



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:40 PM GMT

PDB ID : 1XXI
Title : ADP Bound E. coli Clamp Loader Complex
Authors : Kazmirski, S.L.; Podobnik, M.; Weitze, T.F.; O'Donnell, M.; Kuriyan, J.
Deposited on : 2004-11-05
Resolution : 4.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

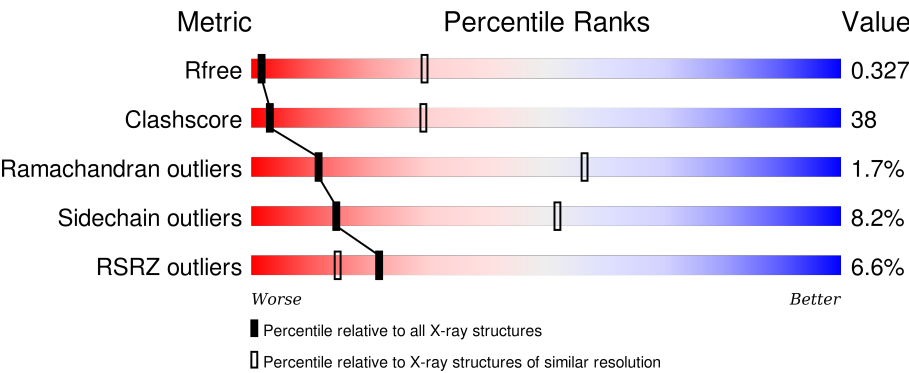
MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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)	Similar resolution (#Entries, resolution range(Å))
R _{free}	91344	1018 (4.60-3.60)
Clashscore	102246	1117 (4.60-3.60)
Ramachandran outliers	100387	1063 (4.60-3.60)
Sidechain outliers	100360	1049 (4.60-3.60)
RSRZ outliers	91569	1022 (4.60-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	343	<div><div>3%</div><div>50%</div><div>39%</div><div>8%</div><div>..</div></div>
1	F	343	<div><div>4%</div><div>45%</div><div>44%</div><div>8%</div><div>..</div></div>
2	B	368	<div><div>5%</div><div>60%</div><div>33%</div><div>5%</div><div>..</div></div>
2	C	368	<div><div>2%</div><div>57%</div><div>41%</div><div>..</div></div>
2	D	368	<div><div>2%</div><div>59%</div><div>35%</div><div>5%</div><div>..</div></div>

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Mol	Chain	Length	Quality of chain
2	G	368	
2	H	368	
2	I	368	
3	E	334	
3	J	334	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	C	1300	-	-	X	-
5	ZN	H	405	-	-	-	X
6	ADP	I	803	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 27688 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 DNA polymerase III, delta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2687	1702	488	487	10			
1	F	338	Total	C	N	O	S	0	0	0
			2687	1702	488	487	10			

- Molecule 2 is a protein called DNA polymerase III subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	364	Total	C	N	O	S	0	0	0
			2829	1779	511	523	16			
2	C	366	Total	C	N	O	S	0	0	0
			2850	1793	514	527	16			
2	D	364	Total	C	N	O	S	0	0	0
			2829	1779	511	523	16			
2	G	364	Total	C	N	O	S	0	0	0
			2829	1779	511	523	16			
2	H	366	Total	C	N	O	S	0	0	0
			2850	1793	514	527	16			
2	I	364	Total	C	N	O	S	0	0	0
			2829	1779	511	523	16			

- Molecule 3 is a protein called DNA polymerase III, delta prime subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	334	Total	C	N	O	S	0	0	0
			2602	1655	468	466	13			
3	J	334	Total	C	N	O	S	0	0	0
			2602	1655	468	466	13			

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	P	0	0
			5	4	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Zn	0	0
			1	1		
5	J	1	Total	Zn	0	0
			1	1		
5	D	1	Total	Zn	0	0
			1	1		
5	E	1	Total	Zn	0	0
			1	1		
5	H	1	Total	Zn	0	0
			1	1		
5	B	1	Total	Zn	0	0
			1	1		
5	I	1	Total	Zn	0	0
			1	1		
5	C	1	Total	Zn	0	0
			1	1		

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

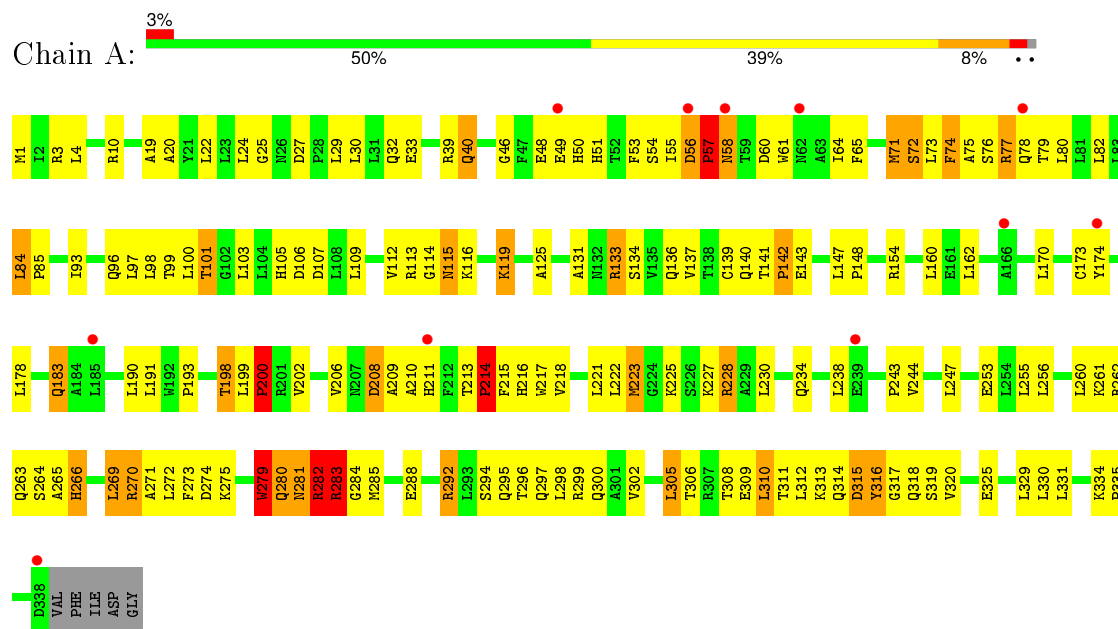


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

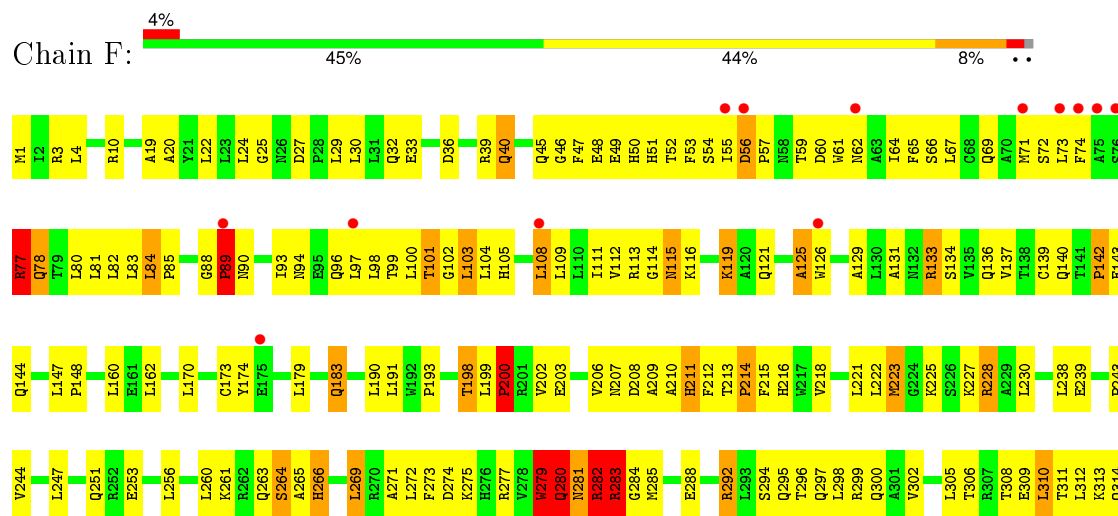
3 Residue-property plots

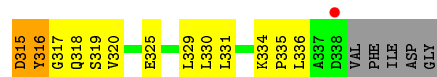
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: DNA polymerase III, delta subunit

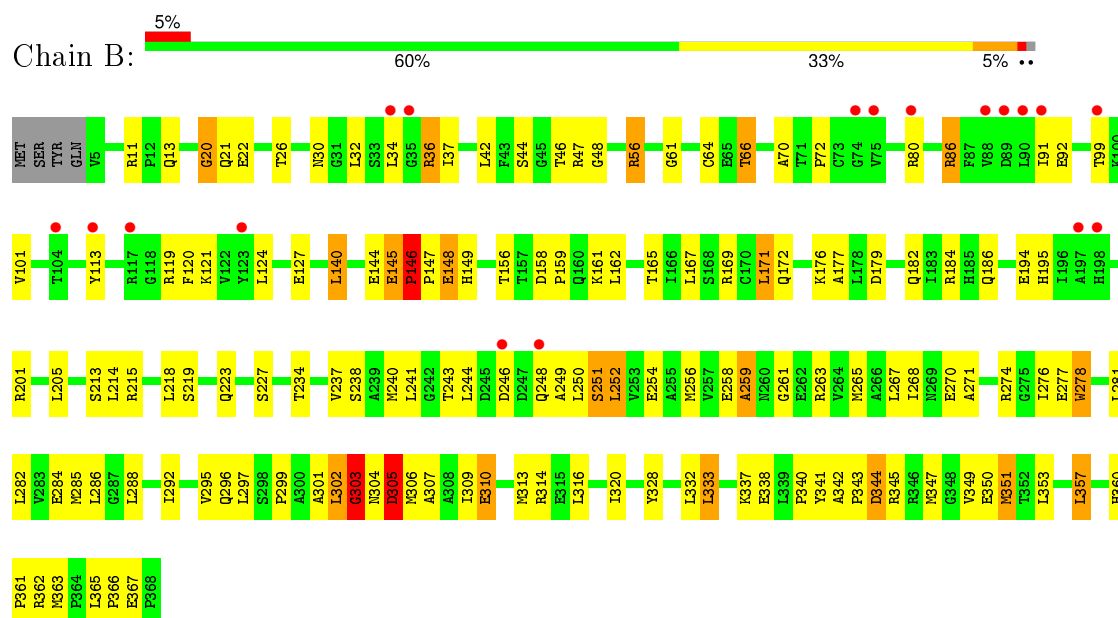


- Molecule 1: DNA polymerase III, delta subunit

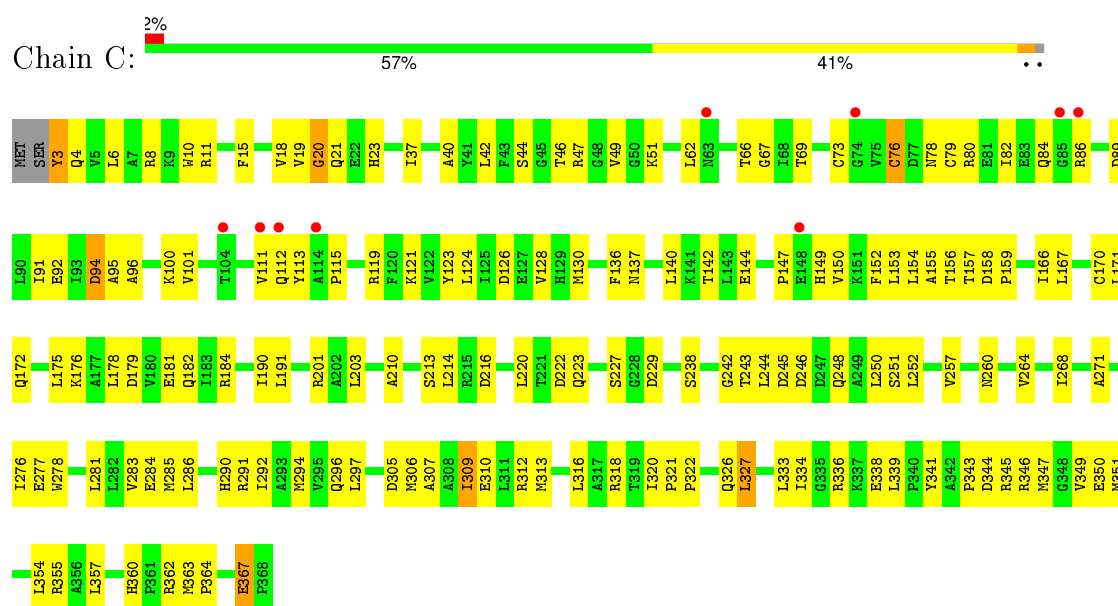




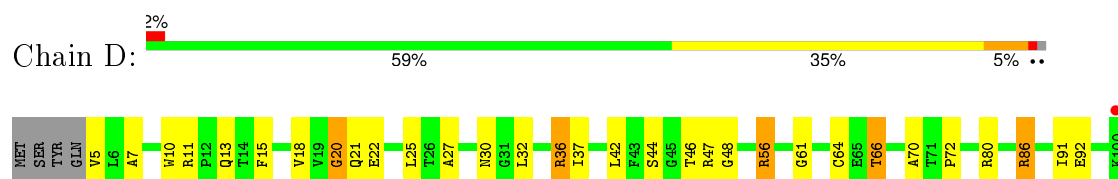
• Molecule 2: DNA polymerase III subunit gamma

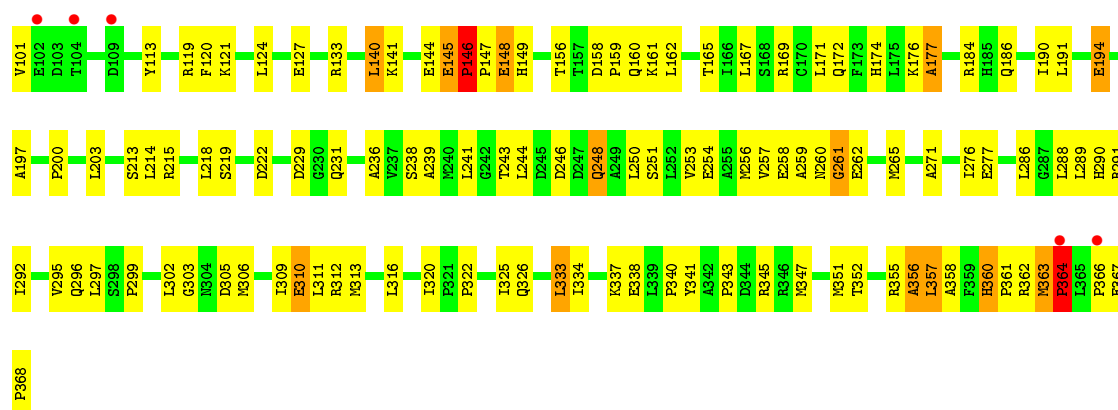


• Molecule 2: DNA polymerase III subunit gamma

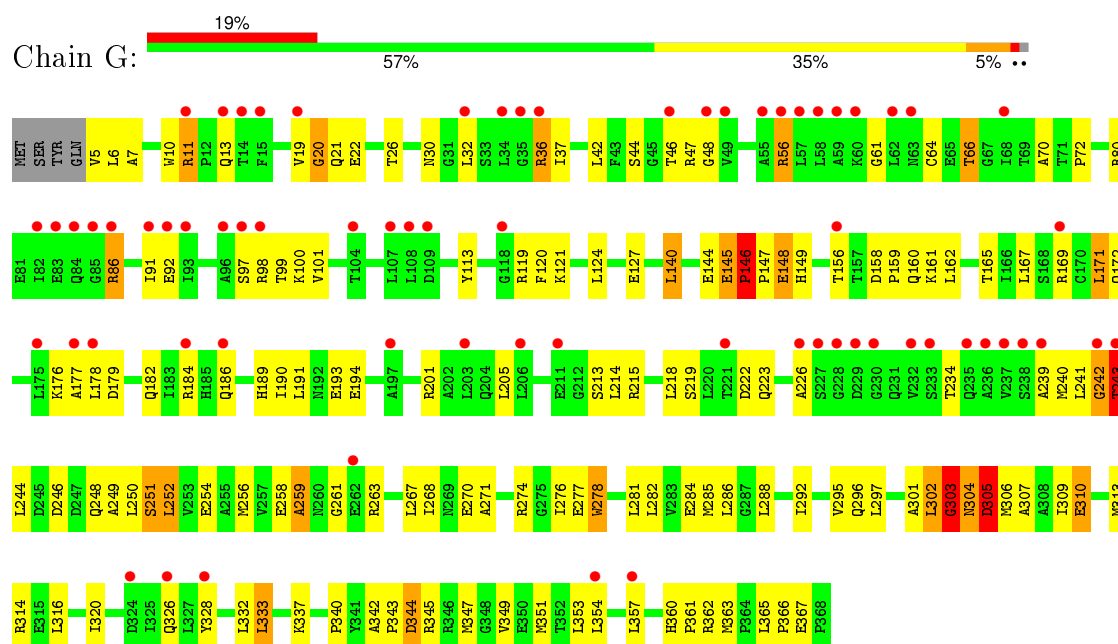


• Molecule 2: DNA polymerase III subunit gamma

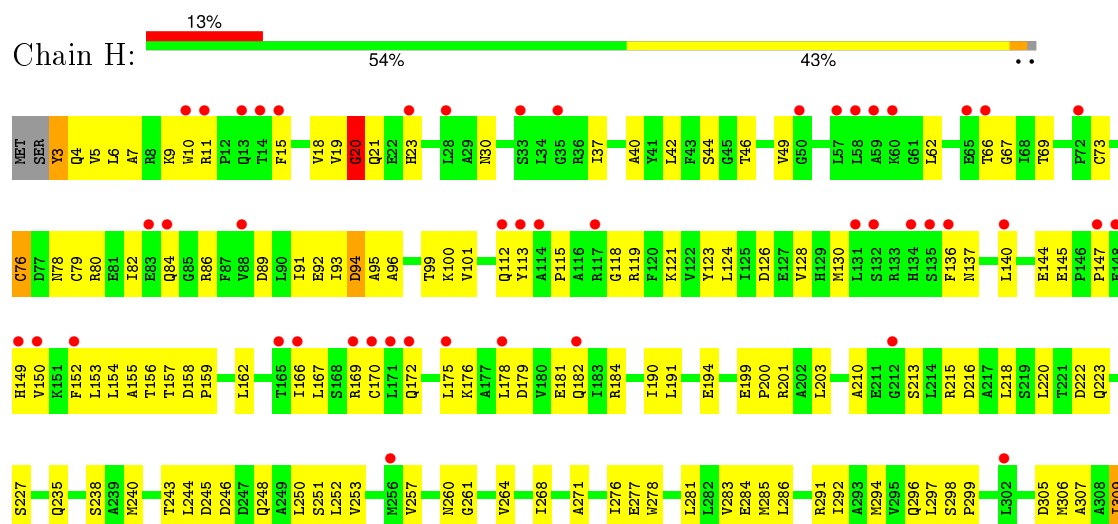




● Molecule 2: DNA polymerase III subunit gamma

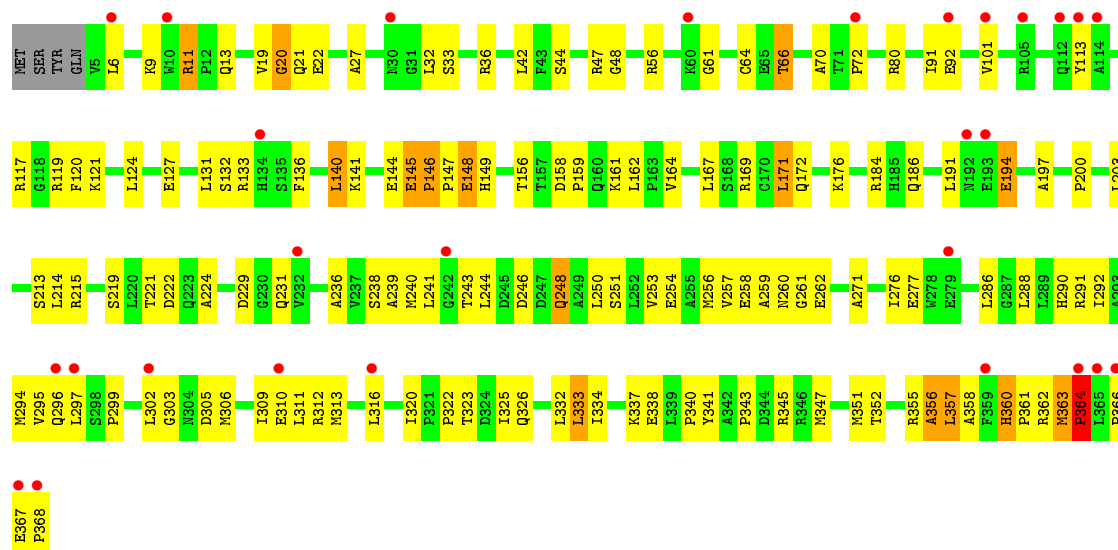


● Molecule 2: DNA polymerase III subunit gamma

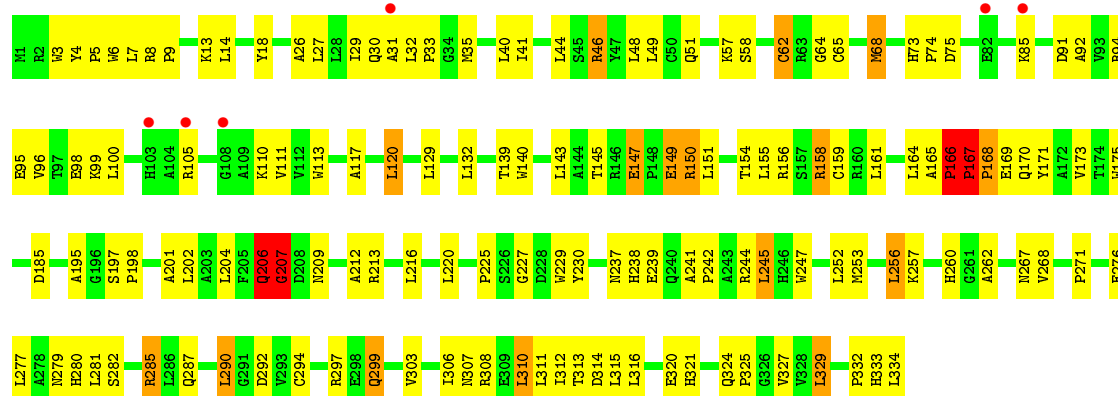




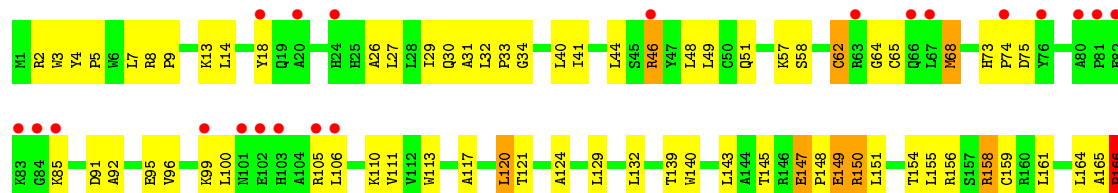
• Molecule 2: DNA polymerase III subunit gamma

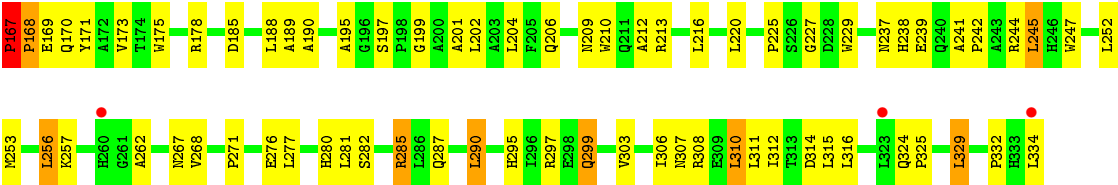


• Molecule 3: DNA polymerase III, delta prime subunit



• Molecule 3: DNA polymerase III, delta prime subunit





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.21Å 106.57Å 535.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.10 49.11 – 4.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-4.10) 88.0 (49.11-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 4.14Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.366 , 0.369 0.334 , 0.327	Depositor DCC
R_{free} test set	3986 reflections (10.11%)	DCC
Wilson B-factor (Å ²)	122.7	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 82.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 42596 reflections	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	27688	wwPDB-VP
Average B, all atoms (Å ²)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PO4, ADP

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 > 5$	RMSZ	# $ Z > 5$
1	A	0.90	9/2735 (0.3%)	1.07	14/3716 (0.4%)
1	F	0.96	11/2735 (0.4%)	1.06	13/3716 (0.3%)
2	B	0.49	0/2876	0.77	8/3900 (0.2%)
2	C	0.48	0/2898	0.75	2/3930 (0.1%)
2	D	0.63	5/2876 (0.2%)	0.88	9/3900 (0.2%)
2	G	0.49	1/2876 (0.0%)	0.86	12/3900 (0.3%)
2	H	0.47	0/2898	0.74	2/3930 (0.1%)
2	I	0.62	5/2876 (0.2%)	0.87	10/3900 (0.3%)
3	E	0.51	0/2667	0.82	5/3639 (0.1%)
3	J	0.50	0/2667	0.82	3/3639 (0.1%)
All	All	0.63	31/28104 (0.1%)	0.87	78/38170 (0.2%)

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	4
1	F	0	4
2	C	0	1
2	H	0	1
All	All	0	10

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	315	ASP	CB-CG	29.11	2.12	1.51
1	F	315	ASP	CB-CG	29.09	2.12	1.51
1	A	310	LEU	CG-CD2	-9.10	1.18	1.51
1	F	310	LEU	CG-CD2	-9.03	1.18	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	363	MET	SD-CE	8.94	2.27	1.77
2	I	363	MET	CG-SD	8.92	2.04	1.81
2	I	363	MET	SD-CE	8.91	2.27	1.77
2	D	363	MET	CG-SD	8.83	2.04	1.81
1	F	316	TYR	CE1-CZ	6.83	1.47	1.38
1	A	283	ARG	CB-CG	6.71	1.70	1.52
1	F	283	ARG	CB-CG	6.62	1.70	1.52
1	A	316	TYR	CE1-CZ	6.57	1.47	1.38
2	I	356	ALA	C-O	-5.79	1.12	1.23
1	F	200	PRO	N-CD	-5.78	1.39	1.47
1	A	142	PRO	N-CA	5.76	1.57	1.47
2	D	360	HIS	CA-CB	5.71	1.66	1.53
2	I	360	HIS	CA-CB	5.71	1.66	1.53
2	D	356	ALA	C-O	-5.65	1.12	1.23
1	F	316	TYR	CZ-OH	5.65	1.47	1.37
1	A	200	PRO	N-CD	-5.54	1.40	1.47
1	A	316	TYR	CZ-OH	5.39	1.47	1.37
1	F	77	ARG	CA-C	5.35	1.66	1.52
1	A	282	ARG	CB-CG	-5.23	1.38	1.52
1	F	78	GLN	N-CA	5.18	1.56	1.46
1	F	316	TYR	CG-CD1	5.17	1.45	1.39
1	A	316	TYR	CG-CD1	5.15	1.45	1.39
2	D	360	HIS	CG-CD2	5.13	1.44	1.35
1	F	77	ARG	C-N	5.10	1.45	1.34
1	F	282	ARG	CB-CG	-5.07	1.38	1.52
2	I	360	HIS	CG-CD2	5.07	1.44	1.35
2	G	304	ASN	C-O	5.02	1.32	1.23

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	363	MET	CG-SD-CE	17.09	127.54	100.20
2	I	363	MET	CG-SD-CE	17.05	127.49	100.20
2	G	242	GLY	C-N-CA	-16.32	80.90	121.70
1	A	214	PRO	CA-N-CD	-15.70	89.52	111.50
1	F	214	PRO	CA-N-CD	-15.29	90.09	111.50
3	J	166	PRO	CA-N-CD	-14.15	91.69	111.50
3	E	166	PRO	CA-N-CD	-13.72	92.30	111.50
1	F	142	PRO	CA-N-CD	-13.56	92.51	111.50
1	A	57	PRO	CA-N-CD	-13.21	93.01	111.50
3	E	167	PRO	CA-N-CD	-13.04	93.24	111.50
3	J	168	PRO	CA-N-CD	-12.55	93.93	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	ARG	C-N-CA	12.47	148.48	122.30
1	F	283	ARG	C-N-CA	12.44	148.42	122.30
1	A	142	PRO	CA-N-CD	-11.61	95.24	111.50
1	A	280	GLN	C-N-CA	11.41	150.23	121.70
1	F	280	GLN	C-N-CA	11.36	150.09	121.70
1	A	315	ASP	CA-CB-CG	-10.74	89.78	113.40
1	F	315	ASP	CA-CB-CG	-10.73	89.79	113.40
3	J	167	PRO	CA-N-CD	-10.56	96.71	111.50
2	D	360	HIS	N-CA-CB	10.30	129.15	110.60
2	I	360	HIS	N-CA-CB	10.19	128.94	110.60
1	A	283	ARG	CA-C-N	-9.29	97.63	116.20
1	F	283	ARG	CA-C-N	-9.27	97.65	116.20
3	E	168	PRO	CA-N-CD	-8.90	99.04	111.50
1	A	283	ARG	NE-CZ-NH1	8.35	124.48	120.30
1	F	283	ARG	NE-CZ-NH1	8.32	124.46	120.30
2	G	243	THR	N-CA-C	8.09	132.84	111.00
1	A	283	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	A	74	PHE	CB-CG-CD1	7.57	126.09	120.80
1	F	283	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	A	74	PHE	CB-CG-CD2	-7.28	115.70	120.80
2	G	243	THR	CA-C-N	-6.89	102.04	117.20
2	I	363	MET	CB-CG-SD	6.80	132.80	112.40
2	D	363	MET	CB-CG-SD	6.75	132.67	112.40
2	I	20	GLY	N-CA-C	6.72	129.89	113.10
2	B	305	ASP	CB-CG-OD2	-6.69	112.28	118.30
2	B	302	LEU	C-N-CA	6.61	136.17	122.30
2	G	305	ASP	CB-CG-OD2	-6.58	112.38	118.30
2	G	302	LEU	C-N-CA	6.55	136.06	122.30
2	B	305	ASP	CB-CG-OD1	6.50	124.14	118.30
2	G	241	LEU	CA-C-N	-6.44	103.33	116.20
2	G	303	GLY	N-CA-C	6.39	129.07	113.10
1	F	310	LEU	CB-CG-CD2	-6.37	100.17	111.00
2	G	305	ASP	CB-CG-OD1	6.36	124.03	118.30
1	A	310	LEU	CB-CG-CD2	-6.33	100.23	111.00
2	B	303	GLY	N-CA-C	6.32	128.89	113.10
2	H	20	GLY	N-CA-C	6.31	128.87	113.10
2	C	20	GLY	N-CA-C	6.30	128.85	113.10
2	G	20	GLY	N-CA-C	6.16	128.50	113.10
2	B	20	GLY	N-CA-C	6.14	128.46	113.10
1	A	280	GLN	O-C-N	-6.09	112.96	122.70
2	D	360	HIS	CA-CB-CG	6.05	123.89	113.60
2	I	360	HIS	CB-CA-C	-6.04	98.32	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	280	GLN	O-C-N	-6.03	113.05	122.70
2	I	360	HIS	CA-CB-CG	5.95	123.72	113.60
2	D	360	HIS	CB-CA-C	-5.95	98.50	110.40
2	D	364	PRO	CA-N-CD	-5.83	103.34	111.50
2	I	364	PRO	CA-N-CD	-5.74	103.47	111.50
2	H	327	LEU	CA-CB-CG	5.72	128.47	115.30
2	C	327	LEU	CA-CB-CG	5.64	128.28	115.30
2	I	360	HIS	CB-CG-ND1	5.55	137.07	123.20
2	D	360	HIS	CB-CG-ND1	5.51	136.97	123.20
1	F	89	PRO	CA-N-CD	-5.50	103.80	111.50
2	G	259	ALA	N-CA-C	5.45	125.73	111.00
2	B	259	ALA	N-CA-C	5.42	125.64	111.00
1	A	282	ARG	CB-CG-CD	-5.32	97.76	111.60
2	I	171	LEU	N-CA-C	-5.28	96.74	111.00
1	F	282	ARG	CB-CG-CD	-5.26	97.92	111.60
2	B	171	LEU	N-CA-C	-5.25	96.84	111.00
2	D	171	LEU	N-CA-C	-5.24	96.84	111.00
2	G	171	LEU	N-CA-C	-5.20	96.97	111.00
2	I	303	GLY	N-CA-C	5.15	125.98	113.10
2	D	303	GLY	N-CA-C	5.10	125.86	113.10
3	E	206	GLN	C-N-CA	-5.09	111.61	122.30
2	G	302	LEU	CA-C-N	-5.07	106.07	116.20
2	B	302	LEU	CA-C-N	-5.06	106.09	116.20
1	F	264	SER	N-CA-C	-5.05	97.36	111.00
3	E	207	GLY	N-CA-C	-5.02	100.55	113.10

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	280	GLN	Peptide
1	A	281	ASN	Mainchain
1	A	282	ARG	Mainchain
1	A	319	SER	Mainchain
2	C	94	ASP	Mainchain
1	F	280	GLN	Peptide
1	F	281	ASN	Mainchain
1	F	282	ARG	Mainchain
1	F	319	SER	Mainchain
2	H	94	ASP	Mainchain

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	2687	0	2741	337	4
1	F	2687	0	2733	391	10
2	B	2829	0	2877	190	6
2	C	2850	0	2896	198	0
2	D	2829	0	2878	270	4
2	G	2829	0	2871	268	0
2	H	2850	0	2894	256	0
2	I	2829	0	2878	327	6
3	E	2602	0	2603	155	6
3	J	2602	0	2603	170	4
4	C	5	0	0	3	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
6	B	27	0	12	8	0
6	D	27	0	12	5	0
6	I	27	0	12	28	0
All	All	27688	0	28010	2129	20

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 38.

All (2129) 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:D:277:GLU:HB3	3:E:149:GLU:CG	1.26	1.66
2:G:10:TRP:HZ2	2:G:193:GLU:CB	0.98	1.59
1:F:71:MET:HB3	1:F:108:LEU:CD1	1.23	1.58
1:A:29:LEU:CD2	1:A:154:ARG:HH12	1.08	1.58
1:A:65:PHE:CE1	1:A:99:THR:HG21	1.06	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:99:THR:HG21	2:I:132:SER:CA	1.30	1.56
1:F:71:MET:CB	1:F:108:LEU:HD12	1.37	1.55
2:G:10:TRP:CZ2	2:G:193:GLU:CB	1.87	1.54
2:C:112:GLN:HB2	2:C:121:LYS:CE	1.08	1.54
2:H:112:GLN:HB2	2:H:121:LYS:CE	1.08	1.54
1:A:65:PHE:CE1	1:A:99:THR:CG2	1.85	1.54
1:A:73:LEU:HD21	1:F:207:ASN:CA	1.32	1.53
1:A:65:PHE:CD1	1:A:99:THR:HG21	1.41	1.52
1:F:210:ALA:CB	2:G:176:LYS:HE2	1.08	1.52
1:F:209:ALA:C	2:G:176:LYS:CE	1.75	1.51
2:H:99:THR:CG2	2:I:132:SER:HA	1.07	1.51
2:I:345:ARG:CZ	3:J:150:ARG:HE	1.22	1.51
1:A:73:LEU:CD2	1:F:207:ASN:CA	1.88	1.50
1:F:210:ALA:HB3	2:G:176:LYS:CE	1.38	1.50
2:H:215:ARG:CZ	2:I:164:VAL:HG11	1.43	1.49
2:I:215:ARG:CG	6:I:803:ADP:H5'1	1.39	1.48
1:F:47:PHE:CE1	1:F:77:ARG:HB3	1.45	1.48
1:F:209:ALA:C	2:G:176:LYS:HE3	1.17	1.48
2:I:363:MET:CG	2:I:363:MET:SD	2.04	1.46
1:F:32:GLN:NE2	2:G:165:THR:HG22	1.30	1.46
2:D:363:MET:SD	2:D:363:MET:CG	2.04	1.46
1:A:53:PHE:CZ	1:A:64:ILE:HB	1.48	1.45
2:D:345:ARG:NE	3:E:150:ARG:HH21	1.10	1.45
2:D:277:GLU:CB	3:E:149:GLU:HG2	1.42	1.45
1:A:193:PRO:CG	2:B:30:ASN:OD1	1.64	1.42
1:F:74:PHE:CD2	1:F:78:GLN:CG	1.84	1.41
2:C:112:GLN:CA	2:C:121:LYS:NZ	1.83	1.41
2:H:112:GLN:CA	2:H:121:LYS:NZ	1.81	1.41
2:I:345:ARG:NE	3:J:150:ARG:HE	1.16	1.40
1:A:73:LEU:CD2	1:F:207:ASN:CB	1.98	1.40
2:H:99:THR:CG2	2:I:132:SER:CA	1.90	1.40
1:A:73:LEU:CD2	1:F:207:ASN:HB3	1.48	1.40
2:H:215:ARG:NH2	2:I:164:VAL:CG1	1.86	1.39
1:F:71:MET:CB	1:F:108:LEU:CD1	1.89	1.38
2:G:98:ARG:H	2:H:169:ARG:NH2	1.17	1.38
1:A:73:LEU:HD23	1:F:207:ASN:CB	1.53	1.38
2:C:112:GLN:CG	2:C:121:LYS:NZ	1.88	1.35
2:H:112:GLN:CG	2:H:121:LYS:NZ	1.87	1.35
2:I:345:ARG:NH2	3:J:150:ARG:CD	1.90	1.35
1:A:107:ASP:CB	1:F:228:ARG:HH12	1.39	1.35
1:F:210:ALA:CB	2:G:176:LYS:CE	1.96	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:98:ARG:N	2:H:169:ARG:HH22	1.26	1.33
1:F:100:LEU:HD23	1:F:103:LEU:CD2	1.57	1.32
1:F:209:ALA:O	2:G:176:LYS:CE	1.72	1.31
1:A:29:LEU:CD2	1:A:154:ARG:NH1	1.93	1.31
2:H:215:ARG:NH2	2:I:164:VAL:HG11	0.99	1.30
2:I:345:ARG:NH2	3:J:150:ARG:CG	1.92	1.30
1:A:53:PHE:CE2	1:A:64:ILE:HB	1.65	1.30
1:F:71:MET:CG	1:F:108:LEU:HD11	1.61	1.29
2:H:112:GLN:CA	2:H:121:LYS:HZ3	1.41	1.29
1:A:73:LEU:CG	1:F:207:ASN:HB3	1.62	1.29
1:A:193:PRO:HG3	2:B:30:ASN:ND2	1.44	1.29
1:A:48:GLU:OE2	1:A:76:SER:HB2	1.31	1.29
1:A:193:PRO:HG3	2:B:30:ASN:CG	1.51	1.28
1:F:100:LEU:HA	1:F:103:LEU:CD2	1.63	1.27
2:I:345:ARG:CZ	3:J:150:ARG:NE	1.95	1.27
2:H:215:ARG:CZ	2:I:164:VAL:CG1	2.09	1.27
2:G:99:THR:HG21	2:H:145:GLU:CB	1.61	1.27
2:G:6:LEU:HD22	2:G:190:ILE:CG2	1.63	1.26
1:A:29:LEU:HD21	1:A:154:ARG:NH1	1.49	1.25
2:G:10:TRP:HZ2	2:G:193:GLU:CG	1.45	1.25
2:G:6:LEU:HD11	2:G:191:LEU:CD2	1.65	1.23
1:A:73:LEU:CD2	1:F:207:ASN:C	2.03	1.23
1:F:210:ALA:HB3	2:G:176:LYS:CD	1.68	1.23
2:C:112:GLN:CA	2:C:121:LYS:HZ3	1.47	1.22
1:A:208:ASP:O	2:B:176:LYS:NZ	1.68	1.22
2:D:363:MET:SD	2:D:363:MET:CE	2.27	1.22
2:I:363:MET:CE	2:I:363:MET:SD	2.27	1.22
1:A:334:LYS:HB2	2:B:297:LEU:CD2	1.68	1.22
1:F:74:PHE:CD2	1:F:78:GLN:HG3	1.55	1.21
2:I:345:ARG:NH2	3:J:150:ARG:NE	1.89	1.20
1:A:193:PRO:HG2	2:B:30:ASN:OD1	1.19	1.20
2:G:6:LEU:CD2	2:G:194:GLU:HG3	1.70	1.20
2:D:345:ARG:HE	3:E:150:ARG:NH2	1.37	1.19
2:D:345:ARG:NE	3:E:150:ARG:NH2	1.86	1.19
2:H:112:GLN:CG	2:H:121:LYS:HZ1	1.48	1.18
1:F:210:ALA:CA	2:G:176:LYS:HE2	1.72	1.18
2:G:6:LEU:CB	2:G:190:ILE:HG21	1.73	1.17
2:H:99:THR:HG21	2:I:132:SER:N	1.59	1.17
1:F:210:ALA:N	2:G:176:LYS:CE	2.07	1.17
1:A:315:ASP:CG	1:A:315:ASP:CB	2.12	1.17
2:C:112:GLN:CG	2:C:121:LYS:HZ3	1.54	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ASP:CB	1:F:228:ARG:NH1	2.01	1.16
1:A:71:MET:HE3	1:A:72:SER:CB	1.75	1.16
1:F:315:ASP:CG	1:F:315:ASP:CB	2.12	1.16
2:I:277:GLU:HB3	3:J:149:GLU:CG	1.76	1.16
1:F:55:ILE:CD1	1:F:82:LEU:HG	1.75	1.16
2:G:6:LEU:HB3	2:G:190:ILE:CG2	1.75	1.15
2:I:345:ARG:NH2	3:J:150:ARG:HG2	1.57	1.15
1:A:73:LEU:CD2	1:F:207:ASN:O	1.94	1.15
2:H:215:ARG:NH1	2:I:164:VAL:CG1	2.09	1.15
1:F:55:ILE:HD11	1:F:82:LEU:HG	1.24	1.15
1:A:334:LYS:HB2	2:B:297:LEU:HD21	1.26	1.15
2:G:242:GLY:O	2:G:243:THR:HG23	1.35	1.15
1:A:71:MET:HE2	1:A:72:SER:C	1.68	1.14
2:B:99:THR:OG1	2:C:144:GLU:HG2	1.44	1.14
2:I:238:SER:CB	2:I:243:THR:HB	1.77	1.14
2:D:47:ARG:HH11	2:D:215:ARG:NH1	1.46	1.14
1:F:334:LYS:HB2	2:G:297:LEU:CD2	1.77	1.14
2:I:215:ARG:HG3	6:I:803:ADP:C5'	1.77	1.14
2:D:360:HIS:HB3	2:D:363:MET:CB	1.77	1.14
2:G:99:THR:CG2	2:H:145:GLU:HB2	1.78	1.14
1:A:190:LEU:O	2:B:30:ASN:ND2	1.82	1.13
1:F:67:LEU:HD11	1:F:80:LEU:CD1	1.79	1.13
2:I:215:ARG:CD	6:I:803:ADP:H5'1	1.77	1.13
1:F:47:PHE:HA	1:F:77:ARG:O	1.47	1.13
2:G:6:LEU:HD23	2:G:194:GLU:HG3	1.25	1.13
2:G:10:TRP:CZ2	2:G:193:GLU:HB3	1.76	1.13
2:I:360:HIS:HB3	2:I:363:MET:CB	1.77	1.13
1:A:71:MET:CE	1:A:72:SER:H	1.62	1.13
1:A:71:MET:CE	1:A:72:SER:CA	2.27	1.13
1:F:209:ALA:C	2:G:176:LYS:NZ	2.01	1.12
2:I:200:PRO:CB	2:I:305:ASP:HB2	1.79	1.12
1:A:71:MET:CE	1:A:72:SER:N	2.11	1.12
2:G:242:GLY:O	2:G:243:THR:CG2	1.79	1.12
2:C:112:GLN:O	2:C:121:LYS:HD3	1.50	1.12
1:A:71:MET:CE	1:A:72:SER:CB	2.27	1.11
1:F:183:GLN:OE1	2:G:172:GLN:NE2	1.84	1.11
1:F:47:PHE:CE2	1:F:78:GLN:O	2.03	1.11
2:G:10:TRP:CZ2	2:G:193:GLU:HB2	1.67	1.11
2:H:112:GLN:O	2:H:121:LYS:HD3	1.51	1.10
1:A:190:LEU:HA	2:B:36:ARG:HH22	1.10	1.10
1:F:100:LEU:CD2	1:F:103:LEU:CD2	2.30	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:33:PRO:O	3:J:197:SER:OG	1.69	1.10
2:G:6:LEU:HD22	2:G:190:ILE:HG22	1.17	1.10
2:I:215:ARG:HG3	6:I:803:ADP:H5'1	1.11	1.10
2:H:99:THR:HG22	2:I:132:SER:HA	1.12	1.09
2:I:214:LEU:HD23	6:I:803:ADP:N3	1.66	1.09
2:I:200:PRO:HB2	2:I:305:ASP:HB2	1.11	1.09
2:I:238:SER:HB2	2:I:243:THR:HB	1.30	1.09
2:G:6:LEU:CD2	2:G:190:ILE:HG22	1.81	1.09
1:A:53:PHE:CE2	1:A:64:ILE:HD12	1.86	1.09
1:F:210:ALA:HB2	2:G:176:LYS:HE2	1.25	1.09
2:I:345:ARG:CZ	3:J:150:ARG:CG	2.29	1.09
2:C:112:GLN:CG	2:C:121:LYS:HZ1	1.57	1.09
2:D:360:HIS:HB3	2:D:363:MET:HB2	1.11	1.09
1:F:100:LEU:CA	1:F:103:LEU:HD22	1.81	1.09
1:F:100:LEU:CD2	1:F:103:LEU:HD23	1.83	1.09
2:C:11:ARG:HH22	2:D:165:THR:HG22	1.15	1.09
2:G:10:TRP:CZ2	2:G:193:GLU:CG	2.14	1.09
1:A:53:PHE:CE2	1:A:64:ILE:CB	2.35	1.09
1:F:74:PHE:CD2	1:F:78:GLN:HG2	1.84	1.08
3:E:35:MET:HE2	3:E:166:PRO:HD3	1.26	1.08
1:A:105:HIS:HB3	1:F:227:LYS:HD2	1.32	1.08
2:I:345:ARG:HH22	3:J:150:ARG:HG2	0.91	1.08
2:I:215:ARG:CG	6:I:803:ADP:C5'	2.30	1.08
1:A:72:SER:OG	1:A:75:ALA:HA	1.52	1.08
1:A:210:ALA:HB3	2:B:176:LYS:HE2	1.16	1.08
1:A:71:MET:HE2	1:A:72:SER:CA	1.83	1.07
1:A:107:ASP:HB2	1:F:228:ARG:NH1	1.31	1.07
1:F:100:LEU:HA	1:F:103:LEU:HD22	1.27	1.07
2:C:351:MET:HE1	2:D:326:GLN:HE22	0.94	1.07
1:A:71:MET:HE2	1:A:72:SER:N	1.69	1.06
2:B:246:ASP:HB3	2:B:274:ARG:HD3	1.37	1.06
2:I:345:ARG:NE	3:J:150:ARG:NE	1.96	1.06
1:F:97:LEU:HD23	1:F:126:TRP:CD2	1.90	1.06
1:A:71:MET:HE3	1:A:72:SER:HB3	1.14	1.06
1:F:47:PHE:CE1	1:F:77:ARG:CB	2.37	1.06
2:C:229:ASP:CG	2:D:30:ASN:HD21	1.57	1.06
2:H:215:ARG:NH1	2:I:164:VAL:HG12	1.70	1.05
2:I:360:HIS:HB3	2:I:363:MET:HB2	1.11	1.05
1:A:106:ASP:H	1:F:225:LYS:HD3	1.10	1.05
1:A:29:LEU:HD22	1:A:154:ARG:HH12	1.17	1.05
1:A:73:LEU:HG	1:F:207:ASN:CG	1.76	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:67:LEU:HD21	1:F:80:LEU:HD13	1.38	1.05
1:A:73:LEU:HG	1:F:207:ASN:CB	1.85	1.04
1:F:100:LEU:HD23	1:F:103:LEU:HD23	1.34	1.04
1:A:49:GLU:O	1:A:78:GLN:HA	1.57	1.04
1:A:71:MET:HE2	1:A:72:SER:H	1.21	1.04
1:F:334:LYS:HB2	2:G:297:LEU:HD23	1.36	1.04
2:I:224:ALA:HB2	2:I:240:MET:HE1	1.39	1.04
2:G:99:THR:HG21	2:H:145:GLU:HB2	1.26	1.04
2:B:215:ARG:HD2	6:B:802:ADP:H5'1	1.38	1.04
1:F:71:MET:CG	1:F:108:LEU:CD1	2.28	1.04
2:I:345:ARG:NH1	3:J:149:GLU:OE1	1.90	1.03
2:H:84:GLN:O	2:I:144:GLU:OE2	1.75	1.03
2:C:112:GLN:CA	2:C:121:LYS:HZ2	1.56	1.03
1:A:223:MET:SD	1:A:292:ARG:HB3	1.99	1.03
1:F:67:LEU:HD11	1:F:80:LEU:HD11	1.41	1.03
1:A:73:LEU:CG	1:F:207:ASN:CB	2.27	1.03
1:A:209:ALA:O	2:B:176:LYS:HE3	1.59	1.03
1:A:73:LEU:HD21	1:F:207:ASN:C	1.71	1.03
2:H:112:GLN:O	2:H:121:LYS:CD	2.07	1.02
2:C:351:MET:CE	2:D:326:GLN:HE22	1.72	1.02
1:F:100:LEU:HD23	1:F:103:LEU:HD21	1.35	1.02
1:F:25:GLY:HA3	1:F:139:CYS:O	1.59	1.02
2:G:6:LEU:HD11	2:G:191:LEU:HD23	1.36	1.02
2:I:345:ARG:HH22	3:J:150:ARG:CG	1.62	1.02
1:A:53:PHE:HE2	1:A:64:ILE:HD12	1.24	1.02
2:C:112:GLN:O	2:C:121:LYS:CD	2.07	1.02
2:G:246:ASP:HB3	2:G:274:ARG:HD3	1.40	1.02
1:F:223:MET:SD	1:F:292:ARG:HB3	1.99	1.02
1:F:71:MET:HG3	1:F:108:LEU:HD11	1.06	1.02
2:B:99:THR:CB	2:C:144:GLU:HG2	1.89	1.01
1:F:100:LEU:HA	1:F:103:LEU:HD21	1.39	1.01
2:I:345:ARG:NH1	3:J:150:ARG:HG3	1.75	1.01
1:A:73:LEU:HD23	1:F:207:ASN:HB3	1.08	1.00
2:H:215:ARG:HH22	2:I:164:VAL:CG1	1.57	1.00
1:A:71:MET:CE	1:A:72:SER:HB3	1.91	1.00
2:H:10:TRP:CE2	2:H:190:ILE:HG23	1.97	1.00
2:D:277:GLU:OE1	3:E:149:GLU:HG3	1.62	1.00
1:A:53:PHE:CZ	1:A:64:ILE:CB	2.45	1.00
2:G:98:ARG:HB2	2:H:169:ARG:HH12	1.21	0.99
1:A:25:GLY:HA3	1:A:139:CYS:O	1.59	0.99
1:F:32:GLN:NE2	2:G:165:THR:CG2	2.25	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LEU:HD22	1:A:314:GLN:HE21	1.27	0.99
1:F:47:PHE:HD2	1:F:78:GLN:C	1.65	0.99
1:F:74:PHE:HD2	1:F:78:GLN:CG	1.37	0.99
1:A:71:MET:CE	1:A:72:SER:O	2.09	0.99
2:I:11:ARG:HH21	2:I:56:ARG:HH21	1.07	0.99
2:I:238:SER:HB2	2:I:243:THR:CB	1.92	0.99
1:F:47:PHE:CD2	1:F:78:GLN:N	2.31	0.99
1:F:74:PHE:HD2	1:F:78:GLN:HG3	0.85	0.99
1:A:64:ILE:HD11	1:A:100:LEU:HD11	1.40	0.99
2:H:351:MET:HE1	2:I:326:GLN:HE22	1.23	0.99
2:D:363:MET:HB3	2:D:364:PRO:HD2	1.43	0.99
1:F:315:ASP:HB2	1:F:318:GLN:CG	1.93	0.99
2:G:6:LEU:HD11	2:G:191:LEU:HD21	1.45	0.98
1:A:119:LYS:H	1:A:119:LYS:HD3	1.26	0.98
1:A:334:LYS:CB	2:B:297:LEU:HD21	1.93	0.98
1:F:47:PHE:CD2	1:F:78:GLN:C	2.37	0.98
1:A:193:PRO:HG3	2:B:30:ASN:OD1	1.47	0.97
1:A:315:ASP:HB2	1:A:318:GLN:CG	1.94	0.97
1:F:119:LYS:H	1:F:119:LYS:HD3	1.26	0.97
1:F:71:MET:HE3	1:F:80:LEU:HD21	1.02	0.97
1:A:106:ASP:H	1:F:225:LYS:CD	1.78	0.97
2:G:6:LEU:CD2	2:G:190:ILE:CG2	2.38	0.97
1:A:49:GLU:HB2	1:A:78:GLN:HG2	1.46	0.97
2:I:363:MET:HB3	2:I:364:PRO:HD2	1.43	0.97
2:H:7:ALA:HA	2:H:218:LEU:CD1	1.95	0.97
2:I:200:PRO:HB2	2:I:305:ASP:CB	1.95	0.97
2:G:11:ARG:HH21	2:G:56:ARG:HH21	1.13	0.97
2:I:277:GLU:HB3	3:J:149:GLU:HG2	1.41	0.96
2:I:215:ARG:CA	6:I:803:ADP:O4'	2.13	0.96
1:F:310:LEU:HD22	1:F:314:GLN:HE21	1.26	0.96
2:C:351:MET:HE1	2:D:326:GLN:NE2	1.79	0.96
1:F:71:MET:HB3	1:F:108:LEU:CG	1.95	0.96
1:F:47:PHE:CA	1:F:77:ARG:O	2.12	0.96
1:F:209:ALA:CA	2:G:176:LYS:NZ	2.22	0.96
2:D:357:LEU:HA	2:D:363:MET:SD	2.06	0.96
1:A:53:PHE:CE2	1:A:64:ILE:CG1	2.48	0.95
1:F:47:PHE:CE2	1:F:78:GLN:N	2.33	0.95
1:F:209:ALA:O	2:G:176:LYS:HE3	0.79	0.95
1:A:61:TRP:O	1:A:64:ILE:HG22	1.66	0.95
1:F:74:PHE:CE2	1:F:78:GLN:CG	2.49	0.95
2:I:357:LEU:HA	2:I:363:MET:SD	2.05	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:277:GLU:CB	3:E:149:GLU:CG	2.17	0.94
1:A:193:PRO:HG3	2:B:30:ASN:HD21	1.19	0.94
1:A:65:PHE:CE1	1:A:99:THR:HG23	2.00	0.94
1:F:32:GLN:HE22	2:G:165:THR:HG22	1.24	0.94
2:H:10:TRP:CZ2	2:H:190:ILE:HG23	2.03	0.94
1:A:213:THR:H	1:A:216:HIS:HD2	1.06	0.94
1:F:71:MET:CB	1:F:108:LEU:HD11	1.82	0.94
2:H:112:GLN:CG	2:H:121:LYS:HZ3	1.61	0.94
3:J:32:LEU:HD12	3:J:166:PRO:HG3	1.48	0.94
2:G:177:ALA:O	2:G:178:LEU:HD23	1.68	0.93
2:C:84:GLN:HB3	2:D:144:GLU:OE2	1.67	0.93
2:G:10:TRP:HZ2	2:G:193:GLU:HB2	1.07	0.93
2:H:5:VAL:HB	2:H:222:ASP:OD2	1.70	0.92
2:H:99:THR:CB	2:I:132:SER:HA	1.99	0.92
1:A:73:LEU:HD22	1:F:207:ASN:O	1.69	0.92
2:G:7:ALA:CB	2:G:218:LEU:HD13	2.00	0.92
2:C:223:GLN:HE22	2:D:174:HIS:CD2	1.87	0.92
2:I:214:LEU:HD23	6:I:803:ADP:C2	2.04	0.92
2:D:47:ARG:HH12	2:D:215:ARG:HH22	1.14	0.92
2:D:334:ILE:HG21	3:E:332:PRO:HB2	1.48	0.92
1:F:71:MET:CE	1:F:80:LEU:HD21	1.98	0.92
1:A:73:LEU:HD23	1:F:207:ASN:C	1.81	0.92
1:F:74:PHE:CE2	1:F:78:GLN:HG2	2.03	0.92
2:H:215:ARG:HH12	2:I:164:VAL:HG12	1.30	0.91
1:F:47:PHE:HE2	1:F:78:GLN:O	1.46	0.91
2:C:227:SER:HB3	2:D:27:ALA:HB2	1.49	0.91
1:F:71:MET:HE3	1:F:80:LEU:CD2	1.98	0.91
1:A:29:LEU:HD21	1:A:154:ARG:HH12	0.77	0.91
2:H:112:GLN:CA	2:H:121:LYS:HZ2	1.58	0.91
1:F:212:PHE:N	1:F:239:GLU:OE2	2.02	0.91
2:G:99:THR:HG21	2:H:145:GLU:CG	2.00	0.91
2:I:215:ARG:CB	6:I:803:ADP:H5'1	2.01	0.91
2:B:215:ARG:CD	6:B:802:ADP:H5'1	2.00	0.91
1:A:71:MET:HE3	1:A:72:SER:N	1.85	0.91
2:D:200:PRO:HB2	2:D:305:ASP:HB2	1.51	0.91
2:I:334:ILE:HG21	3:J:332:PRO:HB2	1.51	0.91
2:B:99:THR:OG1	2:C:144:GLU:CG	2.18	0.91
1:A:29:LEU:HD22	1:A:154:ARG:NH1	1.75	0.90
2:H:201:ARG:NH2	2:H:305:ASP:O	2.04	0.90
2:G:6:LEU:HD22	2:G:190:ILE:HG23	1.52	0.90
1:A:53:PHE:CE2	1:A:64:ILE:CD1	2.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:224:ALA:HB2	2:I:240:MET:CE	2.02	0.90
1:A:71:MET:CE	1:A:72:SER:C	2.39	0.90
3:E:32:LEU:HD11	3:E:195:ALA:O	1.71	0.90
3:J:32:LEU:HD11	3:J:195:ALA:O	1.70	0.90
1:F:62:ASN:HA	1:F:65:PHE:HD1	1.37	0.90
2:I:215:ARG:HA	6:I:803:ADP:O4'	1.70	0.90
2:I:200:PRO:HD2	2:I:305:ASP:CG	1.92	0.89
2:C:113:TYR:CD2	2:C:147:PRO:HG3	2.07	0.89
2:D:47:ARG:NH1	2:D:215:ARG:HH22	1.69	0.89
1:F:55:ILE:HD11	1:F:82:LEU:CG	2.01	0.89
2:H:113:TYR:CD2	2:H:147:PRO:HG3	2.08	0.89
2:C:51:LYS:HE2	4:C:1300:PO4:O3	1.73	0.89
2:H:215:ARG:NH1	2:I:164:VAL:HG11	1.79	0.89
2:D:47:ARG:NH1	2:D:215:ARG:HH12	1.70	0.89
2:H:7:ALA:HA	2:H:218:LEU:HD13	1.51	0.89
2:G:99:THR:CG2	2:H:145:GLU:CB	2.42	0.89
2:I:345:ARG:CZ	3:J:150:ARG:HG3	1.98	0.89
2:H:215:ARG:HH12	2:I:164:VAL:CG1	1.83	0.89
2:I:215:ARG:HD2	6:I:803:ADP:H5'1	1.54	0.89
2:D:20:GLY:HA2	2:D:22:GLU:OE2	1.73	0.89
2:H:351:MET:CE	2:I:326:GLN:HE22	1.85	0.89
2:C:11:ARG:NH2	2:D:165:THR:HG22	1.86	0.89
1:A:73:LEU:CD2	1:F:207:ASN:HA	1.73	0.88
2:C:113:TYR:HB3	2:C:149:HIS:NE2	1.87	0.88
2:I:6:LEU:N	2:I:222:ASP:OD2	2.05	0.88
2:I:357:LEU:O	2:I:363:MET:SD	2.31	0.88
2:G:99:THR:H	2:H:144:GLU:CG	1.82	0.88
1:F:210:ALA:HB3	2:G:176:LYS:HE2	0.97	0.88
1:F:32:GLN:HE21	2:G:165:THR:HG22	1.07	0.88
2:G:10:TRP:CG	2:G:190:ILE:HG12	2.09	0.88
2:D:357:LEU:O	2:D:363:MET:SD	2.30	0.88
2:D:363:MET:CB	2:D:364:PRO:HD2	2.04	0.88
1:A:55:ILE:HD11	1:A:84:LEU:HD12	1.54	0.88
2:I:244:LEU:HD21	2:I:276:ILE:HG12	1.56	0.88
2:I:363:MET:CB	2:I:364:PRO:HD2	2.04	0.87
2:G:99:THR:HG21	2:H:145:GLU:N	1.88	0.87
1:A:72:SER:HG	1:A:75:ALA:HA	1.36	0.87
1:A:65:PHE:CD1	1:A:99:THR:CG2	2.32	0.87
1:A:73:LEU:HD21	1:F:207:ASN:HA	0.90	0.87
1:F:47:PHE:CD2	1:F:78:GLN:O	2.27	0.87
2:H:10:TRP:CZ3	2:H:190:ILE:HG12	2.10	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:11:ARG:HH21	2:G:56:ARG:NH2	1.72	0.87
1:F:334:LYS:HB2	2:G:297:LEU:HD21	1.53	0.87
1:A:49:GLU:CB	1:A:78:GLN:HG2	2.05	0.87
2:D:355:ARG:NH1	3:E:287:GLN:HB3	1.89	0.87
1:A:71:MET:HE1	1:A:72:SER:O	1.72	0.87
2:G:7:ALA:HA	2:G:218:LEU:HD13	1.57	0.87
1:A:210:ALA:HB3	2:B:176:LYS:CE	2.04	0.86
1:A:334:LYS:CB	2:B:297:LEU:CD2	2.52	0.86
1:F:47:PHE:CD1	1:F:77:ARG:HB3	2.10	0.86
1:F:47:PHE:CD2	1:F:78:GLN:CA	2.57	0.86
2:D:309:ILE:CG2	2:D:313:MET:HG2	2.05	0.86
1:F:47:PHE:HE1	1:F:77:ARG:HB3	1.34	0.86
2:H:271:ALA:HB1	2:H:276:ILE:HD11	1.56	0.86
1:F:71:MET:HG3	1:F:108:LEU:CD1	1.95	0.86
2:G:7:ALA:CA	2:G:218:LEU:HD13	2.04	0.86
1:A:55:ILE:HG13	1:A:85:PRO:HD3	1.57	0.86
2:H:112:GLN:HB2	2:H:121:LYS:HE2	1.56	0.86
1:A:65:PHE:HE1	1:A:99:THR:CG2	1.54	0.86
2:G:148:GLU:CD	2:G:149:HIS:H	1.79	0.86
2:I:309:ILE:CG2	2:I:313:MET:HG2	2.05	0.86
2:D:47:ARG:HH11	2:D:215:ARG:HH12	0.89	0.85
2:H:113:TYR:HB3	2:H:149:HIS:NE2	1.87	0.85
1:A:57:PRO:O	1:A:58:ASN:HB2	1.73	0.85
2:C:271:ALA:HB1	2:C:276:ILE:HD11	1.57	0.85
1:A:65:PHE:HE1	1:A:99:THR:HG21	1.07	0.85
1:F:47:PHE:CD2	1:F:77:ARG:C	2.50	0.85
1:A:190:LEU:HA	2:B:36:ARG:NH2	1.90	0.85
3:J:204:LEU:O	3:J:209:ASN:HB2	1.75	0.85
2:G:6:LEU:CB	2:G:190:ILE:CG2	2.45	0.85
2:I:238:SER:HB3	2:I:243:THR:HB	1.57	0.85
1:F:211:HIS:CG	1:F:211:HIS:O	2.30	0.84
1:F:97:LEU:HB3	1:F:126:TRP:HB2	1.56	0.84
1:F:84:LEU:HG	1:F:89:PRO:HD3	1.60	0.84
2:G:6:LEU:HD13	2:G:190:ILE:HG22	1.59	0.84
2:C:112:GLN:HB2	2:C:121:LYS:HE2	1.54	0.84
1:A:141:THR:HG23	1:A:178:LEU:HG	1.59	0.84
2:I:11:ARG:HH21	2:I:56:ARG:NH2	1.75	0.84
2:C:223:GLN:HE22	2:D:174:HIS:HD2	1.22	0.84
2:D:148:GLU:CD	2:D:149:HIS:H	1.79	0.84
2:B:148:GLU:CD	2:B:149:HIS:H	1.79	0.84
1:F:312:LEU:HB2	1:F:320:VAL:HG21	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:PHE:CD2	1:A:64:ILE:HG13	2.12	0.84
1:A:193:PRO:CG	2:B:30:ASN:CG	2.24	0.84
2:C:112:GLN:C	2:C:121:LYS:HZ2	1.81	0.84
1:F:210:ALA:CA	2:G:176:LYS:CE	2.43	0.84
1:F:55:ILE:CD1	1:F:82:LEU:CG	2.56	0.84
1:F:238:LEU:HD13	2:G:177:ALA:HB3	1.58	0.84
2:I:355:ARG:NH1	3:J:287:GLN:HB3	1.93	0.84
1:F:47:PHE:CG	1:F:77:ARG:O	2.31	0.83
1:A:105:HIS:HB3	1:F:227:LYS:CD	2.08	0.83
2:I:277:GLU:CB	3:J:149:GLU:HG2	2.07	0.83
1:A:334:LYS:HB2	2:B:297:LEU:HD23	1.58	0.83
1:A:106:ASP:N	1:F:225:LYS:HD3	1.92	0.83
3:E:35:MET:CE	3:E:166:PRO:HD3	2.09	0.83
2:I:345:ARG:HH21	3:J:150:ARG:NE	1.75	0.83
1:A:71:MET:HE3	1:A:72:SER:CA	2.03	0.83
3:J:8:ARG:HG3	3:J:9:PRO:HD3	1.59	0.83
2:B:362:ARG:HE	2:B:363:MET:HE2	1.44	0.83
1:F:213:THR:H	1:F:216:HIS:HD2	1.26	0.83
1:F:100:LEU:O	1:F:103:LEU:HD22	1.79	0.83
2:G:6:LEU:CG	2:G:190:ILE:CG2	2.56	0.83
2:D:214:LEU:HD23	6:D:801:ADP:C4	2.14	0.82
3:E:8:ARG:HG3	3:E:9:PRO:HD3	1.59	0.82
2:H:99:THR:CG2	2:I:132:SER:CB	2.57	0.82
1:F:210:ALA:N	2:G:176:LYS:HE3	1.85	0.82
2:I:345:ARG:NH1	3:J:150:ARG:CG	2.41	0.82
2:D:357:LEU:HA	2:D:363:MET:CE	2.09	0.82
1:F:71:MET:SD	1:F:108:LEU:HG	2.19	0.82
1:A:64:ILE:CD1	1:A:100:LEU:HD11	2.10	0.82
2:I:357:LEU:HA	2:I:363:MET:CE	2.09	0.82
2:G:99:THR:HG21	2:H:145:GLU:CA	2.10	0.82
2:G:6:LEU:CD2	2:G:194:GLU:CG	2.56	0.82
1:F:210:ALA:HB3	2:G:176:LYS:CG	2.09	0.82
2:G:6:LEU:CD1	2:G:190:ILE:HG22	2.10	0.82
1:F:52:THR:HG23	1:F:81:LEU:HD23	1.62	0.82
2:H:215:ARG:CZ	2:I:164:VAL:CB	2.58	0.82
2:D:215:ARG:HG3	6:D:801:ADP:H5'1	1.60	0.82
2:G:98:ARG:N	2:H:169:ARG:NH2	1.99	0.81
2:G:6:LEU:CG	2:G:190:ILE:HG22	2.10	0.81
1:A:73:LEU:HG	1:F:207:ASN:OD1	1.78	0.81
2:D:253:VAL:O	2:D:257:VAL:HG23	1.80	0.81
2:G:5:VAL:CG1	2:G:222:ASP:OD1	2.29	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:360:HIS:HB3	2:I:363:MET:CG	2.11	0.81
2:I:360:HIS:ND1	2:I:363:MET:HE2	1.96	0.81
3:E:32:LEU:CD1	3:E:195:ALA:O	2.28	0.81
2:C:229:ASP:CG	2:D:30:ASN:ND2	2.32	0.81
1:A:312:LEU:HB2	1:A:320:VAL:HG21	1.59	0.81
2:I:360:HIS:ND1	2:I:363:MET:CE	2.44	0.81
2:G:98:ARG:HB2	2:H:169:ARG:NH1	1.94	0.81
2:I:238:SER:CB	2:I:243:THR:CB	2.57	0.81
1:A:213:THR:H	1:A:216:HIS:CD2	1.97	0.81
3:E:58:SER:HB3	3:E:65:CYS:SG	2.21	0.81
2:D:277:GLU:HB3	3:E:149:GLU:HG3	1.58	0.81
2:D:21:GLN:HE22	2:D:176:LYS:H	1.26	0.81
2:C:309:ILE:HG13	2:C:313:MET:HG2	1.62	0.81
1:A:74:PHE:O	1:A:74:PHE:CD2	2.33	0.81
1:A:71:MET:HE2	1:A:72:SER:O	1.73	0.81
2:B:113:TYR:HE2	2:B:147:PRO:HG3	1.46	0.80
2:D:360:HIS:ND1	2:D:363:MET:CE	2.44	0.80
2:I:253:VAL:O	2:I:257:VAL:HG23	1.80	0.80
1:F:51:HIS:HB2	1:F:80:LEU:HD23	1.61	0.80
3:J:58:SER:HB3	3:J:65:CYS:SG	2.22	0.80
1:A:51:HIS:N	1:A:79:THR:O	2.12	0.80
1:A:315:ASP:HB2	1:A:318:GLN:HG3	1.63	0.80
2:H:93:ILE:HG12	2:I:133:ARG:HH12	1.45	0.80
1:F:61:TRP:HA	1:F:64:ILE:HD13	1.64	0.80
2:H:309:ILE:HG13	2:H:313:MET:HG2	1.62	0.80
2:D:360:HIS:HB3	2:D:363:MET:CG	2.11	0.80
1:F:67:LEU:HD11	1:F:80:LEU:CD2	2.12	0.80
2:H:112:GLN:C	2:H:121:LYS:HZ2	1.84	0.80
1:F:244:VAL:HG22	1:F:312:LEU:HD21	1.64	0.80
2:C:100:LYS:NZ	2:D:133:ARG:HG3	1.96	0.80
3:J:33:PRO:O	3:J:197:SER:CB	2.30	0.79
2:H:10:TRP:CE3	2:H:190:ILE:HG12	2.17	0.79
2:I:345:ARG:HE	3:J:150:ARG:NE	1.79	0.79
2:C:67:GLY:HA2	2:C:119:ARG:HH12	1.47	0.79
2:H:215:ARG:NH2	2:I:164:VAL:CB	2.46	0.79
2:D:113:TYR:HE2	2:D:147:PRO:HG3	1.46	0.79
1:F:71:MET:HB2	1:F:108:LEU:HD12	1.59	0.79
1:F:100:LEU:C	1:F:103:LEU:HD22	2.01	0.79
2:G:7:ALA:HB2	2:G:218:LEU:HD13	1.64	0.79
2:I:259:ALA:HB2	2:I:363:MET:CG	2.12	0.79
2:D:47:ARG:NH1	2:D:215:ARG:NH2	2.29	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:80:ARG:O	2:C:84:GLN:HG3	1.82	0.79
1:F:53:PHE:CZ	1:F:67:LEU:HD22	2.17	0.79
2:H:271:ALA:CB	2:H:276:ILE:HD11	2.13	0.79
2:G:6:LEU:HB3	2:G:190:ILE:HG21	0.86	0.79
2:H:67:GLY:HA2	2:H:119:ARG:HH12	1.47	0.79
1:F:315:ASP:HB2	1:F:318:GLN:HG3	1.63	0.79
1:A:222:LEU:O	1:A:223:MET:HB2	1.83	0.79
2:B:179:ASP:HB3	2:B:182:GLN:HB2	1.65	0.79
2:G:242:GLY:CA	2:G:243:THR:OG1	2.21	0.78
2:H:80:ARG:O	2:H:84:GLN:HG3	1.83	0.78
1:F:310:LEU:HD22	1:F:314:GLN:NE2	1.98	0.78
1:A:107:ASP:HB3	1:F:228:ARG:HH12	1.43	0.78
2:D:214:LEU:HD23	6:D:801:ADP:N3	1.97	0.78
1:A:244:VAL:HG22	1:A:312:LEU:HD21	1.64	0.78
2:G:113:TYR:HE2	2:G:147:PRO:HG3	1.46	0.78
2:G:6:LEU:HD13	2:G:190:ILE:CG2	2.13	0.78
1:A:190:LEU:HD11	2:B:171:LEU:HD21	1.64	0.78
2:I:200:PRO:CG	2:I:305:ASP:HB2	2.13	0.78
1:F:56:ASP:HB2	1:F:57:PRO:HD3	1.66	0.78
1:A:310:LEU:HD22	1:A:314:GLN:NE2	1.98	0.78
2:B:248:GLN:HG3	2:B:267:LEU:HB3	1.65	0.78
1:A:55:ILE:CD1	1:A:84:LEU:HD12	2.13	0.78
2:C:271:ALA:CB	2:C:276:ILE:HD11	2.13	0.78
2:I:360:HIS:CB	2:I:363:MET:CG	2.61	0.78
2:I:277:GLU:CB	3:J:149:GLU:CG	2.61	0.78
2:D:259:ALA:HB2	2:D:363:MET:CG	2.12	0.78
2:D:363:MET:HB3	2:D:364:PRO:CD	2.14	0.78
1:A:49:GLU:HB2	1:A:78:GLN:CG	2.13	0.78
2:G:248:GLN:HG3	2:G:267:LEU:HB3	1.65	0.78
2:B:261:GLY:HA3	2:C:297:LEU:HD21	1.66	0.78
2:G:10:TRP:CE2	2:G:193:GLU:HB3	2.18	0.77
2:H:281:LEU:HD23	2:H:285:MET:HE2	1.67	0.77
2:D:61:GLY:HA2	2:D:72:PRO:HG3	1.66	0.77
2:G:259:ALA:HB3	2:G:363:MET:HE3	1.67	0.77
2:D:360:HIS:CB	2:D:363:MET:CG	2.62	0.77
1:F:210:ALA:N	2:G:176:LYS:HE2	1.83	0.77
2:G:362:ARG:HE	2:G:363:MET:HE2	1.48	0.77
1:A:55:ILE:CG1	1:A:85:PRO:HD3	2.15	0.77
2:I:345:ARG:HE	3:J:150:ARG:HE	1.22	0.77
1:F:97:LEU:HD23	1:F:126:TRP:CE3	2.18	0.77
1:F:222:LEU:O	1:F:223:MET:HB2	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:128:VAL:HG11	2:H:154:LEU:HD22	1.67	0.77
2:B:48:GLY:O	2:B:213:SER:HB2	1.84	0.77
2:D:337:LYS:HD3	3:E:334:LEU:HB2	1.67	0.77
2:D:244:LEU:HD21	2:D:276:ILE:HG12	1.67	0.77
2:H:6:LEU:HB3	2:H:218:LEU:HD22	1.65	0.77
3:J:32:LEU:CD1	3:J:195:ALA:O	2.32	0.77
2:H:112:GLN:HB3	2:H:121:LYS:NZ	1.11	0.77
2:I:277:GLU:HB3	3:J:149:GLU:CB	2.14	0.77
2:I:215:ARG:CB	6:I:803:ADP:C5'	2.61	0.77
2:B:61:GLY:HA2	2:B:72:PRO:HG3	1.66	0.77
1:A:234:GLN:OE1	2:B:304:ASN:ND2	2.17	0.77
2:C:128:VAL:HG11	2:C:154:LEU:HD22	1.67	0.77
1:F:300:GLN:OE1	1:F:335:PRO:CG	2.32	0.77
2:C:281:LEU:HD23	2:C:285:MET:HE2	1.66	0.77
1:A:300:GLN:OE1	1:A:335:PRO:CG	2.33	0.76
2:G:61:GLY:HA2	2:G:72:PRO:HG3	1.66	0.76
1:A:73:LEU:HD23	1:F:207:ASN:CA	1.80	0.76
2:G:56:ARG:HG3	2:G:56:ARG:HH11	1.50	0.76
2:D:56:ARG:HG3	2:D:56:ARG:HH11	1.50	0.76
1:A:53:PHE:CD2	1:A:64:ILE:CG1	2.68	0.76
2:H:99:THR:HG22	2:I:132:SER:CB	2.14	0.76
2:D:360:HIS:HB2	2:D:363:MET:SD	2.26	0.76
1:F:100:LEU:CA	1:F:103:LEU:CD2	2.47	0.76
1:A:209:ALA:O	2:B:176:LYS:CE	2.33	0.76
2:I:61:GLY:HA2	2:I:72:PRO:HG3	1.66	0.76
2:I:345:ARG:HH21	3:J:150:ARG:CD	1.96	0.76
1:F:99:THR:O	1:F:103:LEU:HD11	1.86	0.76
1:F:100:LEU:HD22	1:F:103:LEU:HD23	1.69	0.75
2:I:215:ARG:HD2	6:I:803:ADP:C5'	2.16	0.75
2:I:360:HIS:HB2	2:I:363:MET:SD	2.26	0.75
2:G:97:SER:HA	2:H:169:ARG:HH21	1.51	0.75
2:D:259:ALA:CB	2:D:363:MET:HG2	2.17	0.75
1:A:55:ILE:HD13	1:A:97:LEU:HD11	1.67	0.75
1:F:48:GLU:OE2	1:F:74:PHE:CE1	2.39	0.75
1:F:99:THR:O	1:F:103:LEU:CD1	2.34	0.75
2:D:47:ARG:NH1	2:D:215:ARG:NH1	2.30	0.75
3:J:165:ALA:O	3:J:167:PRO:HD3	1.86	0.75
2:C:276:ILE:HD13	2:C:281:LEU:HD12	1.69	0.75
1:F:67:LEU:CD2	1:F:80:LEU:HD13	2.14	0.75
2:D:257:VAL:O	2:D:360:HIS:HE1	1.69	0.75
1:A:147:LEU:HB3	1:A:148:PRO:HD3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:99:THR:HG22	2:I:132:SER:CA	1.84	0.75
2:I:215:ARG:HB2	6:I:803:ADP:C5'	2.16	0.74
2:I:257:VAL:O	2:I:360:HIS:HE1	1.69	0.74
2:H:276:ILE:HD13	2:H:281:LEU:HD12	1.68	0.74
3:J:5:PRO:O	3:J:8:ARG:HG2	1.87	0.74
1:A:190:LEU:CD1	2:B:171:LEU:HD21	2.17	0.74
2:C:341:TYR:HB2	2:D:333:LEU:HD11	1.68	0.74
2:B:265:MET:HE1	2:C:294:MET:SD	2.27	0.74
2:H:93:ILE:HA	2:I:133:ARG:NH2	2.01	0.74
2:G:99:THR:CG2	2:H:145:GLU:CG	2.65	0.74
2:I:345:ARG:NH2	3:J:150:ARG:HD3	1.99	0.74
1:A:190:LEU:O	2:B:30:ASN:CG	2.25	0.74
1:A:310:LEU:HD13	1:A:314:GLN:NE2	2.01	0.74
3:E:5:PRO:O	3:E:8:ARG:HG2	1.87	0.74
2:C:112:GLN:HB3	2:C:121:LYS:NZ	1.08	0.74
2:G:271:ALA:HB1	2:G:276:ILE:HD12	1.68	0.74
2:I:277:GLU:CA	3:J:149:GLU:HG2	2.18	0.74
1:A:238:LEU:HD13	2:B:177:ALA:HB3	1.70	0.74
2:H:112:GLN:N	2:H:121:LYS:HZ3	1.86	0.74
2:I:259:ALA:CB	2:I:363:MET:HG2	2.17	0.74
2:I:363:MET:HB3	2:I:364:PRO:CD	2.14	0.74
2:I:148:GLU:CD	2:I:149:HIS:H	1.90	0.74
2:I:360:HIS:CG	2:I:363:MET:HG3	2.23	0.74
2:D:357:LEU:CA	2:D:363:MET:SD	2.75	0.74
1:F:273:PHE:HB3	1:F:279:TRP:CB	2.18	0.73
2:I:357:LEU:CA	2:I:363:MET:SD	2.75	0.73
1:F:310:LEU:HD13	1:F:314:GLN:NE2	2.02	0.73
2:H:113:TYR:HD2	2:H:147:PRO:HG3	1.54	0.73
2:H:93:ILE:HA	2:I:133:ARG:CZ	2.18	0.73
3:E:117:ALA:O	3:E:120:LEU:HD22	1.89	0.73
2:I:358:ALA:HA	2:I:364:PRO:HG2	1.70	0.73
2:C:156:THR:HG22	2:C:158:ASP:H	1.53	0.73
2:D:277:GLU:HB3	3:E:149:GLU:CB	2.15	0.73
1:A:82:LEU:HD21	1:A:100:LEU:HD12	1.69	0.73
3:J:49:LEU:HD23	3:J:68:MET:SD	2.29	0.73
2:H:156:THR:HG22	2:H:158:ASP:H	1.53	0.73
2:B:271:ALA:HB1	2:B:276:ILE:HD12	1.69	0.73
2:I:215:ARG:HG3	6:I:803:ADP:C4'	2.19	0.73
2:D:360:HIS:CG	2:D:363:MET:HG3	2.23	0.73
3:E:49:LEU:HD23	3:E:68:MET:SD	2.29	0.72
1:A:273:PHE:HB3	1:A:279:TRP:CB	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:336:LEU:CD1	2:G:326:GLN:NE2	2.52	0.72
2:D:271:ALA:HB1	2:D:276:ILE:CD1	2.19	0.72
2:G:99:THR:N	2:H:144:GLU:CG	2.38	0.72
1:F:147:LEU:HB3	1:F:148:PRO:HD3	1.69	0.72
2:D:259:ALA:HB1	2:D:363:MET:HG2	1.71	0.72
2:D:47:ARG:HH11	2:D:215:ARG:CZ	2.02	0.72
2:I:337:LYS:HD3	3:J:334:LEU:HB2	1.71	0.72
2:C:113:TYR:HD2	2:C:147:PRO:HG3	1.53	0.72
3:J:117:ALA:O	3:J:120:LEU:HD22	1.89	0.72
1:F:310:LEU:HD21	3:J:306:ILE:HD13	1.71	0.72
2:H:238:SER:HB2	2:H:243:THR:O	1.90	0.72
2:I:241:LEU:O	3:J:156:ARG:HD2	1.90	0.72
1:A:190:LEU:O	2:B:30:ASN:CB	2.38	0.72
2:I:271:ALA:HB1	2:I:276:ILE:CD1	2.19	0.71
2:C:86:ARG:CZ	2:D:141:LYS:HD2	2.20	0.71
2:I:244:LEU:HD21	2:I:276:ILE:CG1	2.21	0.71
1:F:74:PHE:CE2	1:F:78:GLN:HG3	2.17	0.71
2:D:358:ALA:HA	2:D:364:PRO:HG2	1.70	0.71
2:B:56:ARG:HH11	2:B:56:ARG:HG3	1.55	0.71
2:G:246:ASP:CB	2:G:274:ARG:HD3	2.20	0.71
2:I:259:ALA:HB1	2:I:363:MET:HG2	1.72	0.71
2:D:277:GLU:CA	3:E:149:GLU:HG2	2.20	0.71
2:C:112:GLN:CB	2:C:121:LYS:NZ	0.56	0.71
2:G:99:THR:N	2:H:144:GLU:HG2	1.90	0.70
1:F:300:GLN:OE1	1:F:335:PRO:HG3	1.91	0.70
1:A:300:GLN:OE1	1:A:335:PRO:HG3	1.91	0.70
2:I:334:ILE:HG12	3:J:334:LEU:OXT	1.90	0.70
2:H:112:GLN:CB	2:H:121:LYS:NZ	0.55	0.70
3:E:35:MET:HE1	3:E:166:PRO:HA	1.73	0.70
2:H:276:ILE:HG22	2:H:277:GLU:H	1.56	0.70
2:G:6:LEU:HD21	2:G:194:GLU:HG3	1.68	0.70
1:F:97:LEU:HD23	1:F:126:TRP:CE2	2.25	0.70
1:F:313:LYS:O	1:F:316:TYR:CZ	2.44	0.70
2:C:360:HIS:HB3	2:C:363:MET:O	1.91	0.70
3:E:31:ALA:HB2	3:E:164:LEU:HB3	1.72	0.70
1:F:334:LYS:CB	2:G:297:LEU:HD21	2.21	0.70
1:A:313:LYS:O	1:A:316:TYR:CZ	2.44	0.70
3:E:169:GLU:O	3:E:173:VAL:HG23	1.92	0.70
1:A:57:PRO:O	1:A:58:ASN:CB	2.39	0.70
2:H:360:HIS:HB3	2:H:363:MET:O	1.91	0.70
3:J:169:GLU:O	3:J:173:VAL:HG23	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:202:VAL:O	1:F:206:VAL:HG23	1.92	0.70
2:D:351:MET:SD	3:E:290:LEU:HD13	2.32	0.70
1:A:64:ILE:HG23	1:A:65:PHE:N	2.06	0.70
1:A:238:LEU:HD22	2:B:177:ALA:CB	2.20	0.70
1:A:53:PHE:CD2	1:A:64:ILE:HD12	2.27	0.69
2:D:345:ARG:CD	3:E:150:ARG:HH21	2.03	0.69
2:H:67:GLY:HA2	2:H:119:ARG:NH1	2.07	0.69
2:H:341:TYR:HB2	2:I:333:LEU:HD11	1.74	0.69
2:C:276:ILE:HG22	2:C:277:GLU:H	1.56	0.69
2:G:10:TRP:CZ3	2:G:189:HIS:CE1	2.79	0.69
2:D:360:HIS:ND1	2:D:363:MET:HE2	2.07	0.69
1:F:97:LEU:HB3	1:F:126:TRP:CB	2.23	0.69
2:I:338:GLU:O	2:I:341:TYR:HB2	1.93	0.69
2:G:47:ARG:O	2:G:213:SER:HB2	1.92	0.69
2:I:144:GLU:C	2:I:146:PRO:HD3	2.13	0.69
1:F:223:MET:SD	1:F:292:ARG:CB	2.78	0.69
2:D:309:ILE:HG22	2:D:313:MET:HG2	1.74	0.69
2:I:113:TYR:HD2	2:I:147:PRO:HB3	1.56	0.69
1:A:202:VAL:O	1:A:206:VAL:HG23	1.92	0.69
2:I:215:ARG:HA	6:I:803:ADP:C4'	2.22	0.69
1:F:67:LEU:HD12	1:F:71:MET:HE2	1.74	0.69
1:A:55:ILE:O	1:A:85:PRO:HG3	1.93	0.69
2:H:215:ARG:NH2	2:I:164:VAL:HG21	2.06	0.69
2:I:309:ILE:HG22	2:I:313:MET:HG2	1.74	0.69
2:C:73:CYS:O	2:C:79:CYS:SG	2.50	0.69
3:J:31:ALA:HB2	3:J:164:LEU:HB3	1.75	0.69
2:H:73:CYS:O	2:H:79:CYS:SG	2.50	0.69
2:D:259:ALA:CB	2:D:363:MET:CG	2.71	0.69
2:D:357:LEU:HA	2:D:363:MET:HE1	1.72	0.69
2:B:215:ARG:CG	6:B:802:ADP:H5'1	2.23	0.69
1:F:119:LYS:H	1:F:119:LYS:CD	2.05	0.69
2:D:338:GLU:O	2:D:341:TYR:HB2	1.93	0.69
2:I:271:ALA:HB1	2:I:276:ILE:HD12	1.75	0.69
2:I:259:ALA:CB	2:I:363:MET:CG	2.72	0.69
1:A:315:ASP:CG	1:A:315:ASP:CA	2.61	0.69
1:F:308:THR:HG23	1:F:320:VAL:HG13	1.75	0.69
3:E:111:VAL:HG12	3:E:140:TRP:HB2	1.75	0.69
2:I:21:GLN:HE22	2:I:176:LYS:H	1.40	0.68
1:F:315:ASP:CA	1:F:315:ASP:CG	2.61	0.68
2:C:67:GLY:HA2	2:C:119:ARG:NH1	2.07	0.68
2:C:112:GLN:HB3	2:C:121:LYS:HZ1	0.79	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:98:ARG:CG	2:H:140:LEU:HB3	1.97	0.68
1:F:222:LEU:HD12	1:F:285:MET:HG2	1.74	0.68
2:B:113:TYR:CE2	2:B:147:PRO:HG3	2.29	0.68
3:J:111:VAL:HG12	3:J:140:TRP:HB2	1.75	0.68
1:A:73:LEU:CB	1:F:207:ASN:HB3	2.23	0.68
1:A:222:LEU:HD12	1:A:285:MET:HG2	1.74	0.68
2:H:112:GLN:CD	2:H:121:LYS:HZ1	1.97	0.68
2:C:227:SER:CB	2:D:27:ALA:HB2	2.22	0.68
2:G:113:TYR:CE2	2:G:147:PRO:HG3	2.29	0.68
2:I:277:GLU:OE1	3:J:149:GLU:HG3	1.94	0.68
2:D:355:ARG:NH1	3:E:287:GLN:CB	2.56	0.68
2:D:254:GLU:OE2	2:D:312:ARG:HD3	1.94	0.68
2:I:254:GLU:OE2	2:I:312:ARG:HD3	1.94	0.68
1:A:308:THR:HG23	1:A:320:VAL:HG13	1.75	0.68
2:C:86:ARG:NH1	2:D:141:LYS:HD2	2.08	0.68
2:H:99:THR:HG21	2:I:132:SER:HA	0.90	0.68
2:B:215:ARG:HB2	6:B:802:ADP:O4'	1.94	0.68
2:G:99:THR:CG2	2:H:145:GLU:N	2.57	0.68
2:I:238:SER:HB2	2:I:243:THR:CA	2.24	0.68
2:B:259:ALA:HB3	2:B:363:MET:HE3	1.74	0.68
2:G:179:ASP:HB3	2:G:182:GLN:HB2	1.74	0.68
1:A:49:GLU:HB2	1:A:78:GLN:CB	2.24	0.68
3:J:204:LEU:O	3:J:209:ASN:CB	2.41	0.68
2:I:260:ASN:O	2:I:262:GLU:N	2.27	0.68
1:F:179:LEU:HD21	2:G:167:LEU:CD2	2.24	0.67
2:I:345:ARG:HE	3:J:150:ARG:NH2	1.92	0.67
1:F:47:PHE:CG	1:F:77:ARG:C	2.68	0.67
1:F:32:GLN:HE21	2:G:165:THR:CG2	1.96	0.67
1:A:223:MET:SD	1:A:292:ARG:CB	2.78	0.67
1:A:255:LEU:HD22	3:E:313:THR:HG21	1.76	0.67
1:A:191:LEU:HD23	2:B:26:THR:HG22	1.77	0.67
3:J:32:LEU:HD22	3:J:195:ALA:HB3	1.75	0.67
2:D:358:ALA:HA	2:D:364:PRO:CG	2.25	0.67
2:D:309:ILE:HG21	2:D:313:MET:HG2	1.77	0.67
1:F:210:ALA:HB3	2:G:176:LYS:HG2	1.76	0.67
2:D:145:GLU:O	2:D:147:PRO:HD3	1.95	0.67
2:I:113:TYR:CD2	2:I:147:PRO:HB3	2.30	0.67
3:J:74:PRO:HB3	3:J:105:ARG:HD2	1.76	0.67
2:G:10:TRP:CZ3	2:G:189:HIS:HE1	2.13	0.67
1:F:67:LEU:HD11	1:F:80:LEU:HD13	1.76	0.67
1:F:67:LEU:CD1	1:F:80:LEU:CD1	2.67	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:357:LEU:HA	2:I:363:MET:HE1	1.76	0.67
2:I:358:ALA:HA	2:I:364:PRO:CG	2.25	0.67
2:H:7:ALA:HA	2:H:218:LEU:HD12	1.75	0.67
2:G:259:ALA:CB	2:G:363:MET:HE3	2.25	0.67
2:H:112:GLN:HB3	2:H:121:LYS:HZ1	0.86	0.67
2:B:145:GLU:O	2:B:147:PRO:HD3	1.95	0.67
2:H:20:GLY:HA3	2:H:182:GLN:NE2	2.10	0.67
2:D:271:ALA:HB1	2:D:276:ILE:HD12	1.75	0.67
2:G:98:ARG:CB	2:H:140:LEU:HB3	2.24	0.67
1:A:234:GLN:HE22	2:B:304:ASN:HD21	1.42	0.67
2:D:244:LEU:HD11	2:D:276:ILE:HD13	1.77	0.67
2:C:112:GLN:CB	2:C:121:LYS:HZ3	0.72	0.67
1:A:73:LEU:HD13	1:F:212:PHE:CZ	2.30	0.67
2:G:21:GLN:HE22	2:G:176:LYS:H	1.41	0.67
2:I:214:LEU:HB3	6:I:803:ADP:N9	2.10	0.67
1:F:334:LYS:CB	2:G:297:LEU:CD2	2.67	0.67
3:J:8:ARG:CG	3:J:9:PRO:HD3	2.25	0.67
1:A:190:LEU:O	2:B:30:ASN:HB3	1.95	0.66
1:A:213:THR:N	1:A:216:HIS:HD2	1.88	0.66
2:D:113:TYR:CE2	2:D:147:PRO:HG3	2.29	0.66
2:I:309:ILE:HG21	2:I:313:MET:HG2	1.77	0.66
1:F:101:THR:HG21	1:F:129:ALA:CB	2.25	0.66
1:A:73:LEU:HD21	1:F:207:ASN:O	1.78	0.66
1:A:27:ASP:OD2	1:A:178:LEU:HD12	1.96	0.66
2:G:145:GLU:O	2:G:147:PRO:HD3	1.95	0.66
2:C:181:GLU:HG2	2:C:184:ARG:HD2	1.78	0.66
2:D:260:ASN:O	2:D:262:GLU:N	2.28	0.66
1:A:55:ILE:HD11	1:A:84:LEU:CD1	2.25	0.66
2:I:277:GLU:HB3	3:J:149:GLU:HB3	1.76	0.66
2:H:354:LEU:CD2	2:I:297:LEU:HD22	2.25	0.66
2:H:181:GLU:HG2	2:H:184:ARG:HD2	1.77	0.66
2:C:229:ASP:OD2	2:D:30:ASN:OD1	2.14	0.66
2:B:20:GLY:HA2	2:B:22:GLU:OE2	1.96	0.66
2:C:354:LEU:CD2	2:D:297:LEU:HD22	2.26	0.66
1:F:179:LEU:HD21	2:G:167:LEU:HD23	1.76	0.66
1:F:183:GLN:OE1	2:G:172:GLN:CD	2.34	0.66
2:G:11:ARG:NH2	2:G:56:ARG:NH2	2.43	0.66
2:B:47:ARG:O	2:B:213:SER:HB3	1.96	0.66
2:D:356:ALA:O	2:D:363:MET:HE1	1.94	0.66
2:D:347:MET:O	2:D:351:MET:HG2	1.96	0.66
3:E:8:ARG:CG	3:E:9:PRO:HD3	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:99:THR:HG21	2:H:145:GLU:HG3	1.75	0.65
3:E:64:GLY:O	3:E:68:MET:HB2	1.96	0.65
2:G:48:GLY:HA3	2:G:215:ARG:HB2	1.77	0.65
2:I:345:ARG:CZ	3:J:150:ARG:CD	2.50	0.65
3:J:32:LEU:CD1	3:J:166:PRO:HG3	2.24	0.65
3:E:74:PRO:HB3	3:E:105:ARG:HD2	1.76	0.65
2:I:347:MET:O	2:I:351:MET:HG2	1.96	0.65
2:H:215:ARG:NH2	2:I:164:VAL:CG2	2.59	0.65
1:F:32:GLN:HE22	2:G:165:THR:CG2	2.01	0.65
2:B:21:GLN:HE22	2:B:176:LYS:H	1.41	0.65
2:I:148:GLU:HA	2:I:148:GLU:OE1	1.97	0.65
3:E:73:HIS:HD2	3:E:75:ASP:H	1.45	0.65
3:J:73:HIS:HD2	3:J:75:ASP:H	1.45	0.65
2:G:56:ARG:NH1	2:G:56:ARG:HG3	2.09	0.65
3:J:64:GLY:O	3:J:68:MET:HB2	1.96	0.65
1:F:306:THR:OG1	3:J:310:LEU:HD22	1.97	0.65
2:I:215:ARG:CB	6:I:803:ADP:O4'	2.45	0.65
1:A:334:LYS:O	2:B:297:LEU:HD23	1.96	0.65
1:F:47:PHE:CE2	1:F:77:ARG:C	2.70	0.65
2:G:7:ALA:HB2	2:G:218:LEU:CD1	2.26	0.65
2:G:20:GLY:HA2	2:G:22:GLU:OE2	1.96	0.65
2:D:356:ALA:O	2:D:363:MET:CE	2.45	0.65
1:A:193:PRO:CG	2:B:30:ASN:HD21	2.05	0.65
2:I:20:GLY:HA2	2:I:22:GLU:OE2	1.97	0.65
2:G:239:ALA:HB1	2:H:23:HIS:CE1	2.32	0.65
1:F:67:LEU:CD1	1:F:80:LEU:CD2	2.75	0.65
1:F:47:PHE:HD2	1:F:78:GLN:CA	2.01	0.65
1:F:55:ILE:HD13	1:F:82:LEU:HG	1.77	0.65
2:C:341:TYR:HB2	2:D:333:LEU:CD1	2.26	0.65
2:G:148:GLU:OE1	2:G:148:GLU:HA	1.97	0.64
1:A:274:ASP:HA	1:A:279:TRP:CE3	2.32	0.64
2:D:277:GLU:CB	3:E:149:GLU:HG3	2.20	0.64
2:I:345:ARG:HE	3:J:150:ARG:HH21	1.43	0.64
1:F:52:THR:CG2	1:F:81:LEU:HD23	2.26	0.64
1:F:273:PHE:HB3	1:F:279:TRP:CG	2.33	0.64
2:H:73:CYS:SG	2:H:73:CYS:O	2.56	0.64
1:A:53:PHE:CD2	1:A:64:ILE:CD1	2.80	0.64
2:H:99:THR:HG21	2:I:131:LEU:C	2.17	0.64
2:D:366:PRO:HB3	3:E:282:SER:HB2	1.79	0.64
2:H:343:PRO:HG2	2:H:347:MET:SD	2.37	0.64
1:F:45:GLN:HB3	1:F:77:ARG:CD	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:56:ARG:HG3	2:D:56:ARG:NH1	2.09	0.64
2:I:360:HIS:CB	2:I:363:MET:CB	2.68	0.64
1:A:48:GLU:HG3	1:A:49:GLU:N	2.12	0.64
2:B:56:ARG:NH1	2:B:56:ARG:HG3	2.10	0.64
2:I:345:ARG:HE	3:J:150:ARG:CZ	2.10	0.64
2:I:214:LEU:HD23	6:I:803:ADP:C4	2.32	0.64
2:G:100:LYS:N	2:H:144:GLU:HG2	2.12	0.64
1:A:273:PHE:HB3	1:A:279:TRP:CG	2.33	0.64
2:D:18:VAL:CG1	2:D:25:LEU:HD11	2.27	0.64
2:I:337:LYS:HG3	2:I:338:GLU:N	2.12	0.64
2:I:356:ALA:O	2:I:363:MET:CE	2.45	0.64
1:A:210:ALA:CB	2:B:176:LYS:HE2	2.10	0.64
2:C:73:CYS:SG	2:C:73:CYS:O	2.55	0.64
3:E:147:GLU:HG2	3:E:147:GLU:O	1.98	0.64
2:G:261:GLY:HA3	2:H:297:LEU:HD21	1.79	0.64
2:C:229:ASP:CB	2:D:30:ASN:HD21	2.10	0.64
2:C:100:LYS:HZ3	2:D:133:ARG:HG3	1.62	0.64
1:A:234:GLN:NE2	2:B:304:ASN:HD21	1.95	0.64
2:B:254:GLU:O	2:B:258:GLU:HG3	1.98	0.64
2:G:6:LEU:CD1	2:G:190:ILE:CG2	2.74	0.64
2:D:360:HIS:CG	2:D:363:MET:CG	2.80	0.64
1:A:48:GLU:OE2	1:A:76:SER:CB	2.27	0.64
3:J:329:LEU:H	3:J:329:LEU:HD23	1.63	0.64
2:C:112:GLN:N	2:C:121:LYS:HZ3	1.93	0.63
2:I:345:ARG:NE	3:J:150:ARG:CZ	2.61	0.63
2:H:215:ARG:CZ	2:I:164:VAL:HB	2.28	0.63
2:I:360:HIS:CG	2:I:363:MET:CG	2.81	0.63
2:C:100:LYS:HZ1	2:D:133:ARG:HG3	1.63	0.63
1:F:274:ASP:HA	1:F:279:TRP:CE3	2.32	0.63
2:G:268:ILE:HD11	2:G:353:LEU:CD1	2.28	0.63
2:B:268:ILE:HD11	2:B:353:LEU:CD1	2.28	0.63
2:C:343:PRO:HG2	2:C:347:MET:SD	2.38	0.63
1:F:67:LEU:CD1	1:F:80:LEU:HD11	2.24	0.63
1:F:48:GLU:HG3	1:F:49:GLU:N	2.12	0.63
2:G:98:ARG:HB3	2:H:140:LEU:HB3	1.81	0.63
2:D:148:GLU:OE1	2:D:148:GLU:HA	1.97	0.63
2:H:235:GLN:HG2	2:H:245:ASP:OD2	1.99	0.63
2:D:5:VAL:HB	2:D:222:ASP:OD2	1.98	0.63
2:D:277:GLU:CD	3:E:149:GLU:HG3	2.19	0.63
1:F:222:LEU:CD1	1:F:285:MET:HG2	2.29	0.63
2:B:148:GLU:OE1	2:B:148:GLU:HA	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:10:TRP:CH2	2:G:193:GLU:HB2	2.29	0.63
1:F:51:HIS:HB2	1:F:80:LEU:CD2	2.28	0.63
1:F:281:ASN:C	1:F:283:ARG:H	2.02	0.63
2:H:215:ARG:HH22	2:I:164:VAL:HG11	0.81	0.63
2:C:100:LYS:HE2	2:D:133:ARG:HB2	1.81	0.63
2:H:19:VAL:HG12	2:H:182:GLN:HE21	1.63	0.63
3:J:147:GLU:O	3:J:147:GLU:HG2	1.97	0.63
2:I:316:LEU:HD22	2:I:320:ILE:HD11	1.81	0.63
2:I:200:PRO:CD	2:I:305:ASP:HB2	2.27	0.63
2:H:7:ALA:CA	2:H:218:LEU:HD13	2.28	0.63
2:G:10:TRP:CD1	2:G:190:ILE:HG23	2.34	0.62
2:I:345:ARG:HG3	3:J:150:ARG:HH21	1.63	0.62
2:H:359:PHE:CE2	2:I:323:THR:HG23	2.34	0.62
1:F:67:LEU:HD11	1:F:80:LEU:HD21	1.80	0.62
1:F:71:MET:HG3	1:F:80:LEU:HD11	1.81	0.62
3:J:129:LEU:HD11	3:J:158:ARG:HH11	1.64	0.62
1:A:222:LEU:CD1	1:A:285:MET:HG2	2.29	0.62
2:H:93:ILE:HG12	2:I:133:ARG:NH1	2.13	0.62
2:G:254:GLU:O	2:G:258:GLU:HG3	1.98	0.62
1:A:256:LEU:O	1:A:260:LEU:HG	2.00	0.62
3:E:129:LEU:HD11	3:E:158:ARG:HH11	1.64	0.62
3:E:161:LEU:HD12	3:E:161:LEU:H	1.64	0.62
1:F:104:LEU:O	1:F:105:HIS:HB3	2.00	0.62
1:F:144:GLN:OE1	1:F:280:GLN:HB3	1.99	0.62
2:D:316:LEU:HD22	2:D:320:ILE:HD11	1.81	0.62
2:D:345:ARG:HE	3:E:150:ARG:HH21	0.64	0.62
2:D:148:GLU:CD	2:D:149:HIS:N	2.53	0.62
3:J:161:LEU:H	3:J:161:LEU:HD12	1.64	0.62
2:B:263:ARG:O	2:B:267:LEU:HG	2.00	0.62
2:D:337:LYS:HG3	2:D:338:GLU:N	2.12	0.62
3:J:73:HIS:CD2	3:J:75:ASP:H	2.18	0.62
2:I:11:ARG:NH2	2:I:56:ARG:NH2	2.46	0.62
2:H:351:MET:HA	2:H:351:MET:CE	2.30	0.62
2:C:250:LEU:HD22	2:C:309:ILE:HD12	1.82	0.62
1:F:24:LEU:HA	1:F:114:GLY:O	2.00	0.62
3:E:329:LEU:HD23	3:E:329:LEU:H	1.63	0.62
2:G:10:TRP:CB	2:G:190:ILE:HG12	2.29	0.62
2:H:215:ARG:HH21	2:I:164:VAL:HG21	1.65	0.62
2:I:200:PRO:HD2	2:I:305:ASP:CB	2.30	0.62
1:F:57:PRO:C	1:F:59:THR:H	2.03	0.62
1:A:50:HIS:HA	1:A:79:THR:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:99:THR:CG2	2:H:145:GLU:HG3	2.30	0.61
1:A:281:ASN:C	1:A:283:ARG:H	2.02	0.61
2:G:226:ALA:HB1	2:H:30:ASN:HD22	1.64	0.61
2:C:351:MET:CE	2:C:351:MET:HA	2.31	0.61
2:H:351:MET:HE3	2:H:351:MET:HA	1.82	0.61
2:B:259:ALA:CB	2:B:363:MET:HE3	2.30	0.61
2:D:265:MET:HE3	3:E:257:LYS:HE2	1.81	0.61
2:D:158:ASP:OD2	2:D:161:LYS:HG2	2.00	0.61
2:G:7:ALA:HB2	2:G:218:LEU:HB3	1.81	0.61
2:H:250:LEU:HD22	2:H:309:ILE:HD12	1.82	0.61
1:A:315:ASP:HB2	1:A:318:GLN:HG2	1.80	0.61
1:F:97:LEU:CD2	1:F:126:TRP:CD2	2.78	0.61
1:F:62:ASN:HA	1:F:65:PHE:CD1	2.29	0.61
2:G:158:ASP:OD2	2:G:161:LYS:HG2	2.00	0.61
2:G:158:ASP:CG	2:G:161:LYS:HG2	2.21	0.61
2:G:328:TYR:O	2:G:332:LEU:HD23	2.00	0.61
2:H:11:ARG:NH1	2:I:169:ARG:HH22	1.97	0.61
2:B:328:TYR:O	2:B:332:LEU:HD23	1.99	0.61
2:C:11:ARG:HH22	2:D:165:THR:CG2	2.02	0.61
2:I:277:GLU:HA	3:J:149:GLU:HG2	1.81	0.61
1:A:24:LEU:HA	1:A:114:GLY:O	2.00	0.61
2:I:56:ARG:HG3	2:I:56:ARG:HH11	1.65	0.61
2:B:271:ALA:HB1	2:B:276:ILE:CD1	2.30	0.61
1:F:256:LEU:O	1:F:260:LEU:HG	2.00	0.61
1:A:116:LYS:HB3	1:A:140:GLN:HE21	1.66	0.61
2:G:5:VAL:HG12	2:G:222:ASP:OD1	2.00	0.61
2:G:271:ALA:HB1	2:G:276:ILE:CD1	2.30	0.61
3:E:117:ALA:HB2	3:E:143:LEU:HD12	1.83	0.61
3:E:73:HIS:CD2	3:E:75:ASP:H	2.18	0.61
2:H:11:ARG:NH1	2:I:169:ARG:NH2	2.48	0.61
2:I:366:PRO:HB3	3:J:282:SER:HB2	1.83	0.61
3:J:117:ALA:HB2	3:J:143:LEU:HD12	1.83	0.61
2:I:229:ASP:O	2:I:231:GLN:N	2.33	0.61
1:F:1:MET:HA	1:F:134:SER:O	2.01	0.61
1:F:315:ASP:HB2	1:F:318:GLN:HG2	1.79	0.61
1:F:94:ASN:HA	1:F:126:TRP:CD1	2.36	0.61
2:B:158:ASP:OD2	2:B:161:LYS:HG2	2.00	0.61
2:B:158:ASP:CG	2:B:161:LYS:HG2	2.21	0.61
2:C:3:TYR:O	2:C:4:GLN:HG3	2.01	0.61
2:H:112:GLN:CB	2:H:121:LYS:HZ3	0.77	0.60
2:H:9:LYS:HZ3	2:H:194:GLU:CD	2.04	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:67:LEU:HD21	1:F:80:LEU:CD1	2.25	0.60
2:H:112:GLN:HB2	2:H:121:LYS:CD	2.19	0.60
2:H:112:GLN:CB	2:H:121:LYS:HZ1	0.84	0.60
2:C:113:TYR:HD2	2:C:147:PRO:CG	2.13	0.60
2:B:148:GLU:CD	2:B:149:HIS:N	2.53	0.60
2:B:113:TYR:HD2	2:B:147:PRO:HB3	1.67	0.60
2:B:246:ASP:HB3	2:B:274:ARG:CD	2.23	0.60
3:J:303:VAL:HB	3:J:306:ILE:HD11	1.84	0.60
2:D:113:TYR:HD2	2:D:147:PRO:HB3	1.67	0.60
2:G:113:TYR:HD2	2:G:147:PRO:HB3	1.67	0.60
2:H:21:GLN:OE1	2:H:175:LEU:HD22	2.01	0.60
3:J:34:GLY:O	3:J:199:GLY:HA3	2.01	0.60
1:A:49:GLU:C	1:A:78:GLN:HA	2.22	0.60
2:H:113:TYR:HD2	2:H:147:PRO:CG	2.13	0.60
1:F:54:SER:O	1:F:57:PRO:HD2	2.02	0.60
2:G:284:GLU:O	2:G:288:LEU:HG	2.02	0.60
2:H:112:GLN:O	2:H:121:LYS:HD2	1.97	0.60
2:I:244:LEU:HD11	2:I:276:ILE:HD13	1.84	0.60
2:I:244:LEU:CD2	2:I:276:ILE:HG12	2.29	0.60
1:F:45:GLN:HB3	1:F:77:ARG:HD3	1.83	0.60
3:E:35:MET:HE2	3:E:166:PRO:CD	2.18	0.60
1:A:269:LEU:HG	1:A:273:PHE:CE1	2.37	0.60
2:G:268:ILE:HD11	2:G:353:LEU:HD12	1.83	0.60
2:D:158:ASP:CG	2:D:161:LYS:HG2	2.21	0.60
2:I:158:ASP:CG	2:I:161:LYS:HG2	2.22	0.60
1:F:71:MET:CG	1:F:108:LEU:CG	2.80	0.60
3:E:149:GLU:C	3:E:151:LEU:H	2.05	0.60
2:I:363:MET:CG	2:I:364:PRO:HD2	2.31	0.60
2:H:10:TRP:CH2	2:H:190:ILE:HG12	2.37	0.60
3:E:303:VAL:HB	3:E:306:ILE:HD11	1.83	0.60
2:G:263:ARG:O	2:G:267:LEU:HG	2.00	0.60
1:F:336:LEU:HD12	2:G:326:GLN:HE22	1.67	0.60
2:G:343:PRO:HG2	2:G:347:MET:SD	2.42	0.60
2:D:357:LEU:HB3	3:E:260:HIS:HE1	1.67	0.60
2:G:242:GLY:HA3	2:G:243:THR:OG1	2.02	0.60
2:C:223:GLN:NE2	2:D:174:HIS:CD2	2.64	0.60
2:B:99:THR:CG2	2:C:144:GLU:HG2	2.31	0.60
2:C:152:PHE:O	2:C:153:LEU:HD23	2.02	0.60
2:H:3:TYR:O	2:H:4:GLN:HG3	2.01	0.60
1:F:71:MET:HB3	1:F:108:LEU:HD12	0.62	0.59
2:B:302:LEU:HD13	2:B:310:GLU:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:292:ILE:O	2:C:296:GLN:HG3	2.02	0.59
2:D:363:MET:CG	2:D:364:PRO:HD2	2.31	0.59
2:D:355:ARG:HA	3:E:287:GLN:NE2	2.16	0.59
1:F:10:ARG:HH12	1:F:40:GLN:NE2	2.01	0.59
2:B:343:PRO:HG2	2:B:347:MET:SD	2.42	0.59
3:J:149:GLU:C	3:J:151:LEU:H	2.05	0.59
2:C:21:GLN:OE1	2:C:175:LEU:HD22	2.02	0.59
2:G:205:LEU:CD1	2:G:234:THR:HG23	2.33	0.59
2:C:112:GLN:CD	2:C:121:LYS:HZ1	2.03	0.59
2:I:214:LEU:HB3	6:I:803:ADP:C4	2.37	0.59
2:I:215:ARG:CB	6:I:803:ADP:C4'	2.80	0.59
2:G:246:ASP:HB3	2:G:274:ARG:CD	2.23	0.59
2:D:246:ASP:HB2	2:D:248:GLN:HG2	1.84	0.59
2:I:241:LEU:O	3:J:156:ARG:NH1	2.36	0.59
2:G:226:ALA:O	2:H:30:ASN:ND2	2.35	0.59
1:F:36:ASP:OD1	2:G:169:ARG:NH2	2.36	0.59
1:A:10:ARG:HH12	1:A:40:GLN:NE2	2.00	0.59
2:G:302:LEU:HD13	2:G:310:GLU:HG2	1.84	0.59
1:A:72:SER:O	1:A:72:SER:OG	2.12	0.59
2:D:47:ARG:NH1	2:D:215:ARG:CZ	2.61	0.59
1:A:222:LEU:HD12	1:A:285:MET:CG	2.33	0.59
2:I:6:LEU:H	2:I:222:ASP:CG	2.04	0.59
2:C:316:LEU:HD22	2:C:320:ILE:HD11	1.85	0.59
2:C:362:ARG:O	2:C:363:MET:HG3	2.02	0.59
2:B:268:ILE:HD11	2:B:353:LEU:HD12	1.83	0.59
2:H:292:ILE:O	2:H:296:GLN:HG3	2.02	0.59
1:F:71:MET:CB	1:F:108:LEU:CG	2.69	0.59
1:A:39:ARG:HE	1:A:79:THR:HG21	1.68	0.59
2:I:6:LEU:HB2	2:I:222:ASP:OD2	2.02	0.59
2:G:259:ALA:HB3	2:G:363:MET:CE	2.33	0.59
2:B:282:LEU:CD2	2:B:332:LEU:HD12	2.33	0.59
3:E:41:ILE:HG21	3:E:113:TRP:CD1	2.38	0.59
2:H:152:PHE:O	2:H:153:LEU:HD23	2.03	0.59
2:B:205:LEU:CD1	2:B:234:THR:HG23	2.33	0.59
2:G:10:TRP:CD1	2:G:190:ILE:HG12	2.37	0.58
2:C:112:GLN:O	2:C:121:LYS:HD2	1.98	0.58
1:F:55:ILE:CD1	1:F:82:LEU:CB	2.81	0.58
1:F:269:LEU:HG	1:F:273:PHE:CE1	2.37	0.58
2:B:284:GLU:O	2:B:288:LEU:HG	2.02	0.58
2:I:246:ASP:HB2	2:I:248:GLN:HG2	1.85	0.58
2:C:291:ARG:HH11	2:C:306:MET:HG3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:41:ILE:HG21	3:J:113:TRP:CD1	2.38	0.58
2:D:186:GLN:HG2	2:D:214:LEU:HD21	1.86	0.58
1:F:56:ASP:H	1:F:57:PRO:CD	2.17	0.58
2:B:304:ASN:OD1	2:B:305:ASP:N	2.37	0.58
1:F:67:LEU:HD12	1:F:71:MET:CE	2.33	0.58
1:A:29:LEU:CD1	1:A:154:ARG:HH22	2.17	0.58
2:I:355:ARG:HH12	3:J:287:GLN:HB3	1.69	0.58
2:G:61:GLY:CA	2:G:72:PRO:HG3	2.33	0.58
2:H:11:ARG:HH12	2:I:169:ARG:HH22	1.52	0.58
1:F:10:ARG:HH22	1:F:40:GLN:HE22	1.51	0.58
1:F:263:GLN:HG2	1:F:266:HIS:HD2	1.68	0.58
1:A:263:GLN:HG2	1:A:266:HIS:HD2	1.68	0.58
1:F:221:LEU:HD13	1:F:331:LEU:HD12	1.86	0.58
2:D:345:ARG:HH12	3:E:150:ARG:HG3	1.68	0.58
2:B:259:ALA:HB3	2:B:363:MET:CE	2.33	0.58
1:A:10:ARG:HH22	1:A:40:GLN:HE22	1.51	0.58
2:I:215:ARG:N	6:I:803:ADP:O4'	2.36	0.58
1:A:49:GLU:O	1:A:78:GLN:CA	2.43	0.58
2:H:257:VAL:HG11	2:H:320:ILE:CD1	2.34	0.58
2:H:362:ARG:O	2:H:363:MET:HG3	2.02	0.58
2:G:282:LEU:CD2	2:G:332:LEU:HD12	2.34	0.58
2:D:229:ASP:O	2:D:231:GLN:N	2.34	0.58
2:D:144:GLU:C	2:D:146:PRO:HD3	2.24	0.58
1:A:32:GLN:HE22	2:B:169:ARG:HH12	1.52	0.58
2:G:304:ASN:OD1	2:G:305:ASP:N	2.37	0.58
2:I:345:ARG:NE	3:J:150:ARG:HH21	2.02	0.58
2:I:186:GLN:HG2	2:I:214:LEU:HD21	1.86	0.58
1:F:222:LEU:HD12	1:F:285:MET:SD	2.44	0.58
3:E:46:ARG:CZ	3:E:68:MET:HG3	2.33	0.58
2:G:343:PRO:CB	2:H:283:VAL:HG13	2.34	0.58
1:A:32:GLN:OE1	2:B:169:ARG:NH2	2.37	0.58
2:D:367:GLU:HB3	2:D:368:PRO:HD2	1.86	0.58
2:I:345:ARG:CG	3:J:150:ARG:HH21	2.16	0.58
1:F:99:THR:O	1:F:103:LEU:HD13	2.03	0.58
2:I:61:GLY:CA	2:I:72:PRO:HG3	2.34	0.57
1:F:273:PHE:CE1	1:F:283:ARG:HG3	2.39	0.57
1:F:281:ASN:C	1:F:283:ARG:N	2.57	0.57
2:H:261:GLY:HA3	2:I:297:LEU:HD11	1.84	0.57
1:F:47:PHE:CE2	1:F:78:GLN:C	2.72	0.57
2:I:224:ALA:CB	2:I:240:MET:CE	2.79	0.57
2:I:338:GLU:OE2	3:J:295:HIS:CE1	2.57	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:93:ILE:CA	2:I:133:ARG:NH2	2.63	0.57
1:A:281:ASN:C	1:A:283:ARG:N	2.57	0.57
1:A:221:LEU:HD13	1:A:331:LEU:HD12	1.85	0.57
1:F:67:LEU:CD1	1:F:80:LEU:HD21	2.34	0.57
1:A:53:PHE:HE2	1:A:64:ILE:CD1	2.02	0.57
1:F:222:LEU:HD12	1:F:285:MET:CG	2.33	0.57
2:G:148:GLU:CD	2:G:149:HIS:N	2.53	0.57
3:J:46:ARG:CZ	3:J:68:MET:HG3	2.33	0.57
3:E:308:ARG:O	3:E:312:ILE:HG13	2.04	0.57
2:I:367:GLU:HB3	2:I:368:PRO:HD2	1.85	0.57
1:A:279:TRP:O	1:A:279:TRP:CG	2.57	0.57
2:H:291:ARG:HH11	2:H:306:MET:HG3	1.69	0.57
2:H:10:TRP:CE2	2:H:190:ILE:CG2	2.83	0.57
1:A:238:LEU:HD22	2:B:177:ALA:HB3	1.86	0.57
2:H:316:LEU:HD22	2:H:320:ILE:HD11	1.85	0.57
2:I:215:ARG:HG3	6:I:803:ADP:H4'	1.87	0.57
2:G:98:ARG:HG2	2:H:140:LEU:HD13	1.86	0.57
2:G:7:ALA:CB	2:G:218:LEU:CD1	2.77	0.57
2:C:257:VAL:HG11	2:C:320:ILE:CD1	2.34	0.57
1:F:144:GLN:OE1	1:F:280:GLN:CB	2.53	0.57
2:I:363:MET:CB	2:I:364:PRO:CD	2.78	0.57
2:G:144:GLU:C	2:G:146:PRO:HD3	2.24	0.57
2:G:328:TYR:OH	2:G:361:PRO:HD2	2.05	0.57
2:I:360:HIS:CB	2:I:363:MET:SD	2.92	0.57
2:D:48:GLY:HA3	2:D:215:ARG:CB	2.34	0.57
1:A:223:MET:HE1	1:A:292:ARG:HB2	1.87	0.57
2:B:144:GLU:C	2:B:146:PRO:HD3	2.24	0.57
2:B:61:GLY:CA	2:B:72:PRO:HG3	2.33	0.57
2:H:20:GLY:HA3	2:H:182:GLN:HE22	1.70	0.57
1:F:71:MET:O	1:F:105:HIS:CE1	2.58	0.57
1:A:74:PHE:O	1:A:74:PHE:CG	2.57	0.57
1:A:107:ASP:HB2	1:F:228:ARG:HH12	0.98	0.57
1:A:282:ARG:HG2	1:A:285:MET:HE2	1.86	0.57
1:F:223:MET:HE1	1:F:292:ARG:HB2	1.86	0.57
2:D:61:GLY:CA	2:D:72:PRO:HG3	2.33	0.57
3:J:308:ARG:O	3:J:312:ILE:HG13	2.04	0.57
1:A:222:LEU:HD12	1:A:285:MET:SD	2.44	0.57
2:D:244:LEU:HD21	2:D:276:ILE:CG1	2.34	0.56
2:D:360:HIS:CB	2:D:363:MET:SD	2.92	0.56
1:A:49:GLU:CB	1:A:78:GLN:CG	2.80	0.56
1:F:279:TRP:O	1:F:279:TRP:CG	2.57	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:48:GLY:CA	2:G:215:ARG:HB2	2.35	0.56
2:I:277:GLU:HB3	3:J:149:GLU:HG3	1.76	0.56
1:A:71:MET:HE1	1:A:72:SER:CB	2.28	0.56
3:J:201:ALA:O	3:J:204:LEU:HB2	2.06	0.56
1:A:29:LEU:HD11	1:A:154:ARG:HH22	1.70	0.56
2:I:345:ARG:HH12	3:J:150:ARG:CG	2.18	0.56
2:I:356:ALA:O	2:I:363:MET:HE3	2.05	0.56
1:A:193:PRO:CG	2:B:30:ASN:ND2	2.40	0.56
1:F:55:ILE:O	1:F:55:ILE:HG22	2.05	0.56
1:A:50:HIS:ND1	1:A:79:THR:HB	2.20	0.56
1:A:105:HIS:CA	1:F:227:LYS:NZ	2.68	0.56
2:C:113:TYR:CD2	2:C:147:PRO:CG	2.84	0.56
1:A:273:PHE:CE1	1:A:283:ARG:HG3	2.39	0.56
2:B:328:TYR:OH	2:B:361:PRO:HD2	2.06	0.56
1:A:218:VAL:HA	1:A:221:LEU:HB2	1.88	0.56
2:I:194:GLU:OE1	2:I:194:GLU:HA	2.05	0.56
2:C:40:ALA:HB1	2:C:170:CYS:SG	2.46	0.56
1:F:67:LEU:HD11	1:F:80:LEU:CG	2.35	0.56
1:A:306:THR:OG1	3:E:310:LEU:HD22	2.06	0.56
2:D:334:ILE:CG2	3:E:332:PRO:HB2	2.29	0.56
1:F:174:TYR:CE2	1:F:211:HIS:HE1	2.23	0.56
2:D:176:LYS:C	2:D:177:ALA:O	2.42	0.56
2:B:205:LEU:HD11	2:B:234:THR:HG23	1.87	0.56
1:F:64:ILE:O	1:F:67:LEU:HB3	2.06	0.56
2:D:261:GLY:HA3	3:E:260:HIS:HB3	1.86	0.56
1:A:310:LEU:HD11	3:E:299:GLN:NE2	2.20	0.56
2:C:51:LYS:CE	4:C:1300:PO4:O3	2.51	0.56
1:F:170:LEU:O	1:F:173:CYS:O	2.24	0.56
1:F:210:ALA:N	2:G:176:LYS:NZ	2.46	0.56
3:J:8:ARG:HG3	3:J:9:PRO:CD	2.32	0.56
2:G:362:ARG:HH21	2:G:363:MET:CE	2.19	0.56
2:G:48:GLY:HA3	2:G:215:ARG:CB	2.36	0.56
3:E:33:PRO:O	3:E:197:SER:OG	2.21	0.56
3:E:280:HIS:O	3:E:281:LEU:HD23	2.05	0.56
2:C:367:GLU:HG3	2:D:322:PRO:HD2	1.87	0.56
2:D:277:GLU:CG	3:E:149:GLU:HG3	2.35	0.56
2:I:215:ARG:HB2	6:I:803:ADP:O4'	2.05	0.56
2:I:9:LYS:NZ	2:I:194:GLU:OE2	2.28	0.56
1:A:170:LEU:O	1:A:173:CYS:O	2.24	0.56
2:I:296:GLN:NE2	2:I:325:ILE:HD12	2.20	0.56
2:G:6:LEU:HD23	2:G:194:GLU:CG	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:355:ARG:NH1	3:J:287:GLN:CB	2.66	0.56
3:J:280:HIS:O	3:J:281:LEU:HD23	2.05	0.56
1:A:64:ILE:HG23	1:A:65:PHE:H	1.70	0.56
1:A:105:HIS:CB	1:F:227:LYS:HD2	2.21	0.56
3:J:32:LEU:HD12	3:J:166:PRO:CG	2.31	0.56
1:F:116:LYS:HB3	1:F:140:GLN:HE21	1.71	0.56
2:G:295:VAL:HG22	2:G:301:ALA:HB3	1.88	0.56
2:I:259:ALA:HB2	2:I:363:MET:SD	2.46	0.56
1:A:49:GLU:CB	1:A:78:GLN:CB	2.84	0.56
2:I:140:LEU:HD22	2:I:144:GLU:HG3	1.87	0.56
1:F:39:ARG:NH2	1:F:50:HIS:HB3	2.21	0.55
2:D:47:ARG:HD2	2:D:215:ARG:NH1	2.22	0.55
1:F:313:LYS:O	1:F:316:TYR:CE2	2.60	0.55
1:F:310:LEU:HD21	3:J:306:ILE:CD1	2.34	0.55
2:D:140:LEU:HD22	2:D:144:GLU:HG3	1.88	0.55
2:G:343:PRO:HB3	2:H:283:VAL:HG13	1.88	0.55
2:B:343:PRO:HB3	2:C:283:VAL:HG13	1.86	0.55
2:B:309:ILE:HG22	2:B:313:MET:HG2	1.88	0.55
1:F:53:PHE:HZ	1:F:67:LEU:HD22	1.69	0.55
2:B:362:ARG:HH21	2:B:363:MET:CE	2.19	0.55
2:B:261:GLY:CA	2:C:297:LEU:HD21	2.36	0.55
2:D:296:GLN:NE2	2:D:325:ILE:HD12	2.20	0.55
3:E:201:ALA:O	3:E:204:LEU:HB2	2.06	0.55
1:F:55:ILE:HD12	1:F:82:LEU:CB	2.37	0.55
2:D:48:GLY:HA3	2:D:215:ARG:HB3	1.87	0.55
2:G:309:ILE:HG22	2:G:313:MET:HG2	1.88	0.55
2:H:40:ALA:HB1	2:H:170:CYS:SG	2.46	0.55
1:F:282:ARG:O	1:F:285:MET:HB3	2.07	0.55
2:H:351:MET:HE1	2:I:326:GLN:NE2	2.08	0.55
1:F:174:TYR:CE2	1:F:211:HIS:CE1	2.94	0.55
2:B:140:LEU:HD22	2:B:144:GLU:HG3	1.89	0.55
2:I:113:TYR:HE2	2:I:147:PRO:HG3	1.71	0.55
2:I:48:GLY:O	2:I:213:SER:HA	2.06	0.55
1:A:106:ASP:N	1:F:225:LYS:CD	2.59	0.55
2:G:140:LEU:HD22	2:G:144:GLU:HG3	1.89	0.55
1:F:57:PRO:C	1:F:59:THR:N	2.60	0.55
2:H:156:THR:HG22	2:H:158:ASP:N	2.21	0.55
2:D:343:PRO:HD3	3:E:294:CYS:SG	2.46	0.55
1:A:271:ALA:O	1:A:275:LYS:HG2	2.07	0.55
1:A:296:THR:HG22	1:A:299:ARG:NH1	2.21	0.55
2:D:238:SER:HB2	2:D:243:THR:HB	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:194:GLU:HA	2:D:194:GLU:OE1	2.05	0.55
2:G:205:LEU:HD11	2:G:234:THR:HG23	1.87	0.55
1:F:218:VAL:HA	1:F:221:LEU:HB2	1.88	0.55
2:I:80:ARG:HG2	2:I:80:ARG:HH11	1.71	0.55
2:I:259:ALA:HB2	2:I:363:MET:HG3	1.89	0.55
1:A:39:ARG:NH2	1:A:50:HIS:HB3	2.21	0.55
2:C:91:ILE:HD12	2:C:123:TYR:CE2	2.42	0.55
3:E:213:ARG:NH2	3:E:267:ASN:OD1	2.40	0.55
2:G:6:LEU:CD1	2:G:191:LEU:HD21	2.28	0.55
3:J:32:LEU:CD1	3:J:166:PRO:CG	2.85	0.55
2:C:281:LEU:HD23	2:C:285:MET:CE	2.36	0.55
2:B:248:GLN:O	2:B:252:LEU:N	2.39	0.55
2:D:271:ALA:HB1	2:D:276:ILE:HD11	1.89	0.55
2:I:360:HIS:HD2	2:I:361:PRO:O	1.90	0.55
2:D:259:ALA:HB2	2:D:363:MET:SD	2.46	0.55
1:A:282:ARG:O	1:A:285:MET:HB3	2.07	0.55
1:F:308:THR:CG2	1:F:320:VAL:HG13	2.37	0.55
2:C:156:THR:HG22	2:C:158:ASP:N	2.21	0.55
2:D:7:ALA:HA	2:D:218:LEU:HD13	1.89	0.55
2:D:244:LEU:HD21	2:D:276:ILE:HG23	1.89	0.54
2:D:360:HIS:CG	2:D:363:MET:CE	2.90	0.54
2:I:56:ARG:NH1	2:I:56:ARG:HG3	2.22	0.54
2:D:113:TYR:CD2	2:D:147:PRO:HB3	2.42	0.54
2:G:248:GLN:O	2:G:252:LEU:N	2.39	0.54
1:A:264:SER:O	1:A:265:ALA:HB3	2.07	0.54
3:J:213:ARG:NH2	3:J:267:ASN:OD1	2.40	0.54
1:A:105:HIS:HB3	1:F:227:LYS:CE	2.37	0.54
2:H:281:LEU:HD23	2:H:285:MET:CE	2.36	0.54
1:A:308:THR:CG2	1:A:320:VAL:HG13	2.37	0.54
1:A:273:PHE:HB3	1:A:279:TRP:HB2	1.90	0.54
2:B:56:ARG:HH11	2:B:56:ARG:CG	2.18	0.54
2:B:295:VAL:HG22	2:B:301:ALA:HB3	1.88	0.54
2:I:360:HIS:CG	2:I:363:MET:CE	2.90	0.54
2:D:360:HIS:CB	2:D:363:MET:CB	2.68	0.54
2:D:345:ARG:NH1	3:E:150:ARG:HG3	2.22	0.54
1:A:193:PRO:HB3	2:B:34:LEU:HD12	1.88	0.54
2:G:98:ARG:CA	2:H:169:ARG:HH22	2.16	0.54
2:C:229:ASP:CB	2:D:30:ASN:ND2	2.69	0.54
3:J:306:ILE:HG22	3:J:307:ASN:H	1.72	0.54
2:I:338:GLU:OE2	3:J:295:HIS:NE2	2.40	0.54
2:B:113:TYR:CD2	2:B:147:PRO:HB3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:33:PRO:O	3:E:197:SER:CB	2.54	0.54
2:G:354:LEU:HD11	2:H:294:MET:SD	2.47	0.54
1:F:296:THR:HG22	1:F:299:ARG:NH1	2.22	0.54
3:E:35:MET:CE	3:E:166:PRO:HA	2.37	0.54
3:J:4:TYR:HB3	3:J:5:PRO:HD2	1.89	0.54
3:E:8:ARG:HG3	3:E:9:PRO:CD	2.33	0.54
1:A:313:LYS:O	1:A:316:TYR:CE2	2.60	0.54
2:G:307:ALA:HA	2:G:310:GLU:HG3	1.89	0.54
2:G:239:ALA:HB1	2:H:23:HIS:NE2	2.23	0.54
3:E:238:HIS:ND1	3:E:239:GLU:N	2.56	0.54
2:C:112:GLN:CB	2:C:121:LYS:CE	2.02	0.54
2:I:214:LEU:CD2	6:I:803:ADP:C2	2.86	0.54
1:F:47:PHE:CD1	1:F:77:ARG:CB	2.82	0.54
1:F:48:GLU:OE2	1:F:74:PHE:HE1	1.90	0.54
1:F:48:GLU:HG3	1:F:49:GLU:H	1.72	0.54
2:D:259:ALA:HB2	2:D:363:MET:HG3	1.88	0.54
2:I:6:LEU:HG	2:I:222:ASP:OD1	2.06	0.54
3:E:4:TYR:HB3	3:E:5:PRO:HD2	1.89	0.54
2:C:307:ALA:HA	2:C:310:GLU:HB2	1.89	0.54
1:F:271:ALA:O	1:F:275:LYS:HG2	2.07	0.54
1:A:1:MET:HA	1:A:134:SER:O	2.08	0.54
3:E:206:GLN:C	3:E:207:GLY:O	2.46	0.54
2:I:356:ALA:O	2:I:363:MET:HE1	2.07	0.54
1:F:103:LEU:N	1:F:103:LEU:HD13	2.22	0.54
1:A:49:GLU:CB	1:A:78:GLN:HB3	2.38	0.54
1:F:25:GLY:O	1:F:115:ASN:HA	2.08	0.54
1:F:211:HIS:ND1	1:F:211:HIS:O	2.41	0.54
1:F:273:PHE:HB3	1:F:279:TRP:HB2	1.90	0.54
2:B:307:ALA:HA	2:B:310:GLU:HG3	1.89	0.54
2:C:346:ARG:O	2:C:350:GLU:HG3	2.08	0.54
2:G:113:TYR:CD2	2:G:147:PRO:HB3	2.42	0.54
2:H:346:ARG:O	2:H:350:GLU:HG3	2.08	0.54
1:F:84:LEU:HG	1:F:89:PRO:CD	2.35	0.54
2:B:341:TYR:O	2:C:336:ARG:NH1	2.38	0.54
1:A:55:ILE:HD12	1:A:93:ILE:HG21	1.90	0.54
2:I:345:ARG:NE	3:J:150:ARG:NH2	2.56	0.54
1:F:264:SER:O	1:F:265:ALA:HB3	2.07	0.54
2:H:367:GLU:HG3	2:I:322:PRO:HD2	1.90	0.54
1:F:71:MET:HB2	1:F:108:LEU:CD1	2.19	0.53
2:D:360:HIS:HD2	2:D:361:PRO:O	1.90	0.53
1:F:310:LEU:HD11	3:J:299:GLN:NE2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:276:ILE:HG22	2:H:277:GLU:N	2.24	0.53
2:B:238:SER:HB2	2:B:243:THR:OG1	2.08	0.53
2:B:243:THR:HG22	2:B:244:LEU:N	2.23	0.53
1:F:103:LEU:CD1	1:F:103:LEU:N	2.71	0.53
1:A:48:GLU:HG3	1:A:49:GLU:H	1.72	0.53
2:C:351:MET:CE	2:D:326:GLN:NE2	2.54	0.53
1:A:25:GLY:O	1:A:115:ASN:HA	2.08	0.53
2:D:291:ARG:HD2	2:D:306:MET:SD	2.49	0.53
2:B:347:MET:HG3	2:C:290:HIS:CD2	2.43	0.53
2:I:302:LEU:HD22	2:I:306:MET:HG2	1.90	0.53
2:D:296:GLN:HE22	2:D:325:ILE:HD12	1.73	0.53
2:H:360:HIS:HD2	2:H:363:MET:H	1.56	0.53
2:C:347:MET:HG2	2:D:290:HIS:ND1	2.23	0.53
2:I:296:GLN:HE22	2:I:325:ILE:HD12	1.73	0.53
2:H:91:ILE:HD12	2:H:123:TYR:CE2	2.42	0.53
2:G:80:ARG:HH11	2:G:80:ARG:HG2	1.74	0.53
3:E:206:GLN:O	3:E:207:GLY:O	2.27	0.53
2:G:159:PRO:O	2:G:162:LEU:HB2	2.09	0.53
2:B:91:ILE:HD11	2:B:121:LYS:HE3	1.91	0.53
1:A:93:ILE:HG23	1:A:97:LEU:HD13	1.91	0.53
2:B:276:ILE:HG22	2:B:277:GLU:N	2.24	0.53
1:F:336:LEU:HD12	2:G:326:GLN:NE2	2.21	0.53
2:B:159:PRO:O	2:B:162:LEU:HB2	2.09	0.53
2:I:159:PRO:O	2:I:162:LEU:HB2	2.08	0.53
2:B:80:ARG:HG2	2:B:80:ARG:HH11	1.74	0.53
2:D:357:LEU:HB3	3:E:260:HIS:CE1	2.43	0.53
2:I:224:ALA:CB	2:I:240:MET:HE1	2.25	0.53
2:G:7:ALA:HB2	2:G:218:LEU:CB	2.39	0.53
1:A:32:GLN:NE2	2:B:165:THR:HG22	2.24	0.53
2:C:10:TRP:CZ2	2:C:190:ILE:HG23	2.43	0.53
3:J:238:HIS:ND1	3:J:239:GLU:N	2.57	0.53
3:J:33:PRO:O	3:J:197:SER:HB2	2.09	0.53
2:H:113:TYR:CD2	2:H:147:PRO:CG	2.84	0.53
2:C:86:ARG:NH2	2:D:141:LYS:HD2	2.23	0.53
2:H:334:ILE:O	2:H:338:GLU:HG3	2.09	0.53
2:D:80:ARG:HG2	2:D:80:ARG:HH11	1.74	0.53
1:A:55:ILE:HD12	1:A:93:ILE:CG2	2.39	0.53
1:A:193:PRO:HB3	2:B:34:LEU:CD1	2.38	0.53
1:F:100:LEU:HD22	1:F:103:LEU:CD2	2.30	0.53
2:H:10:TRP:CH2	2:H:190:ILE:HA	2.44	0.53
2:I:250:LEU:HD23	2:I:312:ARG:HH11	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:THR:CG2	1:A:178:LEU:HG	2.35	0.53
1:F:59:THR:O	1:F:60:ASP:HB2	2.09	0.53
2:H:307:ALA:HA	2:H:310:GLU:HB2	1.90	0.53
2:H:191:LEU:HD12	2:H:203:LEU:HD21	1.91	0.53
2:D:277:GLU:CG	3:E:149:GLU:CG	2.86	0.52
1:F:300:GLN:OE1	1:F:335:PRO:HG2	2.09	0.52
1:A:309:GLU:O	1:A:313:LYS:HG3	2.09	0.52
1:F:71:MET:O	1:F:105:HIS:HE1	1.92	0.52
2:I:360:HIS:O	2:I:363:MET:HB2	2.09	0.52
2:D:360:HIS:O	2:D:363:MET:HB2	2.09	0.52
2:D:360:HIS:CG	2:D:363:MET:SD	3.03	0.52
1:A:49:GLU:HB3	1:A:78:GLN:HB3	1.91	0.52
2:G:276:ILE:HG22	2:G:277:GLU:N	2.24	0.52
2:D:244:LEU:CD1	2:D:276:ILE:HD13	2.39	0.52
2:D:244:LEU:CD2	2:D:276:ILE:HG12	2.38	0.52
1:F:71:MET:SD	1:F:108:LEU:CG	2.96	0.52
1:A:64:ILE:CG2	1:A:65:PHE:N	2.71	0.52
1:F:47:PHE:N	1:F:77:ARG:O	2.42	0.52
2:I:200:PRO:HD2	2:I:305:ASP:HB2	1.90	0.52
3:E:306:ILE:HG22	3:E:307:ASN:H	1.72	0.52
2:C:276:ILE:HG22	2:C:277:GLU:N	2.24	0.52
2:H:181:GLU:HA	2:H:184:ARG:HB3	1.90	0.52
1:A:218:VAL:HG11	1:A:253:GLU:HG3	1.91	0.52
2:I:259:ALA:CB	2:I:363:MET:SD	2.97	0.52
1:F:10:ARG:HH22	1:F:40:GLN:NE2	2.08	0.52
2:C:334:ILE:O	2:C:338:GLU:HG3	2.09	0.52
2:D:159:PRO:O	2:D:162:LEU:HB2	2.09	0.52
1:F:210:ALA:CB	2:G:176:LYS:CD	2.59	0.52
2:C:271:ALA:HB1	2:C:276:ILE:CD1	2.36	0.52
2:I:360:HIS:CG	2:I:363:MET:SD	3.03	0.52
2:I:360:HIS:HB2	2:I:363:MET:CE	2.39	0.52
2:D:352:THR:O	2:D:355:ARG:HB3	2.10	0.52
1:F:336:LEU:HD13	2:G:326:GLN:NE2	2.24	0.52
2:C:360:HIS:HD2	2:C:363:MET:H	1.57	0.52
1:A:10:ARG:HH22	1:A:40:GLN:NE2	2.08	0.52
2:C:191:LEU:HD12	2:C:203:LEU:HD21	1.91	0.52
2:H:6:LEU:O	2:H:218:LEU:HD13	2.08	0.52
3:J:165:ALA:O	3:J:167:PRO:CD	2.57	0.52
2:C:278:TRP:HB3	2:C:349:VAL:HG21	1.91	0.52
2:I:244:LEU:HD21	2:I:276:ILE:HG23	1.90	0.52
1:A:191:LEU:CD2	2:B:26:THR:HG22	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:97:LEU:CD2	1:F:126:TRP:CE2	2.93	0.52
1:F:294:SER:H	1:F:297:GLN:NE2	2.08	0.52
2:D:259:ALA:CB	2:D:363:MET:SD	2.98	0.52
3:E:311:LEU:O	3:E:314:ASP:HB3	2.10	0.52
1:F:309:GLU:O	1:F:313:LYS:HG3	2.09	0.52
2:G:91:ILE:HD11	2:G:121:LYS:HE3	1.91	0.52
3:E:268:VAL:O	3:E:271:PRO:HD3	2.09	0.52
2:I:345:ARG:HH12	3:J:150:ARG:HG3	1.64	0.52
2:D:360:HIS:HB2	2:D:363:MET:CE	2.39	0.52
2:C:84:GLN:O	2:D:140:LEU:HD11	2.10	0.52
2:I:291:ARG:HD2	2:I:306:MET:SD	2.49	0.52
1:F:98:LEU:HG	1:F:125:ALA:HB1	1.91	0.52
3:J:268:VAL:O	3:J:271:PRO:HD3	2.09	0.52
2:I:257:VAL:HG11	2:I:320:ILE:CD1	2.40	0.51
2:D:257:VAL:HG11	2:D:320:ILE:CD1	2.40	0.51
3:E:32:LEU:HD13	3:E:195:ALA:HB3	1.93	0.51
2:C:113:TYR:HD2	2:C:147:PRO:CB	2.23	0.51
2:D:302:LEU:HD22	2:D:306:MET:HG2	1.91	0.51
2:H:252:LEU:HD13	2:H:281:LEU:HD21	1.92	0.51
2:I:148:GLU:CD	2:I:149:HIS:N	2.62	0.51
2:I:236:ALA:O	2:I:239:ALA:HB3	2.09	0.51
2:H:278:TRP:HB3	2:H:349:VAL:HG21	1.91	0.51
1:A:294:SER:H	1:A:297:GLN:NE2	2.08	0.51
2:I:271:ALA:HB1	2:I:276:ILE:HD11	1.90	0.51
1:F:45:GLN:HB3	1:F:77:ARG:HD2	1.92	0.51
2:B:343:PRO:CG	2:B:347:MET:SD	2.99	0.51
3:J:189:ALA:HB3	3:J:210:TRP:HH2	1.75	0.51
2:I:345:ARG:CZ	3:J:150:ARG:HG2	2.20	0.51
2:C:229:ASP:OD1	2:D:30:ASN:ND2	2.35	0.51
1:F:67:LEU:CD1	1:F:71:MET:CE	2.89	0.51
3:J:151:LEU:HD21	3:J:155:LEU:HD12	1.93	0.51
2:C:351:MET:HE3	2:C:351:MET:HA	1.92	0.51
1:F:93:ILE:HG23	1:F:97:LEU:HD13	1.90	0.51
2:I:145:GLU:N	2:I:146:PRO:HD3	2.25	0.51
1:F:310:LEU:O	1:F:314:GLN:HG3	2.10	0.51
2:D:351:MET:SD	3:E:290:LEU:HD22	2.51	0.51
2:G:343:PRO:CG	2:G:347:MET:SD	2.99	0.51
3:E:151:LEU:HD21	3:E:155:LEU:HD12	1.93	0.51
2:C:89:ASP:HB3	2:C:121:LYS:HA	1.93	0.51
2:D:363:MET:CB	2:D:364:PRO:CD	2.79	0.51
3:E:165:ALA:O	3:E:167:PRO:HD3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:GLN:NE2	2:B:304:ASN:ND2	2.59	0.51
2:D:265:MET:CE	3:E:257:LYS:HE2	2.40	0.51
1:F:27:ASP:HB3	1:F:30:LEU:HB2	1.93	0.51
1:A:312:LEU:HB2	1:A:320:VAL:CG2	2.35	0.51
2:D:91:ILE:HD11	2:D:121:LYS:HE3	1.91	0.51
2:G:5:VAL:HB	2:G:222:ASP:OD1	2.10	0.51
2:G:362:ARG:HH21	2:G:363:MET:HE1	1.76	0.51
2:G:302:LEU:HG	2:G:314:ARG:NH1	2.26	0.51
2:B:201:ARG:O	2:B:205:LEU:HG	2.11	0.51
1:F:218:VAL:HG11	1:F:253:GLU:HG3	1.91	0.51
3:E:204:LEU:O	3:E:209:ASN:HB2	2.10	0.51
2:D:64:CYS:SG	2:D:66:THR:HB	2.51	0.51
2:B:64:CYS:SG	2:B:66:THR:HB	2.51	0.51
1:F:71:MET:CG	1:F:80:LEU:HD11	2.41	0.51
2:H:6:LEU:CB	2:H:218:LEU:HD22	2.39	0.51
2:I:352:THR:O	2:I:355:ARG:HB3	2.10	0.51
2:H:113:TYR:HD2	2:H:147:PRO:CB	2.23	0.51
3:J:139:THR:HG22	3:J:140:TRP:N	2.26	0.51
2:D:357:LEU:C	2:D:363:MET:SD	2.88	0.51
1:A:48:GLU:HG3	1:A:49:GLU:HG2	1.92	0.51
2:I:334:ILE:HG21	3:J:332:PRO:CB	2.33	0.51
1:F:84:LEU:CG	1:F:89:PRO:HD3	2.37	0.51
2:C:181:GLU:HA	2:C:184:ARG:HB3	1.93	0.51
3:E:145:THR:HG22	3:E:147:GLU:N	2.26	0.51
2:B:347:MET:HG3	2:C:290:HIS:CG	2.46	0.51
2:C:213:SER:OG	2:C:216:ASP:HB2	2.11	0.51
1:F:55:ILE:HD12	1:F:82:LEU:HB3	1.93	0.50
2:B:246:ASP:CB	2:B:274:ARG:HD3	2.23	0.50
2:B:215:ARG:HG3	6:B:802:ADP:H4'	1.92	0.50
2:D:250:LEU:HD23	2:D:312:ARG:HH11	1.75	0.50
2:C:252:LEU:HD13	2:C:281:LEU:HD21	1.93	0.50
2:G:201:ARG:O	2:G:205:LEU:HG	2.11	0.50
1:A:261:LYS:HE3	1:A:295:GLN:HE21	1.76	0.50
2:C:44:SER:HB2	2:C:159:PRO:HG3	1.94	0.50
2:H:7:ALA:N	2:H:218:LEU:HB3	2.26	0.50
1:F:312:LEU:HB2	1:F:320:VAL:CG2	2.35	0.50
3:E:100:LEU:HD13	3:E:139:THR:HG21	1.93	0.50
1:A:22:LEU:HD22	1:A:112:VAL:HB	1.93	0.50
2:H:99:THR:HG22	2:I:132:SER:HB2	1.93	0.50
2:H:112:GLN:C	2:H:121:LYS:NZ	2.52	0.50
3:E:6:TRP:CB	3:E:167:PRO:HG3	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:MET:CE	2:C:294:MET:SD	2.96	0.50
2:G:47:ARG:O	2:G:213:SER:CB	2.58	0.50
1:A:20:ALA:O	1:A:134:SER:HB2	2.11	0.50
2:D:92:GLU:HG2	2:D:124:LEU:HD12	1.94	0.50
2:B:303:GLY:HA3	2:B:306:MET:HG2	1.94	0.50
3:E:35:MET:HE1	3:E:166:PRO:CA	2.39	0.50
3:J:311:LEU:O	3:J:314:ASP:HB3	2.10	0.50
2:I:357:LEU:C	2:I:363:MET:SD	2.89	0.50
1:A:310:LEU:O	1:A:314:GLN:HG3	2.11	0.50
1:F:20:ALA:O	1:F:134:SER:HB2	2.12	0.50
2:H:213:SER:OG	2:H:216:ASP:HB2	2.11	0.50
2:I:277:GLU:HA	3:J:149:GLU:CG	2.42	0.50
2:C:242:GLY:O	2:C:276:ILE:HG23	2.11	0.50
1:A:27:ASP:HB3	1:A:30:LEU:HB2	1.92	0.50
2:H:9:LYS:NZ	2:H:194:GLU:OE2	2.45	0.50
3:J:34:GLY:O	3:J:199:GLY:N	2.43	0.50
2:H:115:PRO:HG2	2:H:119:ARG:O	2.11	0.50
2:H:360:HIS:CD2	2:H:362:ARG:H	2.30	0.50
3:J:145:THR:HG22	3:J:147:GLU:N	2.27	0.50
2:D:302:LEU:HD11	2:D:313:MET:HB2	1.94	0.50
1:A:234:GLN:CD	2:B:304:ASN:HD21	2.15	0.50
3:E:46:ARG:NH1	3:E:68:MET:HG3	2.27	0.50
2:D:18:VAL:HG11	2:D:25:LEU:HD11	1.94	0.50
2:I:91:ILE:HD11	2:I:121:LYS:HE3	1.94	0.50
2:B:366:PRO:C	2:B:367:GLU:HG3	2.32	0.50
2:I:288:LEU:O	2:I:292:ILE:HG13	2.11	0.50
2:D:288:LEU:O	2:D:292:ILE:HG13	2.12	0.50
3:J:32:LEU:HD22	3:J:195:ALA:CB	2.39	0.50
2:C:360:HIS:CD2	2:C:362:ARG:H	2.30	0.50
1:F:199:LEU:HB3	1:F:200:PRO:HD3	1.94	0.50
2:G:64:CYS:SG	2:G:66:THR:HB	2.51	0.50
2:H:92:GLU:HG2	2:H:124:LEU:HD23	1.94	0.50
2:D:277:GLU:HB3	3:E:149:GLU:HG2	0.53	0.49
1:F:48:GLU:CG	1:F:49:GLU:N	2.75	0.49
2:G:97:SER:HA	2:H:169:ARG:NH2	2.22	0.49
2:C:11:ARG:HH12	2:D:169:ARG:HH12	1.58	0.49
1:F:238:LEU:HD13	2:G:177:ALA:CB	2.35	0.49
3:E:139:THR:HG22	3:E:140:TRP:N	2.26	0.49
3:J:34:GLY:O	3:J:199:GLY:CA	2.59	0.49
2:B:302:LEU:HG	2:B:314:ARG:NH1	2.27	0.49
2:G:92:GLU:HG2	2:G:124:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LEU:HB3	1:A:200:PRO:HD3	1.94	0.49
2:C:115:PRO:HG2	2:C:119:ARG:O	2.12	0.49
2:I:6:LEU:HD12	2:I:221:THR:HB	1.92	0.49
1:A:300:GLN:OE1	1:A:335:PRO:HG2	2.09	0.49
3:J:46:ARG:NH1	3:J:68:MET:HG3	2.27	0.49
2:G:303:GLY:HA3	2:G:306:MET:HG2	1.93	0.49
2:G:366:PRO:C	2:G:367:GLU:HG3	2.32	0.49
2:G:6:LEU:CD1	2:G:191:LEU:CD2	2.61	0.49
2:I:302:LEU:HD11	2:I:313:MET:HB2	1.94	0.49
3:J:85:LYS:NZ	3:J:85:LYS:HB3	2.28	0.49
2:D:44:SER:HA	2:D:156:THR:O	2.13	0.49
1:F:61:TRP:HE1	1:F:96:GLN:HE21	1.61	0.49
1:A:55:ILE:CD1	1:A:85:PRO:HD3	2.42	0.49
3:J:57:LYS:HG3	3:J:58:SER:H	1.78	0.49
1:F:274:ASP:HA	1:F:279:TRP:CZ3	2.47	0.49
1:A:274:ASP:HA	1:A:279:TRP:CZ3	2.47	0.49
3:J:100:LEU:HD13	3:J:139:THR:HG21	1.93	0.49
3:E:41:ILE:HG21	3:E:113:TRP:CG	2.47	0.49
1:A:296:THR:HG22	1:A:299:ARG:HH12	1.77	0.49
1:F:296:THR:HG22	1:F:299:ARG:HH12	1.77	0.49
2:C:92:GLU:HG2	2:C:124:LEU:HD23	1.94	0.49
2:C:244:LEU:HB3	2:C:248:GLN:HB2	1.94	0.49
1:F:67:LEU:CD1	1:F:71:MET:HE3	2.43	0.49
1:A:96:GLN:O	1:A:100:LEU:HG	2.12	0.49
2:H:271:ALA:HB1	2:H:276:ILE:CD1	2.36	0.49
2:C:201:ARG:HD3	2:C:246:ASP:OD2	2.13	0.49
2:D:11:ARG:CZ	2:D:56:ARG:HE	2.24	0.49
3:E:312:ILE:O	3:E:316:LEU:HG	2.12	0.49
3:E:85:LYS:NZ	3:E:85:LYS:HB3	2.28	0.49
2:C:112:GLN:HB2	2:C:121:LYS:CD	2.19	0.49
1:F:261:LYS:HE3	1:F:295:GLN:HE21	1.76	0.49
1:F:22:LEU:HD22	1:F:112:VAL:HB	1.94	0.49
1:F:88:GLY:HA3	1:F:121:GLN:HE22	1.77	0.49
2:H:244:LEU:HB3	2:H:248:GLN:HB2	1.95	0.49
2:I:158:ASP:OD2	2:I:161:LYS:HG2	2.11	0.49
3:E:33:PRO:O	3:E:197:SER:HB2	2.13	0.49
2:D:345:ARG:HH12	3:E:150:ARG:CG	2.26	0.49
2:I:200:PRO:CG	2:I:305:ASP:CB	2.87	0.49
2:B:350:GLU:HB2	2:C:290:HIS:HE1	1.78	0.49
2:B:44:SER:HA	2:B:156:THR:O	2.12	0.49
3:J:145:THR:HG22	3:J:147:GLU:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:44:SER:HA	2:G:156:THR:O	2.13	0.49
1:A:71:MET:HE1	1:A:72:SER:OG	2.12	0.49
1:F:183:GLN:HA	1:F:183:GLN:HE21	1.78	0.49
1:A:234:GLN:CD	2:B:304:ASN:ND2	2.66	0.49
3:E:145:THR:HG22	3:E:147:GLU:H	1.78	0.49
3:J:41:ILE:HG21	3:J:113:TRP:CG	2.47	0.49
2:B:270:GLU:HG2	2:B:274:ARG:NH1	2.29	0.48
2:H:11:ARG:HH12	2:I:169:ARG:HH12	1.59	0.48
2:H:44:SER:HB2	2:H:159:PRO:HG3	1.94	0.48
2:G:246:ASP:HB3	2:G:274:ARG:NH1	2.27	0.48
1:A:310:LEU:HD21	3:E:306:ILE:HD13	1.94	0.48
2:B:256:MET:CE	2:B:332:LEU:HD21	2.44	0.48
2:B:286:LEU:HD11	2:B:333:LEU:HA	1.96	0.48
2:D:236:ALA:O	2:D:239:ALA:HB3	2.13	0.48
2:D:360:HIS:HB2	2:D:363:MET:HE3	1.95	0.48
3:E:57:LYS:HG3	3:E:58:SER:H	1.78	0.48
2:H:261:GLY:HA3	2:I:297:LEU:HD21	1.95	0.48
2:H:11:ARG:HH12	2:I:169:ARG:NH2	2.10	0.48
2:B:127:GLU:OE1	2:B:127:GLU:HA	2.14	0.48
2:B:92:GLU:HG2	2:B:124:LEU:HD12	1.94	0.48
2:I:64:CYS:SG	2:I:66:THR:HB	2.54	0.48
2:I:276:ILE:HG22	2:I:277:GLU:N	2.28	0.48
1:F:47:PHE:CZ	1:F:77:ARG:CA	2.96	0.48
1:F:311:THR:HG23	1:F:318:GLN:CD	2.34	0.48
2:I:338:GLU:HA	2:I:341:TYR:CD1	2.48	0.48
2:D:338:GLU:HA	2:D:341:TYR:CD1	2.48	0.48
3:J:27:LEU:O	3:J:143:LEU:N	2.39	0.48
1:A:10:ARG:NH2	1:A:40:GLN:HE22	2.11	0.48
3:J:312:ILE:O	3:J:316:LEU:HG	2.12	0.48
2:D:32:LEU:HD13	2:D:70:ALA:HA	1.95	0.48
2:D:276:ILE:HG22	2:D:277:GLU:N	2.28	0.48
1:A:48:GLU:CG	1:A:49:GLU:N	2.75	0.48
2:G:243:THR:HG22	2:G:244:LEU:H	1.77	0.48
3:E:306:ILE:HG22	3:E:307:ASN:N	2.28	0.48
1:A:281:ASN:O	1:A:283:ARG:N	2.47	0.48
2:H:66:THR:O	2:H:66:THR:HG22	2.14	0.48
2:D:127:GLU:OE1	2:D:127:GLU:HA	2.13	0.48
1:F:209:ALA:O	2:G:176:LYS:CD	2.55	0.48
2:D:257:VAL:HG11	2:D:320:ILE:HD13	1.95	0.48
2:I:302:LEU:HD11	2:I:313:MET:CB	2.44	0.48
1:A:310:LEU:HD13	1:A:314:GLN:HE22	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:6:LEU:CB	2:I:222:ASP:OD2	2.61	0.48
1:A:234:GLN:HE22	2:B:304:ASN:ND2	2.09	0.48
2:B:351:MET:SD	2:C:326:GLN:NE2	2.87	0.48
3:J:241:ALA:O	3:J:245:LEU:HD22	2.14	0.48
2:B:32:LEU:HD13	2:B:70:ALA:HA	1.96	0.48
1:A:64:ILE:HD11	1:A:100:LEU:CD1	2.29	0.48
2:C:112:GLN:CB	2:C:121:LYS:HZ1	0.89	0.48
2:C:201:ARG:NH2	2:C:305:ASP:O	2.46	0.48
2:I:260:ASN:OD1	2:I:260:ASN:O	2.32	0.48
2:D:10:TRP:CD1	2:D:190:ILE:HG23	2.49	0.48
2:I:360:HIS:HB2	2:I:363:MET:HE3	1.95	0.48
1:A:105:HIS:HA	1:F:227:LYS:NZ	2.28	0.48
2:D:302:LEU:HD11	2:D:313:MET:CB	2.43	0.48
2:G:148:GLU:O	2:G:149:HIS:HB2	2.14	0.48
2:G:5:VAL:HG11	2:G:222:ASP:OD1	2.12	0.48
3:E:241:ALA:O	3:E:245:LEU:HD22	2.14	0.48
1:A:183:GLN:HA	1:A:183:GLN:HE21	1.79	0.48
2:B:215:ARG:HG3	6:B:802:ADP:C4'	2.44	0.48
1:F:251:GLN:OE1	3:J:307:ASN:ND2	2.47	0.48
2:D:260:ASN:OD1	2:D:260:ASN:O	2.32	0.48
2:G:256:MET:CE	2:G:332:LEU:HD21	2.44	0.48
2:I:47:ARG:O	2:I:213:SER:HB3	2.14	0.48
2:C:126:ASP:HA	2:C:155:ALA:HB3	1.96	0.48
2:G:270:GLU:HG2	2:G:274:ARG:NH1	2.29	0.47
2:C:316:LEU:HB3	2:C:320:ILE:HD12	1.96	0.47
2:G:292:ILE:O	2:G:296:GLN:HG3	2.14	0.47
1:F:47:PHE:CZ	1:F:77:ARG:HA	2.49	0.47
3:J:306:ILE:HG22	3:J:307:ASN:N	2.29	0.47
2:I:355:ARG:HA	3:J:287:GLN:NE2	2.28	0.47
2:D:56:ARG:HH11	2:D:56:ARG:CG	2.22	0.47
2:H:126:ASP:HA	2:H:155:ALA:HB3	1.96	0.47
1:F:64:ILE:HD12	1:F:64:ILE:N	2.30	0.47
1:A:73:LEU:HB3	1:F:207:ASN:HB3	1.94	0.47
2:D:48:GLY:CA	2:D:215:ARG:HB2	2.45	0.47
2:D:355:ARG:HH12	3:E:287:GLN:HB3	1.73	0.47
2:B:148:GLU:O	2:B:149:HIS:HB2	2.14	0.47
1:A:174:TYR:CE2	1:A:211:HIS:CE1	3.03	0.47
2:I:44:SER:HA	2:I:156:THR:O	2.14	0.47
2:H:89:ASP:HB3	2:H:121:LYS:HA	1.95	0.47
2:I:257:VAL:HG11	2:I:320:ILE:HD13	1.95	0.47
1:F:174:TYR:CD2	1:F:211:HIS:HE1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:281:ASN:O	1:F:283:ARG:N	2.47	0.47
1:A:64:ILE:CG2	1:A:65:PHE:H	2.27	0.47
1:A:72:SER:OG	1:A:75:ALA:CA	2.43	0.47
3:E:32:LEU:HD12	3:E:166:PRO:CG	2.44	0.47
1:A:106:ASP:H	1:F:225:LYS:CE	2.28	0.47
1:F:282:ARG:HG2	1:F:285:MET:HE2	1.95	0.47
2:H:147:PRO:HG2	2:H:150:VAL:HB	1.95	0.47
2:H:359:PHE:CE2	2:I:323:THR:CG2	2.97	0.47
3:J:241:ALA:N	3:J:242:PRO:HD2	2.30	0.47
3:E:241:ALA:N	3:E:242:PRO:HD2	2.29	0.47
2:G:127:GLU:HA	2:G:127:GLU:OE1	2.14	0.47
2:I:200:PRO:CB	2:I:305:ASP:N	2.77	0.47
2:D:148:GLU:O	2:D:149:HIS:HB2	2.14	0.47
2:B:343:PRO:CB	2:C:283:VAL:HG13	2.45	0.47
2:D:361:PRO:O	2:D:362:ARG:HB2	2.15	0.47
2:I:200:PRO:CB	2:I:305:ASP:H	2.27	0.47
1:A:106:ASP:N	1:F:225:LYS:CE	2.77	0.47
1:A:119:LYS:CD	1:A:119:LYS:H	2.05	0.47
2:D:355:ARG:HA	3:E:287:GLN:HE21	1.79	0.47
1:F:312:LEU:O	1:F:312:LEU:HG	2.15	0.47
2:G:5:VAL:CB	2:G:222:ASP:OD1	2.62	0.47
2:H:257:VAL:HG11	2:H:320:ILE:HD13	1.97	0.47
2:C:291:ARG:NH1	2:C:306:MET:HG3	2.29	0.47
1:A:98:LEU:O	1:A:101:THR:HG22	2.14	0.47
2:B:292:ILE:O	2:B:296:GLN:HG3	2.14	0.47
2:C:66:THR:O	2:C:66:THR:HG22	2.14	0.47
2:I:215:ARG:CG	6:I:803:ADP:C4'	2.86	0.47
2:C:347:MET:CG	2:D:290:HIS:CE1	2.98	0.47
1:F:67:LEU:CD1	1:F:80:LEU:HD13	2.41	0.47
2:D:256:MET:HA	2:D:357:LEU:HD11	1.97	0.47
2:D:355:ARG:HH11	3:E:287:GLN:CB	2.27	0.47
1:F:56:ASP:H	1:F:57:PRO:HD2	1.79	0.47
2:D:343:PRO:HG3	2:D:347:MET:SD	2.55	0.47
2:H:341:TYR:HB2	2:I:333:LEU:CD1	2.42	0.47
2:H:216:ASP:O	2:H:220:LEU:HG	2.15	0.47
2:D:10:TRP:NE1	2:D:190:ILE:HG23	2.29	0.47
2:G:333:LEU:CD1	2:G:337:LYS:HE3	2.45	0.47
3:E:14:LEU:HD13	3:E:44:LEU:HD11	1.97	0.47
2:G:316:LEU:HD22	2:G:320:ILE:HD11	1.97	0.47
2:H:149:HIS:CD2	2:H:149:HIS:H	2.33	0.47
1:F:19:ALA:CB	1:F:133:ARG:HD3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:THR:HG23	1:A:318:GLN:CD	2.34	0.46
1:F:98:LEU:O	1:F:101:THR:HG22	2.14	0.46
1:A:263:GLN:HB2	1:A:272:LEU:HD21	1.97	0.46
2:B:333:LEU:CD1	2:B:337:LYS:HE3	2.45	0.46
3:E:227:GLY:O	3:E:229:TRP:HD1	1.98	0.46
1:A:55:ILE:HG13	1:A:85:PRO:CD	2.37	0.46
1:F:228:ARG:HG2	1:F:228:ARG:H	1.52	0.46
1:A:315:ASP:HB2	1:A:318:GLN:CD	2.36	0.46
1:A:315:ASP:CB	1:A:318:GLN:HG2	2.45	0.46
2:I:338:GLU:HA	2:I:341:TYR:HD1	1.80	0.46
2:D:291:ARG:O	2:D:295:VAL:HG23	2.16	0.46
2:D:148:GLU:O	2:D:149:HIS:CB	2.63	0.46
2:G:286:LEU:HD11	2:G:333:LEU:HA	1.96	0.46
3:E:95:GLU:O	3:E:99:LYS:HB2	2.15	0.46
3:E:57:LYS:HA	3:E:57:LYS:HD2	1.67	0.46
2:C:246:ASP:O	2:C:250:LEU:HB2	2.15	0.46
2:H:354:LEU:HD11	2:I:294:MET:SD	2.55	0.46
3:E:51:GLN:HB2	3:E:62:CYS:HB2	1.97	0.46
1:A:61:TRP:O	1:A:64:ILE:CG2	2.52	0.46
1:F:47:PHE:CE1	1:F:77:ARG:CA	2.97	0.46
1:A:279:TRP:O	1:A:279:TRP:CD2	2.69	0.46
2:C:257:VAL:HG11	2:C:320:ILE:HD13	1.97	0.46
3:E:257:LYS:HB3	3:E:262:ALA:HB3	1.98	0.46
2:D:246:ASP:HB2	2:D:248:GLN:CG	2.45	0.46
2:I:246:ASP:HB2	2:I:248:GLN:CG	2.45	0.46
1:F:263:GLN:OE1	1:F:272:LEU:HD11	2.15	0.46
2:C:216:ASP:O	2:C:220:LEU:HG	2.15	0.46
3:J:95:GLU:O	3:J:99:LYS:HB2	2.15	0.46
2:G:10:TRP:HB2	2:G:190:ILE:HG12	1.98	0.46
2:I:215:ARG:CA	6:I:803:ADP:C4'	2.87	0.46
2:I:316:LEU:HD22	2:I:320:ILE:CD1	2.45	0.46
1:F:309:GLU:HG3	3:J:306:ILE:HG23	1.97	0.46
2:C:147:PRO:HG2	2:C:150:VAL:HB	1.96	0.46
1:A:312:LEU:O	1:A:312:LEU:HG	2.15	0.46
2:B:48:GLY:C	2:B:213:SER:HB2	2.34	0.46
3:J:227:GLY:O	3:J:229:TRP:HD1	1.98	0.46
2:B:99:THR:HG21	2:C:144:GLU:HG2	1.96	0.46
2:H:10:TRP:CD2	2:H:190:ILE:HG12	2.50	0.46
1:A:306:THR:HG23	3:E:311:LEU:HD12	1.98	0.46
2:D:302:LEU:HA	2:D:302:LEU:HD23	1.54	0.46
2:B:148:GLU:O	2:B:149:HIS:CB	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:140:LEU:HD22	2:G:144:GLU:CG	2.45	0.46
2:D:338:GLU:HA	2:D:341:TYR:HD1	1.81	0.46
2:H:316:LEU:HB3	2:H:320:ILE:HD12	1.96	0.46
2:I:343:PRO:HG3	2:I:347:MET:SD	2.56	0.46
2:B:344:ASP:O	2:B:347:MET:HB3	2.16	0.46
1:A:221:LEU:HA	1:A:221:LEU:HD23	1.47	0.46
3:J:51:GLN:HB2	3:J:62:CYS:HB2	1.97	0.46
2:B:365:LEU:HB2	2:C:322:PRO:HG3	1.98	0.46
1:F:298:LEU:O	1:F:302:VAL:HG23	2.16	0.46
1:A:76:SER:O	1:A:76:SER:OG	2.34	0.46
1:A:311:THR:HG23	1:A:318:GLN:OE1	2.15	0.46
1:F:315:ASP:CB	1:F:318:GLN:HG2	2.45	0.46
1:F:279:TRP:CD2	1:F:279:TRP:O	2.69	0.46
2:C:354:LEU:HD21	2:D:297:LEU:HD22	1.98	0.46
2:C:21:GLN:NE2	2:C:176:LYS:O	2.49	0.46
2:G:32:LEU:HD13	2:G:70:ALA:HA	1.96	0.46
3:J:14:LEU:HD13	3:J:44:LEU:HD11	1.97	0.46
1:A:315:ASP:HB2	1:A:318:GLN:NE2	2.31	0.46
2:D:140:LEU:HD22	2:D:144:GLU:CG	2.45	0.46
2:D:200:PRO:HB2	2:D:305:ASP:CB	2.35	0.46
2:I:355:ARG:HH21	3:J:332:PRO:HD3	1.80	0.46
3:E:27:LEU:CD2	3:E:29:ILE:HD11	2.46	0.46
3:J:282:SER:OG	3:J:285:ARG:HB2	2.16	0.46
2:I:197:ALA:HB3	2:I:231:GLN:HG2	1.98	0.46
2:I:32:LEU:HD13	2:I:70:ALA:HA	1.97	0.46
2:B:140:LEU:HD22	2:B:144:GLU:CG	2.45	0.46
3:E:282:SER:OG	3:E:285:ARG:HB2	2.16	0.46
2:I:256:MET:HA	2:I:357:LEU:HD11	1.97	0.46
2:G:98:ARG:CD	2:H:140:LEU:CA	2.69	0.46
1:A:305:LEU:HD22	3:E:310:LEU:HD11	1.98	0.46
1:F:310:LEU:HA	1:F:310:LEU:HD23	1.60	0.46
3:E:253:MET:O	3:E:256:LEU:N	2.49	0.46
1:F:10:ARG:NH2	1:F:40:GLN:HE22	2.11	0.46
1:A:198:THR:HB	1:A:200:PRO:HD2	1.98	0.46
1:F:222:LEU:CD1	1:F:285:MET:SD	3.04	0.45
1:F:310:LEU:HD13	1:F:314:GLN:HE22	1.77	0.45
2:C:149:HIS:CD2	2:C:149:HIS:H	2.33	0.45
2:D:15:PHE:O	2:D:18:VAL:HB	2.17	0.45
2:B:219:SER:O	2:B:223:GLN:HG3	2.16	0.45
1:A:298:LEU:O	1:A:302:VAL:HG23	2.16	0.45
2:I:127:GLU:OE1	2:I:127:GLU:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:86:ARG:HH11	2:D:86:ARG:HG2	1.81	0.45
2:H:260:ASN:OD1	2:H:260:ASN:O	2.34	0.45
1:A:48:GLU:CG	1:A:49:GLU:H	2.30	0.45
2:G:148:GLU:O	2:G:149:HIS:CB	2.63	0.45
2:C:257:VAL:O	2:C:360:HIS:HE1	1.99	0.45
2:H:291:ARG:NH1	2:H:306:MET:HG3	2.29	0.45
2:C:10:TRP:CE2	2:C:190:ILE:HG23	2.51	0.45
1:F:190:LEU:HD22	2:G:30:ASN:HD22	1.80	0.45
2:D:360:HIS:CG	2:D:363:MET:HE3	2.51	0.45
2:I:302:LEU:HA	2:I:302:LEU:HD23	1.54	0.45
2:B:113:TYR:CE2	2:B:147:PRO:CG	3.00	0.45
2:D:197:ALA:HB3	2:D:231:GLN:HG2	1.98	0.45
2:C:245:ASP:HB2	2:C:248:GLN:HG3	1.98	0.45
2:D:119:ARG:HG3	2:D:120:PHE:CD2	2.51	0.45
1:A:228:ARG:HG2	1:A:228:ARG:H	1.52	0.45
1:A:191:LEU:HD23	1:A:191:LEU:HA	1.80	0.45
1:F:315:ASP:HB2	1:F:318:GLN:NE2	2.31	0.45
2:G:362:ARG:HE	2:G:363:MET:CE	2.24	0.45
3:E:27:LEU:HG	3:E:29:ILE:CD1	2.47	0.45
2:H:21:GLN:NE2	2:H:176:LYS:O	2.48	0.45
1:A:263:GLN:OE1	1:A:272:LEU:HD11	2.15	0.45
2:G:119:ARG:HG3	2:G:120:PHE:CD2	2.51	0.45
2:I:291:ARG:O	2:I:295:VAL:HG23	2.16	0.45
1:F:263:GLN:HB2	1:F:272:LEU:HD21	1.97	0.45
1:A:19:ALA:CB	1:A:133:ARG:HD3	2.46	0.45
2:H:100:LYS:HG2	2:I:133:ARG:H	1.51	0.45
2:H:73:CYS:SG	2:H:76:CYS:HB3	2.56	0.45
2:H:245:ASP:HB2	2:H:248:GLN:HG3	1.99	0.45
2:H:9:LYS:CE	2:H:194:GLU:OE2	2.64	0.45
2:B:186:GLN:HG2	2:B:214:LEU:HD21	1.98	0.45
2:B:270:GLU:HG2	2:B:274:ARG:CZ	2.46	0.45
2:G:270:GLU:HG2	2:G:274:ARG:CZ	2.46	0.45
2:H:113:TYR:HD2	2:H:147:PRO:HB3	1.82	0.45
2:C:51:LYS:HE3	2:C:51:LYS:HB2	1.77	0.45
2:G:140:LEU:O	2:G:144:GLU:HG3	2.17	0.45
3:J:27:LEU:HG	3:J:29:ILE:CD1	2.47	0.45
1:F:284:GLY:O	1:F:288:GLU:HB2	2.16	0.45
3:J:253:MET:O	3:J:256:LEU:N	2.50	0.45
3:J:257:LYS:HB3	3:J:262:ALA:HB3	1.98	0.45
2:I:244:LEU:CD1	2:I:276:ILE:HD13	2.46	0.45
2:I:361:PRO:O	2:I:362:ARG:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LEU:HD11	1:A:285:MET:CE	2.47	0.45
2:H:147:PRO:HB2	2:H:149:HIS:CD2	2.52	0.45
2:B:140:LEU:O	2:B:144:GLU:HG3	2.17	0.45
2:I:119:ARG:HG3	2:I:120:PHE:CD2	2.52	0.45
2:D:191:LEU:HD12	2:D:203:LEU:HD21	1.99	0.45
2:H:37:ILE:HD12	2:H:62:LEU:HD21	1.98	0.45
1:F:69:GLN:O	1:F:73:LEU:N	2.50	0.45
2:C:260:ASN:O	2:C:260:ASN:OD1	2.35	0.45
2:D:36:ARG:C	2:D:37:ILE:HD13	2.37	0.45
1:F:209:ALA:HA	2:G:176:LYS:NZ	2.27	0.45
2:B:36:ARG:C	2:B:37:ILE:HD13	2.37	0.45
2:G:98:ARG:HD3	2:H:140:LEU:CA	1.82	0.45
1:F:225:LYS:HE3	1:F:227:LYS:HD2	1.99	0.45
1:F:94:ASN:HA	1:F:126:TRP:HD1	1.82	0.45
1:A:222:LEU:CD1	1:A:285:MET:SD	3.04	0.45
2:H:252:LEU:CD1	2:H:281:LEU:HD21	2.47	0.45
2:C:252:LEU:CD1	2:C:281:LEU:HD21	2.47	0.45
2:G:248:GLN:HA	2:G:251:SER:OG	2.17	0.45
3:J:27:LEU:CD2	3:J:29:ILE:HD11	2.46	0.45
2:B:360:HIS:CD2	2:B:361:PRO:HD2	2.52	0.45
2:I:277:GLU:OE1	3:J:148:PRO:HG2	2.17	0.45
2:I:257:VAL:O	2:I:257:VAL:HG12	2.17	0.45
2:D:356:ALA:O	2:D:363:MET:HE3	2.17	0.45
1:F:315:ASP:HB2	1:F:318:GLN:CD	2.36	0.45
2:B:215:ARG:CB	6:B:802:ADP:O4'	2.64	0.45
2:D:140:LEU:O	2:D:144:GLU:HG3	2.17	0.45
1:A:247:LEU:HD11	1:A:308:THR:HG22	1.98	0.45
2:H:246:ASP:O	2:H:250:LEU:HB2	2.16	0.45
2:B:11:ARG:CZ	2:B:56:ARG:HE	2.29	0.45
2:H:21:GLN:HE22	2:H:49:VAL:HG13	1.81	0.45
2:B:316:LEU:HD22	2:B:320:ILE:HD11	1.97	0.45
2:C:112:GLN:CD	2:C:121:LYS:NZ	2.65	0.44
1:A:74:PHE:HB3	1:F:207:ASN:HD21	1.82	0.44
2:D:258:GLU:O	2:D:259:ALA:HB3	2.17	0.44
2:D:360:HIS:CB	2:D:363:MET:HE3	2.47	0.44
1:A:49:GLU:OE1	1:A:49:GLU:HA	2.16	0.44
1:A:315:ASP:H	1:A:318:GLN:HE21	1.66	0.44
3:E:32:LEU:HD12	3:E:166:PRO:HG2	1.99	0.44
1:F:306:THR:HG23	3:J:311:LEU:HD12	1.99	0.44
3:E:27:LEU:O	3:E:143:LEU:N	2.39	0.44
2:H:261:GLY:CA	2:I:297:LEU:HD21	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:360:HIS:CD2	2:G:361:PRO:HD2	2.52	0.44
2:G:344:ASP:O	2:G:347:MET:HB3	2.16	0.44
2:G:307:ALA:HA	2:G:310:GLU:CG	2.47	0.44
2:G:186:GLN:HG2	2:G:214:LEU:HD21	1.98	0.44
1:F:191:LEU:HD23	2:G:26:THR:HG22	1.97	0.44
2:B:119:ARG:HG3	2:B:120:PHE:CD2	2.52	0.44
2:D:244:LEU:HD11	2:D:276:ILE:CG2	2.48	0.44
1:F:48:GLU:CG	1:F:49:GLU:H	2.29	0.44
1:F:311:THR:HG23	1:F:318:GLN:OE1	2.15	0.44
2:C:73:CYS:SG	2:C:76:CYS:HB3	2.57	0.44
2:I:351:MET:SD	3:J:290:LEU:HD13	2.57	0.44
2:H:11:ARG:HH12	2:I:169:ARG:NH1	2.16	0.44
1:F:198:THR:HB	1:F:200:PRO:HD2	1.98	0.44
2:G:36:ARG:C	2:G:37:ILE:HD13	2.37	0.44
1:A:284:GLY:O	1:A:288:GLU:HB2	2.16	0.44
2:G:86:ARG:HH11	2:G:86:ARG:HG2	1.82	0.44
2:G:219:SER:O	2:G:223:GLN:HG3	2.17	0.44
3:J:57:LYS:HD2	3:J:57:LYS:HA	1.68	0.44
2:B:338:GLU:HB3	2:C:333:LEU:CD2	2.47	0.44
1:A:71:MET:CE	1:A:72:SER:OG	2.65	0.44
2:D:343:PRO:CD	3:E:294:CYS:SG	3.06	0.44
2:I:229:ASP:C	2:I:231:GLN:N	2.71	0.44
2:G:250:LEU:HD13	2:G:288:LEU:HD13	2.00	0.44
2:C:21:GLN:HE22	2:C:49:VAL:HG13	1.81	0.44
2:G:340:PRO:HB3	2:G:345:ARG:HH21	1.83	0.44
2:B:340:PRO:HB3	2:B:345:ARG:HH21	1.82	0.44
1:F:325:GLU:O	1:F:329:LEU:HG	2.18	0.44
1:A:325:GLU:O	1:A:329:LEU:HG	2.18	0.44
2:H:112:GLN:CB	2:H:121:LYS:CE	2.02	0.44
1:F:222:LEU:HD11	1:F:285:MET:CE	2.47	0.44
2:B:265:MET:HE2	2:C:294:MET:CE	2.47	0.44
3:J:117:ALA:HB2	3:J:143:LEU:CD1	2.47	0.44
2:B:307:ALA:HA	2:B:310:GLU:CD	2.38	0.44
2:B:307:ALA:HA	2:B:310:GLU:CG	2.47	0.44
2:G:307:ALA:HA	2:G:310:GLU:CD	2.38	0.44
2:H:333:LEU:O	2:H:336:ARG:N	2.49	0.44
2:I:191:LEU:HD12	2:I:203:LEU:HD21	1.99	0.44
1:F:55:ILE:HD11	1:F:82:LEU:HA	2.00	0.44
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.61	0.44
3:J:299:GLN:HE21	3:J:311:LEU:HD21	1.83	0.44
1:F:247:LEU:HD11	1:F:308:THR:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:30:GLN:HA	3:J:145:THR:O	2.17	0.44
2:B:86:ARG:HH11	2:B:86:ARG:HG2	1.81	0.44
2:D:167:LEU:HD21	2:D:172:GLN:OE1	2.18	0.44
1:F:71:MET:CG	1:F:108:LEU:HG	2.46	0.44
3:E:299:GLN:HE21	3:E:311:LEU:HD21	1.83	0.44
2:C:113:TYR:HD2	2:C:147:PRO:HB3	1.82	0.44
2:C:47:ARG:HA	4:C:1300:PO4:O3	2.18	0.44
2:G:113:TYR:CE2	2:G:147:PRO:CG	3.00	0.44
2:H:238:SER:O	2:H:243:THR:N	2.35	0.44
2:C:333:LEU:O	2:C:336:ARG:N	2.49	0.44
2:D:316:LEU:HD22	2:D:320:ILE:CD1	2.45	0.44
1:F:315:ASP:H	1:F:318:GLN:HE21	1.65	0.44
2:C:8:ARG:HD2	2:D:169:ARG:HG3	2.00	0.44
1:F:174:TYR:CD2	1:F:211:HIS:CE1	3.06	0.44
2:C:42:LEU:HD12	2:C:154:LEU:HB2	2.00	0.44
3:E:204:LEU:O	3:E:209:ASN:CB	2.65	0.44
3:E:7:LEU:HD22	3:E:40:LEU:HB2	2.00	0.44
2:I:167:LEU:HD21	2:I:172:GLN:OE1	2.17	0.44
2:G:10:TRP:NE1	2:G:193:GLU:HB3	2.33	0.44
2:I:258:GLU:O	2:I:259:ALA:HB3	2.17	0.44
1:A:49:GLU:O	1:A:79:THR:N	2.51	0.44
2:I:200:PRO:HG2	2:I:305:ASP:N	2.32	0.44
2:G:167:LEU:HD21	2:G:172:GLN:OE1	2.18	0.44
2:B:265:MET:CE	2:C:294:MET:CE	2.96	0.44
2:H:257:VAL:O	2:H:360:HIS:HE1	2.00	0.44
2:B:250:LEU:HD13	2:B:288:LEU:HD13	2.00	0.44
3:E:209:ASN:O	3:E:212:ALA:HB3	2.18	0.44
3:E:51:GLN:HG2	3:E:62:CYS:SG	2.58	0.44
2:C:37:ILE:HD12	2:C:62:LEU:HD21	1.98	0.44
2:B:167:LEU:HD21	2:B:172:GLN:OE1	2.18	0.44
1:A:100:LEU:O	1:A:103:LEU:HB3	2.18	0.43
2:H:243:THR:HG21	2:H:284:GLU:OE2	2.17	0.43
2:C:347:MET:HG2	2:D:290:HIS:CE1	2.53	0.43
2:H:345:ARG:O	2:H:349:VAL:HG23	2.18	0.43
2:H:264:VAL:O	2:H:268:ILE:HG13	2.18	0.43
2:D:160:GLN:HE21	2:D:160:GLN:HB3	1.61	0.43
1:F:104:LEU:HB3	1:F:133:ARG:NH1	2.34	0.43
2:D:257:VAL:O	2:D:257:VAL:HG12	2.17	0.43
2:D:214:LEU:HD23	6:D:801:ADP:C2	2.54	0.43
3:E:6:TRP:HB2	3:E:167:PRO:HG3	1.99	0.43
1:F:97:LEU:CB	1:F:126:TRP:CB	2.93	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:10:TRP:NE1	2:H:190:ILE:HG23	2.32	0.43
2:C:100:LYS:CE	2:D:133:ARG:HB2	2.46	0.43
2:B:248:GLN:O	2:B:252:LEU:HB2	2.17	0.43
2:C:347:MET:HG3	2:D:290:HIS:CE1	2.53	0.43
3:J:149:GLU:C	3:J:151:LEU:N	2.71	0.43
2:C:147:PRO:HB2	2:C:149:HIS:CD2	2.53	0.43
2:D:229:ASP:C	2:D:231:GLN:N	2.71	0.43
2:B:237:VAL:O	2:B:241:LEU:HB2	2.18	0.43
3:J:18:TYR:HB3	3:J:48:LEU:HD21	2.00	0.43
1:A:25:GLY:N	1:A:114:GLY:O	2.41	0.43
2:D:113:TYR:CE2	2:D:147:PRO:CG	3.00	0.43
2:G:248:GLN:O	2:G:252:LEU:HB2	2.17	0.43
3:J:30:GLN:O	3:J:30:GLN:HG3	2.18	0.43
3:J:51:GLN:HG2	3:J:62:CYS:SG	2.58	0.43
2:B:278:TRP:CE3	2:B:349:VAL:HG21	2.53	0.43
1:A:3:ARG:HG2	1:A:136:GLN:NE2	2.33	0.43
1:A:56:ASP:O	1:A:61:TRP:CZ2	2.71	0.43
1:A:61:TRP:HA	1:A:61:TRP:CE3	2.53	0.43
2:C:112:GLN:C	2:C:121:LYS:NZ	2.52	0.43
2:D:47:ARG:O	2:D:213:SER:HB3	2.18	0.43
2:B:215:ARG:HG3	6:B:802:ADP:H5'1	1.98	0.43
2:H:351:MET:CE	2:I:326:GLN:NE2	2.69	0.43
2:B:248:GLN:HA	2:B:251:SER:OG	2.18	0.43
3:E:30:GLN:HA	3:E:145:THR:O	2.18	0.43
2:G:250:LEU:HD22	2:G:309:ILE:CG2	2.48	0.43
2:B:250:LEU:HD22	2:B:309:ILE:CG2	2.48	0.43
1:F:221:LEU:HA	1:F:221:LEU:HD23	1.46	0.43
3:J:190:ALA:HB2	3:J:210:TRP:CZ3	2.54	0.43
3:J:7:LEU:HD22	3:J:40:LEU:HB2	2.00	0.43
2:G:278:TRP:CE3	2:G:349:VAL:HG21	2.53	0.43
3:E:92:ALA:O	3:E:96:VAL:HG23	2.19	0.43
2:C:167:LEU:HB3	2:C:172:GLN:NE2	2.33	0.43
1:F:3:ARG:HG2	1:F:136:GLN:NE2	2.33	0.43
2:G:6:LEU:CD1	2:G:191:LEU:HD23	2.27	0.43
1:F:55:ILE:HD11	1:F:82:LEU:CB	2.47	0.43
2:D:48:GLY:HA3	2:D:215:ARG:HB2	2.00	0.43
2:I:337:LYS:O	2:I:340:PRO:HD2	2.19	0.43
1:A:32:GLN:HE22	2:B:169:ARG:NH1	2.14	0.43
1:F:191:LEU:O	1:F:193:PRO:HD3	2.18	0.43
2:C:6:LEU:HG	2:C:222:ASP:OD1	2.18	0.43
1:A:262:ARG:CZ	3:E:230:TYR:HB3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:171:LEU:HD12	2:I:171:LEU:HA	1.92	0.43
2:G:342:ALA:HB1	2:G:343:PRO:HD2	2.01	0.43
1:A:225:LYS:HE3	1:A:227:LYS:HD2	2.00	0.43
1:A:334:LYS:CB	2:B:297:LEU:HD23	2.33	0.43
2:I:140:LEU:HD22	2:I:144:GLU:CG	2.47	0.43
2:H:362:ARG:C	2:H:363:MET:HG3	2.39	0.43
2:C:243:THR:HG21	2:C:284:GLU:OE2	2.19	0.43
3:J:92:ALA:O	3:J:96:VAL:HG23	2.19	0.43
1:A:55:ILE:O	1:A:55:ILE:HG13	2.19	0.43
2:G:100:LYS:H	2:H:144:GLU:HG2	1.84	0.43
2:H:201:ARG:HH21	2:H:305:ASP:C	2.15	0.43
3:E:18:TYR:HB3	3:E:48:LEU:HD21	2.01	0.43
2:H:136:PHE:CZ	2:H:166:ILE:HD12	2.54	0.43
1:F:50:HIS:O	1:F:51:HIS:CD2	2.72	0.43
2:H:167:LEU:HB3	2:H:172:GLN:NE2	2.33	0.43
3:E:171:TYR:N	3:E:171:TYR:CD2	2.87	0.43
2:B:357:LEU:HA	2:B:357:LEU:HD12	1.91	0.43
2:C:171:LEU:HA	2:C:171:LEU:HD12	1.91	0.43
1:A:191:LEU:O	1:A:193:PRO:HD3	2.18	0.42
2:H:100:LYS:HE3	2:I:136:PHE:HD2	1.84	0.42
3:J:73:HIS:HA	3:J:74:PRO:HD3	1.77	0.42
1:A:64:ILE:CG1	1:A:100:LEU:HD11	2.49	0.42
2:I:345:ARG:HG3	3:J:150:ARG:NH2	2.33	0.42
3:E:35:MET:HE1	3:E:167:PRO:HD2	2.01	0.42
2:G:56:ARG:CG	2:G:56:ARG:HH11	2.22	0.42
3:E:117:ALA:HB2	3:E:143:LEU:CD1	2.47	0.42
2:B:276:ILE:CG2	2:B:277:GLU:N	2.82	0.42
3:E:30:GLN:HG3	3:E:30:GLN:O	2.18	0.42
3:J:245:LEU:HB2	3:J:297:ARG:HG3	2.01	0.42
1:A:262:ARG:NH2	3:E:320:GLU:OE1	2.53	0.42
2:H:86:ARG:HH21	2:I:141:LYS:CB	2.15	0.42
2:C:264:VAL:O	2:C:268:ILE:HG13	2.18	0.42
1:F:102:GLY:C	1:F:103:LEU:HD13	2.40	0.42
2:D:47:ARG:HH12	2:D:215:ARG:NH2	1.91	0.42
1:F:90:ASN:O	1:F:94:ASN:ND2	2.53	0.42
2:I:140:LEU:O	2:I:144:GLU:HG3	2.18	0.42
1:A:243:PRO:HG2	1:A:244:VAL:H	1.85	0.42
2:C:100:LYS:HE2	2:D:133:ARG:CB	2.48	0.42
2:I:158:ASP:CG	2:I:161:LYS:CG	2.87	0.42
2:B:342:ALA:HB1	2:B:343:PRO:HD2	2.01	0.42
2:C:345:ARG:O	2:C:349:VAL:HG23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:324:GLN:HA	3:E:325:PRO:HD3	1.86	0.42
2:I:19:VAL:N	6:I:803:ADP:N1	2.45	0.42
2:D:358:ALA:C	2:D:360:HIS:H	2.22	0.42
1:A:50:HIS:O	1:A:51:HIS:CD2	2.72	0.42
1:A:334:LYS:HB3	2:B:297:LEU:HD21	1.89	0.42
2:C:147:PRO:HB2	2:C:149:HIS:NE2	2.35	0.42
2:D:355:ARG:HH12	3:E:287:GLN:CB	2.31	0.42
1:F:88:GLY:O	1:F:89:PRO:C	2.55	0.42
2:D:337:LYS:O	2:D:340:PRO:HD2	2.19	0.42
2:G:276:ILE:CG2	2:G:277:GLU:N	2.82	0.42
2:C:362:ARG:C	2:C:363:MET:HG3	2.40	0.42
2:I:113:TYR:HE2	2:I:147:PRO:CG	2.32	0.42
3:E:329:LEU:HD23	3:E:329:LEU:N	2.34	0.42
2:I:257:VAL:O	2:I:360:HIS:CE1	2.60	0.42
1:A:77:ARG:HB3	1:A:107:ASP:O	2.20	0.42
2:G:99:THR:C	2:H:144:GLU:HG2	2.14	0.42
2:H:147:PRO:HB2	2:H:149:HIS:NE2	2.34	0.42
2:H:42:LEU:HD12	2:H:154:LEU:HB2	2.00	0.42
2:C:156:THR:HG22	2:C:157:THR:N	2.34	0.42
2:D:311:LEU:HA	2:D:311:LEU:HD12	1.88	0.42
1:F:47:PHE:CD2	1:F:77:ARG:O	2.66	0.42
2:D:215:ARG:CG	6:D:801:ADP:H5'1	2.40	0.42
2:D:145:GLU:N	2:D:146:PRO:HD3	2.34	0.42
2:D:355:ARG:HH11	3:E:287:GLN:HB3	1.78	0.42
2:B:145:GLU:N	2:B:146:PRO:HD3	2.34	0.42
2:D:337:LYS:NZ	3:E:333:HIS:HB2	2.34	0.42
3:E:197:SER:HA	3:E:198:PRO:HD3	1.87	0.42
2:C:18:VAL:HG12	2:C:19:VAL:N	2.35	0.42
1:F:47:PHE:CB	1:F:77:ARG:O	2.65	0.42
2:G:98:ARG:CD	2:H:140:LEU:HA	2.46	0.42
2:D:355:ARG:HD3	3:E:287:GLN:NE2	2.34	0.42
2:B:362:ARG:HH21	2:B:363:MET:HE1	1.83	0.42
2:H:156:THR:HG22	2:H:157:THR:N	2.34	0.42
2:G:19:VAL:HG12	2:G:182:GLN:HE21	1.84	0.42
3:J:188:LEU:HD23	3:J:268:VAL:HG21	2.00	0.42
2:G:160:GLN:HE21	2:G:160:GLN:HB3	1.61	0.42
1:F:98:LEU:HG	1:F:125:ALA:CB	2.50	0.42
2:I:92:GLU:HG2	2:I:124:LEU:HD12	2.02	0.42
1:A:80:LEU:HD12	1:A:80:LEU:HA	1.88	0.42
2:D:244:LEU:HD11	2:D:276:ILE:HG21	2.02	0.42
1:A:29:LEU:O	1:A:33:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ILE:O	1:A:56:ASP:OD1	2.37	0.42
2:G:145:GLU:N	2:G:146:PRO:HD3	2.34	0.42
2:H:94:ASP:C	2:H:96:ALA:N	2.71	0.42
2:C:78:ASN:O	2:C:82:ILE:HG13	2.20	0.42
3:J:225:PRO:HB3	3:J:276:GLU:OE2	2.20	0.42
2:C:214:LEU:HD12	2:C:214:LEU:HA	1.91	0.42
1:F:80:LEU:CD1	1:F:108:LEU:HD21	2.49	0.42
2:D:358:ALA:HA	2:D:364:PRO:HG3	2.02	0.42
2:H:137:ASN:HA	2:H:140:LEU:HD12	2.02	0.42
2:C:229:ASP:CG	2:D:30:ASN:OD1	2.58	0.42
2:H:243:THR:HG22	2:H:284:GLU:HG3	2.02	0.42
2:G:286:LEU:HD23	2:G:286:LEU:HA	1.91	0.42
1:A:214:PRO:O	1:A:217:TRP:HB3	2.20	0.42
2:G:281:LEU:O	2:G:285:MET:HG3	2.20	0.42
1:A:4:LEU:CD1	1:A:137:VAL:HG22	2.50	0.42
2:H:112:GLN:HB3	2:H:121:LYS:HZ2	1.02	0.41
2:I:244:LEU:HD11	2:I:276:ILE:CG2	2.50	0.41
2:D:345:ARG:NH1	3:E:150:ARG:CG	2.83	0.41
1:A:49:GLU:CG	1:A:78:GLN:HG2	2.50	0.41
1:A:311:THR:O	1:A:318:GLN:NE2	2.53	0.41
1:F:311:THR:O	1:F:318:GLN:NE2	2.53	0.41
2:I:238:SER:HB3	2:I:243:THR:CB	2.38	0.41
1:F:179:LEU:CD2	2:G:167:LEU:HD22	2.50	0.41
1:F:84:LEU:HG	1:F:89:PRO:HG3	2.02	0.41
2:C:100:LYS:NZ	2:D:133:ARG:CG	2.77	0.41
2:C:136:PHE:CZ	2:C:166:ILE:HD12	2.54	0.41
2:D:241:LEU:O	3:E:156:ARG:NH1	2.52	0.41
1:F:39:ARG:CZ	1:F:50:HIS:HB3	2.51	0.41
1:A:29:LEU:HD21	1:A:154:ARG:CZ	2.37	0.41
2:I:113:TYR:CE2	2:I:147:PRO:CG	3.03	0.41
1:F:4:LEU:CD1	1:F:137:VAL:HG22	2.50	0.41
3:J:32:LEU:HD13	3:J:195:ALA:O	2.19	0.41
2:D:246:ASP:CB	2:D:248:GLN:HG2	2.50	0.41
1:A:264:SER:O	1:A:265:ALA:CB	2.68	0.41
1:F:191:LEU:HD23	2:G:26:THR:CG2	2.50	0.41
1:F:71:MET:CB	1:F:108:LEU:HG	2.47	0.41
1:F:67:LEU:O	1:F:71:MET:HG2	2.21	0.41
1:F:48:GLU:OE2	1:F:74:PHE:CZ	2.73	0.41
1:A:39:ARG:CZ	1:A:50:HIS:HB3	2.51	0.41
3:E:35:MET:CE	3:E:166:PRO:CD	2.87	0.41
2:C:210:ALA:HB1	2:C:213:SER:OG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:245:LEU:HB2	3:E:297:ARG:HG3	2.01	0.41
1:F:29:LEU:O	1:F:33:GLU:HG3	2.19	0.41
2:C:137:ASN:HA	2:C:140:LEU:HD12	2.02	0.41
2:B:281:LEU:O	2:B:285:MET:HG3	2.20	0.41
2:H:78:ASN:O	2:H:82:ILE:HG13	2.20	0.41
2:I:271:ALA:O	2:I:276:ILE:HG13	2.20	0.41
1:F:102:GLY:C	1:F:103:LEU:CD1	2.89	0.41
2:I:224:ALA:CB	2:I:240:MET:HE2	2.49	0.41
1:F:243:PRO:HG2	1:F:244:VAL:H	1.84	0.41
2:D:347:MET:O	2:D:351:MET:CG	2.65	0.41
2:H:18:VAL:HG12	2:H:19:VAL:N	2.35	0.41
2:I:246:ASP:CB	2:I:248:GLN:HG2	2.50	0.41
1:F:272:LEU:HD12	1:F:272:LEU:HA	1.91	0.41
2:C:321:PRO:HA	2:C:322:PRO:HD2	1.93	0.41
2:H:227:SER:HB3	2:I:27:ALA:HB2	2.01	0.41
2:B:227:SER:HB2	2:C:23:HIS:ND1	2.35	0.41
2:C:94:ASP:OD1	2:C:96:ALA:HB3	2.21	0.41
3:J:26:ALA:HB2	3:J:132:LEU:HD22	2.03	0.41
2:D:289:LEU:HD23	2:D:289:LEU:HA	1.81	0.41
2:G:365:LEU:HG	2:G:365:LEU:H	1.73	0.41
3:J:171:TYR:CD2	3:J:171:TYR:N	2.88	0.41
2:H:355:ARG:HG3	2:I:326:GLN:OE1	2.21	0.41
2:H:250:LEU:HD23	2:H:312:ARG:CZ	2.51	0.41
2:G:256:MET:HE2	2:G:332:LEU:HD21	2.03	0.41
2:H:21:GLN:HE22	2:H:49:VAL:CG1	2.34	0.41
2:B:338:GLU:HB3	2:C:333:LEU:HD22	2.03	0.41
2:C:94:ASP:C	2:C:96:ALA:N	2.71	0.41
3:E:225:PRO:HB3	3:E:276:GLU:OE2	2.20	0.41
2:D:271:ALA:O	2:D:276:ILE:HG13	2.20	0.41
3:J:311:LEU:HA	3:J:311:LEU:HD12	1.86	0.41
1:F:65:PHE:O	1:F:66:SER:C	2.59	0.41
3:J:209:ASN:O	3:J:212:ALA:HB3	2.21	0.41
2:I:148:GLU:O	2:I:149:HIS:HB2	2.21	0.41
2:H:360:HIS:CD2	2:H:363:MET:H	2.37	0.41
2:B:158:ASP:CG	2:B:161:LYS:CG	2.89	0.41
2:C:21:GLN:HE22	2:C:49:VAL:CG1	2.34	0.41
3:J:121:THR:O	3:J:124:ALA:HB3	2.21	0.41
2:H:162:LEU:HA	2:H:162:LEU:HD23	1.92	0.41
3:E:149:GLU:C	3:E:151:LEU:N	2.71	0.41
3:E:149:GLU:O	3:E:151:LEU:N	2.52	0.41
1:F:64:ILE:HD12	1:F:64:ILE:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ILE:HD11	1:A:85:PRO:HD3	2.02	0.41
2:C:115:PRO:HD3	2:C:149:HIS:HB2	2.03	0.41
3:J:73:HIS:HE1	3:J:106:LEU:HD22	1.86	0.41
2:C:238:SER:HB2	2:C:243:THR:O	2.21	0.41
2:I:360:HIS:CB	2:I:363:MET:HE3	2.50	0.41
1:A:49:GLU:HB2	1:A:78:GLN:CA	2.50	0.41
1:F:85:PRO:HG2	1:F:93:ILE:CD1	2.51	0.41
3:E:311:LEU:HA	3:E:311:LEU:HD12	1.86	0.41
1:A:310:LEU:HB3	1:A:314:GLN:NE2	2.35	0.41
1:F:310:LEU:HB3	1:F:314:GLN:NE2	2.35	0.41
2:H:115:PRO:HB2	2:H:118:GLY:O	2.21	0.41
2:D:302:LEU:HD13	2:D:310:GLU:HA	2.03	0.41
1:F:84:LEU:HA	1:F:84:LEU:HD12	1.84	0.41
1:F:81:LEU:HA	1:F:111:ILE:O	2.20	0.41
2:C:250:LEU:HD23	2:C:312:ARG:CZ	2.51	0.41
2:B:47:ARG:O	2:B:213:SER:CB	2.68	0.41
2:C:360:HIS:CD2	2:C:363:MET:H	2.37	0.41
3:E:256:LEU:HD12	3:E:290:LEU:HD12	2.03	0.41
3:J:73:HIS:CE1	3:J:106:LEU:HD22	2.56	0.41
2:I:351:MET:SD	3:J:290:LEU:HD22	2.60	0.41
3:J:329:LEU:N	3:J:329:LEU:HD23	2.33	0.41
2:C:283:VAL:HA	2:C:286:LEU:HD12	2.03	0.41
1:F:191:LEU:HD23	1:F:191:LEU:HA	1.80	0.41
2:H:199:GLU:HA	2:H:200:PRO:HD2	1.94	0.41
3:J:244:ARG:O	3:J:247:TRP:HB2	2.21	0.41
3:E:244:ARG:O	3:E:247:TRP:HB2	2.21	0.41
1:A:84:LEU:HA	1:A:84:LEU:HD12	1.84	0.41
2:G:100:LYS:HG2	2:H:145:GLU:OE2	2.21	0.41
2:G:244:LEU:HA	2:G:244:LEU:HD23	1.81	0.41
1:A:270:ARG:HG2	1:A:283:ARG:NH2	2.36	0.41
2:D:343:PRO:CG	2:D:347:MET:SD	3.09	0.41
2:B:218:LEU:HD23	2:B:218:LEU:HA	1.88	0.41
1:F:306:THR:HG23	3:J:311:LEU:CD1	2.51	0.40
2:H:253:VAL:O	2:H:257:VAL:HG23	2.21	0.40
1:A:32:GLN:NE2	2:B:169:ARG:HH12	2.17	0.40
2:H:210:ALA:HB1	2:H:213:SER:OG	2.20	0.40
2:H:94:ASP:OD1	2:H:96:ALA:HB3	2.21	0.40
3:J:324:GLN:HA	3:J:325:PRO:HD3	1.86	0.40
1:A:53:PHE:HZ	1:A:60:ASP:O	2.04	0.40
1:A:73:LEU:CG	1:F:207:ASN:HA	2.42	0.40
2:G:246:ASP:HB3	2:G:274:ARG:HH11	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:250:LEU:CD2	2:D:309:ILE:HG23	2.51	0.40
2:I:343:PRO:CG	2:I:347:MET:SD	3.10	0.40
1:A:32:GLN:HE21	2:B:165:THR:HG22	1.86	0.40
2:I:80:ARG:NH1	2:I:80:ARG:HG2	2.36	0.40
2:H:298:SER:HA	2:H:299:PRO:HD2	1.93	0.40
2:D:286:LEU:HD23	2:D:286:LEU:HA	1.90	0.40
1:F:179:LEU:HD21	2:G:167:LEU:HD22	2.01	0.40
2:H:178:LEU:HD22	2:H:182:GLN:NE2	2.36	0.40
2:D:18:VAL:HB	2:D:25:LEU:HD11	2.03	0.40
1:F:199:LEU:O	1:F:203:GLU:HB2	2.22	0.40
2:C:178:LEU:HD22	2:C:182:GLN:NE2	2.36	0.40
2:I:311:LEU:HA	2:I:311:LEU:HD12	1.88	0.40
2:G:171:LEU:HA	2:G:171:LEU:HD12	1.92	0.40
2:I:286:LEU:HD21	2:I:332:LEU:HB2	2.03	0.40
1:F:82:LEU:HD21	1:F:100:LEU:HD12	2.04	0.40
2:I:250:LEU:CD2	2:I:309:ILE:HG23	2.51	0.40
2:B:363:MET:HB2	2:B:363:MET:HE3	1.78	0.40
2:G:363:MET:HE3	2:G:363:MET:HB2	1.87	0.40
2:C:257:VAL:O	2:C:257:VAL:HG12	2.21	0.40
2:H:347:MET:HG2	2:I:290:HIS:ND1	2.36	0.40
2:G:158:ASP:CG	2:G:161:LYS:CG	2.89	0.40
2:H:223:GLN:NE2	2:I:172:GLN:O	2.54	0.40
2:C:111:VAL:HG21	2:C:142:THR:HG21	2.03	0.40
3:E:321:HIS:O	3:E:327:VAL:HG21	2.22	0.40
1:A:190:LEU:C	2:B:30:ASN:HD22	2.16	0.40
1:F:55:ILE:HB	1:F:83:LEU:O	2.20	0.40
1:F:315:ASP:CB	1:F:318:GLN:CG	2.82	0.40
2:H:115:PRO:HD3	2:H:149:HIS:HB2	2.02	0.40
3:J:27:LEU:HG	3:J:29:ILE:HD11	2.03	0.40
2:H:283:VAL:HA	2:H:286:LEU:HD12	2.03	0.40
2:B:243:THR:CG2	2:B:244:LEU:N	2.85	0.40
3:E:26:ALA:HB2	3:E:132:LEU:HD22	2.03	0.40
3:E:94:ARG:O	3:E:98:GLU:HG2	2.22	0.40

All (20) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LYS:NZ	2:D:368:PRO:CG[4_455]	0.40	1.80
2:B:299:PRO:CG	3:E:279:ASN:ND2[4_455]	1.13	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:119:LYS:CB	2:I:117:ARG:NH2[1_455]	1.25	0.95
1:A:227:LYS:NZ	2:D:368:PRO:CD[4_455]	1.29	0.91
1:A:227:LYS:CE	2:D:368:PRO:CG[4_455]	1.51	0.69
2:B:195:HIS:CB	3:E:8:ARG:NH2[1_455]	1.55	0.65
2:B:194:GLU:O	3:E:8:ARG:NH2[1_455]	1.70	0.50
1:F:119:LYS:CB	2:I:117:ARG:CZ[1_455]	1.77	0.43
1:A:227:LYS:NZ	2:D:368:PRO:CB[4_455]	1.78	0.42
2:B:299:PRO:CB	3:E:279:ASN:ND2[4_455]	1.81	0.39
1:F:65:PHE:CE2	3:J:178:ARG:CZ[3_655]	1.88	0.32
1:F:279:TRP:CH2	2:I:33:SER:O[1_455]	1.90	0.30
1:F:279:TRP:CZ2	2:I:33:SER:O[1_455]	1.94	0.26
1:F:65:PHE:CD2	3:J:178:ARG:NH1[3_655]	1.97	0.23
1:F:73:LEU:O	3:J:2:ARG:NH2[3_655]	1.97	0.23
1:F:65:PHE:CE2	3:J:178:ARG:NH1[3_655]	2.00	0.20
1:F:277:ARG:NE	2:I:66:THR:O[1_455]	2.05	0.15
1:F:119:LYS:CA	2:I:117:ARG:NH2[1_455]	2.05	0.15
2:B:194:GLU:C	3:E:8:ARG:NH2[1_455]	2.15	0.05
2:B:195:HIS:CA	3:E:8:ARG:NH2[1_455]	2.17	0.03

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 X-ray entries followed by that with respect to entries of similar resolution.

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	336/343 (98%)	302 (90%)	24 (7%)	10 (3%)	5	45
1	F	336/343 (98%)	294 (88%)	32 (10%)	10 (3%)	5	45
2	B	362/368 (98%)	340 (94%)	16 (4%)	6 (2%)	11	56
2	C	364/368 (99%)	336 (92%)	24 (7%)	4 (1%)	17	64
2	D	362/368 (98%)	335 (92%)	19 (5%)	8 (2%)	8	51
2	G	362/368 (98%)	338 (93%)	18 (5%)	6 (2%)	11	56
2	H	364/368 (99%)	336 (92%)	24 (7%)	4 (1%)	17	64
2	I	362/368 (98%)	335 (92%)	22 (6%)	5 (1%)	14	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	332/334 (99%)	301 (91%)	28 (8%)	3 (1%)	21	67
3	J	332/334 (99%)	300 (90%)	30 (9%)	2 (1%)	30	73
All	All	3512/3562 (99%)	3217 (92%)	237 (7%)	58 (2%)	11	56

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	TRP
2	B	310	GLU
2	C	20	GLY
2	C	364	PRO
2	D	261	GLY
2	D	310	GLU
1	F	279	TRP
1	F	282	ARG
2	G	310	GLU
2	H	20	GLY
2	H	364	PRO
2	I	261	GLY
2	I	310	GLU
1	A	58	ASN
1	A	71	MET
1	A	131	ALA
1	A	282	ARG
2	B	303	GLY
2	D	20	GLY
1	F	108	LEU
1	F	131	ALA
2	G	303	GLY
1	A	46	GLY
1	A	269	LEU
2	B	46	THR
2	B	146	PRO
2	C	95	ALA
2	D	46	THR
2	D	146	PRO
2	D	177	ALA
3	E	62	CYS
1	F	46	GLY
1	F	77	ARG
1	F	269	LEU

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Mol	Chain	Res	Type
2	G	46	THR
2	G	146	PRO
2	G	249	ALA
2	H	95	ALA
2	I	146	PRO
3	J	62	CYS
1	A	125	ALA
2	B	249	ALA
3	E	150	ARG
1	F	125	ALA
3	J	150	ARG
2	B	278	TRP
2	C	339	LEU
2	D	364	PRO
1	F	56	ASP
2	G	278	TRP
2	H	339	LEU
2	I	364	PRO
1	A	270	ARG
2	D	299	PRO
2	I	299	PRO
1	A	317	GLY
3	E	207	GLY
1	F	317	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 X-ray entries followed by that with respect to entries of similar resolution.

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	287/291 (99%)	255 (89%)	32 (11%)	8	38
1	F	287/291 (99%)	256 (89%)	31 (11%)	8	39
2	B	301/305 (99%)	281 (93%)	20 (7%)	21	61
2	C	303/305 (99%)	287 (95%)	16 (5%)	28	67
2	D	301/305 (99%)	283 (94%)	18 (6%)	24	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	301/305 (99%)	279 (93%)	22 (7%)	17	57
2	H	303/305 (99%)	286 (94%)	17 (6%)	26	66
2	I	301/305 (99%)	285 (95%)	16 (5%)	28	67
3	E	270/270 (100%)	236 (87%)	34 (13%)	5	32
3	J	270/270 (100%)	237 (88%)	33 (12%)	6	33
All	All	2924/2952 (99%)	2685 (92%)	239 (8%)	14	52

All (239) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	54	SER
1	A	56	ASP
1	A	57	PRO
1	A	72	SER
1	A	77	ARG
1	A	84	LEU
1	A	101	THR
1	A	109	LEU
1	A	113	ARG
1	A	115	ASN
1	A	119	LYS
1	A	133	ARG
1	A	142	PRO
1	A	143	GLU
1	A	160	LEU
1	A	162	LEU
1	A	183	GLN
1	A	198	THR
1	A	200	PRO
1	A	208	ASP
1	A	214	PRO
1	A	215	PHE
1	A	223	MET
1	A	228	ARG
1	A	230	LEU
1	A	266	HIS
1	A	279	TRP
1	A	283	ARG
1	A	292	ARG

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Mol	Chain	Res	Type
1	A	305	LEU
1	A	330	LEU
2	B	13	GLN
2	B	36	ARG
2	B	42	LEU
2	B	56	ARG
2	B	66	THR
2	B	86	ARG
2	B	101	VAL
2	B	140	LEU
2	B	145	GLU
2	B	146	PRO
2	B	148	GLU
2	B	184	ARG
2	B	240	MET
2	B	251	SER
2	B	252	LEU
2	B	305	ASP
2	B	333	LEU
2	B	344	ASP
2	B	351	MET
2	B	357	LEU
2	C	3	TYR
2	C	15	PHE
2	C	46	THR
2	C	69	THR
2	C	76	CYS
2	C	101	VAL
2	C	130	MET
2	C	179	ASP
2	C	251	SER
2	C	309	ILE
2	C	318	ARG
2	C	327	LEU
2	C	344	ASP
2	C	355	ARG
2	C	357	LEU
2	C	367	GLU
2	D	13	GLN
2	D	36	ARG
2	D	42	LEU
2	D	56	ARG

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Mol	Chain	Res	Type
2	D	66	THR
2	D	86	ARG
2	D	101	VAL
2	D	140	LEU
2	D	145	GLU
2	D	146	PRO
2	D	148	GLU
2	D	184	ARG
2	D	194	GLU
2	D	219	SER
2	D	248	GLN
2	D	251	SER
2	D	333	LEU
2	D	357	LEU
3	E	3	TRP
3	E	13	LYS
3	E	46	ARG
3	E	68	MET
3	E	91	ASP
3	E	110	LYS
3	E	120	LEU
3	E	147	GLU
3	E	149	GLU
3	E	154	THR
3	E	158	ARG
3	E	159	CYS
3	E	166	PRO
3	E	167	PRO
3	E	168	PRO
3	E	170	GLN
3	E	175	TRP
3	E	185	ASP
3	E	202	LEU
3	E	206	GLN
3	E	216	LEU
3	E	220	LEU
3	E	237	ASN
3	E	245	LEU
3	E	252	LEU
3	E	256	LEU
3	E	277	LEU
3	E	285	ARG

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Mol	Chain	Res	Type
3	E	290	LEU
3	E	292	ASP
3	E	299	GLN
3	E	310	LEU
3	E	315	LEU
3	E	329	LEU
1	F	40	GLN
1	F	72	SER
1	F	84	LEU
1	F	89	PRO
1	F	101	THR
1	F	103	LEU
1	F	109	LEU
1	F	113	ARG
1	F	115	ASN
1	F	119	LYS
1	F	133	ARG
1	F	142	PRO
1	F	143	GLU
1	F	160	LEU
1	F	162	LEU
1	F	183	GLN
1	F	198	THR
1	F	200	PRO
1	F	208	ASP
1	F	211	HIS
1	F	214	PRO
1	F	215	PHE
1	F	223	MET
1	F	228	ARG
1	F	230	LEU
1	F	266	HIS
1	F	279	TRP
1	F	283	ARG
1	F	292	ARG
1	F	305	LEU
1	F	330	LEU
2	G	11	ARG
2	G	13	GLN
2	G	36	ARG
2	G	42	LEU
2	G	56	ARG

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Mol	Chain	Res	Type
2	G	66	THR
2	G	86	ARG
2	G	101	VAL
2	G	140	LEU
2	G	145	GLU
2	G	146	PRO
2	G	148	GLU
2	G	184	ARG
2	G	240	MET
2	G	243	THR
2	G	251	SER
2	G	252	LEU
2	G	305	ASP
2	G	333	LEU
2	G	344	ASP
2	G	351	MET
2	G	357	LEU
2	H	3	TYR
2	H	15	PHE
2	H	46	THR
2	H	69	THR
2	H	76	CYS
2	H	101	VAL
2	H	130	MET
2	H	179	ASP
2	H	240	MET
2	H	251	SER
2	H	309	ILE
2	H	318	ARG
2	H	327	LEU
2	H	344	ASP
2	H	355	ARG
2	H	357	LEU
2	H	367	GLU
2	I	11	ARG
2	I	13	GLN
2	I	36	ARG
2	I	42	LEU
2	I	66	THR
2	I	101	VAL
2	I	140	LEU
2	I	145	GLU

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Mol	Chain	Res	Type
2	I	148	GLU
2	I	184	ARG
2	I	194	GLU
2	I	219	SER
2	I	248	GLN
2	I	251	SER
2	I	333	LEU
2	I	357	LEU
3	J	3	TRP
3	J	13	LYS
3	J	46	ARG
3	J	68	MET
3	J	91	ASP
3	J	110	LYS
3	J	120	LEU
3	J	147	GLU
3	J	149	GLU
3	J	154	THR
3	J	158	ARG
3	J	159	CYS
3	J	166	PRO
3	J	167	PRO
3	J	168	PRO
3	J	170	GLN
3	J	175	TRP
3	J	185	ASP
3	J	202	LEU
3	J	206	GLN
3	J	216	LEU
3	J	220	LEU
3	J	237	ASN
3	J	245	LEU
3	J	252	LEU
3	J	256	LEU
3	J	277	LEU
3	J	285	ARG
3	J	290	LEU
3	J	299	GLN
3	J	310	LEU
3	J	315	LEU
3	J	329	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	51	HIS
1	A	94	ASN
1	A	105	HIS
1	A	136	GLN
1	A	211	HIS
1	A	216	HIS
1	A	234	GLN
1	A	259	ASN
1	A	266	HIS
1	A	276	HIS
1	A	295	GLN
1	A	297	GLN
1	A	314	GLN
1	A	318	GLN
2	B	21	GLN
2	B	160	GLN
2	B	198	HIS
2	B	304	ASN
2	B	360	HIS
2	C	149	HIS
2	C	198	HIS
2	C	360	HIS
2	D	21	GLN
2	D	30	ASN
2	D	174	HIS
2	D	198	HIS
2	D	248	GLN
2	D	304	ASN
2	D	326	GLN
3	E	73	HIS
3	E	237	ASN
3	E	260	HIS
3	E	280	HIS
3	E	287	GLN
3	E	299	GLN
3	E	307	ASN
1	F	40	GLN
1	F	51	HIS
1	F	94	ASN
1	F	105	HIS
1	F	136	GLN

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Mol	Chain	Res	Type
1	F	140	GLN
1	F	211	HIS
1	F	216	HIS
1	F	266	HIS
1	F	276	HIS
1	F	295	GLN
1	F	297	GLN
1	F	314	GLN
1	F	318	GLN
2	G	21	GLN
2	G	30	ASN
2	G	160	GLN
2	G	172	GLN
2	G	189	HIS
2	G	198	HIS
2	G	326	GLN
2	G	360	HIS
2	H	30	ASN
2	H	149	HIS
2	H	182	GLN
2	H	198	HIS
2	H	223	GLN
2	H	360	HIS
2	I	21	GLN
2	I	160	GLN
2	I	198	HIS
2	I	248	GLN
2	I	304	ASN
2	I	326	GLN
3	J	73	HIS
3	J	237	ASN
3	J	260	HIS
3	J	299	GLN
3	J	307	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\# Z > 2$
6	ADP	B	802	-	22,29,29	1.48	4 (18%)	27,45,45	1.50	3 (11%)
4	PO4	C	1300	-	4,4,4	0.72	0	6,6,6	0.30	0
6	ADP	D	801	-	22,29,29	1.49	4 (18%)	27,45,45	1.48	3 (11%)
6	ADP	I	803	-	22,29,29	1.49	4 (18%)	27,45,45	1.50	3 (11%)

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
6	ADP	B	802	-	-	0/12/32/32	0/3/3/3
4	PO4	C	1300	-	-	0/0/0/0	0/0/0/0
6	ADP	D	801	-	-	0/12/32/32	0/3/3/3
6	ADP	I	803	-	-	0/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	801	ADP	C4-N3	2.58	1.39	1.35
6	I	803	ADP	C4-N3	2.58	1.39	1.35
6	B	802	ADP	C4-N3	2.59	1.39	1.35
6	I	803	ADP	O4'-C1'	2.63	1.44	1.41
6	B	802	ADP	O4'-C1'	2.63	1.44	1.41
6	D	801	ADP	C2-N1	2.69	1.39	1.33
6	D	801	ADP	O4'-C1'	2.70	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	802	ADP	C2-N1	2.75	1.39	1.33
6	I	803	ADP	C2-N1	2.77	1.39	1.33
6	B	802	ADP	C2-N3	2.92	1.37	1.32
6	I	803	ADP	C2-N3	2.94	1.37	1.32
6	D	801	ADP	C2-N3	2.95	1.37	1.32

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	802	ADP	N3-C2-N1	-2.98	126.61	128.89
6	I	803	ADP	N3-C2-N1	-2.95	126.63	128.89
6	D	801	ADP	N3-C2-N1	-2.86	126.70	128.89
6	B	802	ADP	O2B-PB-O1B	2.30	117.98	110.58
6	I	803	ADP	O2B-PB-O1B	2.30	117.98	110.58
6	D	801	ADP	O2B-PB-O1B	2.30	117.98	110.58
6	D	801	ADP	C1'-N9-C4	5.14	134.69	126.94
6	B	802	ADP	C1'-N9-C4	5.17	134.74	126.94
6	I	803	ADP	C1'-N9-C4	5.19	134.77	126.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	802	ADP	8	0
4	C	1300	PO4	3	0
6	D	801	ADP	5	0
6	I	803	ADP	28	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	338/343 (98%)	0.20	11 (3%)	50	38	78, 150, 164, 164	0
1	F	338/343 (98%)	0.27	14 (4%)	41	31	149, 189, 201, 201	0
2	B	364/368 (98%)	0.25	18 (4%)	33	25	41, 130, 151, 151	0
2	C	366/368 (99%)	0.05	9 (2%)	61	49	21, 41, 132, 132	0
2	D	364/368 (98%)	0.05	6 (1%)	74	64	36, 43, 73, 73	0
2	G	364/368 (98%)	0.99	69 (18%)	2	3	176, 263, 290, 290	0
2	H	366/368 (99%)	0.69	48 (13%)	5	5	180, 199, 272, 272	0
2	I	364/368 (98%)	0.46	28 (7%)	16	12	198, 201, 205, 205	0
3	E	334/334 (100%)	0.13	6 (1%)	71	61	37, 55, 98, 98	0
3	J	334/334 (100%)	0.45	24 (7%)	18	13	138, 169, 221, 221	0
All	All	3532/3562 (99%)	0.36	233 (6%)	22	14	21, 150, 272, 290	0

All (233) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	60	LYS	8.0
2	G	59	ALA	7.0
2	H	170	CYS	6.9
3	J	82	GLU	6.7
2	I	366	PRO	6.5
1	F	75	ALA	6.4
3	J	83	LYS	6.2
2	I	367	GLU	5.8
3	J	102	GLU	5.7
2	G	104	THR	5.5
2	G	15	PHE	5.3
2	B	74	GLY	5.3
2	G	49	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
2	G	56	ARG	4.9
2	G	108	LEU	4.8
2	G	98	ARG	4.7
2	H	175	LEU	4.7
2	H	15	PHE	4.7
1	F	338	ASP	4.5
2	G	63	ASN	4.4
2	B	91	ILE	4.4
2	I	242	GLY	4.4
2	G	324	ASP	4.4
3	J	103	HIS	4.3
2	B	89	ASP	4.3
2	B	117	ARG	4.3
2	G	55	ALA	4.3
2	H	35	GLY	4.3
1	F	76	SER	4.3
3	J	85	LYS	4.2
2	G	35	GLY	4.2
2	G	239	ALA	4.1
3	J	66	GLN	4.1
2	B	246	ASP	4.1
2	H	169	ARG	4.1
2	G	203	LEU	4.1
1	A	211	HIS	4.0
2	H	135	SER	4.0
2	H	60	LYS	4.0
1	F	56	ASP	4.0
2	G	84	GLN	4.0
2	G	232	VAL	3.9
2	G	237	VAL	3.8
2	H	148	GLU	3.8
2	G	229	ASP	3.8
2	H	11	ARG	3.8
3	J	81	PRO	3.8
2	H	147	PRO	3.8
2	I	72	PRO	3.7
2	I	193	GLU	3.7
2	B	90	LEU	3.7
2	I	368	PRO	3.7
2	G	83	GLU	3.7
2	G	57	LEU	3.7
2	D	104	THR	3.6

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Mol	Chain	Res	Type	RSRZ
2	G	184	ARG	3.6
2	G	13	GLN	3.6
2	G	62	LEU	3.6
3	J	18	TYR	3.6
2	H	66	THR	3.6
3	E	85	LYS	3.6
2	G	85	GLY	3.5
2	B	88	VAL	3.5
2	B	75	VAL	3.5
2	H	59	ALA	3.5
2	D	366	PRO	3.5
2	G	357	LEU	3.5
2	H	112	GLN	3.4
2	G	221	THR	3.4
2	H	171	LEU	3.4
2	H	65	GLU	3.4
2	C	112	GLN	3.3
2	G	235	GLN	3.3
2	G	177	ALA	3.3
2	G	96	ALA	3.3
2	H	132	SER	3.3
3	E	105	ARG	3.3
2	G	86	ARG	3.3
2	B	34	LEU	3.3
3	J	105	ARG	3.2
1	F	97	LEU	3.2
2	G	354	LEU	3.2
2	H	13	GLN	3.2
2	D	100	LYS	3.2
2	H	313	MET	3.2
2	G	186	GLN	3.1
2	H	182	GLN	3.1
1	A	58	ASN	3.1
3	J	80	ALA	3.1
2	D	109	ASP	3.1
2	C	63	ASN	3.1
3	J	106	LEU	3.1
2	B	113	TYR	3.1
2	G	48	GLY	3.1
2	H	212	GLY	3.1
2	H	131	LEU	3.0
2	B	99	THR	3.0

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Mol	Chain	Res	Type	RSRZ
3	E	82	GLU	3.0
2	G	236	ALA	3.0
3	J	101	ASN	3.0
2	H	113	TYR	3.0
2	C	111	VAL	2.9
3	J	20	ALA	2.9
3	J	74	PRO	2.9
3	J	67	LEU	2.9
2	H	165	THR	2.9
2	H	57	LEU	2.9
1	A	78	GLN	2.9
1	F	74	PHE	2.9
2	I	296	GLN	2.9
2	H	134	HIS	2.8
2	B	35	GLY	2.8
2	G	107	LEU	2.8
2	H	83	GLU	2.8
2	I	302	LEU	2.8
2	C	86	ARG	2.8
2	H	172	GLN	2.8
2	G	197	ALA	2.8
2	H	117	ARG	2.8
2	G	233	SER	2.8
1	A	62	ASN	2.8
2	H	302	LEU	2.8
2	G	328	TYR	2.7
2	H	33	SER	2.7
2	H	84	GLN	2.7
2	G	326	GLN	2.7
2	D	102	GLU	2.7
2	G	109	ASP	2.7
3	J	84	GLY	2.7
2	G	227	SER	2.7
1	F	73	LEU	2.6
1	F	89	PRO	2.6
1	F	71	MET	2.6
1	A	49	GLU	2.6
2	H	14	THR	2.6
1	A	239	GLU	2.6
1	F	126	TRP	2.6
2	B	80	ARG	2.6
2	G	243	THR	2.6

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Mol	Chain	Res	Type	RSRZ
3	E	31	ALA	2.6
2	G	32	LEU	2.6
2	G	242	GLY	2.6
2	H	88	VAL	2.5
2	I	192	ASN	2.5
3	J	99	LYS	2.5
2	H	140	LEU	2.5
2	G	228	GLY	2.5
2	G	169	ARG	2.5
3	J	323	LEU	2.5
2	G	11	ARG	2.5
2	B	104	THR	2.5
2	I	30	ASN	2.5
2	H	178	LEU	2.5
2	I	297	LEU	2.5
2	C	114	ALA	2.5
2	G	93	ILE	2.5
2	G	58	LEU	2.5
2	G	175	LEU	2.4
2	H	166	ILE	2.4
2	G	82	ILE	2.4
2	I	365	LEU	2.4
2	H	23	HIS	2.4
2	H	114	ALA	2.4
2	C	148	GLU	2.4
2	I	92	GLU	2.4
1	F	108	LEU	2.4
2	I	232	VAL	2.4
3	J	24	HIS	2.4
3	E	108	GLY	2.4
2	H	28	LEU	2.4
2	G	238	SER	2.4
1	A	185	LEU	2.4
2	G	226	ALA	2.4
3	E	103	HIS	2.4
2	G	262	GLU	2.4
2	I	310	GLU	2.4
2	G	97	SER	2.4
2	H	72	PRO	2.3
2	H	150	VAL	2.3
2	I	364	PRO	2.3
2	C	85	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	149	HIS	2.3
2	H	10	TRP	2.3
2	G	46	THR	2.3
2	B	198	HIS	2.3
2	I	113	TYR	2.3
2	G	178	LEU	2.3
2	H	136	PHE	2.2
2	B	197	ALA	2.2
2	I	112	GLN	2.2
2	G	14	THR	2.2
2	H	256	MET	2.2
1	A	166	ALA	2.2
2	G	92	GLU	2.2
2	I	359	PHE	2.2
2	G	19	VAL	2.2
2	H	50	GLY	2.2
1	F	175	GLU	2.2
2	H	58	LEU	2.2
2	G	68	ILE	2.2
2	G	230	GLY	2.2
3	J	260	HIS	2.2
2	G	91	ILE	2.2
1	A	338	ASP	2.2
2	G	118	GLY	2.2
2	C	104	THR	2.2
2	I	114	ALA	2.2
3	J	76	TYR	2.1
2	H	152	PHE	2.1
2	D	364	PRO	2.1
1	F	55	ILE	2.1
2	I	316	LEU	2.1
2	C	74	GLY	2.1
2	B	123	TYR	2.1
2	G	36	ARG	2.1
2	G	211	GLU	2.1
3	J	63	ARG	2.1
2	G	206	LEU	2.1
2	I	101	VAL	2.1
2	I	60	LYS	2.1
2	I	134	HIS	2.1
3	J	334	LEU	2.1
1	A	174	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
3	J	46	ARG	2.1
2	I	279	GLU	2.0
2	I	105	ARG	2.0
2	B	248	GLN	2.0
2	G	34	LEU	2.0
2	I	6	LEU	2.0
2	I	10	TRP	2.0
1	F	62	ASN	2.0
1	A	56	ASP	2.0
2	G	156	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	ADP	B	802	27/27	0.84	0.31	-0.70	68,68,68,68	0
5	ZN	H	405	1/1	0.54	0.47	-0.70	395,395,395,395	0
6	ADP	D	801	27/27	0.89	0.29	-0.78	27,27,27,27	0
6	ADP	I	803	27/27	0.83	0.24	-1.03	203,203,203,203	0
5	ZN	B	403	1/1	0.93	0.06	-1.17	138,138,138,138	0
5	ZN	I	406	1/1	0.79	0.06	-1.18	119,119,119,119	0
5	ZN	E	404	1/1	0.91	0.04	-1.56	124,124,124,124	0
5	ZN	D	402	1/1	0.96	0.10	-1.57	43,43,43,43	0
5	ZN	J	408	1/1	0.78	0.08	-1.66	228,228,228,228	0
5	ZN	C	401	1/1	0.90	0.05	-1.69	147,147,147,147	0
5	ZN	G	407	1/1	0.50	0.04	-1.73	350,350,350,350	0
4	PO4	C	1300	5/5	0.91	0.16	-2.11	58,58,58,58	0

6.5 Other polymers

There are no such residues in this entry.