



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 01:12 pm GMT

PDB ID : 5T9V
EMDB ID: : EMD-8376
Title : Structure of rabbit RyR1 (Caffeine/ATP/Ca²⁺ dataset, class 1)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-09
Resolution : 4.40 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

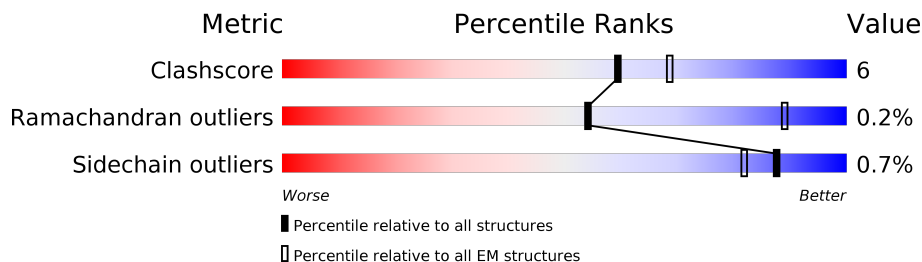
1 Overall quality at a glance

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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	108	81% 18% .
1	F	108	81% 18% .
1	H	108	81% 18% .
1	J	108	81% 19% .
2	B	4416	83% 12% 5%
2	E	4416	83% 11% 5%
2	G	4416	83% 11% 5%
2	I	4416	83% 12% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 121456 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called Ryanodine receptor 1.

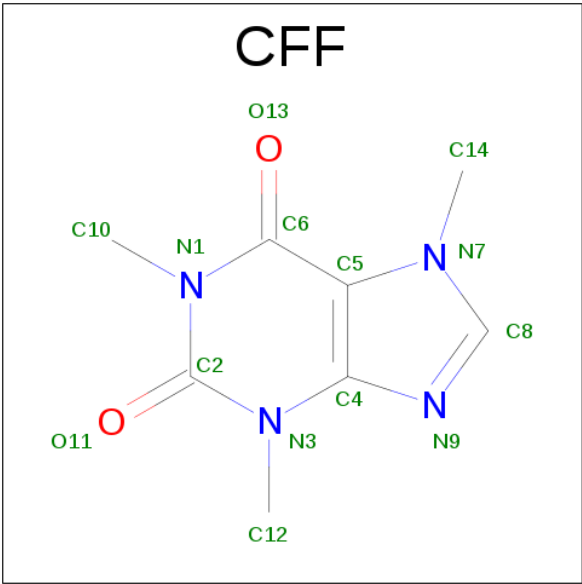
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

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



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

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



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

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

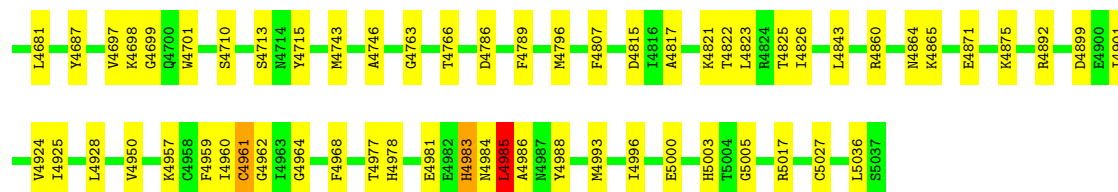
Mol	Chain	Residues	Atoms		AltConf
5	G	1	Total	Zn	0
			1	1	
5	B	1	Total	Zn	0
			1	1	
5	I	1	Total	Zn	0
			1	1	
5	E	1	Total	Zn	0
			1	1	

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

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

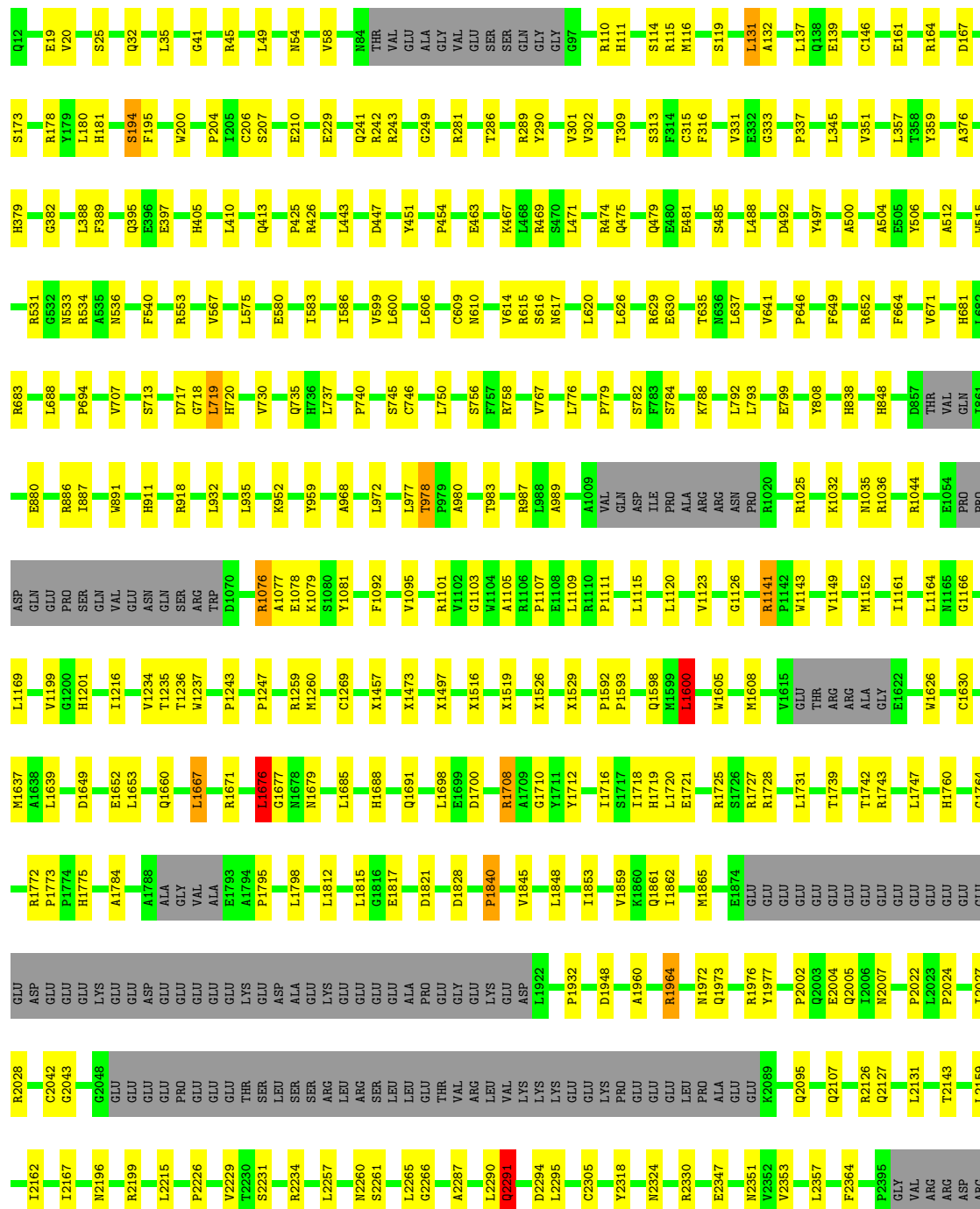

WORLDWIDE PDB
 PROTEIN DATA BANK

EMDataBank
 Unified Data Resource for 3DEM



• Molecule 2: Ryanodine receptor 1

Chain G: 83% 11% 5%











4 Experimental information

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 ($e^-/\text{\AA}^2$)	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	0.53	0/1123
1	F	0.31	0/834	0.53	0/1123
1	H	0.31	0/834	0.53	0/1123
1	J	0.31	0/834	0.53	0/1123
2	B	0.30	0/25428	0.54	10/34534 (0.0%)
2	E	0.30	0/25428	0.54	10/34534 (0.0%)
2	G	0.30	0/25428	0.54	10/34534 (0.0%)
2	I	0.30	0/25428	0.54	10/34534 (0.0%)
All	All	0.30	0/105048	0.54	40/142628 (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 (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	131	LEU	CA-CB-CG	7.69	132.98	115.30
2	B	131	LEU	CA-CB-CG	7.67	132.95	115.30
2	E	131	LEU	CA-CB-CG	7.67	132.93	115.30
2	G	131	LEU	CA-CB-CG	7.65	132.90	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	4985	LEU	CA-CB-CG	6.48	130.20	115.30
2	B	4985	LEU	CA-CB-CG	6.47	130.19	115.30
2	G	4985	LEU	CA-CB-CG	6.46	130.16	115.30
2	E	4985	LEU	CA-CB-CG	6.46	130.16	115.30
2	I	1676	LEU	CA-CB-CG	6.45	130.14	115.30
2	B	1676	LEU	CA-CB-CG	6.45	130.14	115.30
2	E	1676	LEU	CA-CB-CG	6.45	130.12	115.30
2	G	1676	LEU	CA-CB-CG	6.44	130.12	115.30
2	G	1600	LEU	CA-CB-CG	6.37	129.95	115.30
2	B	1600	LEU	CA-CB-CG	6.37	129.94	115.30
2	I	1600	LEU	CA-CB-CG	6.37	129.94	115.30
2	E	1600	LEU	CA-CB-CG	6.35	129.91	115.30
2	G	4901	ILE	CG1-CB-CG2	-6.05	98.08	111.40
2	B	4901	ILE	CG1-CB-CG2	-6.05	98.08	111.40
2	I	4901	ILE	CG1-CB-CG2	-6.05	98.09	111.40
2	E	4901	ILE	CG1-CB-CG2	-6.05	98.10	111.40
2	G	977	LEU	CA-CB-CG	5.51	127.97	115.30
2	E	977	LEU	CA-CB-CG	5.50	127.95	115.30
2	B	977	LEU	CA-CB-CG	5.50	127.94	115.30
2	I	977	LEU	CA-CB-CG	5.49	127.93	115.30
2	G	719	LEU	CA-CB-CG	5.26	127.40	115.30
2	I	719	LEU	CA-CB-CG	5.25	127.39	115.30
2	B	719	LEU	CA-CB-CG	5.25	127.38	115.30
2	E	719	LEU	CA-CB-CG	5.24	127.35	115.30
2	I	4639	MET	C-N-CA	5.15	134.57	121.70
2	B	4639	MET	C-N-CA	5.15	134.57	121.70
2	E	4639	MET	C-N-CA	5.15	134.57	121.70
2	G	4639	MET	C-N-CA	5.13	134.52	121.70
2	G	1667	LEU	CA-CB-CG	5.09	127.01	115.30
2	B	1667	LEU	CA-CB-CG	5.08	126.99	115.30
2	E	1667	LEU	CA-CB-CG	5.08	126.98	115.30
2	I	688	LEU	CA-CB-CG	5.07	126.97	115.30
2	I	1667	LEU	CA-CB-CG	5.07	126.96	115.30
2	E	688	LEU	CA-CB-CG	5.06	126.94	115.30
2	B	688	LEU	CA-CB-CG	5.06	126.93	115.30
2	G	688	LEU	CA-CB-CG	5.05	126.93	115.30

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	B	1676	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	1840	PRO	Peptide
2	B	194	SER	Peptide
2	B	2291	GLN	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	3971	GLY	Peptide
2	B	4641	PRO	Peptide
2	B	4807	PHE	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	1840	PRO	Peptide
2	E	194	SER	Peptide
2	E	2291	GLN	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	3971	GLY	Peptide
2	E	4641	PRO	Peptide
2	E	4807	PHE	Peptide
2	E	694	PRO	Peptide
2	E	808	TYR	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	1840	PRO	Peptide
2	G	194	SER	Peptide
2	G	2291	GLN	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	3971	GLY	Peptide
2	G	4641	PRO	Peptide
2	G	4807	PHE	Peptide
2	G	694	PRO	Peptide
2	G	808	TYR	Peptide
2	I	139	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	I	1676	LEU	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	1840	PRO	Peptide
2	I	194	SER	Peptide
2	I	2291	GLN	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	3971	GLY	Peptide
2	I	4641	PRO	Peptide
2	I	4807	PHE	Peptide
2	I	694	PRO	Peptide
2	I	808	TYR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	13	0
1	F	818	0	824	13	0
1	H	818	0	824	12	0
1	J	818	0	824	15	0
2	B	29499	0	24748	311	0
2	E	29499	0	24748	298	0
2	G	29499	0	24748	300	0
2	I	29499	0	24748	305	0
3	B	31	0	12	1	0
3	E	31	0	12	1	0
3	G	31	0	12	1	0
3	I	31	0	12	1	0
4	B	14	0	10	0	0
4	E	14	0	10	0	0
4	G	14	0	10	0	0
4	I	14	0	10	0	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	102376	1234	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 6.

All (1234) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4968:PHE:CE2	2:E:4978:HIS:CE1	2.64	0.86
2:I:4968:PHE:CE2	2:I:4978:HIS:CE1	2.64	0.86
2:B:4968:PHE:CE2	2:B:4978:HIS:CE1	2.64	0.85
2:G:4968:PHE:CE2	2:G:4978:HIS:CE1	2.64	0.85
2:I:2318:TYR:HH	2:I:2414:ASN:N	1.81	0.78
2:G:2318:TYR:HH	2:G:2414:ASN:N	1.82	0.78
2:G:4968:PHE:HE2	2:G:4978:HIS:CE1	2.02	0.78
2:B:2318:TYR:HH	2:B:2414:ASN:N	1.83	0.77
2:E:4968:PHE:HE2	2:E:4978:HIS:CE1	2.02	0.77
2:E:2318:TYR:HH	2:E:2414:ASN:N	1.82	0.77
2:B:4968:PHE:HE2	2:B:4978:HIS:CE1	2.02	0.77
2:I:4968:PHE:HE2	2:I:4978:HIS:CE1	2.02	0.76
2:G:4985:LEU:HB2	3:G:5101:ATP:HN61	1.51	0.75
2:I:4985:LEU:HB2	3:I:5101:ATP:HN61	1.51	0.75
2:E:4985:LEU:HB2	3:E:5101:ATP:HN61	1.51	0.75
2:B:4985:LEU:HB2	3:B:5101:ATP:HN61	1.51	0.74
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.72	0.72
2:E:4957:LYS:HG2	2:E:4964:GLY:HA2	1.72	0.71
2:G:4957:LYS:HG2	2:G:4964:GLY:HA2	1.73	0.71
2:I:4957:LYS:HG2	2:I:4964:GLY:HA2	1.72	0.71
2:B:4957:LYS:HG2	2:B:4964:GLY:HA2	1.73	0.69
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.76	0.68
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.76	0.68
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.76	0.67
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.76	0.67
2:B:2266:GLY:O	2:B:2330:ARG:NH2	2.28	0.67
2:E:379:HIS:HD2	2:E:382:GLY:H	1.43	0.66
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.60	0.66
2:I:2266:GLY:O	2:I:2330:ARG:NH2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2266:GLY:O	2:E:2330:ARG:NH2	2.28	0.66
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.60	0.66
2:G:2266:GLY:O	2:G:2330:ARG:NH2	2.28	0.65
2:B:379:HIS:HD2	2:B:382:GLY:H	1.43	0.65
2:B:4823:LEU:HD23	2:I:4843:LEU:HD12	1.79	0.65
2:G:379:HIS:HD2	2:G:382:GLY:H	1.43	0.65
2:G:4860:ARG:HD2	2:I:4582:VAL:HG11	1.79	0.65
2:B:4983:HIS:H	2:B:4983:HIS:CD2	2.16	0.64
2:E:4983:HIS:H	2:E:4983:HIS:CD2	2.16	0.64
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.61	0.64
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.80	0.63
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.81	0.63
2:G:4983:HIS:H	2:G:4983:HIS:CD2	2.16	0.63
2:I:379:HIS:HD2	2:I:382:GLY:H	1.43	0.63
2:B:4843:LEU:HD12	2:E:4823:LEU:HD23	1.80	0.63
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.81	0.63
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.80	0.63
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.81	0.63
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.81	0.63
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.60	0.63
2:I:4983:HIS:H	2:I:4983:HIS:CD2	2.16	0.62
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.82	0.62
2:B:3762:ARG:O	2:B:3766:GLN:NE2	2.33	0.62
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.82	0.62
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.82	0.62
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.33	0.62
2:E:132:ALA:HA	2:E:194:SER:HB2	1.82	0.62
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.81	0.62
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.33	0.62
2:G:626:LEU:HD23	2:G:630:GLU:H	1.65	0.61
2:I:626:LEU:HD23	2:I:630:GLU:H	1.65	0.61
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.82	0.61
2:E:626:LEU:HD23	2:E:630:GLU:H	1.65	0.61
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.82	0.61
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.82	0.61
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.82	0.61
2:B:132:ALA:HA	2:B:194:SER:HB2	1.82	0.61
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.33	0.61
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.81	0.61
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.82	0.61
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:132:ALA:HA	2:I:194:SER:HB2	1.82	0.61
2:E:111:HIS:HD2	2:E:114:SER:H	1.48	0.61
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.33	0.61
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.82	0.61
2:B:626:LEU:HD23	2:B:630:GLU:H	1.65	0.61
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.82	0.61
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.82	0.61
2:E:3762:ARG:O	2:E:3766:GLN:NE2	2.33	0.61
2:G:111:HIS:HD2	2:G:114:SER:H	1.48	0.61
2:I:4978:HIS:CE1	2:I:5027:CYS:SG	2.94	0.61
2:B:4978:HIS:CE1	2:B:5027:CYS:SG	2.94	0.61
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.82	0.61
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.34	0.61
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.34	0.61
2:E:4978:HIS:CE1	2:E:5027:CYS:SG	2.94	0.60
2:G:132:ALA:HA	2:G:194:SER:HB2	1.82	0.60
2:G:4978:HIS:CE1	2:G:5027:CYS:SG	2.94	0.60
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.83	0.60
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.82	0.60
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.82	0.60
2:B:111:HIS:HD2	2:B:114:SER:H	1.48	0.60
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.82	0.60
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.67	0.60
2:B:2452:ARG:HH12	2:I:177:GLU:HG3	1.66	0.60
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.83	0.60
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.82	0.60
2:B:609:CYS:SG	2:B:610:ASN:N	2.75	0.60
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.34	0.60
2:E:609:CYS:SG	2:E:610:ASN:N	2.75	0.60
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.67	0.60
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.67	0.60
2:E:1731:LEU:HA	2:E:1772:ARG:HH12	1.67	0.60
2:B:1731:LEU:HA	2:B:1772:ARG:HH12	1.67	0.60
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.83	0.60
2:I:1731:LEU:HA	2:I:1772:ARG:HH12	1.67	0.60
2:I:359:TYR:HA	2:I:376:ALA:HA	1.84	0.60
2:G:1731:LEU:HA	2:G:1772:ARG:HH12	1.67	0.59
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.83	0.59
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.84	0.59
1:F:34:LYS:HD3	2:E:629:ARG:HD2	1.85	0.59
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.34	0.59
2:B:359:TYR:HA	2:B:376:ALA:HA	1.84	0.59
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.84	0.59
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.36	0.59
2:G:609:CYS:SG	2:G:610:ASN:N	2.75	0.59
2:E:3733:CYS:HA	2:E:3766:GLN:HG2	1.85	0.59
2:G:4823:LEU:HD23	2:E:4843:LEU:HD12	1.85	0.59
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.85	0.59
2:G:359:TYR:HA	2:G:376:ALA:HA	1.84	0.59
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.67	0.59
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.84	0.59
2:G:3762:ARG:O	2:G:3766:GLN:NE2	2.33	0.59
2:I:3762:ARG:O	2:I:3766:GLN:NE2	2.33	0.59
2:I:609:CYS:SG	2:I:610:ASN:N	2.75	0.59
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.85	0.59
2:B:4957:LYS:HG2	2:B:4964:GLY:CA	2.33	0.59
2:G:4960:ILE:HD11	2:G:4985:LEU:HD23	1.84	0.59
2:I:111:HIS:HD2	2:I:114:SER:H	1.49	0.59
2:I:4960:ILE:HD11	2:I:4985:LEU:HD23	1.84	0.59
2:B:4960:ILE:HD11	2:B:4985:LEU:HD23	1.84	0.58
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.34	0.58
2:E:641:VAL:HG11	2:E:681:HIS:HD1	1.68	0.58
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.36	0.58
2:I:3981:ALA:HA	2:I:3986:TRP:HE1	1.67	0.58
2:E:359:TYR:HA	2:E:376:ALA:HA	1.84	0.58
2:G:4582:VAL:HG11	2:E:4860:ARG:HD2	1.85	0.58
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.36	0.58
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.36	0.58
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.37	0.58
2:E:3981:ALA:HA	2:E:3986:TRP:HE1	1.67	0.58
2:E:4977:THR:HG23	2:E:4981:GLU:HG3	1.85	0.58
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.36	0.58
2:G:3981:ALA:HA	2:G:3986:TRP:HE1	1.67	0.58
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.85	0.58
2:E:4957:LYS:HG2	2:E:4964:GLY:CA	2.33	0.58
2:G:4977:THR:HG23	2:G:4981:GLU:HG3	1.85	0.58
2:I:313:SER:HB3	2:I:351:VAL:HB	1.86	0.58
2:I:3733:CYS:HA	2:I:3766:GLN:HG2	1.85	0.58
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.85	0.58
2:B:4977:THR:HG23	2:B:4981:GLU:HG3	1.85	0.58
2:B:35:LEU:HD13	2:B:49:LEU:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.86	0.58
2:E:313:SER:HB3	2:E:351:VAL:HB	1.86	0.58
2:E:4960:ILE:HD11	2:E:4985:LEU:HD23	1.84	0.58
2:G:3733:CYS:HA	2:G:3766:GLN:HG2	1.85	0.58
2:G:4924:VAL:HA	2:G:4928:LEU:HB2	1.86	0.58
2:G:35:LEU:HD13	2:G:49:LEU:HD13	1.85	0.58
2:B:3981:ALA:HA	2:B:3986:TRP:HE1	1.67	0.57
2:B:641:VAL:HG11	2:B:681:HIS:HD1	1.68	0.57
2:E:35:LEU:HD13	2:E:49:LEU:HD13	1.85	0.57
2:G:2287:ALA:HA	2:G:2290:LEU:HD13	1.86	0.57
2:G:313:SER:HB3	2:G:351:VAL:HB	1.86	0.57
2:G:4957:LYS:HG2	2:G:4964:GLY:CA	2.33	0.57
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.86	0.57
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.86	0.57
2:B:3733:CYS:HA	2:B:3766:GLN:HG2	1.85	0.57
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.70	0.57
2:I:4957:LYS:HG2	2:I:4964:GLY:CA	2.33	0.57
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.87	0.57
2:E:4924:VAL:HA	2:E:4928:LEU:HB2	1.86	0.57
2:G:173:SER:HB3	2:G:178:ARG:H	1.70	0.57
2:I:4977:THR:HG23	2:I:4981:GLU:HG3	1.85	0.57
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.86	0.57
2:B:2287:ALA:HA	2:B:2290:LEU:HD13	1.86	0.57
2:E:2287:ALA:HA	2:E:2290:LEU:HD13	1.86	0.57
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.86	0.57
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.70	0.57
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.86	0.57
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.86	0.57
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.37	0.57
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.37	0.57
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.87	0.57
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.86	0.57
2:I:173:SER:HB3	2:I:178:ARG:H	1.70	0.57
2:I:4924:VAL:HA	2:I:4928:LEU:HB2	1.86	0.57
2:B:313:SER:HB3	2:B:351:VAL:HB	1.86	0.57
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.86	0.57
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.34	0.57
2:G:641:VAL:HG11	2:G:681:HIS:HD1	1.68	0.57
2:I:2287:ALA:HA	2:I:2290:LEU:HD13	1.86	0.57
2:I:35:LEU:HD13	2:I:49:LEU:HD13	1.85	0.57
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4978:HIS:HE1	2:B:5027:CYS:SG	2.28	0.57
2:E:173:SER:HB3	2:E:178:ARG:H	1.70	0.57
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.87	0.57
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.87	0.56
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.70	0.56
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.86	0.56
2:B:4924:VAL:HA	2:B:4928:LEU:HB2	1.86	0.56
2:E:4978:HIS:HE1	2:E:5027:CYS:SG	2.28	0.56
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.87	0.56
2:G:4843:LEU:HD12	2:I:4823:LEU:HD23	1.86	0.56
2:I:641:VAL:HG11	2:I:681:HIS:HD1	1.68	0.56
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.86	0.56
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.86	0.56
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.86	0.56
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.87	0.56
2:I:1637:MET:SD	2:I:1708:ARG:NH1	2.79	0.56
2:B:1637:MET:SD	2:B:1708:ARG:NH1	2.79	0.56
2:B:173:SER:HB3	2:B:178:ARG:H	1.70	0.56
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.34	0.56
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.87	0.56
2:G:1637:MET:SD	2:G:1708:ARG:NH1	2.79	0.56
2:B:241:GLN:O	2:B:289:ARG:NH1	2.37	0.56
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.86	0.56
2:G:4978:HIS:HE1	2:G:5027:CYS:SG	2.28	0.56
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.71	0.56
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.38	0.56
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.86	0.56
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.38	0.56
2:I:4978:HIS:HE1	2:I:5027:CYS:SG	2.28	0.56
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.87	0.56
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.38	0.56
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.39	0.56
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.71	0.56
2:E:1637:MET:SD	2:E:1708:ARG:NH1	2.79	0.56
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.71	0.56
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.71	0.56
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.38	0.56
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.39	0.56
2:E:683:ARG:NH1	2:E:707:VAL:O	2.37	0.56
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	1.88	0.56
1:A:34:LYS:HD3	2:B:629:ARG:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	1.88	0.56
2:G:241:GLN:O	2:G:289:ARG:NH1	2.37	0.56
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.88	0.56
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.39	0.56
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.71	0.56
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.71	0.56
2:G:1164:LEU:HB3	2:G:1169:LEU:HD21	1.88	0.56
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.88	0.56
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.88	0.56
2:I:683:ARG:NH1	2:I:707:VAL:O	2.37	0.56
2:B:1164:LEU:HB3	2:B:1169:LEU:HD21	1.88	0.55
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.71	0.55
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.70	0.55
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	1.87	0.55
2:I:1164:LEU:HB3	2:I:1169:LEU:HD21	1.88	0.55
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.88	0.55
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.39	0.55
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.72	0.55
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	1.87	0.55
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.88	0.55
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.40	0.55
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.89	0.55
2:E:1164:LEU:HB3	2:E:1169:LEU:HD21	1.88	0.55
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.88	0.55
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.88	0.55
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.71	0.55
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.72	0.55
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.88	0.55
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.40	0.55
2:E:241:GLN:O	2:E:289:ARG:NH1	2.37	0.54
2:E:4180:ARG:NH1	2:E:4981:GLU:OE1	2.41	0.54
2:G:395:GLN:HG3	2:G:397:GLU:H	1.72	0.54
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.40	0.54
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.40	0.54
2:E:395:GLN:HG3	2:E:397:GLU:H	1.73	0.54
2:I:4180:ARG:NH1	2:I:4981:GLU:OE1	2.41	0.54
2:E:1032:LYS:O	2:E:1036:ARG:N	2.40	0.54
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.41	0.54
2:E:111:HIS:CD2	2:E:114:SER:H	2.26	0.54
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.90	0.54
1:J:55:VAL:HA	2:I:1784:ALA:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3733:CYS:HB2	2:E:3803:SER:HB3	1.90	0.54
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.72	0.54
2:I:241:GLN:O	2:I:289:ARG:NH1	2.37	0.54
2:E:4983:HIS:H	2:E:4983:HIS:HD2	1.56	0.54
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.90	0.54
2:I:2911:LEU:HB2	2:I:2916:LYS:HE3	1.90	0.54
2:E:2095:GLN:NE2	2:E:2127:GLN:O	2.39	0.54
2:G:242:ARG:NH1	2:G:481:GLU:OE1	2.41	0.54
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.41	0.53
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.90	0.53
2:G:111:HIS:CD2	2:G:114:SER:H	2.26	0.53
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.91	0.53
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.72	0.53
2:I:242:ARG:NH1	2:I:481:GLU:OE1	2.41	0.53
2:B:2911:LEU:HB2	2:B:2916:LYS:HE3	1.90	0.53
2:B:3733:CYS:HB2	2:B:3803:SER:HB3	1.90	0.53
2:G:2107:GLN:HG3	2:G:3681:GLY:HA2	1.90	0.53
2:G:4993:MET:HA	2:G:4996:ILE:HD12	1.90	0.53
2:I:2107:GLN:HG3	2:I:3681:GLY:HA2	1.90	0.53
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.90	0.53
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.42	0.53
2:E:243:ARG:NH1	2:E:301:VAL:O	2.38	0.53
2:G:4983:HIS:H	2:G:4983:HIS:HD2	1.56	0.53
2:B:4993:MET:HA	2:B:4996:ILE:HD12	1.90	0.53
2:G:3733:CYS:HB2	2:G:3803:SER:HB3	1.90	0.53
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.91	0.53
2:B:395:GLN:HG3	2:B:397:GLU:H	1.73	0.53
2:B:4180:ARG:NH1	2:B:4981:GLU:OE1	2.41	0.53
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.91	0.53
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.91	0.53
1:H:7:ILE:HB	1:H:71:ARG:HB3	1.91	0.53
2:I:395:GLN:HG3	2:I:397:GLU:H	1.73	0.53
2:E:2911:LEU:HB2	2:E:2916:LYS:HE3	1.90	0.53
2:I:3733:CYS:HB2	2:I:3803:SER:HB3	1.90	0.53
2:B:242:ARG:NH1	2:B:481:GLU:OE1	2.41	0.53
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.42	0.53
2:E:242:ARG:NH1	2:E:481:GLU:OE1	2.41	0.53
2:E:606:LEU:O	2:E:617:ASN:ND2	2.42	0.53
2:G:4180:ARG:NH1	2:G:4981:GLU:OE1	2.41	0.53
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.74	0.53
2:I:180:LEU:O	2:I:200:TRP:NE1	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:SER:O	2:B:32:GLN:NE2	2.42	0.53
2:E:2107:GLN:HG3	2:E:3681:GLY:HA2	1.90	0.53
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.42	0.53
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.74	0.53
2:B:2265:LEU:O	2:B:2330:ARG:NH1	2.42	0.53
2:E:4231:MET:CE	2:E:4960:ILE:HA	2.39	0.53
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.41	0.53
2:G:606:LEU:O	2:G:617:ASN:ND2	2.42	0.53
2:I:2265:LEU:O	2:I:2330:ARG:NH1	2.42	0.53
2:I:606:LEU:O	2:I:617:ASN:ND2	2.42	0.53
2:B:4231:MET:CE	2:B:4960:ILE:HA	2.39	0.52
2:E:1259:ARG:HH12	2:E:1593:PRO:HA	1.73	0.52
2:E:4993:MET:HA	2:E:4996:ILE:HD12	1.90	0.52
2:G:180:LEU:O	2:G:200:TRP:NE1	2.37	0.52
2:B:683:ARG:NH1	2:B:707:VAL:O	2.37	0.52
2:I:1259:ARG:HH12	2:I:1593:PRO:HA	1.73	0.52
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.41	0.52
2:B:4983:HIS:H	2:B:4983:HIS:HD2	1.56	0.52
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.43	0.52
2:I:4231:MET:CE	2:I:4960:ILE:HA	2.39	0.52
2:B:606:LEU:O	2:B:617:ASN:ND2	2.42	0.52
2:E:4865:LYS:HG3	2:E:4875:LYS:HZ3	1.74	0.52
2:G:1259:ARG:HH12	2:G:1593:PRO:HA	1.73	0.52
2:G:2911:LEU:HB2	2:G:2916:LYS:HE3	1.90	0.52
2:G:243:ARG:NH1	2:G:301:VAL:O	2.38	0.52
2:G:25:SER:O	2:G:32:GLN:NE2	2.42	0.52
2:G:776:LEU:HG	2:G:848:HIS:HA	1.92	0.52
2:B:111:HIS:CD2	2:B:114:SER:H	2.26	0.52
2:B:180:LEU:O	2:B:200:TRP:NE1	2.37	0.52
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.91	0.52
2:G:683:ARG:NH1	2:G:707:VAL:O	2.37	0.52
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.92	0.52
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.92	0.52
2:G:1653:LEU:HB3	2:G:1660:GLN:HB2	1.91	0.52
2:I:25:SER:O	2:I:32:GLN:NE2	2.42	0.52
2:I:4865:LYS:HG3	2:I:4875:LYS:HZ3	1.73	0.52
1:J:21:THR:HA	1:J:49:ARG:HA	1.92	0.52
2:B:2318:TYR:OH	2:B:2414:ASN:N	2.42	0.52
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.92	0.52
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.91	0.52
2:G:2265:LEU:O	2:G:2330:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:793:LEU:HD11	2:G:1626:TRP:HE1	1.75	0.52
2:I:4993:MET:HA	2:I:4996:ILE:HD12	1.90	0.52
2:I:793:LEU:HD11	2:I:1626:TRP:HE1	1.75	0.52
2:B:776:LEU:HG	2:B:848:HIS:HA	1.92	0.52
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.41	0.52
1:A:7:ILE:HB	1:A:71:ARG:HB3	1.91	0.52
2:B:1259:ARG:HH12	2:B:1593:PRO:HA	1.73	0.52
2:B:1653:LEU:HB3	2:B:1660:GLN:HB2	1.91	0.52
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.92	0.52
2:E:25:SER:O	2:E:32:GLN:NE2	2.42	0.52
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.41	0.52
2:I:243:ARG:NH1	2:I:301:VAL:O	2.38	0.52
2:I:776:LEU:HG	2:I:848:HIS:HA	1.92	0.52
1:A:82:TYR:O	1:A:86:GLY:N	2.43	0.52
2:B:1032:LYS:O	2:B:1036:ARG:N	2.40	0.52
2:E:2265:LEU:O	2:E:2330:ARG:NH1	2.42	0.52
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.43	0.52
2:G:4231:MET:CE	2:G:4960:ILE:HA	2.39	0.52
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.92	0.52
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.74	0.51
2:B:20:VAL:HG12	2:B:204:PRO:HA	1.92	0.51
2:B:179:TYR:OH	2:E:2359:ARG:NH1	2.43	0.51
2:E:776:LEU:HG	2:E:848:HIS:HA	1.92	0.51
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.92	0.51
2:G:20:VAL:HG12	2:G:204:PRO:HA	1.92	0.51
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.92	0.51
2:I:4983:HIS:HD2	2:I:4983:HIS:H	1.56	0.51
1:J:7:ILE:HB	1:J:71:ARG:HB3	1.91	0.51
2:E:1653:LEU:HB3	2:E:1660:GLN:HB2	1.91	0.51
2:E:2479:LEU:O	2:E:2487:UNK:N	2.44	0.51
1:F:7:ILE:HB	1:F:71:ARG:HB3	1.91	0.51
1:H:21:THR:HA	1:H:49:ARG:HA	1.92	0.51
2:I:111:HIS:CD2	2:I:114:SER:H	2.26	0.51
2:I:880:GLU:OE1	2:I:968:ALA:N	2.43	0.51
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.91	0.51
2:B:2107:GLN:HG3	2:B:3681:GLY:HA2	1.90	0.51
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.43	0.51
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.43	0.51
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.40	0.51
2:E:331:VAL:HG12	2:E:333:GLY:H	1.76	0.51
2:E:793:LEU:HD11	2:E:1626:TRP:HE1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1032:LYS:O	2:G:1036:ARG:N	2.40	0.51
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.43	0.51
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.74	0.51
2:E:20:VAL:HG12	2:E:204:PRO:HA	1.92	0.51
2:E:2318:TYR:OH	2:E:2414:ASN:N	2.42	0.51
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.43	0.51
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.93	0.51
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.92	0.51
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.44	0.51
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.76	0.51
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.43	0.51
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.92	0.51
1:F:21:THR:HA	1:F:49:ARG:HA	1.92	0.51
2:G:2318:TYR:OH	2:G:2414:ASN:N	2.42	0.51
2:G:2430:ILE:HG21	2:G:2502:UNK:HA	1.92	0.51
2:G:331:VAL:HG12	2:G:333:GLY:H	1.76	0.51
2:I:1032:LYS:O	2:I:1036:ARG:N	2.40	0.51
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.92	0.51
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.44	0.51
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.76	0.51
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.93	0.51
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.76	0.51
2:I:1653:LEU:HB3	2:I:1660:GLN:HB2	1.92	0.51
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.40	0.51
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.44	0.51
2:B:1727:ARG:NH2	2:B:1773:PRO:O	2.44	0.51
2:E:1865:MET:SD	2:E:1865:MET:N	2.84	0.51
2:I:345:LEU:HD23	2:I:389:PHE:HB3	1.93	0.51
2:B:164:ARG:N	2:B:167:ASP:OD2	2.43	0.51
1:F:55:VAL:HA	2:E:1784:ALA:HA	1.93	0.51
2:E:345:LEU:HD23	2:E:389:PHE:HB3	1.93	0.51
2:G:1865:MET:SD	2:G:1865:MET:N	2.84	0.51
2:I:2430:ILE:HG21	2:I:2502:UNK:HA	1.92	0.51
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.43	0.51
1:J:82:TYR:O	1:J:86:GLY:N	2.43	0.51
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.93	0.51
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.43	0.51
2:B:793:LEU:HD11	2:B:1626:TRP:HE1	1.75	0.51
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.43	0.51
2:G:911:HIS:O	2:G:918:ARG:NH2	2.44	0.51
1:H:55:VAL:HA	2:G:1784:ALA:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1865:MET:SD	2:B:1865:MET:N	2.84	0.51
1:F:82:TYR:O	1:F:86:GLY:N	2.43	0.51
2:G:315:CYS:SG	2:G:316:PHE:N	2.84	0.51
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.43	0.51
2:I:20:VAL:HG12	2:I:204:PRO:HA	1.92	0.51
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.44	0.50
2:B:345:LEU:HD23	2:B:389:PHE:HB3	1.93	0.50
2:B:4983:HIS:HB2	2:B:4988:TYR:HE2	1.77	0.50
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.43	0.50
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.93	0.50
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.91	0.50
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.91	0.50
2:B:2430:ILE:HG21	2:B:2502:UNK:HA	1.92	0.50
2:B:315:CYS:SG	2:B:316:PHE:N	2.84	0.50
2:E:315:CYS:SG	2:E:316:PHE:N	2.84	0.50
2:E:4081:VAL:HB	2:E:4088:ILE:HD12	1.94	0.50
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.93	0.50
2:G:345:LEU:HD23	2:G:389:PHE:HB3	1.93	0.50
2:I:315:CYS:SG	2:I:316:PHE:N	2.84	0.50
2:B:652:ARG:HD2	2:B:750:LEU:HB3	1.94	0.50
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.44	0.50
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.40	0.50
2:G:3903:LEU:HG	2:G:3915:ILE:HD12	1.94	0.50
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.44	0.50
2:B:2359:ARG:NH1	2:I:179:TYR:OH	2.44	0.50
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.93	0.50
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.92	0.50
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	1.93	0.50
2:E:3903:LEU:HG	2:E:3915:ILE:HD12	1.93	0.50
2:I:1457:UNK:N	2:I:1497:UNK:O	2.45	0.50
2:I:2159:LEU:HA	2:I:2162:ILE:HD12	1.94	0.50
2:I:4231:MET:HE1	2:I:4960:ILE:HA	1.94	0.50
2:I:4983:HIS:HB2	2:I:4988:TYR:HE2	1.77	0.50
2:I:652:ARG:HD2	2:I:750:LEU:HB3	1.93	0.50
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	1.93	0.50
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.44	0.50
2:E:206:CYS:SG	2:E:207:SER:N	2.84	0.50
2:E:2430:ILE:HG21	2:E:2502:UNK:HA	1.92	0.50
2:I:1865:MET:SD	2:I:1865:MET:N	2.84	0.50
2:I:4081:VAL:HB	2:I:4088:ILE:HD12	1.94	0.50
2:B:2364:PHE:HD1	2:B:2429:LEU:HD21	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2364:PHE:HD1	2:G:2429:LEU:HD21	1.76	0.50
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.93	0.50
1:A:21:THR:HA	1:A:49:ARG:HA	1.92	0.50
2:B:1457:UNK:N	2:B:1497:UNK:O	2.45	0.50
2:B:2159:LEU:HA	2:B:2162:ILE:HD12	1.94	0.50
2:B:290:TYR:O	2:B:302:VAL:N	2.45	0.50
2:B:331:VAL:HG12	2:B:333:GLY:H	1.76	0.50
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.44	0.50
2:I:2479:LEU:O	2:I:2487:UNK:N	2.44	0.50
2:E:1457:UNK:N	2:E:1497:UNK:O	2.45	0.50
2:E:4983:HIS:HB2	2:E:4988:TYR:HE2	1.77	0.50
1:H:34:LYS:HD3	2:G:629:ARG:HD2	1.94	0.50
2:I:1126:GLY:HA3	2:I:1143:TRP:CE2	2.47	0.50
2:E:911:HIS:O	2:E:918:ARG:NH2	2.44	0.50
2:G:2479:LEU:O	2:G:2487:UNK:N	2.44	0.50
1:H:82:TYR:O	1:H:86:GLY:N	2.44	0.50
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.93	0.50
2:B:2479:LEU:O	2:B:2487:UNK:N	2.44	0.49
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.94	0.49
2:G:1457:UNK:N	2:G:1497:UNK:O	2.45	0.49
2:G:164:ARG:N	2:G:167:ASP:OD2	2.43	0.49
2:G:206:CYS:SG	2:G:207:SER:N	2.84	0.49
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.45	0.49
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.45	0.49
2:B:978:THR:HB	2:B:980:ALA:H	1.78	0.49
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.93	0.49
2:I:2364:PHE:HD1	2:I:2429:LEU:HD21	1.76	0.49
2:E:164:ARG:N	2:E:167:ASP:OD2	2.43	0.49
2:E:652:ARG:HB2	2:E:750:LEU:HD13	1.94	0.49
2:G:652:ARG:HB2	2:G:750:LEU:HD13	1.94	0.49
2:G:880:GLU:OE1	2:G:968:ALA:N	2.43	0.49
2:I:978:THR:HB	2:I:980:ALA:H	1.78	0.49
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.94	0.49
2:B:3903:LEU:HG	2:B:3915:ILE:HD12	1.94	0.49
2:E:1126:GLY:HA3	2:E:1143:TRP:CE2	2.47	0.49
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.44	0.49
2:E:290:TYR:O	2:E:302:VAL:N	2.45	0.49
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.45	0.49
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.94	0.49
2:G:3900:GLN:NE2	2:G:3967:GLU:O	2.46	0.49
2:G:652:ARG:HD2	2:G:750:LEU:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:290:TYR:O	2:I:302:VAL:N	2.45	0.49
2:I:331:VAL:HG12	2:I:333:GLY:H	1.76	0.49
2:I:3903:LEU:HG	2:I:3915:ILE:HD12	1.94	0.49
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.93	0.49
2:B:1126:GLY:HA3	2:B:1143:TRP:CE2	2.47	0.49
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.40	0.49
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.84	0.49
2:B:3759:GLU:HA	2:B:3762:ARG:HE	1.78	0.49
2:B:3900:GLN:NE2	2:B:3967:GLU:O	2.46	0.49
2:E:3759:GLU:HA	2:E:3762:ARG:HE	1.78	0.49
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.76	0.49
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.41	0.49
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.93	0.49
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.95	0.49
2:I:649:PHE:HB3	2:I:776:LEU:HD13	1.95	0.49
2:B:206:CYS:SG	2:B:207:SER:N	2.84	0.49
2:E:2159:LEU:HA	2:E:2162:ILE:HD12	1.94	0.49
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.95	0.49
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.44	0.49
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.84	0.49
2:G:45:ARG:HG2	2:G:443:LEU:HD21	1.95	0.49
2:I:2095:GLN:NE2	2:I:2127:GLN:O	2.39	0.49
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.78	0.49
2:E:652:ARG:HD2	2:E:750:LEU:HB3	1.93	0.49
2:E:978:THR:HB	2:E:980:ALA:H	1.78	0.49
2:G:4081:VAL:HB	2:G:4088:ILE:HD12	1.94	0.49
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.95	0.49
2:I:3759:GLU:HA	2:I:3762:ARG:HE	1.78	0.49
2:B:652:ARG:HB2	2:B:750:LEU:HD13	1.94	0.49
2:E:3900:GLN:NE2	2:E:3967:GLU:O	2.46	0.49
2:G:1126:GLY:HA3	2:G:1143:TRP:CE2	2.47	0.49
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	1.93	0.49
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.78	0.49
2:I:3850:GLN:HA	2:I:3853:ALA:HB3	1.93	0.49
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.95	0.49
2:I:45:ARG:HG2	2:I:443:LEU:HD21	1.95	0.49
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.93	0.49
2:E:2364:PHE:HD1	2:E:2429:LEU:HD21	1.76	0.49
2:E:4983:HIS:N	2:E:4983:HIS:CD2	2.81	0.49
2:G:290:TYR:O	2:G:302:VAL:N	2.45	0.49
2:G:4983:HIS:HB2	2:G:4988:TYR:HE2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4786:ASP:OD2	2:I:4789:PHE:N	2.39	0.49
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.95	0.49
2:B:4081:VAL:HB	2:B:4088:ILE:HD12	1.94	0.49
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	1.95	0.49
2:E:2024:PRO:HB2	2:E:2027:ILE:HG12	1.95	0.49
2:G:649:PHE:HB3	2:G:776:LEU:HD13	1.95	0.49
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.95	0.49
2:B:4786:ASP:OD2	2:B:4789:PHE:N	2.39	0.48
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.95	0.48
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.84	0.48
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.94	0.48
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	1.95	0.48
2:B:2758:PHE:O	2:B:2762:THR:N	2.46	0.48
2:B:45:ARG:HG2	2:B:443:LEU:HD21	1.95	0.48
2:E:41:GLY:O	2:E:45:ARG:NH1	2.47	0.48
2:B:1676:LEU:HD23	2:B:2167:ILE:HG23	1.96	0.48
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.95	0.48
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.93	0.48
2:E:880:GLU:OE1	2:E:968:ALA:N	2.43	0.48
2:G:2159:LEU:HA	2:G:2162:ILE:HD12	1.94	0.48
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.95	0.48
2:I:2024:PRO:HB2	2:I:2027:ILE:HG12	1.95	0.48
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.94	0.48
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.45	0.48
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.78	0.48
2:E:1676:LEU:HD23	2:E:2167:ILE:HG23	1.95	0.48
2:E:180:LEU:O	2:E:200:TRP:NE1	2.37	0.48
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.78	0.48
2:G:2024:PRO:HB2	2:G:2027:ILE:HG12	1.95	0.48
2:G:3759:GLU:HA	2:G:3762:ARG:HE	1.78	0.48
2:I:1676:LEU:HD23	2:I:2167:ILE:HG23	1.96	0.48
2:I:3900:GLN:NE2	2:I:3967:GLU:O	2.46	0.48
2:B:41:GLY:O	2:B:45:ARG:NH1	2.47	0.48
2:B:649:PHE:HB3	2:B:776:LEU:HD13	1.95	0.48
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.44	0.48
2:I:2318:TYR:OH	2:I:2414:ASN:N	2.42	0.48
2:E:1243:PRO:HB2	2:E:1600:LEU:HD22	1.95	0.48
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.95	0.48
2:G:1243:PRO:HB2	2:G:1600:LEU:HD22	1.95	0.48
2:G:1676:LEU:HD23	2:G:2167:ILE:HG23	1.96	0.48
2:G:4865:LYS:HG3	2:G:4875:LYS:HZ3	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:978:THR:HB	2:G:980:ALA:H	1.77	0.48
2:B:2024:PRO:HB2	2:B:2027:ILE:HG12	1.95	0.48
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.95	0.48
2:E:45:ARG:HG2	2:E:443:LEU:HD21	1.95	0.48
2:E:4968:PHE:CE2	2:E:4978:HIS:ND1	2.82	0.48
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	1.95	0.48
2:I:41:GLY:O	2:I:45:ARG:NH1	2.47	0.48
2:E:649:PHE:HB3	2:E:776:LEU:HD13	1.95	0.48
2:I:206:CYS:SG	2:I:207:SER:N	2.84	0.48
2:I:652:ARG:HB2	2:I:750:LEU:HD13	1.94	0.48
2:B:4968:PHE:CE2	2:B:4978:HIS:ND1	2.82	0.48
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.42	0.48
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.96	0.48
2:G:1948:ASP:OD1	2:G:2126:ARG:NH2	2.46	0.48
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.95	0.48
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.95	0.48
2:I:164:ARG:N	2:I:167:ASP:OD2	2.43	0.48
2:I:4817:ALA:HA	2:I:4823:LEU:HD22	1.96	0.48
2:G:41:GLY:O	2:G:45:ARG:NH1	2.47	0.48
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.96	0.48
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.96	0.48
2:E:2758:PHE:O	2:E:2762:THR:N	2.46	0.47
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.95	0.47
2:E:4571:PHE:O	2:E:4575:PHE:N	2.46	0.47
2:E:4817:ALA:HA	2:E:4823:LEU:HD22	1.96	0.47
2:G:3994:HIS:O	2:G:3998:HIS:ND1	2.39	0.47
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.96	0.47
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.94	0.47
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.47	0.47
2:I:4968:PHE:CE2	2:I:4978:HIS:ND1	2.82	0.47
2:B:54:ASN:O	2:B:58:VAL:N	2.44	0.47
2:E:1516:UNK:N	2:E:1529:UNK:O	2.48	0.47
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.47	0.47
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.95	0.47
2:G:2095:GLN:NE2	2:G:2127:GLN:O	2.39	0.47
2:G:4817:ALA:HA	2:G:4823:LEU:HD22	1.96	0.47
2:I:500:ALA:HB1	2:I:504:ALA:HB2	1.96	0.47
2:B:116:MET:HB2	2:B:137:LEU:HD12	1.97	0.47
2:B:177:GLU:HG3	2:E:2452:ARG:HH12	1.79	0.47
2:G:500:ALA:HB1	2:G:504:ALA:HB2	1.97	0.47
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1516:UNK:N	2:I:1529:UNK:O	2.48	0.47
2:B:4066:LEU:HD12	2:B:4169:SER:HB2	1.96	0.47
2:G:1516:UNK:N	2:G:1529:UNK:O	2.48	0.47
2:G:4998:LYS:NZ	2:G:5007:GLU:OE1	2.38	0.47
2:I:1236:THR:OG1	2:I:1608:MET:SD	2.73	0.47
2:B:1243:PRO:HB2	2:B:1600:LEU:HD22	1.95	0.47
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.96	0.47
2:B:4075:GLU:HA	2:B:4078:GLN:HB2	1.97	0.47
2:B:4817:ALA:HA	2:B:4823:LEU:HD22	1.96	0.47
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.97	0.47
2:E:500:ALA:HB1	2:E:504:ALA:HB2	1.97	0.47
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.97	0.47
2:B:1516:UNK:N	2:B:1529:UNK:O	2.48	0.47
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.47	0.47
2:B:500:ALA:HB1	2:B:504:ALA:HB2	1.96	0.47
2:E:4075:GLU:HA	2:E:4078:GLN:HB2	1.97	0.47
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.97	0.47
2:G:4983:HIS:N	2:G:4983:HIS:CD2	2.81	0.47
2:I:3674:ILE:HD11	2:I:3728:ILE:HG22	1.97	0.47
2:B:4983:HIS:N	2:B:4983:HIS:CD2	2.81	0.47
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.96	0.47
2:G:1236:THR:OG1	2:G:1608:MET:SD	2.73	0.47
2:E:116:MET:HB2	2:E:137:LEU:HD12	1.96	0.47
2:E:3994:HIS:O	2:E:3998:HIS:ND1	2.39	0.47
2:E:4066:LEU:HD12	2:E:4169:SER:HB2	1.97	0.47
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	1.95	0.47
2:I:4075:GLU:HA	2:I:4078:GLN:HB2	1.97	0.47
2:B:2231:SER:HA	2:B:2234:ARG:HG2	1.97	0.47
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.97	0.47
2:B:3842:LEU:O	2:B:3929:SER:OG	2.33	0.47
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.80	0.47
2:E:2869:ARG:HA	2:E:2872:GLN:HB3	1.97	0.47
2:E:479:GLN:HE21	2:E:536:ASN:ND2	2.13	0.47
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.97	0.47
2:G:4075:GLU:HA	2:G:4078:GLN:HB2	1.97	0.47
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.80	0.47
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.84	0.47
2:I:2215:LEU:HD23	2:I:2260:ASN:HB3	1.97	0.47
2:B:1236:THR:OG1	2:B:1608:MET:SD	2.73	0.47
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.97	0.47
2:G:2215:LEU:HD23	2:G:2260:ASN:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.47	0.47
2:G:479:GLN:HE21	2:G:536:ASN:ND2	2.13	0.47
2:I:2353:VAL:O	2:I:2357:LEU:N	2.48	0.47
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.97	0.47
2:B:614:VAL:HG22	2:B:616:SER:H	1.80	0.47
2:E:2215:LEU:HD23	2:E:2260:ASN:HB3	1.97	0.47
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.96	0.47
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.96	0.47
2:G:116:MET:HB2	2:G:137:LEU:HD12	1.97	0.47
2:I:2347:GLU:O	2:I:2351:ASN:N	2.48	0.47
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.40	0.47
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.97	0.47
2:B:3994:HIS:O	2:B:3998:HIS:ND1	2.39	0.46
2:B:4571:PHE:O	2:B:4575:PHE:N	2.46	0.46
2:B:4823:LEU:HA	2:B:4826:ILE:HD12	1.97	0.46
2:E:4823:LEU:HA	2:E:4826:ILE:HD12	1.97	0.46
2:G:4152:GLU:OE1	2:G:4192:ARG:NH2	2.48	0.46
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.96	0.46
2:I:2231:SER:HA	2:I:2234:ARG:HG2	1.97	0.46
2:I:3980:LEU:HD22	2:I:3985:LEU:HD22	1.98	0.46
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.80	0.46
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.96	0.46
2:E:3674:ILE:HD11	2:E:3728:ILE:HG22	1.97	0.46
2:E:3842:LEU:O	2:E:3929:SER:OG	2.33	0.46
2:E:4152:GLU:OE1	2:E:4192:ARG:NH2	2.48	0.46
2:I:3971:GLY:N	2:I:4032:GLU:OE2	2.48	0.46
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.96	0.46
2:B:2347:GLU:O	2:B:2351:ASN:N	2.48	0.46
2:B:3980:LEU:HD22	2:B:3985:LEU:HD22	1.97	0.46
2:G:4968:PHE:CE2	2:G:4978:HIS:ND1	2.82	0.46
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.81	0.46
2:I:1948:ASP:OD1	2:I:2126:ARG:NH2	2.46	0.46
2:I:614:VAL:HG22	2:I:616:SER:H	1.80	0.46
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.95	0.46
2:B:3674:ILE:HD11	2:B:3728:ILE:HG22	1.97	0.46
2:B:880:GLU:OE1	2:B:968:ALA:N	2.43	0.46
2:E:1948:ASP:OD1	2:E:2126:ARG:NH2	2.46	0.46
2:G:2353:VAL:O	2:G:2357:LEU:N	2.48	0.46
2:I:1243:PRO:HB2	2:I:1600:LEU:HD22	1.95	0.46
2:I:4066:LEU:HD12	2:I:4169:SER:HB2	1.96	0.46
2:B:3971:GLY:N	2:B:4032:GLU:OE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4152:GLU:OE1	2:B:4192:ARG:NH2	2.48	0.46
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.50	0.46
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.96	0.46
2:I:4961:CYS:HB3	2:I:4983:HIS:CE1	2.51	0.46
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.49	0.46
2:B:2215:LEU:HD23	2:B:2260:ASN:HB3	1.97	0.46
2:B:2868:SER:O	2:B:2872:GLN:N	2.49	0.46
2:B:2869:ARG:HA	2:B:2872:GLN:HB3	1.97	0.46
2:B:243:ARG:NH1	2:B:301:VAL:O	2.38	0.46
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.49	0.46
2:E:2231:SER:HA	2:E:2234:ARG:HG2	1.97	0.46
2:E:2868:SER:O	2:E:2872:GLN:N	2.49	0.46
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.49	0.46
2:G:1077:ALA:HB1	2:G:1234:VAL:HG11	1.98	0.46
2:G:2868:SER:O	2:G:2872:GLN:N	2.49	0.46
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.97	0.46
2:G:3674:ILE:HD11	2:G:3728:ILE:HG22	1.97	0.46
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.49	0.46
2:I:2869:ARG:HA	2:I:2872:GLN:HB3	1.97	0.46
2:I:4152:GLU:OE1	2:I:4192:ARG:NH2	2.48	0.46
2:B:3773:ARG:HG3	2:B:3815:LYS:HZ3	1.81	0.46
2:B:4961:CYS:HB3	2:B:4983:HIS:CE1	2.51	0.46
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.49	0.46
2:G:2452:ARG:HH12	2:E:177:GLU:HG3	1.81	0.46
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.81	0.46
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.49	0.46
2:G:3980:LEU:HD22	2:G:3985:LEU:HD22	1.98	0.46
2:G:4066:LEU:HD12	2:G:4169:SER:HB2	1.96	0.46
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	1.98	0.46
2:G:4961:CYS:HB3	2:G:4983:HIS:CE1	2.51	0.46
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.50	0.46
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.81	0.46
2:B:1948:ASP:OD1	2:B:2126:ARG:NH2	2.46	0.46
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.98	0.46
2:E:838:HIS:HA	2:E:1201:HIS:HB3	1.98	0.46
2:E:1236:THR:OG1	2:E:1608:MET:SD	2.73	0.46
2:E:4961:CYS:HB3	2:E:4983:HIS:CE1	2.51	0.46
2:G:4843:LEU:HD22	2:G:4928:LEU:HD11	1.98	0.46
2:G:54:ASN:O	2:G:58:VAL:N	2.44	0.46
2:I:1077:ALA:HB1	2:I:1234:VAL:HG11	1.98	0.46
2:B:2095:GLN:NE2	2:B:2127:GLN:O	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.50	0.46
2:B:911:HIS:O	2:B:918:ARG:NH2	2.44	0.46
2:G:3361:UNK:O	2:G:3365:UNK:N	2.49	0.46
2:I:2868:SER:O	2:I:2872:GLN:N	2.49	0.46
2:I:4998:LYS:NZ	2:I:5007:GLU:OE1	2.38	0.46
2:B:838:HIS:HA	2:B:1201:HIS:HB3	1.98	0.45
2:B:1077:ALA:HB1	2:B:1234:VAL:HG11	1.98	0.45
2:B:4899:ASP:OD1	2:E:4892:ARG:NH2	2.48	0.45
2:E:3980:LEU:HD22	2:E:3985:LEU:HD22	1.98	0.45
2:E:4843:LEU:HD22	2:E:4928:LEU:HD11	1.98	0.45
2:E:614:VAL:HG22	2:E:616:SER:H	1.80	0.45
2:G:2231:SER:HA	2:G:2234:ARG:HG2	1.97	0.45
2:G:471:LEU:O	2:G:475:GLN:N	2.47	0.45
2:G:580:GLU:HG3	2:G:620:LEU:HD22	1.99	0.45
2:I:3361:UNK:O	2:I:3365:UNK:N	2.49	0.45
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.81	0.45
2:E:2353:VAL:O	2:E:2357:LEU:N	2.48	0.45
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.98	0.45
2:I:116:MET:HB2	2:I:137:LEU:HD12	1.96	0.45
2:B:2353:VAL:O	2:B:2357:LEU:N	2.48	0.45
2:B:2950:UNK:O	2:B:2954:UNK:N	2.50	0.45
2:B:3361:UNK:O	2:B:3365:UNK:N	2.49	0.45
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.33	0.45
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.81	0.45
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.80	0.45
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.99	0.45
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	1.99	0.45
2:G:2347:GLU:O	2:G:2351:ASN:N	2.48	0.45
2:G:4571:PHE:O	2:G:4575:PHE:N	2.46	0.45
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.49	0.45
2:I:1025:ARG:O	2:I:1032:LYS:NZ	2.41	0.45
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.97	0.45
2:I:3842:LEU:O	2:I:3929:SER:OG	2.33	0.45
2:I:4823:LEU:HA	2:I:4826:ILE:HD12	1.97	0.45
1:J:34:LYS:HD3	2:I:629:ARG:HD2	1.97	0.45
2:E:1077:ALA:HB1	2:E:1234:VAL:HG11	1.98	0.45
2:E:2347:GLU:O	2:E:2351:ASN:N	2.48	0.45
2:E:4231:MET:HE1	2:E:4960:ILE:HA	1.98	0.45
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.81	0.45
2:G:451:TYR:O	2:G:474:ARG:NH1	2.49	0.45
2:I:911:HIS:O	2:I:918:ARG:NH2	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3773:ARG:HG3	2:E:3815:LYS:HZ3	1.81	0.45
2:G:2950:UNK:O	2:G:2954:UNK:N	2.50	0.45
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.50	0.45
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.97	0.45
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	1.99	0.45
2:B:580:GLU:HG3	2:B:620:LEU:HD22	1.99	0.45
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.35	0.45
2:E:2950:UNK:O	2:E:2954:UNK:N	2.50	0.45
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.35	0.45
2:G:4823:LEU:HA	2:G:4826:ILE:HD12	1.97	0.45
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.98	0.45
2:G:614:VAL:HG22	2:G:616:SER:H	1.80	0.45
2:I:2950:UNK:O	2:I:2954:UNK:N	2.50	0.45
2:I:4822:THR:O	2:I:4825:THR:OG1	2.31	0.45
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	1.99	0.45
2:B:1973:GLN:O	2:B:1977:TYR:N	2.49	0.45
2:B:2810:LYS:HE2	2:B:2814:LYS:HE3	1.99	0.45
2:B:479:GLN:HE21	2:B:536:ASN:ND2	2.13	0.45
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	1.98	0.45
2:G:2758:PHE:O	2:G:2762:THR:N	2.46	0.45
2:G:2869:ARG:HA	2:G:2872:GLN:HB3	1.97	0.45
2:G:3971:GLY:N	2:G:4032:GLU:OE2	2.48	0.45
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.49	0.45
2:I:4697:VAL:O	2:I:4701:TRP:N	2.49	0.45
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.99	0.45
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.97	0.45
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.99	0.45
2:I:2810:LYS:HE2	2:I:2814:LYS:HE3	1.99	0.45
2:B:410:LEU:HD12	2:B:413:GLN:HE21	1.82	0.45
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.99	0.45
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	1.99	0.45
2:E:3361:UNK:O	2:E:3365:UNK:N	2.49	0.45
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	1.97	0.45
2:G:1078:GLU:HB3	2:G:1081:TYR:HD2	1.82	0.45
2:G:4959:PHE:CG	2:G:4959:PHE:O	2.70	0.45
2:I:1078:GLU:HB3	2:I:1081:TYR:HD2	1.82	0.45
2:I:2196:ASN:OD1	2:I:2199:ARG:NH1	2.43	0.45
2:I:580:GLU:HG3	2:I:620:LEU:HD22	1.99	0.45
2:B:3971:GLY:H	2:B:5005:GLY:HA3	1.82	0.45
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.99	0.45
2:E:2004:GLU:HA	2:E:2007:ASN:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4697:VAL:O	2:E:4701:TRP:N	2.50	0.45
2:E:471:LEU:O	2:E:475:GLN:N	2.47	0.45
2:G:838:HIS:HA	2:G:1201:HIS:HB3	1.98	0.45
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.81	0.45
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.35	0.45
2:I:2758:PHE:O	2:I:2762:THR:N	2.47	0.45
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.34	0.45
2:I:3971:GLY:H	2:I:5005:GLY:HA3	1.82	0.45
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	1.99	0.44
2:B:4843:LEU:HD22	2:B:4928:LEU:HD11	1.98	0.44
2:B:4959:PHE:O	2:B:4959:PHE:CG	2.70	0.44
2:G:3773:ARG:HG3	2:G:3815:LYS:HZ3	1.82	0.44
2:G:3842:LEU:O	2:G:3929:SER:OG	2.33	0.44
2:G:4959:PHE:CD1	2:G:4959:PHE:O	2.70	0.44
2:I:2004:GLU:HA	2:I:2007:ASN:HB2	1.99	0.44
2:I:410:LEU:HD12	2:I:413:GLN:HE21	1.82	0.44
2:B:4892:ARG:NH2	2:I:4899:ASP:OD1	2.49	0.44
2:I:54:ASN:O	2:I:58:VAL:N	2.44	0.44
2:I:838:HIS:HA	2:I:1201:HIS:HB3	1.98	0.44
2:B:2196:ASN:OD1	2:B:2199:ARG:NH1	2.43	0.44
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	1.99	0.44
2:E:410:LEU:HD12	2:E:413:GLN:HE21	1.82	0.44
2:G:3971:GLY:H	2:G:5005:GLY:HA3	1.82	0.44
2:I:451:TYR:O	2:I:474:ARG:NH1	2.49	0.44
2:I:4571:PHE:O	2:I:4575:PHE:N	2.46	0.44
2:I:4843:LEU:HD22	2:I:4928:LEU:HD11	1.98	0.44
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	1.98	0.44
2:I:887:ILE:HG21	2:I:959:TYR:HA	2.00	0.44
1:A:7:ILE:N	1:A:71:ARG:O	2.47	0.44
2:B:1247:PRO:HA	2:B:1598:GLN:HA	2.00	0.44
2:B:4231:MET:HE1	2:B:4960:ILE:HA	2.00	0.44
2:E:2810:LYS:HE2	2:E:2814:LYS:HE3	1.99	0.44
2:E:357:LEU:HD12	2:E:388:LEU:HD11	2.00	0.44
2:E:3971:GLY:H	2:E:5005:GLY:HA3	1.82	0.44
2:I:3891:LEU:HB3	2:I:3899:PHE:CE2	2.53	0.44
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.41	0.44
2:B:1078:GLU:HB3	2:B:1081:TYR:HD2	1.82	0.44
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.35	0.44
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.42	0.44
2:E:4158:PRO:HA	2:E:4161:ARG:HB2	2.00	0.44
2:E:4959:PHE:CG	2:E:4959:PHE:O	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.99	0.44
2:G:2810:LYS:HE2	2:G:2814:LYS:HE3	1.99	0.44
2:G:3891:LEU:HB3	2:G:3899:PHE:CE2	2.53	0.44
2:G:4697:VAL:O	2:G:4701:TRP:N	2.49	0.44
2:G:583:ILE:HA	2:G:586:ILE:HD12	2.00	0.44
2:G:756:SER:HB3	2:G:767:VAL:HG22	2.00	0.44
1:H:87:HIS:HA	1:H:88:PRO:HD3	1.88	0.44
2:I:479:GLN:HE21	2:I:536:ASN:ND2	2.13	0.44
2:B:357:LEU:HD12	2:B:388:LEU:HD11	2.00	0.44
2:B:887:ILE:HG21	2:B:959:TYR:HA	2.00	0.44
2:G:4786:ASP:OD2	2:G:4789:PHE:N	2.39	0.44
2:G:485:SER:HA	2:G:488:LEU:HB2	1.99	0.44
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.98	0.44
2:B:2004:GLU:HA	2:B:2007:ASN:HB2	1.99	0.44
2:B:3552:UNK:O	2:B:3556:UNK:N	2.51	0.44
2:E:3552:UNK:O	2:E:3556:UNK:N	2.51	0.44
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.83	0.44
2:E:887:ILE:HG21	2:E:959:TYR:HA	2.00	0.44
1:F:87:HIS:HA	1:F:88:PRO:HD3	1.88	0.44
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.99	0.44
2:I:583:ILE:HA	2:I:586:ILE:HD12	2.00	0.44
2:B:583:ILE:HA	2:B:586:ILE:HD12	2.00	0.44
2:E:1247:PRO:HA	2:E:1598:GLN:HA	2.00	0.44
2:E:4563:ARG:NH1	2:E:4815:ASP:OD1	2.51	0.44
2:E:756:SER:HB3	2:E:767:VAL:HG22	2.00	0.44
2:G:1973:GLN:O	2:G:1977:TYR:N	2.49	0.44
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	1.99	0.44
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.41	0.44
2:I:485:SER:HA	2:I:488:LEU:HB2	1.99	0.44
2:G:3552:UNK:O	2:G:3556:UNK:N	2.51	0.44
2:G:4231:MET:HE1	2:G:4960:ILE:HA	2.00	0.44
2:I:3552:UNK:O	2:I:3556:UNK:N	2.51	0.44
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.81	0.44
2:I:4959:PHE:CG	2:I:4959:PHE:O	2.70	0.44
1:J:92:PRO:HD3	2:I:627:PRO:HB2	2.00	0.44
2:B:4924:VAL:HG23	2:B:4925:ILE:HG12	2.00	0.44
2:E:1973:GLN:O	2:E:1977:TYR:N	2.49	0.44
2:E:3891:LEU:HB3	2:E:3899:PHE:CE2	2.53	0.44
2:G:1247:PRO:HA	2:G:1598:GLN:HA	2.00	0.44
2:G:2257:LEU:O	2:G:2261:SER:N	2.51	0.44
2:G:4563:ARG:NH1	2:G:4815:ASP:OD1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:887:ILE:HG21	2:G:959:TYR:HA	2.00	0.44
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	1.99	0.44
2:I:4563:ARG:NH1	2:I:4815:ASP:OD1	2.51	0.44
2:B:3891:LEU:HB3	2:B:3899:PHE:CE2	2.53	0.43
2:E:286:THR:HA	2:E:405:HIS:HB2	2.00	0.43
2:E:4786:ASP:OD2	2:E:4789:PHE:N	2.39	0.43
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.82	0.43
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.42	0.43
2:G:488:LEU:O	2:G:492:ASP:N	2.48	0.43
1:A:55:VAL:HA	2:B:1784:ALA:HA	1.99	0.43
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.83	0.43
2:B:4959:PHE:O	2:B:4959:PHE:CD1	2.70	0.43
2:E:485:SER:HA	2:E:488:LEU:HB2	1.99	0.43
2:E:580:GLU:HG3	2:E:620:LEU:HD22	1.99	0.43
2:G:410:LEU:HD12	2:G:413:GLN:HE21	1.82	0.43
2:I:357:LEU:HD12	2:I:388:LEU:HD11	2.00	0.43
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.82	0.43
2:I:4959:PHE:CD1	2:I:4959:PHE:O	2.70	0.43
2:I:756:SER:HB3	2:I:767:VAL:HG22	2.00	0.43
2:B:45:ARG:NH2	2:B:447:ASP:OD1	2.48	0.43
2:B:451:TYR:O	2:B:474:ARG:NH1	2.49	0.43
2:E:4959:PHE:CD1	2:E:4959:PHE:O	2.70	0.43
2:E:5000:GLU:HA	2:E:5003:HIS:CD2	2.53	0.43
2:E:425:PRO:HA	2:E:506:TYR:HD1	1.83	0.43
2:I:2257:LEU:O	2:I:2261:SER:N	2.51	0.43
2:I:475:GLN:NE2	2:I:531:ARG:O	2.42	0.43
2:B:4763:GLY:O	2:B:4766:THR:OG1	2.34	0.43
2:E:2257:LEU:O	2:E:2261:SER:N	2.51	0.43
2:E:488:LEU:O	2:E:492:ASP:N	2.48	0.43
2:E:583:ILE:HA	2:E:586:ILE:HD12	2.00	0.43
2:G:1166:GLY:HA3	2:G:1216:ILE:HD13	2.01	0.43
2:G:357:LEU:HD12	2:G:388:LEU:HD11	2.00	0.43
2:G:4158:PRO:HA	2:G:4161:ARG:HB2	2.00	0.43
2:G:4822:THR:O	2:G:4825:THR:OG1	2.31	0.43
2:G:5000:GLU:HA	2:G:5003:HIS:CD2	2.53	0.43
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.54	0.43
2:I:681:HIS:HB3	2:I:784:SER:HB3	2.01	0.43
2:I:876:GLU:O	2:I:880:GLU:N	2.50	0.43
2:B:161:GLU:HA	2:E:3984:ARG:HH22	1.84	0.43
2:B:2257:LEU:O	2:B:2261:SER:N	2.51	0.43
2:B:4563:ARG:NH1	2:B:4815:ASP:OD1	2.51	0.43

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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	0.43
2:B:5000:GLU:HA	2:B:5003:HIS:CD2	2.53	0.43
2:E:1078:GLU:HB3	2:E:1081:TYR:HD2	1.82	0.43
2:E:4822:THR:O	2:E:4825:THR:OG1	2.31	0.43
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.54	0.43
2:G:286:THR:HA	2:G:405:HIS:HB2	2.00	0.43
2:E:1166:GLY:HA3	2:E:1216:ILE:HD13	2.01	0.43
2:G:2004:GLU:HA	2:G:2007:ASN:HB2	1.99	0.43
2:I:4924:VAL:HG23	2:I:4925:ILE:HG12	2.00	0.43
2:I:4983:HIS:N	2:I:4983:HIS:CD2	2.81	0.43
2:I:5000:GLU:HA	2:I:5003:HIS:CD2	2.53	0.43
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.99	0.43
2:B:425:PRO:HA	2:B:506:TYR:HD1	1.83	0.43
2:E:309:THR:O	2:E:313:SER:OG	2.37	0.43
2:G:161:GLU:HA	2:I:3984:ARG:HH22	1.83	0.43
2:I:1247:PRO:HA	2:I:1598:GLN:HA	2.00	0.43
2:I:1973:GLN:O	2:I:1977:TYR:N	2.49	0.43
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.33	0.43
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.54	0.43
2:B:1848:LEU:HD22	2:B:1853:ILE:HG13	2.01	0.43
2:B:3771:HIS:O	2:B:3774:GLY:N	2.48	0.43
2:E:681:HIS:HB3	2:E:784:SER:HB3	2.01	0.43
2:G:1848:LEU:HD22	2:G:1853:ILE:HG13	2.01	0.43
2:I:45:ARG:NH2	2:I:447:ASP:OD1	2.48	0.43
2:B:4158:PRO:HA	2:B:4161:ARG:HB2	2.00	0.43
2:B:485:SER:HA	2:B:488:LEU:HB2	1.99	0.43
2:B:681:HIS:HB3	2:B:784:SER:HB3	2.01	0.43
2:E:4236:SER:OG	2:E:4675:LYS:NZ	2.46	0.43
2:G:181:HIS:CE1	2:G:195:PHE:HB2	2.54	0.43
2:B:1166:GLY:HA3	2:B:1216:ILE:HD13	2.01	0.43
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.54	0.43
2:E:181:HIS:CE1	2:E:195:PHE:HB2	2.54	0.43
2:G:2107:GLN:NE2	2:G:3680:ALA:O	2.52	0.43
2:G:425:PRO:HA	2:G:506:TYR:HD1	1.83	0.43
1:J:23:VAL:H	1:J:105:ASN:HB3	1.84	0.43
1:J:87:HIS:HA	1:J:88:PRO:HD3	1.88	0.43
2:B:286:THR:HA	2:B:405:HIS:HB2	2.00	0.42
2:B:2107:GLN:NE2	2:B:3680:ALA:O	2.52	0.42
2:E:3771:HIS:O	2:E:3774:GLY:N	2.48	0.42
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.33	0.42
2:G:309:THR:O	2:G:313:SER:OG	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:707:VAL:HG23	2:G:713:SER:HB2	2.01	0.42
2:I:1848:LEU:HD22	2:I:1853:ILE:HG13	2.01	0.42
2:I:2107:GLN:NE2	2:I:3680:ALA:O	2.52	0.42
2:E:4924:VAL:HG23	2:E:4925:ILE:HG12	2.00	0.42
2:I:425:PRO:HA	2:I:506:TYR:HD1	1.83	0.42
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.84	0.42
2:B:1817:GLU:O	2:B:1821:ASP:N	2.49	0.42
2:B:181:HIS:CE1	2:B:195:PHE:HB2	2.54	0.42
2:B:4658:ILE:HD11	2:B:4796:MET:HG3	2.01	0.42
2:B:488:LEU:O	2:B:492:ASP:N	2.48	0.42
2:B:756:SER:HB3	2:B:767:VAL:HG22	2.00	0.42
2:E:3897:ASN:O	2:E:3901:ASN:ND2	2.52	0.42
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.41	0.42
2:G:4658:ILE:HD11	2:G:4796:MET:HG3	2.00	0.42
2:I:1817:GLU:O	2:I:1821:ASP:N	2.49	0.42
2:E:707:VAL:HG23	2:E:713:SER:HB2	2.01	0.42
2:G:3804:ILE:HG22	2:G:3812:VAL:HG21	2.02	0.42
2:I:1166:GLY:HA3	2:I:1216:ILE:HD13	2.01	0.42
2:I:181:HIS:CE1	2:I:195:PHE:HB2	2.54	0.42
2:I:4158:PRO:HA	2:I:4161:ARG:HB2	2.00	0.42
2:I:707:VAL:HG23	2:I:713:SER:HB2	2.01	0.42
2:E:1848:LEU:HD22	2:E:1853:ILE:HG13	2.01	0.42
2:E:3971:GLY:N	2:E:4032:GLU:OE2	2.48	0.42
2:G:4892:ARG:NH2	2:E:4899:ASP:OD1	2.52	0.42
1:F:23:VAL:H	1:F:105:ASN:HB3	1.85	0.42
2:G:1739:THR:H	2:G:1742:THR:HB	1.84	0.42
2:G:2196:ASN:OD1	2:G:2199:ARG:NH1	2.43	0.42
2:G:454:PRO:HG2	2:G:531:ARG:HH12	1.85	0.42
2:G:681:HIS:HB3	2:G:784:SER:HB3	2.01	0.42
1:A:23:VAL:H	1:A:105:ASN:HB3	1.84	0.42
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.53	0.42
2:B:983:THR:O	2:B:987:ARG:N	2.52	0.42
2:E:2107:GLN:NE2	2:E:3680:ALA:O	2.52	0.42
2:E:475:GLN:NE2	2:E:531:ARG:O	2.42	0.42
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.53	0.42
2:G:1815:LEU:HD22	2:G:1845:VAL:HG21	2.02	0.42
2:I:3362:UNK:O	2:I:3366:UNK:N	2.53	0.42
2:I:3804:ILE:HG22	2:I:3812:VAL:HG21	2.02	0.42
1:J:34:LYS:HE3	2:I:634:GLN:HB3	2.00	0.42
2:B:3804:ILE:HG22	2:B:3812:VAL:HG21	2.02	0.42
2:B:4017:LEU:HD22	2:B:4139:ILE:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1078:GLU:HB2	2:E:1235:THR:HG22	2.02	0.42
2:E:3362:UNK:O	2:E:3366:UNK:N	2.53	0.42
2:E:4017:LEU:HD22	2:E:4139:ILE:HG12	2.02	0.42
2:G:1972:ASN:HD21	2:G:2024:PRO:HB3	1.85	0.42
2:G:475:GLN:NE2	2:G:531:ARG:O	2.42	0.42
2:G:792:LEU:HD22	2:G:799:GLU:H	1.83	0.42
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.53	0.42
2:I:1739:THR:H	2:I:1742:THR:HB	1.85	0.42
2:I:286:THR:HA	2:I:405:HIS:HB2	2.00	0.42
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.42	0.42
2:B:309:THR:O	2:B:313:SER:OG	2.37	0.42
2:B:3362:UNK:O	2:B:3366:UNK:N	2.53	0.42
2:B:471:LEU:O	2:B:475:GLN:N	2.47	0.42
2:B:540:PHE:HD2	2:B:567:VAL:HG11	1.85	0.42
2:B:792:LEU:HD22	2:B:799:GLU:H	1.83	0.42
2:E:1739:THR:H	2:E:1742:THR:HB	1.85	0.42
2:E:1815:LEU:HD22	2:E:1845:VAL:HG21	2.02	0.42
2:E:3804:ILE:HG22	2:E:3812:VAL:HG21	2.02	0.42
2:G:3362:UNK:O	2:G:3366:UNK:N	2.53	0.42
2:G:3897:ASN:O	2:G:3901:ASN:ND2	2.52	0.42
2:G:4231:MET:HE3	2:G:4960:ILE:HA	2.02	0.42
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.84	0.42
1:H:23:VAL:H	1:H:105:ASN:HB3	1.85	0.42
1:A:87:HIS:HA	1:A:88:PRO:HD3	1.88	0.42
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.41	0.42
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.53	0.42
2:E:1972:ASN:HD21	2:E:2024:PRO:HB3	1.85	0.42
2:G:4017:LEU:HD22	2:G:4139:ILE:HG12	2.02	0.42
2:G:4924:VAL:HG23	2:G:4925:ILE:HG12	2.00	0.42
2:I:540:PHE:HD2	2:I:567:VAL:HG11	1.85	0.42
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	2.02	0.42
2:B:454:PRO:HG2	2:B:531:ARG:HH12	1.85	0.42
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.84	0.42
2:B:707:VAL:HG23	2:B:713:SER:HB2	2.01	0.42
2:E:45:ARG:NH2	2:E:447:ASP:OD1	2.48	0.42
2:E:454:PRO:HG2	2:E:531:ARG:HH12	1.85	0.42
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	2.02	0.42
2:E:54:ASN:O	2:E:58:VAL:N	2.44	0.42
2:E:792:LEU:HD22	2:E:799:GLU:H	1.83	0.42
2:G:730:VAL:O	2:G:735:GLN:NE2	2.53	0.42
2:G:932:LEU:HA	2:G:935:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1747:LEU:HD13	2:I:1760:HIS:CE1	2.55	0.42
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	2.02	0.42
2:I:924:MET:O	2:I:928:THR:OG1	2.34	0.42
1:J:57:LYS:HB2	1:J:80:VAL:HB	2.02	0.42
2:B:1972:ASN:HD21	2:B:2024:PRO:HB3	1.85	0.41
2:B:4984:ASN:C	2:B:4986:ALA:H	2.23	0.41
2:B:730:VAL:O	2:B:735:GLN:NE2	2.53	0.41
2:E:730:VAL:O	2:E:735:GLN:NE2	2.53	0.41
2:I:3897:ASN:O	2:I:3901:ASN:ND2	2.52	0.41
2:B:1078:GLU:HB2	2:B:1235:THR:HG22	2.02	0.41
2:B:1747:LEU:HD13	2:B:1760:HIS:CE1	2.55	0.41
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.86	0.41
2:G:1817:GLU:O	2:G:1821:ASP:N	2.49	0.41
1:A:57:LYS:HB2	1:A:80:VAL:HB	2.02	0.41
2:B:2467:VAL:HA	2:B:2470:ILE:HD12	2.03	0.41
2:E:2467:VAL:HA	2:E:2470:ILE:HD12	2.03	0.41
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	2.02	0.41
2:I:1972:ASN:HD21	2:I:2024:PRO:HB3	1.85	0.41
2:I:3677:LEU:O	2:I:3698:LEU:N	2.51	0.41
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	2.02	0.41
2:B:3897:ASN:O	2:B:3901:ASN:ND2	2.52	0.41
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	2.02	0.41
2:E:451:TYR:O	2:E:474:ARG:NH1	2.49	0.41
2:E:4658:ILE:HD11	2:E:4796:MET:HG3	2.01	0.41
2:G:2143:THR:O	2:G:3651:ASN:ND2	2.49	0.41
2:G:540:PHE:HD2	2:G:567:VAL:HG11	1.85	0.41
2:I:1101:ARG:HH21	2:I:1115:LEU:HB3	1.86	0.41
2:I:792:LEU:HD22	2:I:799:GLU:H	1.83	0.41
2:B:1269:CYS:HA	2:B:1473:UNK:HA	2.02	0.41
2:B:4231:MET:HE3	2:B:4960:ILE:HA	2.02	0.41
2:B:475:GLN:NE2	2:B:531:ARG:O	2.42	0.41
2:E:3847:PHE:HD1	2:E:3850:GLN:HE21	1.69	0.41
2:G:4899:ASP:OD1	2:I:4892:ARG:NH2	2.52	0.41
2:G:4984:ASN:C	2:G:4986:ALA:H	2.23	0.41
2:I:1815:LEU:HD22	2:I:1845:VAL:HG21	2.02	0.41
2:I:2305:CYS:HA	2:I:2324:ASN:HD22	1.86	0.41
2:I:599:VAL:HG23	2:I:600:LEU:HD12	2.03	0.41
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	2.02	0.41
2:E:1101:ARG:HH21	2:E:1115:LEU:HB3	1.86	0.41
2:E:1747:LEU:HD13	2:E:1760:HIS:CE1	2.55	0.41
2:G:1269:CYS:HA	2:G:1473:UNK:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	2.03	0.41
2:G:3847:PHE:HD1	2:G:3850:GLN:HE21	1.69	0.41
2:G:45:ARG:NH2	2:G:447:ASP:OD1	2.48	0.41
2:G:599:VAL:HG23	2:G:600:LEU:HD12	2.02	0.41
2:I:309:THR:O	2:I:313:SER:OG	2.37	0.41
2:I:3847:PHE:HD1	2:I:3850:GLN:HE21	1.69	0.41
2:I:4984:ASN:C	2:I:4986:ALA:H	2.23	0.41
1:J:7:ILE:N	1:J:71:ARG:O	2.47	0.41
2:B:1101:ARG:HH21	2:B:1115:LEU:HB3	1.86	0.41
2:B:4821:LYS:HB3	2:B:4821:LYS:HE2	1.95	0.41
2:E:4848:VAL:O	2:E:4852:THR:OG1	2.28	0.41
2:E:4928:LEU:HA	2:E:4928:LEU:HD13	1.90	0.41
2:E:932:LEU:HA	2:E:935:LEU:HD12	2.02	0.41
2:G:1078:GLU:HB2	2:G:1235:THR:HG22	2.02	0.41
2:G:1747:LEU:HD13	2:G:1760:HIS:CE1	2.55	0.41
2:I:1078:GLU:HB2	2:I:1235:THR:HG22	2.02	0.41
2:I:4658:ILE:HD11	2:I:4796:MET:HG3	2.01	0.41
2:B:1815:LEU:HD22	2:B:1845:VAL:HG21	2.02	0.41
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	2.03	0.41
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.85	0.41
2:I:4017:LEU:HD22	2:I:4139:ILE:HG12	2.02	0.41
2:I:454:PRO:HG2	2:I:531:ARG:HH12	1.85	0.41
2:I:892:THR:N	2:I:902:ARG:O	2.52	0.41
2:B:1739:THR:H	2:B:1742:THR:HB	1.85	0.41
2:B:4222:VAL:HG23	2:B:4950:VAL:HG12	2.02	0.41
2:B:932:LEU:HA	2:B:935:LEU:HD12	2.02	0.41
2:E:540:PHE:HD2	2:E:567:VAL:HG11	1.85	0.41
2:G:1859:VAL:HA	2:G:1862:ILE:HG12	2.03	0.41
2:I:1716:ILE:HG23	2:I:1720:LEU:HD13	2.03	0.41
2:I:3771:HIS:O	2:I:3774:GLY:N	2.48	0.41
2:B:1859:VAL:HA	2:B:1862:ILE:HG12	2.03	0.41
2:B:3677:LEU:O	2:B:3698:LEU:N	2.51	0.41
2:E:1859:VAL:HA	2:E:1862:ILE:HG12	2.03	0.41
2:E:2034:PHE:O	2:E:2038:LEU:N	2.54	0.41
1:F:7:ILE:N	1:F:71:ARG:O	2.47	0.41
2:G:2305:CYS:HA	2:G:2324:ASN:HD22	1.86	0.41
2:G:4558:ASN:OD1	2:G:4558:ASN:N	2.54	0.41
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.33	0.41
2:I:730:VAL:O	2:I:735:GLN:NE2	2.53	0.41
2:B:3676:ASP:N	2:B:3676:ASP:OD1	2.54	0.41
2:B:3847:PHE:HD1	2:B:3850:GLN:HE21	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2196:ASN:OD1	2:E:2199:ARG:NH1	2.44	0.41
2:E:3677:LEU:O	2:E:3698:LEU:N	2.51	0.41
2:E:4998:LYS:NZ	2:E:5007:GLU:OE1	2.38	0.41
2:G:119:SER:HA	2:G:146:CYS:HA	2.03	0.41
1:H:57:LYS:HB2	1:H:80:VAL:HB	2.02	0.41
2:I:1808:ARG:NH1	2:I:1853:ILE:O	2.54	0.41
2:I:2143:THR:O	2:I:3651:ASN:ND2	2.49	0.41
2:B:1657:LEU:HD13	2:B:1657:LEU:HA	1.95	0.40
2:B:4822:THR:O	2:B:4825:THR:OG1	2.31	0.40
2:B:512:ALA:HA	2:B:515:TRP:HB2	2.03	0.40
2:B:16:THR:OG1	2:B:97:GLY:O	2.39	0.40
2:E:1269:CYS:HA	2:E:1473:UNK:HA	2.02	0.40
2:E:2305:CYS:HA	2:E:2324:ASN:HD22	1.86	0.40
2:G:1141:ARG:HD2	2:G:1141:ARG:H	1.86	0.40
2:G:615:ARG:NH2	2:G:1677:GLY:O	2.41	0.40
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.85	0.40
2:I:1641:ILE:HA	2:I:1642:PRO:HD3	1.92	0.40
2:I:16:THR:OG1	2:I:97:GLY:O	2.39	0.40
2:B:2029:GLN:O	2:B:2033:ASP:N	2.50	0.40
2:B:4697:VAL:O	2:B:4701:TRP:N	2.50	0.40
1:F:57:LYS:HB2	1:F:80:VAL:HB	2.02	0.40
2:G:1973:GLN:HA	2:G:1976:ARG:HB3	2.04	0.40
2:G:3781:GLN:HA	2:G:3784:SER:HB3	2.04	0.40
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	2.02	0.40
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	2.03	0.40
2:I:2029:GLN:O	2:I:2033:ASP:N	2.50	0.40
2:I:3994:HIS:O	2:I:3998:HIS:ND1	2.39	0.40
2:B:1685:LEU:HD22	2:B:1718:ILE:HG21	2.03	0.40
2:B:2305:CYS:HA	2:B:2324:ASN:HD22	1.86	0.40
2:B:2437:ALA:HA	2:B:2438:PRO:HD3	1.95	0.40
2:B:4710:SER:HB3	2:B:4713:SER:HB3	2.03	0.40
2:G:983:THR:O	2:G:987:ARG:N	2.52	0.40
2:I:1685:LEU:HD22	2:I:1718:ILE:HG21	2.03	0.40
2:I:471:LEU:O	2:I:475:GLN:N	2.47	0.40
2:B:3923:LEU:HD13	2:B:3961:VAL:HG11	2.04	0.40
2:B:4681:LEU:HD21	2:B:4687:TYR:HD2	1.86	0.40
2:E:4984:ASN:C	2:E:4986:ALA:H	2.23	0.40
2:G:1592:PRO:HA	2:G:1593:PRO:HD3	1.98	0.40
2:G:1716:ILE:HG23	2:G:1720:LEU:HD13	2.03	0.40
2:G:4681:LEU:HD21	2:G:4687:TYR:HD2	1.86	0.40
2:G:512:ALA:HA	2:G:515:TRP:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3781:GLN:HA	2:I:3784:SER:HB3	2.04	0.40
2:I:3773:ARG:HG3	2:I:3815:LYS:HZ3	1.86	0.40
2:I:932:LEU:HA	2:I:935:LEU:HD12	2.02	0.40
2:I:983:THR:O	2:I:987:ARG:N	2.52	0.40
2:B:119:SER:HA	2:B:146:CYS:HA	2.03	0.40
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	2.03	0.40
2:B:2587:UNK:O	2:B:2591:UNK:N	2.55	0.40
2:B:594:GLY:H	2:B:1594:ARG:HD3	1.87	0.40
2:B:907:LEU:O	2:B:963:ASN:ND2	2.40	0.40
2:E:2029:GLN:O	2:E:2033:ASP:N	2.50	0.40
2:E:321:GLU:HB3	2:E:322:LYS:H	1.76	0.40
2:E:472:ARG:HA	2:E:475:GLN:HB2	2.03	0.40
2:E:599:VAL:HG23	2:E:600:LEU:HD12	2.02	0.40
2:G:1101:ARG:HH21	2:G:1115:LEU:HB3	1.86	0.40
2:I:2034:PHE:O	2:I:2038:LEU:N	2.54	0.40
2:I:2467:VAL:HA	2:I:2470:ILE:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	F	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	B	3235/4416 (73%)	2890 (89%)	338 (10%)	7 (0%)	51	85
2	E	3235/4416 (73%)	2888 (89%)	340 (10%)	7 (0%)	51	85
2	G	3235/4416 (73%)	2889 (89%)	339 (10%)	7 (0%)	51	85

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	3235/4416 (73%)	2889 (89%)	339 (10%)	7 (0%)	51	85
All	All	13360/18096 (74%)	11932 (89%)	1400 (10%)	28 (0%)	54	85

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	G	1708	ARG
2	I	1708	ARG
2	E	1708	ARG
2	E	4985	LEU
2	B	4962	GLY
2	B	4985	LEU
2	G	4641	PRO
2	G	4962	GLY
2	G	4985	LEU
2	I	4641	PRO
2	I	4962	GLY
2	I	4985	LEU
2	E	4962	GLY
2	B	1840	PRO
2	B	4641	PRO
2	G	1840	PRO
2	I	1840	PRO
2	E	1840	PRO
2	E	4641	PRO
2	B	2291	GLN
2	G	2291	GLN
2	I	2291	GLN
2	E	2291	GLN
2	B	1932	PRO
2	G	1932	PRO
2	I	1932	PRO
2	E	1932	PRO

5.3.2 Protein sidechains ⓘ

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%)	2474 (99%)	19 (1%)	85	92
2	E	2493/3022 (82%)	2474 (99%)	19 (1%)	85	92
2	G	2493/3022 (82%)	2474 (99%)	19 (1%)	85	92
2	I	2493/3022 (82%)	2474 (99%)	19 (1%)	85	92
All	All	10324/12444 (83%)	10248 (99%)	76 (1%)	87	93

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	534	ARG
2	B	553	ARG
2	B	978	THR
2	B	1076	ARG
2	B	1141	ARG
2	B	1600	LEU
2	B	1676	LEU
2	B	1964	ARG
2	B	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	4166	LEU
2	B	4961	CYS
2	B	4983	HIS
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	978	THR
2	G	1076	ARG
2	G	1141	ARG

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Mol	Chain	Res	Type
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	4166	LEU
2	G	4961	CYS
2	G	4983	HIS
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	978	THR
2	I	1076	ARG
2	I	1141	ARG
2	I	1600	LEU
2	I	1676	LEU
2	I	1964	ARG
2	I	3663	LEU
2	I	3787	LYS
2	I	3805	LEU
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4166	LEU
2	I	4961	CYS
2	I	4983	HIS
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
2	E	978	THR
2	E	1076	ARG
2	E	1141	ARG
2	E	1600	LEU
2	E	1676	LEU
2	E	1964	ARG
2	E	3663	LEU

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Mol	Chain	Res	Type
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	4166	LEU
2	E	4961	CYS
2	E	4983	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (132) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	43	ASN
1	F	87	HIS
1	A	43	ASN
1	A	87	HIS
1	H	43	ASN
1	H	87	HIS
1	J	43	ASN
1	J	87	HIS
2	B	57	ASN
2	B	71	GLN
2	B	111	HIS
2	B	224	HIS
2	B	273	HIS
2	B	379	HIS
2	B	413	GLN
2	B	479	GLN
2	B	725	HIS
2	B	838	HIS
2	B	1598	GLN
2	B	1691	GLN
2	B	1719	HIS
2	B	1760	HIS
2	B	1775	HIS
2	B	2127	GLN
2	B	3809	ASN
2	B	3889	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN

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Mol	Chain	Res	Type
2	B	3960	GLN
2	B	4034	ASN
2	B	4054	ASN
2	B	4120	ASN
2	B	4142	ASN
2	B	4806	ASN
2	B	4833	ASN
2	B	4978	HIS
2	B	4983	HIS
2	B	5003	HIS
2	G	57	ASN
2	G	71	GLN
2	G	111	HIS
2	G	224	HIS
2	G	273	HIS
2	G	379	HIS
2	G	413	GLN
2	G	479	GLN
2	G	725	HIS
2	G	838	HIS
2	G	1598	GLN
2	G	1691	GLN
2	G	1719	HIS
2	G	1760	HIS
2	G	1775	HIS
2	G	2127	GLN
2	G	3809	ASN
2	G	3889	GLN
2	G	3896	ASN
2	G	3900	GLN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	4034	ASN
2	G	4054	ASN
2	G	4120	ASN
2	G	4142	ASN
2	G	4806	ASN
2	G	4833	ASN
2	G	4978	HIS
2	G	4983	HIS
2	G	5003	HIS

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Mol	Chain	Res	Type
2	I	57	ASN
2	I	71	GLN
2	I	111	HIS
2	I	224	HIS
2	I	273	HIS
2	I	379	HIS
2	I	413	GLN
2	I	479	GLN
2	I	725	HIS
2	I	838	HIS
2	I	1598	GLN
2	I	1691	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	2127	GLN
2	I	3809	ASN
2	I	3889	GLN
2	I	3896	ASN
2	I	3900	GLN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	4034	ASN
2	I	4054	ASN
2	I	4120	ASN
2	I	4142	ASN
2	I	4806	ASN
2	I	4833	ASN
2	I	4978	HIS
2	I	4983	HIS
2	I	5003	HIS
2	E	57	ASN
2	E	71	GLN
2	E	111	HIS
2	E	224	HIS
2	E	273	HIS
2	E	379	HIS
2	E	413	GLN
2	E	479	GLN
2	E	725	HIS
2	E	838	HIS
2	E	1598	GLN

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Mol	Chain	Res	Type
2	E	1691	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	2127	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	4034	ASN
2	E	4054	ASN
2	E	4120	ASN
2	E	4142	ASN
2	E	4806	ASN
2	E	4833	ASN
2	E	4978	HIS
2	E	4983	HIS
2	E	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	-	27,33,33	0.90	1 (3%)	25,52,52	1.63	3 (12%)
4	CFF	B	5102	-	7,15,15	2.00	2 (28%)	8,23,23	1.27	1 (12%)
3	ATP	E	5101	-	27,33,33	0.90	1 (3%)	25,52,52	1.64	3 (12%)
4	CFF	E	5102	-	7,15,15	1.99	2 (28%)	8,23,23	1.27	1 (12%)
3	ATP	G	5101	-	27,33,33	0.90	1 (3%)	25,52,52	1.63	3 (12%)
4	CFF	G	5102	-	7,15,15	2.00	2 (28%)	8,23,23	1.28	1 (12%)
3	ATP	I	5101	-	27,33,33	0.90	1 (3%)	25,52,52	1.63	3 (12%)
4	CFF	I	5102	-	7,15,15	2.00	2 (28%)	8,23,23	1.27	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 (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	5102	CFF	C6-N1	-4.10	1.32	1.38
4	B	5102	CFF	C6-N1	-4.07	1.32	1.38
4	E	5102	CFF	C6-N1	-4.07	1.32	1.38
4	I	5102	CFF	C6-N1	-4.06	1.32	1.38
4	I	5102	CFF	O13-C6	-2.38	1.18	1.24
4	B	5102	CFF	O13-C6	-2.36	1.18	1.24
4	G	5102	CFF	O13-C6	-2.35	1.18	1.24
4	E	5102	CFF	O13-C6	-2.34	1.18	1.24
3	G	5101	ATP	C5-C4	2.94	1.47	1.40
3	E	5101	ATP	C5-C4	2.95	1.47	1.40
3	B	5101	ATP	C5-C4	2.95	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	5101	ATP	C5-C4	2.96	1.47	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5101	ATP	N3-C2-N1	-5.35	124.20	128.86
3	B	5101	ATP	N3-C2-N1	-5.31	124.23	128.86
3	G	5101	ATP	N3-C2-N1	-5.30	124.25	128.86
3	I	5101	ATP	N3-C2-N1	-5.28	124.26	128.86
3	E	5101	ATP	C4-C5-N7	-3.32	106.20	109.41
3	I	5101	ATP	C4-C5-N7	-3.32	106.21	109.41
3	B	5101	ATP	C4-C5-N7	-3.28	106.24	109.41
3	G	5101	ATP	C4-C5-N7	-3.27	106.25	109.41
4	E	5102	CFF	C14-N7-C8	-2.84	111.94	125.45
4	B	5102	CFF	C14-N7-C8	-2.84	111.96	125.45
4	G	5102	CFF	C14-N7-C8	-2.83	111.98	125.45
4	I	5102	CFF	C14-N7-C8	-2.83	111.99	125.45
3	G	5101	ATP	C4'-O4'-C1'	2.11	112.02	109.77
3	B	5101	ATP	C4'-O4'-C1'	2.14	112.04	109.77
3	I	5101	ATP	C4'-O4'-C1'	2.16	112.07	109.77
3	E	5101	ATP	C4'-O4'-C1'	2.17	112.08	109.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

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

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	73.47
1	G	4345:UNK	C	4540:PHE	N	73.47
1	I	4345:UNK	C	4540:PHE	N	73.47
1	E	4345:UNK	C	4540:PHE	N	73.47
1	B	3613:UNK	C	3639:THR	N	45.62
1	G	3613:UNK	C	3639:THR	N	45.62
1	I	3613:UNK	C	3639:THR	N	45.62
1	E	3613:UNK	C	3639:THR	N	45.62
1	B	4253:GLU	C	4320:UNK	N	27.90
1	G	4253:GLU	C	4320:UNK	N	27.90
1	I	4253:GLU	C	4320:UNK	N	27.90
1	E	4253:GLU	C	4320:UNK	N	27.90
1	B	3163:UNK	C	3170:UNK	N	15.83
1	G	3163:UNK	C	3170:UNK	N	15.83
1	I	3163:UNK	C	3170:UNK	N	15.83
1	E	3163:UNK	C	3170:UNK	N	15.83
1	B	3063:UNK	C	3134:UNK	N	14.87
1	G	3063:UNK	C	3134:UNK	N	14.87
1	I	3063:UNK	C	3134:UNK	N	14.87
1	E	3063:UNK	C	3134:UNK	N	14.87
1	B	3468:UNK	C	3511:UNK	N	14.52
1	G	3468:UNK	C	3511:UNK	N	14.52
1	I	3468:UNK	C	3511:UNK	N	14.52
1	E	3468:UNK	C	3511:UNK	N	14.52
1	B	2703:UNK	C	2734:ASN	N	13.45
1	G	2703:UNK	C	2734:ASN	N	13.45
1	I	2703:UNK	C	2734:ASN	N	13.45
1	E	2703:UNK	C	2734:ASN	N	13.45
1	B	3236:UNK	C	3241:UNK	N	12.87
1	G	3236:UNK	C	3241:UNK	N	12.87
1	I	3236:UNK	C	3241:UNK	N	12.87
1	E	3236:UNK	C	3241:UNK	N	12.87

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1564:UNK	C	1573:MET	N	12.40
1	G	1564:UNK	C	1573:MET	N	12.40
1	I	1564:UNK	C	1573:MET	N	12.40
1	E	1564:UNK	C	1573:MET	N	12.40
1	B	2976:UNK	C	2995:UNK	N	12.24
1	G	2976:UNK	C	2995:UNK	N	12.24
1	I	2976:UNK	C	2995:UNK	N	12.24
1	E	2976:UNK	C	2995:UNK	N	12.24
1	B	3254:UNK	C	3261:UNK	N	8.57
1	G	3254:UNK	C	3261:UNK	N	8.57
1	I	3254:UNK	C	3261:UNK	N	8.57
1	E	3254:UNK	C	3261:UNK	N	8.57
1	B	1297:UNK	C	1430:UNK	N	5.81
1	G	1297:UNK	C	1430:UNK	N	5.81
1	I	1297:UNK	C	1430:UNK	N	5.81
1	E	1297:UNK	C	1430:UNK	N	5.81
1	B	2939:ARG	C	2942:UNK	N	3.33
1	G	2939:ARG	C	2942:UNK	N	3.33
1	I	2939:ARG	C	2942:UNK	N	3.33
1	E	2939:ARG	C	2942:UNK	N	3.33
1	B	2479:LEU	C	2487:UNK	N	3.30
1	G	2479:LEU	C	2487:UNK	N	3.30
1	I	2479:LEU	C	2487:UNK	N	3.30
1	E	2479:LEU	C	2487:UNK	N	3.30