I:4928:LEU:HA	1.84	0.41
1:J:6:THR:HA	1:J:72:ALA:HA	2.02	0.41
2:B:3362:UNK:O	2:B:3366:UNK:N	2.54	0.41
2:B:247:TYR:HE2	2:B:359:TYR:HB3	1.85	0.41
2:B:580:GLU:HG3	2:B:620:LEU:HD22	2.02	0.41
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.38	0.41
2:E:2155:LEU:HD13	2:E:2188:ASN:HD21	1.85	0.41
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.38	0.41
2:G:1674:CYS:HB2	2:G:1685:LEU:HD13	2.03	0.41
2:I:119:SER:HA	2:I:146:CYS:HA	2.01	0.41
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.38	0.41
2:I:2102:VAL:HB	2:I:2124:LEU:HD12	2.01	0.41
2:B:1675:ALA:HB1	2:B:1676:LEU:HD13	2.01	0.41
2:B:3676:ASP:N	2:B:3676:ASP:OD1	2.53	0.41
2:E:119:SER:HA	2:E:146:CYS:HA	2.01	0.41
2:E:1674:CYS:HB2	2:E:1685:LEU:HD13	2.03	0.41
2:E:4804:TYR:HB3	2:E:4806:ASN:HD22	1.85	0.41
2:G:615:ARG:NH2	2:G:1677:GLY:O	2.41	0.41
2:G:2869:ARG:HA	2:G:2872:GLN:HB3	2.02	0.41
2:G:3780:LEU:HD11	2:G:3816:MET:HG3	2.02	0.41
2:G:689:THR:H	2:G:778:PHE:HE2	1.67	0.41
2:B:479:GLN:HE21	2:B:536:ASN:ND2	2.17	0.41
2:E:1244:GLN:OE1	2:E:1646:ARG:NH1	2.54	0.41
2:E:681:HIS:HB3	2:E:784:SER:HB3	2.03	0.41
2:G:3971:GLY:N	2:G:4032:GLU:OE2	2.52	0.41
1:H:7:ILE:N	1:H:71:ARG:O	2.45	0.41
2:I:1674:CYS:HB2	2:I:1685:LEU:HD13	2.03	0.41
2:I:346:CYS:N	2:I:388:LEU:O	2.52	0.41
2:I:689:THR:H	2:I:778:PHE:HE2	1.67	0.41
1:J:23:VAL:H	1:J:105:ASN:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.38	0.41
2:B:4163:PHE:HA	2:B:4166:LEU:HB2	2.03	0.41
2:B:599:VAL:HG23	2:B:600:LEU:HD12	2.02	0.41
2:E:3880:PHE:O	2:E:3884:LEU:N	2.54	0.41
1:F:23:VAL:H	1:F:105:ASN:HB3	1.85	0.41
2:G:1728:ARG:HA	2:G:1731:LEU:HB2	2.03	0.41
2:I:247:TYR:HE2	2:I:359:TYR:HB3	1.86	0.41
2:I:3842:LEU:O	2:I:3929:SER:OG	2.37	0.41
1:J:35:LYS:HD3	2:I:636:ASN:ND2	2.35	0.41
2:B:1771:LEU:HB3	2:B:2153:MET:HE1	2.03	0.41
2:E:1728:ARG:HA	2:E:1731:LEU:HB2	2.03	0.41
2:E:3362:UNK:O	2:E:3366:UNK:N	2.53	0.41
1:F:92:PRO:HD3	2:E:627:PRO:HB2	2.03	0.41
2:G:2430:ILE:HG21	2:G:2502:UNK:HA	2.02	0.41
2:G:3694:LYS:HA	2:G:3695:PRO:HD3	1.95	0.41
2:I:681:HIS:HB3	2:I:784:SER:HB3	2.03	0.41
2:B:4914:VAL:HG23	2:E:4888:TYR:CD1	2.54	0.41
2:E:346:CYS:N	2:E:388:LEU:O	2.52	0.41
2:G:4163:PHE:HA	2:G:4166:LEU:HB2	2.03	0.41
2:G:681:HIS:HB3	2:G:784:SER:HB3	2.03	0.41
1:H:23:VAL:H	1:H:105:ASN:HB3	1.85	0.41
1:H:6:THR:HA	1:H:72:ALA:HA	2.02	0.41
1:H:87:HIS:HA	1:H:88:PRO:HD3	1.91	0.41
2:I:500:ALA:HB1	2:I:504:ALA:HB2	2.01	0.41
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.54	0.41
2:B:1728:ARG:HA	2:B:1731:LEU:HB2	2.03	0.41
2:B:4180:ARG:NH1	2:B:4981:GLU:OE1	2.54	0.41
2:G:1725:ARG:HH21	2:G:1725:ARG:HD2	1.71	0.41
2:I:4163:PHE:HA	2:I:4166:LEU:HB2	2.03	0.41
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.38	0.41
2:I:4804:TYR:HB3	2:I:4806:ASN:HD22	1.86	0.41
2:B:1244:GLN:OE1	2:B:1646:ARG:NH1	2.54	0.41
2:B:345:LEU:HD23	2:B:389:PHE:HB3	2.01	0.41
2:E:599:VAL:HG23	2:E:600:LEU:HD12	2.01	0.41
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.55	0.41
2:G:3362:UNK:O	2:G:3366:UNK:N	2.53	0.41
2:G:3880:PHE:O	2:G:3884:LEU:N	2.54	0.41
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.86	0.41
2:I:1244:GLN:OE1	2:I:1646:ARG:NH1	2.54	0.41
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.55	0.41
2:I:3780:LEU:HD11	2:I:3816:MET:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:403:MET:O	2:I:407:THR:OG1	2.33	0.41
2:I:4180:ARG:NH1	2:I:4981:GLU:OE1	2.54	0.41
2:B:2144:ILE:HG13	2:B:2144:ILE:H	1.79	0.41
2:B:4685:GLY:HA3	2:B:4689:THR:HB	2.03	0.41
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.54	0.41
2:E:2810:LYS:HE2	2:E:2814:LYS:HE3	2.03	0.41
2:E:2869:ARG:HA	2:E:2872:GLN:HB3	2.02	0.41
2:E:3971:GLY:N	2:E:4032:GLU:OE2	2.52	0.41
2:E:4180:ARG:NH1	2:E:4981:GLU:OE1	2.54	0.41
2:E:77:ALA:O	2:E:81:MET:N	2.49	0.41
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	2.03	0.41
2:G:1141:ARG:HD2	2:G:1141:ARG:H	1.86	0.41
2:G:2155:LEU:HD13	2:G:2188:ASN:HD21	1.85	0.41
2:G:4180:ARG:NH1	2:G:4981:GLU:OE1	2.54	0.41
2:G:580:GLU:HG3	2:G:620:LEU:HD22	2.02	0.41
2:I:4886:HIS:O	2:I:4890:GLY:N	2.46	0.41
2:I:681:HIS:HE2	2:I:683:ARG:NE	2.19	0.41
1:A:87:HIS:HA	1:A:88:PRO:HD3	1.91	0.41
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	2.03	0.41
2:E:1720:LEU:HD23	2:E:1721:GLU:HA	2.03	0.41
2:G:1720:LEU:HD23	2:G:1721:GLU:HA	2.03	0.41
2:G:2102:VAL:HB	2:G:2124:LEU:HD12	2.01	0.41
2:G:500:ALA:HB1	2:G:504:ALA:HB2	2.01	0.41
2:I:2288:LEU:O	2:I:3849:ARG:NH1	2.49	0.41
2:I:580:GLU:HG3	2:I:620:LEU:HD22	2.02	0.41
2:B:1674:CYS:HB2	2:B:1685:LEU:HD13	2.03	0.40
2:E:2102:VAL:HB	2:E:2124:LEU:HD12	2.01	0.40
2:B:177:GLU:HG3	2:E:2452:ARG:HH12	1.87	0.40
2:E:3891:LEU:HB3	2:E:3899:PHE:CE2	2.56	0.40
2:E:4822:THR:O	2:E:4825:THR:OG1	2.29	0.40
2:E:4913:ARG:O	2:E:4917:ASP:N	2.48	0.40
1:F:34:LYS:HE3	2:E:634:GLN:HB3	2.01	0.40
2:E:689:THR:H	2:E:778:PHE:HE2	1.67	0.40
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.38	0.40
2:I:1728:ARG:HA	2:I:1731:LEU:HB2	2.03	0.40
2:I:2302:LEU:HD12	2:I:2305:CYS:HB3	2.03	0.40
1:A:23:VAL:H	1:A:105:ASN:HB3	1.85	0.40
2:B:2674:UNK:O	2:B:2676:UNK:N	2.55	0.40
2:B:4041:ALA:HA	2:B:4044:MET:HB2	2.04	0.40
2:E:2587:UNK:O	2:E:2591:UNK:N	2.54	0.40
2:E:4163:PHE:HA	2:E:4166:LEU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.54	0.40
2:G:2305:CYS:HA	2:G:2324:ASN:HD22	1.84	0.40
2:G:2810:LYS:HE2	2:G:2814:LYS:HE3	2.03	0.40
2:G:4041:ALA:HA	2:G:4044:MET:HB2	2.04	0.40
2:I:1078:GLU:HB3	2:I:1081:TYR:HD2	1.87	0.40
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.54	0.40
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.51	0.40
2:I:2587:UNK:O	2:I:2591:UNK:N	2.54	0.40
2:I:3677:LEU:O	2:I:3698:LEU:N	2.52	0.40
2:I:875:ALA:HB2	2:I:925:SER:HB2	2.03	0.40
1:J:87:HIS:HA	1:J:88:PRO:HD3	1.91	0.40
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	2.03	0.40
2:B:2302:LEU:HD12	2:B:2305:CYS:HB3	2.03	0.40
2:E:1141:ARG:HD2	2:E:1141:ARG:H	1.86	0.40
2:E:2302:LEU:HD12	2:E:2305:CYS:HB3	2.03	0.40
2:E:3677:LEU:O	2:E:3698:LEU:N	2.52	0.40
2:E:4156:HIS:CE1	2:E:5036:LEU:HD11	2.56	0.40
2:G:1244:GLN:OE1	2:G:1646:ARG:NH1	2.54	0.40
2:G:913:LEU:O	2:G:918:ARG:NH2	2.55	0.40
2:B:2959:UNK:O	2:B:2963:UNK:N	2.54	0.40
2:B:3880:PHE:O	2:B:3884:LEU:N	2.54	0.40
2:B:4215:ARG:NH2	3:B:5101:ATP:O2A	2.55	0.40
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	2.04	0.40
2:B:472:ARG:HA	2:B:475:GLN:HB2	2.04	0.40
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	2.04	0.40
1:F:15:PHE:HA	1:F:16:PRO:HD3	1.97	0.40
2:I:2810:LYS:HE2	2:I:2814:LYS:HE3	2.03	0.40
2:I:3891:LEU:HB3	2:I:3899:PHE:CE2	2.56	0.40
2:I:4041:ALA:HA	2:I:4044:MET:HB2	2.04	0.40
2:I:4685:GLY:HA3	2:I:4689:THR:HB	2.04	0.40
2:B:2587:UNK:O	2:B:2591:UNK:N	2.55	0.40
2:B:2810:LYS:HE2	2:B:2814:LYS:HE3	2.03	0.40
2:B:803:LEU:HA	2:B:804:PRO:HD3	1.98	0.40
2:E:247:TYR:HE2	2:E:359:TYR:HB3	1.85	0.40
2:E:2674:UNK:O	2:E:2676:UNK:N	2.54	0.40
2:G:2810:LYS:O	2:G:2814:LYS:N	2.45	0.40
2:G:4804:TYR:HB3	2:G:4806:ASN:HD22	1.85	0.40
2:I:3880:PHE:O	2:I:3884:LEU:N	2.54	0.40
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	2.03	0.40
2:I:913:LEU:O	2:I:918:ARG:NH2	2.55	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%)	2882 (89%)	348 (11%)	5 (0%)	52	86
2	E	3235/4416 (73%)	2882 (89%)	348 (11%)	5 (0%)	52	86
2	G	3235/4416 (73%)	2881 (89%)	349 (11%)	5 (0%)	52	86
2	I	3235/4416 (73%)	2882 (89%)	348 (11%)	5 (0%)	52	86
All	All	13360/18096 (74%)	11903 (89%)	1437 (11%)	20 (0%)	59	90

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	G	1708	ARG
2	I	1708	ARG
2	E	1708	ARG
2	B	4641	PRO
2	G	4641	PRO
2	I	4641	PRO
2	E	4641	PRO
2	B	1840	PRO
2	B	1932	PRO
2	B	2292	GLU
2	G	1840	PRO
2	G	1932	PRO
2	G	2292	GLU
2	I	1840	PRO
2	I	1932	PRO
2	I	2292	GLU

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Mol	Chain	Res	Type
2	E	1840	PRO
2	E	1932	PRO
2	E	2292	GLU

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%)	2476 (99%)	17 (1%)	88 94
2	E	2493/3022 (82%)	2476 (99%)	17 (1%)	88 94
2	G	2493/3022 (82%)	2476 (99%)	17 (1%)	88 94
2	I	2493/3022 (82%)	2476 (99%)	17 (1%)	88 94
All	All	10324/12444 (83%)	10256 (99%)	68 (1%)	89 94

All (68) 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	3762	ARG
2	B	3787	LYS
2	B	3896	ASN
2	B	4034	ASN

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Mol	Chain	Res	Type
2	B	4085	ARG
2	B	4120	ASN
2	B	4131	ARG
2	B	4166	LEU
2	B	4201	ASN
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	3762	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	4166	LEU
2	G	4201	ASN
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	3762	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	4166	LEU
2	I	4201	ASN
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG

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Mol	Chain	Res	Type
2	E	1076	ARG
2	E	1141	ARG
2	E	1600	LEU
2	E	1676	LEU
2	E	1964	ARG
2	E	3762	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	4166	LEU
2	E	4201	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (126) 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	111	HIS
2	B	113	HIS
2	B	273	HIS
2	B	379	HIS
2	B	395	GLN
2	B	479	GLN
2	B	520	ASN
2	B	725	HIS
2	B	797	HIS
2	B	921	ASN
2	B	949	ASN
2	B	1598	GLN
2	B	1679	ASN
2	B	1693	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	2127	GLN
2	B	2291	GLN
2	B	3809	ASN

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Mol	Chain	Res	Type
2	B	3889	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN
2	B	3976	ASN
2	B	4120	ASN
2	B	4201	ASN
2	B	4209	GLN
2	B	4806	ASN
2	G	57	ASN
2	G	111	HIS
2	G	113	HIS
2	G	273	HIS
2	G	379	HIS
2	G	395	GLN
2	G	479	GLN
2	G	520	ASN
2	G	725	HIS
2	G	797	HIS
2	G	921	ASN
2	G	949	ASN
2	G	1598	GLN
2	G	1679	ASN
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	4120	ASN
2	G	4201	ASN
2	G	4209	GLN
2	G	4806	ASN
2	I	57	ASN
2	I	111	HIS

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Mol	Chain	Res	Type
2	I	113	HIS
2	I	273	HIS
2	I	379	HIS
2	I	395	GLN
2	I	479	GLN
2	I	495	ASN
2	I	520	ASN
2	I	725	HIS
2	I	797	HIS
2	I	921	ASN
2	I	949	ASN
2	I	1598	GLN
2	I	1679	ASN
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	4120	ASN
2	I	4201	ASN
2	I	4209	GLN
2	I	4806	ASN
2	E	57	ASN
2	E	111	HIS
2	E	113	HIS
2	E	273	HIS
2	E	379	HIS
2	E	395	GLN
2	E	479	GLN
2	E	495	ASN
2	E	520	ASN
2	E	725	HIS
2	E	797	HIS
2	E	921	ASN
2	E	949	ASN

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Mol	Chain	Res	Type
2	E	1598	GLN
2	E	1679	ASN
2	E	1693	GLN
2	E	1719	HIS
2	E	1775	HIS
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	4120	ASN
2	E	4201	ASN
2	E	4209	GLN
2	E	4806	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	0.91	1 (3%)	26,52,52	1.77	2 (7%)
4	CFF	B	5102	-	8,15,15	2.42	3 (37%)	8,23,23	1.19	1 (12%)
3	ATP	E	5101	-	26,33,33	0.91	1 (3%)	26,52,52	1.75	3 (11%)
4	CFF	E	5102	-	8,15,15	2.43	3 (37%)	8,23,23	1.19	1 (12%)
3	ATP	G	5101	-	26,33,33	0.91	1 (3%)	26,52,52	1.77	3 (11%)
4	CFF	G	5102	-	8,15,15	2.46	3 (37%)	8,23,23	1.18	1 (12%)
3	ATP	I	5101	-	26,33,33	0.91	1 (3%)	26,52,52	1.76	3 (11%)
4	CFF	I	5102	-	8,15,15	2.47	3 (37%)	8,23,23	1.19	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	G	5102	CFF	C4-N3	-4.77	1.33	1.39
4	I	5102	CFF	C4-N3	-4.76	1.33	1.39
4	E	5102	CFF	C4-N3	-4.62	1.33	1.39
4	B	5102	CFF	C4-N3	-4.58	1.33	1.39
4	I	5102	CFF	C6-N1	-4.05	1.32	1.38
4	E	5102	CFF	C6-N1	-4.03	1.32	1.38
4	B	5102	CFF	C6-N1	-4.00	1.32	1.38
4	G	5102	CFF	C6-N1	-3.98	1.32	1.38
4	B	5102	CFF	O13-C6	-2.32	1.18	1.24
4	E	5102	CFF	O13-C6	-2.32	1.18	1.24
4	G	5102	CFF	O13-C6	-2.31	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	5102	CFF	O13-C6	-2.28	1.18	1.24
3	G	5101	ATP	C5-C4	2.87	1.47	1.40
3	B	5101	ATP	C5-C4	2.87	1.47	1.40
3	I	5101	ATP	C5-C4	2.88	1.47	1.40
3	E	5101	ATP	C5-C4	2.89	1.47	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	5101	ATP	N3-C2-N1	-7.00	123.38	128.87
3	G	5101	ATP	N3-C2-N1	-6.97	123.40	128.87
3	I	5101	ATP	N3-C2-N1	-6.95	123.42	128.87
3	E	5101	ATP	N3-C2-N1	-6.89	123.46	128.87
4	G	5102	CFF	C14-N7-C8	-2.63	111.56	125.31
4	I	5102	CFF	C14-N7-C8	-2.63	111.57	125.31
4	E	5102	CFF	C14-N7-C8	-2.62	111.61	125.31
4	B	5102	CFF	C14-N7-C8	-2.62	111.62	125.31
3	G	5101	ATP	C2'-C1'-N9	-2.11	107.83	113.47
3	I	5101	ATP	C2'-C1'-N9	-2.08	107.90	113.47
3	E	5101	ATP	C2'-C1'-N9	-2.04	107.99	113.47
3	E	5101	ATP	C2-N1-C6	2.04	122.41	118.77
3	B	5101	ATP	C2-N1-C6	2.05	122.42	118.77
3	I	5101	ATP	C2-N1-C6	2.10	122.51	118.77
3	G	5101	ATP	C2-N1-C6	2.11	122.54	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	ATP	2	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
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	E	4345:UNK	C	4540:PHE	N	73.04
1	B	4345:UNK	C	4540:PHE	N	73.02
1	I	4345:UNK	C	4540:PHE	N	73.01
1	G	4345:UNK	C	4540:PHE	N	73.00
1	E	3613:UNK	C	3639:THR	N	45.97
1	B	3613:UNK	C	3639:THR	N	45.94
1	G	3613:UNK	C	3639:THR	N	45.92
1	I	3613:UNK	C	3639:THR	N	45.92
1	E	4253:GLU	C	4320:UNK	N	28.30
1	B	4253:GLU	C	4320:UNK	N	28.29
1	I	4253:GLU	C	4320:UNK	N	28.27
1	G	4253:GLU	C	4320:UNK	N	28.26
1	B	3163:UNK	C	3170:UNK	N	16.28
1	G	3163:UNK	C	3170:UNK	N	16.26
1	I	3163:UNK	C	3170:UNK	N	16.26
1	E	3163:UNK	C	3170:UNK	N	16.25
1	E	3063:UNK	C	3134:UNK	N	14.92
1	G	3063:UNK	C	3134:UNK	N	14.91
1	I	3063:UNK	C	3134:UNK	N	14.91
1	B	3063:UNK	C	3134:UNK	N	14.90
1	B	3468:UNK	C	3511:UNK	N	14.45
1	G	3468:UNK	C	3511:UNK	N	14.45
1	I	3468:UNK	C	3511:UNK	N	14.45
1	E	3468:UNK	C	3511:UNK	N	14.44
1	B	2703:UNK	C	2734:ASN	N	13.67
1	E	2703:UNK	C	2734:ASN	N	13.63
1	I	2703:UNK	C	2734:ASN	N	13.61

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	2703:UNK	C	2734:ASN	N	13.60
1	I	3236:UNK	C	3241:UNK	N	12.64
1	E	3236:UNK	C	3241:UNK	N	12.64
1	B	3236:UNK	C	3241:UNK	N	12.63
1	G	3236:UNK	C	3241:UNK	N	12.63
1	B	1564:UNK	C	1573:MET	N	12.50
1	E	1564:UNK	C	1573:MET	N	12.50
1	G	1564:UNK	C	1573:MET	N	12.48
1	I	1564:UNK	C	1573:MET	N	12.48
1	E	2976:UNK	C	2995:UNK	N	11.98
1	I	2976:UNK	C	2995:UNK	N	11.97
1	G	2976:UNK	C	2995:UNK	N	11.96
1	B	2976:UNK	C	2995:UNK	N	11.94
1	B	3254:UNK	C	3261:UNK	N	8.41
1	G	3254:UNK	C	3261:UNK	N	8.40
1	I	3254:UNK	C	3261:UNK	N	8.40
1	E	3254:UNK	C	3261:UNK	N	8.40
1	I	1297:UNK	C	1430:UNK	N	6.01
1	B	1297:UNK	C	1430:UNK	N	6.00
1	E	1297:UNK	C	1430:UNK	N	5.99
1	G	1297:UNK	C	1430:UNK	N	5.97
1	G	2479:LEU	C	2487:UNK	N	3.26
1	I	2479:LEU	C	2487:UNK	N	3.26
1	B	2479:LEU	C	2487:UNK	N	3.25
1	E	2479:LEU	C	2487:UNK	N	3.25
1	E	2939:ARG	C	2942:UNK	N	3.23
1	B	2939:ARG	C	2942:UNK	N	3.22
1	G	2939:ARG	C	2942:UNK	N	3.21
1	I	2939:ARG	C	2942:UNK	N	3.21