wwPDB EM Map/Model Validation Report (i)

Oct 17, 2016 – 07:38 PM EDT

PDB ID	:	5TAW
EMDB ID:	:	EMD-8387
Title	:	Structure of rabbit RyR1 (ryanodine dataset, all particles)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-10
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

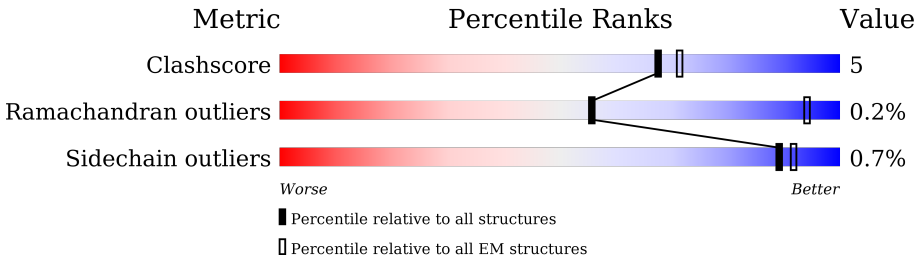
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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	83% 16% .
1	F	108	81% 18% .
1	H	108	81% 18% .
1	J	108	81% 18% .
2	B	4416	84% 11% 5%
2	E	4416	84% 10% 5%
2	G	4416	84% 11% 5%
2	I	4416	84% 11% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 121276 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 ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

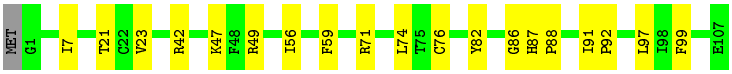
Mol	Chain	Residues	Atoms	AltConf
4	G	1	Total Ca 1 1	0
4	B	1	Total Ca 1 1	0
4	I	1	Total Ca 1 1	0
4	E	1	Total Ca 1 1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

Chain F:



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

Chain A:

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

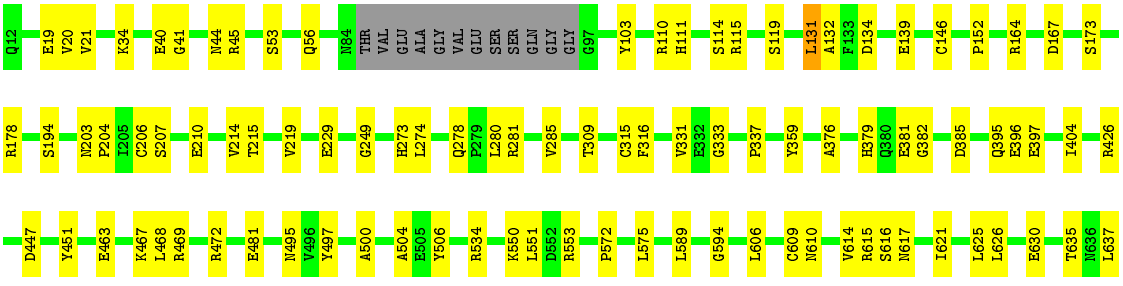
Chain H:

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

Chain J:

- Molecule 2: Ryanodine receptor 1

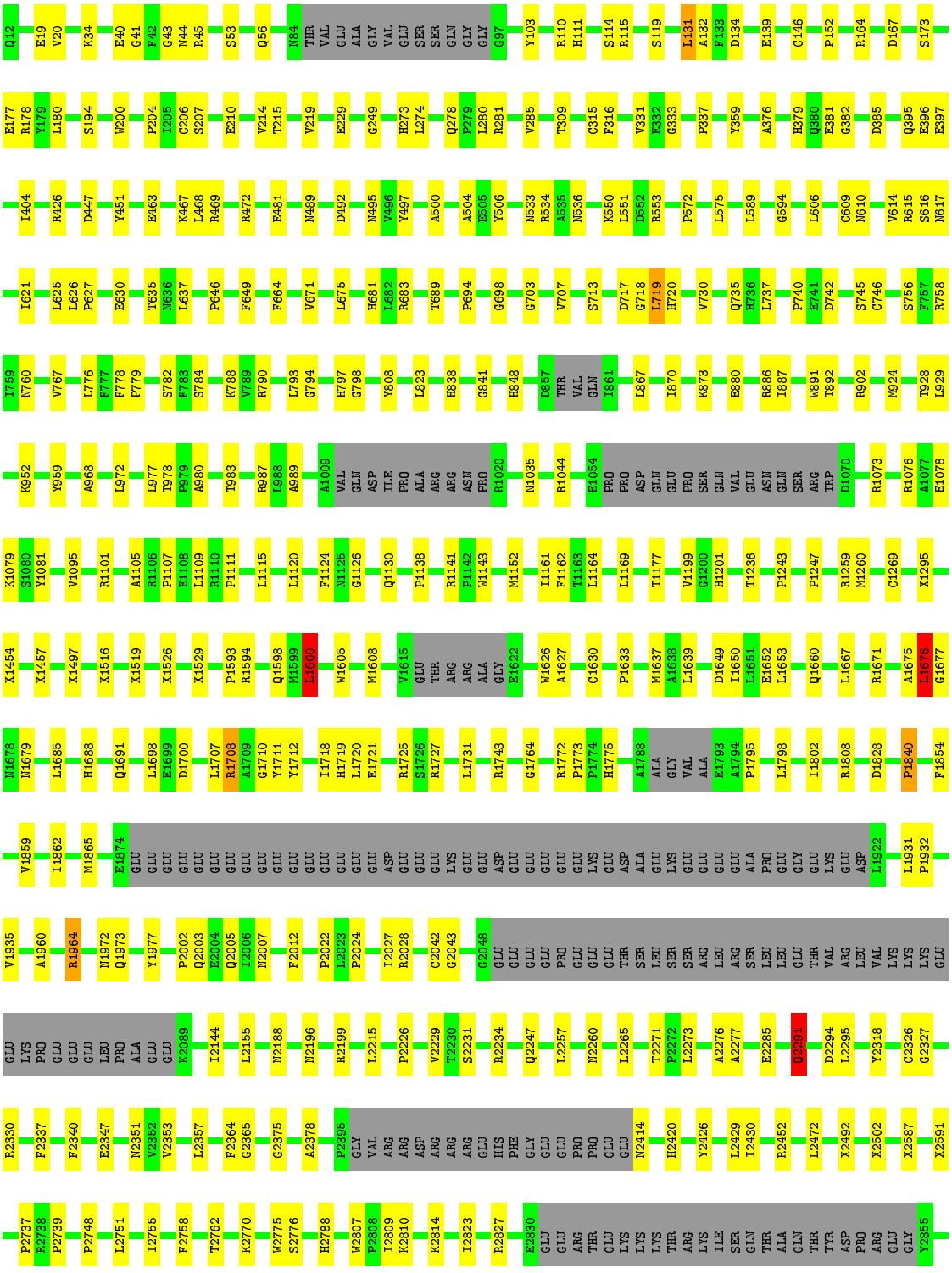
Chain B:

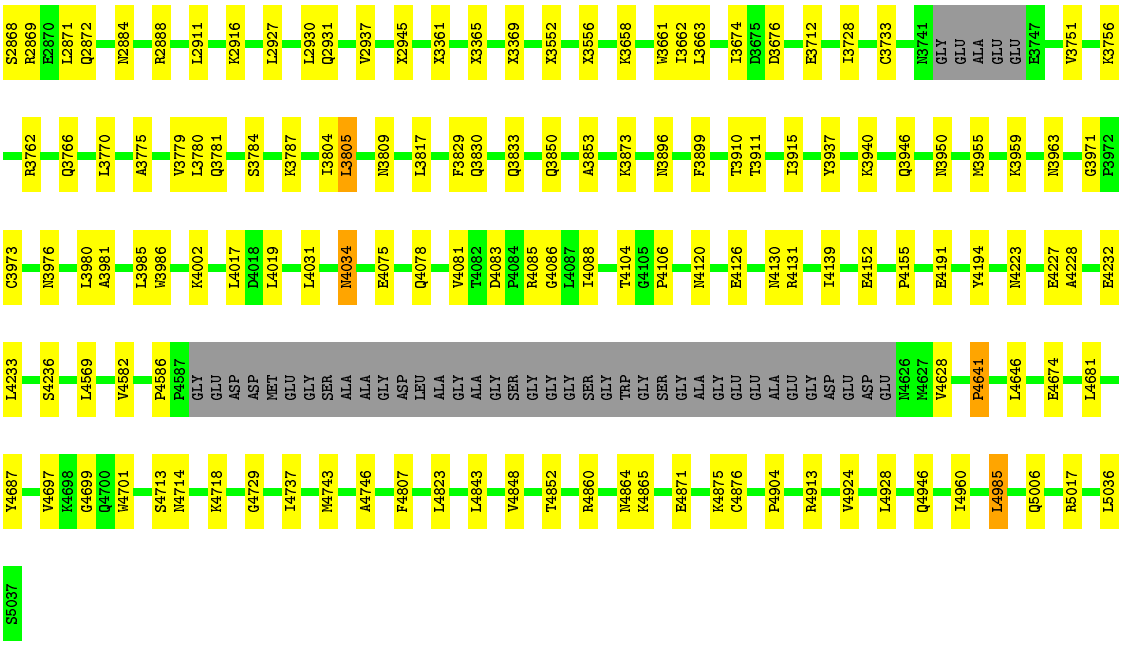


R645 P646 F649 F664 V671 L675 H681 L682 R683 T689 P694 G698 G703 V707 S713 D717 G718 L719 H720 V730 Q735 H736 L737 P740 E741 D742 S745 C746 R758 L759 N760 L776 F777 F778 P779 S782 F783 S784 K788
V789 R790 L793 G794 H797 G798 Y808 L823 E824 H838 G841 H848 D857 THR VAL GLN I861 H866 L867 I870 K873 E880 R886 I887 W891 T892 R902 P914 R918 L929 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 Y1051 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
A1105 R1106 P1107 E1108 L1109 R1110 P1111 L1115 L1120 G1126 Q1130 P1138 R1141 P1142 W1143 V1149 M1152 I1161 L1164 L1169 T1177 V1199 G1200 H1201 T1236 P1243 P1247 R1259 M1260 C1269 X1295 X1454 X1457 X1497 X1516 X1519
X1526 X1529 P1593 R1594 Q1598 M1599 L1600 W1605 M1608 V1615 GLU THR ARG ARG ALA GLY E1622 W1626 A1627 C1630 P1633 M1637 A1638 L1639 D1649 I1650 L1651 E1652 L1653 Q1660 L1667 R1671 A1675 L1676 G1677 N1678 N1679 L1685 H1688 Q1691
L1698 E1699 D1700 L1707 R1708 A1709 G1710 Y1711 Y1712 I1718 H1719 L1720 E1721 R1725 S1726 R1727 L1731 I1735 R1743 G1764 L1771 R1772 P1773 P1774 H1775 A1788 ALA GLY VAL ALA E1793 A1794 P1795 L1798 I1802 R1808 D1828 P1840 F1854 V1859 I1862 M1865
E1874 GLU GLU GLU

- Molecule 2: Ryanodine receptor 1

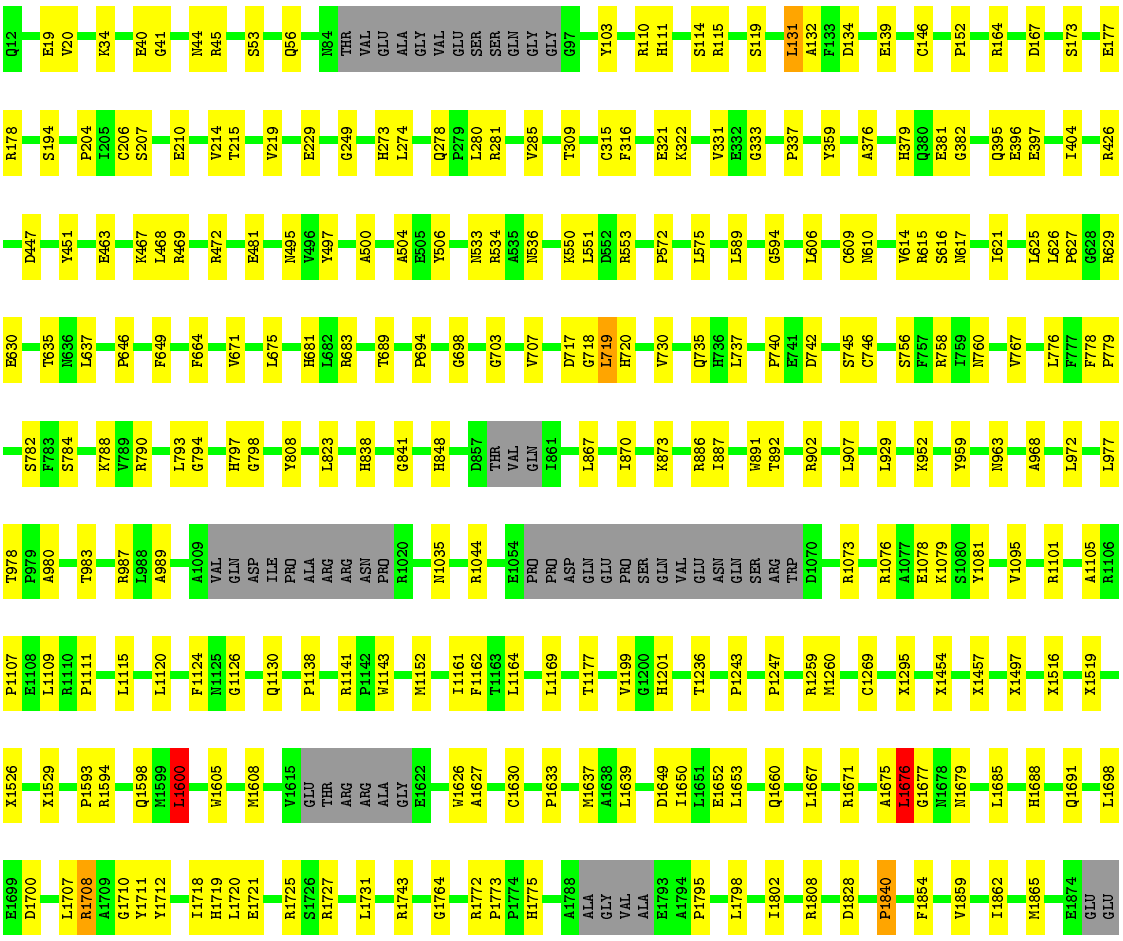
Chain G:

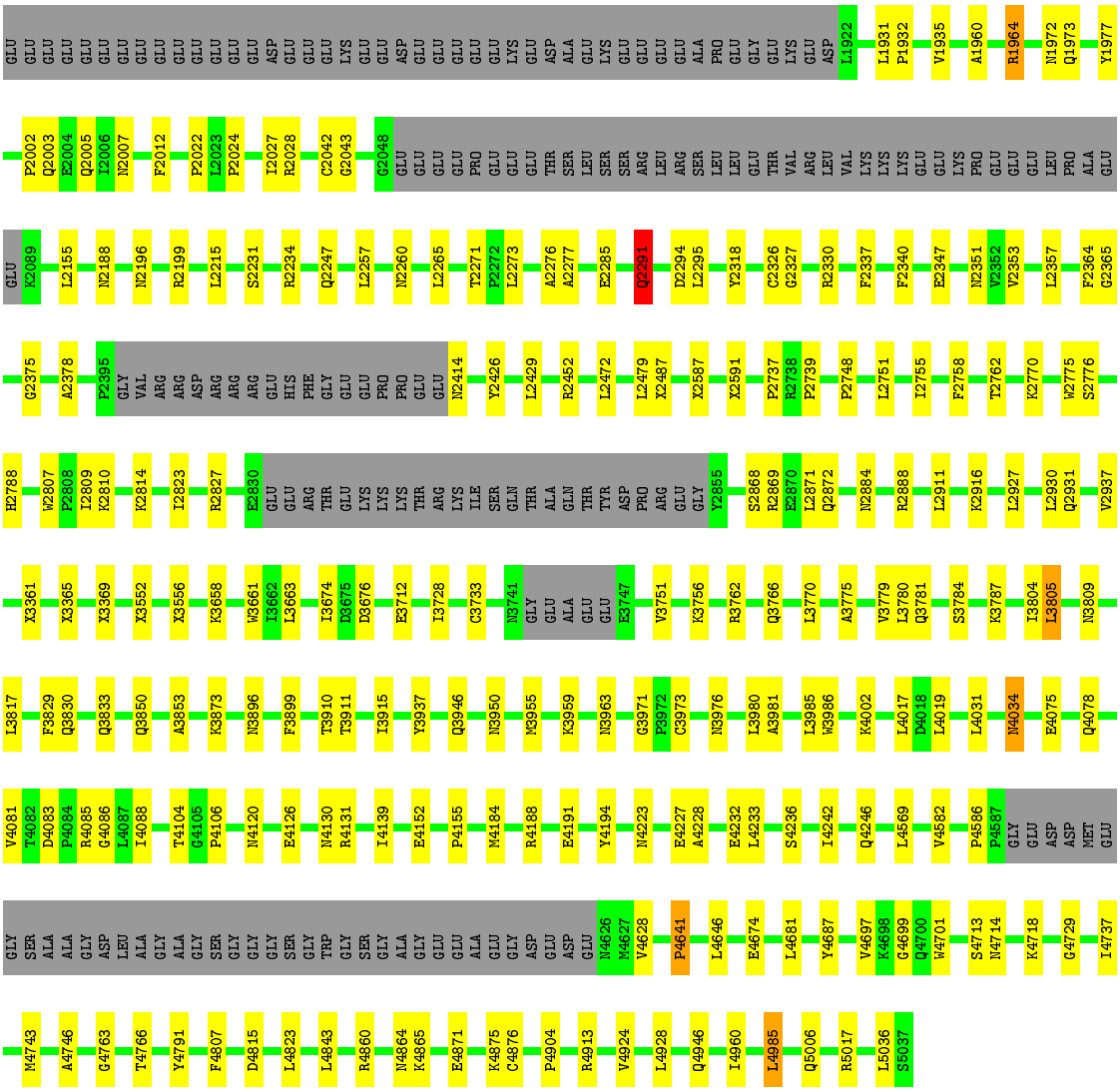




- Molecule 2: Ryanodine receptor 1

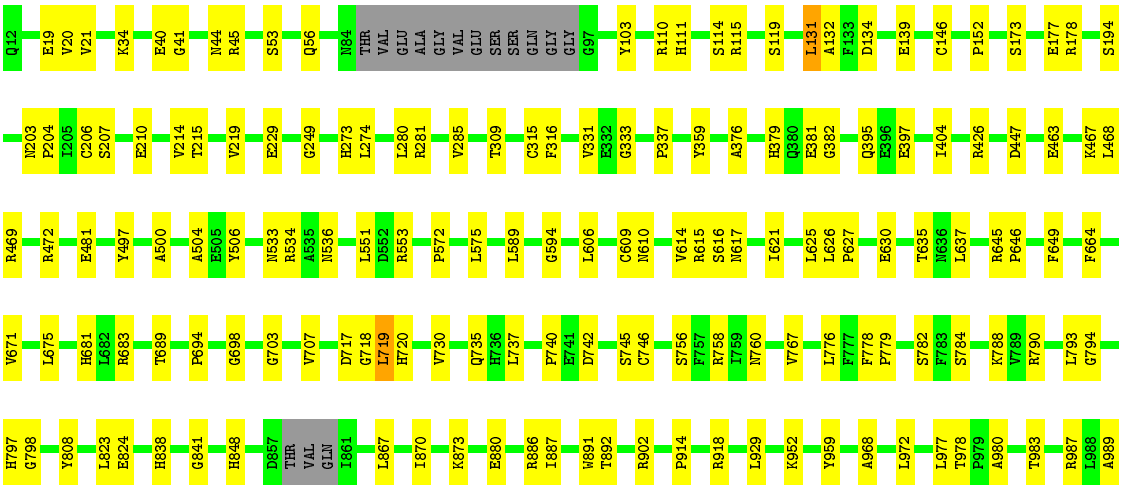
Chain I:

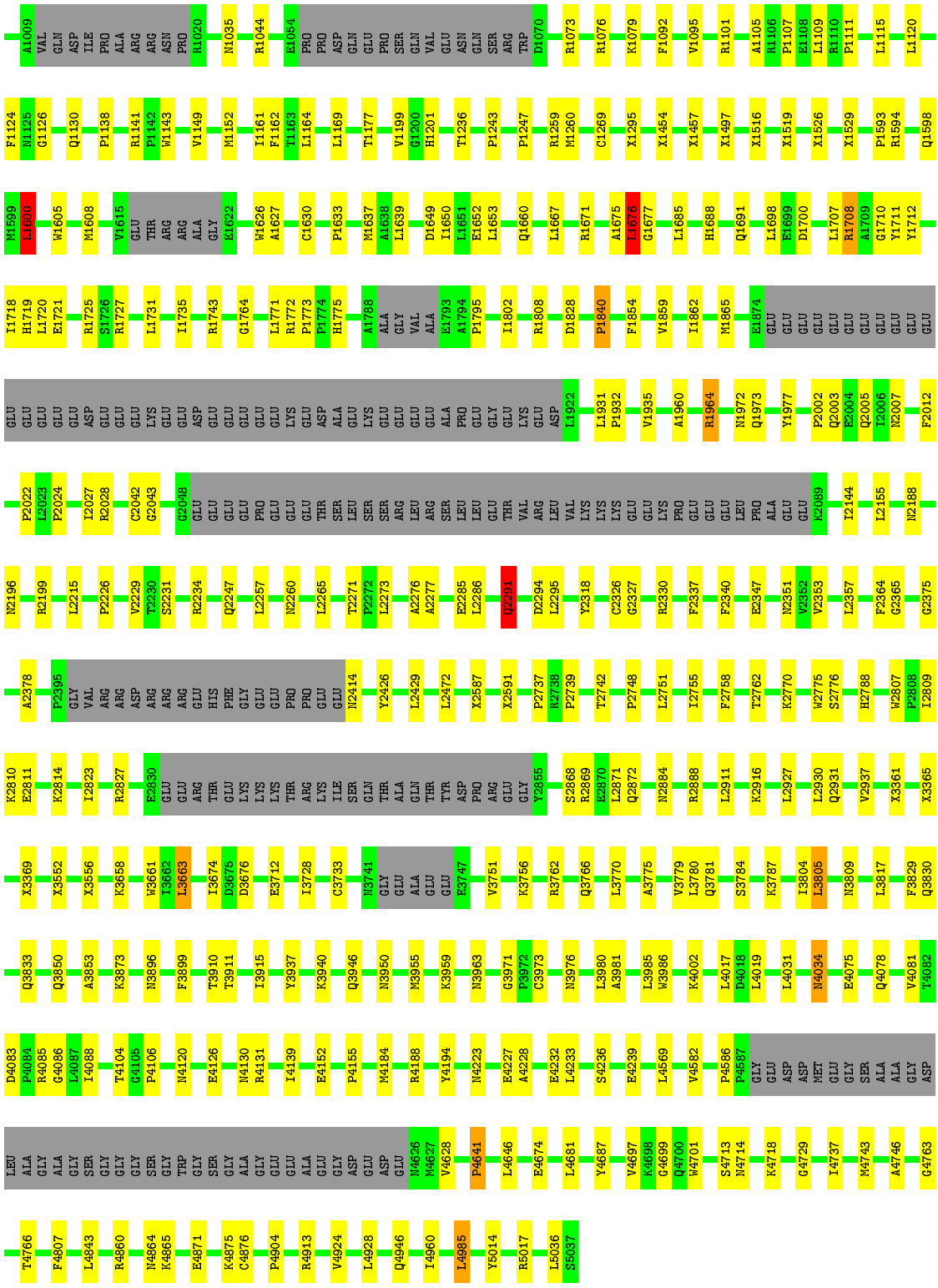




• Molecule 2: Ryanodine receptor 1

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: ZN, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.31	0/834	0.54	0/1123
1	F	0.31	0/834	0.54	0/1123
1	H	0.31	0/834	0.54	0/1123
1	J	0.31	0/834	0.54	0/1123
2	B	0.30	0/25428	0.54	5/34534 (0.0%)
2	E	0.30	0/25428	0.54	5/34534 (0.0%)
2	G	0.30	0/25428	0.54	5/34534 (0.0%)
2	I	0.30	0/25428	0.54	5/34534 (0.0%)
All	All	0.30	0/105048	0.54	20/142628 (0.0%)

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

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

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	131	LEU	CA-CB-CG	7.62	132.81	115.30
2	I	131	LEU	CA-CB-CG	7.61	132.79	115.30
2	B	131	LEU	CA-CB-CG	7.59	132.75	115.30
2	G	131	LEU	CA-CB-CG	7.59	132.75	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1600	LEU	CA-CB-CG	6.68	130.67	115.30
2	E	1600	LEU	CA-CB-CG	6.67	130.64	115.30
2	I	1600	LEU	CA-CB-CG	6.67	130.63	115.30
2	G	1600	LEU	CA-CB-CG	6.66	130.61	115.30
2	G	1676	LEU	CA-CB-CG	6.63	130.54	115.30
2	E	1676	LEU	CA-CB-CG	6.63	130.54	115.30
2	B	1676	LEU	CA-CB-CG	6.62	130.53	115.30
2	I	1676	LEU	CA-CB-CG	6.61	130.50	115.30
2	B	4985	LEU	CA-CB-CG	6.05	129.21	115.30
2	G	4985	LEU	CA-CB-CG	6.03	129.17	115.30
2	I	4985	LEU	CA-CB-CG	6.03	129.17	115.30
2	E	4985	LEU	CA-CB-CG	6.03	129.16	115.30
2	E	977	LEU	CA-CB-CG	5.79	128.62	115.30
2	B	977	LEU	CA-CB-CG	5.79	128.61	115.30
2	I	977	LEU	CA-CB-CG	5.79	128.61	115.30
2	G	977	LEU	CA-CB-CG	5.78	128.59	115.30

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1720	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	1840	PRO	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	1840	PRO	Peptide
2	E	2291	GLN	Peptide

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Mol	Chain	Res	Type	Group
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
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	1840	PRO	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
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	1840	PRO	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

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	10	0
1	F	818	0	824	12	0
1	H	818	0	824	12	0
1	J	818	0	824	12	0
2	B	29499	0	24749	281	0
2	E	29499	0	24749	253	0
2	G	29499	0	24750	262	0
2	I	29499	0	24749	257	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	121276	0	102293	1081	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 (1081) 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:4968:PHE:CE2	2:B:4978:HIS:CE1	2.28	1.20
2:B:4230:LYS:HD2	2:B:4959:PHE:HE2	0.99	1.10
2:B:4230:LYS:HD2	2:B:4959:PHE:CE2	1.92	1.04
2:B:4983:HIS:CE1	2:B:5027:CYS:SG	2.57	0.98
2:B:4230:LYS:CD	2:B:4959:PHE:HE2	1.87	0.87
2:B:4983:HIS:HE1	2:B:5027:CYS:SG	1.98	0.85
2:I:2318:TYR:HH	2:I:2414:ASN:N	1.86	0.74
2:B:4968:PHE:HE2	2:B:4978:HIS:CE1	1.98	0.72
2:E:2318:TYR:HH	2:E:2414:ASN:N	1.86	0.72
2:G:2318:TYR:HH	2:G:2414:ASN:N	1.87	0.71
2:B:2318:TYR:HH	2:B:2414:ASN:N	1.86	0.71
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.57	0.69
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.57	0.69
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.57	0.68
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.57	0.68
2:B:4968:PHE:HE2	2:B:4978:HIS:NE2	1.93	0.67
2:E:111:HIS:HD2	2:E:114:SER:H	1.43	0.67
2:E:379:HIS:HD2	2:E:382:GLY:H	1.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:379:HIS:HD2	2:B:382:GLY:H	1.43	0.66
2:G:111:HIS:HD2	2:G:114:SER:H	1.43	0.66
2:B:111:HIS:HD2	2:B:114:SER:H	1.43	0.66
2:G:379:HIS:HD2	2:G:382:GLY:H	1.43	0.65
2:I:111:HIS:HD2	2:I:114:SER:H	1.43	0.65
2:B:4968:PHE:CE2	2:B:4978:HIS:NE2	2.64	0.64
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.63	0.64
2:I:379:HIS:HD2	2:I:382:GLY:H	1.43	0.64
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.63	0.63
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.63	0.62
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.63	0.62
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.33	0.62
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.33	0.62
2:G:4860:ARG:HD2	2:I:4582:VAL:HG11	1.81	0.62
2:B:1637:MET:SD	2:B:1708:ARG:NH1	2.74	0.61
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.34	0.61
2:E:1637:MET:SD	2:E:1708:ARG:NH1	2.74	0.61
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.33	0.61
2:B:683:ARG:NH1	2:B:707:VAL:O	2.34	0.61
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.33	0.61
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.34	0.60
2:E:614:VAL:HG22	2:E:616:SER:H	1.66	0.60
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.67	0.60
2:I:1637:MET:SD	2:I:1708:ARG:NH1	2.74	0.60
2:G:1637:MET:SD	2:G:1708:ARG:NH1	2.74	0.60
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.34	0.60
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.67	0.60
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.34	0.60
2:B:614:VAL:HG22	2:B:616:SER:H	1.66	0.60
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.35	0.60
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.34	0.60
2:G:683:ARG:NH1	2:G:707:VAL:O	2.34	0.60
2:I:132:ALA:HA	2:I:194:SER:HB2	1.83	0.60
2:G:614:VAL:HG22	2:G:616:SER:H	1.66	0.60
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.34	0.60
2:G:132:ALA:HA	2:G:194:SER:HB2	1.83	0.60
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.34	0.60
2:I:173:SER:HB3	2:I:178:ARG:H	1.67	0.60
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.34	0.59
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.35	0.59
2:I:683:ARG:NH1	2:I:707:VAL:O	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:173:SER:HB3	2:G:178:ARG:H	1.67	0.59
2:B:173:SER:HB3	2:B:178:ARG:H	1.67	0.59
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.67	0.59
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.83	0.59
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.67	0.59
2:B:132:ALA:HA	2:B:194:SER:HB2	1.83	0.59
2:E:132:ALA:HA	2:E:194:SER:HB2	1.83	0.59
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.68	0.59
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.68	0.59
2:I:315:CYS:SG	2:I:316:PHE:N	2.76	0.59
2:I:614:VAL:HG22	2:I:616:SER:H	1.66	0.59
2:E:683:ARG:NH1	2:E:707:VAL:O	2.34	0.58
2:G:315:CYS:SG	2:G:316:PHE:N	2.76	0.58
2:I:40:GLU:HB3	2:I:44:ASN:HB3	1.85	0.58
2:E:4674:GLU:HG3	2:E:4714:ASN:HB3	1.85	0.58
2:B:40:GLU:HB3	2:B:44:ASN:HB3	1.85	0.58
2:E:315:CYS:SG	2:E:316:PHE:N	2.76	0.58
2:E:173:SER:HB3	2:E:178:ARG:H	1.67	0.58
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.35	0.58
2:B:315:CYS:SG	2:B:316:PHE:N	2.76	0.58
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.86	0.58
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.86	0.58
2:I:4674:GLU:HG3	2:I:4714:ASN:HB3	1.85	0.58
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.68	0.58
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.84	0.58
2:E:4223:ASN:OD1	2:E:4946:GLN:NE2	2.37	0.58
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.86	0.57
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.35	0.57
2:I:4223:ASN:OD1	2:I:4946:GLN:NE2	2.37	0.57
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.87	0.57
2:B:4674:GLU:HG3	2:B:4714:ASN:HB3	1.85	0.57
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.86	0.57
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.87	0.57
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.87	0.57
2:G:4674:GLU:HG3	2:G:4714:ASN:HB3	1.85	0.57
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.87	0.57
2:B:4223:ASN:OD1	2:B:4946:GLN:NE2	2.37	0.57
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.87	0.57
2:E:40:GLU:HB3	2:E:44:ASN:HB3	1.85	0.57
2:G:3762:ARG:O	2:G:3766:GLN:NE2	2.38	0.57
2:G:4223:ASN:OD1	2:G:4946:GLN:NE2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3762:ARG:O	2:I:3766:GLN:NE2	2.38	0.57
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.86	0.57
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.87	0.57
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.87	0.57
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.38	0.57
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.87	0.57
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.68	0.57
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.87	0.57
2:E:609:CYS:SG	2:E:610:ASN:N	2.78	0.57
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.78	0.56
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.87	0.56
2:B:3762:ARG:O	2:B:3766:GLN:NE2	2.38	0.56
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.87	0.56
2:B:609:CYS:SG	2:B:610:ASN:N	2.78	0.56
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.87	0.56
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.88	0.56
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.78	0.56
2:B:2827:ARG:HH21	2:B:2931:GLN:HG3	1.70	0.56
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.87	0.56
2:B:1259:ARG:HH12	2:B:1593:PRO:HA	1.70	0.56
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.88	0.56
2:E:2827:ARG:HH21	2:E:2931:GLN:HG3	1.70	0.56
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.87	0.56
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.87	0.56
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.87	0.56
2:E:1259:ARG:HH12	2:E:1593:PRO:HA	1.70	0.56
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.71	0.56
2:G:40:GLU:HB3	2:G:44:ASN:HB3	1.85	0.56
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.88	0.56
2:G:609:CYS:SG	2:G:610:ASN:N	2.78	0.56
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.88	0.56
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.87	0.56
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.88	0.56
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.87	0.56
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.78	0.56
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.38	0.56
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.39	0.56
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.78	0.56
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.88	0.56
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.87	0.56
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.87	0.56
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.88	0.56
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.87	0.56
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.87	0.56
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.88	0.56
2:I:609:CYS:SG	2:I:610:ASN:N	2.78	0.56
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.71	0.55
2:B:4982:GLU:OE1	2:B:4982:GLU:HA	2.06	0.55
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.89	0.55
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.71	0.55
2:E:3762:ARG:O	2:E:3766:GLN:NE2	2.38	0.55
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.87	0.55
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.88	0.55
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.71	0.55
2:B:626:LEU:HD23	2:B:630:GLU:H	1.71	0.55
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.71	0.55
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.88	0.55
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.39	0.55
2:G:1259:ARG:HH12	2:G:1593:PRO:HA	1.70	0.55
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.88	0.55
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.88	0.55
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.88	0.55
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.87	0.55
2:E:2347:GLU:O	2:E:2351:ASN:N	2.40	0.55
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.89	0.55
2:E:626:LEU:HD23	2:E:630:GLU:H	1.71	0.55
2:G:2827:ARG:HH21	2:G:2931:GLN:HG3	1.70	0.55
2:G:626:LEU:HD23	2:G:630:GLU:H	1.71	0.55
2:I:1259:ARG:HH12	2:I:1593:PRO:HA	1.70	0.55
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.88	0.55
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.71	0.55
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.87	0.55
2:G:2347:GLU:O	2:G:2351:ASN:N	2.40	0.55
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.39	0.55
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.40	0.55
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.89	0.55
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.88	0.55
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.40	0.55
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.87	0.55
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.87	0.55
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.40	0.54
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.71	0.54
2:I:626:LEU:HD23	2:I:630:GLU:H	1.71	0.54
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.89	0.54
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.88	0.54
2:B:3981:ALA:HA	2:B:3986:TRP:HE1	1.72	0.54
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.38	0.54
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.90	0.54
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.40	0.54
2:I:2827:ARG:HH21	2:I:2931:GLN:HG3	1.70	0.54
2:E:730:VAL:O	2:E:735:GLN:NE2	2.41	0.54
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.89	0.54
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.40	0.54
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.40	0.54
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.39	0.54
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.90	0.54
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.90	0.54
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.40	0.54
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.38	0.54
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.40	0.54
2:G:730:VAL:O	2:G:735:GLN:NE2	2.41	0.54
2:E:3981:ALA:HA	2:E:3986:TRP:HE1	1.72	0.54
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.90	0.54
2:I:2347:GLU:O	2:I:2351:ASN:N	2.40	0.54
2:I:730:VAL:O	2:I:735:GLN:NE2	2.41	0.54
2:B:359:TYR:HA	2:B:376:ALA:HA	1.90	0.54
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.89	0.54
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.89	0.54
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.90	0.54
2:E:1164:LEU:HB3	2:E:1169:LEU:HD21	1.90	0.53
2:E:359:TYR:HA	2:E:376:ALA:HA	1.90	0.53
2:E:4924:VAL:HA	2:E:4928:LEU:HB2	1.90	0.53
2:G:395:GLN:HG3	2:G:397:GLU:H	1.74	0.53
2:G:41:GLY:O	2:G:45:ARG:NH1	2.42	0.53
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.71	0.53
2:I:359:TYR:HA	2:I:376:ALA:HA	1.90	0.53
2:B:4924:VAL:HA	2:B:4928:LEU:HB2	1.90	0.53
2:G:1731:LEU:HA	2:G:1772:ARG:HH12	1.73	0.53
2:I:1731:LEU:HA	2:I:1772:ARG:HH12	1.73	0.53
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.91	0.53
2:I:3981:ALA:HA	2:I:3986:TRP:HE1	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1164:LEU:HB3	2:B:1169:LEU:HD21	1.90	0.53
2:B:2347:GLU:O	2:B:2351:ASN:N	2.40	0.53
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.90	0.53
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.91	0.53
2:G:359:TYR:HA	2:G:376:ALA:HA	1.90	0.53
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.89	0.53
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.91	0.53
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.90	0.53
2:B:730:VAL:O	2:B:735:GLN:NE2	2.41	0.53
2:I:41:GLY:O	2:I:45:ARG:NH1	2.42	0.53
2:B:1243:PRO:HB2	2:B:1600:LEU:HD22	1.91	0.53
2:E:41:GLY:O	2:E:45:ARG:NH1	2.42	0.53
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.91	0.53
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.91	0.53
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.91	0.53
2:I:4924:VAL:HA	2:I:4928:LEU:HB2	1.90	0.53
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.91	0.53
2:B:395:GLN:HG3	2:B:397:GLU:H	1.74	0.53
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.90	0.53
2:B:867:LEU:HB3	2:B:929:LEU:HD13	1.91	0.53
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.90	0.53
2:E:1650:ILE:HG13	2:E:1707:LEU:HD21	1.91	0.53
2:E:395:GLN:HG3	2:E:397:GLU:H	1.74	0.53
2:E:867:LEU:HB3	2:E:929:LEU:HD13	1.91	0.53
2:G:3981:ALA:HA	2:G:3986:TRP:HE1	1.72	0.53
2:G:4924:VAL:HA	2:G:4928:LEU:HB2	1.90	0.53
2:B:1650:ILE:HG13	2:B:1707:LEU:HD21	1.91	0.52
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.91	0.52
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.91	0.52
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.91	0.52
2:G:1164:LEU:HB3	2:G:1169:LEU:HD21	1.90	0.52
2:I:823:LEU:HD23	2:I:1626:TRP:HB3	1.91	0.52
2:E:823:LEU:HD23	2:E:1626:TRP:HB3	1.92	0.52
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.92	0.52
2:G:867:LEU:HB3	2:G:929:LEU:HD13	1.91	0.52
2:I:1164:LEU:HB3	2:I:1169:LEU:HD21	1.90	0.52
2:B:838:HIS:HA	2:B:1201:HIS:HB3	1.92	0.52
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.91	0.52
2:E:1731:LEU:HA	2:E:1772:ARG:HH12	1.73	0.52
2:E:2911:LEU:HB2	2:E:2916:LYS:HE3	1.91	0.52
2:I:1243:PRO:HB2	2:I:1600:LEU:HD22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.92	0.52
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.91	0.52
2:B:776:LEU:HG	2:B:848:HIS:HA	1.92	0.52
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.91	0.52
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.92	0.52
2:E:838:HIS:HA	2:E:1201:HIS:HB3	1.92	0.52
2:G:823:LEU:HD23	2:G:1626:TRP:HB3	1.92	0.52
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.91	0.52
2:G:4582:VAL:HG11	2:E:4860:ARG:HD2	1.89	0.52
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.91	0.52
2:G:776:LEU:HG	2:G:848:HIS:HA	1.92	0.52
2:B:823:LEU:HD23	2:B:1626:TRP:HB3	1.92	0.52
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.91	0.52
2:G:2452:ARG:HH12	2:E:177:GLU:HG3	1.73	0.52
2:I:1650:ILE:HG13	2:I:1707:LEU:HD21	1.91	0.52
2:B:41:GLY:O	2:B:45:ARG:NH1	2.41	0.52
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.92	0.52
2:B:1731:LEU:HA	2:B:1772:ARG:HH12	1.73	0.52
2:E:1243:PRO:HB2	2:E:1600:LEU:HD22	1.91	0.52
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.92	0.52
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.43	0.52
2:B:2364:PHE:HD1	2:B:2429:LEU:HD21	1.75	0.52
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.92	0.52
2:E:3751:VAL:O	2:E:3756:LYS:NZ	2.43	0.52
2:E:4681:LEU:HD21	2:E:4687:TYR:HD2	1.75	0.52
2:G:2911:LEU:HB2	2:G:2916:LYS:HE3	1.91	0.52
2:I:776:LEU:HG	2:I:848:HIS:HA	1.92	0.52
2:I:838:HIS:HA	2:I:1201:HIS:HB3	1.92	0.52
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.92	0.51
2:E:776:LEU:HG	2:E:848:HIS:HA	1.92	0.51
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.92	0.51
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.92	0.51
2:G:838:HIS:HA	2:G:1201:HIS:HB3	1.92	0.51
2:I:2364:PHE:HD1	2:I:2429:LEU:HD21	1.75	0.51
2:B:3751:VAL:O	2:B:3756:LYS:NZ	2.44	0.51
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.44	0.51
2:G:1243:PRO:HB2	2:G:1600:LEU:HD22	1.91	0.51
2:G:1650:ILE:HG13	2:G:1707:LEU:HD21	1.91	0.51
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.76	0.51
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.91	0.51
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.43	0.51
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.44	0.51
2:E:2364:PHE:HD1	2:E:2429:LEU:HD21	1.75	0.51
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.76	0.51
2:G:56:GLN:O	2:G:309:THR:OG1	2.26	0.51
2:I:2911:LEU:HB2	2:I:2916:LYS:HE3	1.91	0.51
2:I:867:LEU:HB3	2:I:929:LEU:HD13	1.91	0.51
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.91	0.51
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.44	0.51
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.81	0.51
2:I:395:GLN:HG3	2:I:397:GLU:H	1.74	0.51
2:B:1516:UNK:N	2:B:1529:UNK:O	2.44	0.51
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.44	0.51
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.81	0.51
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.93	0.51
2:B:2911:LEU:HB2	2:B:2916:LYS:HE3	1.91	0.51
2:E:2365:GLY:HA3	2:E:2426:TYR:HE1	1.76	0.51
2:G:1516:UNK:N	2:G:1529:UNK:O	2.44	0.51
2:I:3751:VAL:O	2:I:3756:LYS:NZ	2.43	0.51
2:I:2318:TYR:OH	2:I:2414:ASN:N	2.44	0.51
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.91	0.51
2:E:1516:UNK:N	2:E:1529:UNK:O	2.44	0.51
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.93	0.51
2:E:3980:LEU:HD22	2:E:3985:LEU:HD22	1.93	0.51
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.44	0.51
2:G:2364:PHE:HD1	2:G:2429:LEU:HD21	1.75	0.51
2:I:4081:VAL:HB	2:I:4088:ILE:HD12	1.93	0.51
2:G:4681:LEU:HD21	2:G:4687:TYR:HD2	1.75	0.51
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.76	0.51
2:E:4904:PRO:HB3	2:E:4913:ARG:HD3	1.93	0.51
2:G:3751:VAL:O	2:G:3756:LYS:NZ	2.43	0.51
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.44	0.51
2:B:2365:GLY:HA3	2:B:2426:TYR:HE1	1.76	0.50
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.93	0.50
2:G:331:VAL:HG12	2:G:333:GLY:H	1.76	0.50
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.91	0.50
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.45	0.50
2:B:45:ARG:NH2	2:B:447:ASP:OD1	2.45	0.50
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.77	0.50
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.94	0.50
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:56:GLN:O	2:E:309:THR:OG1	2.26	0.50
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.43	0.50
2:G:3980:LEU:HD22	2:G:3985:LEU:HD22	1.93	0.50
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.77	0.50
2:G:794:GLY:H	2:G:798:GLY:HA3	1.76	0.50
2:I:4904:PRO:HB3	2:I:4913:ARG:HD3	1.93	0.50
2:I:794:GLY:H	2:I:798:GLY:HA3	1.76	0.50
2:E:331:VAL:HG12	2:E:333:GLY:H	1.76	0.50
2:G:2265:LEU:HD22	2:G:2330:ARG:HB3	1.94	0.50
2:I:1516:UNK:N	2:I:1529:UNK:O	2.44	0.50
1:A:21:THR:HA	1:A:49:ARG:HA	1.94	0.50
2:B:4681:LEU:HD21	2:B:4687:TYR:HD2	1.75	0.50
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.93	0.50
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.93	0.50
2:E:4729:GLY:HA2	2:E:4737:ILE:HG13	1.93	0.50
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.77	0.50
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.44	0.50
1:J:21:THR:HA	1:J:49:ARG:HA	1.94	0.50
2:B:4983:HIS:N	2:B:4983:HIS:ND1	2.59	0.50
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.94	0.50
1:F:21:THR:HA	1:F:49:ARG:HA	1.94	0.50
2:G:45:ARG:NH2	2:G:447:ASP:OD1	2.44	0.50
2:I:2365:GLY:HA3	2:I:2426:TYR:HE1	1.76	0.50
2:I:4681:LEU:HD21	2:I:4687:TYR:HD2	1.75	0.50
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.94	0.50
2:E:2265:LEU:HD22	2:E:2330:ARG:HB3	1.94	0.50
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.81	0.50
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.94	0.50
2:B:4081:VAL:HB	2:B:4088:ILE:HD12	1.93	0.50
2:B:4904:PRO:HB3	2:B:4913:ARG:HD3	1.93	0.50
2:B:794:GLY:H	2:B:798:GLY:HA3	1.76	0.50
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.76	0.50
2:E:4081:VAL:HB	2:E:4088:ILE:HD12	1.93	0.50
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.94	0.50
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.45	0.50
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.94	0.50
2:E:794:GLY:H	2:E:798:GLY:HA3	1.76	0.50
2:G:4904:PRO:HB3	2:G:4913:ARG:HD3	1.93	0.50
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.93	0.50
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.94	0.50
2:I:3980:LEU:HD22	2:I:3985:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2265:LEU:HD22	2:B:2330:ARG:HB3	1.94	0.49
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.94	0.49
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.94	0.49
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.94	0.49
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.93	0.49
2:I:331:VAL:HG12	2:I:333:GLY:H	1.76	0.49
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	1.94	0.49
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.77	0.49
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.93	0.49
1:H:21:THR:HA	1:H:49:ARG:HA	1.94	0.49
2:I:45:ARG:NH2	2:I:447:ASP:OD1	2.44	0.49
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.77	0.49
2:B:331:VAL:HG12	2:B:333:GLY:H	1.76	0.49
2:B:4968:PHE:CD2	2:B:4978:HIS:CE1	2.94	0.49
2:G:2758:PHE:HD2	2:G:2809:ILE:HG12	1.77	0.49
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.94	0.49
2:B:3980:LEU:HD22	2:B:3985:LEU:HD22	1.93	0.49
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.94	0.49
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.77	0.49
2:E:45:ARG:NH2	2:E:447:ASP:OD1	2.45	0.49
2:G:2318:TYR:OH	2:G:2414:ASN:N	2.44	0.49
2:G:4081:VAL:HB	2:G:4088:ILE:HD12	1.93	0.49
2:I:3850:GLN:HA	2:I:3853:ALA:HB3	1.95	0.49
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.94	0.49
2:B:615:ARG:NH2	2:B:1677:GLY:O	2.43	0.49
2:E:111:HIS:CD2	2:E:114:SER:H	2.29	0.49
2:G:2365:GLY:HA3	2:G:2426:TYR:HE1	1.76	0.49
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.46	0.49
2:I:2265:LEU:HD22	2:I:2330:ARG:HB3	1.94	0.49
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.94	0.49
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	1.94	0.49
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	1.95	0.49
2:G:4729:GLY:HA2	2:G:4737:ILE:HG13	1.93	0.49
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.77	0.49
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.77	0.49
2:B:2758:PHE:HD2	2:B:2809:ILE:HG12	1.77	0.49
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.78	0.49
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.93	0.49
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.81	0.49
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.31	0.49
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:56:GLN:O	2:I:309:THR:OG1	2.26	0.49
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	1.95	0.48
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.93	0.48
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.31	0.48
2:B:4729:GLY:HA2	2:B:4737:ILE:HG13	1.94	0.48
2:B:4962:GLY:H	2:B:5025:GLY:N	2.12	0.48
2:E:2758:PHE:HD2	2:E:2809:ILE:HG12	1.77	0.48
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.94	0.48
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.47	0.48
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.44	0.48
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.31	0.48
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.47	0.48
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.47	0.48
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.30	0.48
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.44	0.48
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.94	0.48
2:B:1126:GLY:HA3	2:B:1143:TRP:CE2	2.49	0.48
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.77	0.48
2:E:34:LYS:H	2:E:53:SER:HG	1.60	0.48
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.94	0.48
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	1.95	0.48
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.95	0.48
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.94	0.48
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.47	0.48
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	1.95	0.48
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.47	0.48
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.77	0.48
2:E:1457:UNK:N	2:E:1497:UNK:O	2.47	0.48
2:E:4697:VAL:O	2:E:4701:TRP:N	2.47	0.48
2:G:1126:GLY:HA3	2:G:1143:TRP:CE2	2.49	0.48
2:I:2257:LEU:HD11	2:I:2276:ALA:HB2	1.94	0.48
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.31	0.48
2:B:4586:PRO:HB3	2:B:4628:VAL:HG21	1.96	0.48
2:I:1126:GLY:HA3	2:I:1143:TRP:CE2	2.49	0.48
2:I:615:ARG:NH2	2:I:1677:GLY:O	2.44	0.48
2:I:4586:PRO:HB3	2:I:4628:VAL:HG21	1.96	0.48
2:I:4729:GLY:HA2	2:I:4737:ILE:HG13	1.94	0.48
2:B:1457:UNK:N	2:B:1497:UNK:O	2.46	0.48
2:B:2257:LEU:HD11	2:B:2276:ALA:HB2	1.94	0.48
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	1.95	0.48
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.96	0.48
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.95	0.48
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.46	0.48
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.30	0.48
2:I:280:LEU:HD21	2:I:316:PHE:HE2	1.79	0.48
2:B:2375:GLY:HA3	2:B:2378:ALA:HB3	1.96	0.48
2:B:280:LEU:HD21	2:B:316:PHE:HE2	1.79	0.48
2:E:1126:GLY:HA3	2:E:1143:TRP:CE2	2.49	0.48
2:E:2375:GLY:HA3	2:E:2378:ALA:HB3	1.96	0.48
2:E:280:LEU:HD21	2:E:316:PHE:HE2	1.79	0.48
2:G:177:GLU:HG3	2:I:2452:ARG:HH12	1.79	0.48
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.95	0.48
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.47	0.47
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.46	0.47
2:E:2318:TYR:OH	2:E:2414:ASN:N	2.44	0.47
2:I:1457:UNK:N	2:I:1497:UNK:O	2.46	0.47
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.47	0.47
2:B:4959:PHE:CD2	2:B:4959:PHE:C	2.86	0.47
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.47	0.47
2:I:2758:PHE:HD2	2:I:2809:ILE:HG12	1.77	0.47
2:I:34:LYS:H	2:I:53:SER:HG	1.60	0.47
2:G:1457:UNK:N	2:G:1497:UNK:O	2.47	0.47
2:G:4586:PRO:HB3	2:G:4628:VAL:HG21	1.96	0.47
2:B:3733:CYS:HA	2:B:3766:GLN:HG2	1.97	0.47
2:E:615:ARG:NH2	2:E:1677:GLY:O	2.44	0.47
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.96	0.47
2:G:111:HIS:CD2	2:G:114:SER:H	2.29	0.47
2:B:1973:GLN:O	2:B:1977:TYR:N	2.45	0.47
2:B:2318:TYR:OH	2:B:2414:ASN:N	2.44	0.47
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.80	0.47
2:E:2868:SER:O	2:E:2872:GLN:N	2.48	0.47
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.96	0.47
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.80	0.47
2:G:4697:VAL:O	2:G:4701:TRP:N	2.47	0.47
1:J:34:LYS:HD3	2:I:629:ARG:HD2	1.95	0.47
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.80	0.47
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.96	0.47
2:G:280:LEU:HD21	2:G:316:PHE:HE2	1.79	0.47
2:G:3733:CYS:HA	2:G:3766:GLN:HG2	1.97	0.47
2:I:111:HIS:CD2	2:I:114:SER:H	2.29	0.47
2:I:2375:GLY:HA3	2:I:2378:ALA:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.96	0.47
2:E:2758:PHE:O	2:E:2762:THR:N	2.47	0.47
2:B:2452:ARG:HH12	2:I:177:GLU:HG3	1.79	0.47
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	1.95	0.47
2:I:4697:VAL:O	2:I:4701:TRP:N	2.47	0.47
2:B:56:GLN:O	2:B:309:THR:OG1	2.26	0.47
2:B:621:ILE:O	2:B:625:LEU:N	2.46	0.47
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.96	0.47
2:I:3733:CYS:HA	2:I:3766:GLN:HG2	1.97	0.47
2:B:20:VAL:HG12	2:B:204:PRO:HA	1.97	0.47
2:E:20:VAL:HG12	2:E:204:PRO:HA	1.97	0.47
2:E:4586:PRO:HB3	2:E:4628:VAL:HG21	1.96	0.47
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.46	0.47
2:G:2353:VAL:O	2:G:2357:LEU:N	2.48	0.47
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	1.97	0.47
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.96	0.47
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.80	0.47
2:B:2868:SER:O	2:B:2872:GLN:N	2.48	0.47
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.95	0.47
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.48	0.47
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.46	0.47
2:G:2868:SER:O	2:G:2872:GLN:N	2.48	0.47
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.79	0.47
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.46	0.47
2:I:20:VAL:HG12	2:I:204:PRO:HA	1.97	0.47
2:I:34:LYS:N	2:I:53:SER:OG	2.44	0.47
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.80	0.46
2:E:2196:ASN:OD1	2:E:2199:ARG:NH1	2.40	0.46
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.98	0.46
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.80	0.46
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	1.97	0.46
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.80	0.46
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.79	0.46
2:I:2810:LYS:O	2:I:2814:LYS:N	2.39	0.46
2:E:1973:GLN:O	2:E:1977:TYR:N	2.46	0.46
2:E:3770:LEU:HD21	2:E:3775:ALA:HB3	1.97	0.46
2:G:615:ARG:NH2	2:G:1677:GLY:O	2.44	0.46
2:G:20:VAL:HG12	2:G:204:PRO:HA	1.97	0.46
2:I:2155:LEU:HD13	2:I:2188:ASN:HD21	1.80	0.46
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.80	0.46
2:B:2758:PHE:O	2:B:2762:THR:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.96	0.46
2:B:978:THR:HB	2:B:980:ALA:H	1.80	0.46
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.49	0.46
2:E:3733:CYS:HA	2:E:3766:GLN:HG2	1.96	0.46
2:G:1973:GLN:O	2:G:1977:TYR:N	2.45	0.46
2:I:2024:PRO:HB2	2:I:2027:ILE:HG12	1.98	0.46
2:I:2247:GLN:NE2	2:I:2285:GLU:OE2	2.49	0.46
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	1.97	0.46
2:B:1808:ARG:HD2	2:B:1854:PHE:HA	1.97	0.46
2:B:2353:VAL:O	2:B:2357:LEU:N	2.48	0.46
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.98	0.46
2:B:551:LEU:HD21	2:B:589:LEU:HD13	1.98	0.46
2:E:214:VAL:HG12	2:E:274:LEU:HD12	1.98	0.46
2:E:683:ARG:HG2	2:E:717:ASP:HB3	1.98	0.46
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.48	0.46
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.49	0.46
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.46	0.46
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.79	0.46
2:G:2758:PHE:O	2:G:2762:THR:N	2.47	0.46
2:I:1808:ARG:HD2	2:I:1854:PHE:HA	1.97	0.46
2:I:1973:GLN:O	2:I:1977:TYR:N	2.46	0.46
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.48	0.46
2:B:2024:PRO:HB2	2:B:2027:ILE:HG12	1.98	0.46
2:B:2247:GLN:NE2	2:B:2285:GLU:OE2	2.49	0.46
2:E:2353:VAL:O	2:E:2357:LEU:N	2.48	0.46
1:F:87:HIS:H	1:F:91:ILE:HB	1.81	0.46
2:G:2247:GLN:NE2	2:G:2285:GLU:OE2	2.49	0.46
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.98	0.46
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.30	0.46
2:I:551:LEU:HD21	2:I:589:LEU:HD13	1.98	0.46
2:E:2247:GLN:NE2	2:E:2285:GLU:OE2	2.49	0.46
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.49	0.46
2:G:2375:GLY:HA3	2:G:2378:ALA:HB3	1.96	0.46
2:G:880:GLU:OE1	2:G:968:ALA:N	2.44	0.46
1:H:87:HIS:H	1:H:91:ILE:HB	1.81	0.46
2:B:111:HIS:CD2	2:B:114:SER:H	2.29	0.46
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	1.98	0.46
2:E:551:LEU:HD21	2:E:589:LEU:HD13	1.98	0.46
2:G:1808:ARG:HD2	2:G:1854:PHE:HA	1.97	0.46
2:G:2155:LEU:HD13	2:G:2188:ASN:HD21	1.81	0.46
2:G:4017:LEU:HB3	2:G:4139:ILE:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:551:LEU:HD21	2:G:589:LEU:HD13	1.98	0.46
2:I:2868:SER:O	2:I:2872:GLN:N	2.48	0.46
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.79	0.46
2:B:4713:SER:HA	2:B:4718:LYS:HE2	1.99	0.45
2:E:2024:PRO:HB2	2:E:2027:ILE:HG12	1.98	0.45
2:E:4184:MET:HE1	2:E:4188:ARG:HE	1.81	0.45
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.48	0.45
2:G:3770:LEU:HD21	2:G:3775:ALA:HB3	1.97	0.45
2:G:978:THR:HB	2:G:980:ALA:H	1.80	0.45
2:I:4017:LEU:HB3	2:I:4139:ILE:HG13	1.98	0.45
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	1.97	0.45
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	1.98	0.45
2:I:3770:LEU:HD21	2:I:3775:ALA:HB3	1.97	0.45
2:B:214:VAL:HG12	2:B:274:LEU:HD12	1.98	0.45
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.98	0.45
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.30	0.45
2:B:683:ARG:HG2	2:B:717:ASP:HB3	1.98	0.45
2:E:4713:SER:HA	2:E:4718:LYS:HE2	1.98	0.45
2:G:2024:PRO:HB2	2:G:2027:ILE:HG12	1.98	0.45
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.98	0.45
2:G:4713:SER:HA	2:G:4718:LYS:HE2	1.98	0.45
2:G:34:LYS:N	2:G:53:SER:OG	2.44	0.45
2:I:978:THR:HB	2:I:980:ALA:H	1.80	0.45
2:B:1865:MET:SD	2:B:1865:MET:N	2.90	0.45
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.49	0.45
2:E:2155:LEU:HD13	2:E:2188:ASN:HD21	1.81	0.45
2:E:4763:GLY:O	2:E:4766:THR:OG1	2.28	0.45
2:E:892:THR:N	2:E:902:ARG:O	2.49	0.45
2:G:4031:LEU:HB3	2:G:4034:ASN:HB2	1.98	0.45
2:E:1865:MET:SD	2:E:1865:MET:N	2.90	0.45
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.49	0.45
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.99	0.45
1:F:7:ILE:HB	1:F:71:ARG:HB3	1.99	0.45
2:G:214:VAL:HG12	2:G:274:LEU:HD12	1.98	0.45
2:G:3361:UNK:O	2:G:3365:UNK:N	2.50	0.45
1:A:87:HIS:H	1:A:91:ILE:HB	1.81	0.45
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.49	0.45
2:B:606:LEU:O	2:B:617:ASN:ND2	2.50	0.45
2:E:1808:ARG:HD2	2:E:1854:PHE:HA	1.97	0.45
2:E:978:THR:HB	2:E:980:ALA:H	1.80	0.45
1:H:7:ILE:HB	1:H:71:ARG:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4031:LEU:HB3	2:I:4034:ASN:HB2	1.98	0.45
2:B:3770:LEU:HD21	2:B:3775:ALA:HB3	1.97	0.45
2:B:359:TYR:OH	2:B:385:ASP:OD2	2.32	0.45
2:E:3365:UNK:O	2:E:3369:UNK:N	2.50	0.45
2:E:621:ILE:O	2:E:625:LEU:N	2.46	0.45
2:I:790:ARG:HG2	2:I:1627:ALA:HA	1.99	0.45
1:J:87:HIS:H	1:J:91:ILE:HB	1.81	0.45
1:J:76:CYS:HB2	1:J:97:LEU:HB2	1.98	0.45
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.99	0.45
2:B:3365:UNK:O	2:B:3369:UNK:N	2.50	0.45
2:B:4697:VAL:O	2:B:4701:TRP:N	2.47	0.45
2:B:4960:ILE:H	2:B:4960:ILE:HG12	1.51	0.45
2:B:4968:PHE:CZ	2:B:4978:HIS:CE1	2.96	0.45
2:E:880:GLU:OE1	2:E:968:ALA:N	2.44	0.45
2:G:2776:SER:O	2:G:2788:HIS:N	2.50	0.45
2:G:34:LYS:H	2:G:53:SER:HG	1.63	0.45
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	1.98	0.45
2:G:606:LEU:O	2:G:617:ASN:ND2	2.50	0.45
2:I:2353:VAL:O	2:I:2357:LEU:N	2.48	0.45
2:I:3365:UNK:O	2:I:3369:UNK:N	2.50	0.45
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	1.98	0.45
2:I:606:LEU:O	2:I:617:ASN:ND2	2.50	0.45
2:B:2155:LEU:HD13	2:B:2188:ASN:HD21	1.81	0.45
2:B:404:ILE:HG21	2:B:481:GLU:HG3	1.99	0.45
2:E:2869:ARG:HA	2:E:2872:GLN:HB3	1.98	0.45
2:G:134:ASP:OD1	2:G:134:ASP:N	2.50	0.45
2:G:3365:UNK:O	2:G:3369:UNK:N	2.50	0.45
2:I:1865:MET:SD	2:I:1865:MET:N	2.90	0.45
2:I:2869:ARG:HA	2:I:2872:GLN:HB3	1.98	0.45
2:B:1247:PRO:HA	2:B:1598:GLN:HA	1.99	0.45
2:E:1092:PHE:N	2:E:1149:VAL:O	2.41	0.45
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.46	0.45
1:F:76:CYS:HB2	1:F:97:LEU:HB2	1.98	0.45
2:G:683:ARG:HG2	2:G:717:ASP:HB3	1.98	0.45
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.99	0.45
2:I:404:ILE:HG21	2:I:481:GLU:HG3	1.99	0.45
2:B:396:GLU:OE2	2:B:451:TYR:OH	2.28	0.44
2:E:2776:SER:O	2:E:2788:HIS:N	2.50	0.44
2:E:4075:GLU:HA	2:E:4078:GLN:HB2	2.00	0.44
1:H:76:CYS:HB2	1:H:97:LEU:HB2	1.98	0.44
2:I:4233:LEU:HA	2:I:4236:SER:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4713:SER:HA	2:I:4718:LYS:HE2	1.98	0.44
2:G:1865:MET:SD	2:G:1865:MET:N	2.90	0.44
2:G:2430:ILE:HG21	2:G:2502:UNK:HA	1.99	0.44
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.98	0.44
2:G:4233:LEU:HA	2:G:4236:SER:HB3	2.00	0.44
2:G:43:GLY:N	2:G:447:ASP:OD2	2.45	0.44
2:G:621:ILE:O	2:G:625:LEU:N	2.46	0.44
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.40	0.44
2:B:2231:SER:HA	2:B:2234:ARG:HG2	2.00	0.44
2:B:4017:LEU:HB3	2:B:4139:ILE:HG13	1.98	0.44
2:E:4017:LEU:HB3	2:E:4139:ILE:HG13	1.98	0.44
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.40	0.44
2:G:790:ARG:HG2	2:G:1627:ALA:HA	1.99	0.44
2:G:3658:LYS:HA	2:G:3661:TRP:CE2	2.53	0.44
2:G:396:GLU:OE2	2:G:451:TYR:OH	2.28	0.44
1:H:74:LEU:HB2	1:H:99:PHE:HB2	2.00	0.44
2:I:134:ASP:OD1	2:I:134:ASP:N	2.50	0.44
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.99	0.44
2:I:683:ARG:HG2	2:I:717:ASP:HB3	1.98	0.44
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.36	0.44
2:B:2776:SER:O	2:B:2788:HIS:N	2.50	0.44
2:B:3973:CYS:SG	2:B:3976:ASN:ND2	2.91	0.44
2:E:3361:UNK:O	2:E:3365:UNK:N	2.50	0.44
2:G:3973:CYS:SG	2:G:3976:ASN:ND2	2.91	0.44
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.36	0.44
1:A:56:ILE:HG13	1:A:59:PHE:H	1.83	0.44
2:B:3658:LYS:HA	2:B:3661:TRP:CE2	2.53	0.44
2:B:4075:GLU:HA	2:B:4078:GLN:HB2	2.00	0.44
2:B:4968:PHE:CE2	2:B:4978:HIS:HE1	2.21	0.44
2:B:892:THR:N	2:B:902:ARG:O	2.49	0.44
2:B:983:THR:O	2:B:987:ARG:N	2.49	0.44
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.99	0.44
2:E:1247:PRO:HA	2:E:1598:GLN:HA	1.99	0.44
2:E:3973:CYS:SG	2:E:3976:ASN:ND2	2.91	0.44
2:E:606:LEU:O	2:E:617:ASN:ND2	2.50	0.44
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.99	0.44
2:G:404:ILE:HG21	2:G:481:GLU:HG3	1.99	0.44
2:I:164:ARG:N	2:I:167:ASP:OD2	2.46	0.44
2:I:214:VAL:HG12	2:I:274:LEU:HD12	1.98	0.44
2:I:3658:LYS:HA	2:I:3661:TRP:CE2	2.53	0.44
2:B:34:LYS:H	2:B:53:SER:HG	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4865:LYS:HG3	2:B:4875:LYS:HZ3	1.82	0.44
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	2.00	0.44
2:E:3940:LYS:O	2:E:4002:LYS:NZ	2.49	0.44
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	2.00	0.44
2:G:1653:LEU:HB3	2:G:1660:GLN:HB2	2.00	0.44
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.36	0.44
2:I:2231:SER:HA	2:I:2234:ARG:HG2	2.00	0.44
2:I:2776:SER:O	2:I:2788:HIS:N	2.50	0.44
2:I:3973:CYS:SG	2:I:3976:ASN:ND2	2.91	0.44
1:A:7:ILE:HB	1:A:71:ARG:HB3	1.99	0.44
2:E:119:SER:HA	2:E:146:CYS:HA	1.99	0.44
2:E:914:PRO:O	2:E:918:ARG:N	2.51	0.44
2:G:2869:ARG:HA	2:G:2872:GLN:HB3	1.98	0.44
2:I:3361:UNK:O	2:I:3365:UNK:N	2.50	0.44
1:A:76:CYS:HB2	1:A:97:LEU:HB2	1.98	0.44
2:B:2869:ARG:HA	2:B:2872:GLN:HB3	1.98	0.44
2:B:4031:LEU:HB3	2:B:4034:ASN:HB2	1.98	0.44
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.36	0.44
2:E:3658:LYS:HA	2:E:3661:TRP:CE2	2.53	0.44
2:E:404:ILE:HG21	2:E:481:GLU:HG3	1.99	0.44
1:F:92:PRO:HD3	2:E:627:PRO:HB2	1.99	0.44
2:G:1247:PRO:HA	2:G:1598:GLN:HA	1.99	0.44
2:G:1972:ASN:HD21	2:G:2024:PRO:HB3	1.83	0.44
2:G:892:THR:N	2:G:902:ARG:O	2.49	0.44
2:I:793:LEU:HB2	2:I:797:HIS:H	1.83	0.44
2:B:3361:UNK:O	2:B:3365:UNK:N	2.50	0.44
2:B:4984:ASN:C	2:B:4986:ALA:H	2.21	0.44
2:E:790:ARG:HG2	2:E:1627:ALA:HA	1.99	0.44
1:F:56:ILE:HG13	1:F:59:PHE:H	1.83	0.44
1:F:74:LEU:HB2	1:F:99:PHE:HB2	2.00	0.44
2:G:2196:ASN:OD1	2:G:2199:ARG:NH1	2.40	0.44
2:G:4075:GLU:HA	2:G:4078:GLN:HB2	1.99	0.44
2:G:793:LEU:HB2	2:G:797:HIS:H	1.83	0.44
2:I:4075:GLU:HA	2:I:4078:GLN:HB2	1.99	0.44
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	2.00	0.44
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.28	0.44
1:J:7:ILE:HB	1:J:71:ARG:HB3	1.99	0.44
2:B:3674:ILE:HD11	2:B:3728:ILE:HG22	1.99	0.43
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	2.00	0.43
2:E:4031:LEU:HB3	2:E:4034:ASN:HB2	1.98	0.43
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:681:HIS:HB3	2:E:784:SER:HB3	2.00	0.43
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.50	0.43
2:I:396:GLU:OE2	2:I:451:TYR:OH	2.28	0.43
2:I:572:PRO:HA	2:I:575:LEU:HD13	2.00	0.43
2:I:681:HIS:HB3	2:I:784:SER:HB3	2.00	0.43
1:J:74:LEU:HB2	1:J:99:PHE:HB2	2.00	0.43
2:B:841:GLY:HA2	2:B:1073:ARG:HD2	2.00	0.43
2:B:572:PRO:HA	2:B:575:LEU:HD13	2.00	0.43
2:E:1236:THR:OG1	2:E:1608:MET:SD	2.76	0.43
2:E:1972:ASN:HD21	2:E:2024:PRO:HB3	1.83	0.43
2:E:3676:ASP:N	2:E:3676:ASP:OD1	2.50	0.43
2:I:3674:ILE:HD11	2:I:3728:ILE:HG22	1.99	0.43
2:B:1859:VAL:HA	2:B:1862:ILE:HG12	2.00	0.43
2:B:1972:ASN:HD21	2:B:2024:PRO:HB3	1.83	0.43
2:B:4233:LEU:HA	2:B:4236:SER:HB3	1.99	0.43
2:B:866:HIS:O	2:B:1051:TYR:OH	2.31	0.43
2:E:1859:VAL:HA	2:E:1862:ILE:HG12	2.01	0.43
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.40	0.43
2:I:1653:LEU:HB3	2:I:1660:GLN:HB2	2.00	0.43
2:B:1130:GLN:HG2	2:B:1138:PRO:HA	2.01	0.43
2:B:790:ARG:HG2	2:B:1627:ALA:HA	1.99	0.43
2:B:793:LEU:HB2	2:B:797:HIS:H	1.83	0.43
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	2.00	0.43
2:G:1130:GLN:HG2	2:G:1138:PRO:HA	2.01	0.43
2:G:681:HIS:HB3	2:G:784:SER:HB3	2.00	0.43
2:I:4569:LEU:HD11	2:I:4646:LEU:HD22	2.00	0.43
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.49	0.43
1:A:7:ILE:HD13	1:A:71:ARG:HG2	2.01	0.43
1:A:82:TYR:O	1:A:86:GLY:N	2.52	0.43
2:E:2231:SER:HA	2:E:2234:ARG:HG2	2.00	0.43
2:G:119:SER:HA	2:G:146:CYS:HA	1.99	0.43
2:G:1236:THR:OG1	2:G:1608:MET:SD	2.76	0.43
2:G:1859:VAL:HA	2:G:1862:ILE:HG12	2.01	0.43
1:H:82:TYR:O	1:H:86:GLY:N	2.52	0.43
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.52	0.43
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	2.01	0.43
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	2.00	0.43
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	2.01	0.43
2:E:206:CYS:SG	2:E:207:SER:N	2.92	0.43
2:E:4233:LEU:HA	2:E:4236:SER:HB3	2.00	0.43
2:E:793:LEU:HB2	2:E:797:HIS:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	2.00	0.43
2:G:3674:ILE:HD11	2:G:3728:ILE:HG22	1.99	0.43
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	2.01	0.43
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.84	0.43
2:I:1972:ASN:HD21	2:I:2024:PRO:HB3	1.83	0.43
2:B:4978:HIS:CE1	2:B:4982:GLU:HG3	2.53	0.43
2:B:914:PRO:O	2:B:918:ARG:N	2.51	0.43
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	2.00	0.43
2:E:1295:UNK:N	2:E:1454:UNK:O	2.52	0.43
2:E:1653:LEU:HB3	2:E:1660:GLN:HB2	2.00	0.43
2:G:3940:LYS:O	2:G:4002:LYS:NZ	2.49	0.43
2:I:1247:PRO:HA	2:I:1598:GLN:HA	1.99	0.43
2:I:1859:VAL:HA	2:I:1862:ILE:HG12	2.00	0.43
2:E:4083:ASP:HB3	2:E:4086:GLY:H	1.84	0.43
2:E:4569:LEU:HD11	2:E:4646:LEU:HD22	2.00	0.43
2:G:2231:SER:HA	2:G:2234:ARG:HG2	2.00	0.43
2:G:4083:ASP:HB3	2:G:4086:GLY:H	1.84	0.43
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	2.00	0.43
2:G:500:ALA:HB1	2:G:504:ALA:HB2	2.01	0.43
2:I:119:SER:HA	2:I:146:CYS:HA	1.99	0.43
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	2.00	0.43
2:I:907:LEU:O	2:I:963:ASN:ND2	2.42	0.43
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.99	0.43
2:B:681:HIS:HB3	2:B:784:SER:HB3	2.00	0.43
2:E:572:PRO:HA	2:E:575:LEU:HD13	2.00	0.43
2:E:645:ARG:N	2:E:824:GLU:O	2.43	0.43
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.52	0.43
2:G:3804:ILE:O	2:G:3809:ASN:ND2	2.52	0.43
2:I:3676:ASP:OD1	2:I:3676:ASP:N	2.51	0.43
2:I:3804:ILE:O	2:I:3809:ASN:ND2	2.52	0.43
2:I:4083:ASP:HB3	2:I:4086:GLY:H	1.84	0.43
1:J:82:TYR:O	1:J:86:GLY:N	2.52	0.43
2:B:1727:ARG:NH2	2:B:1773:PRO:O	2.50	0.43
2:B:2587:UNK:O	2:B:2591:UNK:N	2.52	0.43
2:B:3804:ILE:O	2:B:3809:ASN:ND2	2.52	0.43
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.84	0.43
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.52	0.43
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	2.01	0.43
2:G:4865:LYS:HG3	2:G:4875:LYS:HZ3	1.84	0.43
1:H:56:ILE:HG13	1:H:59:PHE:H	1.83	0.43
1:H:7:ILE:HD13	1:H:71:ARG:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:206:CYS:SG	2:I:207:SER:N	2.92	0.43
2:I:500:ALA:HB1	2:I:504:ALA:HB2	2.01	0.43
1:J:56:ILE:HG13	1:J:59:PHE:H	1.83	0.43
2:B:1295:UNK:N	2:B:1454:UNK:O	2.52	0.42
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.52	0.42
2:B:206:CYS:SG	2:B:207:SER:N	2.92	0.42
2:B:2810:LYS:O	2:B:2814:LYS:N	2.39	0.42
2:B:719:LEU:HD22	2:B:735:GLN:HG2	2.01	0.42
2:E:134:ASP:OD1	2:E:134:ASP:N	2.50	0.42
2:E:2742:THR:OG1	2:E:2811:GLU:OE1	2.31	0.42
2:E:3674:ILE:HD11	2:E:3728:ILE:HG22	1.99	0.42
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	2.00	0.42
1:F:82:TYR:O	1:F:86:GLY:N	2.52	0.42
2:I:1295:UNK:N	2:I:1454:UNK:O	2.52	0.42
2:I:1236:THR:OG1	2:I:1608:MET:SD	2.76	0.42
2:B:134:ASP:OD1	2:B:134:ASP:N	2.50	0.42
2:B:119:SER:HA	2:B:146:CYS:HA	2.00	0.42
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.84	0.42
2:G:2810:LYS:O	2:G:2814:LYS:N	2.39	0.42
2:G:572:PRO:HA	2:G:575:LEU:HD13	2.00	0.42
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	2.00	0.42
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	2.01	0.42
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	2.02	0.42
2:B:3734:HIS:O	2:B:3738:GLY:N	2.43	0.42
2:B:4083:ASP:HB3	2:B:4086:GLY:H	1.84	0.42
2:B:500:ALA:HB1	2:B:504:ALA:HB2	2.01	0.42
2:B:742:ASP:HA	2:B:760:ASN:HD21	1.84	0.42
2:B:870:ILE:HD12	2:B:873:LYS:HB2	2.01	0.42
2:E:594:GLY:H	2:E:1594:ARG:HD3	1.85	0.42
2:E:719:LEU:HD22	2:E:735:GLN:HG2	2.01	0.42
2:G:870:ILE:HD12	2:G:873:LYS:HB2	2.02	0.42
2:I:675:LEU:HD11	2:I:1633:PRO:HB3	2.02	0.42
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.85	0.42
2:I:2871:LEU:HD22	2:I:2927:LEU:HD22	2.02	0.42
2:I:742:ASP:HA	2:I:760:ASN:HD21	1.84	0.42
1:J:7:ILE:HD13	1:J:71:ARG:HG2	2.01	0.42
2:B:1653:LEU:HB3	2:B:1660:GLN:HB2	2.00	0.42
2:B:2871:LEU:HD22	2:B:2927:LEU:HD22	2.02	0.42
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.50	0.42
2:B:4569:LEU:HD11	2:B:4646:LEU:HD22	2.00	0.42
2:B:880:GLU:OE1	2:B:968:ALA:N	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2871:LEU:HD22	2:E:2927:LEU:HD22	2.01	0.42
2:G:210:GLU:HG3	2:G:337:PRO:HG3	2.02	0.42
2:I:1130:GLN:HG2	2:I:1138:PRO:HA	2.01	0.42
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.55	0.42
2:I:594:GLY:H	2:I:1594:ARG:HD3	1.85	0.42
2:I:621:ILE:O	2:I:625:LEU:N	2.46	0.42
2:I:870:ILE:HD12	2:I:873:LYS:HB2	2.01	0.42
2:B:1675:ALA:HB1	2:B:1676:LEU:HD13	2.02	0.42
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.84	0.42
2:B:2823:ILE:HG12	2:B:2937:VAL:HG22	2.02	0.42
2:B:594:GLY:H	2:B:1594:ARG:HD3	1.85	0.42
2:E:2215:LEU:HD23	2:E:2260:ASN:HB3	2.01	0.42
2:E:3804:ILE:O	2:E:3809:ASN:ND2	2.52	0.42
2:E:649:PHE:HB3	2:E:776:LEU:HD13	2.02	0.42
2:G:1295:UNK:N	2:G:1454:UNK:O	2.52	0.42
2:G:2871:LEU:HD22	2:G:2927:LEU:HD22	2.02	0.42
2:G:3676:ASP:N	2:G:3676:ASP:OD1	2.51	0.42
2:G:4960:ILE:HD11	2:G:4985:LEU:HD23	2.02	0.42
2:B:1236:THR:OG1	2:B:1608:MET:SD	2.76	0.42
2:B:675:LEU:HD11	2:B:1633:PRO:HB3	2.02	0.42
2:E:1130:GLN:HG2	2:E:1138:PRO:HA	2.00	0.42
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.50	0.42
2:E:870:ILE:HD12	2:E:873:LYS:HB2	2.02	0.42
2:G:594:GLY:H	2:G:1594:ARG:HD3	1.85	0.42
2:G:215:THR:HG22	2:G:273:HIS:HA	2.02	0.42
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	2.00	0.42
2:G:742:ASP:HA	2:G:760:ASN:HD21	1.84	0.42
2:I:2479:LEU:O	2:I:2487:UNK:N	2.53	0.42
2:I:4960:ILE:HD11	2:I:4985:LEU:HD23	2.02	0.42
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.55	0.42
2:E:210:GLU:HG3	2:E:337:PRO:HG3	2.02	0.42
2:E:2587:UNK:O	2:E:2591:UNK:N	2.53	0.42
2:E:3663:LEU:H	2:E:3663:LEU:HG	1.72	0.42
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.55	0.42
2:G:2012:PHE:CG	2:G:2022:PRO:HD3	2.55	0.42
2:G:206:CYS:SG	2:G:207:SER:N	2.92	0.42
2:I:2012:PHE:CG	2:I:2022:PRO:HD3	2.55	0.42
2:I:2587:UNK:O	2:I:2591:UNK:N	2.53	0.42
2:B:2215:LEU:HD23	2:B:2260:ASN:HB3	2.01	0.42
2:B:649:PHE:HB3	2:B:776:LEU:HD13	2.02	0.42
2:E:2823:ILE:HG12	2:E:2937:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:500:ALA:HB1	2:E:504:ALA:HB2	2.01	0.42
2:G:3829:PHE:HD1	2:G:3915:ILE:HD11	1.85	0.42
2:I:2823:ILE:HG12	2:I:2937:VAL:HG22	2.02	0.42
2:I:379:HIS:CD2	2:I:381:GLU:H	2.38	0.42
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	2.00	0.42
2:I:4791:TYR:OH	2:I:4815:ASP:OD1	2.32	0.42
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.85	0.42
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	2.02	0.42
1:J:92:PRO:HD3	2:I:627:PRO:HB2	2.02	0.42
2:G:675:LEU:HD11	2:G:1633:PRO:HB3	2.02	0.42
2:G:379:HIS:CD2	2:G:381:GLU:H	2.38	0.42
2:G:689:THR:H	2:G:778:PHE:HE2	1.68	0.42
2:I:4865:LYS:HG3	2:I:4875:LYS:HZ3	1.85	0.42
2:B:215:THR:HG22	2:B:273:HIS:HA	2.02	0.41
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	2.00	0.41
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	2.01	0.41
2:E:3829:PHE:HD1	2:E:3915:ILE:HD11	1.85	0.41
2:E:468:LEU:HB3	2:E:472:ARG:HH12	1.85	0.41
2:E:34:LYS:N	2:E:53:SER:OG	2.44	0.41
2:G:1124:PHE:HB2	2:G:1162:PHE:CE2	2.55	0.41
2:I:689:THR:H	2:I:778:PHE:HE2	1.68	0.41
2:I:719:LEU:HD22	2:I:735:GLN:HG2	2.01	0.41
2:B:3552:UNK:O	2:B:3556:UNK:N	2.54	0.41
2:B:698:GLY:HA2	2:B:703:GLY:HA2	2.02	0.41
2:E:675:LEU:HD11	2:E:1633:PRO:HB3	2.02	0.41
1:F:7:ILE:HD13	1:F:71:ARG:HG2	2.01	0.41
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	2.01	0.41
2:I:1675:ALA:HB1	2:I:1676:LEU:HD13	2.02	0.41
2:I:210:GLU:HG3	2:I:337:PRO:HG3	2.02	0.41
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.84	0.41
2:I:4184:MET:HE1	2:I:4188:ARG:HE	1.85	0.41
2:B:164:ARG:N	2:B:167:ASP:OD2	2.46	0.41
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	2.01	0.41
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	2.01	0.41
2:E:983:THR:O	2:E:987:ARG:N	2.49	0.41
2:G:1161:ILE:HA	2:G:1177:THR:HB	2.02	0.41
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	2.02	0.41
2:G:2420:HIS:HB2	2:G:2492:UNK:C	2.50	0.41
2:G:2587:UNK:O	2:G:2591:UNK:N	2.52	0.41
2:G:4569:LEU:HD11	2:G:4646:LEU:HD22	2.00	0.41
2:G:983:THR:O	2:G:987:ARG:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.50	0.41
2:I:215:THR:HG22	2:I:273:HIS:HA	2.02	0.41
2:I:2196:ASN:OD1	2:I:2199:ARG:NH1	2.40	0.41
2:I:3552:UNK:O	2:I:3556:UNK:N	2.54	0.41
2:I:892:THR:N	2:I:902:ARG:O	2.49	0.41
2:B:1708:ARG:HG2	2:B:1711:TYR:CE2	2.55	0.41
2:B:4763:GLY:O	2:B:4766:THR:OG1	2.28	0.41
2:B:34:LYS:N	2:B:53:SER:OG	2.44	0.41
2:E:215:THR:HG22	2:E:273:HIS:HA	2.02	0.41
2:E:4960:ILE:HD11	2:E:4985:LEU:HD23	2.02	0.41
2:E:742:ASP:HA	2:E:760:ASN:HD21	1.84	0.41
2:G:359:TYR:OH	2:G:385:ASP:OD2	2.32	0.41
2:G:468:LEU:HB3	2:G:472:ARG:HH12	1.85	0.41
2:I:278:GLN:N	2:I:315:CYS:SG	2.94	0.41
2:I:321:GLU:HB3	2:I:322:LYS:H	1.75	0.41
2:B:4982:GLU:HB3	2:B:4983:HIS:H	1.63	0.41
2:E:1708:ARG:HG2	2:E:1711:TYR:CE2	2.55	0.41
2:E:3552:UNK:O	2:E:3556:UNK:N	2.54	0.41
2:E:3959:LYS:O	2:E:3963:ASN:ND2	2.53	0.41
2:G:1708:ARG:HG2	2:G:1711:TYR:CE2	2.55	0.41
2:G:3959:LYS:O	2:G:3963:ASN:ND2	2.53	0.41
2:B:4823:LEU:HD23	2:I:4843:LEU:HD12	2.02	0.41
2:I:495:ASN:HD21	2:I:550:LYS:HG3	1.86	0.41
2:B:1092:PHE:N	2:B:1149:VAL:O	2.41	0.41
2:B:2012:PHE:CG	2:B:2022:PRO:HD3	2.55	0.41
2:B:379:HIS:CD2	2:B:381:GLU:H	2.38	0.41
2:E:698:GLY:HA2	2:E:703:GLY:HA2	2.02	0.41
2:G:1078:GLU:HB3	2:G:1081:TYR:HD2	1.86	0.41
2:G:1675:ALA:HB1	2:G:1676:LEU:HD13	2.02	0.41
2:G:2823:ILE:HG12	2:G:2937:VAL:HG22	2.02	0.41
2:G:649:PHE:HB3	2:G:776:LEU:HD13	2.02	0.41
2:G:4843:LEU:HD12	2:I:4823:LEU:HD23	2.03	0.41
2:B:468:LEU:HB3	2:B:472:ARG:HH12	1.85	0.41
2:G:4848:VAL:O	2:G:4852:THR:OG1	2.29	0.41
2:G:698:GLY:HA2	2:G:703:GLY:HA2	2.02	0.41
2:G:924:MET:O	2:G:928:THR:OG1	2.30	0.41
2:I:1101:ARG:HH21	2:I:1115:LEU:HB3	1.86	0.41
2:I:1708:ARG:HG2	2:I:1711:TYR:CE2	2.55	0.41
2:I:2215:LEU:HD23	2:I:2260:ASN:HB3	2.01	0.41
2:I:698:GLY:HA2	2:I:703:GLY:HA2	2.02	0.41
2:I:983:THR:O	2:I:987:ARG:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1124:PHE:HB2	2:E:1162:PHE:CE2	2.55	0.41
2:E:1161:ILE:HA	2:E:1177:THR:HB	2.02	0.41
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.55	0.41
2:E:2285:GLU:HG3	2:E:2286:LEU:HG	2.03	0.41
2:G:4823:LEU:HD23	2:E:4843:LEU:HD12	2.03	0.41
2:E:756:SER:HB3	2:E:767:VAL:HG22	2.03	0.41
2:G:1101:ARG:HH21	2:G:1115:LEU:HB3	1.86	0.41
2:G:2215:LEU:HD23	2:G:2260:ASN:HB3	2.01	0.41
2:G:495:ASN:HD21	2:G:550:LYS:HG3	1.86	0.41
2:I:1124:PHE:HB2	2:I:1162:PHE:CE2	2.55	0.41
2:I:3829:PHE:HD1	2:I:3915:ILE:HD11	1.85	0.41
2:B:2196:ASN:OD1	2:B:2199:ARG:NH1	2.40	0.41
2:B:278:GLN:N	2:B:315:CYS:SG	2.94	0.41
2:B:3829:PHE:HD1	2:B:3915:ILE:HD11	1.85	0.41
2:E:2012:PHE:CG	2:E:2022:PRO:HD3	2.55	0.41
2:E:379:HIS:CD2	2:E:381:GLU:H	2.38	0.41
2:G:180:LEU:O	2:G:200:TRP:NE1	2.41	0.41
2:G:3552:UNK:O	2:G:3556:UNK:N	2.54	0.41
2:I:756:SER:HB3	2:I:767:VAL:HG22	2.03	0.41
2:B:210:GLU:HG3	2:B:337:PRO:HG3	2.02	0.41
2:E:1735:ILE:HG23	2:E:1771:LEU:HD23	2.03	0.41
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	2.03	0.41
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.84	0.41
2:E:4239:GLU:OE2	2:E:5014:TYR:OH	2.36	0.41
2:G:2869:ARG:NH1	2:G:2945:UNK:O	2.53	0.41
2:G:719:LEU:HD22	2:G:735:GLN:HG2	2.01	0.41
2:G:756:SER:HB3	2:G:767:VAL:HG22	2.03	0.41
2:I:1161:ILE:HA	2:I:1177:THR:HB	2.02	0.41
2:I:649:PHE:HB3	2:I:776:LEU:HD13	2.02	0.41
2:B:1101:ARG:HH21	2:B:1115:LEU:HB3	1.86	0.41
2:B:1161:ILE:HA	2:B:1177:THR:HB	2.02	0.41
2:B:2430:ILE:HG21	2:B:2502:UNK:HA	2.02	0.41
2:B:2927:LEU:HA	2:B:2930:LEU:HD12	2.03	0.41
2:E:1675:ALA:HB1	2:E:1676:LEU:HD13	2.02	0.41
2:E:21:VAL:HG22	2:E:203:ASN:HB2	2.03	0.41
2:G:2144:ILE:H	2:G:2144:ILE:HG13	1.81	0.41
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	2.03	0.41
2:I:2758:PHE:O	2:I:2762:THR:N	2.47	0.41
2:I:468:LEU:HB3	2:I:472:ARG:HH12	1.85	0.41
2:B:707:VAL:HG23	2:B:713:SER:HB2	2.03	0.40
2:B:645:ARG:N	2:B:824:GLU:O	2.43	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.54	0.40
2:B:1735:ILE:HG23	2:B:1771:LEU:HD23	2.03	0.40
2:B:2144:ILE:HG13	2:B:2144:ILE:H	1.81	0.40
2:B:495:ASN:HD21	2:B:550:LYS:HG3	1.86	0.40
2:E:1101:ARG:HH21	2:E:1115:LEU:HB3	1.86	0.40
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.54	0.40
2:G:4191:GLU:OE1	2:G:5006:GLN:NE2	2.54	0.40
1:H:92:PRO:HD3	2:G:627:PRO:HB2	2.02	0.40
2:G:707:VAL:HG23	2:G:713:SER:HB2	2.03	0.40
2:I:1078:GLU:HB3	2:I:1081:TYR:HD2	1.86	0.40
2:I:3959:LYS:O	2:I:3963:ASN:ND2	2.53	0.40
2:I:4242:ILE:O	2:I:4246:GLN:N	2.54	0.40
2:I:4928:LEU:HD13	2:I:4928:LEU:HA	1.92	0.40
2:B:21:VAL:HG22	2:B:203:ASN:HB2	2.03	0.40
2:B:2291:GLN:HE21	2:B:2294:ASP:H	1.70	0.40
2:B:3959:LYS:O	2:B:3963:ASN:ND2	2.53	0.40
2:B:4913:ARG:O	2:B:4917:ASP:N	2.48	0.40
1:F:87:HIS:HA	1:F:88:PRO:HD3	1.90	0.40
2:G:164:ARG:N	2:G:167:ASP:OD2	2.46	0.40
2:G:278:GLN:N	2:G:315:CYS:SG	2.94	0.40
2:I:4191:GLU:OE1	2:I:5006:GLN:NE2	2.54	0.40
2:B:1078:GLU:HB3	2:B:1081:TYR:HD2	1.86	0.40
2:B:2674:UNK:O	2:B:2676:UNK:N	2.55	0.40
2:E:2144:ILE:HG13	2:E:2144:ILE:H	1.80	0.40
2:E:4865:LYS:HG3	2:E:4875:LYS:HZ3	1.86	0.40
2:E:689:THR:H	2:E:778:PHE:HE2	1.68	0.40
2:G:489:ASN:HA	2:G:492:ASP:HB2	2.03	0.40
1:H:87:HIS:HA	1:H:88:PRO:HD3	1.90	0.40
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	2.03	0.40
2:B:4191:GLU:OE1	2:B:5006:GLN:NE2	2.54	0.40
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.87	0.40
2:B:4821:LYS:HE2	2:B:4821:LYS:HB3	1.95	0.40
2:B:689:THR:H	2:B:778:PHE:HE2	1.68	0.40
2:B:870:ILE:HD12	2:B:870:ILE:HA	1.98	0.40
2:E:2810:LYS:O	2:E:2814:LYS:N	2.39	0.40
2:G:3662:ILE:HG13	2:G:3662:ILE:H	1.78	0.40
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.54	0.40
2:I:395:GLN:NE2	2:I:397:GLU:OE1	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%)	2894 (90%)	333 (10%)	8 (0%)	52	86
2	E	3235/4416 (73%)	2898 (90%)	332 (10%)	5 (0%)	52	86
2	G	3235/4416 (73%)	2896 (90%)	334 (10%)	5 (0%)	52	86
2	I	3235/4416 (73%)	2898 (90%)	332 (10%)	5 (0%)	52	86
All	All	13360/18096 (74%)	11962 (90%)	1375 (10%)	23 (0%)	56	86

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	4962	GLY
2	B	1708	ARG
2	G	1708	ARG
2	I	1708	ARG
2	E	1708	ARG
2	B	1932	PRO
2	B	4982	GLU
2	B	4985	LEU
2	G	1932	PRO
2	I	1932	PRO
2	E	1932	PRO
2	B	1840	PRO
2	B	4641	PRO
2	G	1840	PRO
2	G	4641	PRO
2	I	1840	PRO
2	I	4641	PRO

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Mol	Chain	Res	Type
2	E	1840	PRO
2	E	4641	PRO
2	B	2291	GLN
2	G	2291	GLN
2	I	2291	GLN
2	E	2291	GLN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	88/89 (99%)	88 (100%)	0	100 100
1	F	88/89 (99%)	88 (100%)	0	100 100
1	H	88/89 (99%)	88 (100%)	0	100 100
1	J	88/89 (99%)	88 (100%)	0	100 100
2	B	2493/3022 (82%)	2473 (99%)	20 (1%)	86 93
2	E	2493/3022 (82%)	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%)	10253 (99%)	71 (1%)	89 94

All (71) 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	719	LEU
2	B	1076	ARG
2	B	1141	ARG
2	B	1600	LEU
2	B	1676	LEU
2	B	1964	ARG

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Mol	Chain	Res	Type
2	B	3663	LEU
2	B	3787	LYS
2	B	3805	LEU
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4131	ARG
2	B	4958	CYS
2	B	4960	ILE
2	B	4983	HIS
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	719	LEU
2	G	1076	ARG
2	G	1141	ARG
2	G	1600	LEU
2	G	1676	LEU
2	G	1964	ARG
2	G	3663	LEU
2	G	3787	LYS
2	G	3805	LEU
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4131	ARG
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	719	LEU
2	I	1076	ARG
2	I	1141	ARG
2	I	1600	LEU
2	I	1676	LEU
2	I	1964	ARG
2	I	3663	LEU
2	I	3787	LYS
2	I	3805	LEU
2	I	3896	ASN
2	I	4034	ASN

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Mol	Chain	Res	Type
2	I	4085	ARG
2	I	4120	ASN
2	I	4131	ARG
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
2	E	719	LEU
2	E	1076	ARG
2	E	1141	ARG
2	E	1600	LEU
2	E	1676	LEU
2	E	1964	ARG
2	E	3663	LEU
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (153) 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	71	GLN
2	B	105	HIS
2	B	111	HIS
2	B	113	HIS
2	B	379	HIS
2	B	395	GLN
2	B	413	GLN
2	B	479	GLN
2	B	797	HIS
2	B	838	HIS
2	B	1041	GLN
2	B	1598	GLN
2	B	1660	GLN

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Mol	Chain	Res	Type
2	B	1679	ASN
2	B	1688	HIS
2	B	1691	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	1972	ASN
2	B	2005	GLN
2	B	2127	GLN
2	B	2291	GLN
2	B	2324	ASN
2	B	3809	ASN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN
2	B	3963	ASN
2	B	3976	ASN
2	B	3994	HIS
2	B	4054	ASN
2	B	4120	ASN
2	B	4806	ASN
2	B	4978	HIS
2	B	4983	HIS
2	G	57	ASN
2	G	71	GLN
2	G	105	HIS
2	G	111	HIS
2	G	113	HIS
2	G	273	HIS
2	G	379	HIS
2	G	395	GLN
2	G	413	GLN
2	G	479	GLN
2	G	797	HIS
2	G	838	HIS
2	G	1041	GLN
2	G	1598	GLN
2	G	1660	GLN
2	G	1679	ASN
2	G	1688	HIS
2	G	1691	GLN
2	G	1719	HIS

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Mol	Chain	Res	Type
2	G	1775	HIS
2	G	1972	ASN
2	G	2005	GLN
2	G	2127	GLN
2	G	2291	GLN
2	G	2324	ASN
2	G	3809	ASN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	3963	ASN
2	G	3976	ASN
2	G	3994	HIS
2	G	4054	ASN
2	G	4120	ASN
2	G	4806	ASN
2	G	4983	HIS
2	I	57	ASN
2	I	71	GLN
2	I	105	HIS
2	I	111	HIS
2	I	113	HIS
2	I	273	HIS
2	I	379	HIS
2	I	395	GLN
2	I	413	GLN
2	I	479	GLN
2	I	797	HIS
2	I	838	HIS
2	I	1041	GLN
2	I	1598	GLN
2	I	1660	GLN
2	I	1679	ASN
2	I	1688	HIS
2	I	1691	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	1972	ASN
2	I	2005	GLN
2	I	2127	GLN
2	I	2291	GLN

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Mol	Chain	Res	Type
2	I	2324	ASN
2	I	3809	ASN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	3963	ASN
2	I	3976	ASN
2	I	3994	HIS
2	I	4054	ASN
2	I	4120	ASN
2	I	4806	ASN
2	I	4946	GLN
2	I	4983	HIS
2	E	57	ASN
2	E	71	GLN
2	E	105	HIS
2	E	111	HIS
2	E	113	HIS
2	E	379	HIS
2	E	395	GLN
2	E	413	GLN
2	E	479	GLN
2	E	797	HIS
2	E	838	HIS
2	E	1041	GLN
2	E	1598	GLN
2	E	1660	GLN
2	E	1679	ASN
2	E	1688	HIS
2	E	1691	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	1972	ASN
2	E	2005	GLN
2	E	2127	GLN
2	E	2291	GLN
2	E	2324	ASN
2	E	3809	ASN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN

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Mol	Chain	Res	Type
2	E	3960	GLN
2	E	3963	ASN
2	E	3976	ASN
2	E	3994	HIS
2	E	4054	ASN
2	E	4120	ASN
2	E	4806	ASN
2	E	4833	ASN
2	E	4983	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 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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	G	4345:UNK	C	4540:PHE	N	73.65
1	B	4345:UNK	C	4540:PHE	N	73.61
1	I	4345:UNK	C	4540:PHE	N	73.61
1	E	4345:UNK	C	4540:PHE	N	73.59
1	G	3613:UNK	C	3639:THR	N	45.21
1	B	3613:UNK	C	3639:THR	N	45.16
1	E	3613:UNK	C	3639:THR	N	45.11
1	I	3613:UNK	C	3639:THR	N	45.10
1	G	4253:GLU	C	4320:UNK	N	28.96
1	I	4253:GLU	C	4320:UNK	N	28.94
1	B	4253:GLU	C	4320:UNK	N	28.93
1	E	4253:GLU	C	4320:UNK	N	28.92
1	B	3163:UNK	C	3170:UNK	N	16.13
1	G	3163:UNK	C	3170:UNK	N	16.13
1	I	3163:UNK	C	3170:UNK	N	16.13
1	E	3163:UNK	C	3170:UNK	N	16.13
1	I	3063:UNK	C	3134:UNK	N	14.80
1	E	3063:UNK	C	3134:UNK	N	14.80
1	B	3063:UNK	C	3134:UNK	N	14.79
1	G	3063:UNK	C	3134:UNK	N	14.79
1	G	3468:UNK	C	3511:UNK	N	14.32
1	B	3468:UNK	C	3511:UNK	N	14.31
1	E	3468:UNK	C	3511:UNK	N	14.31
1	I	3468:UNK	C	3511:UNK	N	14.30
1	I	2703:UNK	C	2734:ASN	N	13.53
1	E	2703:UNK	C	2734:ASN	N	13.51
1	B	2703:UNK	C	2734:ASN	N	13.49
1	G	2703:UNK	C	2734:ASN	N	13.47
1	I	3236:UNK	C	3241:UNK	N	12.90
1	E	3236:UNK	C	3241:UNK	N	12.90
1	B	3236:UNK	C	3241:UNK	N	12.89
1	G	3236:UNK	C	3241:UNK	N	12.89

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	2976:UNK	C	2995:UNK	N	12.39
1	I	2976:UNK	C	2995:UNK	N	12.39
1	E	2976:UNK	C	2995:UNK	N	12.39
1	G	2976:UNK	C	2995:UNK	N	12.38
1	E	1564:UNK	C	1573:MET	N	12.31
1	I	1564:UNK	C	1573:MET	N	12.30
1	B	1564:UNK	C	1573:MET	N	12.29
1	G	1564:UNK	C	1573:MET	N	12.23
1	B	3254:UNK	C	3261:UNK	N	8.56
1	G	3254:UNK	C	3261:UNK	N	8.56
1	I	3254:UNK	C	3261:UNK	N	8.56
1	E	3254:UNK	C	3261:UNK	N	8.56
1	B	1297:UNK	C	1430:UNK	N	5.76
1	G	1297:UNK	C	1430:UNK	N	5.76
1	I	1297:UNK	C	1430:UNK	N	5.75
1	E	1297:UNK	C	1430:UNK	N	5.75
1	G	2479:LEU	C	2487:UNK	N	3.50
1	B	2479:LEU	C	2487:UNK	N	3.44
1	E	2479:LEU	C	2487:UNK	N	3.38
1	I	2479:LEU	C	2487:UNK	N	3.34
1	I	2939:ARG	C	2942:UNK	N	3.22
1	E	2939:ARG	C	2942:UNK	N	3.21
1	B	2939:ARG	C	2942:UNK	N	3.20
1	G	2939:ARG	C	2942:UNK	N	3.20