



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Sep 3, 2017 – 05:55 PM EDT

PDB ID : 5T15
EMDB ID: : EMD-8342
Title : Structural basis for gating and activation of RyR1 (30 uM Ca²⁺ dataset, all particles)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on : unknown
Resolution : 3.60 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
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) : rb-20029824

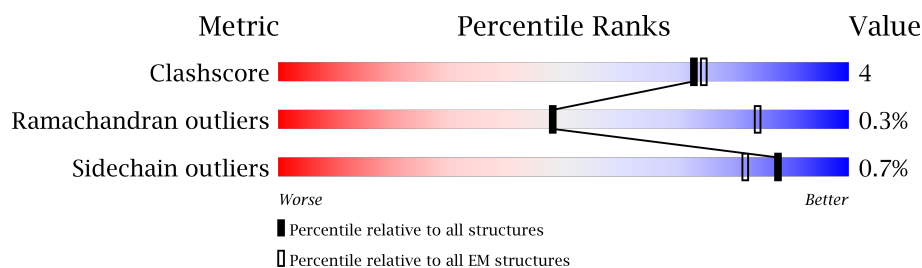
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	87% 12% .
1	F	108	89% 10% .
1	H	108	88% 11% .
1	J	108	89% 10% .
2	B	4676	80% 8% 11%
2	E	4676	81% 8% 11%
2	G	4676	80% 8% 11%
2	I	4676	80% 8% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 120796 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,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4170	Total	C	N	O	S	0	0
			29379	18614	5204	5404	157		
2	E	4170	Total	C	N	O	S	0	0
			29379	18614	5204	5404	157		
2	I	4170	Total	C	N	O	S	0	0
			29379	18614	5204	5404	157		
2	G	4170	Total	C	N	O	S	0	0
			29379	18614	5204	5404	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	

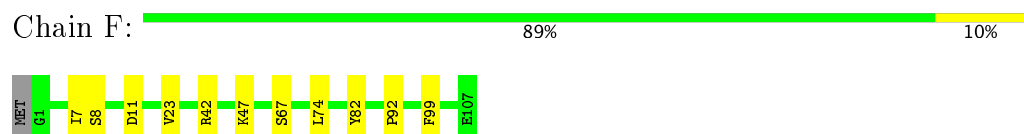
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

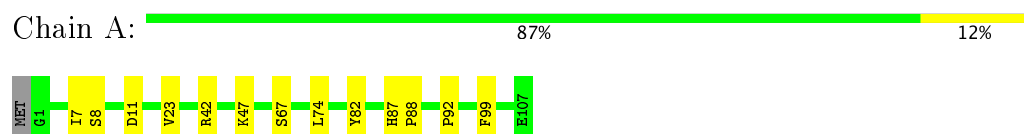
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

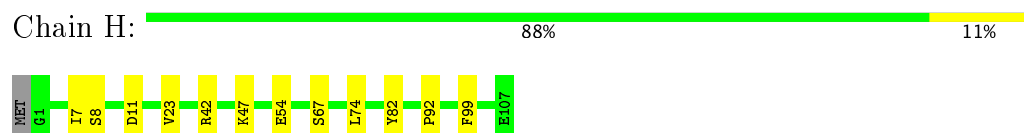
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



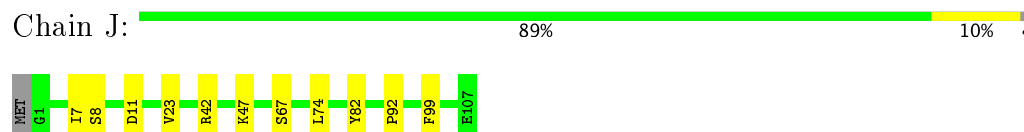
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



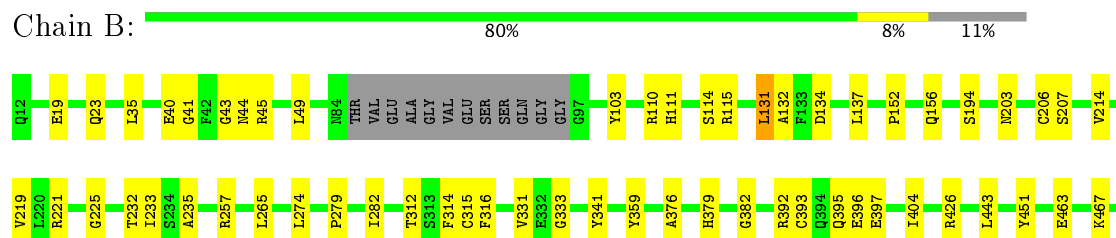
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



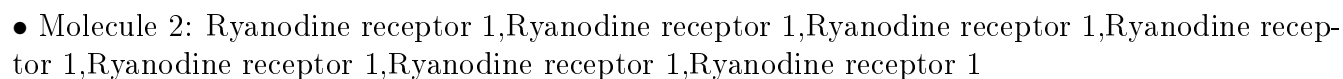
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



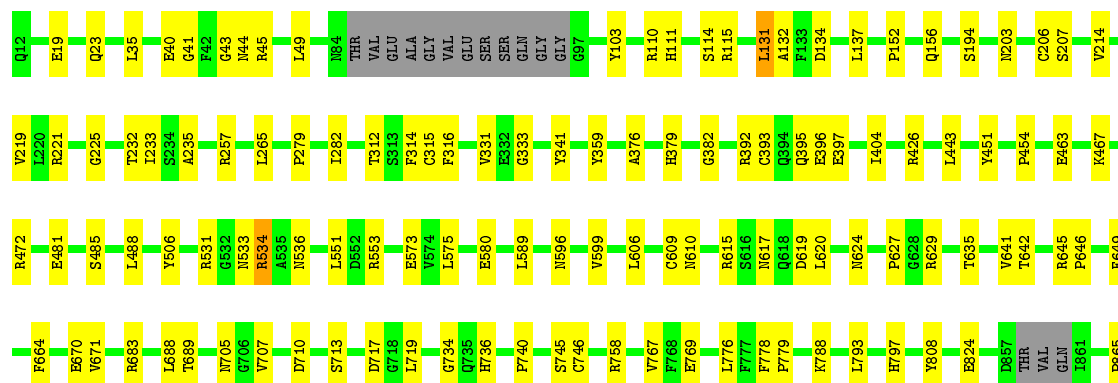
- Molecule 2: Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1



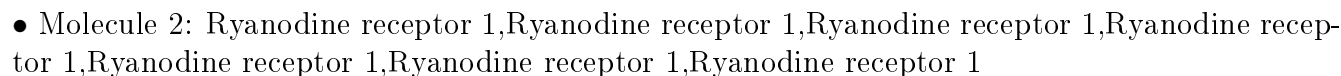


Response	Percentage
Yes	80%
No	8%
Don't know	11%





Response	Percentage
Yes	80%
No	8%
Don't know	11%






4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	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	0.37	0/834	0.55	0/1123
1	F	0.37	0/834	0.55	0/1123
1	H	0.37	0/834	0.55	0/1123
1	J	0.37	0/834	0.55	0/1123
2	B	0.40	0/25438	0.60	11/34548 (0.0%)
2	E	0.40	0/25438	0.60	11/34548 (0.0%)
2	G	0.40	0/25438	0.60	11/34548 (0.0%)
2	I	0.40	0/25438	0.60	11/34548 (0.0%)
All	All	0.40	0/105088	0.59	44/142684 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	F	0	3
1	H	0	3
1	J	0	3
2	B	0	22
2	E	0	22
2	G	0	22
2	I	0	22
All	All	0	100

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	131	LEU	CA-CB-CG	7.90	133.47	115.30
2	I	131	LEU	CA-CB-CG	7.90	133.47	115.30
2	E	131	LEU	CA-CB-CG	7.89	133.46	115.30
2	G	131	LEU	CA-CB-CG	7.89	133.44	115.30
2	B	2290	LEU	CA-CB-CG	7.21	131.87	115.30
2	E	2290	LEU	CA-CB-CG	7.19	131.84	115.30
2	G	2290	LEU	CA-CB-CG	7.19	131.83	115.30
2	I	2290	LEU	CA-CB-CG	7.18	131.82	115.30
2	I	1600	LEU	CA-CB-CG	7.10	131.63	115.30
2	B	1600	LEU	CA-CB-CG	7.10	131.63	115.30
2	G	1600	LEU	CA-CB-CG	7.10	131.62	115.30
2	E	1600	LEU	CA-CB-CG	7.09	131.61	115.30
2	I	1676	LEU	CA-CB-CG	6.48	130.20	115.30
2	G	1676	LEU	CA-CB-CG	6.47	130.18	115.30
2	B	1676	LEU	CA-CB-CG	6.47	130.18	115.30
2	E	1676	LEU	CA-CB-CG	6.47	130.17	115.30
2	E	4639	MET	C-N-CA	6.20	137.21	121.70
2	B	4639	MET	C-N-CA	6.20	137.20	121.70
2	G	4639	MET	C-N-CA	6.19	137.18	121.70
2	I	4639	MET	C-N-CA	6.18	137.15	121.70
2	I	688	LEU	CA-CB-CG	6.08	129.28	115.30
2	E	688	LEU	CA-CB-CG	6.05	129.22	115.30
2	B	688	LEU	CA-CB-CG	6.05	129.22	115.30
2	G	688	LEU	CA-CB-CG	6.05	129.22	115.30
2	G	1712	TYR	CA-CB-CG	-5.99	102.02	113.40
2	I	1712	TYR	CA-CB-CG	-5.98	102.03	113.40
2	B	1712	TYR	CA-CB-CG	-5.97	102.06	113.40
2	E	1712	TYR	CA-CB-CG	-5.96	102.07	113.40
2	B	977	LEU	CA-CB-CG	5.81	128.66	115.30
2	G	977	LEU	CA-CB-CG	5.81	128.66	115.30
2	E	977	LEU	CA-CB-CG	5.81	128.66	115.30
2	I	977	LEU	CA-CB-CG	5.80	128.63	115.30
2	E	1698	LEU	CA-CB-CG	5.42	127.77	115.30
2	G	1698	LEU	CA-CB-CG	5.42	127.77	115.30
2	B	1698	LEU	CA-CB-CG	5.42	127.76	115.30
2	I	1698	LEU	CA-CB-CG	5.42	127.76	115.30
2	I	2291	GLN	C-N-CA	5.22	134.76	121.70
2	B	2291	GLN	C-N-CA	5.20	134.71	121.70
2	E	2291	GLN	C-N-CA	5.20	134.70	121.70
2	G	2291	GLN	C-N-CA	5.20	134.69	121.70
2	E	4133	GLN	C-N-CA	5.08	134.39	121.70
2	B	4133	GLN	C-N-CA	5.06	134.35	121.70
2	I	4133	GLN	C-N-CA	5.04	134.31	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	4133	GLN	C-N-CA	5.04	134.31	121.70

There are no chirality outliers.

All (100) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	7	ILE	Peptide
1	A	8	SER	Peptide
1	A	82	TYR	Peptide
2	B	137	LEU	Peptide
2	B	1676	LEU	Peptide
2	B	1690	ASP	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	2342	ASN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	312	THR	Peptide
2	B	3771	HIS	Peptide
2	B	3971	GLY	Peptide
2	B	4096	ALA	Peptide
2	B	4175	ARG	Peptide
2	B	4198	SER	Peptide
2	B	4228	ALA	Peptide
2	B	4666	VAL	Peptide
2	B	4807	PHE	Peptide
2	B	4958	CYS	Peptide
2	B	624	ASN	Peptide
2	B	808	TYR	Peptide
2	B	977	LEU	Peptide
2	E	137	LEU	Peptide
2	E	1676	LEU	Peptide
2	E	1690	ASP	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	2342	ASN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	312	THR	Peptide
2	E	3771	HIS	Peptide

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Mol	Chain	Res	Type	Group
2	E	3971	GLY	Peptide
2	E	4096	ALA	Peptide
2	E	4175	ARG	Peptide
2	E	4198	SER	Peptide
2	E	4228	ALA	Peptide
2	E	4666	VAL	Peptide
2	E	4807	PHE	Peptide
2	E	4958	CYS	Peptide
2	E	624	ASN	Peptide
2	E	808	TYR	Peptide
2	E	977	LEU	Peptide
1	F	7	ILE	Peptide
1	F	8	SER	Peptide
1	F	82	TYR	Peptide
2	G	137	LEU	Peptide
2	G	1676	LEU	Peptide
2	G	1690	ASP	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	2342	ASN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	312	THR	Peptide
2	G	3771	HIS	Peptide
2	G	3971	GLY	Peptide
2	G	4096	ALA	Peptide
2	G	4175	ARG	Peptide
2	G	4198	SER	Peptide
2	G	4228	ALA	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	4958	CYS	Peptide
2	G	624	ASN	Peptide
2	G	808	TYR	Peptide
2	G	977	LEU	Peptide
1	H	7	ILE	Peptide
1	H	8	SER	Peptide
1	H	82	TYR	Peptide
2	I	137	LEU	Peptide
2	I	1676	LEU	Peptide
2	I	1690	ASP	Peptide

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Mol	Chain	Res	Type	Group
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	2342	ASN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	312	THR	Peptide
2	I	3771	HIS	Peptide
2	I	3971	GLY	Peptide
2	I	4096	ALA	Peptide
2	I	4175	ARG	Peptide
2	I	4198	SER	Peptide
2	I	4228	ALA	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	4958	CYS	Peptide
2	I	624	ASN	Peptide
2	I	808	TYR	Peptide
2	I	977	LEU	Peptide
1	J	7	ILE	Peptide
1	J	8	SER	Peptide
1	J	82	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	6	0
1	F	818	0	824	5	0
1	H	818	0	824	6	0
1	J	818	0	824	5	0
2	B	29379	0	24730	221	0
2	E	29379	0	24729	219	0
2	G	29379	0	24730	223	0
2	I	29379	0	24729	221	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	120796	0	102214	875	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 4.

All (875) 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:G:379:HIS:HD2	2:G:382:GLY:H	1.40	0.70
2:I:379:HIS:HD2	2:I:382:GLY:H	1.40	0.70
2:G:2287:ALA:HA	2:G:2290:LEU:HD13	1.75	0.69
2:B:2287:ALA:HA	2:B:2290:LEU:HD13	1.75	0.69
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.74	0.69
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.74	0.69
2:B:379:HIS:HD2	2:B:382:GLY:H	1.40	0.67
2:I:2287:ALA:HA	2:I:2290:LEU:HD13	1.75	0.67
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.74	0.67
2:E:2287:ALA:HA	2:E:2290:LEU:HD13	1.75	0.67
2:E:379:HIS:HD2	2:E:382:GLY:H	1.40	0.67
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.74	0.67
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.77	0.67
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.78	0.66
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.77	0.66
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.78	0.66
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.78	0.66
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.77	0.66
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.78	0.65
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.77	0.65
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.71	0.64
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.71	0.64
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.79	0.64
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.79	0.64
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.71	0.64
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.71	0.64
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.81	0.63
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:670:GLU:HG3	2:I:788:LYS:H	1.64	0.63
2:G:670:GLU:HG3	2:G:788:LYS:H	1.64	0.63
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.81	0.63
2:B:670:GLU:HG3	2:B:788:LYS:H	1.64	0.63
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.79	0.62
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.81	0.62
2:E:670:GLU:HG3	2:E:788:LYS:H	1.64	0.62
2:B:3767:GLN:OE1	2:B:3809:ASN:ND2	2.33	0.62
2:E:3767:GLN:OE1	2:E:3809:ASN:ND2	2.33	0.62
1:H:92:PRO:HD3	2:G:627:PRO:HB2	1.81	0.62
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.81	0.62
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.33	0.61
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.34	0.61
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.33	0.61
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.34	0.61
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.34	0.61
2:G:3767:GLN:OE1	2:G:3809:ASN:ND2	2.33	0.61
2:I:4567:LEU:HA	2:I:4816:ILE:HD12	1.83	0.61
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.33	0.60
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.33	0.60
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.34	0.60
2:E:4567:LEU:HA	2:E:4816:ILE:HD12	1.83	0.60
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.66	0.60
2:I:645:ARG:HH11	2:I:778:PHE:HE1	1.49	0.60
2:G:4567:LEU:HA	2:G:4816:ILE:HD12	1.83	0.60
2:B:41:GLY:O	2:B:45:ARG:NH1	2.35	0.60
2:B:1148:VAL:HG21	2:B:1212:ARG:HG2	1.84	0.59
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.66	0.59
2:I:3767:GLN:OE1	2:I:3809:ASN:ND2	2.33	0.59
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.85	0.59
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.66	0.59
2:B:4567:LEU:HA	2:B:4816:ILE:HD12	1.83	0.59
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.85	0.59
2:B:645:ARG:HH11	2:B:778:PHE:HE1	1.49	0.59
2:G:1148:VAL:HG21	2:G:1212:ARG:HG2	1.84	0.59
2:I:41:GLY:O	2:I:45:ARG:NH1	2.35	0.59
2:B:2764:GLU:HG3	2:B:2857:PRO:HB2	1.84	0.59
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.85	0.59
2:I:2764:GLU:HG3	2:I:2857:PRO:HB2	1.84	0.59
2:E:41:GLY:O	2:E:45:ARG:NH1	2.35	0.59
2:E:2764:GLU:HG3	2:E:2857:PRO:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.85	0.59
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.67	0.59
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.66	0.59
2:E:1148:VAL:HG21	2:E:1212:ARG:HG2	1.84	0.58
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.67	0.58
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.85	0.58
2:E:645:ARG:HH11	2:E:778:PHE:HE1	1.49	0.58
2:G:41:GLY:O	2:G:45:ARG:NH1	2.35	0.58
2:I:1148:VAL:HG21	2:I:1212:ARG:HG2	1.84	0.58
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.35	0.58
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.36	0.58
2:G:2764:GLU:HG3	2:G:2857:PRO:HB2	1.84	0.58
2:G:645:ARG:HH11	2:G:778:PHE:HE1	1.49	0.58
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.85	0.58
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.67	0.58
2:B:2758:PHE:O	2:B:2762:THR:N	2.36	0.58
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.86	0.58
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.85	0.58
2:E:359:TYR:HA	2:E:376:ALA:HA	1.85	0.58
2:I:359:TYR:HA	2:I:376:ALA:HA	1.85	0.58
2:B:359:TYR:HA	2:B:376:ALA:HA	1.85	0.58
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.67	0.58
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.85	0.58
2:G:359:TYR:HA	2:G:376:ALA:HA	1.85	0.57
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.85	0.57
2:I:2758:PHE:O	2:I:2762:THR:N	2.36	0.57
2:B:3809:ASN:HB3	2:B:3812:VAL:HG22	1.86	0.57
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.37	0.57
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.86	0.57
2:B:1703:LEU:HD12	2:B:1708:ARG:HB2	1.87	0.57
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.37	0.57
2:G:1244:GLN:OE1	2:G:1646:ARG:NH1	2.38	0.57
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.85	0.57
2:B:35:LEU:HD13	2:B:49:LEU:HD13	1.86	0.57
2:E:1244:GLN:OE1	2:E:1646:ARG:NH1	2.38	0.57
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.85	0.57
2:G:1703:LEU:HD12	2:G:1708:ARG:HB2	1.87	0.57
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.35	0.57
2:B:4933:GLN:OE1	2:E:4933:GLN:NE2	2.37	0.57
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.85	0.57
2:I:4933:GLN:NE2	2:G:4933:GLN:OE1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.38	0.57
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.78	0.57
2:B:4914:VAL:HG21	2:E:4884:LEU:HD11	1.87	0.57
2:I:1244:GLN:OE1	2:I:1646:ARG:NH1	2.38	0.57
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.78	0.57
2:G:35:LEU:HD13	2:G:49:LEU:HD13	1.86	0.57
2:I:1703:LEU:HD12	2:I:1708:ARG:HB2	1.87	0.57
2:I:627:PRO:O	2:I:629:ARG:NH1	2.38	0.57
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.37	0.56
2:G:2758:PHE:O	2:G:2762:THR:N	2.36	0.56
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.38	0.56
2:G:627:PRO:O	2:G:629:ARG:NH1	2.38	0.56
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.38	0.56
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.85	0.56
2:E:627:PRO:O	2:E:629:ARG:NH1	2.38	0.56
2:G:3809:ASN:HB3	2:G:3812:VAL:HG22	1.86	0.56
2:I:3809:ASN:HB3	2:I:3812:VAL:HG22	1.86	0.56
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.87	0.56
2:B:23:GLN:OE1	2:B:203:ASN:ND2	2.38	0.56
2:E:23:GLN:OE1	2:E:203:ASN:ND2	2.38	0.56
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.38	0.56
2:G:23:GLN:OE1	2:G:203:ASN:ND2	2.38	0.56
2:I:35:LEU:HD13	2:I:49:LEU:HD13	1.86	0.56
2:B:132:ALA:HA	2:B:194:SER:HB2	1.87	0.56
2:B:4933:GLN:NE2	2:I:4933:GLN:OE1	2.38	0.56
2:E:1703:LEU:HD12	2:E:1708:ARG:HB2	1.87	0.56
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.37	0.56
2:E:132:ALA:HA	2:E:194:SER:HB2	1.88	0.56
2:E:35:LEU:HD13	2:E:49:LEU:HD13	1.86	0.56
2:E:3809:ASN:HB3	2:E:3812:VAL:HG22	1.86	0.56
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.88	0.56
2:E:4933:GLN:OE1	2:G:4933:GLN:NE2	2.37	0.56
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.86	0.56
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.88	0.56
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.86	0.56
2:B:1244:GLN:OE1	2:B:1646:ARG:NH1	2.38	0.56
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.87	0.56
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.38	0.56
2:I:793:LEU:HD12	2:I:797:HIS:H	1.71	0.56
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.38	0.56
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.38	0.56
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.88	0.56
2:B:627:PRO:O	2:B:629:ARG:NH1	2.38	0.56
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.88	0.56
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.35	0.55
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.88	0.55
2:I:609:CYS:SG	2:I:610:ASN:N	2.80	0.55
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.78	0.55
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.38	0.55
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.88	0.55
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.80	0.55
2:E:331:VAL:HG12	2:E:333:GLY:H	1.72	0.55
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.87	0.55
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.88	0.55
2:I:23:GLN:OE1	2:I:203:ASN:ND2	2.38	0.55
2:B:4581:LYS:HD2	2:B:4632:LEU:HD22	1.89	0.55
2:G:609:CYS:SG	2:G:610:ASN:N	2.79	0.55
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.38	0.55
2:B:609:CYS:SG	2:B:610:ASN:N	2.79	0.55
2:E:2758:PHE:O	2:E:2762:THR:N	2.36	0.55
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.80	0.55
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.80	0.55
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.87	0.55
2:E:4914:VAL:HG21	2:G:4884:LEU:HD11	1.89	0.55
2:G:793:LEU:HD12	2:G:797:HIS:H	1.71	0.55
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.80	0.55
2:G:331:VAL:HG12	2:G:333:GLY:H	1.72	0.55
2:I:132:ALA:HA	2:I:194:SER:HB2	1.88	0.55
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.88	0.55
2:B:4079:ASP:OD2	2:I:4736:ARG:NH1	2.40	0.55
2:I:4171:LEU:O	2:I:4175:ARG:NH2	2.41	0.54
2:E:609:CYS:SG	2:E:610:ASN:N	2.79	0.54
2:G:132:ALA:HA	2:G:194:SER:HB2	1.88	0.54
2:G:4171:LEU:O	2:G:4175:ARG:NH2	2.41	0.54
2:I:4884:LEU:HD11	2:G:4914:VAL:HG21	1.88	0.54
2:I:4581:LYS:HD2	2:I:4632:LEU:HD22	1.89	0.54
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	1.90	0.54
2:B:793:LEU:HD12	2:B:797:HIS:H	1.71	0.54
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.78	0.54
2:B:331:VAL:HG12	2:B:333:GLY:H	1.72	0.54
2:I:331:VAL:HG12	2:I:333:GLY:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.38	0.54
2:B:4171:LEU:O	2:B:4175:ARG:NH2	2.41	0.54
2:E:793:LEU:HD12	2:E:797:HIS:H	1.71	0.54
2:I:4198:SER:OG	2:I:4199:GLU:N	2.41	0.54
2:B:2347:GLU:O	2:B:2351:ASN:N	2.41	0.54
2:B:4198:SER:OG	2:B:4199:GLU:N	2.41	0.53
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	1.90	0.53
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	1.90	0.53
2:G:2347:GLU:O	2:G:2351:ASN:N	2.41	0.53
2:I:2347:GLU:O	2:I:2351:ASN:N	2.41	0.53
2:B:4884:LEU:HD11	2:I:4914:VAL:HG21	1.90	0.53
2:G:4581:LYS:HD2	2:G:4632:LEU:HD22	1.89	0.53
2:B:4736:ARG:NH1	2:E:4079:ASP:OD2	2.41	0.53
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.90	0.53
2:I:1663:HIS:HD2	2:I:1707:LEU:HD11	1.73	0.53
2:E:4171:LEU:O	2:E:4175:ARG:NH2	2.41	0.53
2:E:4581:LYS:HD2	2:E:4632:LEU:HD22	1.89	0.53
2:E:683:ARG:HG2	2:E:717:ASP:HB3	1.91	0.53
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	1.90	0.53
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.90	0.53
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.42	0.53
2:E:2342:ASN:OD1	2:E:2342:ASN:N	2.34	0.53
2:E:2347:GLU:O	2:E:2351:ASN:N	2.41	0.53
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.38	0.53
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.42	0.53
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.42	0.53
2:I:606:LEU:O	2:I:617:ASN:ND2	2.42	0.53
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.90	0.52
2:B:1663:HIS:HD2	2:B:1707:LEU:HD11	1.74	0.52
2:E:606:LEU:O	2:E:617:ASN:ND2	2.42	0.52
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.42	0.52
2:I:4956:THR:O	2:I:4965:SER:N	2.43	0.52
2:B:156:GLN:HE22	2:E:225:GLY:HA2	1.75	0.52
2:E:4198:SER:OG	2:E:4199:GLU:N	2.41	0.52
2:G:4198:SER:OG	2:G:4199:GLU:N	2.41	0.52
2:I:1973:GLN:O	2:I:1977:TYR:N	2.43	0.52
2:G:606:LEU:O	2:G:617:ASN:ND2	2.42	0.52
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.43	0.52
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.90	0.52
2:B:683:ARG:HG2	2:B:717:ASP:HB3	1.91	0.52
2:G:1663:HIS:HD2	2:G:1707:LEU:HD11	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1131:ARG:HH12	2:G:1178:ALA:HB3	1.75	0.52
2:B:4956:THR:O	2:B:4965:SER:N	2.43	0.52
2:E:1131:ARG:HH12	2:E:1178:ALA:HB3	1.75	0.52
2:B:606:LEU:O	2:B:617:ASN:ND2	2.42	0.52
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.43	0.52
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	1.92	0.52
2:I:225:GLY:HA2	2:G:156:GLN:HE22	1.74	0.52
2:G:1973:GLN:O	2:G:1977:TYR:N	2.43	0.52
2:G:4956:THR:O	2:G:4965:SER:N	2.43	0.52
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.91	0.51
2:G:2815:ALA:HB3	2:G:2881:ASN:HD21	1.75	0.51
2:I:683:ARG:HG2	2:I:717:ASP:HB3	1.91	0.51
2:B:1131:ARG:HH12	2:B:1178:ALA:HB3	1.75	0.51
2:I:1738:LEU:HB3	2:I:2146:PRO:HD3	1.93	0.51
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.34	0.51
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	1.91	0.51
2:E:1663:HIS:HD2	2:E:1707:LEU:HD11	1.74	0.51
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.43	0.51
2:G:683:ARG:HG2	2:G:717:ASP:HB3	1.91	0.51
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.93	0.51
2:B:225:GLY:HA2	2:I:156:GLN:HE22	1.74	0.51
2:E:1738:LEU:HB3	2:E:2146:PRO:HD3	1.93	0.51
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.92	0.51
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	1.91	0.51
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.91	0.51
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.92	0.51
2:B:1973:GLN:O	2:B:1977:TYR:N	2.43	0.51
2:B:2290:LEU:HG	2:B:2291:GLN:H	1.76	0.51
2:B:2131:LEU:HB3	2:B:3662:ILE:HD13	1.93	0.51
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.93	0.51
2:E:1973:GLN:O	2:E:1977:TYR:N	2.43	0.51
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.92	0.51
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.91	0.51
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.93	0.51
2:G:1738:LEU:HB3	2:G:2146:PRO:HD3	1.92	0.51
2:E:156:GLN:HE22	2:G:225:GLY:HA2	1.76	0.51
2:I:2131:LEU:HB3	2:I:3662:ILE:HD13	1.93	0.51
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.46	0.51
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.43	0.51
2:E:2290:LEU:HG	2:E:2291:GLN:H	1.76	0.51
2:G:1729:SER:HB3	2:G:2163:ARG:HH11	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.91	0.50
2:E:4956:THR:O	2:E:4965:SER:N	2.43	0.50
2:G:551:LEU:HD21	2:G:589:LEU:HD13	1.93	0.50
2:B:1738:LEU:HB3	2:B:2146:PRO:HD3	1.92	0.50
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	1.91	0.50
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.44	0.50
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.45	0.50
2:B:2815:ALA:HB3	2:B:2881:ASN:HD21	1.75	0.50
2:G:1245:PHE:HD1	2:G:1600:LEU:HB3	1.76	0.50
2:I:1729:SER:HB3	2:I:2163:ARG:HH11	1.76	0.50
2:I:4079:ASP:OD2	2:G:4736:ARG:NH1	2.41	0.50
2:E:235:ALA:HA	2:E:257:ARG:HD3	1.93	0.50
2:I:1131:ARG:HH12	2:I:1178:ALA:HB3	1.75	0.50
2:I:2236:LEU:HD23	2:I:2275:VAL:HG21	1.94	0.50
2:I:2290:LEU:HG	2:I:2291:GLN:H	1.76	0.50
2:B:4848:VAL:O	2:B:4852:THR:OG1	2.28	0.50
2:E:2236:LEU:HD23	2:E:2275:VAL:HG21	1.94	0.50
2:E:2815:ALA:HB3	2:E:2881:ASN:HD21	1.76	0.50
2:E:551:LEU:HD21	2:E:589:LEU:HD13	1.94	0.50
2:G:2131:LEU:HB3	2:G:3662:ILE:HD13	1.93	0.50
2:G:2236:LEU:HD23	2:G:2275:VAL:HG21	1.94	0.50
2:B:2236:LEU:HD23	2:B:2275:VAL:HG21	1.94	0.50
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.93	0.50
2:I:551:LEU:HD21	2:I:589:LEU:HD13	1.94	0.50
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.92	0.50
2:B:1729:SER:HB3	2:B:2163:ARG:HH11	1.76	0.50
2:B:235:ALA:HA	2:B:257:ARG:HD3	1.93	0.50
2:I:1245:PHE:HD1	2:I:1600:LEU:HB3	1.76	0.50
2:I:235:ALA:HA	2:I:257:ARG:HD3	1.93	0.50
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.46	0.50
2:B:1245:PHE:HD1	2:B:1600:LEU:HB3	1.76	0.50
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.46	0.50
2:E:2131:LEU:HB3	2:E:3662:ILE:HD13	1.93	0.50
2:G:1675:ALA:HB1	2:G:1676:LEU:HD13	1.94	0.50
2:I:1730:MET:O	2:I:1772:ARG:NH1	2.45	0.50
2:B:551:LEU:HD21	2:B:589:LEU:HD13	1.94	0.49
2:E:1675:ALA:HB1	2:E:1676:LEU:HD13	1.94	0.49
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.45	0.49
2:G:4092:ASP:OD1	2:G:4092:ASP:N	2.45	0.49
2:I:1840:PRO:O	2:I:1844:LEU:N	2.45	0.49
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1840:PRO:O	2:G:1844:LEU:N	2.45	0.49
2:G:2290:LEU:HG	2:G:2291:GLN:H	1.76	0.49
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.45	0.49
2:B:1840:PRO:O	2:B:1844:LEU:N	2.45	0.49
2:E:1245:PHE:HD1	2:E:1600:LEU:HB3	1.76	0.49
2:E:1729:SER:HB3	2:E:2163:ARG:HH11	1.76	0.49
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.46	0.49
2:I:2815:ALA:HB3	2:I:2881:ASN:HD21	1.75	0.49
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.31	0.49
2:I:3889:GLN:HG3	2:I:3967:GLU:HG3	1.95	0.49
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.45	0.49
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.45	0.49
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.31	0.49
1:F:92:PRO:HD3	2:E:627:PRO:HB2	1.95	0.49
2:B:4092:ASP:OD1	2:B:4092:ASP:N	2.45	0.49
2:E:1730:MET:O	2:E:1772:ARG:NH1	2.45	0.49
2:I:2868:SER:O	2:I:2872:GLN:N	2.46	0.49
2:E:580:GLU:HG3	2:E:620:LEU:HD22	1.94	0.49
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.95	0.49
2:G:1730:MET:O	2:G:1772:ARG:NH1	2.45	0.49
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.45	0.49
2:I:1096:THR:HG23	2:I:1199:VAL:HG22	1.95	0.49
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.95	0.49
2:B:1096:THR:HG23	2:B:1199:VAL:HG22	1.95	0.49
2:B:1730:MET:O	2:B:1772:ARG:NH1	2.45	0.49
2:E:2159:LEU:HD22	2:E:2201:LEU:HD23	1.94	0.49
2:G:221:ARG:NH2	2:G:397:GLU:OE2	2.45	0.49
2:G:580:GLU:HG3	2:G:620:LEU:HD22	1.94	0.49
2:I:580:GLU:HG3	2:I:620:LEU:HD22	1.94	0.49
2:E:2823:ILE:HG12	2:E:2937:VAL:HG22	1.95	0.49
2:G:3889:GLN:HG3	2:G:3967:GLU:HG3	1.95	0.49
2:I:1675:ALA:HB1	2:I:1676:LEU:HD13	1.94	0.49
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.45	0.49
2:I:2823:ILE:HG12	2:I:2937:VAL:HG22	1.95	0.49
2:I:4634:GLU:HG3	2:I:4636:THR:H	1.77	0.49
2:B:1675:ALA:HB1	2:B:1676:LEU:HD13	1.94	0.48
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.95	0.48
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.95	0.48
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.95	0.48
2:E:3889:GLN:HG3	2:E:3967:GLU:HG3	1.95	0.48
2:G:1096:THR:HG23	2:G:1199:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:11:ASP:OD1	1:H:67:SER:OG	2.31	0.48
2:B:4634:GLU:HG3	2:B:4636:THR:H	1.77	0.48
2:G:235:ALA:HA	2:G:257:ARG:HD3	1.93	0.48
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.31	0.48
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.95	0.48
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.78	0.48
2:E:1096:THR:HG23	2:E:1199:VAL:HG22	1.95	0.48
2:E:1840:PRO:O	2:E:1844:LEU:N	2.45	0.48
2:G:4634:GLU:HG3	2:G:4636:THR:H	1.77	0.48
2:B:2823:ILE:HG12	2:B:2937:VAL:HG22	1.95	0.48
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.31	0.48
2:E:4634:GLU:HG3	2:E:4636:THR:H	1.77	0.48
2:G:2823:ILE:HG12	2:G:2937:VAL:HG22	1.95	0.48
2:I:2159:LEU:HD22	2:I:2201:LEU:HD23	1.94	0.48
2:E:940:GLY:O	2:E:1052:ASN:N	2.47	0.48
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	1.96	0.48
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	1.96	0.48
2:B:2159:LEU:HD22	2:B:2201:LEU:HD23	1.94	0.48
2:B:3889:GLN:HG3	2:B:3967:GLU:HG3	1.95	0.48
2:B:2342:ASN:N	2:B:2342:ASN:OD1	2.34	0.48
2:E:645:ARG:O	2:E:824:GLU:N	2.47	0.48
2:I:940:GLY:O	2:I:1052:ASN:N	2.47	0.48
2:B:940:GLY:O	2:B:1052:ASN:N	2.47	0.48
2:E:4680:LYS:HD3	2:E:4686:LEU:HD22	1.96	0.48
2:G:2159:LEU:HD22	2:G:2201:LEU:HD23	1.94	0.48
2:E:2868:SER:O	2:E:2872:GLN:N	2.46	0.48
2:G:2868:SER:O	2:G:2872:GLN:N	2.46	0.48
2:G:3552:UNK:O	2:G:3556:UNK:N	2.47	0.48
2:G:689:THR:H	2:G:778:PHE:HE2	1.62	0.48
2:B:645:ARG:O	2:B:824:GLU:N	2.47	0.47
2:B:734:GLY:O	2:B:736:HIS:ND1	2.47	0.47
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.96	0.47
2:I:4092:ASP:OD1	2:I:4092:ASP:N	2.45	0.47
2:I:4629:TYR:OH	2:G:4860:ARG:NH2	2.42	0.47
2:E:4092:ASP:N	2:E:4092:ASP:OD1	2.45	0.47
2:I:3552:UNK:O	2:I:3556:UNK:N	2.47	0.47
2:B:221:ARG:NH2	2:B:397:GLU:OE2	2.45	0.47
2:B:689:THR:H	2:B:778:PHE:HE2	1.61	0.47
2:G:940:GLY:O	2:G:1052:ASN:N	2.47	0.47
2:G:265:LEU:HD12	2:G:279:PRO:HB2	1.97	0.47
2:B:2022:PRO:HB2	2:B:2024:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	1.96	0.47
2:E:4736:ARG:NH1	2:G:4079:ASP:OD2	2.42	0.47
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.78	0.47
2:B:219:VAL:O	2:B:392:ARG:NH1	2.48	0.47
2:E:265:LEU:HD12	2:E:279:PRO:HB2	1.96	0.47
2:I:219:VAL:O	2:I:392:ARG:NH1	2.48	0.47
2:I:534:ARG:NH2	2:I:573:GLU:OE2	2.42	0.47
2:B:580:GLU:HG3	2:B:620:LEU:HD22	1.94	0.47
2:E:1839:VAL:O	2:E:1841:VAL:N	2.48	0.47
2:I:4228:ALA:O	2:I:4232:GLU:N	2.48	0.47
2:B:2868:SER:O	2:B:2872:GLN:N	2.46	0.47
2:G:219:VAL:O	2:G:392:ARG:NH1	2.48	0.47
2:G:645:ARG:O	2:G:824:GLU:N	2.47	0.47
2:I:734:GLY:O	2:I:736:HIS:ND1	2.47	0.47
2:E:3552:UNK:O	2:E:3556:UNK:N	2.47	0.47
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.95	0.47
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.78	0.47
2:G:4978:HIS:ND1	2:G:4982:GLU:OE1	2.32	0.47
2:E:4978:HIS:ND1	2:E:4982:GLU:OE1	2.32	0.47
2:G:3770:LEU:HD12	2:G:3770:LEU:HA	1.74	0.47
2:G:4228:ALA:O	2:G:4232:GLU:N	2.48	0.47
2:I:1839:VAL:O	2:I:1841:VAL:N	2.48	0.47
2:B:111:HIS:CD2	2:B:114:SER:H	2.33	0.47
2:B:615:ARG:NH1	2:B:1677:GLY:O	2.39	0.47
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.97	0.47
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.80	0.47
2:E:2022:PRO:HB2	2:E:2024:PRO:HD2	1.96	0.47
2:E:4181:ILE:HG22	2:E:4193:ILE:HB	1.97	0.47
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.95	0.47
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.80	0.47
2:I:1792:ALA:HB2	2:I:2173:GLN:HG3	1.97	0.47
2:I:265:LEU:HD12	2:I:279:PRO:HB2	1.97	0.47
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.80	0.47
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.96	0.47
2:E:111:HIS:CD2	2:E:114:SER:H	2.33	0.47
2:G:111:HIS:CD2	2:G:114:SER:H	2.33	0.47
2:I:111:HIS:CD2	2:I:114:SER:H	2.33	0.47
2:I:2022:PRO:HB2	2:I:2024:PRO:HD2	1.96	0.47
2:I:221:ARG:NH2	2:I:397:GLU:OE2	2.45	0.47
2:I:689:THR:H	2:I:778:PHE:HE2	1.62	0.47
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1839:VAL:O	2:B:1841:VAL:N	2.48	0.46
2:E:1715:LEU:HD12	2:E:1719:HIS:HD2	1.80	0.46
2:E:877:ASN:HD22	2:E:1045:THR:HG23	1.78	0.46
2:G:1792:ALA:HB2	2:G:2173:GLN:HG3	1.97	0.46
2:B:3552:UNK:O	2:B:3556:UNK:N	2.48	0.46
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.80	0.46
2:G:1715:LEU:HD12	2:G:1719:HIS:HD2	1.80	0.46
2:G:734:GLY:O	2:G:736:HIS:ND1	2.47	0.46
2:B:265:LEU:HD12	2:B:279:PRO:HB2	1.96	0.46
2:B:4228:ALA:O	2:B:4232:GLU:N	2.48	0.46
2:E:689:THR:H	2:E:778:PHE:HE2	1.62	0.46
2:E:898:ASP:HB3	2:E:901:LYS:HB2	1.98	0.46
2:G:1839:VAL:O	2:G:1841:VAL:N	2.48	0.46
2:G:2022:PRO:HB2	2:G:2024:PRO:HD2	1.96	0.46
2:G:4181:ILE:HG22	2:G:4193:ILE:HB	1.97	0.46
2:G:898:ASP:HB3	2:G:901:LYS:HB2	1.98	0.46
2:I:645:ARG:O	2:I:824:GLU:N	2.47	0.46
2:B:396:GLU:OE2	2:B:451:TYR:OH	2.34	0.46
2:G:4848:VAL:O	2:G:4852:THR:OG1	2.28	0.46
1:J:92:PRO:HD3	2:I:627:PRO:HB2	1.97	0.46
2:B:1715:LEU:HD12	2:B:1719:HIS:HD2	1.80	0.46
2:G:534:ARG:NH2	2:G:573:GLU:OE2	2.42	0.46
2:G:617:ASN:OD1	2:G:617:ASN:N	2.49	0.46
2:G:619:ASP:OD1	2:G:1680:ARG:NH1	2.40	0.46
2:I:2827:ARG:HH21	2:I:2931:GLN:HG3	1.81	0.46
2:G:2827:ARG:HH21	2:G:2931:GLN:HG3	1.81	0.46
2:I:898:ASP:HB3	2:I:901:LYS:HB2	1.98	0.46
2:B:2827:ARG:HH21	2:B:2931:GLN:HG3	1.81	0.46
2:B:898:ASP:HB3	2:B:901:LYS:HB2	1.98	0.46
2:E:219:VAL:O	2:E:392:ARG:NH1	2.48	0.46
2:G:2745:VAL:HG21	2:G:2818:ALA:HB2	1.98	0.46
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.96	0.46
2:I:1772:ARG:HH21	2:I:1952:GLN:NE2	2.14	0.46
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.97	0.46
2:I:396:GLU:OE2	2:I:451:TYR:OH	2.34	0.46
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.98	0.46
2:B:1772:ARG:HH21	2:B:1952:GLN:NE2	2.14	0.46
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.98	0.46
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.98	0.46
2:E:111:HIS:HD2	2:E:114:SER:H	1.64	0.46
2:E:2745:VAL:HG21	2:E:2818:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.98	0.46
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.97	0.46
2:I:1715:LEU:HD12	2:I:1719:HIS:HD2	1.80	0.46
2:I:4181:ILE:HG22	2:I:4193:ILE:HB	1.97	0.46
2:I:485:SER:HA	2:I:488:LEU:HB2	1.98	0.46
2:B:1792:ALA:HB2	2:B:2173:GLN:HG3	1.97	0.45
2:E:1772:ARG:HH21	2:E:1952:GLN:NE2	2.14	0.45
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.81	0.45
1:J:11:ASP:OD1	1:J:67:SER:OG	2.31	0.45
2:B:4181:ILE:HG22	2:B:4193:ILE:HB	1.97	0.45
2:B:4629:TYR:OH	2:I:4860:ARG:NH2	2.41	0.45
2:B:4860:ARG:NH2	2:E:4629:TYR:OH	2.40	0.45
2:E:4791:TYR:OH	2:E:4815:ASP:O	2.33	0.45
2:G:485:SER:HA	2:G:488:LEU:HB2	1.98	0.45
2:I:2029:GLN:O	2:I:2033:ASP:N	2.49	0.45
2:E:1099:GLU:OE2	2:E:1127:HIS:ND1	2.38	0.45
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.98	0.45
2:E:2827:ARG:HH21	2:E:2931:GLN:HG3	1.81	0.45
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.97	0.45
2:E:5027:CYS:O	2:E:5029:ARG:N	2.48	0.45
2:B:668:VAL:O	2:B:741:GLU:N	2.47	0.45
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.82	0.45
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.50	0.45
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.82	0.45
2:I:2024:PRO:O	2:I:2028:ARG:NE	2.40	0.45
2:B:619:ASP:OD1	2:B:1680:ARG:NH1	2.40	0.45
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.81	0.45
2:E:1792:ALA:HB2	2:E:2173:GLN:HG3	1.97	0.45
2:E:485:SER:HA	2:E:488:LEU:HB2	1.98	0.45
2:G:596:ASN:HB3	2:G:599:VAL:HG22	1.99	0.45
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.82	0.45
2:I:596:ASN:HB3	2:I:599:VAL:HG22	1.99	0.45
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.50	0.45
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.98	0.45
2:E:221:ARG:NH2	2:E:397:GLU:OE2	2.45	0.45
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.98	0.45
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.82	0.45
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.98	0.45
2:B:596:ASN:HB3	2:B:599:VAL:HG22	1.99	0.45
2:E:4228:ALA:O	2:E:4232:GLU:N	2.48	0.45
2:E:396:GLU:OE2	2:E:451:TYR:OH	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:596:ASN:HB3	2:E:599:VAL:HG22	1.99	0.45
2:E:668:VAL:O	2:E:741:GLU:N	2.47	0.45
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.98	0.45
2:B:617:ASN:N	2:B:617:ASN:OD1	2.49	0.45
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	1.98	0.45
2:E:2747:ILE:HG12	2:E:2817:ILE:HD12	1.99	0.45
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.50	0.45
2:I:111:HIS:HD2	2:I:114:SER:H	1.64	0.45
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	1.98	0.45
2:B:485:SER:HA	2:B:488:LEU:HB2	1.98	0.45
2:B:534:ARG:NH2	2:B:573:GLU:OE2	2.42	0.45
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.81	0.45
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.25	0.45
1:A:11:ASP:OD1	1:A:67:SER:OG	2.31	0.44
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.50	0.44
2:B:2765:LYS:HA	2:B:2859:PRO:HG3	1.99	0.44
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.99	0.44
2:E:40:GLU:HB3	2:E:44:ASN:HB3	1.99	0.44
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.98	0.44
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.98	0.44
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.50	0.44
2:I:232:THR:OG1	2:I:233:ILE:N	2.50	0.44
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.98	0.44
2:B:1855:GLY:H	2:B:1858:ASP:HB2	1.83	0.44
2:E:615:ARG:NH1	2:E:1677:GLY:O	2.39	0.44
2:E:788:LYS:HG2	2:E:1629:GLN:HA	1.99	0.44
2:G:1855:GLY:H	2:G:1858:ASP:HB2	1.82	0.44
2:G:396:GLU:OE2	2:G:451:TYR:OH	2.34	0.44
2:G:40:GLU:HB3	2:G:44:ASN:HB3	1.99	0.44
2:G:788:LYS:HG2	2:G:1629:GLN:HA	1.99	0.44
2:I:1099:GLU:OE2	2:I:1127:HIS:ND1	2.38	0.44
2:B:2231:SER:HA	2:B:2234:ARG:HG2	2.00	0.44
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.99	0.44
2:G:2024:PRO:O	2:G:2028:ARG:NE	2.40	0.44
2:I:1855:GLY:H	2:I:1858:ASP:HB2	1.82	0.44
2:I:2231:SER:HA	2:I:2234:ARG:HG2	2.00	0.44
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	1.98	0.44
2:B:111:HIS:HD2	2:B:114:SER:H	1.64	0.44
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.99	0.44
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.81	0.44
2:B:2029:GLN:O	2:B:2033:ASP:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2745:VAL:HG21	2:B:2818:ALA:HB2	1.98	0.44
2:B:40:GLU:HB3	2:B:44:ASN:HB3	1.99	0.44
2:G:2342:ASN:N	2:G:2342:ASN:OD1	2.34	0.44
2:I:2188:ASN:OD1	2:I:2188:ASN:N	2.49	0.44
2:I:2745:VAL:HG21	2:I:2818:ALA:HB2	1.98	0.44
2:I:2747:ILE:HG12	2:I:2817:ILE:HD12	1.99	0.44
2:I:40:GLU:HB3	2:I:44:ASN:HB3	1.99	0.44
2:B:788:LYS:HG2	2:B:1629:GLN:HA	1.99	0.44
2:E:1855:GLY:H	2:E:1858:ASP:HB2	1.82	0.44
2:G:111:HIS:HD2	2:G:114:SER:H	1.64	0.44
2:G:4138:ASP:N	2:G:4138:ASP:OD1	2.51	0.44
2:I:4642:ALA:HA	2:I:4645:CYS:HB2	2.00	0.44
2:B:5027:CYS:O	2:B:5029:ARG:N	2.48	0.44
2:E:4642:ALA:HA	2:E:4645:CYS:HB2	2.00	0.44
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.50	0.44
2:G:2029:GLN:O	2:G:2033:ASP:N	2.49	0.44
2:G:43:GLY:HA2	2:G:443:LEU:HG	2.00	0.44
2:B:3770:LEU:HD12	2:B:3770:LEU:HA	1.74	0.44
2:E:2231:SER:HA	2:E:2234:ARG:HG2	2.00	0.44
2:E:617:ASN:N	2:E:617:ASN:OD1	2.49	0.44
2:G:2102:VAL:HB	2:G:2124:LEU:HD12	1.99	0.44
2:I:2765:LYS:HA	2:I:2859:PRO:HG3	1.99	0.44
2:E:2102:VAL:HB	2:E:2124:LEU:HD12	1.99	0.44
2:E:2765:LYS:HA	2:E:2859:PRO:HG3	1.98	0.44
2:G:1772:ARG:HH21	2:G:1952:GLN:NE2	2.14	0.44
2:G:2747:ILE:HG12	2:G:2817:ILE:HD12	1.99	0.44
2:G:4642:ALA:HA	2:G:4645:CYS:HB2	2.00	0.44
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	2.00	0.44
2:B:134:ASP:OD1	2:B:134:ASP:N	2.51	0.44
2:B:2747:ILE:HG12	2:B:2817:ILE:HD12	1.99	0.44
2:B:3365:UNK:O	2:B:3369:UNK:N	2.51	0.44
2:E:134:ASP:N	2:E:134:ASP:OD1	2.51	0.44
2:E:4138:ASP:N	2:E:4138:ASP:OD1	2.51	0.44
1:F:11:ASP:OD1	1:F:67:SER:OG	2.31	0.44
2:G:232:THR:OG1	2:G:233:ILE:N	2.50	0.44
2:G:4815:ASP:N	2:G:4815:ASP:OD1	2.50	0.44
2:I:615:ARG:NH1	2:I:1677:GLY:O	2.39	0.44
2:I:2739:PRO:HD2	2:I:2888:ARG:HH21	1.83	0.44
2:I:788:LYS:HG2	2:I:1629:GLN:HA	1.99	0.44
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.50	0.44
2:B:4642:ALA:HA	2:B:4645:CYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4924:VAL:HA	2:B:4928:LEU:HB2	2.00	0.43
2:E:43:GLY:HA2	2:E:443:LEU:HG	2.00	0.43
2:G:2231:SER:HA	2:G:2234:ARG:HG2	2.00	0.43
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.98	0.43
2:B:2447:LYS:HG3	2:B:2449:GLU:H	1.83	0.43
2:B:2739:PRO:HD2	2:B:2888:ARG:HH21	1.83	0.43
2:E:2447:LYS:HG3	2:E:2449:GLU:H	1.83	0.43
2:E:4063:ASP:OD1	2:E:4169:SER:OG	2.28	0.43
2:G:206:CYS:SG	2:G:207:SER:N	2.92	0.43
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	1.98	0.43
2:G:668:VAL:O	2:G:741:GLU:N	2.47	0.43
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	2.00	0.43
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	2.00	0.43
2:G:1707:LEU:O	2:G:1709:ALA:N	2.51	0.43
2:I:4138:ASP:N	2:I:4138:ASP:OD1	2.51	0.43
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	2.00	0.43
2:E:4681:LEU:HD21	2:E:4687:TYR:HD2	1.84	0.43
2:E:734:GLY:O	2:E:736:HIS:ND1	2.47	0.43
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.99	0.43
2:I:206:CYS:SG	2:I:207:SER:N	2.92	0.43
2:B:1707:LEU:O	2:B:1709:ALA:N	2.51	0.43
2:E:206:CYS:SG	2:E:207:SER:N	2.92	0.43
2:G:2188:ASN:OD1	2:G:2188:ASN:N	2.49	0.43
2:G:2765:LYS:HA	2:G:2859:PRO:HG3	1.98	0.43
2:B:206:CYS:SG	2:B:207:SER:N	2.92	0.43
2:B:2102:VAL:HB	2:B:2124:LEU:HD12	1.99	0.43
1:A:92:PRO:HD3	2:B:627:PRO:HB2	2.00	0.43
2:E:1707:LEU:O	2:E:1709:ALA:N	2.51	0.43
2:E:2739:PRO:HD2	2:E:2888:ARG:HH21	1.83	0.43
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.52	0.43
2:G:4924:VAL:HA	2:G:4928:LEU:HB2	2.00	0.43
2:I:2447:LYS:HG3	2:I:2449:GLU:H	1.83	0.43
2:I:43:GLY:HA2	2:I:443:LEU:HG	2.00	0.43
2:B:43:GLY:HA2	2:B:443:LEU:HG	2.00	0.43
2:E:635:THR:HG23	2:E:1693:GLN:HE22	1.84	0.43
2:E:2188:ASN:OD1	2:E:2188:ASN:N	2.49	0.43
2:E:232:THR:OG1	2:E:233:ILE:N	2.51	0.43
2:G:5027:CYS:O	2:G:5029:ARG:N	2.48	0.43
2:G:635:THR:HG23	2:G:1693:GLN:HE22	1.84	0.43
2:I:4681:LEU:HD21	2:I:4687:TYR:HD2	1.84	0.43
2:E:1126:GLY:HA3	2:E:1143:TRP:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4142:ASN:HA	2:E:4145:VAL:HG12	2.01	0.43
2:E:4924:VAL:HA	2:E:4928:LEU:HB2	2.00	0.43
2:G:134:ASP:OD1	2:G:134:ASP:N	2.51	0.43
2:G:3905:THR:HA	2:G:3912:THR:HG23	2.01	0.43
2:G:4681:LEU:HD21	2:G:4687:TYR:HD2	1.84	0.43
2:I:2102:VAL:HB	2:I:2124:LEU:HD12	1.99	0.43
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.54	0.43
2:B:232:THR:OG1	2:B:233:ILE:N	2.50	0.43
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	2.00	0.43
2:G:2447:LYS:HG3	2:G:2449:GLU:H	1.83	0.43
2:I:710:ASP:OD1	2:I:710:ASP:N	2.52	0.43
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.25	0.43
2:B:4681:LEU:HD21	2:B:4687:TYR:HD2	1.84	0.43
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.50	0.43
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	2.00	0.43
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.54	0.43
2:G:4791:TYR:OH	2:G:4815:ASP:O	2.33	0.43
2:I:4063:ASP:OD1	2:I:4169:SER:OG	2.28	0.43
2:B:1126:GLY:HA3	2:B:1143:TRP:CE2	2.54	0.42
2:B:710:ASP:N	2:B:710:ASP:OD1	2.52	0.42
2:G:2739:PRO:HD2	2:G:2888:ARG:HH21	1.83	0.42
2:G:4063:ASP:OD1	2:G:4169:SER:OG	2.28	0.42
2:I:3804:ILE:HG22	2:I:3812:VAL:HG21	2.01	0.42
2:B:2188:ASN:N	2:B:2188:ASN:OD1	2.49	0.42
2:B:4063:ASP:OD1	2:B:4169:SER:OG	2.28	0.42
2:G:315:CYS:SG	2:G:316:PHE:N	2.92	0.42
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	2.01	0.42
2:E:2788:HIS:HE1	2:E:2790:MET:HB2	1.84	0.42
2:E:534:ARG:NH2	2:E:573:GLU:OE2	2.43	0.42
2:G:2827:ARG:H	2:G:2934:GLY:HA3	1.85	0.42
2:G:3365:UNK:O	2:G:3369:UNK:N	2.52	0.42
2:I:1707:LEU:O	2:I:1709:ALA:N	2.51	0.42
2:I:2788:HIS:HE1	2:I:2790:MET:HB2	1.84	0.42
2:I:2827:ARG:H	2:I:2934:GLY:HA3	1.85	0.42
2:I:315:CYS:SG	2:I:316:PHE:N	2.92	0.42
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.40	0.42
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.52	0.42
2:E:2029:GLN:O	2:E:2033:ASP:N	2.49	0.42
2:E:2339:VAL:HG12	2:E:2345:SER:H	1.85	0.42
2:E:3365:UNK:O	2:E:3369:UNK:N	2.52	0.42
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1840:PRO:HB3	2:I:1843:LYS:HB3	2.02	0.42
2:I:3365:UNK:O	2:I:3369:UNK:N	2.52	0.42
2:I:3905:THR:HA	2:I:3912:THR:HG23	2.01	0.42
2:I:4142:ASN:HA	2:I:4145:VAL:HG12	2.01	0.42
2:I:4815:ASP:N	2:I:4815:ASP:OD1	2.50	0.42
2:I:4924:VAL:HA	2:I:4928:LEU:HB2	2.00	0.42
1:A:87:HIS:HA	1:A:88:PRO:HD3	1.94	0.42
2:B:1840:PRO:HB3	2:B:1843:LYS:HB3	2.02	0.42
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.49	0.42
2:B:2788:HIS:HE1	2:B:2790:MET:HB2	1.84	0.42
2:B:2827:ARG:H	2:B:2934:GLY:HA3	1.85	0.42
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.49	0.42
2:G:3804:ILE:HG22	2:G:3812:VAL:HG21	2.01	0.42
2:G:4922:PHE:HA	2:G:4926:VAL:HG12	2.01	0.42
2:I:2215:LEU:HD21	2:I:2272:PRO:HG3	2.02	0.42
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	2.01	0.42
2:B:4142:ASN:HA	2:B:4145:VAL:HG12	2.01	0.42
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.52	0.42
2:E:3676:ASP:N	2:E:3676:ASP:OD1	2.52	0.42
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.52	0.42
2:G:4142:ASN:HA	2:G:4145:VAL:HG12	2.01	0.42
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	2.01	0.42
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.52	0.42
2:I:4922:PHE:HA	2:I:4926:VAL:HG12	2.01	0.42
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	2.00	0.42
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	2.01	0.42
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	2.00	0.42
2:B:635:THR:HG23	2:B:1693:GLN:HE22	1.84	0.42
2:E:2827:ARG:H	2:E:2934:GLY:HA3	1.85	0.42
2:E:315:CYS:SG	2:E:316:PHE:N	2.92	0.42
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	2.01	0.42
2:E:710:ASP:N	2:E:710:ASP:OD1	2.52	0.42
2:G:1099:GLU:OE2	2:G:1127:HIS:ND1	2.38	0.42
2:G:2788:HIS:CE1	2:G:2790:MET:HB2	2.55	0.42
2:G:2788:HIS:HE1	2:G:2790:MET:HB2	1.85	0.42
2:G:282:ILE:HD12	2:G:314:PHE:HD2	1.85	0.42
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	2.01	0.42
2:B:3905:THR:HA	2:B:3912:THR:HG23	2.01	0.42
2:B:4922:PHE:HA	2:B:4926:VAL:HG12	2.01	0.42
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	2.01	0.42
2:E:2788:HIS:CE1	2:E:2790:MET:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	2.00	0.42
2:I:635:THR:HG23	2:I:1693:GLN:HE22	1.84	0.42
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.54	0.42
2:I:2788:HIS:CE1	2:I:2790:MET:HB2	2.55	0.42
2:I:886:ARG:HB3	2:I:891:TRP:HB2	2.02	0.42
2:B:2215:LEU:HD21	2:B:2272:PRO:HG3	2.02	0.42
2:B:282:ILE:HD12	2:B:314:PHE:HD2	1.85	0.42
2:B:3891:LEU:HB3	2:B:3899:PHE:CE2	2.55	0.42
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.54	0.42
2:G:3891:LEU:HB3	2:G:3899:PHE:CE2	2.55	0.42
2:I:1126:GLY:HA3	2:I:1143:TRP:CE2	2.54	0.42
2:I:3676:ASP:OD1	2:I:3676:ASP:N	2.52	0.42
2:I:5027:CYS:O	2:I:5029:ARG:N	2.48	0.42
2:B:642:THR:HG23	2:B:1613:LEU:HD12	2.02	0.42
2:B:2339:VAL:HG12	2:B:2345:SER:H	1.85	0.42
2:B:599:VAL:HG23	2:B:600:LEU:HD12	2.02	0.42
2:E:2290:LEU:HD21	2:E:2349:ASN:HA	2.01	0.42
2:E:3891:LEU:HB3	2:E:3899:PHE:CE2	2.55	0.42
1:H:54:GLU:O	2:G:1785:ALA:N	2.53	0.42
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	2.01	0.42
2:G:3676:ASP:OD1	2:G:3676:ASP:N	2.52	0.42
2:G:886:ARG:HB3	2:G:891:TRP:HB2	2.02	0.42
2:B:1727:ARG:HH12	2:B:1772:ARG:HB3	1.85	0.41
2:B:2290:LEU:HD21	2:B:2349:ASN:HA	2.01	0.41
2:B:2346:VAL:O	2:B:2349:ASN:ND2	2.53	0.41
2:E:282:ILE:HD12	2:E:314:PHE:HD2	1.85	0.41
2:E:864:PRO:HA	2:E:865:PRO:HD3	1.89	0.41
2:G:1126:GLY:HA3	2:G:1143:TRP:CE2	2.54	0.41
2:G:2215:LEU:HD21	2:G:2272:PRO:HG3	2.02	0.41
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.49	0.41
2:I:2290:LEU:HD21	2:I:2349:ASN:HA	2.01	0.41
2:B:1099:GLU:OE2	2:B:1127:HIS:ND1	2.38	0.41
2:E:1245:PHE:CD1	2:E:1600:LEU:HB3	2.54	0.41
2:E:395:GLN:HG3	2:E:397:GLU:H	1.85	0.41
2:E:474:ARG:HD2	2:E:474:ARG:HH11	1.75	0.41
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	2.02	0.41
2:I:282:ILE:HD12	2:I:314:PHE:HD2	1.85	0.41
2:B:2155:LEU:HD13	2:B:2188:ASN:HD21	1.85	0.41
2:B:2788:HIS:CE1	2:B:2790:MET:HB2	2.54	0.41
2:E:2215:LEU:HD21	2:E:2272:PRO:HG3	2.02	0.41
2:E:2346:VAL:O	2:E:2349:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1141:ARG:HD2	2:G:1141:ARG:H	1.86	0.41
2:G:3844:LEU:HD23	2:G:3844:LEU:HA	1.88	0.41
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	2.02	0.41
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.86	0.41
2:I:1245:PHE:CD1	2:I:1600:LEU:HB3	2.54	0.41
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.25	0.41
2:I:3844:LEU:HA	2:I:3844:LEU:HD23	1.88	0.41
2:B:3804:ILE:HG22	2:B:3812:VAL:HG21	2.01	0.41
2:B:4152:GLU:OE2	2:B:4180:ARG:NH1	2.50	0.41
2:G:1840:PRO:HB3	2:G:1843:LYS:HB3	2.02	0.41
2:G:2290:LEU:HD21	2:G:2349:ASN:HA	2.01	0.41
2:G:426:ARG:HB2	2:G:506:TYR:HA	2.03	0.41
2:G:599:VAL:HG23	2:G:600:LEU:HD12	2.02	0.41
2:I:1727:ARG:HH12	2:I:1772:ARG:HB3	1.85	0.41
2:I:2339:VAL:HG12	2:I:2345:SER:H	1.85	0.41
2:B:315:CYS:SG	2:B:316:PHE:N	2.92	0.41
2:B:3842:LEU:O	2:B:3929:SER:OG	2.39	0.41
2:E:1727:ARG:HH12	2:E:1772:ARG:HB3	1.85	0.41
2:I:642:THR:HG23	2:I:1613:LEU:HD12	2.02	0.41
2:I:426:ARG:HB2	2:I:506:TYR:HA	2.03	0.41
2:B:3844:LEU:HA	2:B:3844:LEU:HD23	1.88	0.41
2:E:3804:ILE:HG22	2:E:3812:VAL:HG21	2.01	0.41
2:E:3905:THR:HA	2:E:3912:THR:HG23	2.01	0.41
2:E:4922:PHE:HA	2:E:4926:VAL:HG12	2.01	0.41
2:G:395:GLN:HG3	2:G:397:GLU:H	1.85	0.41
2:G:4232:GLU:OE1	2:G:5019:TRP:NE1	2.53	0.41
2:I:3891:LEU:HB3	2:I:3899:PHE:CE2	2.55	0.41
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	2.01	0.41
2:E:3658:LYS:HA	2:E:3661:TRP:CE2	2.56	0.41
2:E:3842:LEU:O	2:E:3929:SER:OG	2.39	0.41
2:G:1727:ARG:HH12	2:G:1772:ARG:HB3	1.85	0.41
2:G:2155:LEU:HD13	2:G:2188:ASN:HD21	1.85	0.41
2:G:2346:VAL:O	2:G:2349:ASN:ND2	2.53	0.41
2:G:642:THR:HG23	2:G:1613:LEU:HD12	2.02	0.41
2:G:647:ASN:N	2:G:647:ASN:OD1	2.53	0.41
2:I:2346:VAL:O	2:I:2349:ASN:ND2	2.53	0.41
2:I:3658:LYS:HA	2:I:3661:TRP:CE2	2.56	0.41
2:B:214:VAL:HG12	2:B:274:LEU:HD12	2.03	0.41
2:B:772:ASN:OD1	2:B:772:ASN:N	2.54	0.41
2:E:214:VAL:HG22	2:E:341:TYR:CE1	2.56	0.41
2:E:2155:LEU:HD13	2:E:2188:ASN:HD21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:214:VAL:HG12	2:E:274:LEU:HD12	2.03	0.41
2:E:4570:ALA:HA	2:E:4573:ILE:HG22	2.03	0.41
2:G:1245:PHE:CD1	2:G:1600:LEU:HB3	2.54	0.41
2:G:955:LEU:O	2:G:966:LYS:NZ	2.43	0.41
2:I:404:ILE:HG21	2:I:481:GLU:HG3	2.03	0.41
2:B:1245:PHE:CD1	2:B:1600:LEU:HB3	2.54	0.41
2:B:214:VAL:HG22	2:B:341:TYR:CE1	2.56	0.41
2:B:404:ILE:HG21	2:B:481:GLU:HG3	2.03	0.41
2:B:886:ARG:HB3	2:B:891:TRP:HB2	2.02	0.41
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.25	0.41
2:E:4247:ILE:HA	2:E:4247:ILE:HD12	1.98	0.41
2:I:134:ASP:OD1	2:I:134:ASP:N	2.51	0.41
2:I:2155:LEU:HD13	2:I:2188:ASN:HD21	1.86	0.41
2:I:865:PRO:HA	2:I:868:GLU:HB2	2.03	0.41
2:B:1141:ARG:H	2:B:1141:ARG:HD2	1.86	0.41
2:B:1725:ARG:HD2	2:B:1725:ARG:HH21	1.72	0.41
2:B:4138:ASP:OD1	2:B:4138:ASP:N	2.51	0.41
2:E:1141:ARG:HD2	2:E:1141:ARG:H	1.86	0.41
2:G:2339:VAL:HG12	2:G:2345:SER:H	1.85	0.41
2:G:710:ASP:OD1	2:G:710:ASP:N	2.52	0.41
2:G:865:PRO:HA	2:G:868:GLU:HB2	2.03	0.41
2:I:214:VAL:HG22	2:I:341:TYR:CE1	2.56	0.41
2:B:426:ARG:HB2	2:B:506:TYR:HA	2.03	0.41
2:B:4570:ALA:HA	2:B:4573:ILE:HG22	2.03	0.41
2:E:1840:PRO:HB3	2:E:1843:LYS:HB3	2.02	0.41
2:E:1972:ASN:HD21	2:E:2024:PRO:HB3	1.86	0.41
2:E:4865:LYS:HD2	2:E:4865:LYS:HA	1.90	0.41
2:E:599:VAL:HG23	2:E:600:LEU:HD12	2.02	0.41
2:I:2095:GLN:NE2	2:I:2127:GLN:O	2.54	0.41
2:I:395:GLN:HG3	2:I:397:GLU:H	1.85	0.41
2:I:767:VAL:HG12	2:I:769:GLU:HG3	2.03	0.41
2:B:395:GLN:HG3	2:B:397:GLU:H	1.85	0.40
2:E:1725:ARG:HD2	2:E:1725:ARG:HH21	1.71	0.40
2:E:2095:GLN:NE2	2:E:2127:GLN:O	2.54	0.40
2:E:426:ARG:HB2	2:E:506:TYR:HA	2.03	0.40
2:G:767:VAL:HG12	2:G:769:GLU:HG3	2.03	0.40
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	2.02	0.40
2:I:4172:GLU:OE1	2:I:4175:ARG:NH1	2.55	0.40
2:I:4570:ALA:HA	2:I:4573:ILE:HG22	2.03	0.40
2:E:1671:ARG:NH2	2:E:1713:ASP:HB3	2.36	0.40
2:E:688:LEU:HB3	2:E:777:PHE:CE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1694:LEU:O	2:G:1712:TYR:OH	2.23	0.40
2:G:214:VAL:HG22	2:G:341:TYR:CE1	2.56	0.40
2:G:3658:LYS:HA	2:G:3661:TRP:CE2	2.56	0.40
2:B:4863:TYR:HA	2:B:4901:ILE:HG23	2.04	0.40
2:B:688:LEU:HB3	2:B:777:PHE:CE1	2.57	0.40
2:E:642:THR:HG23	2:E:1613:LEU:HD12	2.03	0.40
2:G:4251:ILE:HG22	2:G:4553:ASN:HD22	1.87	0.40
2:I:4152:GLU:OE2	2:I:4180:ARG:NH1	2.50	0.40
2:I:4251:ILE:HG22	2:I:4553:ASN:HD22	1.87	0.40
2:I:5036:LEU:HD12	2:I:5036:LEU:HA	1.91	0.40
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	2.03	0.40
2:B:1972:ASN:HD21	2:B:2024:PRO:HB3	1.86	0.40
2:B:2878:LEU:HD23	2:B:2878:LEU:HA	1.94	0.40
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	2.02	0.40
2:G:2095:GLN:NE2	2:G:2127:GLN:O	2.54	0.40
2:G:4172:GLU:OE1	2:G:4175:ARG:NH1	2.55	0.40
2:G:864:PRO:HA	2:G:865:PRO:HD3	1.89	0.40
2:I:454:PRO:HG2	2:I:531:ARG:HH12	1.87	0.40
2:I:649:PHE:HB3	2:I:776:LEU:HB3	2.04	0.40
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	2.02	0.40
2:B:4172:GLU:OE1	2:B:4175:ARG:NH1	2.55	0.40
2:E:4017:LEU:HA	2:E:4017:LEU:HD23	1.87	0.40
2:E:886:ARG:HB3	2:E:891:TRP:HB2	2.02	0.40
2:G:1651:LEU:HD23	2:G:1651:LEU:HA	1.86	0.40
2:I:1658:ASP:N	2:I:1658:ASP:OD1	2.55	0.40
2:I:3787:LYS:HB2	2:I:3831:SER:HA	2.04	0.40
2:I:4863:TYR:HA	2:I:4901:ILE:HG23	2.04	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%)	91 (87%)	14 (13%)	0	100	100
1	F	105/108 (97%)	91 (87%)	14 (13%)	0	100	100
1	H	105/108 (97%)	91 (87%)	14 (13%)	0	100	100
1	J	105/108 (97%)	91 (87%)	14 (13%)	0	100	100
2	B	3237/4676 (69%)	2857 (88%)	371 (12%)	9 (0%)	44	80
2	E	3237/4676 (69%)	2859 (88%)	369 (11%)	9 (0%)	44	80
2	G	3237/4676 (69%)	2858 (88%)	370 (11%)	9 (0%)	44	80
2	I	3237/4676 (69%)	2859 (88%)	369 (11%)	9 (0%)	44	80
All	All	13368/19136 (70%)	11797 (88%)	1535 (12%)	36 (0%)	48	80

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	B	1932	PRO
2	E	1708	ARG
2	E	1932	PRO
2	I	1708	ARG
2	I	1932	PRO
2	G	1708	ARG
2	G	1932	PRO
2	B	1840	PRO
2	B	4641	PRO
2	B	5028	PHE
2	E	1840	PRO
2	E	4641	PRO
2	E	5028	PHE
2	I	1840	PRO
2	I	4641	PRO
2	I	5028	PHE
2	G	1840	PRO
2	G	4641	PRO
2	G	5028	PHE
2	B	2291	GLN
2	E	2291	GLN
2	I	2291	GLN
2	G	2291	GLN
2	B	4640	GLU
2	E	4135	PRO
2	E	4640	GLU

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Mol	Chain	Res	Type
2	I	4135	PRO
2	I	4640	GLU
2	G	4640	GLU
2	B	4135	PRO
2	G	4135	PRO
2	B	2343	GLY
2	E	2343	GLY
2	I	2343	GLY
2	G	2343	GLY

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	2493/3202 (78%)	2476 (99%)	17 (1%)	87	95
2	E	2493/3202 (78%)	2476 (99%)	17 (1%)	87	95
2	G	2493/3202 (78%)	2476 (99%)	17 (1%)	87	95
2	I	2493/3202 (78%)	2476 (99%)	17 (1%)	87	95
All	All	10324/13164 (78%)	10256 (99%)	68 (1%)	87	95

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	534	ARG
2	B	553	ARG
2	B	719	LEU
2	B	1076	ARG
2	B	1141	ARG

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Mol	Chain	Res	Type
2	B	1600	LEU
2	B	1676	LEU
2	B	1964	ARG
2	B	2339	VAL
2	B	2342	ASN
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	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	2339	VAL
2	E	2342	ASN
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	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	2339	VAL
2	I	2342	ASN
2	I	3787	LYS
2	I	3805	LEU
2	I	3896	ASN

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Mol	Chain	Res	Type
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
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	2339	VAL
2	G	2342	ASN
2	G	3787	LYS
2	G	3805	LEU
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (136) 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	105	HIS
2	B	111	HIS
2	B	113	HIS
2	B	156	GLN
2	B	203	ASN
2	B	224	HIS
2	B	379	HIS
2	B	383	HIS
2	B	395	GLN
2	B	479	GLN
2	B	520	ASN
2	B	949	ASN
2	B	1158	ASN

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Mol	Chain	Res	Type
2	B	1598	GLN
2	B	1663	HIS
2	B	1688	HIS
2	B	1691	GLN
2	B	1693	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	1952	GLN
2	B	1972	ASN
2	B	2005	GLN
2	B	2881	ASN
2	B	3781	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	4034	ASN
2	B	4120	ASN
2	B	4553	ASN
2	B	4728	HIS
2	E	57	ASN
2	E	105	HIS
2	E	111	HIS
2	E	113	HIS
2	E	156	GLN
2	E	203	ASN
2	E	224	HIS
2	E	379	HIS
2	E	383	HIS
2	E	395	GLN
2	E	479	GLN
2	E	520	ASN
2	E	1158	ASN
2	E	1598	GLN
2	E	1663	HIS
2	E	1688	HIS
2	E	1691	GLN
2	E	1693	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	1952	GLN
2	E	1972	ASN
2	E	2005	GLN

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Mol	Chain	Res	Type
2	E	2127	GLN
2	E	2881	ASN
2	E	3781	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	4034	ASN
2	E	4120	ASN
2	E	4142	ASN
2	E	4553	ASN
2	E	4728	HIS
2	I	57	ASN
2	I	105	HIS
2	I	111	HIS
2	I	113	HIS
2	I	156	GLN
2	I	203	ASN
2	I	224	HIS
2	I	379	HIS
2	I	383	HIS
2	I	395	GLN
2	I	479	GLN
2	I	520	ASN
2	I	949	ASN
2	I	1158	ASN
2	I	1598	GLN
2	I	1663	HIS
2	I	1688	HIS
2	I	1691	GLN
2	I	1693	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	1952	GLN
2	I	2005	GLN
2	I	2881	ASN
2	I	3781	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	4034	ASN
2	I	4120	ASN
2	I	4553	ASN

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Mol	Chain	Res	Type
2	I	4728	HIS
2	G	57	ASN
2	G	105	HIS
2	G	111	HIS
2	G	113	HIS
2	G	156	GLN
2	G	203	ASN
2	G	224	HIS
2	G	379	HIS
2	G	383	HIS
2	G	395	GLN
2	G	479	GLN
2	G	520	ASN
2	G	949	ASN
2	G	1158	ASN
2	G	1598	GLN
2	G	1663	HIS
2	G	1691	GLN
2	G	1693	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	1952	GLN
2	G	1972	ASN
2	G	2005	GLN
2	G	2127	GLN
2	G	2881	ASN
2	G	3781	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	4034	ASN
2	G	4120	ASN
2	G	4553	ASN
2	G	4728	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	G	12
2	B	12
2	I	12
2	E	12

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3613:UNK	C	3639:THR	N	42.64
1	G	3613:UNK	C	3639:THR	N	42.57
1	I	3613:UNK	C	3639:THR	N	42.56
1	E	3613:UNK	C	3639:THR	N	42.54
1	E	3163:UNK	C	3170:UNK	N	16.55
1	I	3163:UNK	C	3170:UNK	N	16.55
1	G	3163:UNK	C	3170:UNK	N	16.55
1	B	3163:UNK	C	3170:UNK	N	16.52
1	E	3468:UNK	C	3511:UNK	N	15.29

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	3468:UNK	C	3511:UNK	N	15.29
1	G	3468:UNK	C	3511:UNK	N	15.29
1	B	3468:UNK	C	3511:UNK	N	15.27
1	E	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	14.86
1	B	3063:UNK	C	3134:UNK	N	14.83
1	E	2703:UNK	C	2734:ASN	N	14.48
1	I	2703:UNK	C	2734:ASN	N	14.47
1	G	2703:UNK	C	2734:ASN	N	14.44
1	B	2703:UNK	C	2734:ASN	N	14.41
1	B	3236:UNK	C	3241:UNK	N	13.70
1	G	3236:UNK	C	3241:UNK	N	13.62
1	I	3236:UNK	C	3241:UNK	N	13.61
1	E	3236:UNK	C	3241:UNK	N	13.60
1	E	1564:UNK	C	1573:MET	N	12.83
1	I	1564:UNK	C	1573:MET	N	12.83
1	G	1564:UNK	C	1573:MET	N	12.81
1	B	1564:UNK	C	1573:MET	N	12.75
1	E	2976:UNK	C	2995:UNK	N	12.39
1	I	2976:UNK	C	2995:UNK	N	12.39
1	G	2976:UNK	C	2995:UNK	N	12.39
1	B	2976:UNK	C	2995:UNK	N	12.36
1	E	3254:UNK	C	3261:UNK	N	8.63
1	I	3254:UNK	C	3261:UNK	N	8.62
1	G	3254:UNK	C	3261:UNK	N	8.62
1	B	3254:UNK	C	3261:UNK	N	8.56
1	B	1297:UNK	C	1430:UNK	N	5.72
1	E	1297:UNK	C	1430:UNK	N	5.72
1	I	1297:UNK	C	1430:UNK	N	5.72
1	G	1297:UNK	C	1430:UNK	N	5.72
1	B	2479:LEU	C	2487:UNK	N	3.59
1	G	2479:LEU	C	2487:UNK	N	3.53
1	I	2479:LEU	C	2487:UNK	N	3.52
1	E	2479:LEU	C	2487:UNK	N	3.51
1	E	2939:ARG	C	2942:UNK	N	3.37
1	I	2939:ARG	C	2942:UNK	N	3.34
1	G	2939:ARG	C	2942:UNK	N	3.33
1	B	2939:ARG	C	2942:UNK	N	3.26