wwPDB EM Map/Model Validation Report (i)

Oct 17, 2016 – 06:17 PM EDT

PDB ID	:	5TAM
EMDB ID:	:	EMD-8379
Title	:	Structure of rabbit RyR1 (Caffeine/ATP/Ca2+ dataset, class 4)
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

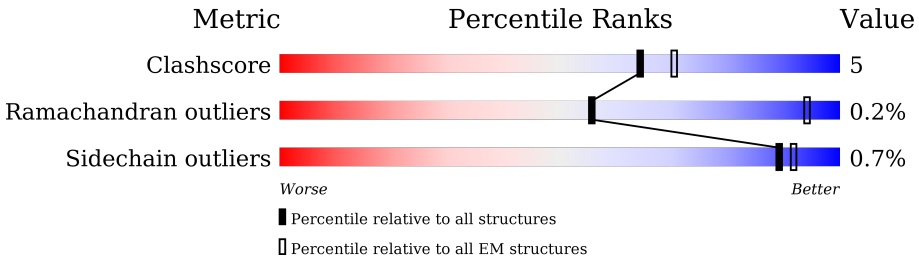
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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	79% 20% .
1	F	108	81% 19% .
1	H	108	81% 19% .
1	J	108	81% 19% .
2	B	4416	83% 11% 5%
2	E	4416	84% 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.

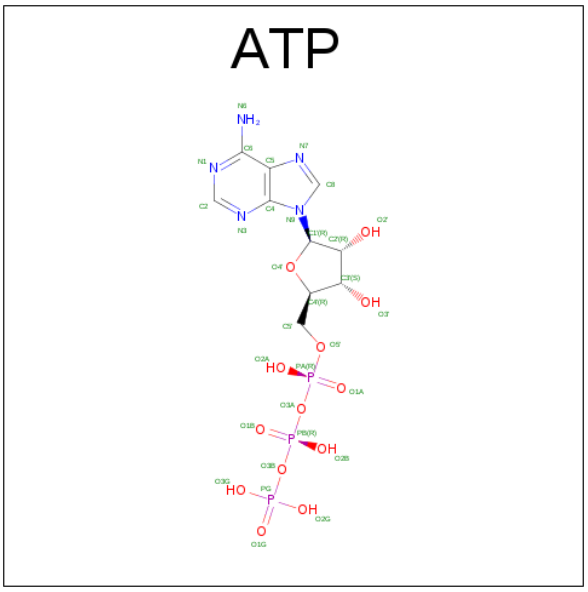
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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.

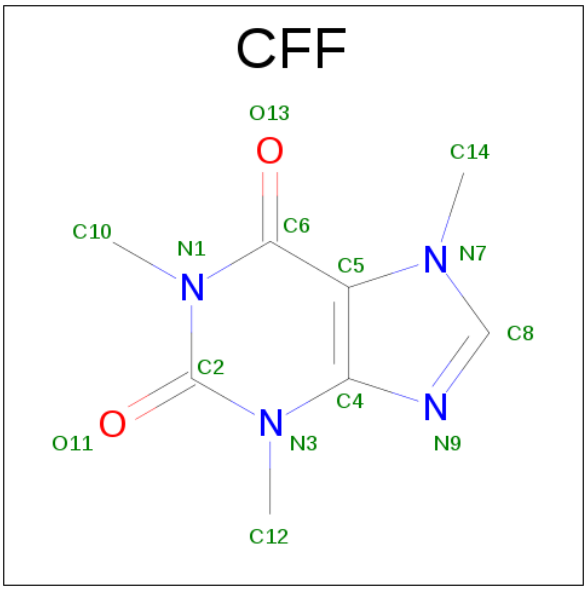
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- 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).

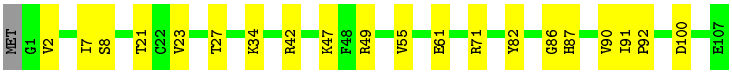
Mol	Chain	Residues	Atoms		AltConf
6	G	1	Total	Ca	0
			1	1	
6	B	1	Total	Ca	0
			1	1	
6	I	1	Total	Ca	0
			1	1	
6	E	1	Total	Ca	0
			1	1	

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.

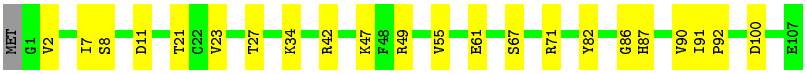
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



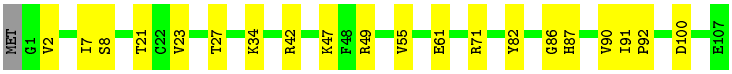
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



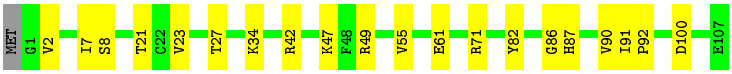
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



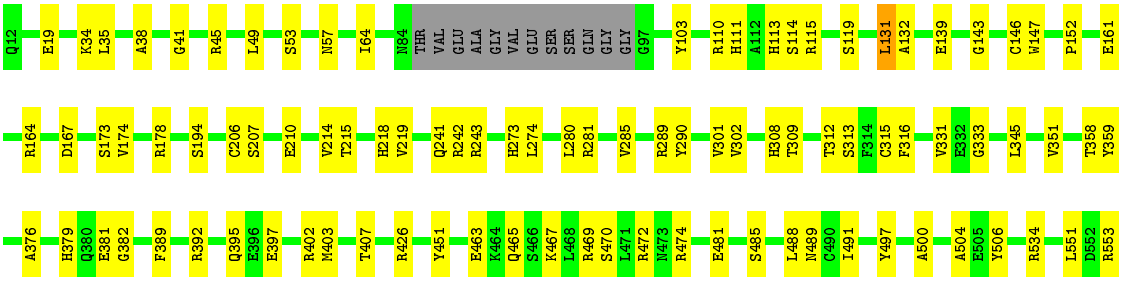
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

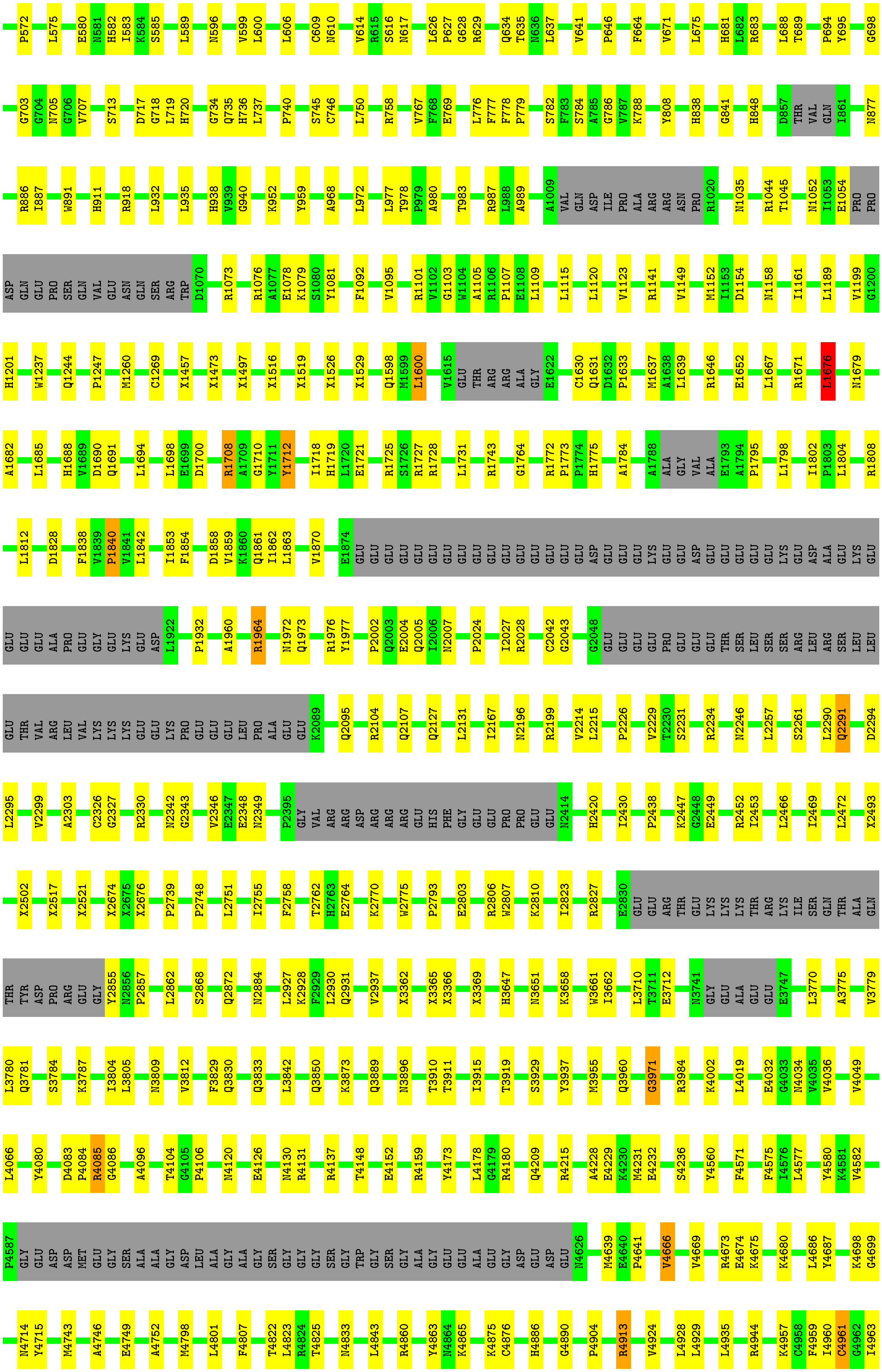
Chain J:



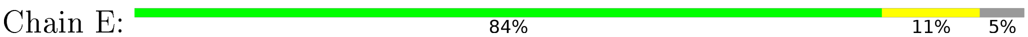
- Molecule 2: Ryanodine receptor 1

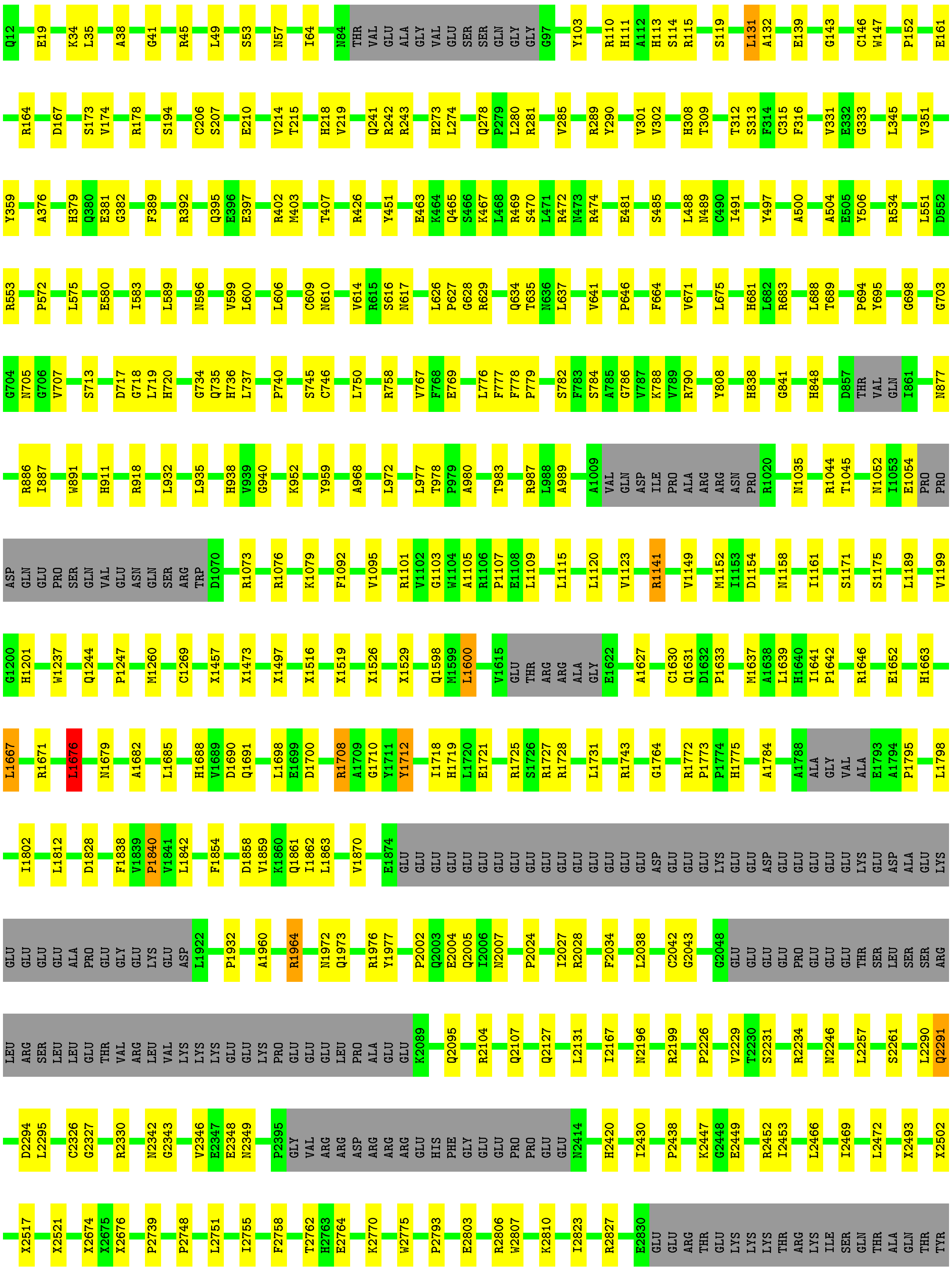
Chain B:

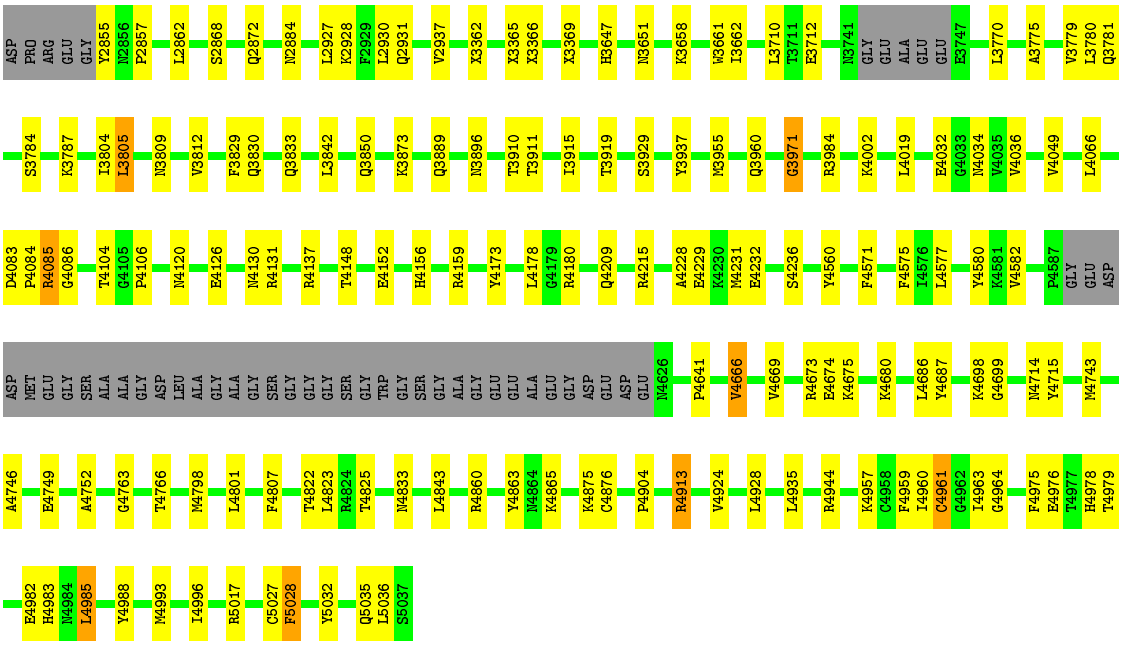



P572 L575 E580 N581 H582 I583 K584 S585 L589 N596 V599 L600 L606 C609 N610 V614 R615 S616 N617 L626 P627 G628 R629 Q634 T635 N636 L637 V641 P646 F664 V671 L675 H681 L682 R683 L688 T689 P694 Y695 G698
G703 G704 N705 G706 V707 S713 D717 G718 L719 H720 G734 Q735 H736 L737 P740 S745 C746 L750 R758 V767 F768 E769 L776 F777 F778 P779 S782 F783 S784 A785 G786 V787 K788 Y808 H838 G841 H848 D857 THR VAL GLN I861 N877
R886 I887 W891 H911 R918 L932 L935 H938 V939 G940 K952 Y959 A968 L972 L977 T978 P979 A980 T983 R987 L988 A989 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO R1020 N1035 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 F1092 V1095 R1101 V1102 G1103 W1104 A1105 R1106 P1107 E1108 L1109 L1115 L1120 V1123 R1141 V1149 M1152 I1153 D1154 N1158 I1161 L1189 V1199 G1200
H1201 W1237 Q1244 P1247 M1260 C1269 X1457 X1473 X1497 X1516 X1519 X1526 X1529 Q1598 M1599 L1600 V1615 GLU THR ARG ARG ALA GLY E1622 C1630 Q1631 D1632 P1633 M1637 A1638 L1639 R1646 E1652 L1667 R1671 L1676 N1679
A1682 L1685 H1688 V1689 D1690 Q1691 L1694 L1698 E1699 D1700 R1708 A1709 G1710 Y1711 Y1712 I1718 H1719 L1720 E1721 R1725 S1726 R1727 R1728 L1731 R1743 G1764 R1772 P1773 P1774 H1775 A1784 A1788 ALA GLY VAL ALA E1793 A1794 P1795 L1798 I1802 P1803 L1804 R1808
L1812 D1828 F1838 V1839 P1840 V1841 L1842 I1853 F1854 D1858 V1859 K1860 Q1861 I1862 L1863 V1870 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 P1932 A1960 R1964 N1972 Q1973 R1976 Y1977 P2002 Q2003 E2004 Q2005 I2006 N2007 P2024 I2027 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 Q2095 R2104 Q2107 Q2127 L2131 I2167 N2196 R2199 V2214 L2215 P2226 V2229 T2230 S2231 R2234 N2246 L2257 S2261 L2290 Q2291 D2294
L2295 V2299 A2303 C2326 G2327 R2330 N2342 G2343 V2346 E2347 E2348 N2349 P2395 GLY VAL ARG ARG ASP ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 H2420 I2430 P2438 K2447 G2448 E2449 R2452 I2453 L2466 I2469 L2472 X2493
X2502 X2517 X2521 X2674 X2675 X2676 P2739 P2748 L2751 I2755 F2758 T2762 H2763 E2764 K2770 W2775 P2793 E2803 R2806 W2807 K2810 I2823 R2827 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN
THR TYR ASP PRO ARG GLU GLY Y2855 N2856 P2857 L2862 S2868 Q2872 N2884 L2927 K2928 F2929 L2930 Q2931 V2937 X3362 X3365 X3366 X3369 H3647 N3651 K3658 W3661 I3662 L3710 T3711 E3712 N3741 GLY GLU ALA GLU GLU E3747 L3770 A3775 V3779
L3780 Q3781 S3784 K3787 I3804 L3805 N3809 V3812 F3829 Q3830 Q3833 L3842 Q3850 K3873 Q3889 N3896 T3910 T3911 I3915 T3919 S3929 Y3937 M3955 Q3960 G3971 R3984 K4002 L4019 E4032 G4033 N4034 V4035 V4036 V4049
L4066 Y4080 D4083 P4084 R4085 G4086 A4096 T4104 G4105 P4106 N4120 E4126 N4130 R4131 R4137 T4148 E4152 R4159 Y4173 L4178 G4179 R4180 Q4209 R4215 A4228 E4229 K4230 M4231 E4232 S4236 Y4560 F4571 F4575 I4576 L4577 Y4580 K4581 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 V4666 V4669 R4673 E4674 K4675 K4680 L4686 Y4687 K4698 G4699
N4714 Y4715 M4743 A4746 E4749 A4752 M4798 L4801 F4807 T4822 L4823 R4824 T4825 N4833 L4843 R4860 Y4863 N4864 K4865 K4875 C4876 H4886 G4890 P4904 R4913 V4924 L4928 L4929 L4935 R4944 K4957 C4958 F4959 I4960 C4961 G4962 I4963

- Molecule 2: Ryanodine receptor 1

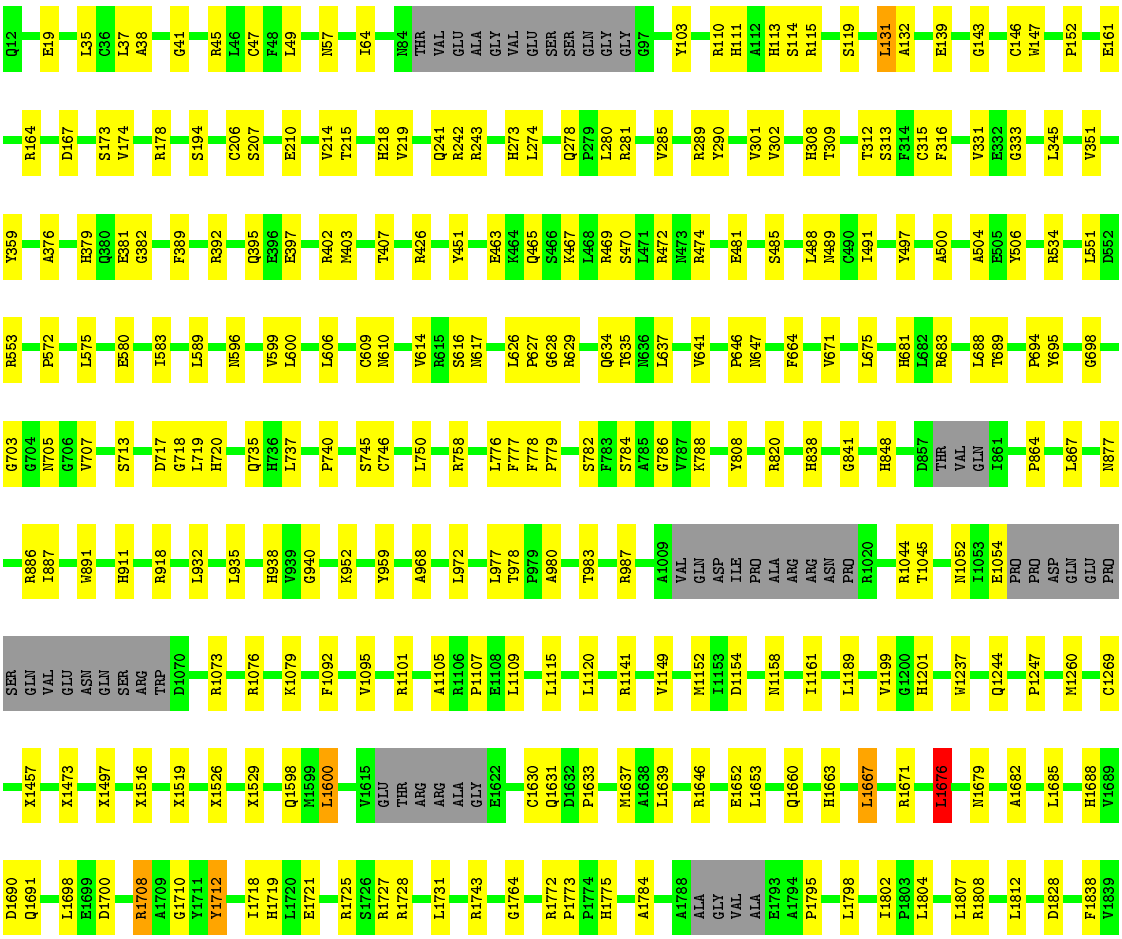


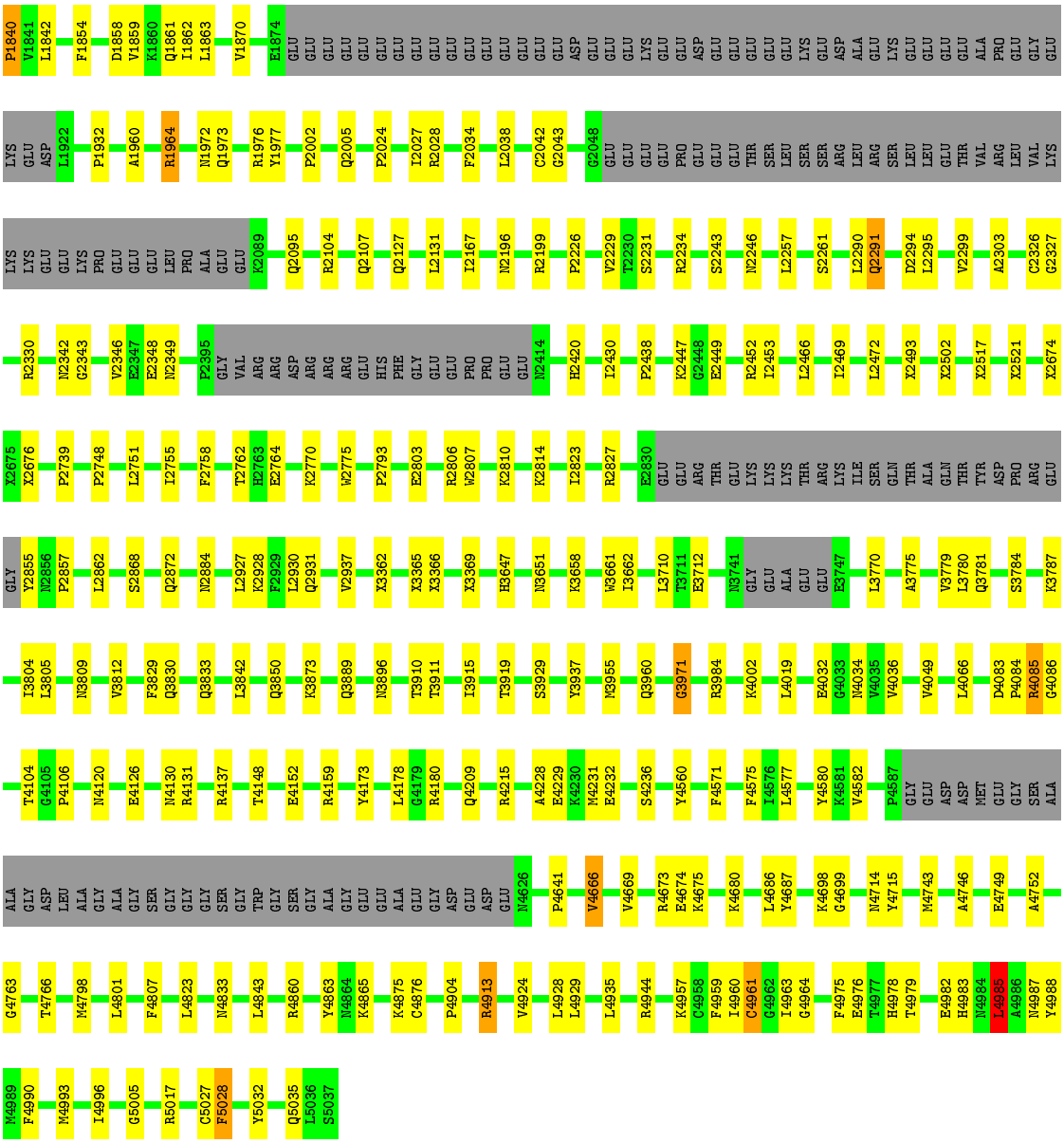




• Molecule 2: Ryanodine receptor 1

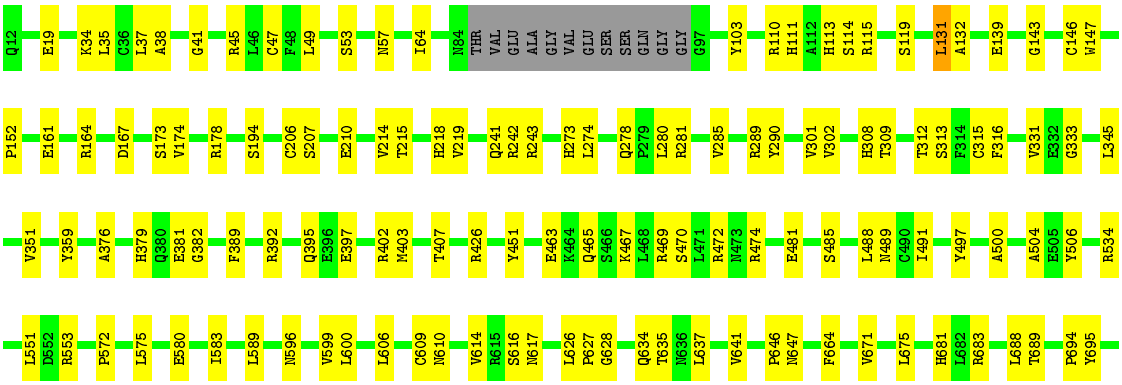
Chain I:

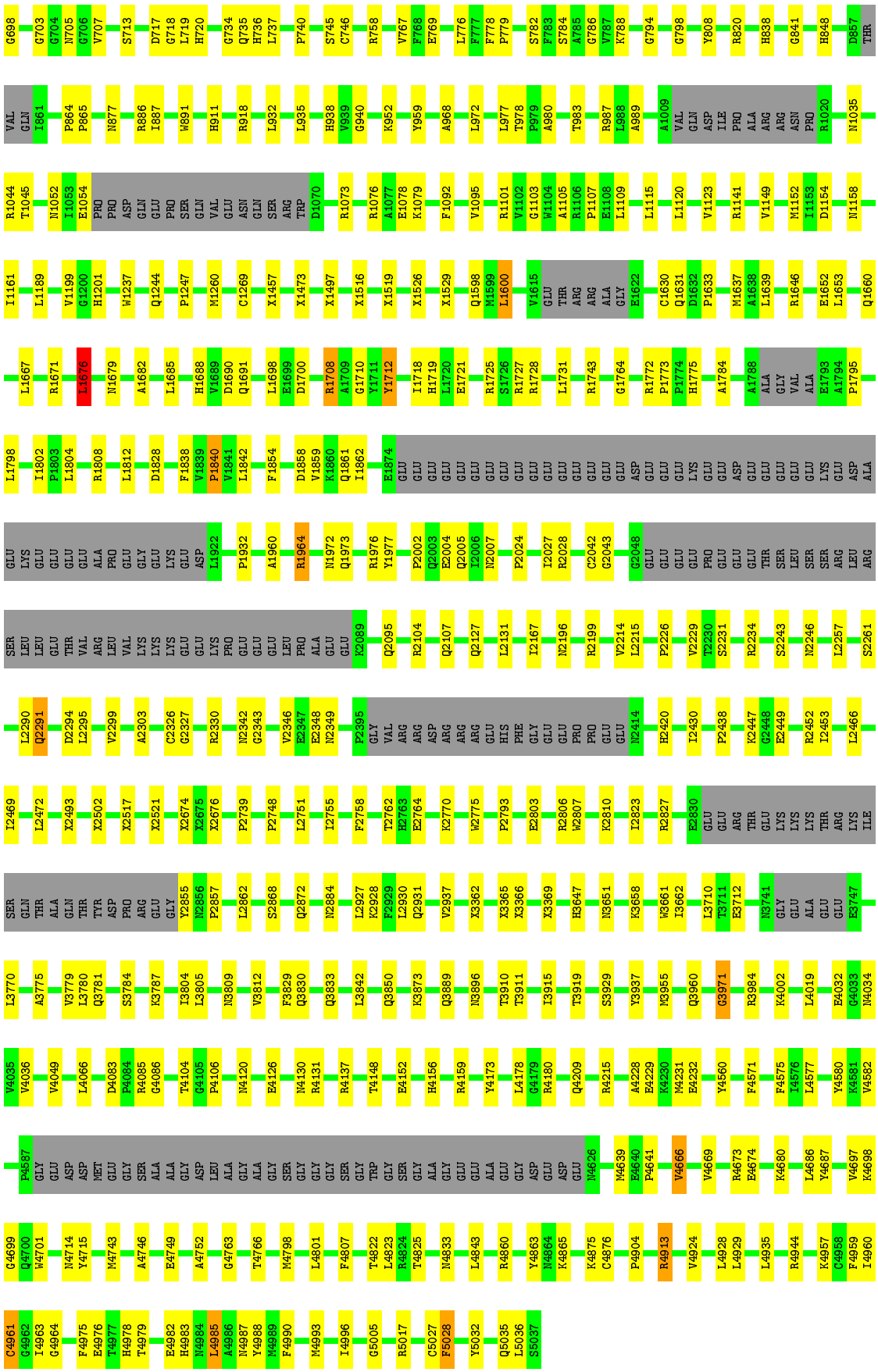




• Molecule 2: Ryanodine receptor 1

Chain G:





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	0.31	0/834	0.52	0/1123
1	F	0.31	0/834	0.52	0/1123
1	H	0.31	0/834	0.52	0/1123
1	J	0.31	0/834	0.52	0/1123
2	B	0.31	0/25428	0.55	9/34534 (0.0%)
2	E	0.31	0/25428	0.55	8/34534 (0.0%)
2	G	0.31	0/25428	0.55	9/34534 (0.0%)
2	I	0.31	0/25428	0.55	8/34534 (0.0%)
All	All	0.31	0/105048	0.55	34/142628 (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	17
2	E	0	17
2	G	0	17
2	I	0	17
All	All	0	72

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	131	LEU	CA-CB-CG	8.16	134.07	115.30
2	G	131	LEU	CA-CB-CG	8.16	134.07	115.30
2	B	131	LEU	CA-CB-CG	8.15	134.04	115.30
2	I	131	LEU	CA-CB-CG	8.13	133.99	115.30
2	E	4985	LEU	CA-CB-CG	7.48	132.50	115.30
2	G	4985	LEU	CA-CB-CG	7.47	132.47	115.30
2	B	4985	LEU	CA-CB-CG	7.46	132.47	115.30
2	I	4985	LEU	CA-CB-CG	7.45	132.44	115.30
2	I	1600	LEU	CA-CB-CG	6.83	131.00	115.30
2	G	1600	LEU	CA-CB-CG	6.82	130.98	115.30
2	B	1600	LEU	CA-CB-CG	6.81	130.97	115.30
2	E	1600	LEU	CA-CB-CG	6.81	130.97	115.30
2	B	1676	LEU	CA-CB-CG	6.66	130.62	115.30
2	G	1676	LEU	CA-CB-CG	6.65	130.60	115.30
2	E	1676	LEU	CA-CB-CG	6.64	130.57	115.30
2	I	1676	LEU	CA-CB-CG	6.64	130.56	115.30
2	G	2290	LEU	CA-CB-CG	6.02	129.14	115.30
2	B	2290	LEU	CA-CB-CG	6.02	129.14	115.30
2	E	2290	LEU	CA-CB-CG	6.02	129.14	115.30
2	I	2290	LEU	CA-CB-CG	6.00	129.10	115.30
2	G	688	LEU	CA-CB-CG	5.72	128.46	115.30
2	G	977	LEU	CA-CB-CG	5.72	128.45	115.30
2	E	977	LEU	CA-CB-CG	5.71	128.44	115.30
2	B	688	LEU	CA-CB-CG	5.71	128.44	115.30
2	E	688	LEU	CA-CB-CG	5.71	128.44	115.30
2	B	977	LEU	CA-CB-CG	5.71	128.43	115.30
2	I	977	LEU	CA-CB-CG	5.71	128.43	115.30
2	I	688	LEU	CA-CB-CG	5.70	128.41	115.30
2	I	1667	LEU	CA-CB-CG	5.34	127.57	115.30
2	G	1667	LEU	CA-CB-CG	5.33	127.57	115.30
2	B	1667	LEU	CA-CB-CG	5.32	127.53	115.30
2	E	1667	LEU	CA-CB-CG	5.32	127.53	115.30
2	G	4639	MET	C-N-CA	5.00	134.21	121.70
2	B	4639	MET	C-N-CA	5.00	134.21	121.70

There are no chirality outliers.

All (72) 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

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Mol	Chain	Res	Type	Group
2	B	1712	TYR	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
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	4666	VAL	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	1690	ASP	Peptide
2	E	1712	TYR	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	4666	VAL	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	1690	ASP	Peptide
2	G	1712	TYR	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

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Mol	Chain	Res	Type	Group
2	G	2807	TRP	Peptide
2	G	312	THR	Peptide
2	G	3971	GLY	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	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	1712	TYR	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	4666	VAL	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 (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	15	0
1	F	818	0	824	13	0
1	H	818	0	824	12	0
1	J	818	0	824	14	0
2	B	29499	0	24747	289	0
2	E	29499	0	24747	286	0
2	G	29499	0	24747	288	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	29499	0	24748	285	0
3	B	31	0	12	2	0
3	E	31	0	12	2	0
3	G	31	0	12	2	0
3	I	31	0	12	2	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	102373	1167	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 (1167) 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:B:4975:PHE:O	2:B:4979:THR:HG23	1.85	0.77
2:I:4975:PHE:O	2:I:4979:THR:HG23	1.85	0.76
2:E:4975:PHE:O	2:E:4979:THR:HG23	1.86	0.76
2:G:4975:PHE:O	2:G:4979:THR:HG23	1.86	0.76
2:G:5028:PHE:CE1	2:G:5032:TYR:CD2	2.78	0.71
2:I:5028:PHE:CE1	2:I:5032:TYR:CD2	2.78	0.71
2:B:5028:PHE:CE1	2:B:5032:TYR:CD2	2.78	0.71
2:E:5028:PHE:CE1	2:E:5032:TYR:CD2	2.78	0.70
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.57	0.70
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.57	0.70
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.57	0.68
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.57	0.67
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.60	0.67
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.60	0.66
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.60	0.66
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.78	0.66
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.78	0.66
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.78	0.66
2:G:173:SER:HB3	2:G:178:ARG:H	1.61	0.65
2:B:173:SER:HB3	2:B:178:ARG:H	1.61	0.65
2:I:173:SER:HB3	2:I:178:ARG:H	1.61	0.65
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.60	0.65
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.78	0.65
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.79	0.65
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.79	0.65
2:G:379:HIS:HD2	2:G:382:GLY:H	1.46	0.64
2:I:5028:PHE:CE1	2:I:5032:TYR:CE2	2.86	0.64
2:B:5028:PHE:CE1	2:B:5032:TYR:CE2	2.86	0.64
2:I:331:VAL:HG12	2:I:333:GLY:H	1.62	0.64
2:I:379:HIS:HD2	2:I:382:GLY:H	1.46	0.64
2:E:938:HIS:HB2	2:E:1054:GLU:HB2	1.79	0.64
2:E:379:HIS:HD2	2:E:382:GLY:H	1.46	0.63
2:E:4674:GLU:HG3	2:E:4714:ASN:HB3	1.81	0.63
2:G:5028:PHE:CE1	2:G:5032:TYR:CE2	2.86	0.63
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.80	0.63
2:B:938:HIS:HB2	2:B:1054:GLU:HB2	1.79	0.63
2:E:173:SER:HB3	2:E:178:ARG:H	1.61	0.63
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.79	0.63
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.80	0.63
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.80	0.63
2:B:4674:GLU:HG3	2:B:4714:ASN:HB3	1.81	0.63
2:E:5028:PHE:CE1	2:E:5032:TYR:CE2	2.86	0.63
2:I:938:HIS:HB2	2:I:1054:GLU:HB2	1.79	0.63
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.80	0.63
2:G:4674:GLU:HG3	2:G:4714:ASN:HB3	1.81	0.63
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.79	0.63
2:G:938:HIS:HB2	2:G:1054:GLU:HB2	1.79	0.63
2:G:331:VAL:HG12	2:G:333:GLY:H	1.62	0.63
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.32	0.63
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.80	0.63
2:E:174:VAL:O	2:G:2452:ARG:NH1	2.31	0.63
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.80	0.63
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.79	0.63
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.80	0.62
2:G:4957:LYS:HG2	2:G:4964:GLY:HA2	1.81	0.62
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:379:HIS:HD2	2:B:382:GLY:H	1.46	0.62
2:E:4957:LYS:HG2	2:E:4964:GLY:HA2	1.81	0.62
2:E:331:VAL:HG12	2:E:333:GLY:H	1.63	0.62
2:B:331:VAL:HG12	2:B:333:GLY:H	1.62	0.62
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.80	0.62
2:I:111:HIS:HD2	2:I:114:SER:H	1.48	0.62
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.32	0.62
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.32	0.62
2:G:111:HIS:HD2	2:G:114:SER:H	1.48	0.62
2:I:4674:GLU:HG3	2:I:4714:ASN:HB3	1.81	0.62
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.32	0.62
2:I:4957:LYS:HG2	2:I:4964:GLY:HA2	1.81	0.62
2:B:111:HIS:HD2	2:B:114:SER:H	1.48	0.61
2:B:4957:LYS:HG2	2:B:4964:GLY:HA2	1.81	0.61
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.34	0.61
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.34	0.61
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.34	0.61
2:E:4985:LEU:HB2	3:E:5101:ATP:HN61	1.66	0.61
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.34	0.61
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.83	0.61
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.34	0.60
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.83	0.60
2:E:111:HIS:HD2	2:E:114:SER:H	1.48	0.60
2:B:4985:LEU:HB2	3:B:5101:ATP:HN61	1.66	0.60
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.34	0.60
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.34	0.60
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.34	0.60
2:G:4985:LEU:HB2	3:G:5101:ATP:HN61	1.66	0.60
2:I:4985:LEU:HB2	3:I:5101:ATP:HN61	1.66	0.60
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.34	0.60
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.34	0.60
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.34	0.60
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.83	0.59
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.67	0.59
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.84	0.59
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.83	0.59
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.85	0.59
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.85	0.59
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.84	0.59
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.85	0.59
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.85	0.59
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.85	0.59
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.85	0.59
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.85	0.58
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.68	0.58
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.84	0.58
2:G:1637:MET:SD	2:G:1708:ARG:NH1	2.77	0.58
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.34	0.58
2:B:1637:MET:SD	2:B:1708:ARG:NH1	2.77	0.58
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.67	0.58
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.86	0.58
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.85	0.58
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.68	0.58
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.86	0.58
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.84	0.58
2:I:1637:MET:SD	2:I:1708:ARG:NH1	2.77	0.58
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.84	0.58
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.85	0.58
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.67	0.58
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.86	0.58
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.67	0.58
2:E:5028:PHE:CE1	2:E:5032:TYR:HD2	2.21	0.58
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.85	0.58
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.84	0.58
2:E:1637:MET:SD	2:E:1708:ARG:NH1	2.77	0.58
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.69	0.58
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.86	0.58
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.69	0.58
2:B:5028:PHE:CE1	2:B:5032:TYR:HD2	2.21	0.58
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.85	0.58
2:B:2452:ARG:NH1	2:I:174:VAL:O	2.37	0.58
2:I:609:CYS:SG	2:I:610:ASN:N	2.77	0.58
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.37	0.58
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.86	0.58
1:H:92:PRO:HD3	2:G:627:PRO:HB2	1.86	0.58
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.84	0.58
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	1.85	0.58
2:G:5028:PHE:CE1	2:G:5032:TYR:HD2	2.21	0.58
2:I:5028:PHE:CE1	2:I:5032:TYR:HD2	2.21	0.58
2:E:609:CYS:SG	2:E:610:ASN:N	2.77	0.57
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:609:CYS:SG	2:G:610:ASN:N	2.77	0.57
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.37	0.57
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.86	0.57
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.86	0.57
2:B:174:VAL:O	2:E:2452:ARG:NH1	2.37	0.57
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	1.85	0.57
2:B:609:CYS:SG	2:B:610:ASN:N	2.77	0.57
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.87	0.57
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.37	0.57
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.69	0.57
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.86	0.57
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.68	0.57
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.38	0.57
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.86	0.57
2:B:683:ARG:NH1	2:B:707:VAL:O	2.37	0.57
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.85	0.57
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.86	0.57
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.86	0.57
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	1.85	0.57
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	1.85	0.57
2:I:2452:ARG:NH1	2:G:174:VAL:O	2.36	0.57
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.86	0.57
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.38	0.57
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.37	0.57
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.86	0.57
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.86	0.57
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.38	0.57
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.86	0.57
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.86	0.57
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.86	0.57
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.85	0.57
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.38	0.57
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.38	0.57
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.86	0.57
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.87	0.56
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.69	0.56
2:G:2420:HIS:ND1	2:G:2493:UNK:O	2.38	0.56
2:I:2420:HIS:ND1	2:I:2493:UNK:O	2.38	0.56
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.39	0.56
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.87	0.56
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.71	0.56
2:E:2420:HIS:ND1	2:E:2493:UNK:O	2.38	0.56
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.88	0.56
2:I:315:CYS:SG	2:I:316:PHE:N	2.79	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	1.88	0.56
2:G:345:LEU:HD23	2:G:389:PHE:HB3	1.88	0.56
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.88	0.56
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.38	0.56
2:E:345:LEU:HD23	2:E:389:PHE:HB3	1.88	0.55
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.39	0.55
2:G:683:ARG:NH1	2:G:707:VAL:O	2.37	0.55
2:B:111:HIS:CD2	2:B:114:SER:H	2.25	0.55
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.71	0.55
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.38	0.55
2:E:683:ARG:NH1	2:E:707:VAL:O	2.37	0.55
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.39	0.55
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.40	0.55
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.71	0.55
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.38	0.55
2:I:111:HIS:CD2	2:I:114:SER:H	2.25	0.55
2:I:4231:MET:HE1	2:I:4960:ILE:HA	1.88	0.55
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.72	0.55
2:G:315:CYS:SG	2:G:316:PHE:N	2.79	0.55
2:G:4983:HIS:HB2	2:G:4988:TYR:HE2	1.72	0.55
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.72	0.55
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.89	0.55
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.89	0.55
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.89	0.55
2:G:111:HIS:CD2	2:G:114:SER:H	2.25	0.55
2:I:345:LEU:HD23	2:I:389:PHE:HB3	1.88	0.55
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.89	0.55
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.40	0.55
2:I:683:ARG:NH1	2:I:707:VAL:O	2.37	0.55
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.88	0.55
2:B:2420:HIS:ND1	2:B:2493:UNK:O	2.38	0.55
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.40	0.55
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.88	0.55
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.39	0.55
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.40	0.55
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.71	0.55
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.80	0.55
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.89	0.55
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.88	0.55
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.80	0.55
2:I:675:LEU:HD11	2:I:1633:PRO:HB3	1.89	0.55
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.88	0.55
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.40	0.55
2:I:4983:HIS:HB2	2:I:4988:TYR:HE2	1.72	0.55
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.39	0.55
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.40	0.54
2:B:345:LEU:HD23	2:B:389:PHE:HB3	1.88	0.54
2:E:4983:HIS:HB2	2:E:4988:TYR:HE2	1.72	0.54
2:G:675:LEU:HD11	2:G:1633:PRO:HB3	1.89	0.54
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.88	0.54
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.39	0.54
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.89	0.54
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.40	0.54
2:B:614:VAL:HG22	2:B:616:SER:H	1.73	0.54
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.72	0.54
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.90	0.54
2:E:4228:ALA:O	2:E:4232:GLU:N	2.40	0.54
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.40	0.54
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.40	0.54
2:B:4209:GLN:HE22	2:B:4560:TYR:HE2	1.56	0.54
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.40	0.54
2:B:315:CYS:SG	2:B:316:PHE:N	2.79	0.54
2:B:4983:HIS:HB2	2:B:4988:TYR:HE2	1.72	0.54
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.89	0.54
2:E:614:VAL:HG22	2:E:616:SER:H	1.73	0.54
2:G:695:TYR:OH	2:G:1073:ARG:NH1	2.40	0.54
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.90	0.54
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.40	0.54
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.90	0.54
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.40	0.54
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.80	0.54
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.40	0.54
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.80	0.54
2:B:580:GLU:HG2	2:B:583:ILE:HD11	1.89	0.54
2:E:395:GLN:HG3	2:E:397:GLU:H	1.73	0.54
2:G:395:GLN:HG3	2:G:397:GLU:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4924:VAL:HA	2:I:4928:LEU:HB2	1.90	0.54
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.89	0.54
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.72	0.54
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.90	0.54
2:G:4982:GLU:HA	2:G:4982:GLU:OE1	2.08	0.54
2:G:689:THR:H	2:G:778:PHE:HE2	1.55	0.54
2:B:689:THR:H	2:B:778:PHE:HE2	1.55	0.54
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.90	0.54
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.40	0.54
2:G:4209:GLN:HE22	2:G:4560:TYR:HE2	1.56	0.54
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.90	0.53
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.89	0.53
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.90	0.53
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.90	0.53
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.73	0.53
2:E:4152:GLU:OE2	2:E:4180:ARG:NH1	2.42	0.53
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.89	0.53
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.88	0.53
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.90	0.53
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.90	0.53
2:E:313:SER:HB3	2:E:351:VAL:HB	1.91	0.53
2:E:580:GLU:HG2	2:E:583:ILE:HD11	1.89	0.53
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.41	0.53
2:G:4924:VAL:HA	2:G:4928:LEU:HB2	1.90	0.53
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.73	0.53
2:B:675:LEU:HD11	2:B:1633:PRO:HB3	1.89	0.53
2:E:111:HIS:CD2	2:E:114:SER:H	2.25	0.53
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.91	0.53
2:I:4152:GLU:OE2	2:I:4180:ARG:NH1	2.42	0.53
2:I:689:THR:H	2:I:778:PHE:HE2	1.55	0.53
2:B:4152:GLU:OE2	2:B:4180:ARG:NH1	2.42	0.53
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.40	0.53
2:B:1247:PRO:HA	2:B:1598:GLN:HA	1.91	0.53
2:E:675:LEU:HD11	2:E:1633:PRO:HB3	1.89	0.53
2:I:313:SER:HB3	2:I:351:VAL:HB	1.91	0.53
2:I:614:VAL:HG22	2:I:616:SER:H	1.73	0.53
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.90	0.53
2:B:4982:GLU:OE1	2:B:4982:GLU:HA	2.08	0.53
2:E:4982:GLU:HA	2:E:4982:GLU:OE1	2.08	0.53
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.90	0.53
2:E:315:CYS:SG	2:E:316:PHE:N	2.79	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4152:GLU:OE2	2:G:4180:ARG:NH1	2.42	0.53
2:I:395:GLN:HG3	2:I:397:GLU:H	1.73	0.53
2:I:4209:GLN:HE22	2:I:4560:TYR:HE2	1.56	0.53
2:I:695:TYR:OH	2:I:1073:ARG:NH1	2.40	0.53
1:J:7:ILE:HB	1:J:71:ARG:HB3	1.91	0.53
1:A:7:ILE:HB	1:A:71:ARG:HB3	1.91	0.53
2:B:4924:VAL:HA	2:B:4928:LEU:HB2	1.90	0.53
2:B:4961:CYS:HB3	2:B:4983:HIS:CE1	2.44	0.53
2:B:4960:ILE:HD11	2:B:4985:LEU:HD23	1.91	0.53
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.90	0.53
2:E:1247:PRO:HA	2:E:1598:GLN:HA	1.91	0.53
2:E:4961:CYS:HB3	2:E:4983:HIS:CE1	2.44	0.53
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.90	0.53
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.91	0.53
2:G:580:GLU:HG2	2:G:583:ILE:HD11	1.89	0.53
2:B:313:SER:HB3	2:B:351:VAL:HB	1.91	0.53
2:B:395:GLN:HG3	2:B:397:GLU:H	1.73	0.53
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.73	0.53
2:E:4231:MET:HE1	2:E:4960:ILE:HA	1.91	0.53
1:F:92:PRO:HD3	2:E:627:PRO:HB2	1.90	0.53
2:I:4961:CYS:HB3	2:I:4983:HIS:CE1	2.44	0.53
2:I:4960:ILE:HD11	2:I:4985:LEU:HD23	1.91	0.53
2:E:4924:VAL:HA	2:E:4928:LEU:HB2	1.90	0.52
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.91	0.52
2:G:313:SER:HB3	2:G:351:VAL:HB	1.91	0.52
2:G:4961:CYS:HB3	2:G:4983:HIS:CE1	2.44	0.52
2:I:911:HIS:O	2:I:918:ARG:NH2	2.42	0.52
2:B:911:HIS:O	2:B:918:ARG:NH2	2.42	0.52
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.91	0.52
1:F:7:ILE:HB	1:F:71:ARG:HB3	1.91	0.52
2:G:4978:HIS:HA	2:G:4982:GLU:HB2	1.91	0.52
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.92	0.52
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.91	0.52
2:I:580:GLU:HG2	2:I:583:ILE:HD11	1.89	0.52
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.91	0.52
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.89	0.52
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.92	0.52
2:G:1247:PRO:HA	2:G:1598:GLN:HA	1.91	0.52
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.90	0.52
2:B:132:ALA:HA	2:B:194:SER:HB2	1.91	0.52
2:G:143:GLY:HA3	2:G:147:TRP:HE1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:143:GLY:HA3	2:I:147:TRP:HE1	1.75	0.52
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.92	0.52
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.92	0.52
1:A:34:LYS:HD3	2:B:629:ARG:HD2	1.92	0.52
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.90	0.52
2:I:4982:GLU:HA	2:I:4982:GLU:OE1	2.08	0.52
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.91	0.52
2:E:143:GLY:HA3	2:E:147:TRP:HE1	1.75	0.52
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.91	0.52
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.92	0.52
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.90	0.52
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.90	0.52
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.73	0.52
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.43	0.52
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.90	0.52
2:G:4960:ILE:HD11	2:G:4985:LEU:HD23	1.91	0.52
2:G:614:VAL:HG22	2:G:616:SER:H	1.73	0.52
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.92	0.52
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.90	0.52
2:E:465:GLN:HG3	2:E:3710:LEU:HB3	1.92	0.52
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.91	0.52
2:E:4960:ILE:HD11	2:E:4985:LEU:HD23	1.91	0.52
2:G:465:GLN:HG3	2:G:3710:LEU:HB3	1.92	0.52
2:E:132:ALA:HA	2:E:194:SER:HB2	1.91	0.52
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.91	0.52
2:B:4749:GLU:HA	2:B:4752:ALA:HB3	1.93	0.51
2:B:4978:HIS:HA	2:B:4982:GLU:HB2	1.91	0.51
2:E:4209:GLN:HE22	2:E:4560:TYR:HE2	1.56	0.51
2:E:4798:MET:HA	2:E:4801:LEU:HB2	1.91	0.51
2:E:4865:LYS:HG3	2:E:4875:LYS:HZ3	1.76	0.51
2:E:4978:HIS:HA	2:E:4982:GLU:HB2	1.91	0.51
2:E:689:THR:H	2:E:778:PHE:HE2	1.55	0.51
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.92	0.51
1:H:55:VAL:HA	2:G:1784:ALA:HA	1.92	0.51
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.92	0.51
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.92	0.51
2:B:143:GLY:HA3	2:B:147:TRP:HE1	1.75	0.51
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.92	0.51
2:E:470:SER:O	2:E:474:ARG:NE	2.40	0.51
2:E:695:TYR:OH	2:E:1073:ARG:NH1	2.40	0.51
2:G:309:THR:O	2:G:313:SER:OG	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.91	0.51
2:G:4798:MET:HA	2:G:4801:LEU:HB2	1.91	0.51
2:I:1247:PRO:HA	2:I:1598:GLN:HA	1.91	0.51
2:I:1516:UNK:N	2:I:1529:UNK:O	2.43	0.51
2:I:465:GLN:HG3	2:I:3710:LEU:HB3	1.92	0.51
2:B:465:GLN:HG3	2:B:3710:LEU:HB3	1.92	0.51
2:B:695:TYR:OH	2:B:1073:ARG:NH1	2.40	0.51
2:E:309:THR:O	2:E:313:SER:OG	2.28	0.51
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.92	0.51
2:G:4749:GLU:HA	2:G:4752:ALA:HB3	1.93	0.51
2:G:5028:PHE:HE1	2:G:5032:TYR:CE2	2.29	0.51
2:G:911:HIS:O	2:G:918:ARG:NH2	2.42	0.51
2:I:164:ARG:N	2:I:167:ASP:OD2	2.44	0.51
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.43	0.51
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.91	0.51
2:B:4798:MET:HA	2:B:4801:LEU:HB2	1.91	0.51
2:B:4865:LYS:HG3	2:B:4875:LYS:HZ3	1.76	0.51
2:E:4749:GLU:HA	2:E:4752:ALA:HB3	1.93	0.51
2:G:132:ALA:HA	2:G:194:SER:HB2	1.91	0.51
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.92	0.51
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.43	0.51
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.43	0.51
2:E:485:SER:O	2:E:489:ASN:N	2.37	0.51
2:I:4749:GLU:HA	2:I:4752:ALA:HB3	1.92	0.51
2:I:4798:MET:HA	2:I:4801:LEU:HB2	1.91	0.51
2:I:4978:HIS:HA	2:I:4982:GLU:HB2	1.91	0.51
2:B:309:THR:O	2:B:313:SER:OG	2.29	0.51
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.92	0.51
2:B:5028:PHE:HE1	2:B:5032:TYR:CE2	2.29	0.51
2:E:1516:UNK:N	2:E:1529:UNK:O	2.43	0.51
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.92	0.51
2:G:1516:UNK:N	2:G:1529:UNK:O	2.43	0.51
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.93	0.51
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.93	0.51
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.93	0.51
1:H:7:ILE:HB	1:H:71:ARG:HB3	1.91	0.51
2:I:4865:LYS:HG3	2:I:4875:LYS:HZ3	1.76	0.51
2:E:2196:ASN:OD1	2:E:2199:ARG:NH1	2.40	0.51
2:G:4231:MET:HE1	2:G:4960:ILE:HA	1.93	0.51
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.92	0.51
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.93	0.51
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.92	0.51
2:I:132:ALA:HA	2:I:194:SER:HB2	1.91	0.51
2:B:1516:UNK:N	2:B:1529:UNK:O	2.43	0.50
2:B:4231:MET:HE1	2:B:4960:ILE:HA	1.92	0.50
2:G:2868:SER:O	2:G:2872:GLN:N	2.45	0.50
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.93	0.50
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.45	0.50
1:A:21:THR:HA	1:A:49:ARG:HA	1.94	0.50
1:A:82:TYR:O	1:A:86:GLY:N	2.45	0.50
2:B:164:ARG:N	2:B:167:ASP:OD2	2.44	0.50
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.93	0.50
2:E:241:GLN:O	2:E:289:ARG:NH1	2.38	0.50
2:E:2868:SER:O	2:E:2872:GLN:N	2.45	0.50
2:E:359:TYR:HA	2:E:376:ALA:HA	1.94	0.50
1:F:21:THR:HA	1:F:49:ARG:HA	1.94	0.50
2:G:359:TYR:HA	2:G:376:ALA:HA	1.93	0.50
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.92	0.50
2:I:470:SER:O	2:I:474:ARG:NE	2.40	0.50
2:I:242:ARG:NH1	2:I:481:GLU:OE1	2.45	0.50
1:J:34:LYS:HD3	2:I:629:ARG:HD2	1.93	0.50
2:B:242:ARG:NH1	2:B:481:GLU:OE1	2.45	0.50
2:E:911:HIS:O	2:E:918:ARG:NH2	2.42	0.50
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.45	0.50
1:J:82:TYR:O	1:J:86:GLY:N	2.45	0.50
2:E:5028:PHE:HE1	2:E:5032:TYR:CE2	2.29	0.50
2:I:309:THR:O	2:I:313:SER:OG	2.29	0.50
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.45	0.50
2:E:242:ARG:NH1	2:E:481:GLU:OE1	2.45	0.50
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.83	0.50
2:B:4996:ILE:HG12	4:B:5102:CFF:H123	1.94	0.50
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.44	0.50
2:I:243:ARG:NH1	2:I:301:VAL:O	2.39	0.50
2:E:4996:ILE:HG12	4:E:5102:CFF:H123	1.94	0.50
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.45	0.49
2:B:4976:GLU:HA	2:B:4979:THR:HG23	1.94	0.49
2:E:243:ARG:NH1	2:E:301:VAL:O	2.39	0.49
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.94	0.49
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.94	0.49
2:G:470:SER:O	2:G:474:ARG:NE	2.40	0.49
2:I:572:PRO:HA	2:I:575:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.94	0.49
1:J:21:THR:HA	1:J:49:ARG:HA	1.94	0.49
2:B:2196:ASN:OD1	2:B:2199:ARG:NH1	2.40	0.49
2:B:572:PRO:HA	2:B:575:LEU:HD13	1.94	0.49
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.93	0.49
2:E:41:GLY:O	2:E:45:ARG:NH1	2.45	0.49
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	1.95	0.49
2:G:4865:LYS:HG3	2:G:4875:LYS:HZ3	1.76	0.49
1:H:82:TYR:O	1:H:86:GLY:N	2.45	0.49
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.94	0.49
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.94	0.49
2:G:164:ARG:N	2:G:167:ASP:OD2	2.44	0.49
2:G:2196:ASN:OD1	2:G:2199:ARG:NH1	2.40	0.49
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.94	0.49
2:I:4228:ALA:O	2:I:4232:GLU:N	2.40	0.49
1:J:92:PRO:HD3	2:I:627:PRO:HB2	1.93	0.49
1:A:55:VAL:HA	2:B:1784:ALA:HA	1.94	0.49
2:B:241:GLN:O	2:B:289:ARG:NH1	2.38	0.49
2:B:470:SER:O	2:B:474:ARG:NE	2.40	0.49
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.44	0.49
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.94	0.49
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	1.94	0.49
2:I:4996:ILE:HG12	4:I:5102:CFF:H123	1.94	0.49
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.93	0.49
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	1.94	0.49
2:B:41:GLY:O	2:B:45:ARG:NH1	2.45	0.49
2:G:4976:GLU:HA	2:G:4979:THR:HG23	1.94	0.49
2:I:596:ASN:HB3	2:I:599:VAL:HG22	1.95	0.49
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.94	0.49
2:B:596:ASN:HB3	2:B:599:VAL:HG22	1.95	0.49
2:E:161:GLU:HA	2:G:3984:ARG:HH22	1.77	0.49
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	1.95	0.49
2:G:4904:PRO:HB3	2:G:4913:ARG:HD2	1.95	0.49
2:I:2196:ASN:OD1	2:I:2199:ARG:NH1	2.40	0.49
2:I:2868:SER:O	2:I:2872:GLN:N	2.44	0.49
2:I:4904:PRO:HB3	2:I:4913:ARG:HD2	1.95	0.49
2:I:500:ALA:HB1	2:I:504:ALA:HB2	1.95	0.49
2:B:290:TYR:O	2:B:302:VAL:N	2.46	0.49
2:E:164:ARG:N	2:E:167:ASP:OD2	2.44	0.49
2:G:2346:VAL:HG22	2:G:2348:GLU:H	1.78	0.49
2:G:500:ALA:HB1	2:G:504:ALA:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:21:THR:HA	1:H:49:ARG:HA	1.94	0.49
1:F:82:TYR:O	1:F:86:GLY:N	2.45	0.49
2:I:359:TYR:HA	2:I:376:ALA:HA	1.93	0.49
2:B:359:TYR:HA	2:B:376:ALA:HA	1.93	0.49
2:E:572:PRO:HA	2:E:575:LEU:HD13	1.94	0.49
2:I:4976:GLU:HA	2:I:4979:THR:HG23	1.94	0.49
2:B:2346:VAL:HG22	2:B:2348:GLU:H	1.78	0.49
2:B:2827:ARG:HH21	2:B:2931:GLN:HG3	1.78	0.49
2:E:5028:PHE:HE1	2:E:5032:TYR:HE2	1.61	0.49
2:G:41:GLY:O	2:G:45:ARG:NH1	2.45	0.49
2:G:596:ASN:HB3	2:G:599:VAL:HG22	1.95	0.49
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.95	0.49
2:I:2346:VAL:HG22	2:I:2348:GLU:H	1.78	0.49
2:E:1731:LEU:HA	2:E:1772:ARG:HH12	1.78	0.48
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.46	0.48
2:G:978:THR:HB	2:G:980:ALA:H	1.78	0.48
2:I:5028:PHE:HE1	2:I:5032:TYR:CE2	2.29	0.48
1:J:55:VAL:HA	2:I:1784:ALA:HA	1.95	0.48
2:B:2868:SER:O	2:B:2872:GLN:N	2.44	0.48
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.94	0.48
2:B:485:SER:O	2:B:489:ASN:N	2.37	0.48
2:E:551:LEU:HD21	2:E:589:LEU:HD13	1.95	0.48
2:I:978:THR:HB	2:I:980:ALA:H	1.78	0.48
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.46	0.48
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.83	0.48
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.96	0.48
2:B:4904:PRO:HB3	2:B:4913:ARG:HD2	1.95	0.48
2:E:290:TYR:O	2:E:302:VAL:N	2.46	0.48
2:E:2827:ARG:HH21	2:E:2931:GLN:HG3	1.78	0.48
2:E:4976:GLU:HA	2:E:4979:THR:HG23	1.94	0.48
2:G:4996:ILE:HG12	4:G:5102:CFF:H123	1.94	0.48
2:G:551:LEU:HD21	2:G:589:LEU:HD13	1.95	0.48
2:B:1731:LEU:HA	2:B:1772:ARG:HH12	1.78	0.48
2:G:243:ARG:NH1	2:G:301:VAL:O	2.39	0.48
2:G:4228:ALA:O	2:G:4232:GLU:N	2.40	0.48
2:G:5028:PHE:HE1	2:G:5032:TYR:HE2	1.61	0.48
2:I:2346:VAL:HG13	2:I:2349:ASN:H	1.79	0.48
2:I:290:TYR:O	2:I:302:VAL:N	2.46	0.48
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.47	0.48
2:B:2346:VAL:HG13	2:B:2349:ASN:H	1.79	0.48
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:978:THR:HB	2:B:980:ALA:H	1.78	0.48
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.96	0.48
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.47	0.48
2:E:4904:PRO:HB3	2:E:4913:ARG:HD2	1.95	0.48
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.95	0.48
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.46	0.48
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.94	0.48
2:G:4577:LEU:HG	2:G:4580:TYR:HE2	1.79	0.48
2:G:4963:ILE:HD13	2:G:5027:CYS:SG	2.54	0.48
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.49	0.48
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.94	0.48
2:B:698:GLY:HA2	2:B:703:GLY:HA2	1.96	0.48
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.49	0.48
2:I:551:LEU:HD21	2:I:589:LEU:HD13	1.95	0.48
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.94	0.48
2:B:4963:ILE:HD13	2:B:5027:CYS:SG	2.54	0.48
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.94	0.48
2:E:4577:LEU:HG	2:E:4580:TYR:HE2	1.79	0.48
2:E:978:THR:HB	2:E:980:ALA:H	1.78	0.48
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.96	0.48
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.47	0.48
2:G:572:PRO:HA	2:G:575:LEU:HD13	1.94	0.48
2:B:551:LEU:HD21	2:B:589:LEU:HD13	1.95	0.48
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.95	0.48
2:E:2346:VAL:HG22	2:E:2348:GLU:H	1.78	0.48
2:E:596:ASN:HB3	2:E:599:VAL:HG22	1.95	0.48
2:I:3984:ARG:HH22	2:G:161:GLU:HA	1.79	0.48
2:G:2346:VAL:HG13	2:G:2349:ASN:H	1.79	0.48
2:B:161:GLU:HA	2:E:3984:ARG:HH22	1.79	0.48
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.49	0.48
2:E:4963:ILE:HD13	2:E:5027:CYS:SG	2.54	0.48
2:E:500:ALA:HB1	2:E:504:ALA:HB2	1.95	0.48
2:E:698:GLY:HA2	2:E:703:GLY:HA2	1.96	0.48
2:G:3770:LEU:HD21	2:G:3775:ALA:HB3	1.96	0.48
2:G:4083:ASP:HB3	2:G:4086:GLY:H	1.79	0.48
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.46	0.48
2:I:4963:ILE:HD13	2:I:5027:CYS:SG	2.54	0.48
2:B:3915:ILE:O	2:B:3919:THR:N	2.45	0.48
2:G:698:GLY:HA2	2:G:703:GLY:HA2	1.96	0.48
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.95	0.48
2:B:500:ALA:HB1	2:B:504:ALA:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4577:LEU:HG	2:I:4580:TYR:HE2	1.79	0.47
2:I:1731:LEU:HA	2:I:1772:ARG:HH12	1.78	0.47
2:I:2827:ARG:HH21	2:I:2931:GLN:HG3	1.78	0.47
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.96	0.47
2:I:41:GLY:O	2:I:45:ARG:NH1	2.45	0.47
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.95	0.47
2:B:4577:LEU:HG	2:B:4580:TYR:HE2	1.79	0.47
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.96	0.47
2:E:4083:ASP:HB3	2:E:4086:GLY:H	1.79	0.47
2:G:3915:ILE:O	2:G:3919:THR:N	2.45	0.47
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.49	0.47
1:A:92:PRO:HD3	2:B:627:PRO:HB2	1.97	0.47
2:G:290:TYR:O	2:G:302:VAL:N	2.46	0.47
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.96	0.47
2:B:4228:ALA:O	2:B:4232:GLU:N	2.40	0.47
2:B:4822:THR:O	2:B:4825:THR:OG1	2.27	0.47
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.96	0.47
2:E:3915:ILE:O	2:E:3919:THR:N	2.45	0.47
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.83	0.47
2:G:242:ARG:NH1	2:G:481:GLU:OE1	2.45	0.47
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.48	0.47
2:B:4083:ASP:HB3	2:B:4086:GLY:H	1.79	0.47
2:G:2827:ARG:HH21	2:G:2931:GLN:HG3	1.78	0.47
2:I:4236:SER:OG	2:I:4675:LYS:NZ	2.36	0.47
2:B:3971:GLY:N	2:B:4032:GLU:OE2	2.47	0.47
2:B:5028:PHE:HE1	2:B:5032:TYR:HE2	1.61	0.47
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.48	0.47
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.96	0.47
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.48	0.47
2:I:4083:ASP:HB3	2:I:4086:GLY:H	1.79	0.47
2:I:698:GLY:HA2	2:I:703:GLY:HA2	1.96	0.47
2:G:1731:LEU:HA	2:G:1772:ARG:HH12	1.78	0.47
2:G:4863:TYR:HD2	2:G:4875:LYS:HB2	1.79	0.47
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.97	0.47
2:B:1727:ARG:NH2	2:B:1773:PRO:O	2.44	0.47
2:B:4236:SER:OG	2:B:4675:LYS:NZ	2.36	0.47
2:E:4822:THR:O	2:E:4825:THR:OG1	2.27	0.47
2:E:4863:TYR:HD2	2:E:4875:LYS:HB2	1.79	0.47
1:F:34:LYS:HE3	2:E:634:GLN:HB3	1.95	0.47
2:G:241:GLN:O	2:G:289:ARG:NH1	2.38	0.47
2:I:451:TYR:O	2:I:474:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.97	0.47
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.80	0.47
2:B:34:LYS:H	2:B:53:SER:HG	1.62	0.47
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.97	0.47
2:E:641:VAL:HG11	2:E:681:HIS:HD1	1.80	0.47
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.44	0.47
2:B:403:MET:O	2:B:407:THR:N	2.49	0.46
2:B:4863:TYR:HD2	2:B:4875:LYS:HB2	1.79	0.46
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.97	0.46
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.80	0.46
2:E:3770:LEU:HD21	2:E:3775:ALA:HB3	1.96	0.46
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.97	0.46
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.80	0.46
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.80	0.46
2:B:683:ARG:HG2	2:B:717:ASP:HB3	1.98	0.46
2:G:451:TYR:O	2:G:474:ARG:NH1	2.47	0.46
2:I:4863:TYR:HD2	2:I:4875:LYS:HB2	1.78	0.46
2:E:1244:GLN:OE1	2:E:1646:ARG:NH1	2.49	0.46
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.97	0.46
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.80	0.46
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.81	0.46
2:B:3770:LEU:HD21	2:B:3775:ALA:HB3	1.96	0.46
2:B:641:VAL:HG11	2:B:681:HIS:HD1	1.80	0.46
2:E:1105:ALA:N	2:E:1189:LEU:O	2.49	0.46
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.81	0.46
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.34	0.46
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.51	0.46
2:E:4571:PHE:O	2:E:4575:PHE:N	2.49	0.46
2:E:4036:VAL:HG11	2:E:5035:GLN:HB3	1.97	0.46
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.80	0.46
2:G:683:ARG:HG2	2:G:717:ASP:HB3	1.98	0.46
2:I:1244:GLN:OE1	2:I:1646:ARG:NH1	2.49	0.46
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.49	0.46
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.96	0.46
1:J:34:LYS:HE3	2:I:634:GLN:HB3	1.97	0.46
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.49	0.46
2:B:3804:ILE:HG22	2:B:3812:VAL:HG21	1.98	0.46
2:B:451:TYR:O	2:B:474:ARG:NH1	2.47	0.46
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.34	0.46
2:G:35:LEU:HD13	2:G:49:LEU:HD13	1.98	0.46
2:G:3804:ILE:HG22	2:G:3812:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.33	0.46
2:G:641:VAL:HG11	2:G:681:HIS:HD1	1.80	0.46
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.48	0.46
2:I:3770:LEU:HD21	2:I:3775:ALA:HB3	1.96	0.46
2:I:403:MET:O	2:I:407:THR:N	2.49	0.46
2:B:1244:GLN:OE1	2:B:1646:ARG:NH1	2.49	0.46
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.34	0.46
2:E:2346:VAL:HG13	2:E:2349:ASN:H	1.79	0.46
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.96	0.46
2:E:683:ARG:HG2	2:E:717:ASP:HB3	1.98	0.46
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.96	0.46
2:B:4036:VAL:HG11	2:B:5035:GLN:HB3	1.97	0.46
2:G:1244:GLN:OE1	2:G:1646:ARG:NH1	2.49	0.46
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.51	0.46
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.34	0.46
2:I:3804:ILE:HG22	2:I:3812:VAL:HG21	1.98	0.46
2:B:1105:ALA:N	2:B:1189:LEU:O	2.49	0.46
2:B:214:VAL:HG12	2:B:274:LEU:HD12	1.98	0.46
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.33	0.46
2:E:35:LEU:HD13	2:E:49:LEU:HD13	1.98	0.46
2:E:3804:ILE:HG22	2:E:3812:VAL:HG21	1.98	0.46
2:E:4236:SER:OG	2:E:4675:LYS:NZ	2.36	0.46
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.80	0.46
2:G:379:HIS:CD2	2:G:381:GLU:H	2.34	0.46
2:G:4571:PHE:O	2:G:4575:PHE:N	2.49	0.46
1:H:87:HIS:H	1:H:91:ILE:HB	1.81	0.46
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.80	0.46
2:I:5028:PHE:HE1	2:I:5032:TYR:HE2	1.61	0.46
2:I:681:HIS:HB3	2:I:784:SER:HB3	1.98	0.46
2:I:683:ARG:HG2	2:I:717:ASP:HB3	1.98	0.46
2:B:606:LEU:O	2:B:617:ASN:ND2	2.49	0.46
2:E:403:MET:O	2:E:407:THR:N	2.49	0.46
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.81	0.46
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.81	0.46
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.51	0.46
2:B:3842:LEU:O	2:B:3929:SER:OG	2.34	0.46
2:B:4571:PHE:O	2:B:4575:PHE:N	2.49	0.46
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	1.98	0.46
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.83	0.46
2:E:218:HIS:HB3	2:E:392:ARG:HD3	1.98	0.46
2:E:214:VAL:HG12	2:E:274:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.49	0.46
2:E:681:HIS:HB3	2:E:784:SER:HB3	1.98	0.46
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.97	0.46
2:I:35:LEU:HD13	2:I:49:LEU:HD13	1.98	0.46
2:B:243:ARG:NH1	2:B:301:VAL:O	2.39	0.45
2:E:983:THR:O	2:E:987:ARG:N	2.48	0.45
1:F:34:LYS:HD3	2:E:629:ARG:HD2	1.98	0.45
2:I:379:HIS:CD2	2:I:381:GLU:H	2.34	0.45
2:I:641:VAL:HG11	2:I:681:HIS:HD1	1.80	0.45
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.97	0.45
2:B:681:HIS:HB3	2:B:784:SER:HB3	1.98	0.45
2:E:3362:UNK:O	2:E:3366:UNK:N	2.50	0.45
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.33	0.45
1:F:87:HIS:H	1:F:91:ILE:HB	1.81	0.45
2:I:206:CYS:SG	2:I:207:SER:N	2.90	0.45
2:I:4036:VAL:HG11	2:I:5035:GLN:HB3	1.97	0.45
2:B:4823:LEU:HD23	2:I:4843:LEU:HD12	1.98	0.45
2:I:606:LEU:O	2:I:617:ASN:ND2	2.49	0.45
2:E:1838:PHE:HB3	2:E:1842:LEU:HD11	1.99	0.45
2:G:3362:UNK:O	2:G:3366:UNK:N	2.50	0.45
2:G:403:MET:O	2:G:407:THR:N	2.49	0.45
2:I:1838:PHE:HB3	2:I:1842:LEU:HD11	1.99	0.45
2:I:3362:UNK:O	2:I:3366:UNK:N	2.50	0.45
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	1.98	0.45
2:B:1457:UNK:N	2:B:1497:UNK:O	2.49	0.45
2:B:1838:PHE:HB3	2:B:1842:LEU:HD11	1.99	0.45
2:B:218:HIS:HB3	2:B:392:ARG:HD3	1.98	0.45
2:E:1457:UNK:N	2:E:1497:UNK:O	2.49	0.45
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.49	0.45
2:I:218:HIS:HB3	2:I:392:ARG:HD3	1.98	0.45
2:I:4571:PHE:O	2:I:4575:PHE:N	2.49	0.45
2:B:1973:GLN:O	2:B:1977:TYR:N	2.45	0.45
2:B:206:CYS:SG	2:B:207:SER:N	2.89	0.45
2:B:379:HIS:CD2	2:B:381:GLU:H	2.34	0.45
2:E:2327:GLY:HA2	2:E:2330:ARG:HD3	1.98	0.45
2:E:3842:LEU:O	2:E:3929:SER:OG	2.34	0.45
2:G:1105:ALA:N	2:G:1189:LEU:O	2.49	0.45
2:G:1838:PHE:HB3	2:G:1842:LEU:HD11	1.99	0.45
2:G:206:CYS:SG	2:G:207:SER:N	2.89	0.45
2:G:214:VAL:HG12	2:G:274:LEU:HD12	1.98	0.45
2:G:4822:THR:O	2:G:4825:THR:OG1	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:606:LEU:O	2:G:617:ASN:ND2	2.49	0.45
2:I:214:VAL:HG12	2:I:274:LEU:HD12	1.98	0.45
2:E:206:CYS:SG	2:E:207:SER:N	2.90	0.45
2:G:1457:UNK:N	2:G:1497:UNK:O	2.49	0.45
2:G:4036:VAL:HG11	2:G:5035:GLN:HB3	1.97	0.45
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	1.98	0.45
2:I:1457:UNK:N	2:I:1497:UNK:O	2.49	0.45
2:B:3362:UNK:O	2:B:3366:UNK:N	2.50	0.45
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	1.98	0.45
2:B:35:LEU:HD13	2:B:49:LEU:HD13	1.98	0.45
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	1.98	0.45
2:G:681:HIS:HB3	2:G:784:SER:HB3	1.98	0.45
2:G:218:HIS:HB3	2:G:392:ARG:HD3	1.98	0.45
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.33	0.45
1:A:87:HIS:H	1:A:91:ILE:HB	1.81	0.45
2:B:2327:GLY:HA2	2:B:2330:ARG:HD3	1.98	0.45
2:E:379:HIS:CD2	2:E:381:GLU:H	2.34	0.45
2:E:4959:PHE:CG	2:E:4959:PHE:O	2.70	0.45
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.81	0.45
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	1.98	0.45
2:G:4959:PHE:CG	2:G:4959:PHE:O	2.70	0.45
2:I:215:THR:HG22	2:I:273:HIS:HA	1.99	0.45
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	1.98	0.45
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.99	0.45
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.99	0.45
2:E:451:TYR:O	2:E:474:ARG:NH1	2.47	0.45
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.81	0.45
2:I:626:LEU:HG	2:I:628:GLY:H	1.82	0.45
1:A:27:THR:HB	1:A:100:ASP:HB3	1.99	0.44
2:E:1972:ASN:HD21	2:E:2024:PRO:HB3	1.83	0.44
1:F:27:THR:HB	1:F:100:ASP:HB3	1.99	0.44
2:B:3984:ARG:HH22	2:I:161:GLU:HA	1.82	0.44
2:I:5028:PHE:O	2:I:5028:PHE:CG	2.70	0.44
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.51	0.44
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	1.99	0.44
2:E:215:THR:HG22	2:E:273:HIS:HA	2.00	0.44
2:E:4680:LYS:HD3	2:E:4686:LEU:HD22	1.98	0.44
2:E:606:LEU:O	2:E:617:ASN:ND2	2.49	0.44
2:G:215:THR:HG22	2:G:273:HIS:HA	2.00	0.44
2:I:1972:ASN:HD21	2:I:2024:PRO:HB3	1.83	0.44
2:I:4959:PHE:O	2:I:4959:PHE:CD1	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:27:THR:HB	1:J:100:ASP:HB3	1.99	0.44
1:J:23:VAL:HG22	1:J:47:LYS:HG2	2.00	0.44
2:B:1972:ASN:HD21	2:B:2024:PRO:HB3	1.83	0.44
2:E:626:LEU:HG	2:E:628:GLY:H	1.82	0.44
2:I:1105:ALA:N	2:I:1189:LEU:O	2.49	0.44
2:I:3842:LEU:O	2:I:3929:SER:OG	2.34	0.44
2:E:2104:ARG:HA	2:E:2107:GLN:HB3	1.99	0.44
2:E:2430:ILE:HG21	2:E:2502:UNK:HA	1.99	0.44
2:E:3829:PHE:HD1	2:E:3915:ILE:HD11	1.82	0.44
2:G:210:GLU:H	2:G:273:HIS:CE1	2.36	0.44
2:G:3829:PHE:HD1	2:G:3915:ILE:HD11	1.82	0.44
2:G:626:LEU:HG	2:G:628:GLY:H	1.82	0.44
2:I:3829:PHE:HD1	2:I:3915:ILE:HD11	1.82	0.44
2:B:4843:LEU:HD12	2:E:4823:LEU:HD23	1.99	0.44
2:E:3971:GLY:N	2:E:4032:GLU:OE2	2.47	0.44
2:G:838:HIS:HA	2:G:1201:HIS:HB3	2.00	0.44
2:G:1804:LEU:O	2:G:1808:ARG:N	2.49	0.44
2:G:2447:LYS:HG3	2:G:2449:GLU:H	1.83	0.44
2:I:838:HIS:HA	2:I:1201:HIS:HB3	2.00	0.44
1:J:87:HIS:H	1:J:91:ILE:HB	1.81	0.44
2:B:2104:ARG:HA	2:B:2107:GLN:HB3	1.99	0.44
2:B:215:THR:HG22	2:B:273:HIS:HA	1.99	0.44
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.51	0.44
2:B:4959:PHE:O	2:B:4959:PHE:CD1	2.71	0.44
2:B:4959:PHE:O	2:B:4959:PHE:CG	2.70	0.44
2:B:626:LEU:HG	2:B:628:GLY:H	1.82	0.44
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.99	0.44
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.81	0.44
2:E:4843:LEU:HD12	2:G:4823:LEU:HD23	2.00	0.44
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	2.00	0.44
1:H:34:LYS:HE3	2:G:634:GLN:HB3	1.98	0.44
2:I:2447:LYS:HG3	2:I:2449:GLU:H	1.83	0.44
2:I:2764:GLU:HG3	2:I:2857:PRO:HB2	2.00	0.44
2:I:3915:ILE:O	2:I:3919:THR:N	2.45	0.44
2:B:5028:PHE:O	2:B:5028:PHE:CG	2.70	0.44
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.51	0.44
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	1.99	0.44
2:G:1973:GLN:HA	2:G:1976:ARG:HB3	2.00	0.44
2:G:2327:GLY:HA2	2:G:2330:ARG:HD3	1.98	0.44
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	2.00	0.44
2:G:4959:PHE:CD1	2:G:4959:PHE:O	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:5028:PHE:O	2:G:5028:PHE:CG	2.70	0.44
2:I:2104:ARG:HA	2:I:2107:GLN:HB3	1.99	0.44
2:I:210:GLU:H	2:I:273:HIS:CE1	2.36	0.44
2:I:2299:VAL:O	2:I:2303:ALA:N	2.50	0.44
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.51	0.44
2:B:1101:ARG:HH21	2:B:1115:LEU:H	1.66	0.44
2:E:210:GLU:H	2:E:273:HIS:CE1	2.36	0.44
2:E:4215:ARG:NH2	3:E:5101:ATP:O1A	2.51	0.44
1:F:23:VAL:HG22	1:F:47:LYS:HG2	2.00	0.44
2:G:1972:ASN:HD21	2:G:2024:PRO:HB3	1.83	0.44
2:G:4229:GLU:HA	2:G:4232:GLU:HB3	1.99	0.44
2:I:2327:GLY:HA2	2:I:2330:ARG:HD3	1.98	0.44
2:I:2758:PHE:O	2:I:2762:THR:N	2.51	0.44
2:I:485:SER:O	2:I:489:ASN:N	2.37	0.44
2:I:647:ASN:ND2	2:I:820:ARG:O	2.50	0.44
1:A:11:ASP:OD1	1:A:67:SER:OG	2.29	0.44
2:B:34:LYS:N	2:B:53:SER:OG	2.40	0.44
2:E:4959:PHE:CD1	2:E:4959:PHE:O	2.70	0.44
2:G:2104:ARG:HA	2:G:2107:GLN:HB3	1.99	0.44
2:G:2257:LEU:O	2:G:2261:SER:N	2.51	0.44
2:I:1663:HIS:O	2:I:1667:LEU:N	2.49	0.44
2:I:2257:LEU:O	2:I:2261:SER:N	2.51	0.44
2:I:241:GLN:O	2:I:289:ARG:NH1	2.38	0.44
2:I:4959:PHE:CG	2:I:4959:PHE:O	2.70	0.44
2:B:3365:UNK:O	2:B:3369:UNK:N	2.51	0.43
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	2.00	0.43
2:E:3365:UNK:O	2:E:3369:UNK:N	2.51	0.43
2:G:2758:PHE:O	2:G:2762:THR:N	2.51	0.43
2:G:3971:GLY:N	2:G:4032:GLU:OE2	2.47	0.43
2:G:4215:ARG:NH2	3:G:5101:ATP:O1A	2.51	0.43
2:I:119:SER:HA	2:I:146:CYS:HA	2.00	0.43
2:I:2430:ILE:HG21	2:I:2502:UNK:HA	1.99	0.43
2:I:3365:UNK:O	2:I:3369:UNK:N	2.51	0.43
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.51	0.43
2:I:4229:GLU:HA	2:I:4232:GLU:HB3	1.99	0.43
2:B:4215:ARG:NH2	3:B:5101:ATP:O1A	2.51	0.43
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	2.00	0.43
2:E:34:LYS:N	2:E:53:SER:OG	2.40	0.43
2:G:2764:GLU:HG3	2:G:2857:PRO:HB2	2.00	0.43
2:G:379:HIS:NE2	2:G:381:GLU:OE1	2.52	0.43
2:B:2764:GLU:HG3	2:B:2857:PRO:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3829:PHE:HD1	2:B:3915:ILE:HD11	1.82	0.43
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.81	0.43
2:E:1663:HIS:O	2:E:1667:LEU:N	2.49	0.43
2:E:4229:GLU:HA	2:E:4232:GLU:HB3	1.99	0.43
2:G:3842:LEU:O	2:G:3929:SER:OG	2.34	0.43
1:H:27:THR:HB	1:H:100:ASP:HB3	1.99	0.43
1:H:23:VAL:HG22	1:H:47:LYS:HG2	2.00	0.43
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.99	0.43
2:I:4673:ARG:HH12	2:I:4698:LYS:HE3	1.84	0.43
2:B:210:GLU:H	2:B:273:HIS:CE1	2.36	0.43
2:B:2342:ASN:N	2:B:2342:ASN:OD1	2.51	0.43
2:B:2430:ILE:HG21	2:B:2502:UNK:HA	1.99	0.43
2:B:2447:LYS:HG3	2:B:2449:GLU:H	1.83	0.43
2:B:2758:PHE:O	2:B:2762:THR:N	2.51	0.43
2:B:4229:GLU:HA	2:B:4232:GLU:HB3	1.99	0.43
2:E:2447:LYS:HG3	2:E:2449:GLU:H	1.83	0.43
2:G:1101:ARG:HH21	2:G:1115:LEU:H	1.65	0.43
2:I:932:LEU:HA	2:I:935:LEU:HD12	2.01	0.43
1:A:34:LYS:HE3	2:B:634:GLN:HB3	2.00	0.43
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	2.00	0.43
2:B:2231:SER:HA	2:B:2234:ARG:HG2	2.01	0.43
2:B:838:HIS:HA	2:B:1201:HIS:HB3	2.00	0.43
2:E:119:SER:HA	2:E:146:CYS:HA	2.00	0.43
2:E:1973:GLN:HA	2:E:1976:ARG:HB3	2.00	0.43
2:E:2231:SER:HA	2:E:2234:ARG:HG2	2.01	0.43
2:E:932:LEU:HA	2:E:935:LEU:HD12	2.01	0.43
2:G:1676:LEU:HD23	2:G:2167:ILE:HG23	2.01	0.43
2:G:3365:UNK:O	2:G:3369:UNK:N	2.51	0.43
2:G:776:LEU:HG	2:G:848:HIS:HA	2.01	0.43
2:G:864:PRO:HA	2:G:865:PRO:HD3	1.92	0.43
2:I:379:HIS:NE2	2:I:381:GLU:OE1	2.52	0.43
2:B:1973:GLN:HA	2:B:1976:ARG:HB3	2.00	0.43
2:E:2758:PHE:O	2:E:2762:THR:N	2.51	0.43
2:E:4673:ARG:HH12	2:E:4698:LYS:HE3	1.84	0.43
2:E:5028:PHE:CG	2:E:5028:PHE:O	2.70	0.43
2:E:887:ILE:HG21	2:E:959:TYR:HA	2.01	0.43
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.99	0.43
2:G:4673:ARG:HH12	2:G:4698:LYS:HE3	1.84	0.43
2:I:1973:GLN:O	2:I:1977:TYR:N	2.45	0.43
2:I:2231:SER:HA	2:I:2234:ARG:HG2	2.01	0.43
2:I:2793:PRO:HG3	2:I:2855:TYR:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:SER:HA	2:B:146:CYS:HA	2.01	0.43
2:B:1854:PHE:HD1	2:B:1858:ASP:HB3	1.84	0.43
2:B:2024:PRO:O	2:B:2028:ARG:NE	2.49	0.43
2:G:1269:CYS:HA	2:G:1473:UNK:HA	2.01	0.43
2:G:2231:SER:HA	2:G:2234:ARG:HG2	2.01	0.43
2:G:887:ILE:HG21	2:G:959:TYR:HA	2.01	0.43
2:I:103:TYR:HB3	2:I:152:PRO:HD3	2.01	0.43
2:I:1854:PHE:HD1	2:I:1858:ASP:HB3	1.84	0.43
2:I:4215:ARG:NH2	3:I:5101:ATP:O1A	2.51	0.43
2:B:841:GLY:HA2	2:B:1073:ARG:HD2	1.99	0.43
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	2.00	0.43
2:B:4983:HIS:CB	2:B:4988:TYR:HE2	2.32	0.43
2:E:734:GLY:O	2:E:736:HIS:ND1	2.51	0.43
2:G:2430:ILE:HG21	2:G:2502:UNK:HA	1.99	0.43
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	2.00	0.43
2:G:932:LEU:HA	2:G:935:LEU:HD12	2.01	0.43
2:I:1859:VAL:HA	2:I:1862:ILE:HG12	2.01	0.43
2:I:599:VAL:HG23	2:I:600:LEU:HD12	2.00	0.43
2:B:932:LEU:HA	2:B:935:LEU:HD12	2.01	0.43
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.51	0.43
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	2.00	0.43
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	2.00	0.43
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	1.99	0.43
2:B:887:ILE:HG21	2:B:959:TYR:HA	2.01	0.43
2:E:1101:ARG:HH21	2:E:1115:LEU:H	1.66	0.43
2:E:2257:LEU:O	2:E:2261:SER:N	2.51	0.43
2:E:838:HIS:HA	2:E:1201:HIS:HB3	2.00	0.43
2:G:2024:PRO:O	2:G:2028:ARG:NE	2.49	0.43
2:G:2299:VAL:O	2:G:2303:ALA:N	2.50	0.43
2:G:4929:LEU:HA	2:G:4929:LEU:HD13	1.91	0.43
2:I:4993:MET:HA	2:I:4996:ILE:HD12	2.00	0.43
2:I:776:LEU:HG	2:I:848:HIS:HA	2.01	0.43
2:B:103:TYR:HB3	2:B:152:PRO:HD3	2.01	0.42
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	2.00	0.42
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	2.00	0.42
2:E:2793:PRO:HG3	2:E:2855:TYR:CZ	2.54	0.42
2:E:4983:HIS:CB	2:E:4988:TYR:HE2	2.32	0.42
2:E:4993:MET:HA	2:E:4996:ILE:HD12	2.01	0.42
2:G:2342:ASN:N	2:G:2342:ASN:OD1	2.51	0.42
2:G:485:SER:O	2:G:489:ASN:N	2.37	0.42
2:I:1101:ARG:HH21	2:I:1115:LEU:H	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4983:HIS:CB	2:I:4988:TYR:HE2	2.32	0.42
2:I:887:ILE:HG21	2:I:959:TYR:HA	2.01	0.42
2:B:2793:PRO:HG3	2:B:2855:TYR:CZ	2.54	0.42
2:E:2764:GLU:HG3	2:E:2857:PRO:HB2	2.00	0.42
2:G:4833:ASN:ND2	2:G:4935:LEU:O	2.52	0.42
2:G:599:VAL:HG23	2:G:600:LEU:HD12	2.00	0.42
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	2.00	0.42
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	2.01	0.42
2:B:379:HIS:NE2	2:B:381:GLU:OE1	2.52	0.42
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	2.02	0.42
2:E:1859:VAL:HA	2:E:1862:ILE:HG12	2.01	0.42
2:E:4763:GLY:O	2:E:4766:THR:OG1	2.33	0.42
2:G:278:GLN:N	2:G:315:CYS:SG	2.92	0.42
2:B:1804:LEU:O	2:B:1808:ARG:N	2.49	0.42
2:B:2257:LEU:O	2:B:2261:SER:N	2.51	0.42
2:B:4673:ARG:HH12	2:B:4698:LYS:HE3	1.84	0.42
2:B:599:VAL:HG23	2:B:600:LEU:HD12	2.00	0.42
2:B:38:ALA:HB1	2:B:64:ILE:HG13	2.02	0.42
2:G:119:SER:HA	2:G:146:CYS:HA	2.01	0.42
2:G:2793:PRO:HG3	2:G:2855:TYR:CZ	2.54	0.42
2:G:38:ALA:HB1	2:G:64:ILE:HG13	2.02	0.42
2:I:38:ALA:HB1	2:I:64:ILE:HG13	2.02	0.42
2:B:1269:CYS:HA	2:B:1473:UNK:HA	2.01	0.42
2:B:1694:LEU:O	2:B:1712:TYR:OH	2.27	0.42
2:B:4993:MET:HA	2:B:4996:ILE:HD12	2.00	0.42
2:E:1679:ASN:HA	2:E:1682:ALA:HB3	2.01	0.42
2:E:4833:ASN:ND2	2:E:4935:LEU:O	2.52	0.42
2:G:1973:GLN:O	2:G:1977:TYR:N	2.45	0.42
2:I:1269:CYS:HA	2:I:1473:UNK:HA	2.01	0.42
2:B:2517:UNK:O	2:B:2521:UNK:N	2.53	0.42
2:E:1676:LEU:HD23	2:E:2167:ILE:HG23	2.01	0.42
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.52	0.42
2:G:940:GLY:O	2:G:1052:ASN:N	2.53	0.42
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	2.02	0.42
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.32	0.42
2:B:983:THR:O	2:B:987:ARG:N	2.48	0.42
2:G:103:TYR:HB3	2:G:152:PRO:HD3	2.01	0.42
2:G:1859:VAL:HA	2:G:1862:ILE:HG12	2.01	0.42
2:G:4983:HIS:CB	2:G:4988:TYR:HE2	2.32	0.42
2:G:4993:MET:HA	2:G:4996:ILE:HD12	2.01	0.42
2:G:34:LYS:N	2:G:53:SER:OG	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2024:PRO:O	2:I:2028:ARG:NE	2.49	0.42
2:I:983:THR:O	2:I:987:ARG:N	2.48	0.42
2:B:1859:VAL:HA	2:B:1862:ILE:HG12	2.01	0.42
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	2.01	0.42
2:E:2024:PRO:HB2	2:E:2027:ILE:HG12	2.02	0.42
2:E:379:HIS:NE2	2:E:381:GLU:OE1	2.51	0.42
2:E:38:ALA:HB1	2:E:64:ILE:HG13	2.02	0.42
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	2.01	0.42
2:B:1676:LEU:HD23	2:B:2167:ILE:HG23	2.01	0.42
2:E:1237:TRP:HH2	2:E:1652:GLU:HA	1.85	0.42
2:E:2024:PRO:O	2:E:2028:ARG:NE	2.49	0.42
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	2.02	0.42
2:G:1854:PHE:HD1	2:G:1858:ASP:HB3	1.84	0.42
2:G:2024:PRO:HB2	2:G:2027:ILE:HG12	2.02	0.42
2:G:2517:UNK:O	2:G:2521:UNK:N	2.53	0.42
2:I:1804:LEU:O	2:I:1808:ARG:N	2.49	0.42
2:I:1973:GLN:HA	2:I:1976:ARG:HB3	2.00	0.42
2:I:940:GLY:O	2:I:1052:ASN:N	2.53	0.42
2:B:4929:LEU:HA	2:B:4929:LEU:HD13	1.91	0.42
2:B:734:GLY:O	2:B:736:HIS:ND1	2.51	0.42
2:B:776:LEU:HG	2:B:848:HIS:HA	2.01	0.42
2:E:1854:PHE:HD1	2:E:1858:ASP:HB3	1.84	0.42
2:E:2342:ASN:OD1	2:E:2342:ASN:N	2.51	0.42
2:E:599:VAL:HG23	2:E:600:LEU:HD12	2.00	0.42
2:G:1679:ASN:HA	2:G:1682:ALA:HB3	2.01	0.42
2:I:4066:LEU:HD11	2:I:4173:TYR:HB2	2.02	0.42
2:E:1269:CYS:HA	2:E:1473:UNK:HA	2.01	0.41
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	2.02	0.41
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	2.02	0.41
2:G:4066:LEU:HD11	2:G:4173:TYR:HB2	2.02	0.41
2:G:734:GLY:O	2:G:736:HIS:ND1	2.51	0.41
2:I:3647:HIS:O	2:I:3651:ASN:ND2	2.53	0.41
2:B:4066:LEU:HD11	2:B:4173:TYR:HB2	2.02	0.41
2:B:582:HIS:O	2:B:585:SER:OG	2.30	0.41
2:G:1154:ASP:O	2:G:1158:ASN:N	2.53	0.41
2:B:1237:TRP:HH2	2:B:1652:GLU:HA	1.85	0.41
2:B:4833:ASN:ND2	2:B:4935:LEU:O	2.52	0.41
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.52	0.41
2:E:1171:SER:OG	2:E:1175:SER:N	2.44	0.41
2:E:2517:UNK:O	2:E:2521:UNK:N	2.53	0.41
2:E:3647:HIS:O	2:E:3651:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2674:UNK:O	2:G:2676:UNK:N	2.54	0.41
2:I:1676:LEU:HD23	2:I:2167:ILE:HG23	2.01	0.41
2:I:2674:UNK:O	2:I:2676:UNK:N	2.53	0.41
2:I:4084:PRO:HD2	2:I:4085:ARG:NH1	2.36	0.41
2:I:4823:LEU:HD23	2:G:4843:LEU:HD12	2.01	0.41
2:I:4929:LEU:HA	2:I:4929:LEU:HD13	1.91	0.41
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	2.02	0.41
2:B:1679:ASN:HA	2:B:1682:ALA:HB3	2.01	0.41
2:E:2823:ILE:HG12	2:E:2937:VAL:HG22	2.03	0.41
2:E:278:GLN:N	2:E:315:CYS:SG	2.92	0.41
2:E:776:LEU:HG	2:E:848:HIS:HA	2.01	0.41
2:G:280:LEU:HD21	2:G:316:PHE:HE2	1.86	0.41
2:I:1154:ASP:O	2:I:1158:ASN:N	2.53	0.41
2:I:2024:PRO:HB2	2:I:2027:ILE:HG12	2.02	0.41
1:A:2:VAL:HG21	1:A:61:GLU:HB2	2.02	0.41
2:B:2466:LEU:HD23	2:B:2469:ILE:HD12	2.03	0.41
2:B:280:LEU:HD21	2:B:316:PHE:HE2	1.86	0.41
2:B:4148:THR:HG21	2:B:4178:LEU:HD21	2.02	0.41
2:E:1973:GLN:O	2:E:1977:TYR:N	2.45	0.41
2:G:1237:TRP:HH2	2:G:1652:GLU:HA	1.85	0.41
2:G:3647:HIS:O	2:G:3651:ASN:ND2	2.53	0.41
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.85	0.41
2:E:113:HIS:CE1	2:E:402:ARG:HB3	2.55	0.41
2:E:280:LEU:HD21	2:E:316:PHE:HE2	1.86	0.41
2:E:4084:PRO:HD2	2:E:4085:ARG:NH1	2.36	0.41
2:E:4148:THR:HG21	2:E:4178:LEU:HD21	2.02	0.41
2:E:4066:LEU:HD11	2:E:4173:TYR:HB2	2.02	0.41
2:G:2214:VAL:HG23	2:G:2215:LEU:HD12	2.03	0.41
2:G:113:HIS:CE1	2:G:402:ARG:HB3	2.55	0.41
2:I:1679:ASN:HA	2:I:1682:ALA:HB3	2.01	0.41
2:I:278:GLN:N	2:I:315:CYS:SG	2.92	0.41
2:B:113:HIS:CE1	2:B:402:ARG:HB3	2.55	0.41
2:B:786:GLY:HA2	2:B:1631:GLN:HA	2.03	0.41
2:B:2299:VAL:O	2:B:2303:ALA:N	2.50	0.41
2:B:940:GLY:O	2:B:1052:ASN:N	2.53	0.41
2:E:1641:ILE:HA	2:E:1642:PRO:HD3	1.93	0.41
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.86	0.41
2:E:2674:UNK:O	2:E:2676:UNK:N	2.54	0.41
2:E:877:ASN:HD22	2:E:1045:THR:HG23	1.85	0.41
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.52	0.41
2:G:983:THR:O	2:G:987:ARG:N	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:786:GLY:HA2	2:I:1631:GLN:HA	2.03	0.41
2:E:103:TYR:HB3	2:E:152:PRO:HD3	2.01	0.41
2:E:750:LEU:HD21	2:E:777:PHE:HE2	1.86	0.41
2:E:940:GLY:O	2:E:1052:ASN:N	2.53	0.41
2:G:4697:VAL:O	2:G:4701:TRP:N	2.52	0.41
2:I:113:HIS:CE1	2:I:402:ARG:HB3	2.55	0.41
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	2.01	0.41
2:I:2810:LYS:O	2:I:2814:LYS:N	2.45	0.41
2:I:2823:ILE:HG12	2:I:2937:VAL:HG22	2.03	0.41
1:A:7:ILE:N	1:A:71:ARG:O	2.50	0.41
2:B:2823:ILE:HG12	2:B:2937:VAL:HG22	2.03	0.41
2:B:4960:ILE:HD11	2:B:4985:LEU:CD2	2.51	0.41
2:B:767:VAL:HG12	2:B:769:GLU:HG3	2.03	0.41
2:E:1154:ASP:O	2:E:1158:ASN:N	2.53	0.41
2:E:1863:LEU:HB3	2:E:1870:VAL:HG21	2.03	0.41
2:G:647:ASN:ND2	2:G:820:ARG:O	2.50	0.41
2:I:4833:ASN:ND2	2:I:4935:LEU:O	2.52	0.41
2:B:2674:UNK:O	2:B:2676:UNK:N	2.54	0.41
2:B:3647:HIS:O	2:B:3651:ASN:ND2	2.53	0.41
2:B:4084:PRO:HD2	2:B:4085:ARG:NH1	2.36	0.41
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.85	0.41
2:E:1141:ARG:HD2	2:E:1141:ARG:H	1.86	0.41
1:F:2:VAL:HG21	1:F:61:GLU:HB2	2.02	0.41
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.86	0.41
2:I:2243:SER:HB3	2:I:2246:ASN:H	1.86	0.41
2:I:3971:GLY:N	2:I:4032:GLU:OE2	2.47	0.41
1:J:7:ILE:N	1:J:71:ARG:O	2.50	0.41
2:B:1863:LEU:HB3	2:B:1870:VAL:HG21	2.03	0.41
2:B:2024:PRO:HB2	2:B:2027:ILE:HG12	2.02	0.41
2:E:790:ARG:HG2	2:E:1627:ALA:HA	2.03	0.41
2:E:4957:LYS:HG2	2:E:4964:GLY:CA	2.51	0.41
2:E:767:VAL:HG12	2:E:769:GLU:HG3	2.03	0.41
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.85	0.41
2:G:2823:ILE:HG12	2:G:2937:VAL:HG22	2.03	0.41
1:H:2:VAL:HG21	1:H:61:GLU:HB2	2.02	0.41
2:I:2517:UNK:O	2:I:2521:UNK:N	2.53	0.41
2:I:3971:GLY:H	2:I:5005:GLY:HA3	1.86	0.41
1:J:2:VAL:HG21	1:J:61:GLU:HB2	2.02	0.41
2:B:4886:HIS:O	2:B:4890:GLY:N	2.52	0.40
2:E:4976:GLU:HA	2:E:4979:THR:CG2	2.52	0.40
2:G:2095:GLN:HA	2:G:2127:GLN:NE2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4763:GLY:O	2:G:4766:THR:OG1	2.32	0.40
2:G:37:LEU:HD11	2:G:47:CYS:HB3	2.04	0.40
2:I:1237:TRP:HH2	2:I:1652:GLU:HA	1.85	0.40
2:I:2466:LEU:HD23	2:I:2469:ILE:HD12	2.03	0.40
2:I:4148:THR:HG21	2:I:4178:LEU:HD21	2.02	0.40
2:I:864:PRO:HD2	2:I:867:LEU:HD12	2.03	0.40
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	2.02	0.40
2:G:1653:LEU:HB3	2:G:1660:GLN:HB2	2.04	0.40
2:G:767:VAL:HG12	2:G:769:GLU:HG3	2.03	0.40
2:I:1802:ILE:HG21	2:I:1807:LEU:HD22	2.04	0.40
2:I:4960:ILE:HD11	2:I:4985:LEU:CD2	2.51	0.40
2:B:1078:GLU:HB3	2:B:1081:TYR:HD2	1.86	0.40
2:B:1808:ARG:HD3	2:B:1853:ILE:HG22	2.04	0.40
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.86	0.40
2:B:358:THR:HG21	2:B:382:GLY:HA2	2.04	0.40
2:B:4080:TYR:CZ	2:B:4096:ALA:HB3	2.56	0.40
2:E:2034:PHE:O	2:E:2038:LEU:N	2.55	0.40
2:G:4976:GLU:HA	2:G:4979:THR:CG2	2.52	0.40
2:I:37:LEU:HD11	2:I:47:CYS:HB3	2.03	0.40
2:B:1154:ASP:O	2:B:1158:ASN:N	2.53	0.40
2:B:750:LEU:HD21	2:B:777:PHE:HE2	1.86	0.40
2:E:2095:GLN:HA	2:E:2127:GLN:NE2	2.36	0.40
2:E:2466:LEU:HA	2:E:2469:ILE:HD12	2.03	0.40
2:E:4156:HIS:CE1	2:E:5036:LEU:HD11	2.56	0.40
2:E:786:GLY:HA2	2:E:1631:GLN:HA	2.03	0.40
2:G:1078:GLU:HG3	2:G:1237:TRP:HE1	1.87	0.40
2:G:2243:SER:HB3	2:G:2246:ASN:H	1.86	0.40
2:G:4987:ASN:HA	2:G:4990:PHE:HD2	1.87	0.40
2:G:786:GLY:HA2	2:G:1631:GLN:HA	2.03	0.40
2:I:2034:PHE:O	2:I:2038:LEU:N	2.55	0.40
2:I:280:LEU:HD21	2:I:316:PHE:HE2	1.86	0.40
2:I:4987:ASN:HA	2:I:4990:PHE:HD2	1.87	0.40
2:B:2095:GLN:HA	2:B:2127:GLN:NE2	2.37	0.40
2:B:2214:VAL:HG23	2:B:2215:LEU:HD12	2.03	0.40
2:B:4984:ASN:C	2:B:4986:ALA:N	2.75	0.40
2:G:2466:LEU:HA	2:G:2469:ILE:HD12	2.03	0.40
2:G:3971:GLY:H	2:G:5005:GLY:HA3	1.86	0.40
2:G:4156:HIS:CE1	2:G:5036:LEU:HD11	2.56	0.40
2:G:4148:THR:HG21	2:G:4178:LEU:HD21	2.02	0.40
2:G:794:GLY:H	2:G:798:GLY:HA3	1.87	0.40
2:I:1653:LEU:HB3	2:I:1660:GLN:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1863:LEU:HB3	2:I:1870:VAL:HG21	2.03	0.40
2:I:2095:GLN:HA	2:I:2127:GLN:NE2	2.36	0.40
2:I:750:LEU:HD21	2:I:777:PHE:HE2	1.86	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%)	98 (93%)	7 (7%)	0	100	100
1	F	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
1	H	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
1	J	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
2	B	3235/4416 (73%)	2891 (89%)	338 (10%)	6 (0%)	52	86
2	E	3235/4416 (73%)	2892 (89%)	338 (10%)	5 (0%)	52	86
2	G	3235/4416 (73%)	2890 (89%)	340 (10%)	5 (0%)	52	86
2	I	3235/4416 (73%)	2889 (89%)	340 (10%)	6 (0%)	52	86
All	All	13360/18096 (74%)	11954 (90%)	1384 (10%)	22 (0%)	56	86

All (22) 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	1932	PRO
2	E	1932	PRO
2	I	1932	PRO

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Mol	Chain	Res	Type
2	G	1932	PRO
2	B	1708	ARG
2	E	1708	ARG
2	I	1708	ARG
2	G	1708	ARG
2	B	1840	PRO
2	B	4641	PRO
2	E	1840	PRO
2	E	4641	PRO
2	I	1840	PRO
2	I	4641	PRO
2	G	1840	PRO
2	G	4641	PRO
2	B	4985	LEU
2	I	4985	LEU

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%)	2475 (99%)	18 (1%)	88 94
2	E	2493/3022 (82%)	2474 (99%)	19 (1%)	86 93
2	G	2493/3022 (82%)	2475 (99%)	18 (1%)	88 94
2	I	2493/3022 (82%)	2475 (99%)	18 (1%)	88 94
All	All	10324/12444 (83%)	10251 (99%)	73 (1%)	89 94

All (73) 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	4944	ARG
2	B	4961	CYS
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	3805	LEU
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4131	ARG
2	E	4137	ARG
2	E	4913	ARG
2	E	4944	ARG
2	E	4961	CYS
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	1076	ARG
2	I	1141	ARG
2	I	1600	LEU

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Mol	Chain	Res	Type
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	4944	ARG
2	I	4961	CYS
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
2	G	4944	ARG
2	G	4961	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (156) 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	113	HIS
2	B	224	HIS
2	B	273	HIS

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Mol	Chain	Res	Type
2	B	379	HIS
2	B	383	HIS
2	B	395	GLN
2	B	413	GLN
2	B	479	GLN
2	B	520	ASN
2	B	582	HIS
2	B	725	HIS
2	B	1598	GLN
2	B	1679	ASN
2	B	1688	HIS
2	B	1691	GLN
2	B	1693	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	1972	ASN
2	B	2005	GLN
2	B	2127	GLN
2	B	3766	GLN
2	B	3809	ASN
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	4034	ASN
2	B	4054	ASN
2	B	4120	ASN
2	B	4142	ASN
2	B	4209	GLN
2	B	4806	ASN
2	B	4983	HIS
2	B	5003	HIS
2	E	57	ASN
2	E	111	HIS
2	E	113	HIS
2	E	224	HIS
2	E	273	HIS
2	E	379	HIS
2	E	383	HIS
2	E	395	GLN

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Mol	Chain	Res	Type
2	E	413	GLN
2	E	479	GLN
2	E	520	ASN
2	E	582	HIS
2	E	725	HIS
2	E	1598	GLN
2	E	1679	ASN
2	E	1688	HIS
2	E	1691	GLN
2	E	1693	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	1972	ASN
2	E	2005	GLN
2	E	2127	GLN
2	E	3766	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	4209	GLN
2	E	4806	ASN
2	E	4983	HIS
2	E	5003	HIS
2	I	57	ASN
2	I	111	HIS
2	I	113	HIS
2	I	224	HIS
2	I	273	HIS
2	I	379	HIS
2	I	383	HIS
2	I	395	GLN
2	I	413	GLN
2	I	479	GLN
2	I	520	ASN
2	I	582	HIS

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Mol	Chain	Res	Type
2	I	725	HIS
2	I	1598	GLN
2	I	1679	ASN
2	I	1688	HIS
2	I	1691	GLN
2	I	1693	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	1972	ASN
2	I	2005	GLN
2	I	2127	GLN
2	I	3766	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	4209	GLN
2	I	4806	ASN
2	I	4983	HIS
2	I	5003	HIS
2	G	57	ASN
2	G	111	HIS
2	G	113	HIS
2	G	224	HIS
2	G	273	HIS
2	G	379	HIS
2	G	383	HIS
2	G	395	GLN
2	G	413	GLN
2	G	479	GLN
2	G	582	HIS
2	G	725	HIS
2	G	1598	GLN
2	G	1679	ASN
2	G	1688	HIS

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Mol	Chain	Res	Type
2	G	1691	GLN
2	G	1693	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	1972	ASN
2	G	2005	GLN
2	G	2127	GLN
2	G	3766	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	4209	GLN
2	G	4806	ASN
2	G	4983	HIS
2	G	5003	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

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	1.59	2 (7%)
4	CFF	B	5102	-	8,15,15	2.55	3 (37%)	8,23,23	1.16	1 (12%)
3	ATP	E	5101	-	26,33,33	0.91	1 (3%)	26,52,52	1.58	2 (7%)
4	CFF	E	5102	-	8,15,15	2.55	3 (37%)	8,23,23	1.16	1 (12%)
3	ATP	G	5101	-	26,33,33	0.91	1 (3%)	26,52,52	1.59	2 (7%)
4	CFF	G	5102	-	8,15,15	2.54	3 (37%)	8,23,23	1.17	1 (12%)
3	ATP	I	5101	-	26,33,33	0.91	1 (3%)	26,52,52	1.59	2 (7%)
4	CFF	I	5102	-	8,15,15	2.55	3 (37%)	8,23,23	1.16	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	B	5102	CFF	C4-N3	-5.03	1.33	1.39
4	I	5102	CFF	C4-N3	-5.03	1.33	1.39
4	E	5102	CFF	C4-N3	-5.03	1.33	1.39
4	G	5102	CFF	C4-N3	-5.00	1.33	1.39
4	G	5102	CFF	C6-N1	-3.95	1.32	1.38
4	I	5102	CFF	C6-N1	-3.94	1.32	1.38
4	B	5102	CFF	C6-N1	-3.92	1.32	1.38
4	E	5102	CFF	C6-N1	-3.92	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	5102	CFF	O13-C6	-2.37	1.18	1.24
4	I	5102	CFF	O13-C6	-2.37	1.18	1.24
4	E	5102	CFF	O13-C6	-2.37	1.18	1.24
4	G	5102	CFF	O13-C6	-2.37	1.18	1.24
3	E	5101	ATP	C5-C4	2.86	1.46	1.40
3	G	5101	ATP	C5-C4	2.88	1.47	1.40
3	I	5101	ATP	C5-C4	2.90	1.47	1.40
3	B	5101	ATP	C5-C4	2.90	1.47	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	5101	ATP	N3-C2-N1	-6.35	123.88	128.87
3	B	5101	ATP	N3-C2-N1	-6.33	123.90	128.87
3	I	5101	ATP	N3-C2-N1	-6.30	123.92	128.87
3	E	5101	ATP	N3-C2-N1	-6.29	123.93	128.87
4	I	5102	CFF	C14-N7-C8	-2.60	111.73	125.31
4	B	5102	CFF	C14-N7-C8	-2.59	111.76	125.31
4	E	5102	CFF	C14-N7-C8	-2.59	111.76	125.31
4	G	5102	CFF	C14-N7-C8	-2.59	111.77	125.31
3	I	5101	ATP	O3G-PG-O2G	2.07	115.02	107.44
3	G	5101	ATP	O3G-PG-O2G	2.07	115.04	107.44
3	B	5101	ATP	O3G-PG-O2G	2.08	115.07	107.44
3	E	5101	ATP	O3G-PG-O2G	2.09	115.12	107.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 12 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	2	0
4	E	5102	CFF	1	0
3	G	5101	ATP	2	0
4	G	5102	CFF	1	0
3	I	5101	ATP	2	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	B	4345:UNK	C	4540:PHE	N	72.88
1	E	4345:UNK	C	4540:PHE	N	72.88
1	I	4345:UNK	C	4540:PHE	N	72.88
1	G	4345:UNK	C	4540:PHE	N	72.88
1	B	3613:UNK	C	3639:THR	N	43.44
1	E	3613:UNK	C	3639:THR	N	43.44
1	I	3613:UNK	C	3639:THR	N	43.44
1	G	3613:UNK	C	3639:THR	N	43.44
1	B	4253:GLU	C	4320:UNK	N	27.19
1	E	4253:GLU	C	4320:UNK	N	27.19
1	I	4253:GLU	C	4320:UNK	N	27.19
1	G	4253:GLU	C	4320:UNK	N	27.19
1	B	3163:UNK	C	3170:UNK	N	15.93
1	E	3163:UNK	C	3170:UNK	N	15.93
1	I	3163:UNK	C	3170:UNK	N	15.93
1	G	3163:UNK	C	3170:UNK	N	15.93
1	E	3063:UNK	C	3134:UNK	N	15.07
1	G	3063:UNK	C	3134:UNK	N	15.07
1	B	3063:UNK	C	3134:UNK	N	15.06
1	I	3063:UNK	C	3134:UNK	N	15.06
1	B	3468:UNK	C	3511:UNK	N	14.28
1	E	3468:UNK	C	3511:UNK	N	14.28
1	I	3468:UNK	C	3511:UNK	N	14.28
1	G	3468:UNK	C	3511:UNK	N	14.28
1	B	2703:UNK	C	2734:ASN	N	14.09
1	E	2703:UNK	C	2734:ASN	N	14.09
1	I	2703:UNK	C	2734:ASN	N	14.09

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	2703:UNK	C	2734:ASN	N	14.09
1	B	3236:UNK	C	3241:UNK	N	13.30
1	E	3236:UNK	C	3241:UNK	N	13.30
1	I	3236:UNK	C	3241:UNK	N	13.30
1	G	3236:UNK	C	3241:UNK	N	13.30
1	B	1564:UNK	C	1573:MET	N	12.36
1	E	1564:UNK	C	1573:MET	N	12.36
1	I	1564:UNK	C	1573:MET	N	12.36
1	G	1564:UNK	C	1573:MET	N	12.36
1	B	2976:UNK	C	2995:UNK	N	12.29
1	E	2976:UNK	C	2995:UNK	N	12.29
1	I	2976:UNK	C	2995:UNK	N	12.29
1	G	2976:UNK	C	2995:UNK	N	12.29
1	B	3254:UNK	C	3261:UNK	N	8.12
1	E	3254:UNK	C	3261:UNK	N	8.12
1	I	3254:UNK	C	3261:UNK	N	8.12
1	G	3254:UNK	C	3261:UNK	N	8.12
1	B	1297:UNK	C	1430:UNK	N	6.33
1	E	1297:UNK	C	1430:UNK	N	6.33
1	I	1297:UNK	C	1430:UNK	N	6.33
1	G	1297:UNK	C	1430:UNK	N	6.33
1	B	2939:ARG	C	2942:UNK	N	3.27
1	E	2939:ARG	C	2942:UNK	N	3.27
1	I	2939:ARG	C	2942:UNK	N	3.27
1	G	2939:ARG	C	2942:UNK	N	3.27
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