



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:58 PM UTC

PDB ID : 1XXH / pdb_00001xxh
Title : ATPgS 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 : 3.45 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

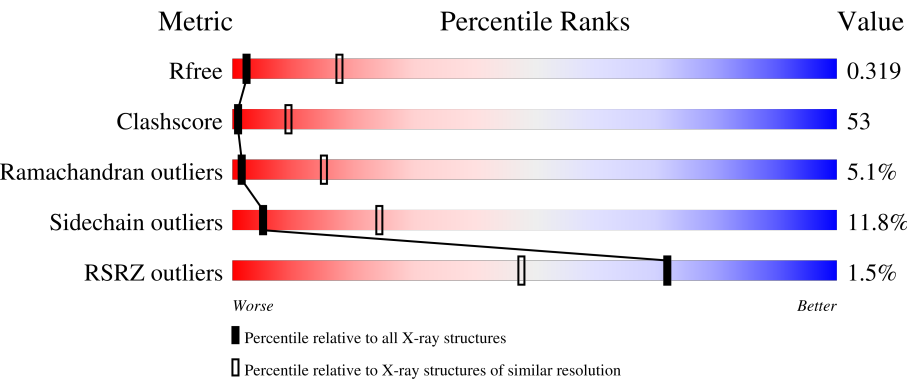
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.45 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}	180053	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	2% 24% 51% 19% ..
1	F	343	% 31% 53% 13% ..
2	B	373	2% 34% 47% 16% ..
2	C	373	% 26% 52% 19% ..
2	D	373	2% 25% 53% 17% ..

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Mol	Chain	Length	Quality of chain
2	G	373	
2	H	373	
2	I	373	
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
5	AGS	I	803	-	-	X	-
6	PO4	C	1300	-	-	X	-
6	PO4	H	1400	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 27736 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	Se	0	0	0
			2687	1702	488	487	5	5			
1	F	338	Total	C	N	O	S	Se	0	0	0
			2687	1702	488	487	5	5			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P28630
A	71	MSE	MET	modified residue	UNP P28630
A	223	MSE	MET	modified residue	UNP P28630
A	285	MSE	MET	modified residue	UNP P28630
A	286	MSE	MET	modified residue	UNP P28630
F	1	MSE	MET	modified residue	UNP P28630
F	71	MSE	MET	modified residue	UNP P28630
F	223	MSE	MET	modified residue	UNP P28630
F	285	MSE	MET	modified residue	UNP P28630
F	286	MSE	MET	modified residue	UNP P28630

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	Se	0	0	0
			2602	1655	468	466	7	6			
3	J	334	Total	C	N	O	S	Se	0	0	0
			2602	1655	468	466	7	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	MSE	MET	modified residue	UNP P28631
E	35	MSE	MET	modified residue	UNP P28631
E	68	MSE	MET	modified residue	UNP P28631
E	182	MSE	MET	modified residue	UNP P28631
E	253	MSE	MET	modified residue	UNP P28631
E	301	MSE	MET	modified residue	UNP P28631
J	1	MSE	MET	modified residue	UNP P28631
J	35	MSE	MET	modified residue	UNP P28631
J	68	MSE	MET	modified residue	UNP P28631
J	182	MSE	MET	modified residue	UNP P28631
J	253	MSE	MET	modified residue	UNP P28631
J	301	MSE	MET	modified residue	UNP P28631

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

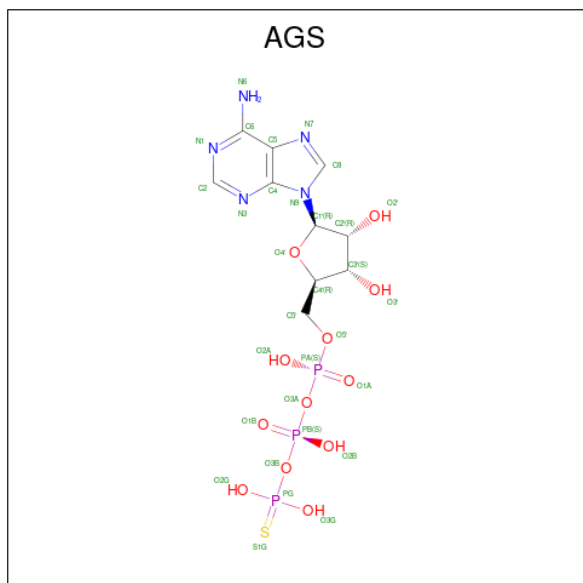
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		
4	E	1	Total	Zn	0	0
			1	1		
4	G	1	Total	Zn	0	0
			1	1		
4	H	1	Total	Zn	0	0
			1	1		

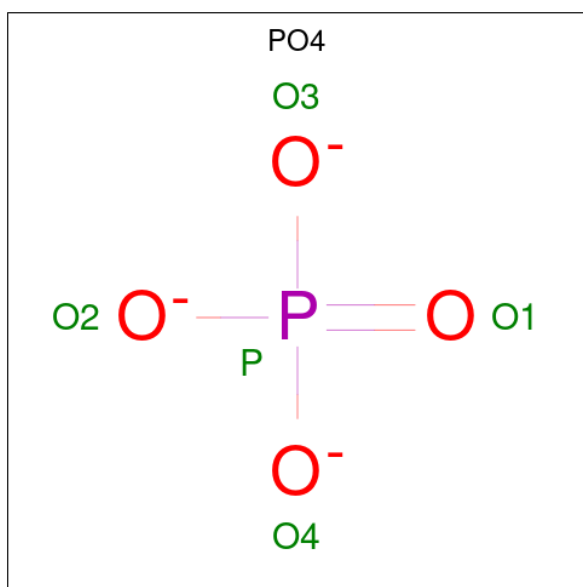
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	1	Total	Zn	0	0
			1	1		
4	J	1	Total	Zn	0	0
			1	1		

- Molecule 5 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



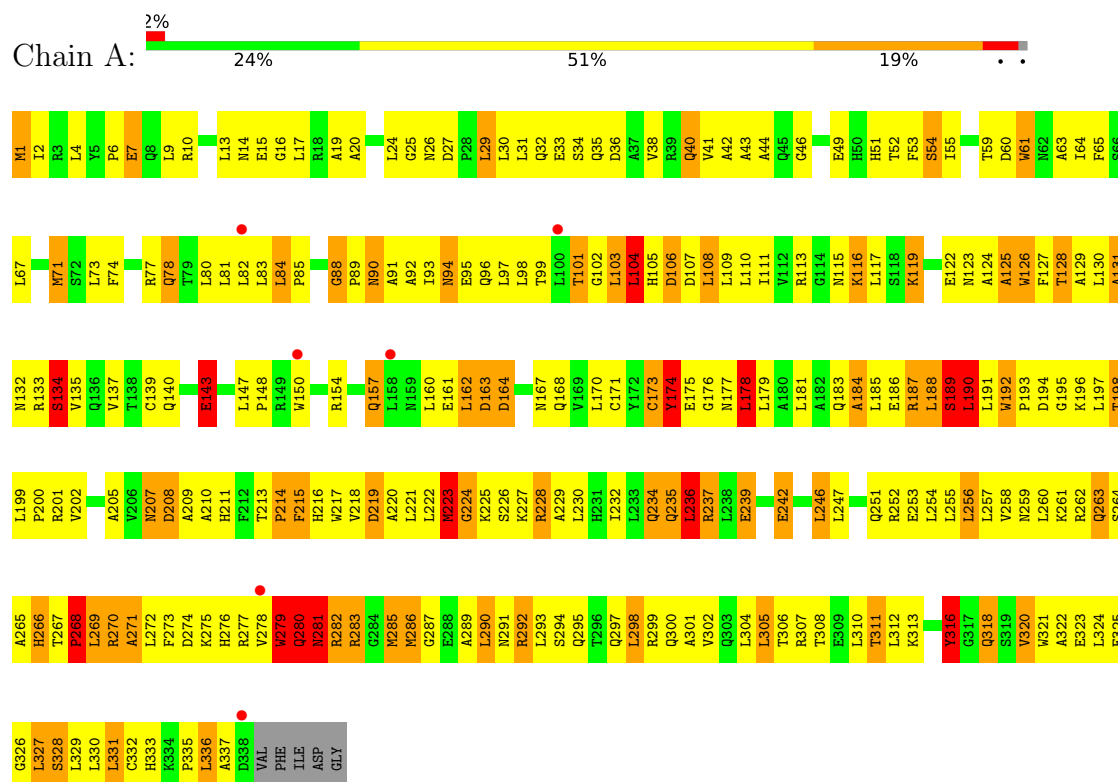


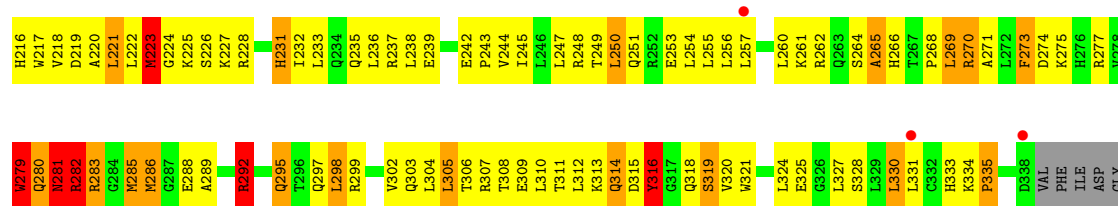
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	P	0	0
			5	4	1		
6	H	1	Total	O	P	0	0
			5	4	1		

3 Residue-property plots

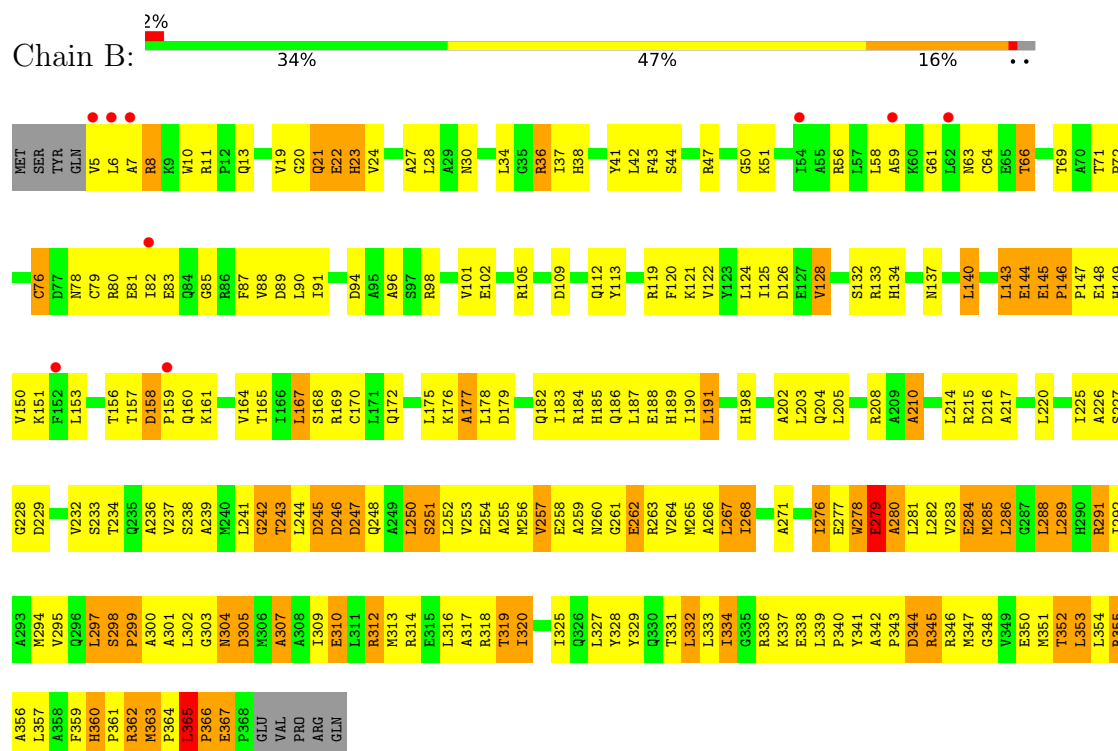
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

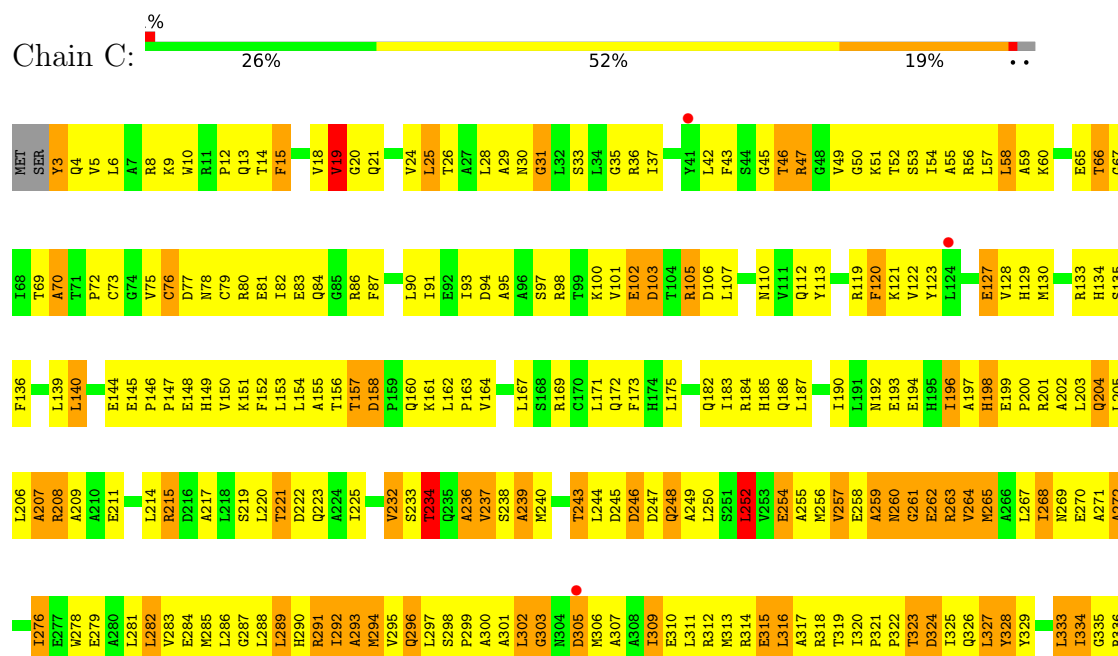




• Molecule 2: DNA polymerase III subunit gamma

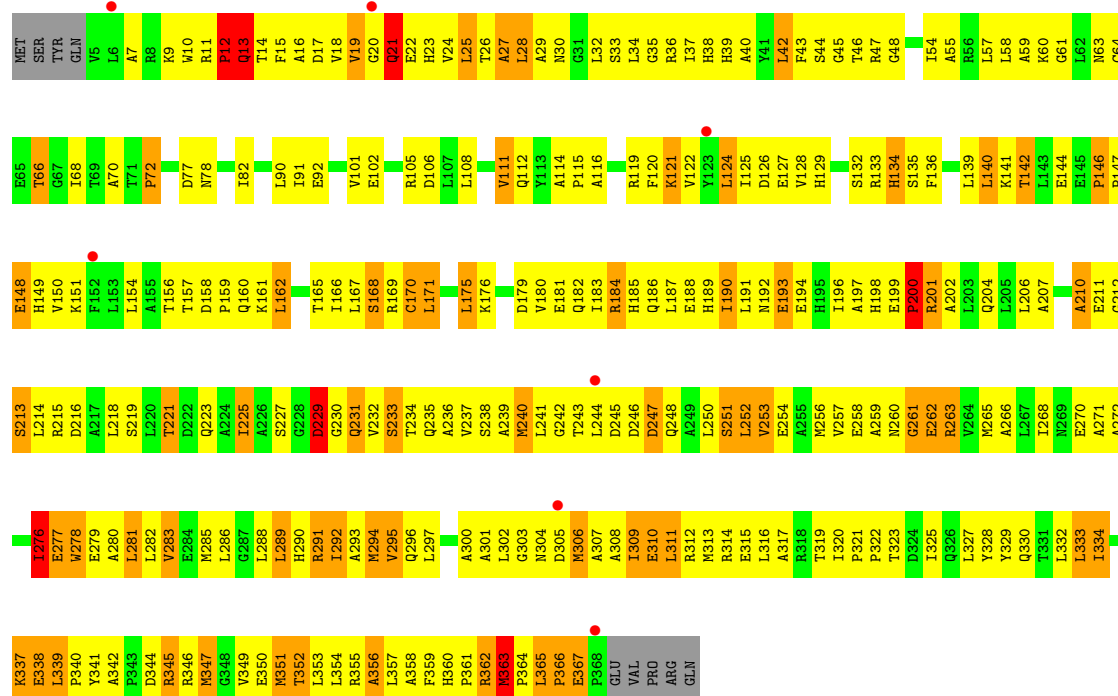


• Molecule 2: DNA polymerase III subunit gamma

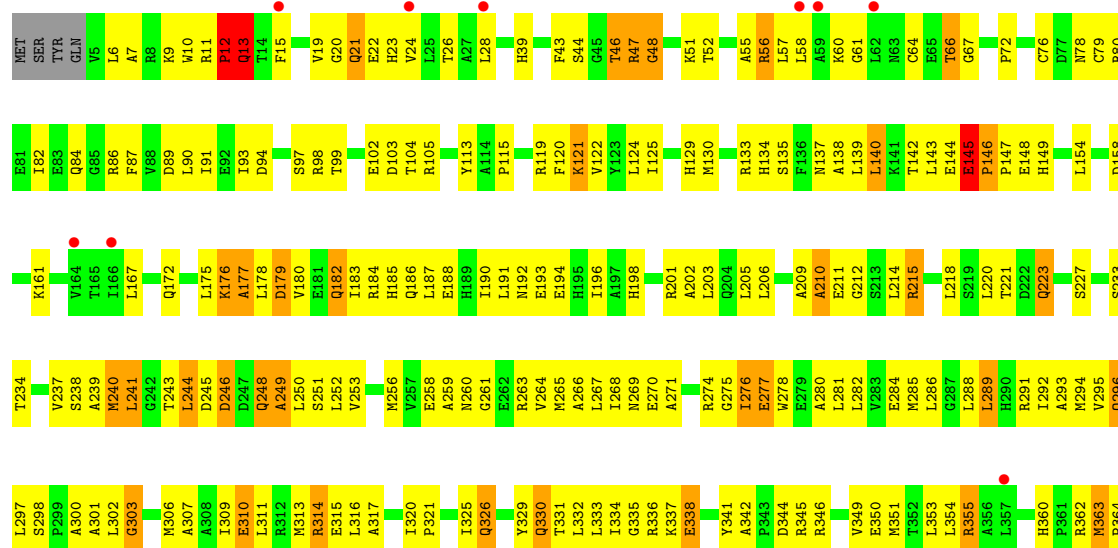




• Molecule 2: DNA polymerase III subunit gamma

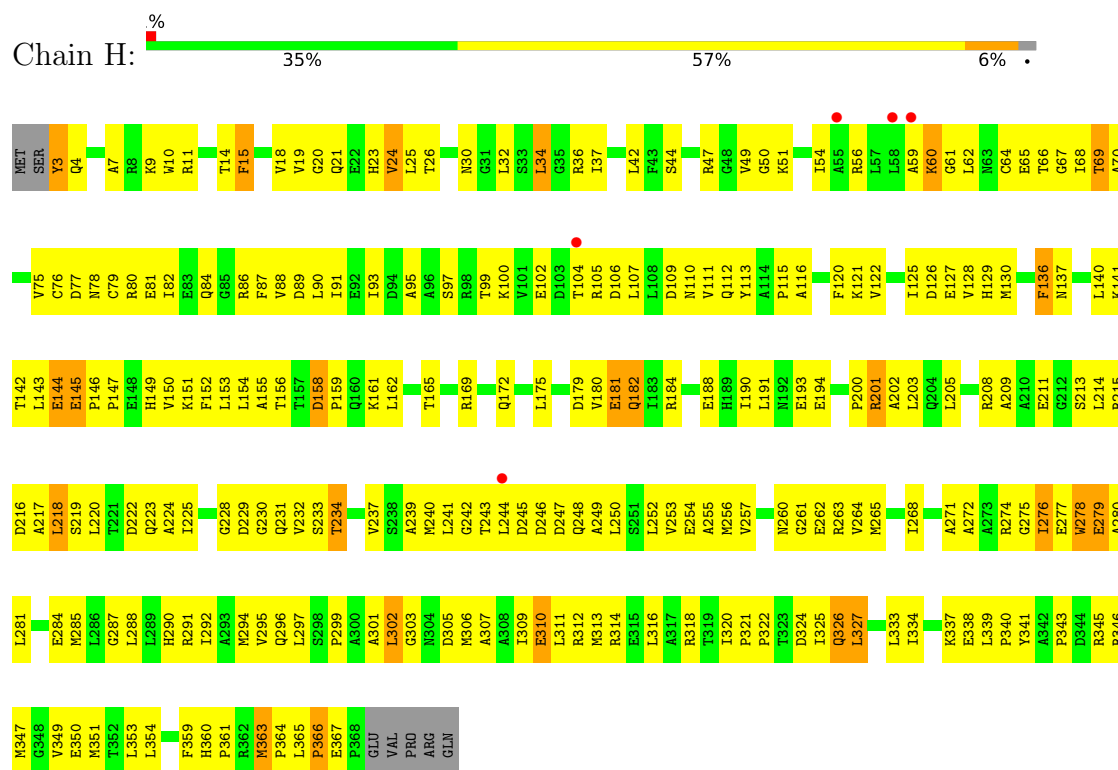


• Molecule 2: DNA polymerase III subunit gamma

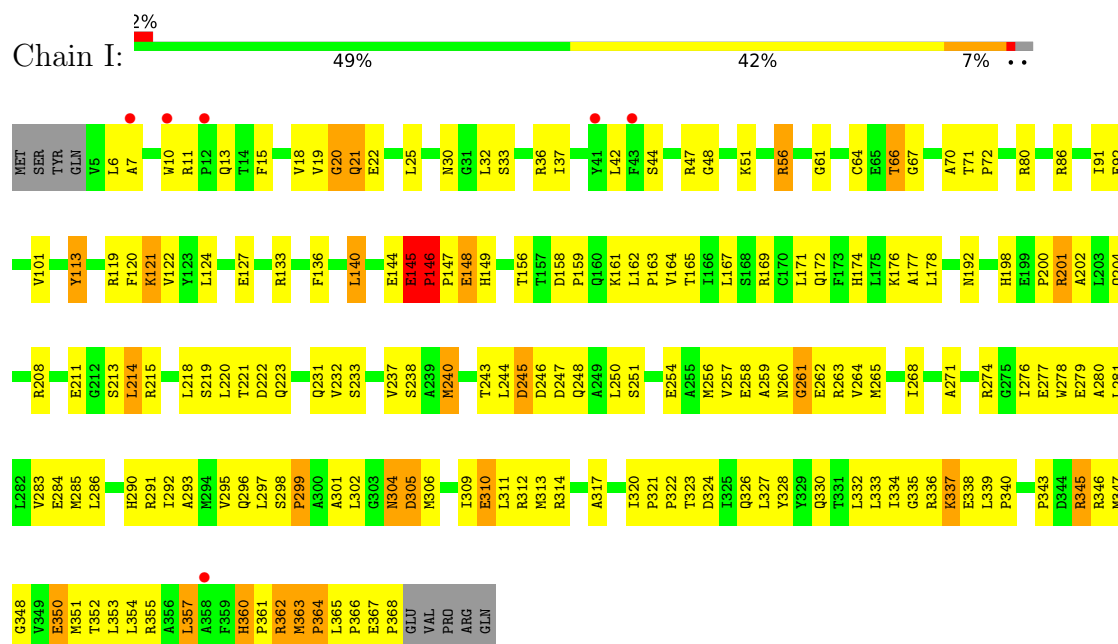


L365
P366
E367
GLU
VAL
PRO
ARG
GLN

• Molecule 2: DNA polymerase III subunit gamma

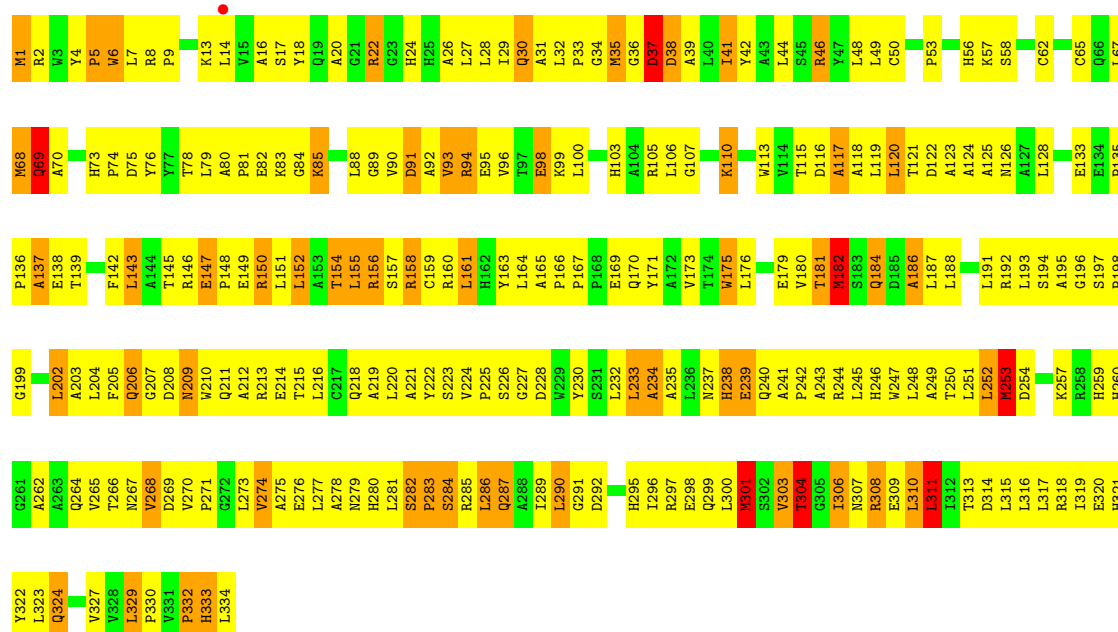


• Molecule 2: DNA polymerase III subunit gamma

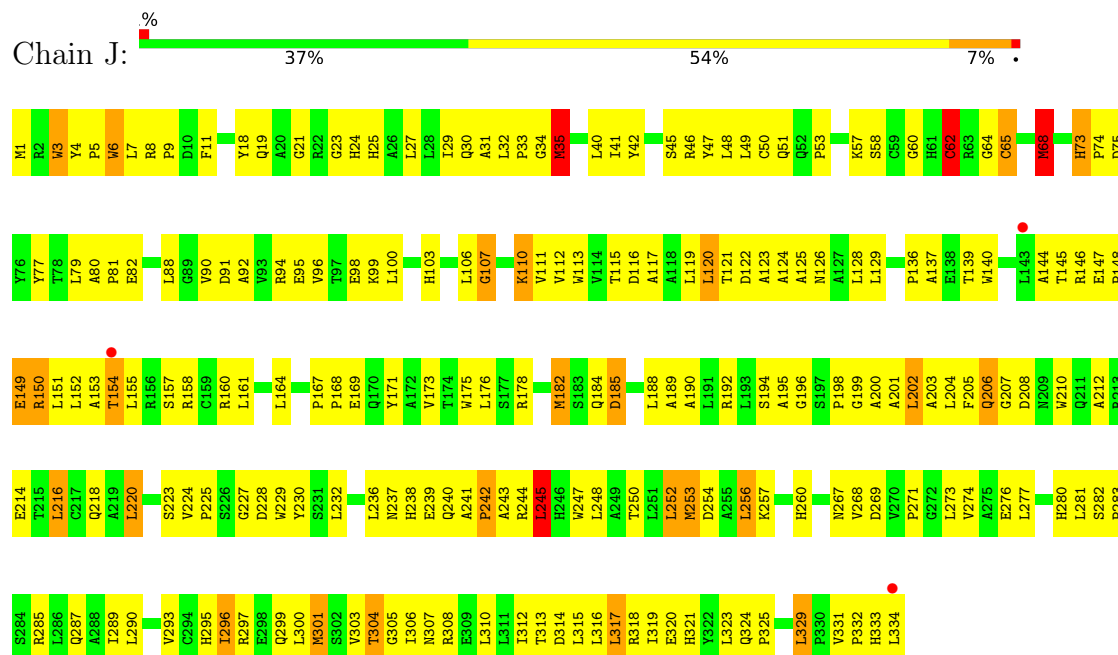


• Molecule 3: DNA polymerase III, delta prime subunit





● 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	98.45Å 106.46Å 535.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 3.45 100.00 – 3.45	Depositor EDS
% Data completeness (in resolution range)	(Not available) (100.00-3.45) 97.7 (100.00-3.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 3.49Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.315 , 0.350 0.280 , 0.319	Depositor DCC
R_{free} test set	7449 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å ²)	106.7	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 138.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27736	wwPDB-VP
Average B, all atoms (Å ²)	158.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, AGS

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	0.84	9/2731 (0.3%)	1.30	45/3704 (1.2%)
1	F	0.88	14/2731 (0.5%)	1.14	34/3704 (0.9%)
2	B	0.74	3/2876 (0.1%)	1.26	35/3900 (0.9%)
2	C	0.86	2/2898 (0.1%)	1.32	39/3930 (1.0%)
2	D	0.89	7/2876 (0.2%)	1.37	43/3900 (1.1%)
2	G	0.54	4/2876 (0.1%)	1.10	21/3900 (0.5%)
2	H	0.39	0/2898	0.97	10/3930 (0.3%)
2	I	0.46	0/2876	1.02	16/3900 (0.4%)
3	E	0.74	11/2662 (0.4%)	1.16	23/3624 (0.6%)
3	J	0.50	8/2662 (0.3%)	0.92	4/3624 (0.1%)
All	All	0.71	58/28086 (0.2%)	1.17	270/38116 (0.7%)

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	285	MSE	SE-CE	32.17	2.92	1.95
1	A	286	MSE	C-N	17.70	1.54	1.33
1	A	285	MSE	SE-CE	11.12	2.28	1.95
2	B	285	MET	SD-CE	10.65	2.06	1.79
1	F	285	MSE	CG-SE	9.22	2.23	1.95
1	A	286	MSE	CG-SE	-9.16	1.68	1.95
1	A	286	MSE	SE-CE	-9.12	1.68	1.95
3	E	253	MSE	SE-CE	-8.23	1.70	1.95
3	E	68	MSE	SE-CE	-8.23	1.70	1.95
3	E	1	MSE	SE-CE	-7.49	1.73	1.95
3	E	253	MSE	CG-SE	-7.22	1.73	1.95
1	F	78	GLN	CA-C	7.14	1.61	1.53
2	D	294	MET	SD-CE	-6.90	1.62	1.79
1	F	77	ARG	C-N	6.82	1.39	1.33
3	J	253	MSE	SE-CE	-6.65	1.75	1.95
2	D	262	GLU	C-N	6.52	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	1	MSE	SE-CE	-6.51	1.75	1.95
2	D	304	ASN	CA-C	-6.51	1.46	1.52
1	A	223	MSE	SE-CE	-6.50	1.75	1.95
1	F	78	GLN	C-N	6.39	1.42	1.33
3	E	301	MSE	SE-CE	-6.38	1.76	1.95
1	F	285	MSE	N-CA	-6.38	1.38	1.46
2	G	245	ASP	N-CA	-6.34	1.38	1.46
2	G	55	ALA	C-O	6.27	1.31	1.24
3	E	182	MSE	SE-CE	-6.16	1.76	1.95
2	D	351	MET	SD-CE	6.07	1.94	1.79
3	E	35	MSE	CG-SE	-6.04	1.77	1.95
2	C	351	MET	SD-CE	-6.00	1.64	1.79
3	J	35	MSE	SE-CE	-5.98	1.77	1.95
1	F	79	THR	N-CA	5.93	1.53	1.46
2	C	265	MET	SD-CE	-5.88	1.64	1.79
1	F	286	MSE	SE-CE	-5.82	1.77	1.95
1	A	1	MSE	CG-SE	-5.64	1.78	1.95
3	J	1	MSE	SE-CE	-5.56	1.78	1.95
2	B	312	ARG	CA-C	-5.50	1.45	1.52
1	A	280	GLN	N-CA	5.49	1.53	1.46
3	E	35	MSE	SE-CE	-5.45	1.79	1.95
3	J	182	MSE	SE-CE	-5.36	1.79	1.95
1	A	71	MSE	SE-CE	-5.34	1.79	1.95
3	J	301	MSE	CG-SE	-5.33	1.79	1.95
3	E	182	MSE	CG-SE	-5.33	1.79	1.95
1	F	1	MSE	CG-SE	-5.32	1.79	1.95
1	F	223	MSE	CG-SE	-5.32	1.79	1.95
1	F	286	MSE	CG-SE	-5.32	1.79	1.95
3	J	253	MSE	CG-SE	-5.30	1.79	1.95
3	J	68	MSE	SE-CE	-5.27	1.79	1.95
1	F	71	MSE	SE-CE	-5.24	1.79	1.95
3	E	274	VAL	CA-CB	5.22	1.61	1.54
3	E	301	MSE	CG-SE	-5.21	1.79	1.95
1	A	283	ARG	CA-C	-5.21	1.46	1.53
2	D	20	GLY	CA-C	5.20	1.56	1.51
2	D	48	GLY	CA-C	5.18	1.56	1.51
2	D	47	ARG	C-O	-5.16	1.17	1.23
2	G	244	LEU	C-N	-5.15	1.26	1.33
2	B	312	ARG	C-N	-5.11	1.27	1.33
1	F	223	MSE	SE-CE	-5.09	1.80	1.95
2	G	47	ARG	C-O	-5.06	1.17	1.23
3	J	301	MSE	SE-CE	-5.02	1.80	1.95

All (270) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	285	MSE	CG-SE-CE	-15.69	64.40	98.92
1	A	268	PRO	CA-N-CD	-13.97	92.44	112.00
2	C	365	LEU	CA-C-N	13.09	134.12	119.99
2	C	365	LEU	C-N-CA	13.09	134.12	119.99
3	E	329	LEU	N-CA-C	11.78	124.92	110.07
2	H	75	VAL	N-CA-C	11.07	121.33	111.81
1	A	280	GLN	OE1-CD-NE2	-10.80	111.80	122.60
1	F	78	GLN	OE1-CD-NE2	-10.79	111.81	122.60
2	G	13	GLN	OE1-CD-NE2	-10.52	112.08	122.60
2	D	307	ALA	N-CA-C	-10.44	100.57	113.20
2	G	248	GLN	OE1-CD-NE2	-10.43	112.17	122.60
2	D	13	GLN	OE1-CD-NE2	-10.08	112.52	122.60
2	D	21	GLN	OE1-CD-NE2	-10.00	112.60	122.60
1	A	157	GLN	OE1-CD-NE2	-9.97	112.63	122.60
1	A	239	GLU	N-CA-C	-9.82	97.70	112.54
1	F	69	GLN	OE1-CD-NE2	-9.81	112.79	122.60
2	G	21	GLN	OE1-CD-NE2	-9.78	112.82	122.60
1	A	263	GLN	OE1-CD-NE2	-9.63	112.97	122.60
1	A	337	ALA	N-CA-C	9.61	125.42	111.87
2	D	347	MET	N-CA-C	-9.60	99.71	111.33
2	D	365	LEU	CA-C-N	9.55	131.78	119.84
2	D	365	LEU	C-N-CA	9.55	131.78	119.84
2	B	21	GLN	OE1-CD-NE2	-9.52	113.08	122.60
2	I	231	GLN	OE1-CD-NE2	-9.50	113.10	122.60
2	H	70	ALA	N-CA-C	-9.49	101.71	113.38
1	F	61	TRP	N-CA-C	-9.39	101.09	112.54
2	I	21	GLN	OE1-CD-NE2	-9.31	113.29	122.60
1	A	78	GLN	OE1-CD-NE2	-9.09	113.51	122.60
2	C	70	ALA	N-CA-C	-9.05	102.25	113.38
1	F	280	GLN	OE1-CD-NE2	-8.97	113.63	122.60
3	E	329	LEU	CA-C-N	8.72	129.26	119.93
3	E	329	LEU	C-N-CA	8.72	129.26	119.93
2	D	12	PRO	CA-N-CD	-8.53	100.06	112.00
2	B	280	ALA	N-CA-C	-8.52	101.96	111.07
2	D	170	CYS	N-CA-C	8.43	122.99	110.52
2	C	360	HIS	CA-C-N	-8.31	111.46	120.94
2	C	360	HIS	C-N-CA	-8.31	111.46	120.94
1	A	286	MSE	O-C-N	8.24	130.86	122.12
2	C	342	ALA	N-CA-C	-8.19	99.34	109.65
2	G	246	ASP	CA-CB-CG	-8.13	104.47	112.60
2	C	75	VAL	N-CA-C	8.09	118.77	111.81
3	E	333	HIS	N-CA-C	8.06	127.97	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	12	PRO	CA-N-CD	-8.00	100.81	112.00
1	F	280	GLN	CA-C-N	7.99	136.81	121.54
1	F	280	GLN	C-N-CA	7.99	136.81	121.54
2	D	225	ILE	N-CA-C	-7.85	103.15	110.53
1	F	283	ARG	CA-C-O	7.83	129.06	120.92
3	E	69	GLN	N-CA-C	-7.81	102.08	111.69
2	I	146	PRO	N-CA-C	7.65	120.03	110.70
2	H	24	VAL	N-CA-C	-7.57	103.92	113.22
1	A	235	GLN	N-CA-C	-7.51	103.03	111.14
3	E	186	ALA	N-CA-C	-7.50	104.13	113.28
1	A	29	LEU	N-CA-C	7.44	119.47	111.36
2	B	365	LEU	CA-C-N	7.43	129.13	119.84
2	B	365	LEU	C-N-CA	7.43	129.13	119.84
2	B	298	SER	CA-C-N	7.38	129.06	119.84
2	B	298	SER	C-N-CA	7.38	129.06	119.84
2	B	363	MET	N-CA-C	7.34	126.04	109.81
1	A	283	ARG	CA-C-O	7.32	128.74	120.84
3	E	286	LEU	N-CA-C	-7.29	95.27	110.80
2	I	145	GLU	CA-C-N	7.28	127.88	120.38
2	I	145	GLU	C-N-CA	7.28	127.88	120.38
2	D	20	GLY	N-CA-C	7.22	124.03	113.48
3	E	235	ALA	N-CA-C	7.22	120.19	111.82
2	C	305	ASP	N-CA-C	-7.20	104.11	114.12
1	A	189	SER	N-CA-C	-7.19	102.48	111.11
1	F	314	GLN	N-CA-C	-7.19	104.13	113.12
2	C	319	THR	N-CA-C	7.14	122.28	113.50
2	H	182	GLN	N-CA-C	-7.11	102.56	112.45
2	C	15	PHE	N-CA-C	-7.07	103.63	112.90
3	J	208	ASP	N-CA-C	-7.05	103.03	113.61
2	B	320	ILE	CA-C-N	7.03	127.62	120.38
2	B	320	ILE	C-N-CA	7.03	127.62	120.38
2	B	360	HIS	CA-C-N	7.03	128.62	119.84
2	B	360	HIS	C-N-CA	7.03	128.62	119.84
1	A	43	ALA	N-CA-C	-6.96	103.71	111.71
3	E	211	GLN	N-CA-C	-6.89	103.87	112.90
2	I	21	GLN	CG-CD-NE2	6.86	126.68	116.40
2	D	162	LEU	CA-C-N	6.84	128.64	120.23
2	D	162	LEU	C-N-CA	6.84	128.64	120.23
1	F	78	GLN	CG-CD-NE2	6.84	126.66	116.40
1	F	283	ARG	O-C-N	6.82	131.34	122.68
2	D	229	ASP	N-CA-C	-6.81	101.74	110.53
2	C	60	LYS	N-CA-C	-6.81	105.13	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	342	ALA	CA-C-N	6.78	128.31	119.84
2	C	342	ALA	C-N-CA	6.78	128.31	119.84
2	C	249	ALA	N-CA-C	-6.75	103.61	110.97
2	I	171	LEU	N-CA-C	-6.74	96.67	108.20
2	C	354	LEU	N-CA-C	-6.73	103.64	110.97
3	E	264	GLN	N-CA-C	6.72	119.37	108.41
2	D	216	ASP	N-CA-C	-6.72	103.76	112.23
2	G	21	GLN	CG-CD-NE2	6.72	126.48	116.40
2	G	248	GLN	CG-CD-NE2	6.71	126.47	116.40
1	F	173	CYS	N-CA-C	-6.70	99.30	109.95
1	A	280	GLN	CB-CG-CD	-6.69	101.23	112.60
2	D	116	ALA	N-CA-C	6.67	119.56	111.82
2	H	102	GLU	N-CA-C	6.67	118.34	111.14
1	A	214	PRO	N-CA-C	-6.61	105.45	113.98
2	G	47	ARG	N-CA-C	6.60	120.63	110.20
3	J	245	LEU	N-CA-C	-6.58	104.03	111.07
2	G	13	GLN	CG-CD-NE2	6.56	126.25	116.40
1	F	69	GLN	CG-CD-NE2	6.53	126.20	116.40
2	C	338	GLU	N-CA-C	6.50	119.36	111.82
1	F	58	ASN	N-CA-C	-6.46	103.90	113.72
1	A	280	GLN	CG-CD-NE2	6.45	126.08	116.40
2	C	328	TYR	N-CA-C	-6.45	104.17	111.07
2	D	292	ILE	CB-CA-C	-6.45	103.55	111.87
2	D	70	ALA	N-CA-C	-6.44	105.17	113.16
1	F	195	GLY	N-CA-C	-6.42	107.05	114.69
2	B	21	GLN	CG-CD-NE2	6.39	125.98	116.40
1	A	173	CYS	N-CA-C	-6.38	100.52	110.42
2	H	60	LYS	N-CA-C	-6.35	105.36	113.23
2	C	282	LEU	N-CA-C	-6.33	104.27	112.68
1	A	78	GLN	CG-CD-NE2	6.32	125.89	116.40
2	B	362	ARG	N-CA-C	-6.32	100.84	109.95
3	E	35	MSE	N-CA-C	-6.32	105.50	113.72
2	D	13	GLN	CG-CD-NE2	6.29	125.84	116.40
2	B	210	ALA	N-CA-C	-6.28	100.74	110.10
1	F	75	ALA	N-CA-C	6.27	120.67	112.89
1	F	273	PHE	CA-C-N	6.27	128.59	120.44
1	F	273	PHE	C-N-CA	6.27	128.59	120.44
2	I	231	GLN	CG-CD-NE2	6.24	125.75	116.40
2	I	245	ASP	N-CA-C	-6.20	106.13	113.38
2	I	47	ARG	N-CA-C	6.18	119.23	109.96
2	B	125	ILE	N-CA-C	6.18	116.28	106.88
2	D	58	LEU	N-CA-C	-6.17	103.28	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	339	LEU	CA-C-N	-6.17	113.87	120.47
2	D	339	LEU	C-N-CA	-6.17	113.87	120.47
1	A	157	GLN	CG-CD-NE2	6.16	125.64	116.40
2	D	303	GLY	N-CA-C	6.15	127.77	113.18
1	A	285	MSE	CG-SE-CE	-6.13	85.43	98.92
2	C	272	ALA	N-CA-C	-6.12	104.91	112.38
2	C	252	LEU	N-CA-C	-6.12	103.33	111.96
1	F	280	GLN	CG-CD-NE2	6.11	125.57	116.40
1	A	263	GLN	CG-CD-NE2	6.11	125.56	116.40
2	D	171	LEU	N-CA-C	-6.08	99.29	108.96
1	A	192	TRP	N-CA-C	6.05	119.60	108.94
2	C	58	LEU	N-CA-C	-6.04	104.64	112.68
2	C	25	LEU	N-CA-C	-6.04	105.57	113.12
2	D	221	THR	N-CA-C	-6.04	104.77	111.36
1	A	283	ARG	O-C-N	6.03	130.28	122.87
2	G	276	ILE	N-CA-C	6.00	116.51	108.11
2	B	353	LEU	N-CA-C	-5.96	104.71	111.14
1	F	158	LEU	N-CA-C	-5.91	104.46	112.26
1	F	231	HIS	N-CA-C	-5.89	104.21	111.40
1	A	283	ARG	CA-C-N	5.88	132.94	121.41
1	A	283	ARG	C-N-CA	5.88	132.94	121.41
2	G	48	GLY	O-C-N	5.88	127.28	122.51
2	B	307	ALA	N-CA-C	5.86	118.17	111.02
2	H	19	VAL	N-CA-C	5.85	117.43	108.71
1	A	134	SER	N-CA-C	5.83	123.22	110.80
2	D	68	ILE	N-CA-C	-5.83	100.30	108.12
3	E	135	PRO	CA-C-N	5.83	127.13	119.84
3	E	135	PRO	C-N-CA	5.83	127.13	119.84
2	G	158	ASP	CA-C-N	5.83	125.70	119.28
2	G	158	ASP	C-N-CA	5.83	125.70	119.28
2	C	157	THR	N-CA-C	-5.80	105.96	113.16
1	A	126	TRP	N-CA-C	5.80	117.29	110.97
1	A	61	TRP	N-CA-C	5.79	119.45	112.38
2	B	288	LEU	N-CA-C	-5.79	103.78	111.24
2	C	66	THR	N-CA-C	-5.78	106.31	113.19
2	B	228	GLY	N-CA-C	-5.78	107.75	115.32
2	D	21	GLN	CG-CD-NE2	5.78	125.07	116.40
2	I	122	VAL	N-CA-C	5.75	116.22	108.17
2	D	262	GLU	O-C-N	5.74	130.23	122.59
1	F	283	ARG	CA-C-N	5.73	132.64	121.41
1	F	283	ARG	C-N-CA	5.73	132.64	121.41
3	E	227	GLY	N-CA-C	-5.72	107.48	114.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	113	TYR	N-CA-C	5.70	119.34	112.38
3	E	133	GLU	N-CA-C	-5.69	104.69	111.69
1	F	76	SER	N-CA-C	5.67	117.24	109.18
2	B	59	ALA	CA-C-N	5.67	128.93	120.31
2	B	59	ALA	C-N-CA	5.67	128.93	120.31
2	B	268	ILE	N-CA-C	-5.67	104.84	110.62
2	C	236	ALA	N-CA-C	-5.67	104.74	111.03
2	D	77	ASP	N-CA-C	5.63	117.42	111.28
1	F	78	GLN	N-CA-C	5.63	115.45	108.19
2	B	122	VAL	N-CA-C	5.61	116.82	109.58
2	B	345	ARG	N-CA-C	5.60	120.61	111.37
1	A	224	GLY	N-CA-C	-5.59	105.50	111.93
1	F	213	THR	N-CA-C	-5.58	103.04	110.07
2	D	356	ALA	N-CA-C	-5.57	106.44	113.18
2	H	363	MET	CA-C-N	5.56	126.79	119.84
2	H	363	MET	C-N-CA	5.56	126.79	119.84
2	C	350	GLU	N-CA-C	-5.55	104.07	111.24
2	I	21	GLN	N-CA-C	-5.55	103.77	110.88
2	D	253	VAL	CB-CA-C	-5.54	104.88	111.81
2	G	365	LEU	N-CA-C	5.54	115.97	109.60
2	B	297	LEU	N-CA-C	-5.53	105.65	112.72
1	A	280	GLN	CB-CA-C	-5.52	99.57	109.24
2	B	69	THR	N-CA-C	5.51	117.56	109.24
2	D	121	LYS	N-CA-C	-5.50	99.55	108.41
1	A	174	TYR	N-CA-C	-5.50	104.64	111.90
3	E	208	ASP	N-CA-C	-5.49	106.56	113.20
1	F	53	PHE	N-CA-C	5.48	118.01	109.52
2	D	240	MET	N-CA-C	-5.48	105.40	112.68
2	D	342	ALA	CA-C-N	5.47	125.56	119.32
2	D	342	ALA	C-N-CA	5.47	125.56	119.32
2	H	136	PHE	N-CA-C	-5.47	105.22	111.07
3	J	73	HIS	CA-C-N	5.47	125.08	119.56
3	J	73	HIS	C-N-CA	5.47	125.08	119.56
2	D	19	VAL	CA-C-N	5.46	128.36	120.11
2	D	19	VAL	C-N-CA	5.46	128.36	120.11
2	I	350	GLU	N-CA-C	-5.46	105.44	111.71
1	A	242	GLU	N-CA-C	-5.45	102.76	110.29
1	A	237	ARG	N-CA-C	-5.45	106.68	113.55
2	D	47	ARG	N-CA-C	5.45	118.35	110.28
2	D	158	ASP	CA-C-N	5.44	124.96	119.19
2	D	158	ASP	C-N-CA	5.44	124.96	119.19
2	C	164	VAL	N-CA-C	-5.44	106.18	112.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	123	ASN	N-CA-C	-5.44	106.78	113.41
1	F	281	ASN	N-CA-CB	5.43	119.66	110.49
2	G	145	GLU	CA-C-N	5.41	125.95	120.38
2	G	145	GLU	C-N-CA	5.41	125.95	120.38
1	F	239	GLU	N-CA-C	-5.41	106.05	113.30
2	C	158	ASP	CA-C-N	5.39	125.48	119.87
2	C	158	ASP	C-N-CA	5.39	125.48	119.87
2	G	122	VAL	N-CA-C	5.38	116.53	109.21
2	C	19	VAL	N-CA-C	5.36	116.20	108.48
2	C	122	VAL	N-CA-C	5.36	116.30	108.58
2	B	85	GLY	N-CA-C	-5.36	107.92	115.32
2	D	352	THR	N-CA-C	5.35	118.28	111.69
2	D	366	PRO	N-CA-C	5.33	123.44	112.47
2	B	144	GLU	N-CA-C	-5.33	105.64	111.82
1	A	71	MSE	N-CA-C	-5.32	102.60	110.48
1	A	88	GLY	CA-C-N	5.32	126.49	119.84
1	A	88	GLY	C-N-CA	5.32	126.49	119.84
1	A	190	LEU	N-CA-C	5.32	117.08	111.28
2	C	259	ALA	CA-C-N	-5.32	115.93	122.84
2	C	259	ALA	C-N-CA	-5.32	115.93	122.84
2	G	241	LEU	N-CA-C	-5.31	100.52	108.96
3	E	56	HIS	N-CA-C	-5.30	107.18	113.97
3	E	39	ALA	N-CA-C	5.28	117.95	111.82
3	E	290	LEU	N-CA-C	-5.26	104.96	111.33
2	C	257	VAL	CB-CA-C	-5.25	105.25	111.97
2	G	172	GLN	N-CA-C	5.25	118.11	109.76
1	A	94	ASN	N-CA-C	-5.25	106.38	112.89
2	C	192	ASN	N-CA-C	-5.25	105.62	112.23
1	A	281	ASN	N-CA-C	-5.24	99.64	110.80
3	E	70	ALA	N-CA-C	-5.24	105.69	111.71
2	C	194	GLU	N-CA-C	-5.22	105.58	112.94
2	B	167	LEU	N-CA-C	-5.22	106.01	112.38
2	B	157	THR	N-CA-C	-5.21	106.24	112.59
2	I	37	ILE	N-CA-C	5.21	115.46	108.17
2	B	336	ARG	N-CA-C	-5.20	105.26	111.03
2	I	177	ALA	N-CA-C	-5.19	103.29	110.35
2	G	60	LYS	N-CA-C	-5.18	106.12	112.90
2	D	291	ARG	N-CA-C	-5.17	105.13	111.75
2	C	296	GLN	N-CA-C	-5.16	106.49	112.89
2	G	103	ASP	N-CA-C	-5.15	105.75	111.36
1	A	287	GLY	N-CA-C	-5.14	106.27	112.49
1	A	7	GLU	N-CA-C	5.13	118.31	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	145	GLU	CA-C-N	5.11	125.64	120.38
2	B	145	GLU	C-N-CA	5.11	125.64	120.38
3	E	184	GLN	N-CA-C	5.11	118.98	112.34
1	F	212	PHE	N-CA-C	5.10	117.70	110.50
2	B	19	VAL	CA-C-N	5.09	131.39	121.41
2	B	19	VAL	C-N-CA	5.09	131.39	121.41
1	F	134	SER	N-CA-C	5.08	118.23	110.36
1	A	280	GLN	CA-C-N	5.07	131.23	121.54
1	A	280	GLN	C-N-CA	5.07	131.23	121.54
2	C	234	THR	N-CA-C	-5.06	105.20	111.33
2	C	309	ILE	N-CA-C	-5.06	108.34	113.20
1	F	292	ARG	N-CA-C	5.05	119.13	112.92
1	A	143	GLU	N-CA-C	5.04	116.44	110.19
3	E	41	ILE	N-CA-C	-5.04	105.94	110.82
1	F	281	ASN	CA-CB-CG	-5.04	107.56	112.60
2	D	168	SER	N-CA-C	5.02	118.18	111.75
3	E	268	VAL	N-CA-C	-5.02	105.02	112.04
1	A	281	ASN	N-CA-CB	5.00	118.95	110.49

There are no chirality outliers.

There are no planarity outliers.

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	2743	401	0
1	F	2687	0	2737	352	6
2	B	2829	0	2881	316	0
2	C	2850	0	2897	355	0
2	D	2829	0	2879	398	0
2	G	2829	0	2881	285	0
2	H	2850	0	2898	294	0
2	I	2829	0	2877	281	6
3	E	2602	0	2605	319	0
3	J	2602	0	2605	251	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
5	B	31	0	12	4	0
5	D	31	0	12	4	0
5	G	31	0	12	2	0
5	I	31	0	12	27	0
6	C	5	0	0	3	0
6	H	5	0	0	4	0
All	All	27736	0	28051	2976	6

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 53.

All (2976) 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)
1:A:71:MSE:SE	1:F:228:ARG:HA	1.53	1.56
2:H:100:LYS:NZ	2:I:133:ARG:CG	1.68	1.54
2:G:10:TRP:CZ2	2:G:193:GLU:HB3	1.47	1.48
1:A:74:PHE:CZ	1:F:206:VAL:HB	1.49	1.47
2:B:285:MET:CE	2:B:285:MET:SD	2.06	1.43
2:G:10:TRP:HZ2	2:G:193:GLU:CB	1.28	1.43
1:A:74:PHE:CD1	1:F:203:GLU:HG3	1.53	1.41
2:I:215:ARG:HD3	5:I:803:AGS:C4'	1.48	1.41
2:I:215:ARG:CD	5:I:803:AGS:H4'	1.52	1.39
2:I:6:LEU:HG	2:I:222:ASP:CG	1.42	1.38
2:I:21:GLN:HE22	2:I:176:LYS:N	1.17	1.36
1:A:73:LEU:HB2	1:F:207:ASN:OD1	1.24	1.36
2:I:21:GLN:NE2	2:I:176:LYS:H	1.18	1.35
1:F:285:MSE:SE	1:F:285:MSE:CG	2.23	1.35
2:I:215:ARG:NH1	5:I:803:AGS:H5'2	1.40	1.33
1:A:285:MSE:CE	1:A:285:MSE:SE	2.28	1.31
2:I:215:ARG:HB2	5:I:803:AGS:C4'	1.59	1.30
1:A:71:MSE:CE	1:F:231:HIS:HB2	1.61	1.29
1:F:45:GLN:OE1	1:F:77:ARG:HD3	1.18	1.26
2:G:10:TRP:CZ2	2:G:193:GLU:CB	2.12	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:LEU:HG	1:A:273:PHE:CE1	1.76	1.21
1:A:74:PHE:CD1	1:F:203:GLU:CG	2.23	1.20
1:F:273:PHE:CD1	1:F:283:ARG:HG3	1.76	1.20
2:I:215:ARG:CZ	5:I:803:AGS:H5'2	1.69	1.20
2:I:200:PRO:CB	2:I:305:ASP:HB2	1.72	1.20
2:G:6:LEU:HB3	2:G:190:ILE:CG2	1.71	1.19
2:D:184:ARG:HH11	2:D:184:ARG:HG3	1.07	1.19
2:G:20:GLY:HA2	2:G:22:GLU:OE2	1.41	1.19
2:I:215:ARG:CB	5:I:803:AGS:O4'	1.91	1.19
1:A:74:PHE:HZ	1:F:206:VAL:CB	1.55	1.18
2:I:215:ARG:HB2	5:I:803:AGS:O4'	1.02	1.18
2:H:326:GLN:HA	2:H:326:GLN:HE21	1.10	1.17
2:D:265:MET:HE1	2:D:354:LEU:HD21	1.22	1.16
1:F:273:PHE:CE1	1:F:283:ARG:HG3	1.80	1.16
2:I:200:PRO:HB2	2:I:305:ASP:CB	1.75	1.15
2:B:276:ILE:HD11	2:B:281:LEU:HB2	1.29	1.15
1:A:71:MSE:SE	1:F:228:ARG:CA	2.45	1.15
1:F:47:PHE:HD2	1:F:78:GLN:O	1.29	1.15
2:I:355:ARG:HH21	3:J:332:PRO:HD3	1.09	1.14
2:H:100:LYS:HG2	2:I:133:ARG:HB2	1.20	1.14
2:I:215:ARG:CZ	5:I:803:AGS:C5'	2.26	1.14
2:B:76:CYS:SG	2:B:78:ASN:HB2	1.88	1.13
1:F:244:VAL:HG22	1:F:312:LEU:HD21	1.27	1.12
2:H:229:ASP:OD2	2:I:30:ASN:ND2	1.83	1.11
1:A:105:HIS:CE1	1:A:108:LEU:HB2	1.85	1.10
2:G:6:LEU:HB3	2:G:190:ILE:HG21	1.17	1.10
2:B:360:HIS:CD2	2:B:361:PRO:HD2	1.86	1.09
2:B:360:HIS:HD2	2:B:361:PRO:HD2	1.06	1.09
1:F:223:MSE:HG3	1:F:289:ALA:HA	1.26	1.09
1:A:71:MSE:HE1	1:F:231:HIS:CB	1.83	1.09
3:J:303:VAL:HB	3:J:306:ILE:HD11	1.33	1.09
1:A:336:LEU:H	1:A:336:LEU:HD22	1.17	1.08
2:H:229:ASP:OD2	2:I:30:ASN:CG	1.96	1.08
2:H:351:MET:HE2	2:I:326:GLN:HE22	1.15	1.08
2:I:223:GLN:CD	2:I:240:MET:HE2	1.78	1.08
2:G:248:GLN:O	2:G:250:LEU:N	1.86	1.08
2:H:100:LYS:NZ	2:I:133:ARG:HG3	0.75	1.07
1:A:74:PHE:CZ	1:F:206:VAL:CB	2.32	1.07
1:F:47:PHE:CD2	1:F:78:GLN:O	2.07	1.07
2:I:19:VAL:HG12	2:I:178:LEU:HD22	1.35	1.07
2:G:11:ARG:HH22	2:G:52:THR:HG22	1.16	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:PHE:HE2	1:F:206:VAL:HG11	1.20	1.06
1:A:119:LYS:HD3	1:A:119:LYS:H	1.19	1.06
1:A:74:PHE:CE1	1:F:203:GLU:O	2.09	1.05
2:G:7:ALA:CB	2:G:218:LEU:HD13	1.86	1.05
2:G:295:VAL:HG22	2:G:301:ALA:HB3	1.38	1.05
2:D:10:TRP:CE2	2:D:190:ILE:HD12	1.90	1.05
2:G:46:THR:HG22	2:G:47:ARG:H	1.20	1.04
2:C:360:HIS:HD2	2:C:361:PRO:HD2	1.17	1.04
2:C:14:THR:HG22	2:C:15:PHE:H	1.22	1.04
1:F:45:GLN:OE1	1:F:77:ARG:CD	2.07	1.02
2:I:215:ARG:NE	5:I:803:AGS:H5'1	1.72	1.02
1:F:166:ALA:HB1	1:F:202:VAL:HG21	1.41	1.02
2:C:254:GLU:O	2:C:258:GLU:HG3	1.58	1.02
2:I:223:GLN:NE2	2:I:240:MET:CE	2.23	1.02
2:I:6:LEU:HG	2:I:222:ASP:OD2	1.60	1.01
2:B:360:HIS:HD2	2:B:361:PRO:CD	1.73	1.01
1:A:71:MSE:CE	1:F:231:HIS:CB	2.38	1.00
2:H:128:VAL:HG11	2:H:154:LEU:HD22	1.42	1.00
2:G:6:LEU:HD11	2:G:191:LEU:HD21	1.43	1.00
1:A:193:PRO:HG3	2:B:36:ARG:HH22	1.27	1.00
1:F:270:ARG:HG2	1:F:283:ARG:NH2	1.77	1.00
2:B:260:ASN:HD22	2:B:263:ARG:HB2	1.24	0.99
3:J:30:GLN:HG3	3:J:148:PRO:HD3	1.40	0.99
1:F:217:TRP:HE1	1:F:233:LEU:HB2	1.28	0.99
2:B:36:ARG:CB	2:B:36:ARG:HH11	1.76	0.99
2:B:351:MET:HE3	2:C:290:HIS:HA	1.44	0.99
2:I:11:ARG:HH21	2:I:56:ARG:HH21	1.07	0.98
2:G:11:ARG:NH2	2:G:52:THR:HG22	1.77	0.98
2:I:215:ARG:CB	5:I:803:AGS:C4'	2.41	0.98
2:H:360:HIS:HD2	2:H:363:MET:H	1.01	0.97
2:I:6:LEU:CG	2:I:222:ASP:CG	2.37	0.97
2:I:271:ALA:HB1	2:I:276:ILE:HD12	1.42	0.97
1:F:24:LEU:HD12	1:F:136:GLN:NE2	1.80	0.97
2:G:7:ALA:HB2	2:G:218:LEU:HD13	1.45	0.97
2:B:260:ASN:ND2	2:B:263:ARG:HB2	1.79	0.97
2:G:11:ARG:HH22	2:G:52:THR:CG2	1.77	0.97
2:I:215:ARG:NE	5:I:803:AGS:C5'	2.28	0.97
2:C:245:ASP:O	2:C:247:ASP:N	1.98	0.96
1:A:73:LEU:CB	1:F:207:ASN:OD1	2.13	0.96
2:G:274:ARG:HE	2:G:276:ILE:HD11	1.30	0.96
2:C:128:VAL:HG11	2:C:154:LEU:HD22	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:304:LEU:HB3	1:F:327:LEU:HD21	1.47	0.95
1:A:74:PHE:CG	1:F:203:GLU:HG3	2.01	0.95
1:F:98:LEU:O	1:F:101:THR:HG22	1.67	0.95
2:H:80:ARG:O	2:H:84:GLN:HG3	1.66	0.95
1:F:282:ARG:HG3	1:F:285:MSE:CE	1.96	0.95
2:H:100:LYS:HZ1	2:I:133:ARG:HG3	1.22	0.95
2:C:360:HIS:CD2	2:C:361:PRO:HD2	2.02	0.94
2:D:363:MET:HB3	2:D:364:PRO:HD2	1.49	0.94
2:G:248:GLN:O	2:G:251:SER:N	2.00	0.94
2:D:265:MET:CE	2:D:354:LEU:HD21	1.97	0.94
1:A:183:GLN:HE21	2:B:172:GLN:H	1.05	0.94
2:B:309:ILE:HG22	2:B:313:MET:HG2	1.50	0.94
2:I:215:ARG:HD3	5:I:803:AGS:C5'	1.97	0.94
3:J:117:ALA:O	3:J:120:LEU:HD22	1.66	0.94
1:A:251:GLN:HE21	1:A:255:LEU:HD11	1.33	0.94
3:E:303:VAL:HB	3:E:306:ILE:HD11	1.49	0.94
1:A:74:PHE:CE2	1:F:206:VAL:CG1	2.50	0.93
1:A:253:GLU:OE1	1:A:286:MSE:HE1	1.68	0.93
1:F:119:LYS:HD3	1:F:119:LYS:H	1.30	0.93
1:A:74:PHE:CE2	1:F:206:VAL:HG11	2.03	0.93
1:F:299:ARG:HG3	3:J:317:LEU:HD11	1.48	0.93
3:J:253:MSE:HG3	3:J:257:LYS:HE3	1.50	0.93
1:F:270:ARG:HG2	1:F:283:ARG:HH21	1.32	0.93
2:I:215:ARG:CD	5:I:803:AGS:C5'	2.46	0.93
1:A:73:LEU:HB2	1:F:207:ASN:CG	1.92	0.92
3:J:49:LEU:HD23	3:J:68:MSE:SE	2.20	0.92
3:E:74:PRO:HB3	3:E:105:ARG:HD3	1.51	0.92
1:F:222:LEU:CD1	1:F:285:MSE:HE3	1.99	0.92
1:F:295:GLN:CD	1:F:295:GLN:H	1.75	0.92
1:A:93:ILE:HG12	1:A:96:GLN:OE1	1.69	0.92
2:C:263:ARG:O	2:C:267:LEU:HG	1.70	0.92
2:D:10:TRP:NE1	2:D:190:ILE:HG23	1.84	0.91
1:F:71:MSE:SE	1:F:80:LEU:HD12	2.20	0.91
3:J:46:ARG:CZ	3:J:68:MSE:HG3	2.01	0.91
2:C:243:THR:HG22	2:C:244:LEU:N	1.83	0.91
2:C:343:PRO:O	2:C:344:ASP:HB2	1.68	0.91
2:G:10:TRP:HZ2	2:G:193:GLU:HB3	0.75	0.91
2:I:363:MET:HB3	2:I:364:PRO:HD2	1.53	0.91
3:J:296:ILE:HG21	3:J:315:LEU:HD12	1.53	0.91
2:G:248:GLN:HA	2:G:251:SER:OG	1.69	0.91
2:B:343:PRO:HG2	2:B:347:MET:SD	2.11	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:291:ARG:NH2	2:G:303:GLY:H	1.67	0.90
3:J:4:TYR:H	3:J:7:LEU:HD12	1.33	0.90
1:F:24:LEU:HD12	1:F:136:GLN:HE21	1.34	0.90
2:D:184:ARG:HD3	2:D:185:HIS:N	1.85	0.90
1:F:80:LEU:HD13	1:F:80:LEU:H	1.37	0.90
1:F:48:GLU:OE2	1:F:74:PHE:HZ	1.53	0.90
1:F:71:MSE:HB3	1:F:108:LEU:HD13	1.54	0.90
2:G:6:LEU:HD21	2:G:196:ILE:HD12	1.54	0.90
3:E:296:ILE:HA	3:E:299:GLN:HG3	1.53	0.90
1:A:150:TRP:CH2	1:A:178:LEU:HD11	2.08	0.89
2:C:243:THR:CG2	2:C:244:LEU:N	2.33	0.89
2:I:354:LEU:HD12	3:J:253:MSE:HE1	1.53	0.89
2:C:316:LEU:HD22	2:C:320:ILE:HD11	1.53	0.89
2:D:10:TRP:CD2	2:D:190:ILE:HD12	2.07	0.89
1:A:336:LEU:HD22	1:A:336:LEU:N	1.86	0.89
1:A:125:ALA:O	1:A:128:THR:HG23	1.71	0.88
1:A:147:LEU:HB3	1:A:148:PRO:HD3	1.55	0.88
3:E:79:LEU:HD11	3:E:96:VAL:HG11	1.54	0.88
3:E:121:THR:HG22	3:E:123:ALA:H	1.39	0.88
2:G:11:ARG:HH21	2:G:56:ARG:NH2	1.72	0.88
2:G:10:TRP:HZ2	2:G:193:GLU:HB2	1.34	0.88
2:D:108:LEU:O	2:D:111:VAL:HG23	1.73	0.88
2:C:156:THR:HG22	2:C:158:ASP:H	1.37	0.87
2:G:11:ARG:NH2	2:G:56:ARG:NH2	2.23	0.87
2:D:184:ARG:HH11	2:D:184:ARG:CG	1.88	0.87
1:F:48:GLU:HG2	1:F:49:GLU:N	1.88	0.87
2:I:215:ARG:CD	5:I:803:AGS:C4'	2.27	0.87
2:B:44:SER:CB	2:B:159:PRO:HG2	2.05	0.87
1:F:27:ASP:OD2	1:F:30:LEU:HG	1.75	0.87
2:I:223:GLN:NE2	2:I:240:MET:HE1	1.88	0.87
1:A:281:ASN:O	1:A:283:ARG:N	2.08	0.86
3:E:58:SER:HB3	3:E:65:CYS:SG	2.16	0.86
2:H:261:GLY:HA3	2:I:297:LEU:HD11	1.58	0.86
1:A:74:PHE:CE1	1:F:203:GLU:HG3	2.09	0.86
1:A:74:PHE:HE1	1:F:203:GLU:O	1.58	0.86
2:G:268:ILE:HD11	2:G:353:LEU:HD12	1.56	0.86
2:I:244:LEU:HD11	2:I:276:ILE:HD13	1.58	0.86
2:D:223:GLN:HB3	2:D:240:MET:HE1	1.57	0.86
2:H:100:LYS:HZ2	2:I:133:ARG:HG3	1.10	0.86
2:C:243:THR:CG2	2:C:244:LEU:H	1.88	0.85
2:B:257:VAL:HG11	2:B:320:ILE:HD13	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:20:GLY:HA2	2:I:22:GLU:OE2	1.76	0.85
2:B:198:HIS:CD2	2:B:203:LEU:HD11	2.11	0.85
3:J:31:ALA:HB2	3:J:164:LEU:HB3	1.59	0.85
1:A:71:MSE:HE1	1:F:231:HIS:HB2	0.89	0.85
1:A:269:LEU:HG	1:A:273:PHE:HE1	1.42	0.85
3:E:186:ALA:HA	3:E:269:ASP:OD1	1.77	0.85
2:H:291:ARG:HA	2:H:294:MET:HB2	1.58	0.85
2:C:198:HIS:HB2	2:C:232:VAL:HG22	1.57	0.85
1:A:1:MSE:HE1	1:A:127:PHE:CZ	2.11	0.85
2:I:248:GLN:HG3	2:I:274:ARG:HH22	1.39	0.85
2:H:88:VAL:HG11	2:H:116:ALA:HB3	1.58	0.84
2:D:363:MET:CB	2:D:364:PRO:HD2	2.05	0.84
1:A:183:GLN:NE2	2:B:172:GLN:H	1.76	0.84
2:G:10:TRP:CZ2	2:G:193:GLU:HB2	2.07	0.84
2:G:248:GLN:O	2:G:249:ALA:C	2.18	0.84
2:C:259:ALA:HB2	2:C:360:HIS:CE1	2.12	0.84
2:I:215:ARG:CG	5:I:803:AGS:H4'	2.07	0.84
1:A:74:PHE:CD1	1:F:207:ASN:OD1	2.07	0.84
2:H:367:GLU:HG3	2:I:321:PRO:HA	1.58	0.84
2:B:165:THR:O	2:B:168:SER:HB3	1.77	0.84
2:D:354:LEU:HD13	3:E:253:MSE:HE1	1.59	0.84
2:H:201:ARG:HD2	2:H:246:ASP:OD2	1.77	0.84
2:I:11:ARG:HH21	2:I:56:ARG:NH2	1.75	0.84
1:F:273:PHE:CE1	1:F:283:ARG:CG	2.61	0.84
1:A:133:ARG:HH21	2:G:300:ALA:CB	1.90	0.83
2:C:200:PRO:HG2	2:C:305:ASP:OD2	1.77	0.83
2:H:360:HIS:CD2	2:H:363:MET:H	1.93	0.83
2:B:351:MET:SD	2:C:326:GLN:NE2	2.49	0.83
2:I:355:ARG:NH2	3:J:332:PRO:HD3	1.93	0.83
1:A:214:PRO:HA	1:A:236:LEU:HD11	1.60	0.83
2:D:306:MET:HG2	2:D:309:ILE:HD11	1.61	0.83
2:D:184:ARG:HG3	2:D:184:ARG:NH1	1.83	0.83
2:H:24:VAL:HG11	2:H:175:LEU:HD21	1.60	0.83
3:E:333:HIS:O	3:E:334:LEU:HB2	1.78	0.83
3:J:317:LEU:HD13	3:J:318:ARG:N	1.93	0.83
3:J:68:MSE:HA	3:J:68:MSE:HE3	1.60	0.83
1:F:144:GLN:HG3	1:F:280:GLN:CD	2.04	0.83
3:J:230:TYR:HE1	3:J:313:THR:HG23	1.42	0.83
2:D:257:VAL:HG11	2:D:320:ILE:HG12	1.60	0.83
3:E:30:GLN:CG	3:E:163:TYR:HD1	1.93	0.82
2:H:100:LYS:NZ	2:I:133:ARG:CB	2.42	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:215:ARG:CZ	5:I:803:AGS:H5'1	2.02	0.82
2:I:223:GLN:CD	2:I:240:MET:CE	2.49	0.82
1:F:282:ARG:HG3	1:F:285:MSE:HE1	1.59	0.82
2:H:339:LEU:HB3	2:H:340:PRO:HD3	1.59	0.82
3:E:30:GLN:HG2	3:E:163:TYR:HD1	1.44	0.82
2:B:261:GLY:HA3	2:C:297:LEU:HD11	1.61	0.82
2:D:223:GLN:HB3	2:D:240:MET:CE	2.10	0.82
2:G:19:VAL:HG21	2:G:186:GLN:OE1	1.80	0.82
3:E:169:GLU:O	3:E:173:VAL:HG23	1.78	0.82
2:B:344:ASP:OD2	2:B:344:ASP:C	2.20	0.82
1:F:45:GLN:CD	1:F:77:ARG:HD3	2.03	0.82
2:H:84:GLN:O	2:I:144:GLU:OE2	1.98	0.81
2:C:197:ALA:O	2:C:198:HIS:HB3	1.80	0.81
2:I:244:LEU:HD21	2:I:276:ILE:HG12	1.61	0.81
1:A:74:PHE:HZ	1:F:206:VAL:HB	0.75	0.81
1:A:262:ARG:NH2	3:E:320:GLU:OE2	2.13	0.81
2:C:119:ARG:HB2	2:C:120:PHE:CD2	2.15	0.81
2:D:358:ALA:O	2:D:360:HIS:N	2.10	0.81
2:D:292:ILE:HG13	2:D:313:MET:HE1	1.62	0.81
1:A:193:PRO:HD3	2:B:30:ASN:HD21	1.45	0.81
1:F:304:LEU:HD13	1:F:327:LEU:HD22	1.61	0.81
2:G:6:LEU:HD11	2:G:191:LEU:CD2	2.10	0.81
2:G:250:LEU:HD23	2:G:288:LEU:HD13	1.61	0.81
2:C:268:ILE:HD11	2:C:353:LEU:HD12	1.63	0.81
2:D:42:LEU:HD23	2:D:154:LEU:HB2	1.62	0.81
1:F:282:ARG:CG	1:F:285:MSE:CE	2.58	0.81
1:F:253:GLU:O	1:F:256:LEU:HB3	1.81	0.81
2:G:291:ARG:HH21	2:G:303:GLY:H	1.27	0.81
2:I:6:LEU:CG	2:I:222:ASP:OD2	2.22	0.81
2:I:223:GLN:NE2	2:I:240:MET:HE2	1.91	0.81
1:A:150:TRP:CZ2	1:A:178:LEU:HD11	2.16	0.80
2:G:20:GLY:CA	2:G:22:GLU:OE2	2.28	0.80
2:D:229:ASP:O	2:D:231:GLN:N	2.12	0.80
2:I:246:ASP:HB3	2:I:248:GLN:HG2	1.63	0.80
1:A:208:ASP:O	2:B:176:LYS:HE2	1.80	0.80
1:F:248:ARG:HH21	1:F:309:GLU:CD	1.89	0.80
2:G:98:ARG:HH11	2:H:140:LEU:HD22	1.46	0.80
1:A:25:GLY:HA3	1:A:139:CYS:O	1.82	0.80
3:J:35:MSE:HE3	3:J:198:PRO:HD2	1.64	0.80
2:B:302:LEU:HD12	2:B:314:ARG:HH21	1.47	0.80
2:C:128:VAL:HG23	2:C:162:LEU:HD21	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:265:MET:HE1	2:D:354:LEU:CD2	2.07	0.80
2:D:10:TRP:CD2	2:D:190:ILE:CD1	2.65	0.80
2:C:236:ALA:O	2:C:239:ALA:HB3	1.81	0.80
2:C:14:THR:HG22	2:C:15:PHE:N	1.98	0.79
2:G:271:ALA:HB1	2:G:276:ILE:HD12	1.62	0.79
1:A:281:ASN:C	1:A:283:ARG:H	1.89	0.79
2:B:259:ALA:HB2	2:B:360:HIS:CE1	2.17	0.79
1:F:223:MSE:HG3	1:F:289:ALA:CA	2.12	0.79
1:F:223:MSE:HE1	1:F:292:ARG:HB2	1.65	0.79
2:H:326:GLN:HA	2:H:326:GLN:NE2	1.91	0.79
1:A:234:GLN:HA	1:A:237:ARG:HE	1.48	0.79
2:B:248:GLN:HA	2:B:251:SER:HB2	1.64	0.79
1:F:119:LYS:HD3	1:F:119:LYS:N	1.97	0.79
1:A:71:MSE:HE3	1:F:231:HIS:CG	2.17	0.79
2:B:351:MET:CE	2:C:290:HIS:HA	2.12	0.79
3:E:161:LEU:HD12	3:E:161:LEU:H	1.45	0.79
2:H:295:VAL:HG22	2:H:301:ALA:HB3	1.65	0.79
1:A:74:PHE:CZ	1:F:203:GLU:O	2.35	0.79
1:F:142:PRO:HD2	1:F:178:LEU:HD11	1.63	0.79
2:I:215:ARG:NH1	5:I:803:AGS:C5'	2.34	0.79
1:A:105:HIS:HB3	1:F:227:LYS:HD3	1.65	0.79
2:H:42:LEU:HD23	2:H:172:GLN:HG2	1.63	0.79
2:B:61:GLY:HA2	2:B:72:PRO:HG3	1.65	0.79
2:G:98:ARG:HD3	2:H:140:LEU:HB3	1.65	0.79
1:A:59:THR:HG22	1:A:60:ASP:N	1.98	0.79
1:A:219:ASP:O	1:A:222:LEU:HB2	1.83	0.79
2:B:140:LEU:HA	2:B:143:LEU:HD22	1.65	0.79
1:A:91:ALA:HA	1:A:94:ASN:ND2	1.98	0.78
2:H:341:TYR:CE2	2:I:337:LYS:HB2	2.18	0.78
2:I:148:GLU:CD	2:I:149:HIS:H	1.90	0.78
3:J:58:SER:HB3	3:J:65:CYS:SG	2.24	0.78
2:G:11:ARG:HH21	2:G:56:ARG:CZ	1.96	0.78
2:G:271:ALA:O	2:G:274:ARG:HG2	1.83	0.78
2:H:351:MET:HE2	2:I:326:GLN:NE2	1.96	0.78
2:B:215:ARG:HD3	5:B:802:AGS:H5'1	1.66	0.78
2:G:239:ALA:HB1	2:H:23:HIS:NE2	1.98	0.78
2:B:42:LEU:HB2	2:B:170:CYS:SG	2.23	0.78
1:F:48:GLU:OE2	1:F:74:PHE:CZ	2.36	0.78
1:F:104:LEU:HB3	1:F:133:ARG:NH1	1.99	0.78
2:G:248:GLN:HA	2:G:251:SER:CB	2.14	0.78
3:E:218:GLN:O	3:E:221:ALA:HB3	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:100:LYS:CG	2:I:133:ARG:HB2	2.06	0.78
1:F:198:THR:HB	1:F:200:PRO:HD2	1.66	0.78
2:H:113:TYR:HA	2:H:149:HIS:CE1	2.19	0.78
1:F:222:LEU:HD12	1:F:285:MSE:HE3	1.66	0.78
1:F:187:ARG:O	1:F:191:LEU:HD23	1.84	0.77
1:F:282:ARG:HG3	1:F:285:MSE:HE2	1.64	0.77
2:I:6:LEU:HG	2:I:222:ASP:OD1	1.85	0.77
2:C:97:SER:OG	2:C:100:LYS:HD2	1.84	0.77
2:H:137:ASN:HA	2:H:140:LEU:HD12	1.66	0.77
2:I:355:ARG:HH21	3:J:332:PRO:CD	1.96	0.77
2:B:156:THR:HG23	2:B:159:PRO:HG3	1.65	0.77
1:A:193:PRO:CD	2:B:30:ASN:HD21	1.98	0.77
2:G:341:TYR:O	2:H:333:LEU:HD11	1.85	0.77
2:I:363:MET:CB	2:I:364:PRO:HD2	2.15	0.77
2:B:263:ARG:HG2	2:B:267:LEU:HD13	1.65	0.77
1:F:242:GLU:O	1:F:245:ILE:HG22	1.84	0.77
2:C:287:GLY:O	2:C:290:HIS:HB3	1.83	0.77
2:G:98:ARG:HD3	2:H:140:LEU:HD13	1.67	0.77
2:D:197:ALA:HB3	2:D:231:GLN:HG2	1.67	0.76
2:I:61:GLY:HA2	2:I:72:PRO:HG3	1.66	0.76
2:D:259:ALA:HA	2:D:363:MET:HE2	1.67	0.76
3:E:283:PRO:HG2	3:E:284:SER:H	1.50	0.76
1:F:1:MSE:HE1	1:F:127:PHE:CZ	2.20	0.76
2:I:215:ARG:HH11	5:I:803:AGS:H5'2	1.44	0.76
1:A:63:ALA:O	1:A:67:LEU:HG	1.85	0.76
1:A:74:PHE:CE1	1:F:203:GLU:CG	2.66	0.76
2:D:285:MET:HE1	2:D:353:LEU:HD21	1.68	0.76
1:F:213:THR:H	1:F:216:HIS:HD2	1.33	0.76
2:D:10:TRP:CE2	2:D:190:ILE:HG23	2.21	0.76
2:H:100:LYS:HG2	2:I:133:ARG:CB	2.09	0.76
3:E:158:ARG:HH11	3:E:158:ARG:HG3	1.49	0.76
2:H:11:ARG:HH12	2:I:169:ARG:HH12	1.28	0.76
2:H:136:PHE:O	2:H:140:LEU:HG	1.84	0.76
2:I:348:GLY:O	2:I:351:MET:HB2	1.86	0.76
2:B:36:ARG:HH11	2:B:36:ARG:HB3	1.49	0.76
2:B:328:TYR:O	2:B:329:TYR:C	2.27	0.76
2:G:46:THR:HG22	2:G:47:ARG:N	2.00	0.76
2:H:179:ASP:HB3	2:H:182:GLN:HB2	1.67	0.76
1:A:74:PHE:CD1	1:F:203:GLU:HG2	2.20	0.75
2:H:359:PHE:CE1	2:I:323:THR:HG23	2.20	0.75
2:H:11:ARG:HH12	2:I:169:ARG:NH1	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:PHE:CZ	1:F:206:VAL:CG1	2.66	0.75
2:C:95:ALA:HB3	2:C:127:GLU:O	1.87	0.75
1:F:304:LEU:HB2	1:F:327:LEU:HD11	1.68	0.75
2:G:355:ARG:HD2	2:G:355:ARG:C	2.12	0.75
2:I:201:ARG:NH2	2:I:284:GLU:OE2	2.19	0.75
2:C:37:ILE:HD13	2:C:120:PHE:CE1	2.20	0.75
2:D:259:ALA:CB	2:D:363:MET:HG2	2.15	0.75
1:F:310:LEU:HB3	1:F:314:GLN:NE2	2.01	0.75
2:I:248:GLN:HG3	2:I:274:ARG:NH2	2.01	0.75
1:A:198:THR:HB	1:A:200:PRO:HD2	1.69	0.75
1:F:80:LEU:HD13	1:F:80:LEU:N	2.01	0.75
1:A:71:MSE:CE	1:F:231:HIS:CG	2.69	0.75
1:A:133:ARG:HH21	2:G:300:ALA:HB2	1.51	0.75
1:A:190:LEU:HD21	2:B:38:HIS:CE1	2.21	0.75
2:B:76:CYS:SG	2:B:78:ASN:CB	2.73	0.75
3:E:246:HIS:O	3:E:250:THR:HG23	1.86	0.75
2:G:9:LYS:HD3	2:G:194:GLU:CD	2.12	0.75
2:B:81:GLU:HB2	2:B:87:PHE:HD1	1.50	0.74
2:G:6:LEU:HB3	2:G:190:ILE:HG22	1.68	0.74
2:I:257:VAL:O	2:I:360:HIS:HE1	1.70	0.74
1:A:279:TRP:CG	1:A:279:TRP:O	2.40	0.74
3:J:57:LYS:HG3	3:J:58:SER:H	1.52	0.74
3:J:303:VAL:HB	3:J:306:ILE:CD1	2.14	0.74
2:C:147:PRO:HG2	2:C:150:VAL:HB	1.69	0.74
2:G:11:ARG:NH2	2:G:56:ARG:HH21	1.84	0.74
1:A:281:ASN:C	1:A:283:ARG:N	2.45	0.74
2:D:78:ASN:O	2:D:82:ILE:HG13	1.85	0.74
2:D:354:LEU:CD1	3:E:253:MSE:HE1	2.17	0.74
2:C:42:LEU:HD12	2:C:154:LEU:HB2	1.69	0.74
2:C:119:ARG:HB2	2:C:120:PHE:HD2	1.51	0.74
2:D:119:ARG:HG3	2:D:120:PHE:CD2	2.21	0.74
1:F:281:ASN:C	1:F:283:ARG:H	1.95	0.74
1:F:13:LEU:HD23	1:F:41:VAL:HG21	1.68	0.74
2:D:148:GLU:CD	2:D:149:HIS:H	1.95	0.74
2:H:202:ALA:HB2	2:H:234:THR:HG23	1.70	0.74
2:I:144:GLU:C	2:I:146:PRO:HD3	2.13	0.74
1:F:53:PHE:HZ	1:F:67:LEU:HD13	1.52	0.74
1:F:188:LEU:HD23	1:F:197:LEU:HD13	1.70	0.74
2:H:271:ALA:O	2:H:274:ARG:HG2	1.88	0.74
1:A:52:THR:HG22	1:A:81:LEU:HB3	1.69	0.74
1:A:55:ILE:O	1:A:85:PRO:HG3	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:292:ASP:OD2	3:E:318:ARG:NH1	2.19	0.74
2:G:274:ARG:NE	2:G:276:ILE:HD11	2.01	0.74
1:A:263:GLN:HB2	1:A:272:LEU:HD21	1.70	0.73
1:F:213:THR:H	1:F:216:HIS:CD2	2.05	0.73
2:G:248:GLN:C	2:G:250:LEU:N	2.44	0.73
2:B:304:ASN:OD1	2:B:305:ASP:N	2.21	0.73
2:G:67:GLY:HA2	2:G:119:ARG:NH2	2.03	0.73
1:A:260:LEU:HB3	1:A:290:LEU:HD11	1.70	0.73
1:A:272:LEU:O	1:A:275:LYS:HB2	1.88	0.73
1:A:269:LEU:HD11	1:A:273:PHE:CZ	2.23	0.73
2:D:10:TRP:CE2	2:D:190:ILE:CD1	2.70	0.73
1:F:217:TRP:NE1	1:F:233:LEU:HB2	2.00	0.73
1:F:310:LEU:O	1:F:314:GLN:HG3	1.88	0.73
2:B:244:LEU:O	2:B:245:ASP:HB3	1.86	0.73
2:C:343:PRO:O	2:C:344:ASP:CB	2.36	0.73
1:F:281:ASN:O	1:F:283:ARG:N	2.22	0.73
2:G:214:LEU:HD23	5:G:804:AGS:N9	2.03	0.73
1:A:184:ALA:HA	1:A:187:ARG:HD2	1.71	0.73
2:D:363:MET:HB3	2:D:364:PRO:CD	2.18	0.73
2:I:248:GLN:HE21	2:I:248:GLN:HA	1.52	0.73
1:F:279:TRP:CG	1:F:279:TRP:O	2.42	0.73
1:A:251:GLN:NE2	1:A:255:LEU:HD11	2.04	0.73
2:D:357:LEU:HA	2:D:363:MET:CE	2.18	0.73
1:F:282:ARG:CG	1:F:285:MSE:HE2	2.17	0.73
2:G:243:THR:HG21	2:G:274:ARG:HD2	1.69	0.73
2:D:246:ASP:HB3	2:D:248:GLN:HE21	1.54	0.73
2:B:156:THR:CG2	2:B:159:PRO:HG3	2.19	0.72
2:I:215:ARG:HD3	5:I:803:AGS:H4'	0.74	0.72
2:D:248:GLN:O	2:D:252:LEU:HB2	1.90	0.72
2:H:271:ALA:HA	2:H:274:ARG:NE	2.04	0.72
2:I:354:LEU:CD1	3:J:253:MSE:HE1	2.18	0.72
1:A:164:ASP:O	1:A:168:GLN:HG3	1.89	0.72
1:A:269:LEU:HG	1:A:273:PHE:CZ	2.24	0.72
3:E:222:TYR:O	3:E:225:PRO:HD2	1.89	0.72
2:I:7:ALA:HB1	2:I:215:ARG:HG3	1.70	0.72
3:J:121:THR:HG22	3:J:123:ALA:H	1.54	0.72
2:D:315:GLU:O	2:D:319:THR:HG23	1.89	0.72
2:I:6:LEU:HB3	2:I:218:LEU:HB3	1.72	0.72
2:D:276:ILE:HG22	2:D:277:GLU:N	2.05	0.72
2:H:327:LEU:HD21	2:H:361:PRO:HD3	1.70	0.72
1:A:27:ASP:OD1	1:A:29:LEU:HD23	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:295:VAL:HA	2:D:301:ALA:HB3	1.71	0.72
3:E:277:LEU:C	3:E:279:ASN:H	1.98	0.72
1:F:80:LEU:HD11	1:F:108:LEU:HD12	1.71	0.72
3:J:230:TYR:CE1	3:J:313:THR:HG23	2.24	0.72
2:G:6:LEU:HD21	2:G:191:LEU:HD23	1.72	0.71
2:H:100:LYS:HE2	2:I:133:ARG:HA	1.72	0.71
1:A:269:LEU:CG	1:A:273:PHE:CE1	2.67	0.71
2:C:243:THR:HG23	2:C:244:LEU:H	1.53	0.71
2:D:9:LYS:NZ	2:D:194:GLU:OE2	2.22	0.71
2:G:10:TRP:CD1	2:G:190:ILE:HG23	2.25	0.71
2:B:56:ARG:HH11	2:B:56:ARG:HG3	1.55	0.71
3:E:253:MSE:HA	3:E:253:MSE:HE3	1.72	0.71
2:I:354:LEU:HD13	3:J:256:LEU:HD22	1.73	0.71
2:I:223:GLN:CG	2:I:240:MET:HE2	2.19	0.71
3:J:116:ASP:HA	3:J:144:ALA:O	1.90	0.71
2:B:278:TRP:O	2:B:281:LEU:N	2.24	0.71
2:D:25:LEU:HD21	2:D:54:ILE:CD1	2.20	0.71
2:D:150:VAL:O	2:D:151:LYS:HD3	1.90	0.71
2:D:285:MET:CE	2:D:353:LEU:HD21	2.21	0.71
2:B:36:ARG:HH11	2:B:36:ARG:HB2	1.55	0.71
2:C:86:ARG:HH12	2:D:141:LYS:HG3	1.55	0.71
2:C:133:ARG:HD3	2:C:133:ARG:N	2.05	0.71
3:E:233:LEU:HD12	3:E:237:ASN:HB2	1.72	0.71
1:F:165:ALA:O	1:F:169:VAL:HG23	1.91	0.71
2:H:213:SER:OG	2:H:216:ASP:HB2	1.91	0.71
2:H:351:MET:HE1	2:I:293:ALA:CB	2.21	0.71
1:A:34:SER:O	1:A:38:VAL:HG23	1.90	0.71
2:C:259:ALA:HB2	2:C:360:HIS:ND1	2.05	0.71
2:I:292:ILE:O	2:I:296:GLN:HG3	1.90	0.71
1:A:181:LEU:O	1:A:185:LEU:HG	1.91	0.70
2:D:10:TRP:NE1	2:D:190:ILE:HD12	2.06	0.70
1:F:299:ARG:HG3	3:J:317:LEU:CD1	2.20	0.70
3:E:181:THR:O	3:E:182:MSE:HG2	1.91	0.70
2:D:32:LEU:O	2:D:34:LEU:N	2.24	0.70
2:H:271:ALA:C	2:H:276:ILE:HD11	2.16	0.70
1:A:308:THR:HG23	1:A:320:VAL:HG22	1.73	0.70
2:I:6:LEU:HD12	2:I:218:LEU:O	1.90	0.70
3:J:41:ILE:HG21	3:J:113:TRP:CD1	2.26	0.70
1:A:140:GLN:OE1	1:A:140:GLN:HA	1.91	0.70
2:C:261:GLY:HA3	2:D:297:LEU:HD21	1.71	0.70
2:G:302:LEU:HD13	2:G:310:GLU:HG2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:351:MET:HA	2:H:351:MET:HE3	1.73	0.70
3:J:273:LEU:O	3:J:277:LEU:HB2	1.91	0.70
1:A:71:MSE:SE	1:F:231:HIS:CB	2.90	0.70
3:E:163:TYR:CD2	3:E:165:ALA:HB2	2.26	0.70
1:F:48:GLU:HG2	1:F:49:GLU:H	1.56	0.70
1:F:84:LEU:HG	1:F:89:PRO:HG3	1.74	0.70
1:A:221:LEU:HD21	1:A:328:SER:CB	2.22	0.70
1:F:25:GLY:HA2	1:F:140:GLN:NE2	2.07	0.70
3:J:252:LEU:HD23	3:J:290:LEU:HA	1.74	0.70
2:C:361:PRO:O	2:C:362:ARG:HD3	1.92	0.70
3:E:74:PRO:HB3	3:E:105:ARG:CD	2.19	0.69
3:E:26:ALA:HB1	3:E:159:CYS:HB3	1.73	0.69
2:H:200:PRO:HG2	2:H:305:ASP:OD2	1.92	0.69
3:J:117:ALA:HB3	3:J:145:THR:OG1	1.92	0.69
1:A:270:ARG:HG2	1:A:283:ARG:NH2	2.07	0.69
2:B:354:LEU:HD11	2:C:294:MET:HG2	1.75	0.69
2:C:186:GLN:OE1	2:C:186:GLN:HA	1.91	0.69
2:I:6:LEU:HD12	2:I:221:THR:HB	1.73	0.69
2:B:333:LEU:HD11	2:B:337:LYS:HE3	1.75	0.69
2:C:360:HIS:HD2	2:C:361:PRO:CD	1.98	0.69
1:F:299:ARG:CG	3:J:317:LEU:HD11	2.21	0.69
2:C:186:GLN:HG3	2:C:190:ILE:HD11	1.73	0.69
3:E:238:HIS:ND1	3:E:239:GLU:N	2.41	0.69
3:J:51:GLN:HG2	3:J:62:CYS:SG	2.32	0.69
2:B:78:ASN:HA	2:B:87:PHE:CE1	2.28	0.69
2:C:28:LEU:HD21	2:C:173:PHE:CE2	2.28	0.69
3:E:29:ILE:HD13	3:E:41:ILE:HD11	1.73	0.69
3:E:237:ASN:O	3:E:238:HIS:HB2	1.91	0.69
2:I:113:TYR:HD2	2:I:147:PRO:HB3	1.56	0.69
2:B:44:SER:HB2	2:B:159:PRO:HG2	1.74	0.69
2:B:158:ASP:O	2:B:158:ASP:CG	2.36	0.69
1:F:218:VAL:O	1:F:222:LEU:HG	1.92	0.69
2:G:220:LEU:HD23	2:G:223:GLN:HE21	1.58	0.69
2:H:287:GLY:O	2:H:290:HIS:HB3	1.92	0.69
1:A:183:GLN:HE21	2:B:172:GLN:N	1.87	0.69
2:C:323:THR:HG22	2:C:324:ASP:N	2.06	0.69
2:D:183:ILE:HG23	2:D:214:LEU:HD12	1.72	0.69
1:F:25:GLY:O	1:F:115:ASN:HA	1.91	0.69
1:F:144:GLN:HG3	1:F:280:GLN:OE1	1.92	0.69
1:F:247:LEU:HD21	1:F:308:THR:HG21	1.75	0.69
2:H:112:GLN:HB2	2:H:121:LYS:NZ	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:GLU:OE1	1:A:286:MSE:CE	2.39	0.69
2:D:366:PRO:HB3	3:E:282:SER:HB2	1.74	0.69
1:F:80:LEU:HD11	1:F:108:LEU:CD1	2.23	0.68
2:G:277:GLU:HG3	2:G:280:ALA:H	1.57	0.68
2:I:10:TRP:HB2	2:I:218:LEU:HD13	1.74	0.68
3:J:45:SER:O	3:J:49:LEU:HB2	1.93	0.68
2:B:360:HIS:CD2	2:B:361:PRO:CD	2.62	0.68
2:C:350:GLU:OE1	2:D:294:MET:HE1	1.93	0.68
3:E:74:PRO:HD2	3:E:106:LEU:HD11	1.75	0.68
3:E:225:PRO:HA	3:E:280:HIS:ND1	2.08	0.68
2:H:142:THR:O	2:H:146:PRO:HB3	1.92	0.68
1:A:55:ILE:HD12	1:A:84:LEU:HD12	1.75	0.68
2:H:88:VAL:CG1	2:H:116:ALA:HB3	2.22	0.68
2:H:242:GLY:HA3	2:H:277:GLU:HG2	1.74	0.68
1:A:193:PRO:HD3	2:B:30:ASN:ND2	2.07	0.68
3:E:179:GLU:O	3:E:180:VAL:HG23	1.94	0.68
2:C:327:LEU:HD12	2:C:327:LEU:O	1.94	0.68
3:E:254:ASP:CG	3:E:265:VAL:HG13	2.18	0.68
2:G:220:LEU:HD23	2:G:223:GLN:NE2	2.08	0.68
3:J:256:LEU:HD11	3:J:287:GLN:HG2	1.74	0.68
1:A:154:ARG:O	1:A:157:GLN:HG2	1.94	0.68
2:C:223:GLN:NE2	2:C:240:MET:HE3	2.08	0.68
2:D:24:VAL:O	2:D:25:LEU:C	2.36	0.68
1:F:285:MSE:SE	1:F:285:MSE:CE	2.92	0.68
2:C:14:THR:CG2	2:C:15:PHE:H	2.04	0.68
1:F:54:SER:O	1:F:57:PRO:HD2	1.94	0.68
2:G:178:LEU:HD22	2:G:182:GLN:HE21	1.59	0.68
2:D:27:ALA:O	2:D:28:LEU:C	2.37	0.68
2:D:184:ARG:CG	2:D:184:ARG:NH1	2.48	0.68
2:D:196:ILE:HG22	2:D:197:ALA:N	2.09	0.68
2:D:296:GLN:HE22	2:D:322:PRO:HA	1.57	0.68
3:E:289:ILE:HG23	3:E:319:ILE:HD13	1.75	0.68
1:F:158:LEU:O	1:F:160:LEU:HD13	1.93	0.68
2:G:7:ALA:HB2	2:G:218:LEU:CD1	2.23	0.68
2:B:304:ASN:CG	2:B:305:ASP:H	2.01	0.68
2:D:184:ARG:HD3	2:D:184:ARG:C	2.19	0.68
1:F:225:LYS:HG3	1:F:227:LYS:H	1.59	0.68
2:G:9:LYS:CD	2:G:194:GLU:OE1	2.42	0.68
2:G:278:TRP:HE3	2:G:349:VAL:HG21	1.58	0.68
2:G:291:ARG:NH2	2:G:303:GLY:N	2.40	0.68
2:I:208:ARG:NH2	2:I:283:VAL:HG11	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:PRO:HB3	1:A:246:LEU:HD22	1.75	0.67
2:C:198:HIS:CB	2:C:232:VAL:HG22	2.24	0.67
2:C:291:ARG:O	2:C:295:VAL:HG23	1.94	0.67
2:C:329:TYR:CE2	2:C:333:LEU:HD12	2.30	0.67
1:A:17:LEU:HD21	1:A:109:LEU:HD12	1.76	0.67
2:B:61:GLY:CA	2:B:72:PRO:HG3	2.24	0.67
2:B:285:MET:HE2	2:B:332:LEU:HD21	1.75	0.67
2:B:333:LEU:HD13	2:B:333:LEU:C	2.19	0.67
3:J:297:ARG:NH1	3:J:301:MSE:SE	2.78	0.67
1:A:25:GLY:O	1:A:115:ASN:HA	1.94	0.67
2:D:24:VAL:O	2:D:26:THR:N	2.27	0.67
3:E:36:GLY:O	3:E:37:ASP:C	2.38	0.67
3:E:125:ALA:O	3:E:128:LEU:N	2.26	0.67
2:H:249:ALA:O	2:H:253:VAL:HG23	1.94	0.67
2:I:260:ASN:O	2:I:262:GLU:N	2.28	0.67
1:A:234:GLN:HB3	1:A:237:ARG:HH21	1.58	0.67
1:A:263:GLN:OE1	1:A:272:LEU:HD11	1.93	0.67
2:B:302:LEU:HD12	2:B:314:ARG:NH2	2.09	0.67
2:C:184:ARG:HG2	2:C:184:ARG:HH11	1.59	0.67
3:E:277:LEU:CD2	3:E:281:LEU:HD12	2.25	0.67
3:E:282:SER:HB2	3:E:283:PRO:HD2	1.77	0.67
2:G:295:VAL:HG22	2:G:301:ALA:CB	2.21	0.67
2:I:278:TRP:HD1	2:I:345:ARG:HD3	1.59	0.67
2:C:21:GLN:OE1	2:C:175:LEU:HD22	1.94	0.67
2:C:265:MET:HE1	2:D:294:MET:HE2	1.77	0.67
2:G:291:ARG:HH21	2:G:303:GLY:N	1.92	0.67
2:I:19:VAL:HG21	2:I:214:LEU:HD21	1.77	0.67
2:C:208:ARG:HG2	2:C:209:ALA:N	2.10	0.67
2:C:261:GLY:O	2:C:264:VAL:N	2.28	0.67
2:D:337:LYS:O	2:D:340:PRO:HD2	1.95	0.67
2:G:238:SER:HA	2:G:241:LEU:O	1.95	0.67
2:H:24:VAL:HG11	2:H:175:LEU:CD2	2.25	0.67
2:I:113:TYR:CD2	2:I:147:PRO:HB3	2.30	0.67
3:E:242:PRO:HG2	3:E:243:ALA:H	1.60	0.67
2:B:264:VAL:CG1	2:B:353:LEU:HD13	2.25	0.67
2:C:65:GLU:HA	2:C:119:ARG:HH21	1.58	0.67
2:C:152:PHE:O	2:C:153:LEU:HD23	1.95	0.67
2:D:277:GLU:HB2	2:D:280:ALA:HB3	1.76	0.67
2:D:292:ILE:HG22	2:D:293:ALA:N	2.08	0.67
1:F:119:LYS:H	1:F:119:LYS:CD	1.95	0.67
2:G:10:TRP:CE2	2:G:193:GLU:HB3	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:LEU:CD1	1:A:273:PHE:CZ	2.78	0.67
2:B:56:ARG:HG3	2:B:56:ARG:NH1	2.09	0.67
2:C:264:VAL:HG12	2:C:265:MET:N	2.09	0.67
2:D:357:LEU:HG	2:D:363:MET:HE1	1.75	0.67
2:H:292:ILE:O	2:H:296:GLN:HG3	1.95	0.67
2:I:265:MET:HE2	3:J:257:LYS:HG2	1.75	0.67
1:A:190:LEU:HD21	2:B:38:HIS:HE1	1.57	0.66
2:C:271:ALA:CB	2:C:276:ILE:HD11	2.25	0.66
3:J:145:THR:HG22	3:J:147:GLU:H	1.60	0.66
2:B:216:ASP:O	2:B:220:LEU:HG	1.96	0.66
3:E:80:ALA:HB1	3:E:81:PRO:HD2	1.77	0.66
2:D:260:ASN:O	2:D:262:GLU:N	2.27	0.66
2:G:248:GLN:O	2:G:250:LEU:C	2.37	0.66
2:H:149:HIS:ND1	2:H:150:VAL:HG23	2.09	0.66
3:J:241:ALA:N	3:J:242:PRO:HD2	2.09	0.66
2:C:43:PHE:O	2:C:155:ALA:HA	1.96	0.66
2:C:144:GLU:HA	2:C:144:GLU:OE1	1.96	0.66
2:D:285:MET:O	2:D:286:LEU:C	2.39	0.66
3:J:201:ALA:HA	3:J:204:LEU:HD22	1.77	0.66
2:B:44:SER:HB3	2:B:159:PRO:HG2	1.77	0.66
2:H:281:LEU:HD23	2:H:285:MET:HE2	1.78	0.66
2:I:238:SER:HB2	2:I:243:THR:HB	1.75	0.66
1:A:234:GLN:HA	1:A:237:ARG:NE	2.11	0.66
2:B:298:SER:O	2:B:300:ALA:N	2.29	0.66
2:D:10:TRP:CD1	2:D:190:ILE:HD12	2.30	0.66
2:D:15:PHE:HE2	2:D:57:LEU:HB3	1.60	0.66
3:E:116:ASP:O	3:E:118:ALA:N	2.29	0.66
2:G:220:LEU:HD22	2:G:241:LEU:HD11	1.76	0.66
1:A:74:PHE:CE2	1:F:206:VAL:HB	2.25	0.66
2:D:254:GLU:OE2	2:D:312:ARG:HD3	1.96	0.66
3:E:193:LEU:HD23	3:E:266:THR:HG21	1.78	0.66
1:F:281:ASN:C	1:F:283:ARG:N	2.50	0.66
2:B:21:GLN:HE22	2:B:175:LEU:HA	1.61	0.66
2:D:180:VAL:O	2:D:181:GLU:C	2.39	0.66
2:D:221:THR:O	2:D:225:ILE:HG13	1.95	0.66
3:E:50:CYS:SG	3:E:53:PRO:HA	2.36	0.66
2:I:21:GLN:OE1	2:I:176:LYS:O	2.13	0.66
1:A:267:THR:CG2	1:A:271:ALA:HB3	2.25	0.66
2:D:42:LEU:HD22	2:D:43:PHE:N	2.11	0.66
2:D:268:ILE:O	2:D:271:ALA:HB3	1.96	0.66
3:E:238:HIS:H	3:E:308:ARG:HD3	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:285:MET:HB2	2:G:332:LEU:HD21	1.77	0.66
2:H:91:ILE:HG21	2:H:107:LEU:HD13	1.78	0.66
1:A:291:ASN:O	1:A:292:ARG:HD2	1.95	0.65
2:D:254:GLU:OE2	2:D:312:ARG:CD	2.44	0.65
2:D:259:ALA:HB2	2:D:363:MET:HG2	1.77	0.65
1:F:166:ALA:CB	1:F:202:VAL:HG21	2.22	0.65
1:F:203:GLU:HG2	1:F:207:ASN:ND2	2.11	0.65
1:F:225:LYS:HD3	1:F:226:SER:N	2.11	0.65
2:I:277:GLU:HB2	2:I:280:ALA:HB3	1.75	0.65
2:C:198:HIS:CD2	2:C:203:LEU:HD11	2.31	0.65
2:C:243:THR:HG23	2:C:284:GLU:HG3	1.78	0.65
3:E:306:ILE:HG21	3:E:311:LEU:HD21	1.77	0.65
2:H:326:GLN:HE21	2:H:326:GLN:CA	1.96	0.65
1:A:74:PHE:CE1	1:F:203:GLU:C	2.74	0.65
1:A:223:MSE:HE2	1:A:292:ARG:HB2	1.77	0.65
1:A:261:LYS:HE3	1:A:293:LEU:O	1.95	0.65
2:D:353:LEU:O	2:D:357:LEU:HD13	1.96	0.65
1:F:222:LEU:HD13	1:F:285:MSE:HE3	1.78	0.65
2:I:243:THR:HG22	2:I:245:ASP:H	1.60	0.65
2:C:260:ASN:HD21	2:C:263:ARG:H	1.43	0.65
3:E:158:ARG:HG3	3:E:158:ARG:NH1	2.12	0.65
2:G:82:ILE:HG23	2:G:90:LEU:HD22	1.79	0.65
2:I:158:ASP:CG	2:I:161:LYS:HG2	2.22	0.65
2:I:215:ARG:CG	5:I:803:AGS:C4'	2.73	0.65
2:I:363:MET:HB3	2:I:364:PRO:CD	2.24	0.65
1:A:221:LEU:HD21	1:A:328:SER:HB3	1.79	0.65
2:B:202:ALA:HB1	2:B:237:VAL:HG21	1.79	0.65
2:B:243:THR:HG22	2:B:246:ASP:HB2	1.76	0.65
3:E:145:THR:HG22	3:E:146:ARG:N	2.10	0.65
2:H:137:ASN:HA	2:H:140:LEU:CD1	2.26	0.65
2:C:198:HIS:HB2	2:C:232:VAL:CG2	2.26	0.65
2:C:265:MET:CE	2:D:294:MET:SD	2.85	0.65
2:G:9:LYS:HD3	2:G:194:GLU:OE1	1.97	0.65
2:I:148:GLU:HA	2:I:148:GLU:OE1	1.97	0.65
1:A:1:MSE:HE1	1:A:127:PHE:CE1	2.31	0.65
1:A:59:THR:CG2	1:A:60:ASP:N	2.60	0.65
2:C:367:GLU:OE2	2:C:368:PRO:N	2.29	0.65
1:F:274:ASP:HA	1:F:279:TRP:CE3	2.31	0.65
1:F:309:GLU:O	1:F:312:LEU:HB3	1.96	0.65
3:J:200:ALA:O	3:J:204:LEU:HD13	1.97	0.65
1:A:124:ALA:O	1:A:126:TRP:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:ALA:HB1	2:B:276:ILE:HG21	1.78	0.65
2:G:6:LEU:HD22	2:G:190:ILE:HG22	1.79	0.65
2:I:351:MET:SD	3:J:290:LEU:HD22	2.36	0.65
3:E:14:LEU:HD13	3:E:44:LEU:HD11	1.78	0.65
3:E:95:GLU:O	3:E:99:LYS:HB2	1.97	0.65
3:E:307:ASN:O	3:E:309:GLU:N	2.30	0.65
2:H:201:ARG:HE	2:H:205:LEU:HD21	1.61	0.65
2:H:271:ALA:HA	2:H:274:ARG:HE	1.61	0.65
2:C:221:THR:O	2:C:225:ILE:HG13	1.97	0.64
1:F:53:PHE:CZ	1:F:67:LEU:HD22	2.32	0.64
2:I:6:LEU:CD1	2:I:221:THR:HB	2.27	0.64
1:A:74:PHE:CE2	1:F:206:VAL:CB	2.78	0.64
2:D:42:LEU:HD23	2:D:154:LEU:CB	2.26	0.64
2:D:329:TYR:C	2:D:329:TYR:CD2	2.75	0.64
2:G:61:GLY:HA2	2:G:72:PRO:HG3	1.79	0.64
2:H:250:LEU:HD22	2:H:309:ILE:HD12	1.79	0.64
2:I:19:VAL:HG12	2:I:178:LEU:CD2	2.21	0.64
2:I:283:VAL:HG22	2:I:336:ARG:NH1	2.13	0.64
2:B:367:GLU:N	2:B:367:GLU:OE2	2.30	0.64
2:C:232:VAL:CG2	2:C:232:VAL:O	2.45	0.64
3:E:232:LEU:O	3:E:233:LEU:C	2.39	0.64
2:G:144:GLU:C	2:G:146:PRO:HD3	2.23	0.64
2:H:279:GLU:HG2	2:H:339:LEU:CD2	2.28	0.64
2:I:268:ILE:HD11	2:I:353:LEU:HD12	1.78	0.64
3:J:238:HIS:ND1	3:J:239:GLU:N	2.45	0.64
1:A:214:PRO:O	1:A:218:VAL:HG23	1.98	0.64
1:A:222:LEU:O	1:A:224:GLY:N	2.31	0.64
2:I:19:VAL:CG1	2:I:178:LEU:HD22	2.22	0.64
2:B:186:GLN:HE21	2:B:190:ILE:HD11	1.63	0.64
2:C:112:GLN:CD	2:C:121:LYS:HE2	2.22	0.64
3:E:31:ALA:HB2	3:E:164:LEU:HB3	1.78	0.64
1:F:25:GLY:HA3	1:F:139:CYS:O	1.97	0.64
2:D:38:HIS:CD2	2:D:40:ALA:H	2.15	0.64
3:E:136:PRO:O	3:E:137:ALA:O	2.15	0.64
1:F:64:ILE:HG12	1:F:96:GLN:HE21	1.61	0.64
2:G:250:LEU:CD2	2:G:288:LEU:HD13	2.28	0.64
2:H:7:ALA:HA	2:H:218:LEU:HD23	1.79	0.64
2:H:93:ILE:HG12	2:I:133:ARG:HH12	1.63	0.64
2:H:279:GLU:HG2	2:H:339:LEU:HD23	1.80	0.64
2:B:260:ASN:HD22	2:B:263:ARG:CB	2.06	0.64
2:B:343:PRO:CG	2:B:347:MET:SD	2.86	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:310:LEU:C	1:F:314:GLN:HG3	2.23	0.64
2:G:76:CYS:SG	2:G:78:ASN:HB2	2.38	0.64
2:H:215:ARG:NH1	6:H:1400:PO4:O1	2.30	0.64
2:B:58:LEU:HD23	2:B:153:LEU:HD22	1.79	0.64
2:B:245:ASP:O	2:B:246:ASP:C	2.40	0.64
2:D:124:LEU:HD22	2:D:124:LEU:C	2.22	0.64
2:D:253:VAL:O	2:D:254:GLU:C	2.41	0.64
2:D:345:ARG:CZ	3:E:150:ARG:HE	2.10	0.64
1:F:295:GLN:H	1:F:295:GLN:NE2	1.96	0.64
2:G:6:LEU:CB	2:G:190:ILE:CG2	2.64	0.64
2:I:246:ASP:CB	2:I:248:GLN:HG2	2.27	0.64
2:B:347:MET:HG3	2:C:290:HIS:CE1	2.33	0.63
1:F:57:PRO:C	1:F:59:THR:H	2.06	0.63
3:J:161:LEU:HD12	3:J:161:LEU:H	1.63	0.63
1:A:269:LEU:CG	1:A:273:PHE:CZ	2.81	0.63
2:D:259:ALA:HA	2:D:363:MET:CE	2.28	0.63
2:D:360:HIS:CD2	2:D:363:MET:HG3	2.33	0.63
1:F:225:LYS:HD3	1:F:226:SER:H	1.63	0.63
2:G:281:LEU:HG	2:G:285:MET:HE2	1.80	0.63
2:H:128:VAL:HG23	2:H:162:LEU:HD21	1.80	0.63
2:I:256:MET:HE2	2:I:353:LEU:HD22	1.80	0.63
1:A:71:MSE:SE	1:F:231:HIS:HB2	2.47	0.63
2:D:281:LEU:CD1	2:D:285:MET:HE2	2.28	0.63
3:E:289:ILE:HG23	3:E:319:ILE:CD1	2.28	0.63
1:F:61:TRP:HA	1:F:64:ILE:HD13	1.81	0.63
2:H:93:ILE:HG12	2:I:133:ARG:NH1	2.13	0.63
2:I:279:GLU:HB3	3:J:149:GLU:OE2	1.97	0.63
2:C:293:ALA:HA	2:C:296:GLN:HG3	1.80	0.63
3:E:151:LEU:HD11	3:E:155:LEU:HD12	1.79	0.63
2:B:179:ASP:HB2	2:B:182:GLN:NE2	2.13	0.63
2:C:65:GLU:HA	2:C:119:ARG:NH2	2.13	0.63
2:C:86:ARG:NH1	2:D:141:LYS:HG3	2.12	0.63
3:E:68:MSE:HE3	3:E:73:HIS:CB	2.28	0.63
2:B:350:GLU:OE1	2:C:294:MET:CE	2.47	0.63
2:C:35:GLY:O	2:C:37:ILE:N	2.31	0.63
1:F:308:THR:HG23	1:F:320:VAL:HG13	1.81	0.63
2:G:316:LEU:HD22	2:G:320:ILE:HD11	1.80	0.63
2:B:13:GLN:NE2	2:B:83:GLU:OE2	2.31	0.63
2:B:41:TYR:C	2:B:170:CYS:SG	2.81	0.63
2:D:263:ARG:O	2:D:266:ALA:HB3	1.99	0.63
1:F:330:LEU:O	1:F:330:LEU:HD13	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:145:THR:HG22	3:E:147:GLU:H	1.64	0.63
2:I:271:ALA:O	2:I:276:ILE:HG13	1.99	0.63
1:A:268:PRO:O	1:A:270:ARG:N	2.30	0.63
2:H:306:MET:HE1	2:H:313:MET:HE2	1.79	0.63
2:I:6:LEU:CB	2:I:218:LEU:HB3	2.29	0.63
2:B:165:THR:HB	2:B:169:ARG:HH12	1.64	0.62
2:D:15:PHE:HD2	2:D:57:LEU:HD13	1.62	0.62
2:G:278:TRP:CE3	2:G:349:VAL:HG21	2.34	0.62
2:C:147:PRO:HB2	2:C:149:HIS:CE1	2.34	0.62
2:D:306:MET:C	2:D:308:ALA:H	2.07	0.62
3:E:253:MSE:O	3:E:257:LYS:HG3	1.99	0.62
1:F:26:ASN:O	1:F:28:PRO:HD3	1.99	0.62
2:G:6:LEU:CD2	2:G:194:GLU:HG3	2.29	0.62
1:A:331:LEU:N	1:A:331:LEU:HD23	2.14	0.62
1:F:99:THR:O	1:F:103:LEU:HD13	1.99	0.62
2:H:215:ARG:CZ	6:H:1400:PO4:O1	2.47	0.62
2:I:215:ARG:HB2	5:I:803:AGS:C5'	2.28	0.62
2:D:144:GLU:C	2:D:146:PRO:HD3	2.24	0.62
2:D:259:ALA:CA	2:D:363:MET:HE2	2.28	0.62
2:D:360:HIS:HD2	2:D:363:MET:N	1.97	0.62
3:E:297:ARG:HG2	3:E:298:GLU:N	2.14	0.62
1:A:263:GLN:HG2	1:A:266:HIS:HD2	1.64	0.62
2:B:42:LEU:HD23	2:B:42:LEU:C	2.24	0.62
2:C:49:VAL:HG11	2:C:175:LEU:HB3	1.80	0.62
2:C:260:ASN:ND2	2:C:263:ARG:H	1.97	0.62
2:D:260:ASN:OD1	2:D:263:ARG:HB2	1.99	0.62
1:F:299:ARG:O	1:F:302:VAL:HB	1.98	0.62
2:H:257:VAL:HG11	2:H:320:ILE:CD1	2.30	0.62
2:I:295:VAL:HG11	2:I:314:ARG:HG2	1.81	0.62
3:J:30:GLN:CG	3:J:148:PRO:HD3	2.22	0.62
3:J:110:LYS:HB2	3:J:139:THR:HG23	1.82	0.62
1:A:278:VAL:O	1:A:280:GLN:OE1	2.18	0.62
3:E:220:LEU:HD21	3:E:248:LEU:HD13	1.82	0.62
3:J:244:ARG:HG2	3:J:247:TRP:CZ3	2.34	0.62
3:E:30:GLN:CG	3:E:163:TYR:CD1	2.81	0.62
1:F:46:GLY:O	1:F:77:ARG:HB2	1.99	0.62
2:G:288:LEU:O	2:G:292:ILE:HG13	1.98	0.62
2:H:100:LYS:HE2	2:I:136:PHE:HD2	1.64	0.62
2:C:97:SER:CB	2:C:100:LYS:HD2	2.30	0.62
1:F:162:LEU:HD11	1:F:185:LEU:HD21	1.82	0.62
2:G:102:GLU:HG3	2:G:105:ARG:NH2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:350:GLU:O	2:H:354:LEU:HD12	2.00	0.62
2:B:309:ILE:CG2	2:B:313:MET:HG2	2.28	0.62
3:E:149:GLU:C	3:E:151:LEU:H	2.08	0.62
1:A:154:ARG:HH11	1:A:157:GLN:HE21	1.46	0.62
2:C:341:TYR:HB2	2:D:333:LEU:HD11	1.81	0.62
2:D:366:PRO:O	2:D:367:GLU:HG3	2.00	0.62
3:E:303:VAL:HB	3:E:306:ILE:CD1	2.26	0.62
2:H:229:ASP:OD2	2:I:30:ASN:OD1	2.18	0.62
3:J:64:GLY:O	3:J:68:MSE:HB2	2.00	0.62
2:C:100:LYS:HD3	2:D:133:ARG:HE	1.65	0.61
2:D:10:TRP:CG	2:D:190:ILE:HD12	2.34	0.61
2:D:129:HIS:HB2	2:D:161:LYS:HB2	1.82	0.61
1:F:93:ILE:HG23	1:F:97:LEU:HD13	1.82	0.61
2:H:343:PRO:HB3	2:I:283:VAL:HG13	1.80	0.61
2:B:5:VAL:HG23	2:B:7:ALA:HB3	1.81	0.61
2:C:77:ASP:O	2:C:81:GLU:HG3	2.00	0.61
1:F:199:LEU:HB3	1:F:200:PRO:HD3	1.82	0.61
1:F:303:GLN:O	1:F:306:THR:HB	2.00	0.61
2:G:316:LEU:HB3	2:G:320:ILE:HD12	1.82	0.61
3:J:90:VAL:HG22	3:J:124:ALA:N	2.15	0.61
3:J:202:LEU:C	3:J:202:LEU:HD22	2.25	0.61
2:C:184:ARG:HG2	2:C:184:ARG:NH1	2.15	0.61
2:C:271:ALA:C	2:C:276:ILE:HD11	2.25	0.61
2:D:277:GLU:HB2	2:D:280:ALA:CB	2.29	0.61
2:H:112:GLN:HB2	2:H:121:LYS:HZ3	1.65	0.61
2:H:306:MET:CE	2:H:313:MET:HE2	2.30	0.61
2:I:363:MET:SD	2:I:364:PRO:HD2	2.40	0.61
2:G:15:PHE:CE2	2:G:57:LEU:HB3	2.36	0.61
2:H:201:ARG:HH21	2:H:205:LEU:HD23	1.64	0.61
2:C:202:ALA:HB2	2:C:234:THR:HA	1.82	0.61
2:B:205:LEU:HD11	2:B:234:THR:HG23	1.82	0.61
2:C:120:PHE:CD2	2:C:120:PHE:N	2.69	0.61
2:C:271:ALA:HB1	2:C:276:ILE:HD11	1.81	0.61
2:D:360:HIS:HD2	2:D:363:MET:H	1.48	0.61
2:G:98:ARG:CG	2:H:169:ARG:HH22	2.13	0.61
2:I:215:ARG:CA	5:I:803:AGS:O4'	2.48	0.61
2:B:44:SER:CB	2:B:159:PRO:CG	2.78	0.61
2:C:15:PHE:CE1	2:C:57:LEU:HB3	2.35	0.61
2:C:58:LEU:HD23	2:C:153:LEU:CD2	2.31	0.61
2:C:351:MET:HA	2:C:351:MET:HE3	1.83	0.61
2:I:11:ARG:NH2	2:I:56:ARG:NH2	2.46	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:VAL:HG11	1:A:111:ILE:HD11	1.82	0.61
2:D:259:ALA:HB2	2:D:363:MET:CG	2.30	0.61
2:G:186:GLN:O	2:G:190:ILE:HG13	2.01	0.61
3:J:126:ASN:HA	3:J:129:LEU:HD13	1.82	0.61
1:F:47:PHE:HA	1:F:77:ARG:O	1.99	0.61
1:F:202:VAL:O	1:F:206:VAL:HG23	2.01	0.61
2:G:6:LEU:CB	2:G:190:ILE:HG21	2.11	0.61
2:B:76:CYS:O	2:B:80:ARG:HG3	2.01	0.61
2:C:285:MET:O	2:C:286:LEU:C	2.43	0.61
1:A:264:SER:O	1:A:265:ALA:HB3	2.01	0.60
1:A:275:LYS:HA	1:A:275:LYS:HE2	1.83	0.60
2:C:265:MET:HE1	2:D:294:MET:CE	2.31	0.60
2:C:354:LEU:O	2:C:357:LEU:N	2.34	0.60
2:H:21:GLN:OE1	2:H:175:LEU:HB3	2.01	0.60
2:I:56:ARG:HH11	2:I:56:ARG:HG3	1.64	0.60
1:A:222:LEU:CD1	1:A:285:MSE:HE3	2.31	0.60
2:C:278:TRP:CZ2	2:C:346:ARG:HD2	2.36	0.60
2:D:355:ARG:HH21	3:E:332:PRO:HD3	1.66	0.60
1:F:27:ASP:OD2	1:F:178:LEU:HD12	2.01	0.60
2:G:341:TYR:CZ	2:H:337:LYS:HG2	2.36	0.60
2:B:44:SER:HB3	2:B:159:PRO:CG	2.32	0.60
2:B:64:CYS:SG	2:B:66:THR:HB	2.41	0.60
2:D:357:LEU:HA	2:D:363:MET:HE1	1.83	0.60
1:F:13:LEU:HD23	1:F:41:VAL:CG2	2.31	0.60
1:F:304:LEU:CB	1:F:327:LEU:HD11	2.32	0.60
2:G:10:TRP:CH2	2:G:193:GLU:CD	2.79	0.60
3:J:188:LEU:HD23	3:J:268:VAL:HG21	1.84	0.60
3:J:320:GLU:HA	3:J:323:LEU:HD12	1.83	0.60
2:B:226:ALA:O	2:C:26:THR:HG22	2.01	0.60
2:C:265:MET:HE1	2:D:294:MET:SD	2.42	0.60
2:G:274:ARG:HE	2:G:276:ILE:CD1	2.09	0.60
1:A:213:THR:HG22	1:A:215:PHE:H	1.65	0.60
2:B:277:GLU:O	2:B:278:TRP:C	2.45	0.60
2:C:347:MET:HG2	2:D:290:HIS:CE1	2.36	0.60
2:D:355:ARG:NH1	3:E:287:GLN:HB3	2.16	0.60
3:E:50:CYS:SG	3:E:53:PRO:CA	2.89	0.60
1:A:130:LEU:O	1:A:132:ASN:N	2.35	0.60
2:C:140:LEU:HD13	2:C:169:ARG:NH1	2.17	0.60
2:D:277:GLU:HB3	3:E:149:GLU:HB2	1.84	0.60
3:E:41:ILE:HD12	3:E:142:PHE:HB3	1.83	0.60
3:E:296:ILE:O	3:E:297:ARG:C	2.44	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:188:LEU:HG	1:F:197:LEU:HD22	1.83	0.60
2:G:341:TYR:C	2:H:333:LEU:HD11	2.26	0.60
3:J:316:LEU:HA	3:J:319:ILE:HD12	1.84	0.60
2:D:332:LEU:CD2	2:D:352:THR:HG22	2.32	0.60
2:G:6:LEU:HD23	2:G:194:GLU:HG3	1.82	0.60
2:I:277:GLU:HB3	3:J:149:GLU:HG3	1.82	0.60
3:J:79:LEU:HD13	3:J:112:VAL:HG13	1.84	0.60
1:A:333:HIS:HB3	2:B:298:SER:OG	2.01	0.60
1:F:46:GLY:C	1:F:77:ARG:HB2	2.27	0.60
2:H:64:CYS:SG	2:H:66:THR:HB	2.41	0.60
2:H:191:LEU:HD12	2:H:203:LEU:HD21	1.84	0.60
2:H:302:LEU:HD12	2:H:314:ARG:HE	1.65	0.60
2:I:200:PRO:HB2	2:I:305:ASP:HB2	0.80	0.60
3:J:214:GLU:HG2	3:J:218:GLN:HE21	1.66	0.60
2:C:245:ASP:O	2:C:246:ASP:C	2.43	0.60
2:H:89:ASP:HB3	2:H:121:LYS:HA	1.83	0.60
2:I:198:HIS:HA	2:I:232:VAL:O	2.02	0.60
2:B:243:THR:CG2	2:B:246:ASP:HB2	2.31	0.60
2:D:60:LYS:HA	2:D:82:ILE:HD12	1.83	0.60
1:F:165:ALA:HB1	1:F:199:LEU:HD13	1.84	0.60
2:I:7:ALA:CB	2:I:215:ARG:HG3	2.31	0.60
2:I:244:LEU:HD21	2:I:276:ILE:CG1	2.31	0.60
3:J:111:VAL:HA	3:J:140:TRP:O	2.01	0.60
3:J:212:ALA:HB1	3:J:244:ARG:NH2	2.16	0.60
1:A:20:ALA:HB2	1:A:110:LEU:HB3	1.84	0.59
2:B:347:MET:HG3	2:C:290:HIS:ND1	2.17	0.59
2:C:52:THR:O	2:C:55:ALA:HB3	2.02	0.59
2:C:261:GLY:O	2:C:262:GLU:C	2.44	0.59
2:G:263:ARG:O	2:G:267:LEU:HG	2.00	0.59
3:J:220:LEU:HA	3:J:232:LEU:HD21	1.83	0.59
1:A:19:ALA:HB3	1:A:133:ARG:HB3	1.85	0.59
2:B:278:TRP:O	2:B:280:ALA:N	2.35	0.59
2:C:18:VAL:HG11	2:C:54:ILE:HD11	1.84	0.59
2:C:59:ALA:O	2:C:82:ILE:HD13	2.00	0.59
2:C:257:VAL:O	2:C:360:HIS:CE1	2.55	0.59
2:C:300:ALA:O	2:C:302:LEU:N	2.35	0.59
2:D:247:ASP:O	2:D:251:SER:HB2	2.02	0.59
2:D:360:HIS:CG	2:D:361:PRO:N	2.70	0.59
1:F:130:LEU:HB3	1:F:134:SER:OG	2.02	0.59
1:F:264:SER:O	1:F:265:ALA:HB3	2.01	0.59
1:F:316:TYR:CG	1:F:316:TYR:O	2.55	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:95:ALA:HB3	2:H:127:GLU:O	2.01	0.59
2:H:129:HIS:HD2	2:H:161:LYS:HD2	1.66	0.59
1:A:119:LYS:O	1:A:123:ASN:ND2	2.35	0.59
1:A:128:THR:O	1:A:131:ALA:HB3	2.02	0.59
3:E:163:TYR:CE2	3:E:165:ALA:HB2	2.36	0.59
1:F:310:LEU:HB3	1:F:314:GLN:CD	2.27	0.59
2:G:179:ASP:HB3	2:G:182:GLN:HB2	1.84	0.59
2:G:286:LEU:HG	2:G:332:LEU:HD23	1.83	0.59
2:H:21:GLN:HE22	2:H:49:VAL:CG1	2.15	0.59
2:H:152:PHE:O	2:H:153:LEU:HD23	2.02	0.59
1:A:73:LEU:HB2	1:F:207:ASN:CB	2.31	0.59
2:C:186:GLN:HG3	2:C:190:ILE:CD1	2.32	0.59
2:D:302:LEU:HD13	2:D:310:GLU:OE2	2.03	0.59
2:D:345:ARG:NH2	3:E:150:ARG:HE	2.00	0.59
1:F:47:PHE:HD2	1:F:78:GLN:C	2.05	0.59
2:I:18:VAL:CG1	2:I:25:LEU:HD11	2.32	0.59
2:B:353:LEU:O	2:B:354:LEU:C	2.44	0.59
2:C:292:ILE:CG1	2:C:313:MET:HE1	2.32	0.59
2:D:111:VAL:CG1	2:D:112:GLN:N	2.65	0.59
2:D:363:MET:CB	2:D:364:PRO:CD	2.79	0.59
1:F:223:MSE:HE1	1:F:292:ARG:CB	2.32	0.59
1:F:251:GLN:HE22	3:J:307:ASN:ND2	2.00	0.59
1:F:315:ASP:O	1:F:316:TYR:C	2.44	0.59
2:H:21:GLN:OE1	2:H:175:LEU:HD22	2.02	0.59
2:H:78:ASN:O	2:H:82:ILE:HG13	2.01	0.59
3:J:229:TRP:CE3	3:J:319:ILE:HG21	2.37	0.59
1:A:193:PRO:CG	2:B:36:ARG:HH22	2.11	0.59
2:B:81:GLU:HB2	2:B:87:PHE:CD1	2.35	0.59
2:C:120:PHE:HB3	2:C:149:HIS:O	2.01	0.59
2:C:200:PRO:HG2	2:C:305:ASP:CG	2.27	0.59
3:E:5:PRO:O	3:E:7:LEU:N	2.35	0.59
1:F:174:TYR:HB2	1:F:181:LEU:CD2	2.33	0.59
2:H:272:ALA:HB2	2:H:278:TRP:HH2	1.68	0.59
3:J:4:TYR:HB3	3:J:5:PRO:HD2	1.83	0.59
3:J:253:MSE:O	3:J:253:MSE:HE3	2.02	0.59
2:C:351:MET:HE1	2:D:293:ALA:CB	2.32	0.59
3:J:18:TYR:HB3	3:J:48:LEU:HD21	1.85	0.59
2:B:276:ILE:CD1	2:B:281:LEU:HB2	2.20	0.59
2:C:264:VAL:HG13	2:C:353:LEU:HD13	1.84	0.59
2:D:357:LEU:O	2:D:360:HIS:HB3	2.01	0.59
3:E:20:ALA:HB3	3:E:22:ARG:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:21:GLN:HE22	2:H:49:VAL:HG13	1.68	0.59
2:I:250:LEU:HD21	2:I:312:ARG:HD2	1.84	0.59
1:F:279:TRP:O	1:F:279:TRP:CD2	2.56	0.59
2:H:111:VAL:CG1	2:H:150:VAL:HG21	2.33	0.59
3:E:279:ASN:C	3:E:281:LEU:H	2.11	0.59
3:E:281:LEU:HD21	3:E:323:LEU:HD21	1.84	0.59
1:F:264:SER:O	1:F:265:ALA:CB	2.51	0.59
2:G:240:MET:HG3	2:G:241:LEU:H	1.68	0.59
2:B:51:LYS:NZ	5:B:802:AGS:S1G	2.71	0.58
2:B:263:ARG:HG2	2:B:267:LEU:CD1	2.32	0.58
2:C:281:LEU:O	2:C:285:MET:HG3	2.02	0.58
2:C:360:HIS:CD2	2:C:361:PRO:CD	2.80	0.58
1:F:211:HIS:CG	1:F:211:HIS:O	2.56	0.58
2:G:295:VAL:HA	2:G:298:SER:O	2.03	0.58
2:H:11:ARG:HH22	2:I:165:THR:HG22	1.68	0.58
2:H:316:LEU:HB3	2:H:320:ILE:HD12	1.85	0.58
2:I:248:GLN:CG	2:I:274:ARG:HH22	2.13	0.58
3:J:92:ALA:O	3:J:96:VAL:HG23	2.03	0.58
1:A:130:LEU:HB3	1:A:134:SER:OG	2.02	0.58
1:A:213:THR:CG2	1:A:215:PHE:HB2	2.33	0.58
2:D:355:ARG:NH2	3:E:332:PRO:HD3	2.17	0.58
3:E:314:ASP:OD2	3:E:318:ARG:NH2	2.37	0.58
1:F:285:MSE:CG	1:F:285:MSE:CE	2.80	0.58
1:F:299:ARG:HG3	3:J:317:LEU:HD21	1.86	0.58
2:G:355:ARG:HD2	2:G:355:ARG:O	2.02	0.58
2:G:363:MET:HE2	2:G:363:MET:HA	1.85	0.58
3:J:29:ILE:HD12	3:J:29:ILE:N	2.17	0.58
2:B:299:PRO:C	2:B:301:ALA:H	2.11	0.58
2:C:133:ARG:HD3	2:C:133:ARG:H	1.66	0.58
2:C:324:ASP:O	2:C:327:LEU:HB3	2.03	0.58
3:E:220:LEU:HA	3:E:223:SER:HB2	1.85	0.58
1:F:59:THR:O	1:F:60:ASP:HB2	2.02	0.58
2:G:210:ALA:HB2	2:G:220:LEU:HD12	1.85	0.58
2:H:51:LYS:HE2	6:H:1400:PO4:O2	2.03	0.58
1:A:85:PRO:HB2	1:A:88:GLY:H	1.68	0.58
1:A:285:MSE:CE	1:A:285:MSE:CG	2.80	0.58
2:D:360:HIS:CG	2:D:363:MET:HG3	2.38	0.58
3:E:209:ASN:O	3:E:212:ALA:HB3	2.04	0.58
2:G:43:PHE:O	2:G:51:LYS:HD2	2.02	0.58
2:G:252:LEU:O	2:G:252:LEU:HD23	2.03	0.58
2:G:277:GLU:HG2	2:G:280:ALA:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:8:ARG:CG	3:J:9:PRO:HD3	2.33	0.58
1:A:54:SER:HA	1:A:83:LEU:HB2	1.86	0.58
1:A:269:LEU:O	1:A:273:PHE:CD1	2.57	0.58
2:B:76:CYS:SG	2:B:78:ASN:N	2.75	0.58
2:B:285:MET:O	2:B:286:LEU:C	2.47	0.58
2:C:201:ARG:HG3	2:C:234:THR:HG23	1.86	0.58
2:D:246:ASP:HB3	2:D:248:GLN:NE2	2.18	0.58
3:E:214:GLU:O	3:E:218:GLN:HG3	2.04	0.58
1:F:71:MSE:HA	1:F:78:GLN:HE22	1.69	0.58
1:F:247:LEU:HD21	1:F:308:THR:CG2	2.33	0.58
2:I:254:GLU:O	2:I:258:GLU:HG2	2.04	0.58
2:I:261:GLY:HA2	2:I:357:LEU:HD21	1.86	0.58
3:J:188:LEU:HD11	3:J:192:ARG:HE	1.68	0.58
2:B:362:ARG:O	2:B:364:PRO:HD3	2.03	0.58
2:C:49:VAL:HG11	2:C:175:LEU:CB	2.32	0.58
2:D:260:ASN:OD1	2:D:263:ARG:CB	2.51	0.58
1:F:250:LEU:N	1:F:250:LEU:HD23	2.18	0.58
2:C:204:GLN:O	2:C:207:ALA:HB3	2.04	0.58
2:C:367:GLU:CG	2:D:321:PRO:HA	2.34	0.58
2:D:278:TRP:CE2	2:D:346:ARG:HB2	2.39	0.58
3:E:204:LEU:O	3:E:209:ASN:HB2	2.03	0.58
1:F:304:LEU:HD13	1:F:327:LEU:CD2	2.32	0.58
2:G:253:VAL:O	2:G:256:MET:HB3	2.04	0.58
1:A:17:LEU:HD21	1:A:109:LEU:CD1	2.34	0.58
1:A:232:ILE:O	1:A:236:LEU:HB2	2.04	0.58
1:A:293:LEU:HB3	1:A:298:LEU:HD11	1.85	0.58
2:B:63:ASN:O	2:B:78:ASN:ND2	2.25	0.58
2:D:15:PHE:CE2	2:D:57:LEU:HB3	2.38	0.58
2:G:61:GLY:CA	2:G:72:PRO:HG3	2.32	0.58
2:G:239:ALA:HB1	2:H:23:HIS:CD2	2.39	0.58
2:I:6:LEU:HB2	2:I:218:LEU:O	2.04	0.58
3:E:194:SER:O	3:E:195:ALA:HB3	2.03	0.58
2:G:177:ALA:HB1	2:G:212:GLY:O	2.03	0.58
2:G:191:LEU:HD22	2:G:196:ILE:HB	1.86	0.58
1:A:196:LYS:H	1:A:201:ARG:NH1	2.01	0.58
2:D:91:ILE:HD11	2:D:121:LYS:HE3	1.86	0.58
2:D:236:ALA:O	2:D:239:ALA:HB3	2.04	0.58
2:G:362:ARG:O	2:G:363:MET:HB2	2.02	0.58
1:A:103:LEU:C	1:A:103:LEU:HD12	2.28	0.57
1:A:119:LYS:HD3	1:A:119:LYS:N	2.04	0.57
2:D:289:LEU:HD12	2:D:329:TYR:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:251:LEU:O	3:E:252:LEU:C	2.46	0.57
3:J:111:VAL:HG12	3:J:140:TRP:HB2	1.84	0.57
1:A:273:PHE:HB3	1:A:279:TRP:CB	2.34	0.57
2:C:244:LEU:HD22	2:C:248:GLN:HB2	1.86	0.57
2:C:314:ARG:HG2	2:C:314:ARG:HH11	1.69	0.57
2:D:19:VAL:HG21	2:D:186:GLN:HG3	1.85	0.57
2:D:185:HIS:ND1	2:D:185:HIS:O	2.37	0.57
2:D:276:ILE:CG2	2:D:277:GLU:N	2.67	0.57
3:E:42:TYR:HE2	3:E:46:ARG:HH12	1.51	0.57
3:E:220:LEU:O	3:E:224:VAL:HG23	2.03	0.57
3:E:321:HIS:CE1	3:E:327:VAL:HG22	2.39	0.57
2:H:21:GLN:O	2:H:25:LEU:HG	2.03	0.57
2:I:309:ILE:HG22	2:I:313:MET:HG2	1.85	0.57
2:B:316:LEU:O	2:B:317:ALA:C	2.46	0.57
2:C:80:ARG:O	2:C:84:GLN:HG3	2.04	0.57
3:E:57:LYS:HG3	3:E:58:SER:H	1.68	0.57
1:F:166:ALA:HB1	1:F:202:VAL:CG2	2.25	0.57
3:J:253:MSE:O	3:J:257:LYS:HG3	2.04	0.57
1:A:90:ASN:OD1	1:A:93:ILE:HG13	2.03	0.57
1:A:106:ASP:OD2	1:F:225:LYS:HB2	2.03	0.57
2:B:10:TRP:CE2	2:B:190:ILE:HG23	2.39	0.57
2:B:143:LEU:HD23	2:B:144:GLU:N	2.20	0.57
2:B:251:SER:HB3	2:B:267:LEU:HD21	1.86	0.57
2:C:102:GLU:HA	2:C:105:ARG:HD3	1.87	0.57
2:D:259:ALA:HB1	2:D:363:MET:HG2	1.84	0.57
2:D:363:MET:CG	2:D:364:PRO:HD2	2.34	0.57
2:H:100:LYS:CE	2:I:133:ARG:HA	2.34	0.57
2:I:61:GLY:CA	2:I:72:PRO:HG3	2.34	0.57
1:A:187:ARG:HG2	1:A:188:LEU:N	2.19	0.57
3:E:152:LEU:HD22	3:E:154:THR:CG2	2.34	0.57
3:E:209:ASN:O	3:E:212:ALA:N	2.37	0.57
3:E:270:VAL:HG23	3:E:270:VAL:O	2.03	0.57
1:F:295:GLN:NE2	1:F:295:GLN:N	2.53	0.57
2:G:6:LEU:CD2	2:G:191:LEU:HD23	2.34	0.57
1:A:24:LEU:HD13	1:A:117:LEU:HG	1.86	0.57
1:A:279:TRP:O	1:A:279:TRP:CD2	2.58	0.57
1:A:293:LEU:HB3	1:A:298:LEU:CD1	2.35	0.57
2:C:30:ASN:O	2:C:33:SER:N	2.38	0.57
2:C:232:VAL:O	2:C:232:VAL:HG23	2.05	0.57
2:D:25:LEU:HD21	2:D:54:ILE:HD11	1.86	0.57
3:E:17:SER:HB2	3:E:22:ARG:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:216:LEU:O	3:E:219:ALA:HB3	2.04	0.57
2:H:360:HIS:HD2	2:H:363:MET:N	1.86	0.57
2:I:10:TRP:HB2	2:I:218:LEU:CD1	2.35	0.57
2:G:19:VAL:HG12	2:G:178:LEU:CD1	2.35	0.57
2:B:36:ARG:CB	2:B:36:ARG:NH1	2.58	0.57
2:B:286:LEU:O	2:B:289:LEU:HB2	2.05	0.57
2:C:271:ALA:HB1	2:C:276:ILE:CD1	2.35	0.57
2:C:309:ILE:HG13	2:C:313:MET:HG2	1.87	0.57
3:E:75:ASP:HB3	3:E:110:LYS:HA	1.87	0.57
2:G:9:LYS:CD	2:G:194:GLU:CD	2.78	0.57
2:G:64:CYS:SG	2:G:66:THR:HB	2.45	0.57
2:G:82:ILE:HG23	2:G:90:LEU:CD2	2.35	0.57
2:G:214:LEU:HD23	5:G:804:AGS:C8	2.34	0.57
2:H:209:ALA:HB2	2:H:241:LEU:HD11	1.86	0.57
1:A:2:ILE:HB	1:A:135:VAL:HG22	1.87	0.57
1:A:289:ALA:C	1:A:291:ASN:H	2.13	0.57
2:C:333:LEU:O	2:C:335:GLY:N	2.38	0.57
3:E:90:VAL:O	3:E:94:ARG:HG3	2.05	0.57
3:E:90:VAL:HG22	3:E:124:ALA:N	2.19	0.57
1:F:222:LEU:O	1:F:223:MSE:HB2	2.04	0.57
2:H:302:LEU:HD13	2:H:310:GLU:HG3	1.86	0.57
2:I:148:GLU:CD	2:I:149:HIS:N	2.62	0.57
2:I:286:LEU:HD23	2:I:332:LEU:HD23	1.85	0.57
2:B:242:GLY:O	2:B:244:LEU:HG	2.05	0.57
2:B:253:VAL:O	2:B:256:MET:HB3	2.05	0.57
2:B:362:ARG:O	2:B:364:PRO:CD	2.53	0.57
2:D:199:GLU:OE1	2:D:233:SER:HB2	2.05	0.57
2:G:10:TRP:HD1	2:G:190:ILE:HG23	1.69	0.57
2:G:98:ARG:CD	2:H:140:LEU:HD13	2.34	0.57
2:G:198:HIS:CD2	2:G:203:LEU:HD11	2.40	0.57
2:I:240:MET:HE1	3:J:157:SER:HB3	1.85	0.57
3:J:214:GLU:HG2	3:J:218:GLN:NE2	2.20	0.57
3:J:317:LEU:HD22	3:J:317:LEU:C	2.30	0.57
2:B:165:THR:HB	2:B:169:ARG:NH1	2.20	0.56
2:C:296:GLN:OE1	2:C:322:PRO:HB3	2.04	0.56
1:A:6:PRO:HG2	1:A:30:LEU:HD13	1.87	0.56
1:A:222:LEU:HD12	1:A:285:MSE:HE3	1.88	0.56
2:B:238:SER:HA	2:B:241:LEU:O	2.05	0.56
2:D:148:GLU:HA	2:D:148:GLU:OE1	2.04	0.56
1:F:218:VAL:HG11	1:F:253:GLU:HG3	1.87	0.56
2:G:10:TRP:CZ2	2:G:193:GLU:CD	2.83	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:250:LEU:HD11	2:G:309:ILE:HD13	1.87	0.56
2:H:143:LEU:O	2:H:146:PRO:HD3	2.04	0.56
3:J:296:ILE:CG2	3:J:315:LEU:HD12	2.31	0.56
1:A:102:GLY:HA3	2:G:310:GLU:CD	2.30	0.56
1:A:222:LEU:C	1:A:224:GLY:H	2.12	0.56
2:B:184:ARG:HG3	2:B:204:GLN:OE1	2.05	0.56
2:B:259:ALA:HB2	2:B:360:HIS:HE1	1.68	0.56
2:C:234:THR:O	2:C:238:SER:OG	2.17	0.56
2:D:25:LEU:CD2	2:D:54:ILE:HD13	2.35	0.56
2:D:364:PRO:HG3	3:E:260:HIS:CE1	2.41	0.56
3:E:155:LEU:C	3:E:157:SER:H	2.13	0.56
1:F:17:LEU:HD21	1:F:109:LEU:HD12	1.86	0.56
1:F:24:LEU:HD13	1:F:117:LEU:HG	1.87	0.56
1:F:57:PRO:C	1:F:59:THR:N	2.63	0.56
1:F:251:GLN:HE22	3:J:307:ASN:HD21	1.52	0.56
2:H:9:LYS:NZ	2:H:194:GLU:OE1	2.39	0.56
2:H:216:ASP:O	2:H:220:LEU:HG	2.05	0.56
2:I:264:VAL:O	2:I:268:ILE:HG13	2.05	0.56
3:J:32:LEU:HB2	3:J:35:MSE:HG3	1.87	0.56
1:A:27:ASP:O	1:A:31:LEU:HG	2.06	0.56
1:A:259:ASN:O	1:A:262:ARG:HB2	2.04	0.56
1:A:270:ARG:HG2	1:A:283:ARG:HH21	1.67	0.56
2:B:210:ALA:CB	2:B:217:ALA:HB2	2.34	0.56
2:B:359:PHE:HE2	2:C:323:THR:HG1	1.52	0.56
2:D:201:ARG:O	2:D:204:GLN:N	2.39	0.56
3:E:20:ALA:CB	3:E:22:ARG:HD3	2.36	0.56
1:A:59:THR:CG2	1:A:60:ASP:H	2.18	0.56
2:B:252:LEU:CD2	2:B:281:LEU:HD21	2.36	0.56
3:E:68:MSE:HE1	3:E:76:TYR:CB	2.36	0.56
3:J:149:GLU:C	3:J:151:LEU:H	2.14	0.56
1:A:27:ASP:OD2	1:A:30:LEU:HG	2.06	0.56
1:A:115:ASN:O	1:A:116:LYS:O	2.24	0.56
1:A:260:LEU:CB	1:A:290:LEU:HD11	2.36	0.56
2:D:361:PRO:O	2:D:362:ARG:HB2	2.06	0.56
1:F:64:ILE:CG1	1:F:96:GLN:HE21	2.17	0.56
2:G:28:LEU:HD22	2:G:58:LEU:HD13	1.87	0.56
2:G:258:GLU:HB3	2:G:260:ASN:ND2	2.21	0.56
2:H:50:GLY:O	2:H:54:ILE:HG13	2.06	0.56
2:H:84:GLN:HB3	2:I:144:GLU:OE2	2.06	0.56
3:J:280:HIS:O	3:J:281:LEU:HD23	2.06	0.56
1:A:117:LEU:HB2	1:A:122:GLU:HG3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:262:GLU:HG3	2:B:263:ARG:N	2.21	0.56
2:G:21:GLN:O	2:G:24:VAL:HB	2.05	0.56
2:H:10:TRP:NE1	2:H:190:ILE:HG23	2.21	0.56
2:I:360:HIS:CD2	2:I:360:HIS:C	2.84	0.56
2:B:140:LEU:O	2:B:143:LEU:HD23	2.05	0.56
2:D:259:ALA:CB	2:D:363:MET:CG	2.84	0.56
2:G:184:ARG:HG3	2:G:185:HIS:N	2.20	0.56
2:H:223:GLN:HE22	2:I:174:HIS:CE1	2.24	0.56
2:I:140:LEU:HD22	2:I:144:GLU:HG3	1.87	0.56
2:D:333:LEU:C	2:D:333:LEU:CD1	2.79	0.56
1:F:156:LYS:O	1:F:156:LYS:HD3	2.06	0.56
2:G:341:TYR:CE2	2:H:337:LYS:HA	2.41	0.56
2:H:32:LEU:HD13	2:H:69:THR:O	2.06	0.56
2:I:220:LEU:HD21	3:J:157:SER:OG	2.06	0.56
1:A:71:MSE:SE	1:F:228:ARG:CB	3.04	0.56
2:B:250:LEU:HD23	2:B:312:ARG:CZ	2.35	0.56
2:D:45:GLY:O	2:D:157:THR:HA	2.06	0.56
2:G:261:GLY:HA3	2:H:297:LEU:HD21	1.88	0.56
3:J:8:ARG:HG2	3:J:9:PRO:HD3	1.88	0.56
2:C:367:GLU:OE2	2:C:367:GLU:C	2.49	0.55
3:E:214:GLU:HG2	3:E:218:GLN:HE21	1.70	0.55
2:G:326:GLN:O	2:G:330:GLN:HB3	2.07	0.55
2:I:251:SER:HB3	2:I:263:ARG:NH2	2.21	0.55
2:I:360:HIS:CG	2:I:363:MET:HG3	2.41	0.55
2:D:272:ALA:HB2	2:D:346:ARG:HH11	1.71	0.55
3:E:216:LEU:HD23	3:E:216:LEU:C	2.32	0.55
1:F:25:GLY:HA2	1:F:140:GLN:HE21	1.69	0.55
2:H:284:GLU:OE1	2:H:284:GLU:HA	2.06	0.55
2:I:248:GLN:HA	2:I:248:GLN:NE2	2.20	0.55
2:I:361:PRO:O	2:I:362:ARG:HB2	2.07	0.55
3:J:220:LEU:O	3:J:220:LEU:HD22	2.05	0.55
2:D:42:LEU:HD22	2:D:42:LEU:C	2.30	0.55
2:D:290:HIS:CE1	2:D:294:MET:HE3	2.40	0.55
3:E:313:THR:O	3:E:313:THR:HG22	2.06	0.55
1:F:24:LEU:HB3	1:F:116:LYS:HA	1.88	0.55
1:F:56:ASP:OD1	1:F:85:PRO:HA	2.06	0.55
1:F:282:ARG:HG2	1:F:285:MSE:CE	2.37	0.55
2:G:11:ARG:HH21	2:G:56:ARG:NE	2.04	0.55
2:G:333:LEU:CD1	2:G:337:LYS:HE3	2.37	0.55
2:I:291:ARG:HD2	2:I:306:MET:SD	2.45	0.55
2:C:350:GLU:O	2:C:351:MET:C	2.47	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:27:ALA:O	2:D:30:ASN:N	2.40	0.55
3:E:280:HIS:O	3:E:281:LEU:HD23	2.07	0.55
2:H:307:ALA:HA	2:H:310:GLU:HB2	1.87	0.55
2:B:119:ARG:HG3	2:B:120:PHE:CD2	2.42	0.55
2:C:18:VAL:HB	2:C:25:LEU:HD11	1.88	0.55
2:G:98:ARG:HD3	2:H:140:LEU:CB	2.35	0.55
2:H:147:PRO:HG2	2:H:150:VAL:HB	1.87	0.55
2:I:56:ARG:HG3	2:I:56:ARG:NH1	2.21	0.55
2:I:80:ARG:HG2	2:I:80:ARG:HH11	1.71	0.55
1:A:274:ASP:HA	1:A:279:TRP:CE3	2.41	0.55
2:B:76:CYS:SG	2:B:79:CYS:N	2.79	0.55
2:C:24:VAL:O	2:C:24:VAL:HG12	2.07	0.55
3:E:151:LEU:HD11	3:E:155:LEU:CD1	2.36	0.55
3:E:249:ALA:O	3:E:250:THR:C	2.50	0.55
2:G:7:ALA:CA	2:G:218:LEU:HD13	2.36	0.55
2:G:306:MET:O	2:G:310:GLU:HG3	2.06	0.55
2:H:291:ARG:CA	2:H:294:MET:HB2	2.34	0.55
2:I:113:TYR:HE2	2:I:147:PRO:HG3	1.71	0.55
2:B:178:LEU:HD22	2:B:178:LEU:N	2.22	0.55
2:C:263:ARG:NH1	2:C:263:ARG:HG3	2.21	0.55
2:C:282:LEU:O	2:C:283:VAL:C	2.49	0.55
2:D:144:GLU:OE1	2:D:144:GLU:HA	2.07	0.55
2:D:354:LEU:CD1	3:E:253:MSE:CE	2.85	0.55
3:E:254:ASP:OD1	3:E:265:VAL:HG13	2.05	0.55
2:G:12:PRO:O	2:G:57:LEU:HD21	2.06	0.55
2:H:115:PRO:HG3	2:H:121:LYS:HB2	1.89	0.55
2:H:250:LEU:CD2	2:H:309:ILE:HB	2.37	0.55
2:I:238:SER:CB	2:I:243:THR:HB	2.37	0.55
3:J:35:MSE:HE3	3:J:198:PRO:CD	2.33	0.55
1:A:73:LEU:HD13	1:F:206:VAL:O	2.06	0.55
2:C:215:ARG:NH2	6:C:1300:PO4:O1	2.40	0.55
2:C:316:LEU:HD22	2:C:320:ILE:CD1	2.31	0.55
2:D:346:ARG:O	2:D:347:MET:C	2.47	0.55
3:E:241:ALA:N	3:E:242:PRO:HD2	2.21	0.55
3:E:276:GLU:O	3:E:279:ASN:HB2	2.07	0.55
1:F:194:ASP:CB	1:F:201:ARG:HH12	2.19	0.55
2:G:9:LYS:HD2	2:G:194:GLU:OE1	2.06	0.55
2:B:158:ASP:OD2	2:B:161:LYS:HG2	2.06	0.55
2:C:201:ARG:HG3	2:C:234:THR:CG2	2.37	0.55
2:C:338:GLU:C	2:C:340:PRO:HD2	2.32	0.55
2:H:11:ARG:NH2	2:I:165:THR:HG22	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:156:THR:HG22	2:H:158:ASP:H	1.72	0.55
3:J:161:LEU:HD12	3:J:161:LEU:N	2.21	0.55
1:A:102:GLY:HA3	2:G:310:GLU:OE1	2.06	0.55
2:B:354:LEU:O	2:B:355:ARG:C	2.49	0.55
2:C:333:LEU:C	2:C:335:GLY:N	2.63	0.55
1:F:270:ARG:CG	1:F:283:ARG:NH2	2.63	0.55
2:G:113:TYR:CD2	2:G:147:PRO:HB3	2.42	0.55
2:H:77:ASP:O	2:H:81:GLU:HG3	2.06	0.55
2:I:215:ARG:CD	5:I:803:AGS:H5'1	2.25	0.55
2:I:347:MET:O	2:I:351:MET:HG2	2.07	0.55
1:A:268:PRO:C	1:A:270:ARG:N	2.65	0.54
2:D:119:ARG:HG3	2:D:120:PHE:HD2	1.67	0.54
2:G:263:ARG:NE	2:G:267:LEU:HD21	2.22	0.54
2:C:258:GLU:O	2:C:259:ALA:HB3	2.05	0.54
1:F:217:TRP:CZ3	1:F:250:LEU:HD22	2.42	0.54
2:H:34:LEU:HD13	2:H:36:ARG:NE	2.22	0.54
2:H:351:MET:HE1	2:I:293:ALA:HB3	1.88	0.54
2:I:240:MET:SD	3:J:157:SER:HA	2.46	0.54
1:A:234:GLN:HA	1:A:237:ARG:HG3	1.89	0.54
1:A:295:GLN:CD	1:A:295:GLN:H	2.15	0.54
2:C:65:GLU:C	2:C:67:GLY:H	2.16	0.54
2:C:100:LYS:HB3	2:D:133:ARG:NE	2.22	0.54
2:C:217:ALA:O	2:C:221:THR:OG1	2.21	0.54
2:D:124:LEU:HD22	2:D:125:ILE:N	2.21	0.54
2:D:309:ILE:O	2:D:310:GLU:C	2.48	0.54
3:E:285:ARG:HD3	3:E:323:LEU:HD23	1.90	0.54
1:F:247:LEU:HD12	1:F:312:LEU:HD22	1.89	0.54
2:G:248:GLN:HA	2:G:251:SER:HB2	1.88	0.54
2:H:87:PHE:HB3	2:H:90:LEU:HB3	1.90	0.54
1:A:161:GLU:OE1	1:A:196:LYS:HE2	2.07	0.54
2:C:354:LEU:O	2:C:355:ARG:C	2.50	0.54
2:D:238:SER:HB2	2:D:243:THR:HB	1.88	0.54
3:E:210:TRP:CH2	3:E:213:ARG:NH1	2.76	0.54
1:F:174:TYR:HB2	1:F:181:LEU:HD23	1.89	0.54
1:F:250:LEU:HD23	1:F:250:LEU:H	1.73	0.54
2:G:23:HIS:CE1	2:G:176:LYS:HE3	2.42	0.54
1:A:52:THR:HG22	1:A:81:LEU:HD23	1.90	0.54
2:B:233:SER:O	2:B:237:VAL:HG23	2.07	0.54
2:C:42:LEU:HB3	2:C:172:GLN:HA	1.90	0.54
2:D:358:ALA:C	2:D:360:HIS:H	2.12	0.54
3:E:296:ILE:CA	3:E:299:GLN:HG3	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:148:GLU:OE1	2:G:148:GLU:HA	2.06	0.54
2:G:248:GLN:O	2:G:250:LEU:CA	2.56	0.54
2:H:91:ILE:CG2	2:H:107:LEU:HD13	2.37	0.54
2:H:93:ILE:HG21	2:H:104:THR:HG23	1.89	0.54
2:C:15:PHE:HE1	2:C:57:LEU:HB3	1.71	0.54
2:D:82:ILE:HG23	2:D:90:LEU:HD22	1.90	0.54
2:D:290:HIS:NE2	2:D:294:MET:HE3	2.23	0.54
3:E:169:GLU:CD	3:E:192:ARG:HH21	2.16	0.54
3:E:199:GLY:O	3:E:202:LEU:HB3	2.08	0.54
3:E:205:PHE:O	3:E:207:GLY:N	2.34	0.54
1:F:299:ARG:HG3	3:J:317:LEU:CG	2.37	0.54
2:G:284:GLU:O	2:G:288:LEU:HG	2.08	0.54
2:H:97:SER:HB3	2:H:100:LYS:HB2	1.89	0.54
3:J:46:ARG:NH1	3:J:68:MSE:HG3	2.22	0.54
2:C:314:ARG:O	2:C:315:GLU:O	2.25	0.54
3:E:13:LYS:O	3:E:16:ALA:HB3	2.06	0.54
3:E:49:LEU:HD23	3:E:68:MSE:SE	2.58	0.54
3:E:192:ARG:C	3:E:194:SER:H	2.16	0.54
3:E:202:LEU:HD13	3:E:203:ALA:N	2.23	0.54
2:H:257:VAL:HG11	2:H:320:ILE:HD13	1.88	0.54
2:I:244:LEU:C	2:I:246:ASP:H	2.15	0.54
3:J:212:ALA:HB1	3:J:244:ARG:HH21	1.73	0.54
1:A:187:ARG:O	1:A:190:LEU:HB2	2.07	0.54
1:A:197:LEU:HB3	1:A:202:VAL:CG2	2.38	0.54
2:C:24:VAL:HG13	2:C:173:PHE:CD1	2.42	0.54
2:C:199:GLU:OE2	2:C:201:ARG:NH2	2.39	0.54
2:D:279:GLU:HB3	3:E:149:GLU:OE2	2.08	0.54
3:E:237:ASN:HD22	3:E:238:HIS:N	2.06	0.54
2:G:6:LEU:CD1	2:G:191:LEU:CD2	2.85	0.54
2:G:227:SER:HA	2:H:26:THR:HG22	1.90	0.54
2:G:354:LEU:HD11	2:H:294:MET:SD	2.47	0.54
2:H:201:ARG:HH21	2:H:205:LEU:CD2	2.21	0.54
2:B:245:ASP:OD1	2:B:246:ASP:N	2.41	0.54
2:B:339:LEU:HG	2:B:345:ARG:HD3	1.90	0.54
2:C:49:VAL:CG1	2:C:175:LEU:HB3	2.38	0.54
2:C:347:MET:O	2:C:348:GLY:C	2.51	0.54
2:D:198:HIS:HA	2:D:232:VAL:O	2.08	0.54
3:E:4:TYR:HB3	3:E:5:PRO:HD2	1.89	0.54
1:F:311:THR:HA	1:F:314:GLN:OE1	2.08	0.54
2:G:338:GLU:HB3	2:H:333:LEU:CD2	2.38	0.54
2:H:100:LYS:CE	2:I:136:PHE:HD2	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:90:VAL:HG21	3:J:123:ALA:HB3	1.90	0.54
3:J:106:LEU:O	3:J:107:GLY:C	2.50	0.54
1:A:316:TYR:N	1:A:316:TYR:CD1	2.76	0.54
2:D:60:LYS:HA	2:D:82:ILE:CD1	2.38	0.54
2:G:188:GLU:O	2:G:192:ASN:ND2	2.41	0.54
2:H:316:LEU:HD22	2:H:320:ILE:HD11	1.90	0.54
2:I:244:LEU:CD1	2:I:276:ILE:HD13	2.34	0.54
3:J:203:ALA:O	3:J:206:GLN:HG2	2.07	0.54
1:A:32:GLN:O	1:A:35:GLN:HB3	2.08	0.53
3:E:213:ARG:NH2	3:E:267:ASN:OD1	2.41	0.53
2:H:295:VAL:CG2	2:H:301:ALA:HB3	2.36	0.53
2:I:244:LEU:C	2:I:246:ASP:N	2.65	0.53
2:I:277:GLU:HB2	2:I:280:ALA:CB	2.38	0.53
2:I:281:LEU:HG	2:I:285:MET:HE2	1.91	0.53
3:J:304:THR:HG22	3:J:305:GLY:N	2.24	0.53
1:A:82:LEU:HD13	1:A:110:LEU:HD11	1.90	0.53
2:D:38:HIS:HD2	2:D:40:ALA:H	1.54	0.53
2:D:61:GLY:CA	2:D:72:PRO:HG3	2.38	0.53
2:D:357:LEU:C	2:D:363:MET:SD	2.91	0.53
3:E:233:LEU:CD1	3:E:237:ASN:HB2	2.37	0.53
3:E:321:HIS:O	3:E:327:VAL:HG21	2.08	0.53
1:F:19:ALA:HB2	1:F:133:ARG:HD3	1.90	0.53
2:G:269:ASN:HA	2:G:346:ARG:HH21	1.71	0.53
2:H:281:LEU:HD23	2:H:281:LEU:C	2.32	0.53
3:J:331:VAL:HG13	3:J:332:PRO:HD2	1.90	0.53
2:B:198:HIS:HD2	2:B:203:LEU:HD11	1.66	0.53
2:B:236:ALA:O	2:B:239:ALA:HB3	2.08	0.53
2:B:362:ARG:C	2:B:364:PRO:CD	2.81	0.53
2:C:101:VAL:HG23	2:C:102:GLU:OE2	2.08	0.53
2:C:292:ILE:HG12	2:C:313:MET:HE1	1.89	0.53
1:F:213:THR:C	1:F:215:PHE:H	2.15	0.53
2:H:111:VAL:HG11	2:H:150:VAL:HG21	1.90	0.53
2:I:214:LEU:HB3	5:I:803:AGS:C4	2.38	0.53
2:C:98:ARG:O	2:C:101:VAL:HG22	2.07	0.53
2:C:327:LEU:HD12	2:C:327:LEU:C	2.32	0.53
2:D:102:GLU:HG2	2:D:106:ASP:OD2	2.07	0.53
2:D:215:ARG:NH1	5:D:801:AGS:O2G	2.41	0.53
3:E:6:TRP:O	3:E:9:PRO:HD2	2.08	0.53
1:F:299:ARG:CG	3:J:317:LEU:HD21	2.39	0.53
2:I:258:GLU:O	2:I:259:ALA:HB3	2.09	0.53
3:J:4:TYR:N	3:J:7:LEU:HD12	2.14	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:51:GLN:HB2	3:J:62:CYS:HB2	1.90	0.53
2:C:302:LEU:O	2:C:303:GLY:O	2.26	0.53
3:E:214:GLU:HG2	3:E:218:GLN:NE2	2.23	0.53
3:E:307:ASN:O	3:E:308:ARG:C	2.51	0.53
3:J:153:ALA:O	3:J:157:SER:OG	2.25	0.53
1:A:213:THR:C	1:A:215:PHE:N	2.62	0.53
1:A:262:ARG:NH1	3:E:230:TYR:HB3	2.24	0.53
2:C:263:ARG:HG3	2:C:263:ARG:HH11	1.73	0.53
3:E:203:ALA:HA	3:E:206:GLN:HB2	1.91	0.53
3:E:251:LEU:O	3:E:254:ASP:N	2.39	0.53
1:F:147:LEU:HB3	1:F:148:PRO:HD3	1.90	0.53
1:F:249:THR:HB	1:F:250:LEU:HD23	1.90	0.53
1:F:318:GLN:O	1:F:319:SER:C	2.52	0.53
2:G:119:ARG:HG3	2:G:120:PHE:CD2	2.44	0.53
2:I:159:PRO:O	2:I:162:LEU:HB2	2.08	0.53
2:B:246:ASP:C	2:B:248:GLN:H	2.16	0.53
2:D:12:PRO:C	2:D:13:GLN:HE21	2.17	0.53
2:D:22:GLU:C	2:D:24:VAL:N	2.62	0.53
2:D:25:LEU:HD21	2:D:54:ILE:HD13	1.89	0.53
2:D:61:GLY:HA2	2:D:72:PRO:HG3	1.91	0.53
3:E:74:PRO:HD2	3:E:106:LEU:CD1	2.38	0.53
3:E:88:LEU:HD23	3:E:89:GLY:N	2.23	0.53
3:E:296:ILE:O	3:E:300:LEU:HD12	2.09	0.53
1:F:1:MSE:HE1	1:F:127:PHE:CE1	2.44	0.53
1:F:96:GLN:OE1	1:F:96:GLN:HA	2.08	0.53
1:F:188:LEU:HD21	1:F:202:VAL:HG22	1.91	0.53
1:F:299:ARG:NH1	3:J:321:HIS:ND1	2.57	0.53
2:G:48:GLY:HA3	2:G:215:ARG:H	1.74	0.53
2:H:351:MET:HE3	2:H:354:LEU:HD13	1.91	0.53
3:J:315:LEU:O	3:J:319:ILE:HG13	2.09	0.53
1:A:237:ARG:HG2	1:A:321:TRP:CZ3	2.43	0.53
2:B:21:GLN:OE1	2:B:175:LEU:HB3	2.09	0.53
2:B:133:ARG:O	2:B:137:ASN:ND2	2.42	0.53
2:B:191:LEU:HD11	2:B:232:VAL:HG21	1.90	0.53
2:G:309:ILE:HG22	2:G:313:MET:HG2	1.91	0.53
1:A:32:GLN:HE21	1:A:113:ARG:HH22	1.56	0.53
2:B:47:ARG:HD2	5:B:802:AGS:O2G	2.09	0.53
3:E:92:ALA:O	3:E:96:VAL:HG23	2.09	0.53
2:H:181:GLU:CD	2:H:184:ARG:HD2	2.33	0.53
2:H:276:ILE:HD12	2:H:278:TRP:CZ3	2.44	0.53
2:H:295:VAL:HG13	2:H:299:PRO:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:232:LEU:O	3:J:236:LEU:HG	2.09	0.53
3:J:333:HIS:O	3:J:334:LEU:OXT	2.27	0.53
1:A:6:PRO:HB2	1:A:7:GLU:OE2	2.08	0.53
2:B:210:ALA:HB2	2:B:217:ALA:HB2	1.90	0.53
2:C:346:ARG:O	2:C:347:MET:C	2.52	0.53
2:G:341:TYR:O	2:H:333:LEU:CD1	2.56	0.53
2:I:257:VAL:HG11	2:I:320:ILE:HD13	1.91	0.53
2:C:307:ALA:HA	2:C:310:GLU:HB2	1.91	0.52
3:E:117:ALA:C	3:E:119:LEU:H	2.17	0.52
3:E:277:LEU:HD23	3:E:281:LEU:HD12	1.91	0.52
1:F:55:ILE:HG22	1:F:55:ILE:O	2.09	0.52
2:G:11:ARG:HH21	2:G:56:ARG:HH21	1.47	0.52
2:G:94:ASP:OD2	2:G:97:SER:HB2	2.08	0.52
2:H:60:LYS:HG2	2:H:79:CYS:SG	2.49	0.52
3:J:50:CYS:SG	3:J:53:PRO:HA	2.49	0.52
1:A:59:THR:HG22	1:A:60:ASP:H	1.72	0.52
2:I:271:ALA:HB1	2:I:276:ILE:CD1	2.28	0.52
2:I:357:LEU:HA	2:I:363:MET:CE	2.39	0.52
2:I:364:PRO:HG3	3:J:260:HIS:CE1	2.43	0.52
1:A:71:MSE:SE	1:F:231:HIS:HB3	2.59	0.52
2:C:220:LEU:O	2:C:222:ASP:N	2.42	0.52
2:D:189:HIS:O	2:D:190:ILE:C	2.50	0.52
2:D:254:GLU:OE2	2:D:312:ARG:HD2	2.08	0.52
1:F:2:ILE:HD11	1:F:18:ARG:HH21	1.73	0.52
3:J:5:PRO:C	3:J:7:LEU:H	2.17	0.52
3:J:94:ARG:O	3:J:98:GLU:HG2	2.09	0.52
1:A:24:LEU:HB3	1:A:116:LYS:HA	1.91	0.52
3:E:118:ALA:HB2	3:E:145:THR:HG23	1.90	0.52
1:F:19:ALA:CB	1:F:133:ARG:HD3	2.40	0.52
3:J:147:GLU:OE2	3:J:150:ARG:HG3	2.08	0.52
2:D:214:LEU:HD23	5:D:801:AGS:N3	2.23	0.52
3:E:202:LEU:HD13	3:E:202:LEU:C	2.35	0.52
2:I:291:ARG:O	2:I:295:VAL:HG23	2.09	0.52
2:C:84:GLN:NE2	2:D:144:GLU:OE2	2.43	0.52
2:C:245:ASP:C	2:C:247:ASP:N	2.66	0.52
2:D:268:ILE:HG23	2:D:278:TRP:CH2	2.45	0.52
3:E:145:THR:HG22	3:E:147:GLU:N	2.24	0.52
2:H:219:SER:HA	2:H:222:ASP:OD2	2.09	0.52
2:I:309:ILE:CG2	2:I:313:MET:HG2	2.39	0.52
3:J:50:CYS:SG	3:J:53:PRO:CA	2.97	0.52
2:D:256:MET:HE2	2:D:353:LEU:CD2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:145:ALA:O	1:F:148:PRO:HD2	2.08	0.52
1:F:221:LEU:HD13	1:F:331:LEU:HD12	1.92	0.52
2:I:21:GLN:NE2	2:I:176:LYS:N	2.00	0.52
2:B:255:ALA:HB2	2:B:263:ARG:HD3	1.92	0.52
2:C:367:GLU:HG3	2:D:321:PRO:HA	1.91	0.52
1:F:269:LEU:HG	1:F:273:PHE:CE1	2.44	0.52
2:G:7:ALA:CB	2:G:218:LEU:CD1	2.76	0.52
2:G:248:GLN:C	2:G:250:LEU:H	2.18	0.52
3:J:31:ALA:CB	3:J:164:LEU:HB3	2.35	0.52
1:A:213:THR:O	1:A:216:HIS:HB2	2.10	0.52
2:B:5:VAL:C	2:B:7:ALA:N	2.67	0.52
2:B:44:SER:HB2	2:B:159:PRO:CG	2.40	0.52
2:B:360:HIS:HD2	2:B:361:PRO:N	2.08	0.52
2:C:5:VAL:O	2:C:5:VAL:HG23	2.10	0.52
2:D:32:LEU:C	2:D:34:LEU:H	2.16	0.52
2:D:268:ILE:HD11	2:D:353:LEU:HD12	1.92	0.52
2:D:288:LEU:C	2:D:290:HIS:N	2.68	0.52
2:D:292:ILE:HD11	2:D:316:LEU:HD12	1.92	0.52
2:G:139:LEU:O	2:G:143:LEU:HG	2.09	0.52
2:H:268:ILE:HD11	2:H:353:LEU:HD12	1.91	0.52
2:I:145:GLU:N	2:I:146:PRO:HD3	2.25	0.52
3:J:155:LEU:C	3:J:157:SER:H	2.17	0.52
2:C:254:GLU:O	2:C:258:GLU:CG	2.47	0.52
2:C:362:ARG:C	2:C:363:MET:HG3	2.35	0.52
2:D:160:GLN:C	2:D:162:LEU:H	2.18	0.52
2:D:218:LEU:O	2:D:221:THR:N	2.42	0.52
2:D:306:MET:C	2:D:308:ALA:N	2.60	0.52
3:E:239:GLU:HA	3:E:308:ARG:NH2	2.25	0.52
1:F:24:LEU:HA	1:F:114:GLY:O	2.10	0.52
2:G:10:TRP:CH2	2:G:193:GLU:OE1	2.63	0.52
2:H:181:GLU:OE1	2:H:184:ARG:HD2	2.10	0.52
1:A:247:LEU:HD23	1:A:324:LEU:HD21	1.92	0.51
2:B:316:LEU:HD22	2:B:320:ILE:CD1	2.40	0.51
2:C:220:LEU:O	2:C:221:THR:C	2.51	0.51
2:D:32:LEU:HD23	2:D:37:ILE:HD11	1.92	0.51
2:D:363:MET:SD	2:D:364:PRO:HD2	2.50	0.51
2:I:339:LEU:N	2:I:340:PRO:HD2	2.25	0.51
3:J:139:THR:HG22	3:J:140:TRP:N	2.23	0.51
3:J:155:LEU:C	3:J:155:LEU:HD13	2.35	0.51
1:A:105:HIS:CD2	1:A:107:ASP:HB2	2.46	0.51
1:A:105:HIS:ND1	1:A:108:LEU:HB2	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:318:ARG:CG	2:B:319:THR:N	2.72	0.51
2:C:10:TRP:CE2	2:C:190:ILE:HG23	2.45	0.51
2:C:37:ILE:HD13	2:C:120:PHE:HE1	1.73	0.51
2:C:100:LYS:HB3	2:D:133:ARG:HE	1.75	0.51
2:D:290:HIS:CE1	2:D:294:MET:CE	2.93	0.51
3:E:110:LYS:HD3	3:E:139:THR:OG1	2.09	0.51
3:E:277:LEU:C	3:E:279:ASN:N	2.64	0.51
3:J:220:LEU:HD23	3:J:232:LEU:HD11	1.92	0.51
3:J:253:MSE:HE2	3:J:257:LYS:HG3	1.93	0.51
3:J:303:VAL:CB	3:J:306:ILE:HD11	2.23	0.51
1:A:223:MSE:HE2	1:A:292:ARG:CB	2.39	0.51
2:B:262:GLU:O	2:B:266:ALA:HB2	2.10	0.51
2:C:233:SER:O	2:C:234:THR:C	2.52	0.51
2:D:244:LEU:HD21	2:D:276:ILE:HD13	1.92	0.51
2:D:265:MET:HG2	3:E:262:ALA:HB2	1.92	0.51
3:E:323:LEU:O	3:E:324:GLN:C	2.51	0.51
1:F:50:HIS:ND1	1:F:79:THR:CG2	2.74	0.51
2:G:342:ALA:C	2:G:344:ASP:H	2.17	0.51
2:H:253:VAL:O	2:H:256:MET:HB3	2.10	0.51
2:I:346:ARG:O	2:I:350:GLU:HG3	2.11	0.51
1:A:4:LEU:CD1	1:A:137:VAL:HG22	2.40	0.51
2:B:342:ALA:O	2:B:343:PRO:C	2.51	0.51
2:D:32:LEU:O	2:D:35:GLY:N	2.41	0.51
2:D:238:SER:O	2:D:242:GLY:N	2.43	0.51
2:D:355:ARG:HH12	3:E:287:GLN:HB3	1.74	0.51
2:D:357:LEU:O	2:D:358:ALA:C	2.53	0.51
2:G:313:MET:O	2:G:314:ARG:C	2.53	0.51
2:H:11:ARG:NH1	2:I:169:ARG:NH1	2.56	0.51
3:J:225:PRO:HB3	3:J:276:GLU:OE2	2.10	0.51
1:A:74:PHE:CZ	1:F:207:ASN:N	2.79	0.51
1:A:133:ARG:HH21	2:G:300:ALA:HB1	1.73	0.51
1:A:143:GLU:H	1:A:143:GLU:CD	2.19	0.51
1:A:154:ARG:HH11	1:A:157:GLN:NE2	2.08	0.51
1:A:306:THR:O	1:A:307:ARG:C	2.54	0.51
1:A:321:TRP:O	1:A:322:ALA:C	2.54	0.51
2:B:28:LEU:HD11	2:B:43:PHE:HE1	1.75	0.51
2:D:44:SER:HA	2:D:156:THR:O	2.11	0.51
2:D:211:GLU:O	2:D:213:SER:N	2.44	0.51
3:E:220:LEU:HD21	3:E:248:LEU:CD1	2.40	0.51
2:I:201:ARG:HA	2:I:204:GLN:HE21	1.76	0.51
2:I:281:LEU:O	2:I:284:GLU:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:293:VAL:HA	3:J:315:LEU:HD11	1.92	0.51
2:B:140:LEU:HA	2:B:143:LEU:CD2	2.35	0.51
2:B:232:VAL:O	2:B:232:VAL:HG12	2.10	0.51
2:B:318:ARG:HG3	2:B:319:THR:N	2.25	0.51
2:C:19:VAL:O	2:C:21:GLN:N	2.44	0.51
3:E:92:ALA:O	3:E:95:GLU:HG2	2.10	0.51
3:E:268:VAL:O	3:E:271:PRO:HD3	2.11	0.51
1:F:82:LEU:HB2	1:F:112:VAL:HG22	1.93	0.51
1:F:217:TRP:HZ3	1:F:250:LEU:HD13	1.75	0.51
1:F:304:LEU:HB3	1:F:327:LEU:CD2	2.31	0.51
2:G:98:ARG:NH1	2:H:140:LEU:HD22	2.21	0.51
1:A:20:ALA:CB	1:A:110:LEU:HB3	2.40	0.51
1:A:80:LEU:HG	1:A:82:LEU:HD12	1.93	0.51
1:A:129:ALA:C	1:A:131:ALA:N	2.68	0.51
2:C:254:GLU:OE1	2:C:312:ARG:NH2	2.41	0.51
3:E:318:ARG:O	3:E:321:HIS:HB3	2.11	0.51
2:H:44:SER:HB2	2:H:159:PRO:HG3	1.91	0.51
2:H:149:HIS:CE1	2:H:150:VAL:HG23	2.46	0.51
3:J:19:GLN:HB2	3:J:47:TYR:OH	2.11	0.51
1:A:29:LEU:O	1:A:33:GLU:HG3	2.11	0.51
1:A:105:HIS:HE1	1:A:108:LEU:HB2	1.63	0.51
1:A:300:GLN:OE1	1:A:335:PRO:HB2	2.11	0.51
2:B:158:ASP:N	2:B:159:PRO:HD3	2.26	0.51
2:C:5:VAL:O	2:C:6:LEU:C	2.53	0.51
2:C:14:THR:O	2:C:57:LEU:HD13	2.11	0.51
2:C:28:LEU:HD13	2:C:58:LEU:HD13	1.92	0.51
3:E:277:LEU:O	3:E:279:ASN:N	2.43	0.51
3:E:286:LEU:O	3:E:289:ILE:N	2.43	0.51
2:G:291:ARG:HH22	2:G:303:GLY:HA3	1.74	0.51
2:I:21:GLN:HE22	2:I:176:LYS:CA	2.13	0.51
1:A:98:LEU:O	1:A:101:THR:HG22	2.11	0.51
2:B:260:ASN:O	2:B:261:GLY:C	2.52	0.51
2:C:279:GLU:HG3	2:C:336:ARG:HD2	1.93	0.51
2:D:366:PRO:HB3	3:E:282:SER:CB	2.41	0.51
3:E:117:ALA:O	3:E:120:LEU:HD23	2.10	0.51
3:E:317:LEU:O	3:E:320:GLU:HB2	2.10	0.51
2:H:156:THR:HG22	2:H:158:ASP:N	2.26	0.51
3:J:253:MSE:CG	3:J:257:LYS:HE3	2.32	0.51
1:A:298:LEU:CD1	1:A:298:LEU:N	2.73	0.51
1:A:299:ARG:O	1:A:302:VAL:N	2.42	0.51
2:B:276:ILE:HG13	2:B:277:GLU:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:291:ARG:HD2	2:C:306:MET:HE2	1.93	0.51
2:C:296:GLN:HE21	2:C:317:ALA:HA	1.76	0.51
2:D:128:VAL:HG13	2:D:162:LEU:HD21	1.91	0.51
3:E:298:GLU:HA	3:E:301:MSE:HG3	1.92	0.51
1:F:93:ILE:CG2	1:F:97:LEU:HD13	2.41	0.51
2:G:98:ARG:HD3	2:H:140:LEU:CD1	2.39	0.51
2:G:205:LEU:CD1	2:G:234:THR:HG23	2.40	0.51
2:G:205:LEU:HD11	2:G:234:THR:HG23	1.91	0.51
3:J:320:GLU:O	3:J:323:LEU:HB2	2.11	0.51
1:A:103:LEU:HD12	1:A:103:LEU:O	2.10	0.50
2:B:357:LEU:HB3	2:B:365:LEU:HD21	1.92	0.50
2:C:220:LEU:O	2:C:223:GLN:N	2.44	0.50
2:C:236:ALA:O	2:C:239:ALA:CB	2.57	0.50
2:C:263:ARG:HH11	2:C:263:ARG:CG	2.25	0.50
2:D:229:ASP:OD1	2:D:229:ASP:N	2.45	0.50
2:D:285:MET:HE1	2:D:353:LEU:CD2	2.39	0.50
3:E:35:MSE:CE	3:E:166:PRO:HA	2.41	0.50
3:E:303:VAL:CG1	3:E:306:ILE:HG12	2.41	0.50
1:F:130:LEU:HB3	1:F:134:SER:HG	1.76	0.50
2:G:178:LEU:HD22	2:G:182:GLN:NE2	2.24	0.50
2:G:227:SER:O	2:H:26:THR:HG21	2.11	0.50
2:H:37:ILE:HD13	2:H:151:LYS:HE3	1.93	0.50
2:H:93:ILE:HD13	2:H:104:THR:HG23	1.92	0.50
2:H:224:ALA:O	2:H:228:GLY:N	2.43	0.50
2:I:250:LEU:CD2	2:I:312:ARG:HD2	2.41	0.50
1:A:74:PHE:CG	1:F:207:ASN:OD1	2.60	0.50
1:A:193:PRO:HB2	2:B:34:LEU:HD12	1.91	0.50
1:A:254:LEU:HD23	1:A:305:LEU:HD12	1.93	0.50
2:C:30:ASN:O	2:C:31:GLY:C	2.53	0.50
2:D:237:VAL:C	2:D:239:ALA:N	2.69	0.50
3:E:143:LEU:HD22	3:E:143:LEU:N	2.26	0.50
3:E:175:TRP:CD1	3:E:176:LEU:HD23	2.46	0.50
2:G:9:LYS:HB3	2:G:194:GLU:OE2	2.11	0.50
2:G:48:GLY:O	2:G:214:LEU:HB3	2.11	0.50
2:G:98:ARG:CZ	2:H:140:LEU:HD13	2.42	0.50
2:G:306:MET:HE2	2:G:306:MET:HA	1.92	0.50
2:H:327:LEU:HD12	2:H:327:LEU:O	2.10	0.50
1:A:119:LYS:H	1:A:119:LYS:CD	2.01	0.50
2:B:191:LEU:CD2	2:B:198:HIS:HB3	2.41	0.50
2:C:310:GLU:O	2:C:311:LEU:C	2.53	0.50
2:D:328:TYR:O	2:D:329:TYR:C	2.53	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:332:LEU:HD23	2:D:352:THR:HG22	1.93	0.50
1:F:162:LEU:HD11	1:F:185:LEU:CD2	2.40	0.50
2:G:46:THR:CG2	2:G:47:ARG:H	2.01	0.50
2:G:309:ILE:CG2	2:G:313:MET:HG2	2.41	0.50
1:A:289:ALA:O	1:A:291:ASN:N	2.44	0.50
2:D:244:LEU:CD2	2:D:276:ILE:HD13	2.42	0.50
3:E:125:ALA:O	3:E:128:LEU:HB3	2.12	0.50
1:F:154:ARG:O	1:F:154:ARG:HD2	2.10	0.50
1:F:188:LEU:CD2	1:F:197:LEU:HD13	2.39	0.50
1:F:217:TRP:CZ3	1:F:250:LEU:HD13	2.45	0.50
2:H:225:ILE:HG23	2:H:230:GLY:HA2	1.94	0.50
1:A:74:PHE:CE1	1:F:203:GLU:HG2	2.44	0.50
1:A:177:ASN:OD1	1:A:179:LEU:HB3	2.12	0.50
1:A:262:ARG:NH2	3:E:230:TYR:HB2	2.26	0.50
1:A:271:ALA:O	1:A:275:LYS:HG2	2.12	0.50
2:B:147:PRO:O	2:B:150:VAL:HB	2.11	0.50
2:B:360:HIS:CD2	2:B:361:PRO:N	2.80	0.50
2:C:269:ASN:C	2:C:271:ALA:N	2.65	0.50
2:D:111:VAL:HG13	2:D:112:GLN:N	2.27	0.50
2:D:196:ILE:HG22	2:D:197:ALA:H	1.75	0.50
3:E:303:VAL:O	3:E:303:VAL:HG12	2.12	0.50
2:G:93:ILE:CG2	2:G:104:THR:HG23	2.42	0.50
2:G:99:THR:HG21	2:H:145:GLU:CB	2.41	0.50
2:I:324:ASP:O	2:I:327:LEU:HB3	2.12	0.50
1:A:226:SER:O	1:A:227:LYS:C	2.54	0.50
2:C:140:LEU:O	2:C:169:ARG:NH1	2.45	0.50
2:D:292:ILE:HG13	2:D:313:MET:CE	2.39	0.50
1:F:71:MSE:HA	1:F:78:GLN:NE2	2.26	0.50
1:F:220:ALA:C	1:F:222:LEU:H	2.20	0.50
1:F:273:PHE:CD1	1:F:283:ARG:CG	2.70	0.50
1:F:285:MSE:HE2	1:F:285:MSE:HB3	1.93	0.50
2:H:245:ASP:HB2	2:H:248:GLN:HG3	1.93	0.50
2:H:277:GLU:O	2:H:279:GLU:N	2.45	0.50
2:I:347:MET:HE1	3:J:250:THR:HA	1.94	0.50
2:B:148:GLU:HG3	2:B:149:HIS:CE1	2.46	0.50
2:B:252:LEU:HD23	2:B:285:MET:SD	2.52	0.50
2:C:112:GLN:HB2	2:C:121:LYS:HE2	1.92	0.50
2:C:250:LEU:HB2	2:C:288:LEU:HD13	1.94	0.50
2:C:293:ALA:HB2	2:C:325:ILE:HG21	1.93	0.50
2:D:13:GLN:C	2:D:57:LEU:HD21	2.37	0.50
2:D:281:LEU:HD11	2:D:285:MET:HE2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:8:ARG:N	3:E:9:PRO:CD	2.74	0.50
3:E:237:ASN:ND2	3:E:308:ARG:HD2	2.27	0.50
3:E:249:ALA:O	3:E:252:LEU:N	2.45	0.50
1:F:179:LEU:HD21	2:G:167:LEU:CD2	2.42	0.50
2:I:91:ILE:HD11	2:I:121:LYS:HE3	1.94	0.50
3:J:202:LEU:C	3:J:202:LEU:CD2	2.84	0.50
3:J:282:SER:HB3	3:J:283:PRO:HD2	1.92	0.50
1:A:93:ILE:HG22	1:A:93:ILE:O	2.10	0.50
1:A:192:TRP:HB3	1:A:195:GLY:HA3	1.94	0.50
2:B:183:ILE:HG12	2:B:214:LEU:HD13	1.94	0.50
2:B:191:LEU:HD21	2:B:198:HIS:HB3	1.94	0.50
2:B:295:VAL:HA	2:B:301:ALA:HB3	1.92	0.50
2:B:341:TYR:CD1	2:C:337:LYS:HG3	2.47	0.50
2:C:281:LEU:HD23	2:C:285:MET:HE2	1.94	0.50
2:C:292:ILE:HG13	2:C:313:MET:HE1	1.93	0.50
3:E:32:LEU:HB3	3:E:33:PRO:HD2	1.94	0.50
1:F:104:LEU:HB3	1:F:133:ARG:HH11	1.74	0.50
1:F:144:GLN:OE1	1:F:280:GLN:HG3	2.12	0.50
1:F:161:GLU:HB2	1:F:196:LYS:HA	1.94	0.50
1:F:168:GLN:HA	1:F:171:CYS:SG	2.52	0.50
3:J:116:ASP:HB3	3:J:119:LEU:HD12	1.93	0.50
3:J:154:THR:O	3:J:157:SER:HB2	2.11	0.50
3:J:196:GLY:O	3:J:198:PRO:HD3	2.10	0.50
1:A:38:VAL:CG1	1:A:111:ILE:HD11	2.42	0.50
1:A:329:LEU:CD1	2:B:291:ARG:HH21	2.25	0.50
2:C:3:TYR:CD2	2:C:3:TYR:N	2.80	0.50
2:C:91:ILE:HD12	2:C:123:TYR:CZ	2.47	0.50
2:D:360:HIS:ND1	2:D:361:PRO:HD2	2.27	0.50
1:F:128:THR:O	1:F:131:ALA:HB3	2.12	0.50
2:H:191:LEU:CD1	2:H:203:LEU:HD21	2.41	0.50
2:I:233:SER:O	2:I:237:VAL:HG23	2.11	0.50
2:I:309:ILE:O	2:I:310:GLU:C	2.55	0.50
1:A:196:LYS:H	1:A:201:ARG:HH12	1.60	0.49
2:B:164:VAL:HG23	2:B:165:THR:N	2.26	0.49
2:C:58:LEU:HD23	2:C:153:LEU:HD21	1.93	0.49
2:C:206:LEU:HD13	2:C:221:THR:HA	1.94	0.49
2:C:343:PRO:HG2	2:C:347:MET:SD	2.52	0.49
2:D:32:LEU:HD23	2:D:37:ILE:CD1	2.42	0.49
2:D:38:HIS:CD2	2:D:39:HIS:H	2.30	0.49
3:E:81:PRO:O	3:E:82:GLU:C	2.55	0.49
3:E:91:ASP:O	3:E:92:ALA:C	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:202:ALA:HB1	2:G:237:VAL:HG21	1.94	0.49
2:H:184:ARG:HH12	2:H:203:LEU:CD1	2.25	0.49
2:H:321:PRO:HB2	2:H:324:ASP:OD1	2.12	0.49
1:A:92:ALA:O	1:A:96:GLN:HG3	2.12	0.49
1:A:188:LEU:HD12	1:A:197:LEU:HD21	1.93	0.49
2:B:42:LEU:C	2:B:42:LEU:CD2	2.85	0.49
2:D:290:HIS:C	2:D:292:ILE:N	2.68	0.49
1:F:330:LEU:O	1:F:330:LEU:CD1	2.61	0.49
2:I:334:ILE:HG21	3:J:332:PRO:CB	2.42	0.49
3:J:77:TYR:HE2	3:J:100:LEU:HD21	1.76	0.49
1:A:81:LEU:HD12	1:A:111:ILE:O	2.12	0.49
1:A:101:THR:OG1	1:A:129:ALA:HB3	2.13	0.49
1:A:105:HIS:HE1	1:A:108:LEU:HD12	1.77	0.49
1:A:207:ASN:HD22	1:A:207:ASN:C	2.20	0.49
2:B:11:ARG:HH21	2:B:56:ARG:HH21	1.60	0.49
2:B:307:ALA:HA	2:B:310:GLU:CD	2.37	0.49
2:C:248:GLN:O	2:C:252:LEU:HD12	2.12	0.49
2:D:281:LEU:HD12	2:D:285:MET:HE2	1.94	0.49
1:F:237:ARG:O	1:F:237:ARG:HG2	2.11	0.49
1:F:257:LEU:HD21	1:F:286:MSE:SE	2.63	0.49
2:H:208:ARG:O	2:H:209:ALA:C	2.55	0.49
2:I:158:ASP:OD2	2:I:161:LYS:HG2	2.11	0.49
2:B:177:ALA:C	2:B:178:LEU:HD22	2.38	0.49
2:B:299:PRO:C	2:B:301:ALA:N	2.69	0.49
2:C:13:GLN:OE1	2:C:83:GLU:OE1	2.30	0.49
2:C:306:MET:O	2:C:309:ILE:HG12	2.12	0.49
2:D:277:GLU:O	2:D:279:GLU:N	2.46	0.49
3:E:118:ALA:HB2	3:E:145:THR:CG2	2.42	0.49
2:H:281:LEU:CD2	2:H:285:MET:HE2	2.42	0.49
2:H:311:LEU:HD13	2:H:312:ARG:N	2.27	0.49
2:I:219:SER:OG	3:J:158:ARG:NH2	2.45	0.49
3:J:7:LEU:HD22	3:J:40:LEU:HB2	1.94	0.49
3:J:297:ARG:HH12	3:J:301:MSE:SE	2.44	0.49
1:A:293:LEU:CB	1:A:298:LEU:HD11	2.42	0.49
1:A:298:LEU:O	1:A:301:ALA:HB3	2.13	0.49
1:A:311:THR:CG2	1:A:318:GLN:HG2	2.42	0.49
2:C:37:ILE:HD11	2:C:151:LYS:HG3	1.93	0.49
2:C:102:GLU:HB3	2:C:105:ARG:NH1	2.27	0.49
2:D:136:PHE:HD1	2:D:166:ILE:HD11	1.77	0.49
1:F:45:GLN:CD	1:F:77:ARG:CD	2.66	0.49
2:G:252:LEU:HD21	2:G:353:LEU:CD1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:LEU:CD2	1:A:324:LEU:HD21	2.42	0.49
2:C:6:LEU:C	2:C:8:ARG:N	2.69	0.49
2:C:367:GLU:HG2	2:D:321:PRO:HA	1.95	0.49
2:D:244:LEU:CD1	2:D:276:ILE:HD13	2.42	0.49
3:E:155:LEU:C	3:E:157:SER:N	2.70	0.49
2:H:250:LEU:HD21	2:H:312:ARG:HB2	1.95	0.49
2:H:296:GLN:OE1	2:H:322:PRO:HB3	2.11	0.49
3:J:317:LEU:HD13	3:J:317:LEU:C	2.36	0.49
1:A:262:ARG:NH1	3:E:228:ASP:OD2	2.46	0.49
1:A:298:LEU:N	1:A:298:LEU:HD13	2.28	0.49
2:B:148:GLU:CD	2:B:149:HIS:H	2.21	0.49
2:C:59:ALA:O	2:C:82:ILE:CD1	2.61	0.49
2:C:261:GLY:CA	2:C:357:LEU:HD21	2.43	0.49
2:D:10:TRP:HE1	2:D:190:ILE:HG23	1.71	0.49
2:D:357:LEU:CG	2:D:363:MET:HE1	2.41	0.49
2:G:10:TRP:CZ2	2:G:193:GLU:CG	2.90	0.49
2:G:179:ASP:OD1	2:G:180:VAL:N	2.46	0.49
2:H:264:VAL:O	2:H:268:ILE:HG13	2.13	0.49
1:A:49:GLU:HB2	1:A:77:ARG:O	2.11	0.49
1:A:143:GLU:O	1:A:147:LEU:HB2	2.13	0.49
1:A:259:ASN:O	1:A:262:ARG:N	2.45	0.49
2:B:5:VAL:C	2:B:7:ALA:H	2.19	0.49
2:D:22:GLU:C	2:D:24:VAL:H	2.21	0.49
2:D:38:HIS:CG	2:D:39:HIS:H	2.31	0.49
2:D:149:HIS:C	2:D:150:VAL:HG23	2.37	0.49
2:D:257:VAL:CG1	2:D:320:ILE:HG12	2.36	0.49
3:E:24:HIS:HB2	3:E:160:ARG:CZ	2.43	0.49
3:E:193:LEU:HD23	3:E:266:THR:CG2	2.43	0.49
1:F:31:LEU:HD23	1:F:139:CYS:SG	2.53	0.49
2:G:7:ALA:HB2	2:G:218:LEU:HB3	1.95	0.49
2:G:7:ALA:HB1	2:G:218:LEU:HD13	1.86	0.49
2:G:293:ALA:HB2	2:G:325:ILE:HG21	1.94	0.49
2:H:81:GLU:HB3	2:H:86:ARG:O	2.12	0.49
2:I:309:ILE:O	2:I:311:LEU:N	2.45	0.49
3:J:223:SER:O	3:J:227:GLY:N	2.41	0.49
1:A:130:LEU:C	1:A:132:ASN:H	2.21	0.49
1:A:170:LEU:HD21	1:A:202:VAL:CG1	2.43	0.49
1:A:264:SER:O	1:A:265:ALA:CB	2.61	0.49
2:D:132:SER:O	2:D:133:ARG:C	2.54	0.49
3:E:237:ASN:O	3:E:238:HIS:CB	2.55	0.49
2:G:252:LEU:HD21	2:G:353:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:334:ILE:O	2:G:337:LYS:HB2	2.11	0.49
2:H:65:GLU:HG3	2:H:78:ASN:ND2	2.28	0.49
2:H:277:GLU:O	2:H:280:ALA:N	2.46	0.49
1:A:164:ASP:O	1:A:167:ASN:HB3	2.13	0.49
1:A:213:THR:H	1:A:216:HIS:CG	2.31	0.49
2:B:36:ARG:HB2	2:B:36:ARG:NH1	2.27	0.49
2:C:51:LYS:HB2	6:C:1300:PO4:O4	2.13	0.49
2:C:58:LEU:HD23	2:C:153:LEU:HD22	1.94	0.49
2:C:134:HIS:ND1	2:C:135:SER:N	2.61	0.49
2:C:255:ALA:HB2	2:C:263:ARG:NH1	2.28	0.49
2:C:269:ASN:O	2:C:272:ALA:N	2.46	0.49
2:D:82:ILE:O	2:D:82:ILE:HG22	2.13	0.49
3:E:196:GLY:O	3:E:198:PRO:HD3	2.12	0.49
1:F:2:ILE:HD11	1:F:18:ARG:NH2	2.28	0.49
2:H:215:ARG:NH1	2:I:164:VAL:HG11	2.28	0.49
2:I:285:MET:HB2	2:I:332:LEU:HD21	1.94	0.49
1:A:55:ILE:CG2	1:A:93:ILE:HD13	2.43	0.48
1:A:267:THR:HG22	1:A:271:ALA:HB3	1.95	0.48
2:C:6:LEU:N	2:C:6:LEU:HD23	2.27	0.48
2:C:202:ALA:HB2	2:C:234:THR:CA	2.42	0.48
2:D:250:LEU:C	2:D:252:LEU:N	2.69	0.48
1:F:53:PHE:CZ	1:F:67:LEU:HD13	2.41	0.48
3:J:3:TRP:HH2	3:J:8:ARG:HB3	1.78	0.48
1:A:255:LEU:O	1:A:258:VAL:N	2.43	0.48
2:B:265:MET:HG3	2:C:297:LEU:HD21	1.94	0.48
2:C:78:ASN:O	2:C:82:ILE:HG13	2.11	0.48
2:C:328:TYR:O	2:C:329:TYR:C	2.56	0.48
2:C:333:LEU:C	2:C:335:GLY:H	2.21	0.48
2:D:37:ILE:HG22	2:D:38:HIS:N	2.28	0.48
2:D:139:LEU:O	2:D:142:THR:N	2.44	0.48
3:E:18:TYR:HB3	3:E:48:LEU:HD21	1.96	0.48
2:H:51:LYS:HB2	6:H:1400:PO4:O4	2.13	0.48
2:H:281:LEU:HD22	2:H:349:VAL:HG11	1.95	0.48
2:I:64:CYS:SG	2:I:66:THR:HB	2.53	0.48
2:I:257:VAL:HG13	2:I:328:TYR:OH	2.13	0.48
1:A:298:LEU:HD13	1:A:298:LEU:H	1.78	0.48
2:B:132:SER:C	2:B:134:HIS:N	2.69	0.48
2:B:250:LEU:HD12	2:B:288:LEU:HD13	1.95	0.48
2:D:7:ALA:HA	2:D:218:LEU:HD13	1.95	0.48
2:D:244:LEU:HD11	2:D:276:ILE:HD13	1.95	0.48
2:D:276:ILE:HG22	2:D:277:GLU:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:344:ASP:HB3	2:D:347:MET:HB2	1.94	0.48
3:E:74:PRO:HB2	3:E:105:ARG:HB2	1.94	0.48
3:E:230:TYR:CD1	3:E:230:TYR:O	2.65	0.48
3:J:314:ASP:OD2	3:J:318:ARG:NH2	2.46	0.48
1:A:304:LEU:O	1:A:305:LEU:C	2.57	0.48
1:A:318:GLN:O	1:A:318:GLN:CG	2.61	0.48
1:A:318:GLN:O	1:A:318:GLN:HG3	2.13	0.48
2:B:124:LEU:HD13	2:B:124:LEU:C	2.39	0.48
2:B:352:THR:O	2:B:355:ARG:HB3	2.13	0.48
2:C:257:VAL:O	2:C:360:HIS:HE1	1.95	0.48
2:D:142:THR:HG22	2:D:147:PRO:HD3	1.96	0.48
2:D:260:ASN:CG	2:D:263:ARG:HB2	2.39	0.48
3:E:137:ALA:O	3:E:138:GLU:C	2.57	0.48
3:E:161:LEU:HD12	3:E:161:LEU:N	2.20	0.48
3:E:295:HIS:O	3:E:296:ILE:C	2.55	0.48
1:F:101:THR:O	1:F:104:LEU:HG	2.13	0.48
2:G:125:ILE:HD12	2:G:154:LEU:CD2	2.44	0.48
2:H:144:GLU:OE2	2:H:169:ARG:HD3	2.13	0.48
2:H:278:TRP:HB3	2:H:349:VAL:HG21	1.94	0.48
3:J:90:VAL:HG13	3:J:124:ALA:HA	1.95	0.48
3:J:169:GLU:O	3:J:173:VAL:HG23	2.14	0.48
1:A:36:ASP:O	1:A:40:GLN:HB2	2.13	0.48
1:A:162:LEU:C	1:A:162:LEU:CD2	2.87	0.48
2:B:179:ASP:HB3	2:B:182:GLN:HB2	1.95	0.48
2:D:196:ILE:CG2	2:D:197:ALA:N	2.77	0.48
2:D:268:ILE:HD12	2:D:350:GLU:HG2	1.94	0.48
2:D:321:PRO:O	2:D:322:PRO:C	2.57	0.48
1:F:191:LEU:HD13	2:G:26:THR:CG2	2.43	0.48
2:G:253:VAL:HA	2:G:256:MET:HE3	1.96	0.48
2:G:310:GLU:O	2:G:314:ARG:HG2	2.14	0.48
1:A:186:GLU:O	1:A:190:LEU:HD23	2.14	0.48
2:B:28:LEU:HD11	2:B:43:PHE:CE1	2.48	0.48
2:B:145:GLU:O	2:B:147:PRO:HD3	2.13	0.48
2:B:205:LEU:CD1	2:B:234:THR:HG23	2.44	0.48
2:B:225:ILE:O	2:B:229:ASP:N	2.47	0.48
2:B:278:TRP:O	2:B:279:GLU:C	2.56	0.48
2:C:291:ARG:CD	2:C:306:MET:HE2	2.43	0.48
2:C:321:PRO:O	2:C:324:ASP:HB2	2.13	0.48
2:D:288:LEU:C	2:D:290:HIS:H	2.19	0.48
1:F:222:LEU:HD12	1:F:285:MSE:CE	2.42	0.48
2:H:288:LEU:C	2:H:290:HIS:H	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:286:LEU:CD2	2:I:332:LEU:HD23	2.43	0.48
3:J:120:LEU:O	3:J:120:LEU:HD23	2.14	0.48
3:J:241:ALA:O	3:J:244:ARG:N	2.47	0.48
1:A:99:THR:C	1:A:101:THR:H	2.20	0.48
1:A:188:LEU:O	1:A:189:SER:C	2.56	0.48
2:B:82:ILE:HG23	2:B:90:LEU:HD22	1.96	0.48
2:C:214:LEU:O	2:C:215:ARG:C	2.54	0.48
2:C:314:ARG:O	2:C:315:GLU:C	2.55	0.48
2:C:341:TYR:HB2	2:D:333:LEU:CD1	2.42	0.48
3:E:149:GLU:C	3:E:151:LEU:N	2.72	0.48
1:F:285:MSE:CE	1:F:285:MSE:HG2	2.44	0.48
2:G:99:THR:HG21	2:H:145:GLU:HB3	1.94	0.48
2:G:289:LEU:HD13	2:G:329:TYR:HA	1.96	0.48
2:G:309:ILE:O	2:G:310:GLU:C	2.56	0.48
3:J:295:HIS:O	3:J:299:GLN:HG3	2.14	0.48
1:A:235:GLN:C	1:A:237:ARG:H	2.22	0.48
1:A:255:LEU:O	1:A:256:LEU:C	2.56	0.48
1:A:301:ALA:CB	1:A:331:LEU:HD21	2.44	0.48
2:D:260:ASN:CG	2:D:263:ARG:CB	2.87	0.48
3:E:285:ARG:O	3:E:289:ILE:HG13	2.14	0.48
1:F:3:ARG:NE	1:F:136:GLN:OE1	2.47	0.48
1:F:98:LEU:HD22	1:F:101:THR:CG2	2.44	0.48
3:J:155:LEU:C	3:J:157:SER:N	2.70	0.48
2:C:37:ILE:O	2:C:37:ILE:HG23	2.14	0.48
2:C:157:THR:HG22	2:C:157:THR:O	2.14	0.48
2:D:140:LEU:HD11	2:D:165:THR:OG1	2.14	0.48
2:D:210:ALA:O	2:D:211:GLU:C	2.56	0.48
2:D:250:LEU:HD23	2:D:309:ILE:HG21	1.94	0.48
2:D:260:ASN:O	2:D:260:ASN:OD1	2.32	0.48
2:D:276:ILE:CG2	2:D:277:GLU:H	2.25	0.48
2:G:113:TYR:HD2	2:G:147:PRO:HB3	1.76	0.48
2:I:304:ASN:C	2:I:306:MET:H	2.21	0.48
3:J:151:LEU:O	3:J:152:LEU:C	2.57	0.48
1:A:26:ASN:ND2	1:A:140:GLN:HE22	2.12	0.48
1:A:52:THR:CG2	1:A:81:LEU:HD23	2.44	0.48
1:A:134:SER:O	1:A:135:VAL:HG23	2.14	0.48
1:A:247:LEU:HD21	1:A:308:THR:HG21	1.95	0.48
2:C:338:GLU:C	2:C:340:PRO:CD	2.87	0.48
2:D:24:VAL:O	2:D:27:ALA:N	2.47	0.48
2:D:156:THR:HG21	2:D:159:PRO:HA	1.96	0.48
2:D:282:LEU:O	2:D:283:VAL:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:290:HIS:NE2	2:D:294:MET:CE	2.77	0.48
1:F:304:LEU:HD12	1:F:327:LEU:HD13	1.95	0.48
2:I:257:VAL:O	2:I:257:VAL:HG12	2.14	0.48
1:A:14:ASN:O	1:A:16:GLY:N	2.47	0.47
2:B:128:VAL:O	2:B:128:VAL:HG22	2.14	0.47
2:C:45:GLY:C	2:C:46:THR:O	2.51	0.47
2:C:128:VAL:CG1	2:C:154:LEU:HD22	2.32	0.47
2:D:262:GLU:O	2:D:266:ALA:HB2	2.13	0.47
3:E:251:LEU:O	3:E:254:ASP:HB2	2.13	0.47
2:H:250:LEU:HD22	2:H:309:ILE:HB	1.95	0.47
2:I:19:VAL:HG21	2:I:214:LEU:CD2	2.44	0.47
3:J:268:VAL:O	3:J:271:PRO:HD3	2.14	0.47
1:A:19:ALA:CB	1:A:133:ARG:HD3	2.44	0.47
2:B:256:MET:HE1	2:B:328:TYR:HB3	1.97	0.47
2:C:139:LEU:O	2:C:140:LEU:C	2.58	0.47
2:C:237:VAL:O	2:C:238:SER:C	2.56	0.47
2:C:245:ASP:O	2:C:248:GLN:N	2.47	0.47
2:D:127:GLU:OE1	2:D:157:THR:HG23	2.14	0.47
3:E:58:SER:CB	3:E:65:CYS:SG	2.97	0.47
1:F:192:TRP:C	1:F:194:ASP:H	2.22	0.47
2:H:14:THR:HG22	2:H:15:PHE:N	2.28	0.47
1:A:274:ASP:O	1:A:277:ARG:N	2.48	0.47
2:B:187:LEU:C	2:B:189:HIS:N	2.71	0.47
2:C:70:ALA:C	2:C:72:PRO:HD3	2.39	0.47
2:C:136:PHE:CZ	2:C:163:PRO:HG2	2.49	0.47
2:C:260:ASN:OD1	2:C:263:ARG:HB2	2.14	0.47
2:D:237:VAL:O	2:D:239:ALA:N	2.47	0.47
3:E:167:PRO:HB2	3:E:171:TYR:HD1	1.79	0.47
2:B:21:GLN:NE2	2:B:175:LEU:HA	2.27	0.47
2:B:176:LYS:C	2:B:177:ALA:O	2.56	0.47
2:B:227:SER:HA	2:C:26:THR:CG2	2.45	0.47
2:B:242:GLY:O	2:B:244:LEU:N	2.47	0.47
2:B:294:MET:HE2	2:B:294:MET:HA	1.97	0.47
2:C:268:ILE:O	2:C:271:ALA:HB3	2.13	0.47
3:E:145:THR:CG2	3:E:146:ARG:N	2.76	0.47
2:H:179:ASP:CG	2:H:180:VAL:N	2.71	0.47
2:I:201:ARG:NH2	2:I:284:GLU:CD	2.72	0.47
2:I:364:PRO:HG3	3:J:260:HIS:HE1	1.79	0.47
3:J:73:HIS:HE1	3:J:106:LEU:HD22	1.80	0.47
3:J:296:ILE:HA	3:J:299:GLN:HG3	1.97	0.47
1:A:199:LEU:N	1:A:200:PRO:CD	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ALA:O	1:A:209:ALA:HB2	2.15	0.47
3:E:42:TYR:CE2	3:E:46:ARG:NH1	2.82	0.47
3:E:82:GLU:OE1	3:E:85:LYS:HD3	2.15	0.47
3:E:152:LEU:HD22	3:E:154:THR:HG23	1.97	0.47
3:E:249:ALA:O	3:E:252:LEU:HB2	2.14	0.47
1:F:192:TRP:C	1:F:194:ASP:N	2.71	0.47
2:G:350:GLU:O	2:G:354:LEU:HG	2.15	0.47
2:H:260:ASN:CG	2:H:260:ASN:O	2.57	0.47
2:I:44:SER:HA	2:I:156:THR:O	2.14	0.47
2:I:158:ASP:CG	2:I:161:LYS:CG	2.87	0.47
3:J:5:PRO:O	3:J:7:LEU:N	2.48	0.47
1:A:167:ASN:O	1:A:171:CYS:SG	2.64	0.47
1:A:207:ASN:C	1:A:207:ASN:ND2	2.73	0.47
2:C:243:THR:HG23	2:C:284:GLU:CG	2.44	0.47
2:C:333:LEU:C	2:C:333:LEU:HD23	2.38	0.47
2:D:18:VAL:HB	2:D:25:LEU:HD11	1.96	0.47
2:D:214:LEU:HD23	5:D:801:AGS:C4	2.45	0.47
2:D:347:MET:O	2:D:351:MET:HG3	2.14	0.47
2:G:140:LEU:HD22	2:G:144:GLU:CD	2.39	0.47
2:G:243:THR:HG22	2:G:243:THR:O	2.14	0.47
2:G:282:LEU:HD13	2:G:336:ARG:HA	1.96	0.47
2:H:295:VAL:O	2:H:295:VAL:HG12	2.14	0.47
3:J:3:TRP:CH2	3:J:8:ARG:HB3	2.50	0.47
1:A:179:LEU:HD21	2:B:167:LEU:HD22	1.96	0.47
2:B:208:ARG:O	2:B:210:ALA:O	2.33	0.47
2:B:299:PRO:O	2:B:301:ALA:N	2.43	0.47
2:C:160:GLN:C	2:C:162:LEU:H	2.23	0.47
2:C:244:LEU:HD11	2:C:281:LEU:HD12	1.97	0.47
2:C:344:ASP:HB3	2:C:347:MET:HB2	1.96	0.47
3:E:125:ALA:O	3:E:126:ASN:C	2.56	0.47
3:E:225:PRO:HA	3:E:280:HIS:CE1	2.49	0.47
1:F:13:LEU:HD12	1:F:21:TYR:OH	2.14	0.47
1:F:71:MSE:O	1:F:105:HIS:HE1	1.97	0.47
2:G:148:GLU:O	2:G:149:HIS:HB2	2.15	0.47
2:H:56:ARG:O	2:H:60:LYS:HB2	2.14	0.47
3:J:32:LEU:HB3	3:J:33:PRO:HD2	1.97	0.47
3:J:73:HIS:CD2	3:J:75:ASP:H	2.31	0.47
3:J:171:TYR:CD2	3:J:171:TYR:N	2.81	0.47
1:A:59:THR:HG21	1:A:64:ILE:HD11	1.97	0.47
1:A:95:GLU:O	1:A:98:LEU:N	2.47	0.47
1:A:326:GLY:O	1:A:327:LEU:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:120:PHE:HD2	2:C:120:PHE:N	2.12	0.47
3:E:122:ASP:O	3:E:126:ASN:OD1	2.33	0.47
2:H:360:HIS:O	2:H:364:PRO:HG3	2.14	0.47
1:A:150:TRP:CH2	1:A:178:LEU:CD1	2.90	0.47
1:A:252:ARG:O	1:A:256:LEU:HB2	2.15	0.47
2:B:179:ASP:HB3	2:B:182:GLN:CB	2.45	0.47
2:B:332:LEU:HD13	2:B:332:LEU:HA	1.73	0.47
2:C:265:MET:HG3	2:D:297:LEU:HD23	1.97	0.47
2:D:22:GLU:O	2:D:24:VAL:N	2.48	0.47
2:D:184:ARG:HD3	2:D:185:HIS:CA	2.45	0.47
2:D:291:ARG:HD2	2:D:306:MET:SD	2.55	0.47
2:H:100:LYS:NZ	2:I:133:ARG:HA	2.30	0.47
2:H:202:ALA:HB2	2:H:234:THR:CG2	2.42	0.47
2:H:346:ARG:O	2:H:350:GLU:HG3	2.15	0.47
3:J:5:PRO:C	3:J:7:LEU:N	2.71	0.47
1:A:31:LEU:HB3	1:A:113:ARG:HD2	1.97	0.47
2:B:140:LEU:O	2:B:143:LEU:CD2	2.62	0.47
2:B:254:GLU:HA	2:B:257:VAL:HG23	1.95	0.47
2:D:188:GLU:O	2:D:189:HIS:C	2.57	0.47
2:D:288:LEU:O	2:D:290:HIS:N	2.47	0.47
3:E:24:HIS:HB2	3:E:160:ARG:NH2	2.30	0.47
1:F:67:LEU:CD1	1:F:71:MSE:HE3	2.46	0.47
1:F:223:MSE:SE	1:F:292:ARG:HB3	2.65	0.47
2:H:47:ARG:O	2:H:47:ARG:HG3	2.14	0.47
2:H:327:LEU:CD2	2:H:361:PRO:HD3	2.43	0.47
1:A:6:PRO:O	1:A:9:LEU:HB3	2.15	0.46
1:A:59:THR:HB	1:A:61:TRP:NE1	2.29	0.46
1:A:262:ARG:NH2	3:E:320:GLU:CD	2.73	0.46
2:B:42:LEU:HD23	2:B:43:PHE:N	2.30	0.46
2:B:259:ALA:HB2	2:B:360:HIS:ND1	2.30	0.46
2:B:265:MET:HA	2:B:265:MET:HE3	1.98	0.46
2:B:286:LEU:HD21	2:B:333:LEU:HA	1.97	0.46
2:C:51:LYS:HB2	2:C:51:LYS:HE3	1.78	0.46
2:D:223:GLN:HB3	2:D:240:MET:HE3	1.94	0.46
2:D:238:SER:CB	2:D:243:THR:HB	2.45	0.46
2:D:355:ARG:HH21	3:E:332:PRO:CD	2.26	0.46
3:E:32:LEU:HD22	3:E:195:ALA:CB	2.45	0.46
3:E:32:LEU:CD1	3:E:166:PRO:HG2	2.45	0.46
2:G:133:ARG:O	2:G:137:ASN:ND2	2.48	0.46
2:G:259:ALA:HB2	2:G:360:HIS:CE1	2.50	0.46
2:G:291:ARG:O	2:G:295:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:62:LEU:HB3	2:H:120:PHE:CD2	2.51	0.46
2:H:231:GLN:C	2:H:233:SER:H	2.23	0.46
2:I:259:ALA:HA	2:I:363:MET:SD	2.55	0.46
3:J:129:LEU:CD1	3:J:129:LEU:H	2.28	0.46
3:J:254:ASP:HA	3:J:257:LYS:HD2	1.97	0.46
1:A:13:LEU:HD12	1:A:13:LEU:HA	1.74	0.46
1:A:190:LEU:HD22	2:B:36:ARG:CZ	2.45	0.46
1:A:226:SER:O	1:A:229:ALA:HB3	2.15	0.46
2:B:98:ARG:O	2:B:101:VAL:HG13	2.14	0.46
2:C:47:ARG:O	2:C:47:ARG:HG3	2.15	0.46
2:C:285:MET:HE1	2:C:353:LEU:HD21	1.97	0.46
2:C:292:ILE:HG12	2:C:313:MET:CE	2.46	0.46
2:D:105:ARG:HG3	2:D:134:HIS:NE2	2.30	0.46
2:D:184:ARG:C	2:D:184:ARG:CD	2.83	0.46
3:E:28:LEU:HA	3:E:143:LEU:O	2.15	0.46
3:E:192:ARG:C	3:E:194:SER:N	2.74	0.46
1:F:80:LEU:CD1	1:F:108:LEU:HD12	2.44	0.46
2:G:98:ARG:HG3	2:H:169:ARG:HH22	1.79	0.46
2:G:227:SER:HA	2:H:26:THR:CG2	2.45	0.46
2:I:32:LEU:HD13	2:I:70:ALA:HA	1.97	0.46
2:I:259:ALA:CB	2:I:363:MET:SD	3.04	0.46
2:I:361:PRO:O	2:I:362:ARG:CB	2.63	0.46
3:J:176:LEU:C	3:J:178:ARG:H	2.22	0.46
1:A:213:THR:HB	1:A:216:HIS:ND1	2.30	0.46
1:A:223:MSE:HG3	1:A:289:ALA:HA	1.97	0.46
2:B:56:ARG:HH11	2:B:56:ARG:CG	2.23	0.46
2:B:113:TYR:CD2	2:B:147:PRO:HB3	2.50	0.46
2:B:226:ALA:HA	2:C:30:ASN:ND2	2.30	0.46
2:D:92:GLU:HG2	2:D:124:LEU:HD12	1.97	0.46
3:E:34:GLY:O	3:E:197:SER:OG	2.34	0.46
3:E:250:THR:O	3:E:251:LEU:C	2.58	0.46
3:E:319:ILE:HA	3:E:322:TYR:CD2	2.49	0.46
2:G:140:LEU:HD22	2:G:144:GLU:HG3	1.97	0.46
2:H:354:LEU:HD22	2:I:293:ALA:HB1	1.97	0.46
3:J:31:ALA:HB2	3:J:164:LEU:CB	2.40	0.46
1:A:102:GLY:HA3	2:G:310:GLU:OE2	2.15	0.46
2:B:81:GLU:CB	2:B:87:PHE:HD1	2.23	0.46
2:D:148:GLU:CD	2:D:149:HIS:N	2.70	0.46
2:D:334:ILE:HG21	3:E:332:PRO:HB2	1.97	0.46
3:E:73:HIS:CE1	3:E:106:LEU:HD22	2.50	0.46
1:F:155:ALA:CB	1:F:162:LEU:HD12	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:199:LEU:N	1:F:200:PRO:CD	2.78	0.46
2:G:209:ALA:CB	2:G:241:LEU:HD13	2.46	0.46
2:H:56:ARG:HG2	2:H:56:ARG:HH11	1.81	0.46
2:I:260:ASN:HB3	2:I:263:ARG:HB3	1.98	0.46
3:J:4:TYR:O	3:J:7:LEU:HB2	2.15	0.46
3:J:80:ALA:HB1	3:J:81:PRO:HD2	1.97	0.46
3:J:240:GLN:O	3:J:244:ARG:HG3	2.15	0.46
3:J:308:ARG:O	3:J:312:ILE:HG13	2.15	0.46
2:B:5:VAL:O	2:B:7:ALA:N	2.48	0.46
2:B:255:ALA:CB	2:B:263:ARG:HD3	2.45	0.46
2:C:37:ILE:CD1	2:C:151:LYS:HE3	2.46	0.46
2:C:289:LEU:H	2:C:289:LEU:CD2	2.28	0.46
2:D:10:TRP:CG	2:D:190:ILE:CD1	2.97	0.46
2:D:64:CYS:SG	2:D:66:THR:HB	2.55	0.46
2:D:341:TYR:CD2	3:E:295:HIS:CE1	3.04	0.46
2:G:309:ILE:O	2:G:311:LEU:N	2.48	0.46
2:I:360:HIS:HD2	2:I:361:PRO:N	2.13	0.46
3:J:317:LEU:HD22	3:J:317:LEU:O	2.15	0.46
1:A:276:HIS:O	1:A:277:ARG:HB2	2.16	0.46
2:C:6:LEU:O	2:C:8:ARG:N	2.48	0.46
2:C:305:ASP:C	2:C:307:ALA:N	2.72	0.46
2:D:24:VAL:C	2:D:26:THR:N	2.72	0.46
2:D:129:HIS:HD2	2:D:161:LYS:HG3	1.81	0.46
2:D:290:HIS:O	2:D:291:ARG:C	2.59	0.46
3:E:13:LYS:O	3:E:16:ALA:N	2.48	0.46
3:E:78:THR:O	3:E:78:THR:HG22	2.14	0.46
3:E:281:LEU:CD2	3:E:323:LEU:HD21	2.45	0.46
1:F:273:PHE:HB3	1:F:279:TRP:CB	2.46	0.46
1:A:126:TRP:CG	1:A:127:PHE:N	2.83	0.46
1:A:213:THR:C	1:A:215:PHE:H	2.23	0.46
1:A:220:ALA:C	1:A:222:LEU:N	2.72	0.46
1:A:269:LEU:HD11	1:A:273:PHE:HZ	1.79	0.46
2:B:140:LEU:CA	2:B:143:LEU:HD22	2.42	0.46
2:C:292:ILE:O	2:C:294:MET:N	2.49	0.46
2:C:302:LEU:CD1	2:C:310:GLU:HG3	2.46	0.46
2:D:10:TRP:NE1	2:D:190:ILE:CG2	2.69	0.46
2:D:11:ARG:O	2:D:13:GLN:NE2	2.48	0.46
3:E:32:LEU:HD12	3:E:166:PRO:CG	2.45	0.46
3:E:233:LEU:O	3:E:234:ALA:C	2.58	0.46
3:E:281:LEU:O	3:E:282:SER:O	2.33	0.46
1:F:20:ALA:HB2	1:F:110:LEU:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:299:ARG:CD	3:J:317:LEU:HD21	2.46	0.46
2:H:184:ARG:HH12	2:H:203:LEU:HD12	1.80	0.46
2:I:334:ILE:HG21	3:J:332:PRO:HB2	1.98	0.46
3:J:50:CYS:SG	3:J:53:PRO:N	2.88	0.46
3:J:185:ASP:OD2	3:J:185:ASP:N	2.49	0.46
3:J:225:PRO:HA	3:J:280:HIS:ND1	2.30	0.46
1:A:221:LEU:HD21	1:A:328:SER:HB2	1.94	0.46
1:A:256:LEU:O	1:A:260:LEU:HG	2.16	0.46
2:B:276:ILE:CD1	2:B:281:LEU:HD13	2.45	0.46
2:B:333:LEU:HD11	2:B:337:LYS:CE	2.45	0.46
2:D:13:GLN:HE21	2:D:13:GLN:N	2.14	0.46
2:D:21:GLN:HE21	2:D:21:GLN:HA	1.81	0.46
2:D:292:ILE:O	2:D:296:GLN:HG3	2.16	0.46
3:E:292:ASP:OD2	3:E:322:TYR:OH	2.33	0.46
2:G:98:ARG:CD	2:H:140:LEU:HB3	2.43	0.46
2:G:330:GLN:HG3	2:G:331:THR:N	2.31	0.46
2:H:223:GLN:NE2	2:I:174:HIS:CE1	2.84	0.46
2:I:333:LEU:C	2:I:333:LEU:HD13	2.41	0.46
1:A:106:ASP:OD2	1:F:225:LYS:HE2	2.15	0.46
2:C:196:ILE:C	2:C:197:ALA:O	2.54	0.46
2:C:205:LEU:O	2:C:206:LEU:C	2.59	0.46
2:C:288:LEU:O	2:C:289:LEU:C	2.59	0.46
2:D:142:THR:HG22	2:D:147:PRO:CD	2.46	0.46
3:E:1:MSE:HE1	3:E:42:TYR:CG	2.51	0.46
3:E:283:PRO:CG	3:E:284:SER:H	2.25	0.46
1:F:181:LEU:O	1:F:185:LEU:HG	2.15	0.46
1:F:223:MSE:CE	1:F:292:ARG:HB2	2.43	0.46
2:G:130:MET:HE1	2:H:165:THR:HG22	1.98	0.46
2:H:18:VAL:HB	2:H:25:LEU:HD11	1.97	0.46
2:H:314:ARG:O	2:H:318:ARG:HG2	2.15	0.46
3:J:182:MSE:HG3	3:J:205:PHE:CE1	2.50	0.46
3:J:205:PHE:O	3:J:207:GLY:N	2.48	0.46
1:A:154:ARG:NH1	1:A:157:GLN:HE21	2.12	0.46
1:A:234:GLN:HB3	1:A:237:ARG:NH2	2.28	0.46
2:B:71:THR:O	2:B:72:PRO:C	2.59	0.46
2:B:140:LEU:HD22	2:B:144:GLU:OE1	2.16	0.46
2:B:179:ASP:HB3	2:B:182:GLN:HG3	1.97	0.46
2:C:106:ASP:O	2:C:110:ASN:HB2	2.15	0.46
2:C:302:LEU:CD2	2:C:306:MET:HG3	2.45	0.46
2:D:197:ALA:CB	2:D:231:GLN:HG2	2.44	0.46
2:D:339:LEU:HD11	2:D:345:ARG:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:37:ASP:CG	3:E:38:ASP:N	2.73	0.46
3:E:69:GLN:HE21	3:E:69:GLN:C	2.24	0.46
3:E:136:PRO:O	3:E:137:ALA:C	2.58	0.46
3:E:142:PHE:C	3:E:143:LEU:HD22	2.41	0.46
3:E:279:ASN:C	3:E:281:LEU:N	2.73	0.46
1:F:147:LEU:N	1:F:148:PRO:CD	2.79	0.46
2:G:246:ASP:O	2:G:246:ASP:CG	2.57	0.46
2:I:354:LEU:HD23	2:I:357:LEU:HD22	1.98	0.46
2:C:42:LEU:HD23	2:C:172:GLN:HG3	1.98	0.45
2:C:220:LEU:C	2:C:222:ASP:N	2.73	0.45
3:E:98:GLU:C	3:E:100:LEU:H	2.24	0.45
3:E:182:MSE:HA	3:E:182:MSE:HE3	1.98	0.45
3:E:318:ARG:O	3:E:319:ILE:C	2.57	0.45
1:F:70:ALA:C	1:F:71:MSE:HE2	2.40	0.45
1:F:242:GLU:O	1:F:245:ILE:CG2	2.60	0.45
2:H:351:MET:SD	2:I:290:HIS:HA	2.56	0.45
2:I:248:GLN:HE21	2:I:248:GLN:CA	2.20	0.45
2:I:286:LEU:HD21	2:I:332:LEU:HB3	1.98	0.45
1:A:20:ALA:HA	1:A:110:LEU:O	2.16	0.45
1:A:254:LEU:O	1:A:258:VAL:HG23	2.15	0.45
1:A:336:LEU:H	1:A:336:LEU:CD2	2.06	0.45
2:B:144:GLU:C	2:B:146:PRO:HD3	2.42	0.45
2:C:315:GLU:O	2:C:316:LEU:C	2.59	0.45
2:D:21:GLN:HE22	2:D:176:LYS:H	1.65	0.45
3:E:88:LEU:HD23	3:E:88:LEU:C	2.40	0.45
2:H:184:ARG:NH1	2:H:188:GLU:HB2	2.31	0.45
3:J:316:LEU:HA	3:J:319:ILE:CD1	2.45	0.45
1:A:19:ALA:CB	1:A:133:ARG:HB3	2.46	0.45
2:B:347:MET:O	2:B:348:GLY:C	2.59	0.45
2:C:73:CYS:SG	2:C:76:CYS:HB3	2.56	0.45
2:D:32:LEU:C	2:D:34:LEU:N	2.74	0.45
2:D:235:GLN:O	2:D:236:ALA:C	2.59	0.45
3:E:120:LEU:HD12	3:E:125:ALA:N	2.31	0.45
1:F:80:LEU:N	1:F:80:LEU:CD1	2.73	0.45
1:F:93:ILE:C	1:F:95:GLU:H	2.23	0.45
1:F:271:ALA:O	1:F:275:LYS:HG2	2.15	0.45
2:H:100:LYS:HE2	2:I:136:PHE:CD2	2.48	0.45
2:I:337:LYS:HD2	2:I:337:LYS:O	2.16	0.45
3:J:129:LEU:H	3:J:129:LEU:HD12	1.80	0.45
3:J:236:LEU:O	3:J:237:ASN:C	2.58	0.45
1:A:105:HIS:CE1	1:A:108:LEU:HD12	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:ARG:O	2:B:109:ASP:OD2	2.34	0.45
2:B:247:ASP:HB2	2:B:312:ARG:HH12	1.82	0.45
2:B:347:MET:HG3	2:C:290:HIS:CG	2.51	0.45
2:C:136:PHE:HZ	2:C:163:PRO:HG2	1.80	0.45
2:D:160:GLN:C	2:D:162:LEU:N	2.74	0.45
2:D:257:VAL:HG11	2:D:320:ILE:CG1	2.39	0.45
2:D:332:LEU:HD23	2:D:332:LEU:HA	1.68	0.45
3:E:316:LEU:HD23	3:E:316:LEU:HA	1.68	0.45
1:F:250:LEU:H	1:F:250:LEU:CD2	2.28	0.45
2:G:268:ILE:HD11	2:G:353:LEU:CD1	2.35	0.45
2:G:342:ALA:C	2:G:344:ASP:N	2.75	0.45
2:H:214:LEU:HD12	2:H:217:ALA:HB3	1.99	0.45
2:I:127:GLU:OE1	2:I:127:GLU:HA	2.16	0.45
2:I:220:LEU:CD2	3:J:157:SER:OG	2.64	0.45
3:J:35:MSE:SE	3:J:167:PRO:HD3	2.66	0.45
2:B:10:TRP:CH2	2:B:190:ILE:HA	2.52	0.45
2:B:50:GLY:HA2	5:B:802:AGS:O1A	2.16	0.45
2:B:338:GLU:O	2:B:339:LEU:C	2.60	0.45
2:B:356:ALA:O	2:B:360:HIS:N	2.49	0.45
2:C:367:GLU:OE2	2:C:368:PRO:CD	2.65	0.45
2:D:21:GLN:CD	2:D:175:LEU:HG	2.41	0.45
2:D:310:GLU:O	2:D:311:LEU:C	2.58	0.45
1:F:56:ASP:N	1:F:57:PRO:CD	2.79	0.45
2:I:15:PHE:O	2:I:18:VAL:HB	2.16	0.45
2:I:248:GLN:NE2	2:I:248:GLN:CA	2.79	0.45
3:J:190:ALA:HB2	3:J:210:TRP:CZ3	2.52	0.45
3:J:271:PRO:O	3:J:274:VAL:HG22	2.16	0.45
1:A:124:ALA:O	1:A:125:ALA:C	2.60	0.45
1:A:280:GLN:H	1:A:280:GLN:HG2	1.43	0.45
2:B:245:ASP:O	2:B:246:ASP:O	2.35	0.45
2:D:15:PHE:O	2:D:17:ASP:N	2.49	0.45
2:D:115:PRO:HG3	2:D:121:LYS:HB2	1.99	0.45
2:D:186:GLN:O	2:D:187:LEU:C	2.59	0.45
2:D:201:ARG:HB2	2:D:305:ASP:OD2	2.17	0.45
2:D:332:LEU:O	2:D:333:LEU:C	2.58	0.45
1:F:299:ARG:HG3	3:J:317:LEU:CD2	2.47	0.45
2:I:330:GLN:O	2:I:334:ILE:HG13	2.15	0.45
3:J:27:LEU:HG	3:J:29:ILE:HD11	1.98	0.45
1:A:117:LEU:CB	1:A:122:GLU:HG3	2.46	0.45
2:B:124:LEU:HA	2:B:153:LEU:O	2.17	0.45
2:B:307:ALA:HA	2:B:310:GLU:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:237:VAL:O	2:D:238:SER:C	2.60	0.45
2:G:148:GLU:OE1	2:G:148:GLU:CA	2.65	0.45
2:H:61:GLY:O	2:H:68:ILE:HA	2.17	0.45
2:H:351:MET:HA	2:H:354:LEU:HD13	1.99	0.45
1:A:294:SER:O	1:A:295:GLN:C	2.60	0.45
2:B:94:ASP:OD1	2:B:96:ALA:HB3	2.16	0.45
2:C:29:ALA:O	2:C:33:SER:OG	2.27	0.45
2:D:27:ALA:O	2:D:29:ALA:N	2.50	0.45
2:D:179:ASP:O	2:D:182:GLN:HB2	2.16	0.45
3:E:6:TRP:CH2	3:E:198:PRO:HB2	2.52	0.45
3:E:222:TYR:CE1	3:E:226:SER:HB3	2.51	0.45
3:E:333:HIS:ND1	3:E:333:HIS:N	2.65	0.45
1:F:214:PRO:HA	1:F:236:LEU:HD11	1.99	0.45
2:G:44:SER:O	2:G:175:LEU:HB2	2.17	0.45
2:G:76:CYS:O	2:G:80:ARG:HG3	2.17	0.45
2:G:93:ILE:HG21	2:G:104:THR:HG23	1.99	0.45
2:I:367:GLU:HB3	2:I:368:PRO:HD2	1.99	0.45
1:A:80:LEU:HG	1:A:82:LEU:CD1	2.47	0.45
1:A:237:ARG:C	1:A:239:GLU:H	2.23	0.45
2:B:158:ASP:C	2:B:160:GLN:H	2.24	0.45
2:B:286:LEU:HD21	2:B:333:LEU:CA	2.47	0.45
2:B:314:ARG:O	2:B:317:ALA:HB3	2.17	0.45
2:C:18:VAL:HG12	2:C:19:VAL:N	2.32	0.45
2:D:328:TYR:HD1	2:D:356:ALA:HB1	1.81	0.45
2:D:352:THR:O	2:D:355:ARG:HB3	2.17	0.45
1:F:168:GLN:HE21	1:F:168:GLN:HB2	1.49	0.45
2:I:119:ARG:HG3	2:I:120:PHE:CD2	2.52	0.45
1:A:228:ARG:H	1:A:228:ARG:HG2	1.42	0.45
1:A:320:VAL:O	1:A:321:TRP:C	2.60	0.45
2:B:8:ARG:HD2	2:B:8:ARG:C	2.41	0.45
2:B:10:TRP:CZ2	2:B:190:ILE:HG23	2.51	0.45
2:B:254:GLU:O	2:B:255:ALA:C	2.60	0.45
2:B:254:GLU:C	2:B:256:MET:N	2.73	0.45
2:C:15:PHE:CE1	2:C:57:LEU:O	2.70	0.45
2:C:163:PRO:O	2:C:167:LEU:HG	2.17	0.45
2:C:276:ILE:H	2:C:276:ILE:HG13	1.52	0.45
2:D:10:TRP:O	2:D:12:PRO:HD3	2.16	0.45
2:D:134:HIS:CG	2:D:135:SER:N	2.84	0.45
1:F:97:LEU:HD23	1:F:126:TRP:CE3	2.50	0.45
2:G:98:ARG:HD2	2:H:169:ARG:NH2	2.32	0.45
2:G:295:VAL:CG2	2:G:301:ALA:HB3	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:129:HIS:CD2	2:H:161:LYS:HD2	2.50	0.45
3:J:121:THR:HG22	3:J:122:ASP:N	2.32	0.45
1:A:220:ALA:O	1:A:224:GLY:N	2.50	0.44
2:C:268:ILE:O	2:C:272:ALA:N	2.45	0.44
2:D:128:VAL:HG13	2:D:129:HIS:N	2.33	0.44
2:D:191:LEU:HD23	2:D:191:LEU:HA	1.68	0.44
2:D:258:GLU:O	2:D:259:ALA:HB3	2.17	0.44
2:D:329:TYR:HD2	2:D:330:GLN:N	2.15	0.44
3:E:98:GLU:H	3:E:98:GLU:HG2	1.61	0.44
3:E:237:ASN:HD22	3:E:237:ASN:C	2.25	0.44
1:F:262:ARG:HH22	3:J:228:ASP:CG	2.25	0.44
1:F:318:GLN:O	1:F:318:GLN:HG3	2.17	0.44
2:H:62:LEU:HB3	2:H:120:PHE:HD2	1.81	0.44
2:H:359:PHE:CZ	2:I:323:THR:HG23	2.52	0.44
2:I:51:LYS:NZ	5:I:803:AGS:S1G	2.80	0.44
3:J:60:GLY:N	3:J:65:CYS:SG	2.89	0.44
3:J:245:LEU:O	3:J:248:LEU:HB3	2.16	0.44
1:A:173:CYS:O	1:A:174:TYR:C	2.59	0.44
1:A:191:LEU:HD23	2:B:27:ALA:HA	1.99	0.44
1:A:223:MSE:CE	1:A:292:ARG:CB	2.96	0.44
2:B:278:TRP:C	2:B:280:ALA:N	2.74	0.44
2:D:302:LEU:HD23	2:D:302:LEU:HA	1.79	0.44
2:D:353:LEU:C	2:D:355:ARG:N	2.73	0.44
3:E:57:LYS:HD2	3:E:57:LYS:HA	1.79	0.44
3:E:219:ALA:O	3:E:220:LEU:C	2.59	0.44
3:E:270:VAL:HG23	3:E:273:LEU:HB3	1.99	0.44
1:F:67:LEU:O	1:F:70:ALA:N	2.50	0.44
1:F:147:LEU:O	1:F:151:VAL:HG23	2.17	0.44
2:G:145:GLU:N	2:G:146:PRO:HD3	2.32	0.44
2:H:365:LEU:HB2	2:I:322:PRO:HG3	1.98	0.44
3:J:35:MSE:HA	3:J:35:MSE:HE2	2.00	0.44
3:J:241:ALA:O	3:J:242:PRO:C	2.59	0.44
2:B:257:VAL:C	2:B:259:ALA:N	2.74	0.44
2:B:333:LEU:HD13	2:B:334:ILE:N	2.32	0.44
2:C:113:TYR:HD2	2:C:147:PRO:HB3	1.82	0.44
2:C:324:ASP:OD1	2:C:362:ARG:NH2	2.46	0.44
2:D:354:LEU:HD13	3:E:253:MSE:CE	2.38	0.44
3:E:68:MSE:HE2	3:E:68:MSE:HA	2.00	0.44
3:E:275:ALA:O	3:E:279:ASN:ND2	2.49	0.44
2:G:313:MET:O	2:G:316:LEU:N	2.50	0.44
2:I:299:PRO:O	2:I:314:ARG:NH2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:345:ARG:NH2	3:J:146:ARG:O	2.50	0.44
3:J:241:ALA:HB3	3:J:242:PRO:CD	2.48	0.44
1:A:308:THR:O	1:A:312:LEU:N	2.49	0.44
2:B:8:ARG:HD2	2:B:8:ARG:O	2.17	0.44
2:B:291:ARG:O	2:B:294:MET:HB3	2.17	0.44
2:B:328:TYR:O	2:B:329:TYR:O	2.36	0.44
2:C:100:LYS:HG2	2:D:133:ARG:HG3	1.99	0.44
2:C:171:LEU:HD12	2:C:171:LEU:HA	1.87	0.44
2:C:237:VAL:C	2:C:239:ALA:N	2.74	0.44
2:C:261:GLY:O	2:C:263:ARG:N	2.51	0.44
2:D:268:ILE:O	2:D:271:ALA:N	2.48	0.44
2:D:295:VAL:HG21	2:D:302:LEU:HG	2.00	0.44
3:E:90:VAL:HA	3:E:124:ALA:HA	2.00	0.44
1:F:237:ARG:O	1:F:238:LEU:HD23	2.17	0.44
2:H:112:GLN:HB2	2:H:121:LYS:HZ2	1.78	0.44
2:H:126:ASP:HA	2:H:155:ALA:HB3	1.98	0.44
2:H:142:THR:O	2:H:142:THR:HG22	2.17	0.44
2:H:265:MET:SD	2:I:297:LEU:HD23	2.56	0.44
3:J:77:TYR:HE1	3:J:99:LYS:HE2	1.82	0.44
3:J:194:SER:O	3:J:195:ALA:HB3	2.18	0.44
1:A:74:PHE:HD1	1:F:203:GLU:CG	2.17	0.44
1:A:274:ASP:HA	1:A:279:TRP:CZ3	2.52	0.44
2:B:316:LEU:HD23	2:B:316:LEU:HA	1.85	0.44
2:C:97:SER:HG	2:C:100:LYS:HD2	1.82	0.44
2:D:278:TRP:CZ2	2:D:346:ARG:HB2	2.52	0.44
3:E:120:LEU:CD1	3:E:125:ALA:HA	2.47	0.44
3:E:310:LEU:O	3:E:311:LEU:C	2.60	0.44
1:F:310:LEU:O	1:F:313:LYS:N	2.47	0.44
2:G:22:GLU:H	2:G:22:GLU:CD	2.25	0.44
2:I:202:ALA:HB1	2:I:237:VAL:HG21	2.00	0.44
2:I:365:LEU:HB3	2:I:366:PRO:HD2	2.00	0.44
3:J:94:ARG:HA	3:J:94:ARG:HD3	1.81	0.44
3:J:95:GLU:O	3:J:99:LYS:HB2	2.18	0.44
3:J:167:PRO:O	3:J:168:PRO:C	2.61	0.44
1:A:327:LEU:C	1:A:327:LEU:CD2	2.90	0.44
2:B:156:THR:HG21	2:B:159:PRO:HG3	2.00	0.44
2:B:158:ASP:O	2:B:158:ASP:OD1	2.36	0.44
2:B:248:GLN:HA	2:B:251:SER:CB	2.42	0.44
2:C:252:LEU:O	2:C:256:MET:N	2.49	0.44
2:C:295:VAL:HG12	2:C:299:PRO:HA	2.00	0.44
2:C:321:PRO:O	2:C:322:PRO:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:136:PHE:HD1	2:D:166:ILE:CD1	2.31	0.44
1:F:174:TYR:HB2	1:F:181:LEU:HD21	1.98	0.44
2:G:307:ALA:HA	2:G:310:GLU:HG3	1.99	0.44
2:H:100:LYS:NZ	2:I:133:ARG:CA	2.80	0.44
2:I:48:GLY:O	2:I:213:SER:HA	2.16	0.44
3:J:317:LEU:HD13	3:J:318:ARG:CA	2.48	0.44
1:A:221:LEU:HD11	1:A:328:SER:HB3	1.98	0.44
1:A:320:VAL:HG12	1:A:321:TRP:N	2.33	0.44
1:A:324:LEU:HD23	1:A:324:LEU:HA	1.73	0.44
2:B:282:LEU:HD23	2:B:282:LEU:HA	1.67	0.44
2:B:319:THR:C	2:B:320:ILE:HG13	2.43	0.44
2:D:13:GLN:HE21	2:D:13:GLN:CA	2.30	0.44
2:D:268:ILE:HG23	2:D:278:TRP:HH2	1.82	0.44
3:E:7:LEU:HD21	3:E:36:GLY:HA3	2.00	0.44
2:H:91:ILE:HD13	2:H:107:LEU:HD22	1.99	0.44
2:I:167:LEU:HD21	2:I:172:GLN:OE1	2.17	0.44
1:A:53:PHE:CD2	1:A:64:ILE:HG12	2.52	0.44
1:A:177:ASN:O	1:A:179:LEU:N	2.49	0.44
1:A:221:LEU:O	1:A:223:MSE:N	2.50	0.44
1:A:259:ASN:O	1:A:260:LEU:C	2.60	0.44
2:B:227:SER:HA	2:C:26:THR:HG21	1.99	0.44
2:C:52:THR:OG1	2:C:53:SER:N	2.51	0.44
2:C:240:MET:HA	2:D:23:HIS:CB	2.48	0.44
1:F:219:ASP:O	1:F:222:LEU:HB2	2.17	0.44
2:G:289:LEU:CD2	2:G:325:ILE:HG23	2.47	0.44
2:H:3:TYR:CD2	2:H:3:TYR:N	2.86	0.44
2:H:44:SER:CB	2:H:159:PRO:HG3	2.48	0.44
2:I:295:VAL:HG22	2:I:301:ALA:HB3	2.00	0.44
3:J:5:PRO:HG2	3:J:6:TRP:H	1.81	0.44
3:J:125:ALA:O	3:J:128:LEU:HB3	2.17	0.44
3:J:253:MSE:CE	3:J:257:LYS:HG3	2.48	0.44
1:A:105:HIS:HB3	1:F:227:LYS:CD	2.42	0.44
1:A:209:ALA:HA	2:B:176:LYS:HZ1	1.82	0.44
2:B:179:ASP:O	2:B:183:ILE:HG13	2.18	0.44
2:C:66:THR:O	2:C:66:THR:HG22	2.18	0.44
2:C:346:ARG:O	2:C:349:VAL:N	2.51	0.44
2:D:215:ARG:HD2	5:D:801:AGS:H5'1	2.00	0.44
3:E:286:LEU:O	3:E:287:GLN:C	2.61	0.44
1:F:297:GLN:HG2	1:F:335:PRO:HD3	2.00	0.44
2:G:345:ARG:O	2:G:349:VAL:HG23	2.18	0.44
2:H:9:LYS:NZ	2:H:194:GLU:CD	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:279:GLU:HG3	2:H:345:ARG:HH12	1.82	0.44
2:I:6:LEU:HB2	2:I:218:LEU:C	2.43	0.44
2:I:277:GLU:O	2:I:280:ALA:N	2.51	0.44
2:I:337:LYS:HE3	2:I:338:GLU:HG2	2.00	0.44
3:J:173:VAL:HG11	3:J:184:GLN:HG3	2.00	0.44
1:A:192:TRP:CH2	1:A:201:ARG:HB3	2.53	0.43
2:C:351:MET:HE1	2:D:293:ALA:HB3	2.00	0.43
2:C:367:GLU:HG3	2:D:321:PRO:CA	2.48	0.43
2:D:192:ASN:O	2:D:193:GLU:C	2.61	0.43
2:D:256:MET:HE2	2:D:353:LEU:HD22	2.00	0.43
3:E:68:MSE:CE	3:E:73:HIS:HB2	2.48	0.43
3:E:318:ARG:HD2	3:E:322:TYR:OH	2.18	0.43
1:F:81:LEU:HD13	1:F:111:ILE:HG22	2.00	0.43
2:G:124:LEU:O	2:G:124:LEU:HD13	2.18	0.43
2:G:129:HIS:HB2	2:G:161:LYS:HB2	2.00	0.43
2:H:60:LYS:O	2:H:64:CYS:HB2	2.18	0.43
3:J:315:LEU:HD22	3:J:319:ILE:HD11	2.00	0.43
1:A:170:LEU:O	1:A:173:CYS:O	2.36	0.43
1:A:217:TRP:NE1	1:A:221:LEU:HD11	2.33	0.43
2:B:102:GLU:HG3	2:B:105:ARG:NH2	2.33	0.43
2:C:281:LEU:CD2	2:C:285:MET:HE2	2.48	0.43
2:C:351:MET:HA	2:C:354:LEU:HD12	2.00	0.43
2:D:201:ARG:O	2:D:202:ALA:C	2.60	0.43
2:D:257:VAL:O	2:D:257:VAL:HG12	2.17	0.43
2:D:358:ALA:C	2:D:360:HIS:N	2.71	0.43
3:E:1:MSE:HA	3:E:38:ASP:OD2	2.18	0.43
1:F:48:GLU:CG	1:F:49:GLU:N	2.71	0.43
1:F:55:ILE:HB	1:F:83:LEU:O	2.18	0.43
1:F:299:ARG:HH12	3:J:321:HIS:CE1	2.35	0.43
2:G:250:LEU:HD11	2:G:309:ILE:CD1	2.48	0.43
2:G:265:MET:HE2	2:H:294:MET:HE1	2.00	0.43
2:H:303:GLY:O	2:H:306:MET:HB2	2.18	0.43
2:I:215:ARG:NH1	5:I:803:AGS:O2A	2.51	0.43
2:I:357:LEU:HD12	2:I:363:MET:HE1	2.00	0.43
1:A:278:VAL:O	1:A:280:GLN:CD	2.61	0.43
2:D:278:TRP:CE3	2:D:349:VAL:HG21	2.53	0.43
3:E:41:ILE:HG21	3:E:113:TRP:CD1	2.54	0.43
3:E:67:LEU:HD23	3:E:67:LEU:HA	1.87	0.43
3:E:333:HIS:HB2	3:E:334:LEU:H	1.54	0.43
1:F:4:LEU:CD1	1:F:137:VAL:HG22	2.48	0.43
1:F:23:LEU:HB2	1:F:113:ARG:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:94:ASN:HA	1:F:126:TRP:CD1	2.54	0.43
1:F:274:ASP:HA	1:F:279:TRP:CZ3	2.52	0.43
2:H:252:LEU:O	2:H:253:VAL:C	2.61	0.43
2:H:339:LEU:HB3	2:H:340:PRO:CD	2.39	0.43
2:I:140:LEU:HD22	2:I:144:GLU:CG	2.47	0.43
1:A:130:LEU:C	1:A:132:ASN:N	2.75	0.43
1:A:176:GLY:O	1:A:178:LEU:N	2.50	0.43
2:B:124:LEU:HD22	2:B:153:LEU:O	2.18	0.43
2:B:179:ASP:HB3	2:B:182:GLN:H	1.83	0.43
2:B:292:ILE:HD13	2:B:316:LEU:HB2	2.00	0.43
2:C:197:ALA:O	2:C:198:HIS:CB	2.54	0.43
3:E:163:TYR:CE2	3:E:165:ALA:CB	3.00	0.43
2:G:48:GLY:HA3	2:G:215:ARG:HB2	2.00	0.43
2:H:288:LEU:C	2:H:290:HIS:N	2.77	0.43
2:H:295:VAL:HG21	2:H:302:LEU:HG	2.01	0.43
3:J:24:HIS:HD2	3:J:160:ARG:CZ	2.31	0.43
3:J:145:THR:HG22	3:J:147:GLU:N	2.31	0.43
1:A:255:LEU:HD13	3:E:309:GLU:OE2	2.18	0.43
2:B:357:LEU:HD12	2:B:357:LEU:N	2.33	0.43
2:C:250:LEU:O	2:C:254:GLU:HB2	2.17	0.43
2:C:338:GLU:O	2:C:339:LEU:C	2.62	0.43
3:E:4:TYR:CD2	3:E:6:TRP:CZ2	3.06	0.43
3:E:17:SER:HB2	3:E:22:ARG:C	2.43	0.43
3:E:32:LEU:HD12	3:E:166:PRO:HG2	2.01	0.43
3:E:68:MSE:HE3	3:E:73:HIS:HB2	2.01	0.43
3:E:89:GLY:O	3:E:93:VAL:HG23	2.18	0.43
3:E:224:VAL:HB	3:E:225:PRO:HD3	2.01	0.43
3:E:296:ILE:HG21	3:E:315:LEU:HD12	2.01	0.43
1:F:248:ARG:CZ	3:J:307:ASN:HB2	2.49	0.43
2:G:56:ARG:HH11	2:G:56:ARG:HG3	1.84	0.43
2:G:206:LEU:HD13	2:G:221:THR:OG1	2.18	0.43
2:H:93:ILE:HB	2:H:125:ILE:HG12	2.01	0.43
2:H:250:LEU:HD13	2:H:313:MET:SD	2.58	0.43
2:H:281:LEU:HD23	2:H:281:LEU:O	2.18	0.43
3:J:316:LEU:O	3:J:317:LEU:C	2.61	0.43
1:A:329:LEU:HD11	2:B:291:ARG:HH21	1.83	0.43
2:B:298:SER:HA	2:B:299:PRO:HD2	1.71	0.43
2:B:318:ARG:CG	2:B:319:THR:H	2.31	0.43
2:B:346:ARG:O	2:B:347:MET:C	2.61	0.43
2:C:133:ARG:H	2:C:133:ARG:CD	2.25	0.43
2:D:244:LEU:HD11	2:D:276:ILE:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:49:LEU:CD2	3:E:68:MSE:SE	3.16	0.43
3:E:121:THR:O	3:E:122:ASP:C	2.61	0.43
1:F:19:ALA:HB3	1:F:133:ARG:HB3	2.00	0.43
1:F:215:PHE:HD2	1:F:215:PHE:HA	1.68	0.43
1:F:235:GLN:C	1:F:237:ARG:H	2.25	0.43
1:F:273:PHE:HB3	1:F:279:TRP:CG	2.53	0.43
1:F:312:LEU:O	1:F:316:TYR:HA	2.18	0.43
1:F:320:VAL:O	1:F:321:TRP:C	2.61	0.43
2:G:91:ILE:HD11	2:G:121:LYS:HE3	2.00	0.43
2:G:233:SER:O	2:G:237:VAL:HG23	2.18	0.43
2:G:286:LEU:HD21	2:G:332:LEU:HB3	2.00	0.43
2:H:242:GLY:O	2:H:276:ILE:HG22	2.18	0.43
2:I:243:THR:HG22	2:I:244:LEU:N	2.33	0.43
1:A:27:ASP:OD1	1:A:27:ASP:C	2.58	0.43
2:B:23:HIS:CE1	2:B:176:LYS:NZ	2.86	0.43
2:B:37:ILE:HG21	2:B:151:LYS:HE3	2.01	0.43
2:B:350:GLU:HB2	2:C:290:HIS:HE1	1.82	0.43
2:D:38:HIS:CG	2:D:39:HIS:N	2.87	0.43
2:D:159:PRO:O	2:D:162:LEU:HB2	2.18	0.43
2:D:320:ILE:HG22	2:D:325:ILE:HG13	2.00	0.43
3:E:30:GLN:HB2	3:E:148:PRO:HD3	2.01	0.43
3:E:68:MSE:CE	3:E:73:HIS:CB	2.95	0.43
3:E:281:LEU:O	3:E:282:SER:C	2.62	0.43
1:F:64:ILE:HD12	1:F:64:ILE:N	2.34	0.43
1:F:221:LEU:HD11	1:F:328:SER:HA	2.01	0.43
2:G:244:LEU:HD23	2:G:244:LEU:HA	1.71	0.43
2:H:291:ARG:O	2:H:294:MET:HB2	2.18	0.43
2:H:354:LEU:HD22	2:I:293:ALA:CB	2.48	0.43
2:I:332:LEU:HA	2:I:352:THR:HG21	1.99	0.43
2:I:366:PRO:O	2:I:367:GLU:HG3	2.18	0.43
1:A:74:PHE:CZ	1:F:203:GLU:HA	2.54	0.43
1:A:150:TRP:CE2	1:A:154:ARG:HG3	2.54	0.43
1:A:213:THR:O	1:A:216:HIS:N	2.44	0.43
2:C:46:THR:HG22	2:C:47:ARG:H	1.83	0.43
2:C:333:LEU:O	2:C:334:ILE:C	2.60	0.43
2:D:333:LEU:C	2:D:333:LEU:HD12	2.44	0.43
3:E:121:THR:O	3:E:124:ALA:N	2.52	0.43
1:F:78:GLN:O	1:F:79:THR:HB	2.19	0.43
2:G:142:THR:HG23	2:G:147:PRO:HG2	2.01	0.43
2:G:314:ARG:O	2:G:317:ALA:HB3	2.18	0.43
2:I:309:ILE:O	2:I:312:ARG:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:303:VAL:HB	3:J:306:ILE:CG1	2.49	0.43
1:A:80:LEU:CD2	1:A:82:LEU:HD11	2.49	0.43
1:A:255:LEU:HD22	3:E:313:THR:HG21	2.01	0.43
2:B:132:SER:O	2:B:133:ARG:C	2.60	0.43
2:B:294:MET:O	2:B:295:VAL:C	2.62	0.43
2:C:347:MET:HG2	2:D:290:HIS:ND1	2.33	0.43
2:D:114:ALA:HA	2:D:115:PRO:HD3	1.83	0.43
2:D:120:PHE:CE1	2:D:151:LYS:HE2	2.54	0.43
2:D:184:ARG:HB2	2:D:207:ALA:HB2	2.00	0.43
2:I:263:ARG:HH11	2:I:263:ARG:HG3	1.82	0.43
3:J:81:PRO:O	3:J:82:GLU:C	2.62	0.43
1:A:129:ALA:C	1:A:131:ALA:H	2.26	0.43
1:A:215:PHE:CD2	1:A:282:ARG:NH2	2.86	0.43
1:A:274:ASP:O	1:A:275:LYS:C	2.62	0.43
1:A:277:ARG:NH1	1:A:277:ARG:HG2	2.33	0.43
1:A:289:ALA:C	1:A:291:ASN:N	2.75	0.43
1:A:332:CYS:C	1:A:333:HIS:CG	2.97	0.43
2:B:347:MET:HE3	2:B:347:MET:HB2	1.58	0.43
2:C:269:ASN:O	2:C:270:GLU:C	2.61	0.43
2:C:285:MET:O	2:C:288:LEU:N	2.51	0.43
2:D:229:ASP:C	2:D:231:GLN:N	2.76	0.43
3:E:121:THR:C	3:E:123:ALA:N	2.72	0.43
3:E:143:LEU:N	3:E:143:LEU:CD2	2.81	0.43
2:H:237:VAL:C	2:H:239:ALA:N	2.75	0.43
2:H:265:MET:HA	2:H:268:ILE:HD12	2.01	0.43
2:H:271:ALA:CB	2:H:276:ILE:HD11	2.48	0.43
2:H:343:PRO:HG2	2:H:347:MET:SD	2.59	0.43
2:H:351:MET:HE3	2:H:354:LEU:HB2	2.01	0.43
2:I:223:GLN:CB	2:I:240:MET:HE2	2.49	0.43
3:J:57:LYS:CG	3:J:58:SER:H	2.28	0.43
3:J:252:LEU:HD23	3:J:290:LEU:CA	2.46	0.43
3:J:296:ILE:HD12	3:J:299:GLN:HE21	1.84	0.43
1:A:230:LEU:HD22	2:B:303:GLY:HA3	2.01	0.42
2:B:254:GLU:O	2:B:257:VAL:HG23	2.19	0.42
2:C:254:GLU:CD	2:C:312:ARG:HH21	2.26	0.42
2:C:342:ALA:C	2:C:344:ASP:H	2.27	0.42
2:D:15:PHE:C	2:D:17:ASP:N	2.77	0.42
2:D:34:LEU:C	2:D:36:ARG:H	2.27	0.42
2:D:281:LEU:O	2:D:281:LEU:HD13	2.18	0.42
2:D:321:PRO:HA	2:D:322:PRO:HD2	1.89	0.42
1:F:47:PHE:CD2	1:F:78:GLN:N	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:223:GLN:HB3	2:I:240:MET:HE2	2.00	0.42
3:J:27:LEU:HD12	3:J:160:ARG:O	2.19	0.42
3:J:41:ILE:HG21	3:J:113:TRP:CG	2.54	0.42
3:J:90:VAL:HG12	3:J:90:VAL:O	2.18	0.42
3:J:289:ILE:O	3:J:293:VAL:HG23	2.19	0.42
3:J:316:LEU:O	3:J:319:ILE:HB	2.19	0.42
1:A:4:LEU:HD11	1:A:137:VAL:HG22	2.01	0.42
1:A:323:GLU:O	1:A:324:LEU:C	2.62	0.42
2:B:351:MET:HG2	2:C:329:TYR:CE1	2.53	0.42
2:C:285:MET:O	2:C:287:GLY:N	2.52	0.42
2:C:336:ARG:O	2:C:337:LYS:C	2.60	0.42
2:D:171:LEU:HD12	2:D:171:LEU:HA	1.83	0.42
2:D:338:GLU:O	2:D:339:LEU:C	2.61	0.42
3:E:155:LEU:O	3:E:157:SER:N	2.52	0.42
2:G:313:MET:O	2:G:315:GLU:N	2.52	0.42
2:H:60:LYS:HA	2:H:82:ILE:HD13	2.00	0.42
2:I:347:MET:SD	3:J:253:MSE:HG2	2.59	0.42
3:J:6:TRP:O	3:J:9:PRO:HD2	2.19	0.42
3:J:11:PHE:CD1	3:J:11:PHE:C	2.97	0.42
1:A:65:PHE:CE1	1:A:99:THR:CG2	3.02	0.42
1:A:105:HIS:O	1:A:107:ASP:N	2.53	0.42
2:B:179:ASP:HB3	2:B:182:GLN:CG	2.49	0.42
2:B:241:LEU:O	2:B:242:GLY:O	2.37	0.42
2:B:304:ASN:OD1	2:B:305:ASP:HB2	2.19	0.42
2:D:132:SER:O	2:D:134:HIS:N	2.52	0.42
2:D:339:LEU:HD11	2:D:345:ARG:CG	2.48	0.42
1:F:144:GLN:HE21	1:F:144:GLN:C	2.26	0.42
2:G:13:GLN:HA	2:G:13:GLN:HE21	1.83	0.42
2:G:115:PRO:HD3	2:G:149:HIS:HB3	2.01	0.42
2:G:261:GLY:O	2:G:265:MET:HG2	2.19	0.42
2:G:335:GLY:O	2:G:336:ARG:C	2.61	0.42
2:H:240:MET:C	2:H:242:GLY:H	2.28	0.42
2:I:113:TYR:HE2	2:I:147:PRO:CG	2.32	0.42
2:I:345:ARG:H	2:I:345:ARG:HG3	1.41	0.42
3:J:24:HIS:CD2	3:J:160:ARG:NE	2.88	0.42
1:A:98:LEU:HD22	1:A:101:THR:HG21	2.01	0.42
1:A:173:CYS:SG	1:A:211:HIS:HE1	2.42	0.42
1:A:177:ASN:C	1:A:179:LEU:N	2.75	0.42
1:A:333:HIS:CB	2:B:298:SER:OG	2.66	0.42
2:C:206:LEU:O	2:C:209:ALA:HB3	2.19	0.42
2:C:260:ASN:HD21	2:C:263:ARG:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:264:VAL:CG1	2:C:353:LEU:HD13	2.47	0.42
2:C:325:ILE:HA	2:C:328:TYR:HD2	1.84	0.42
2:D:126:ASP:OD1	2:D:127:GLU:HG2	2.20	0.42
2:D:280:ALA:N	3:E:149:GLU:OE2	2.50	0.42
3:E:238:HIS:HB3	3:E:244:ARG:NH1	2.34	0.42
1:F:213:THR:C	1:F:215:PHE:N	2.78	0.42
1:F:220:ALA:C	1:F:222:LEU:N	2.76	0.42
1:F:231:HIS:O	1:F:235:GLN:HG2	2.20	0.42
1:F:248:ARG:HD2	1:F:251:GLN:OE1	2.20	0.42
1:F:282:ARG:CG	1:F:285:MSE:HE1	2.33	0.42
2:G:220:LEU:O	2:G:240:MET:HE1	2.19	0.42
2:G:316:LEU:HB3	2:G:320:ILE:CD1	2.48	0.42
2:I:343:PRO:HB3	3:J:297:ARG:HE	1.85	0.42
3:J:58:SER:CB	3:J:65:CYS:SG	3.03	0.42
3:J:250:THR:CB	3:J:267:ASN:HD21	2.33	0.42
1:A:27:ASP:OD2	1:A:30:LEU:CB	2.67	0.42
1:A:147:LEU:HB3	1:A:148:PRO:CD	2.38	0.42
1:A:222:LEU:C	1:A:224:GLY:N	2.75	0.42
1:A:285:MSE:HB3	1:A:285:MSE:HE2	2.01	0.42
1:A:305:LEU:O	1:A:308:THR:HB	2.18	0.42
2:B:91:ILE:HD11	2:B:112:GLN:NE2	2.34	0.42
2:C:351:MET:SD	2:D:329:TYR:CD1	3.13	0.42
3:E:283:PRO:HG2	3:E:284:SER:N	2.27	0.42
1:F:57:PRO:O	1:F:58:ASN:HB2	2.19	0.42
1:F:108:LEU:O	1:F:108:LEU:HG	2.19	0.42
2:G:124:LEU:HD13	2:G:124:LEU:C	2.44	0.42
2:G:148:GLU:O	2:G:149:HIS:CB	2.66	0.42
2:H:44:SER:HB2	2:H:159:PRO:CG	2.50	0.42
2:H:122:VAL:HG13	2:H:153:LEU:HG	2.02	0.42
2:H:243:THR:HG22	2:H:244:LEU:N	2.34	0.42
2:H:276:ILE:HG22	2:H:277:GLU:H	1.84	0.42
2:H:353:LEU:HD23	2:H:353:LEU:HA	1.90	0.42
3:J:25:HIS:ND1	3:J:25:HIS:N	2.62	0.42
3:J:88:LEU:HB3	3:J:120:LEU:HA	2.01	0.42
3:J:329:LEU:N	3:J:329:LEU:HD23	2.34	0.42
1:A:257:LEU:HD23	1:A:257:LEU:HA	1.82	0.42
2:B:37:ILE:CG2	2:B:151:LYS:HE3	2.49	0.42
2:B:132:SER:O	2:B:134:HIS:N	2.52	0.42
2:B:244:LEU:O	2:B:245:ASP:CB	2.59	0.42
2:B:256:MET:HE3	2:B:328:TYR:CD1	2.54	0.42
2:B:258:GLU:O	2:B:259:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:9:LYS:NZ	2:D:194:GLU:CD	2.77	0.42
2:D:102:GLU:HG3	2:D:105:ARG:NH2	2.34	0.42
2:D:112:GLN:OE1	2:D:112:GLN:HA	2.19	0.42
2:D:250:LEU:O	2:D:252:LEU:N	2.53	0.42
2:D:320:ILE:HA	2:D:321:PRO:HD3	1.91	0.42
3:E:73:HIS:CE1	3:E:106:LEU:CD2	3.02	0.42
3:E:289:ILE:CG2	3:E:319:ILE:HD13	2.46	0.42
1:F:93:ILE:C	1:F:95:GLU:N	2.77	0.42
2:G:326:GLN:O	2:G:326:GLN:HG2	2.17	0.42
2:H:34:LEU:HD13	2:H:36:ARG:CZ	2.50	0.42
1:A:209:ALA:O	2:B:176:LYS:HE3	2.19	0.42
2:B:187:LEU:O	2:B:188:GLU:C	2.62	0.42
2:C:269:ASN:O	2:C:271:ALA:N	2.52	0.42
3:E:68:MSE:SE	3:E:76:TYR:CD2	3.23	0.42
3:E:247:TRP:O	3:E:248:LEU:C	2.62	0.42
1:F:26:ASN:O	1:F:26:ASN:OD1	2.38	0.42
1:F:217:TRP:HZ3	1:F:250:LEU:HD22	1.83	0.42
2:I:140:LEU:O	2:I:144:GLU:HG3	2.18	0.42
2:I:192:ASN:OD1	2:I:198:HIS:HE1	2.03	0.42
3:J:42:TYR:O	3:J:46:ARG:HG2	2.19	0.42
1:A:51:HIS:HB3	1:A:53:PHE:HE1	1.85	0.42
1:A:134:SER:HB2	1:A:135:VAL:H	1.68	0.42
1:A:213:THR:HG22	1:A:215:PHE:HB2	2.02	0.42
2:B:184:ARG:C	2:B:184:ARG:HD3	2.45	0.42
2:B:264:VAL:HG11	2:B:353:LEU:HD13	2.01	0.42
3:E:50:CYS:SG	3:E:53:PRO:N	2.93	0.42
3:E:74:PRO:CD	3:E:106:LEU:HD11	2.47	0.42
3:E:117:ALA:HA	3:E:120:LEU:HD23	2.01	0.42
3:E:187:LEU:HA	3:E:187:LEU:HD23	1.80	0.42
3:E:238:HIS:CB	3:E:244:ARG:NH1	2.83	0.42
3:E:303:VAL:O	3:E:304:THR:C	2.63	0.42
1:F:27:ASP:HB2	1:F:141:THR:OG1	2.20	0.42
1:F:268:PRO:O	1:F:270:ARG:N	2.53	0.42
2:G:10:TRP:O	2:G:12:PRO:HD3	2.20	0.42
2:G:264:VAL:CG1	2:G:353:LEU:HD13	2.50	0.42
2:H:137:ASN:O	2:H:141:LYS:HG3	2.20	0.42
2:H:245:ASP:C	2:H:247:ASP:N	2.76	0.42
2:H:260:ASN:ND2	2:H:263:ARG:HB3	2.35	0.42
3:J:220:LEU:HD22	3:J:224:VAL:HG23	2.01	0.42
3:J:225:PRO:HA	3:J:280:HIS:CE1	2.54	0.42
1:A:7:GLU:CD	1:A:7:GLU:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:ALA:HB2	1:A:331:LEU:HD21	2.02	0.42
2:B:42:LEU:HD21	2:B:156:THR:HG22	2.01	0.42
2:B:309:ILE:O	2:B:312:ARG:N	2.50	0.42
2:B:333:LEU:C	2:B:333:LEU:CD1	2.92	0.42
2:D:136:PHE:O	2:D:140:LEU:HB2	2.20	0.42
2:D:353:LEU:C	2:D:355:ARG:H	2.27	0.42
3:E:158:ARG:HA	3:E:158:ARG:HD2	1.81	0.42
3:E:188:LEU:O	3:E:191:LEU:HB3	2.20	0.42
3:E:218:GLN:O	3:E:219:ALA:C	2.62	0.42
3:E:334:LEU:HD13	3:E:334:LEU:HA	1.78	0.42
1:F:47:PHE:HA	1:F:77:ARG:C	2.45	0.42
1:F:303:GLN:OE1	3:J:314:ASP:OD1	2.38	0.42
2:G:98:ARG:NE	2:H:140:LEU:HD13	2.35	0.42
2:G:209:ALA:O	2:G:211:GLU:N	2.52	0.42
2:G:266:ALA:O	2:G:270:GLU:HB2	2.20	0.42
2:I:92:GLU:HG2	2:I:124:LEU:HD12	2.02	0.42
2:I:276:ILE:HG22	2:I:277:GLU:N	2.32	0.42
2:I:352:THR:O	2:I:355:ARG:HB3	2.20	0.42
3:J:189:ALA:HB3	3:J:210:TRP:HH2	1.84	0.42
3:J:267:ASN:C	3:J:269:ASP:H	2.28	0.42
1:A:268:PRO:O	1:A:269:LEU:C	2.62	0.42
2:B:76:CYS:SG	2:B:78:ASN:CA	3.08	0.42
2:B:164:VAL:CG2	2:B:165:THR:N	2.83	0.42
2:B:185:HIS:O	2:B:185:HIS:ND1	2.50	0.42
2:B:334:ILE:O	2:B:338:GLU:HG3	2.19	0.42
2:C:286:LEU:O	2:C:287:GLY:C	2.60	0.42
2:C:320:ILE:HA	2:C:321:PRO:HD3	1.94	0.42
2:D:54:ILE:O	2:D:55:ALA:C	2.61	0.42
2:D:250:LEU:C	2:D:252:LEU:H	2.28	0.42
1:F:40:GLN:HE21	1:F:40:GLN:HB3	1.60	0.42
1:F:174:TYR:CD2	1:F:180:ALA:HB1	2.55	0.42
1:F:334:LYS:H	1:F:334:LYS:HG3	1.66	0.42
2:G:19:VAL:HG12	2:G:178:LEU:HD13	2.01	0.42
2:G:294:MET:C	2:G:296:GLN:N	2.74	0.42
2:H:106:ASP:O	2:H:110:ASN:ND2	2.52	0.42
2:I:11:ARG:HH12	5:I:803:AGS:PA	2.42	0.42
2:I:302:LEU:HD13	2:I:310:GLU:HA	2.01	0.42
2:B:88:VAL:HG13	2:B:89:ASP:N	2.35	0.41
2:B:178:LEU:HD13	2:B:178:LEU:HA	1.69	0.41
2:B:179:ASP:HB2	2:B:182:GLN:HE21	1.81	0.41
2:B:359:PHE:HE2	2:C:323:THR:OG1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:51:LYS:HE2	6:C:1300:PO4:O3	2.20	0.41
2:D:34:LEU:C	2:D:36:ARG:N	2.78	0.41
2:D:128:VAL:CG1	2:D:129:HIS:N	2.83	0.41
2:D:132:SER:O	2:D:135:SER:N	2.53	0.41
2:D:206:LEU:O	2:D:207:ALA:C	2.61	0.41
2:D:314:ARG:O	2:D:317:ALA:HB3	2.20	0.41
2:D:332:LEU:HD23	2:D:352:THR:CG2	2.50	0.41
2:D:361:PRO:O	2:D:362:ARG:CB	2.68	0.41
3:E:42:TYR:HE2	3:E:46:ARG:NH1	2.17	0.41
1:F:191:LEU:HD13	2:G:26:THR:HG21	2.00	0.41
1:F:220:ALA:O	1:F:222:LEU:N	2.53	0.41
2:H:301:ALA:O	2:H:302:LEU:C	2.62	0.41
2:I:113:TYR:CE2	2:I:147:PRO:CG	3.03	0.41
2:I:296:GLN:HE21	2:I:317:ALA:C	2.28	0.41
3:J:158:ARG:CG	3:J:158:ARG:HH11	2.33	0.41
3:J:176:LEU:C	3:J:178:ARG:N	2.78	0.41
1:A:221:LEU:HA	1:A:221:LEU:HD23	1.63	0.41
2:B:41:TYR:N	2:B:41:TYR:CD1	2.88	0.41
2:C:56:ARG:HG2	2:C:56:ARG:HH11	1.85	0.41
2:C:65:GLU:CA	2:C:119:ARG:HH21	2.30	0.41
2:C:102:GLU:HB3	2:C:105:ARG:HH11	1.84	0.41
2:D:243:THR:HG22	2:D:244:LEU:N	2.36	0.41
2:D:259:ALA:CB	2:D:363:MET:SD	3.08	0.41
2:D:260:ASN:CG	2:D:263:ARG:HB3	2.45	0.41
2:D:316:LEU:HA	2:D:316:LEU:HD23	1.67	0.41
1:F:81:LEU:HA	1:F:111:ILE:O	2.20	0.41
2:G:99:THR:HB	2:H:145:GLU:HB2	2.02	0.41
2:G:201:ARG:HB2	2:G:234:THR:OG1	2.20	0.41
2:G:277:GLU:CG	2:G:280:ALA:HB2	2.49	0.41
2:I:343:PRO:HA	3:J:297:ARG:HH21	1.85	0.41
3:J:116:ASP:HB3	3:J:119:LEU:CD1	2.50	0.41
3:J:324:GLN:HA	3:J:325:PRO:HD3	1.93	0.41
1:A:26:ASN:CG	1:A:140:GLN:OE1	2.63	0.41
1:A:74:PHE:CZ	1:F:206:VAL:HG12	2.54	0.41
1:A:98:LEU:HG	1:A:125:ALA:HB1	2.02	0.41
2:D:200:PRO:O	2:D:201:ARG:C	2.61	0.41
2:D:202:ALA:HB2	2:D:233:SER:C	2.45	0.41
2:D:237:VAL:C	2:D:239:ALA:H	2.28	0.41
3:E:281:LEU:C	3:E:282:SER:O	2.63	0.41
1:F:51:HIS:O	1:F:81:LEU:N	2.53	0.41
1:F:55:ILE:HD11	1:F:82:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:254:LEU:O	1:F:255:LEU:C	2.62	0.41
3:J:73:HIS:HA	3:J:74:PRO:HD3	1.82	0.41
3:J:216:LEU:HD11	3:J:236:LEU:HD21	2.03	0.41
1:A:143:GLU:O	1:A:147:LEU:N	2.50	0.41
1:A:162:LEU:C	1:A:162:LEU:HD23	2.45	0.41
1:A:173:CYS:C	1:A:175:GLU:N	2.77	0.41
2:B:365:LEU:HA	2:B:366:PRO:HD3	1.81	0.41
2:C:185:HIS:O	2:C:186:GLN:C	2.61	0.41
2:C:245:ASP:HB3	2:C:248:GLN:CG	2.50	0.41
2:C:292:ILE:C	2:C:294:MET:H	2.28	0.41
2:C:305:ASP:O	2:C:306:MET:C	2.62	0.41
2:D:149:HIS:C	2:D:150:VAL:CG2	2.93	0.41
3:E:88:LEU:HD21	3:E:93:VAL:HG22	2.02	0.41
1:F:4:LEU:O	1:F:137:VAL:HA	2.20	0.41
1:F:225:LYS:HZ3	1:F:333:HIS:HE1	1.68	0.41
1:F:310:LEU:O	1:F:311:THR:C	2.62	0.41
2:G:98:ARG:CB	2:H:169:ARG:HH22	2.33	0.41
2:G:285:MET:CB	2:G:332:LEU:HD21	2.47	0.41
2:H:59:ALA:CB	2:H:122:VAL:HG21	2.51	0.41
1:A:128:THR:O	1:A:131:ALA:CB	2.67	0.41
2:B:186:GLN:O	2:B:190:ILE:HG13	2.20	0.41
2:B:338:GLU:C	2:B:340:PRO:HD2	2.45	0.41
2:C:187:LEU:HD22	2:C:221:THR:OG1	2.20	0.41
2:D:285:MET:HE3	2:D:353:LEU:HD21	1.98	0.41
3:E:161:LEU:H	3:E:161:LEU:CD1	2.23	0.41
3:E:307:ASN:O	3:E:310:LEU:N	2.51	0.41
2:G:87:PHE:CE2	2:G:89:ASP:HB2	2.55	0.41
2:G:278:TRP:CH2	2:G:346:ARG:HG3	2.55	0.41
2:I:71:THR:O	2:I:72:PRO:C	2.63	0.41
2:I:148:GLU:O	2:I:149:HIS:HB2	2.21	0.41
2:B:22:GLU:O	2:B:24:VAL:N	2.53	0.41
2:B:247:ASP:OD2	2:B:312:ARG:NH1	2.44	0.41
2:C:183:ILE:HD13	2:C:217:ALA:HB2	2.01	0.41
2:C:351:MET:HG2	2:D:329:TYR:CE1	2.56	0.41
3:E:31:ALA:CB	3:E:164:LEU:HB3	2.49	0.41
1:F:308:THR:O	1:F:309:GLU:C	2.64	0.41
2:G:7:ALA:HA	2:G:218:LEU:HD13	2.02	0.41
2:G:183:ILE:O	2:G:187:LEU:HG	2.20	0.41
2:H:65:GLU:C	2:H:67:GLY:H	2.28	0.41
2:H:311:LEU:HD13	2:H:311:LEU:C	2.45	0.41
3:J:267:ASN:C	3:J:269:ASP:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:297:ARG:O	3:J:300:LEU:HB2	2.21	0.41
1:A:105:HIS:CB	1:F:227:LYS:HD3	2.41	0.41
1:A:208:ASP:C	1:A:210:ALA:N	2.76	0.41
2:B:283:VAL:O	2:B:284:GLU:C	2.63	0.41
2:C:144:GLU:OE1	2:C:144:GLU:CA	2.68	0.41
2:C:202:ALA:HB2	2:C:234:THR:N	2.35	0.41
2:D:15:PHE:C	2:D:17:ASP:H	2.28	0.41
2:D:357:LEU:HG	2:D:363:MET:CE	2.49	0.41
1:F:50:HIS:ND1	1:F:79:THR:HG23	2.36	0.41
1:F:260:LEU:O	1:F:261:LYS:C	2.64	0.41
1:F:275:LYS:HA	1:F:275:LYS:HD3	1.91	0.41
1:F:298:LEU:O	1:F:299:ARG:C	2.64	0.41
2:G:11:ARG:O	2:G:12:PRO:C	2.59	0.41
2:I:304:ASN:C	2:I:306:MET:N	2.79	0.41
1:A:103:LEU:O	1:A:104:LEU:C	2.64	0.41
1:A:162:LEU:HD21	1:A:167:ASN:N	2.35	0.41
2:B:179:ASP:CB	2:B:182:GLN:HB2	2.50	0.41
2:B:250:LEU:C	2:B:252:LEU:N	2.77	0.41
2:B:253:VAL:O	2:B:257:VAL:HG22	2.21	0.41
2:C:93:ILE:HG23	2:D:133:ARG:HH22	1.84	0.41
2:C:103:ASP:O	2:C:107:LEU:HG	2.21	0.41
2:D:59:ALA:HB2	2:D:122:VAL:HG11	2.01	0.41
2:D:199:GLU:O	2:D:200:PRO:C	2.63	0.41
3:E:13:LYS:O	3:E:14:LEU:C	2.64	0.41
3:E:27:LEU:HB3	3:E:142:PHE:CD1	2.56	0.41
3:E:84:GLY:C	3:E:85:LYS:O	2.63	0.41
3:E:242:PRO:CG	3:E:243:ALA:H	2.31	0.41
1:F:174:TYR:O	1:F:181:LEU:HD21	2.20	0.41
1:F:247:LEU:HD22	1:F:305:LEU:CD2	2.51	0.41
2:G:10:TRP:CH2	2:G:193:GLU:HB2	2.52	0.41
2:H:261:GLY:O	2:H:262:GLU:C	2.63	0.41
2:I:200:PRO:HD2	2:I:305:ASP:CG	2.46	0.41
3:J:254:ASP:O	3:J:257:LYS:HB2	2.21	0.41
3:J:296:ILE:HD12	3:J:299:GLN:NE2	2.36	0.41
1:A:41:VAL:O	1:A:41:VAL:HG12	2.19	0.41
1:A:115:ASN:O	1:A:116:LYS:C	2.63	0.41
1:A:125:ALA:C	1:A:128:THR:HG23	2.40	0.41
2:B:286:LEU:HD21	2:B:333:LEU:N	2.36	0.41
2:C:87:PHE:HB3	2:C:90:LEU:HB3	2.03	0.41
2:C:94:ASP:HB3	2:C:97:SER:HB2	2.02	0.41
2:C:129:HIS:ND1	2:C:156:THR:HG23	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:302:LEU:HD23	2:C:302:LEU:HA	1.73	0.41
2:C:367:GLU:HG2	2:D:322:PRO:HD2	2.03	0.41
2:D:132:SER:C	2:D:134:HIS:N	2.77	0.41
2:D:234:THR:HG22	2:D:245:ASP:OD1	2.20	0.41
2:D:272:ALA:CB	2:D:346:ARG:HH11	2.34	0.41
2:D:316:LEU:HD22	2:D:320:ILE:CD1	2.51	0.41
3:E:98:GLU:C	3:E:100:LEU:N	2.79	0.41
3:E:175:TRP:CD1	3:E:175:TRP:C	2.99	0.41
3:E:218:GLN:O	3:E:221:ALA:CB	2.61	0.41
3:E:241:ALA:O	3:E:242:PRO:C	2.61	0.41
3:E:329:LEU:HA	3:E:330:PRO:HD3	1.71	0.41
1:F:109:LEU:HD23	1:F:110:LEU:N	2.36	0.41
1:F:223:MSE:HE2	1:F:288:GLU:O	2.21	0.41
2:G:285:MET:O	2:G:289:LEU:HB2	2.21	0.41
2:G:333:LEU:HD11	2:G:337:LYS:HE3	2.03	0.41
2:H:93:ILE:HG21	2:H:104:THR:CG2	2.51	0.41
2:H:93:ILE:HG23	2:H:104:THR:OG1	2.20	0.41
2:H:288:LEU:O	2:H:292:ILE:HG13	2.21	0.41
2:H:292:ILE:HG22	2:H:325:ILE:CD1	2.51	0.41
2:I:240:MET:SD	3:J:157:SER:CA	3.09	0.41
2:I:298:SER:HA	2:I:299:PRO:HD2	1.84	0.41
2:I:335:GLY:O	2:I:338:GLU:N	2.53	0.41
3:J:34:GLY:O	3:J:199:GLY:HA3	2.21	0.41
3:J:41:ILE:HG21	3:J:113:TRP:NE1	2.36	0.41
3:J:77:TYR:CE1	3:J:99:LYS:HE2	2.56	0.41
3:J:90:VAL:HG21	3:J:123:ALA:CB	2.51	0.41
3:J:242:PRO:HG2	3:J:243:ALA:H	1.86	0.41
1:A:310:LEU:C	1:A:312:LEU:N	2.79	0.41
1:A:322:ALA:O	1:A:325:GLU:HB3	2.20	0.41
2:C:6:LEU:C	2:C:8:ARG:H	2.28	0.41
2:C:261:GLY:CA	2:D:297:LEU:HD21	2.44	0.41
2:D:134:HIS:ND1	2:D:135:SER:N	2.68	0.41
2:D:148:GLU:O	2:D:149:HIS:HB2	2.21	0.41
3:E:169:GLU:OE1	3:E:192:ARG:NE	2.49	0.41
3:E:173:VAL:CG1	3:E:184:GLN:HE21	2.34	0.41
1:F:188:LEU:HG	1:F:197:LEU:CD2	2.49	0.41
1:F:233:LEU:HD23	1:F:325:GLU:HG3	2.02	0.41
1:F:281:ASN:O	1:F:282:ARG:C	2.64	0.41
2:G:243:THR:HG21	2:G:274:ARG:CD	2.44	0.41
2:H:231:GLN:C	2:H:233:SER:N	2.79	0.41
3:J:21:GLY:C	3:J:23:GLY:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:15:PHE:CD1	2:C:57:LEU:HB3	2.55	0.40
2:C:302:LEU:HD13	2:C:310:GLU:HG3	2.02	0.40
2:D:297:LEU:O	2:D:297:LEU:HG	2.20	0.40
2:D:365:LEU:HB3	2:D:366:PRO:HD2	2.02	0.40
3:E:80:ALA:HA	3:E:115:THR:OG1	2.21	0.40
3:E:94:ARG:HH11	3:E:94:ARG:CB	2.33	0.40
3:E:230:TYR:O	3:E:230:TYR:HD1	2.04	0.40
2:H:254:GLU:C	2:H:256:MET:N	2.77	0.40
2:H:272:ALA:N	2:H:276:ILE:HD11	2.35	0.40
2:H:309:ILE:O	2:H:310:GLU:C	2.64	0.40
2:H:309:ILE:O	2:H:311:LEU:N	2.54	0.40
1:A:42:ALA:C	1:A:44:ALA:N	2.76	0.40
1:A:55:ILE:HD11	1:A:82:LEU:HD23	2.02	0.40
1:A:163:ASP:O	1:A:167:ASN:N	2.54	0.40
1:A:297:GLN:HG2	1:A:335:PRO:HG3	2.02	0.40
1:A:327:LEU:C	1:A:327:LEU:HD23	2.46	0.40
2:C:43:PHE:CD1	2:C:173:PHE:HB2	2.56	0.40
2:C:100:LYS:CB	2:D:133:ARG:HE	2.33	0.40
2:D:15:PHE:CD2	2:D:57:LEU:HD13	2.48	0.40
2:D:322:PRO:O	2:D:323:THR:C	2.63	0.40
2:D:329:TYR:C	2:D:329:TYR:HD2	2.28	0.40
3:E:73:HIS:HE1	3:E:106:LEU:CD2	2.34	0.40
3:E:230:TYR:CD1	3:E:230:TYR:C	2.99	0.40
1:F:232:ILE:O	1:F:236:LEU:N	2.50	0.40
2:G:6:LEU:CB	2:G:190:ILE:HG22	2.45	0.40
2:G:125:ILE:HD12	2:G:154:LEU:HD21	2.04	0.40
2:H:334:ILE:O	2:H:338:GLU:HG3	2.22	0.40
2:I:178:LEU:HD13	2:I:214:LEU:HD22	2.02	0.40
2:I:201:ARG:HH22	2:I:284:GLU:CD	2.29	0.40
3:J:57:LYS:HD2	3:J:57:LYS:HA	1.91	0.40
3:J:158:ARG:HH11	3:J:158:ARG:HG3	1.86	0.40
1:A:91:ALA:HA	1:A:94:ASN:HD21	1.83	0.40
1:A:273:PHE:HB3	1:A:279:TRP:HB2	2.04	0.40
1:A:295:GLN:HA	1:A:298:LEU:HD22	2.04	0.40
1:A:304:LEU:HD23	1:A:304:LEU:HA	1.88	0.40
2:C:9:LYS:HG2	2:C:9:LYS:O	2.21	0.40
2:C:65:GLU:C	2:C:67:GLY:N	2.72	0.40
2:C:73:CYS:O	2:C:79:CYS:SG	2.78	0.40
2:D:63:ASN:C	2:D:119:ARG:NH1	2.80	0.40
2:D:261:GLY:O	2:D:265:MET:HB2	2.21	0.40
3:E:8:ARG:H	3:E:9:PRO:CD	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:68:MSE:HE3	3:E:73:HIS:CG	2.55	0.40
3:E:238:HIS:C	3:E:308:ARG:CZ	2.95	0.40
1:F:105:HIS:CE1	1:F:108:LEU:HB3	2.56	0.40
1:F:144:GLN:CG	1:F:280:GLN:CD	2.86	0.40
1:F:211:HIS:O	1:F:211:HIS:ND1	2.55	0.40
1:F:324:LEU:O	1:F:325:GLU:C	2.64	0.40
2:G:135:SER:O	2:G:138:ALA:HB3	2.21	0.40
2:G:363:MET:N	2:G:364:PRO:CD	2.85	0.40
2:H:243:THR:CG2	2:H:284:GLU:HG3	2.50	0.40
3:J:35:MSE:HE1	3:J:167:PRO:CD	2.51	0.40
1:A:14:ASN:C	1:A:16:GLY:N	2.76	0.40
1:A:105:HIS:C	1:A:107:ASP:H	2.30	0.40
1:A:268:PRO:C	1:A:270:ARG:H	2.28	0.40
1:A:292:ARG:HD2	1:A:292:ARG:HA	1.66	0.40
1:A:318:GLN:O	1:A:318:GLN:NE2	2.54	0.40
2:B:331:THR:HG23	2:B:355:ARG:HG2	2.02	0.40
2:C:15:PHE:HE1	2:C:57:LEU:O	2.05	0.40
2:C:291:ARG:CG	2:C:291:ARG:HH11	2.34	0.40
2:D:235:GLN:HG2	2:D:236:ALA:N	2.31	0.40
2:D:268:ILE:O	2:D:272:ALA:N	2.51	0.40
3:E:94:ARG:HH11	3:E:94:ARG:HB3	1.87	0.40
3:E:156:ARG:HE	3:E:156:ARG:HB3	1.46	0.40
3:E:222:TYR:CE1	3:E:226:SER:CB	3.04	0.40
3:E:238:HIS:CG	3:E:239:GLU:N	2.88	0.40
1:F:243:PRO:HG2	1:F:244:VAL:H	1.85	0.40
2:G:193:GLU:O	2:G:193:GLU:HG2	2.21	0.40
2:G:320:ILE:HA	2:G:321:PRO:HD3	1.90	0.40
2:H:15:PHE:HD1	2:H:15:PHE:HA	1.76	0.40
2:H:88:VAL:HG11	2:H:116:ALA:CB	2.41	0.40
2:H:105:ARG:O	2:H:109:ASP:OD2	2.40	0.40
2:H:145:GLU:N	2:H:146:PRO:CD	2.84	0.40
2:H:255:ALA:CB	2:H:264:VAL:HG22	2.51	0.40
2:I:80:ARG:HG2	2:I:80:ARG:NH1	2.36	0.40
3:J:29:ILE:N	3:J:29:ILE:CD1	2.84	0.40
1:A:177:ASN:O	1:A:178:LEU:C	2.64	0.40
1:A:277:ARG:HG2	1:A:277:ARG:HH11	1.85	0.40
2:B:143:LEU:CD1	2:B:169:ARG:HB2	2.51	0.40
2:B:265:MET:HG3	2:C:297:LEU:CD2	2.51	0.40
2:G:51:LYS:HG2	2:G:175:LEU:HD22	2.02	0.40
2:G:99:THR:CG2	2:H:145:GLU:HB2	2.51	0.40
2:G:234:THR:O	2:G:234:THR:HG22	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:240:MET:HE3	2:G:241:LEU:CD1	2.51	0.40
2:H:261:GLY:O	2:H:264:VAL:N	2.51	0.40
2:H:366:PRO:O	2:H:367:GLU:HG2	2.22	0.40
3:J:289:ILE:O	3:J:290:LEU:C	2.64	0.40

All (6) 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:F:274:ASP:OD2	2:I:33:SER:O[1_455]	1.82	0.38
1:F:277:ARG:NH2	2:I:67:GLY:CA[1_455]	1.82	0.38
1:F:277:ARG:NE	2:I:66:THR:O[1_455]	1.87	0.33
1:F:277:ARG:CZ	2:I:67:GLY:CA[1_455]	2.03	0.17
1:F:277:ARG:NH2	2:I:67:GLY:C[1_455]	2.10	0.10
1:F:277:ARG:NH2	2:I:67:GLY:N[1_455]	2.19	0.01

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%)	244 (73%)	70 (21%)	22 (6%)	1	11
1	F	336/343 (98%)	270 (80%)	47 (14%)	19 (6%)	1	13
2	B	362/373 (97%)	278 (77%)	62 (17%)	22 (6%)	1	12
2	C	364/373 (98%)	283 (78%)	54 (15%)	27 (7%)	1	9
2	D	362/373 (97%)	261 (72%)	77 (21%)	24 (7%)	1	11
2	G	362/373 (97%)	312 (86%)	39 (11%)	11 (3%)	3	25
2	H	364/373 (98%)	312 (86%)	44 (12%)	8 (2%)	5	30
2	I	362/373 (97%)	335 (92%)	18 (5%)	9 (2%)	4	28
3	E	332/334 (99%)	237 (71%)	68 (20%)	27 (8%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	J	332/334 (99%)	271 (82%)	50 (15%)	11 (3%)	3	23
All	All	3512/3592 (98%)	2803 (80%)	529 (15%)	180 (5%)	1	15

All (180) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	LEU
1	A	116	LYS
1	A	125	ALA
1	A	131	ALA
1	A	223	MSE
1	A	269	LEU
1	A	270	ARG
1	A	279	TRP
1	A	282	ARG
1	A	290	LEU
1	A	316	TYR
2	B	245	ASP
2	B	246	ASP
2	B	278	TRP
2	B	279	GLU
2	B	299	PRO
2	B	304	ASN
2	B	310	GLU
2	B	363	MET
2	C	36	ARG
2	C	198	HIS
2	C	246	ASP
2	C	262	GLU
2	C	301	ALA
2	C	303	GLY
2	C	315	GLU
2	C	344	ASP
2	D	27	ALA
2	D	33	SER
2	D	261	GLY
2	D	278	TRP
2	D	359	PHE
3	E	62	CYS
3	E	117	ALA
3	E	137	ALA
3	E	206	GLN

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Mol	Chain	Res	Type
3	E	303	VAL
3	E	304	THR
3	E	308	ARG
1	F	279	TRP
1	F	281	ASN
2	G	179	ASP
2	G	249	ALA
2	G	310	GLU
2	H	278	TRP
2	H	302	LEU
2	I	261	GLY
2	I	310	GLU
2	I	362	ARG
3	J	62	CYS
3	J	137	ALA
3	J	304	THR
1	A	15	GLU
1	A	134	SER
1	A	178	LEU
1	A	236	LEU
2	B	20	GLY
2	B	242	GLY
2	B	243	THR
2	B	319	THR
2	C	4	GLN
2	C	20	GLY
2	C	50	GLY
2	C	207	ALA
2	C	237	VAL
2	C	316	LEU
2	D	25	LEU
2	D	28	LEU
2	D	190	ILE
2	D	212	GLY
2	D	227	SER
2	D	230	GLY
3	E	2	ARG
3	E	6	TRP
3	E	85	LYS
3	E	107	GLY
3	E	156	ARG
3	E	238	HIS

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Mol	Chain	Res	Type
3	E	278	ALA
3	E	284	SER
1	F	132	ASN
1	F	210	ALA
1	F	269	LEU
1	F	282	ARG
1	F	316	TYR
1	F	335	PRO
2	G	275	GLY
2	H	275	GLY
3	J	103	HIS
3	J	107	GLY
3	J	206	GLN
1	A	106	ASP
1	A	184	ALA
1	A	281	ASN
2	B	6	LEU
2	B	23	HIS
2	B	366	PRO
2	C	221	THR
2	C	261	GLY
2	C	293	ALA
2	C	333	LEU
2	D	16	ALA
2	D	46	THR
2	D	247	ASP
3	E	37	ASP
3	E	83	LYS
3	E	150	ARG
3	E	287	GLN
1	F	46	GLY
1	F	79	THR
1	F	108	LEU
1	F	131	ALA
1	F	143	GLU
1	F	221	LEU
1	F	270	ARG
2	G	46	THR
2	G	177	ALA
2	G	303	GLY
2	H	211	GLU
2	H	310	GLU

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Mol	Chain	Res	Type
2	I	146	PRO
2	I	299	PRO
2	I	304	ASN
2	I	305	ASP
2	I	364	PRO
3	J	6	TRP
3	J	115	THR
1	A	46	GLY
1	A	90	ASN
2	B	22	GLU
2	B	247	ASP
2	B	286	LEU
2	C	127	GLU
2	C	334	ILE
2	D	306	MET
3	E	38	ASP
1	F	319	SER
2	G	146	PRO
2	G	210	ALA
2	G	314	ARG
3	J	150	ARG
1	A	271	ALA
2	B	146	PRO
2	B	177	ALA
2	B	355	ARG
2	C	46	THR
2	C	239	ALA
2	C	264	VAL
2	C	292	ILE
2	C	343	PRO
2	D	276	ILE
2	D	289	LEU
2	D	300	ALA
2	D	362	ARG
2	D	363	MET
3	E	209	ASN
3	E	291	GLY
3	E	311	LEU
1	F	106	ASP
2	H	232	VAL
1	A	89	PRO
2	C	161	LYS

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Mol	Chain	Res	Type
2	D	210	ALA
3	E	234	ALA
1	F	265	ALA
2	G	363	MET
2	H	20	GLY
2	D	101	VAL
2	H	366	PRO
3	J	136	PRO
2	D	146	PRO
3	E	282	SER
3	J	242	PRO
2	D	200	PRO
3	E	5	PRO
3	E	283	PRO
1	F	224	GLY
2	B	128	VAL
2	C	31	GLY
2	I	20	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	287/286 (100%)	234 (82%)	53 (18%)	1	9
1	F	287/286 (100%)	256 (89%)	31 (11%)	6	27
2	B	301/310 (97%)	270 (90%)	31 (10%)	7	28
2	C	303/310 (98%)	256 (84%)	47 (16%)	2	15
2	D	301/310 (97%)	253 (84%)	48 (16%)	2	15
2	G	301/310 (97%)	274 (91%)	27 (9%)	9	33
2	H	303/310 (98%)	282 (93%)	21 (7%)	14	41
2	I	301/310 (97%)	279 (93%)	22 (7%)	13	39
3	E	270/264 (102%)	229 (85%)	41 (15%)	3	16
3	J	270/264 (102%)	247 (92%)	23 (8%)	10	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2924/2960 (99%)	2580 (88%)	344 (12%)	5 24

All (344) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	40	GLN
1	A	54	SER
1	A	78	GLN
1	A	84	LEU
1	A	97	LEU
1	A	101	THR
1	A	103	LEU
1	A	104	LEU
1	A	108	LEU
1	A	119	LYS
1	A	128	THR
1	A	143	GLU
1	A	160	LEU
1	A	162	LEU
1	A	163	ASP
1	A	164	ASP
1	A	174	TYR
1	A	178	LEU
1	A	187	ARG
1	A	188	LEU
1	A	189	SER
1	A	190	LEU
1	A	194	ASP
1	A	198	THR
1	A	207	ASN
1	A	208	ASP
1	A	215	PHE
1	A	219	ASP
1	A	225	LYS
1	A	228	ARG
1	A	234	GLN
1	A	236	LEU
1	A	242	GLU
1	A	246	LEU
1	A	256	LEU
1	A	266	HIS

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Mol	Chain	Res	Type
1	A	268	PRO
1	A	279	TRP
1	A	280	GLN
1	A	292	ARG
1	A	298	LEU
1	A	305	LEU
1	A	311	THR
1	A	313	LYS
1	A	316	TYR
1	A	318	GLN
1	A	320	VAL
1	A	327	LEU
1	A	328	SER
1	A	330	LEU
1	A	331	LEU
1	A	336	LEU
2	B	8	ARG
2	B	36	ARG
2	B	66	THR
2	B	76	CYS
2	B	121	LYS
2	B	126	ASP
2	B	140	LEU
2	B	143	LEU
2	B	158	ASP
2	B	191	LEU
2	B	250	LEU
2	B	251	SER
2	B	257	VAL
2	B	262	GLU
2	B	267	LEU
2	B	268	ILE
2	B	276	ILE
2	B	279	GLU
2	B	284	GLU
2	B	289	LEU
2	B	291	ARG
2	B	297	LEU
2	B	305	ASP
2	B	325	ILE
2	B	327	LEU
2	B	332	LEU

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Mol	Chain	Res	Type
2	B	334	ILE
2	B	344	ASP
2	B	352	THR
2	B	365	LEU
2	B	367	GLU
2	C	3	TYR
2	C	12	PRO
2	C	19	VAL
2	C	47	ARG
2	C	69	THR
2	C	76	CYS
2	C	102	GLU
2	C	103	ASP
2	C	105	ARG
2	C	120	PHE
2	C	130	MET
2	C	140	LEU
2	C	145	GLU
2	C	146	PRO
2	C	148	GLU
2	C	182	GLN
2	C	193	GLU
2	C	196	ILE
2	C	204	GLN
2	C	208	ARG
2	C	211	GLU
2	C	215	ARG
2	C	219	SER
2	C	232	VAL
2	C	234	THR
2	C	243	THR
2	C	248	GLN
2	C	252	LEU
2	C	254	GLU
2	C	260	ASN
2	C	263	ARG
2	C	268	ILE
2	C	276	ILE
2	C	289	LEU
2	C	291	ARG
2	C	294	MET
2	C	298	SER

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Mol	Chain	Res	Type
2	C	302	LEU
2	C	318	ARG
2	C	323	THR
2	C	324	ASP
2	C	327	LEU
2	C	338	GLU
2	C	352	THR
2	C	357	LEU
2	C	366	PRO
2	C	367	GLU
2	D	12	PRO
2	D	13	GLN
2	D	14	THR
2	D	21	GLN
2	D	42	LEU
2	D	66	THR
2	D	72	PRO
2	D	111	VAL
2	D	124	LEU
2	D	134	HIS
2	D	140	LEU
2	D	142	THR
2	D	148	GLU
2	D	167	LEU
2	D	168	SER
2	D	169	ARG
2	D	170	CYS
2	D	175	LEU
2	D	184	ARG
2	D	193	GLU
2	D	200	PRO
2	D	201	ARG
2	D	213	SER
2	D	219	SER
2	D	229	ASP
2	D	231	GLN
2	D	233	SER
2	D	241	LEU
2	D	251	SER
2	D	252	LEU
2	D	263	ARG
2	D	270	GLU

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Mol	Chain	Res	Type
2	D	276	ILE
2	D	277	GLU
2	D	281	LEU
2	D	283	VAL
2	D	295	VAL
2	D	309	ILE
2	D	310	GLU
2	D	311	LEU
2	D	327	LEU
2	D	333	LEU
2	D	334	ILE
2	D	337	LYS
2	D	338	GLU
2	D	345	ARG
2	D	363	MET
2	D	367	GLU
3	E	22	ARG
3	E	30	GLN
3	E	37	ASP
3	E	46	ARG
3	E	69	GLN
3	E	91	ASP
3	E	93	VAL
3	E	94	ARG
3	E	98	GLU
3	E	103	HIS
3	E	110	LYS
3	E	120	LEU
3	E	143	LEU
3	E	147	GLU
3	E	152	LEU
3	E	154	THR
3	E	155	LEU
3	E	158	ARG
3	E	161	LEU
3	E	170	GLN
3	E	175	TRP
3	E	181	THR
3	E	182	MSE
3	E	202	LEU
3	E	215	THR
3	E	233	LEU

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Mol	Chain	Res	Type
3	E	239	GLU
3	E	240	GLN
3	E	245	LEU
3	E	252	LEU
3	E	253	MSE
3	E	259	HIS
3	E	274	VAL
3	E	290	LEU
3	E	301	MSE
3	E	304	THR
3	E	306	ILE
3	E	310	LEU
3	E	311	LEU
3	E	324	GLN
3	E	332	PRO
1	F	33	GLU
1	F	40	GLN
1	F	48	GLU
1	F	80	LEU
1	F	84	LEU
1	F	100	LEU
1	F	108	LEU
1	F	115	ASN
1	F	119	LYS
1	F	144	GLN
1	F	156	LYS
1	F	158	LEU
1	F	160	LEU
1	F	168	GLN
1	F	194	ASP
1	F	198	THR
1	F	208	ASP
1	F	211	HIS
1	F	215	PHE
1	F	223	MSE
1	F	250	LEU
1	F	266	HIS
1	F	279	TRP
1	F	282	ARG
1	F	292	ARG
1	F	295	GLN
1	F	298	LEU

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Mol	Chain	Res	Type
1	F	305	LEU
1	F	307	ARG
1	F	316	TYR
1	F	330	LEU
2	G	12	PRO
2	G	13	GLN
2	G	39	HIS
2	G	56	ARG
2	G	66	THR
2	G	79	CYS
2	G	84	GLN
2	G	86	ARG
2	G	121	LYS
2	G	134	HIS
2	G	140	LEU
2	G	145	GLU
2	G	176	LYS
2	G	182	GLN
2	G	215	ARG
2	G	223	GLN
2	G	240	MET
2	G	277	GLU
2	G	289	LEU
2	G	296	GLN
2	G	297	LEU
2	G	326	GLN
2	G	330	GLN
2	G	338	GLU
2	G	351	MET
2	G	355	ARG
2	G	367	GLU
2	H	3	TYR
2	H	4	GLN
2	H	15	PHE
2	H	30	ASN
2	H	34	LEU
2	H	69	THR
2	H	76	CYS
2	H	99	THR
2	H	130	MET
2	H	144	GLU
2	H	145	GLU

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Mol	Chain	Res	Type
2	H	158	ASP
2	H	181	GLU
2	H	193	GLU
2	H	201	ARG
2	H	218	LEU
2	H	234	THR
2	H	276	ILE
2	H	279	GLU
2	H	326	GLN
2	H	327	LEU
2	I	13	GLN
2	I	36	ARG
2	I	42	LEU
2	I	56	ARG
2	I	66	THR
2	I	86	ARG
2	I	101	VAL
2	I	121	LYS
2	I	140	LEU
2	I	145	GLU
2	I	148	GLU
2	I	163	PRO
2	I	201	ARG
2	I	211	GLU
2	I	214	LEU
2	I	240	MET
2	I	247	ASP
2	I	337	LYS
2	I	345	ARG
2	I	357	LEU
2	I	360	HIS
2	I	363	MET
3	J	3	TRP
3	J	35	MSE
3	J	62	CYS
3	J	65	CYS
3	J	68	MSE
3	J	91	ASP
3	J	110	LYS
3	J	120	LEU
3	J	149	GLU
3	J	154	THR

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Mol	Chain	Res	Type
3	J	175	TRP
3	J	185	ASP
3	J	202	LEU
3	J	216	LEU
3	J	220	LEU
3	J	245	LEU
3	J	252	LEU
3	J	256	LEU
3	J	285	ARG
3	J	296	ILE
3	J	310	LEU
3	J	317	LEU
3	J	329	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (112) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	35	GLN
1	A	58	ASN
1	A	105	HIS
1	A	157	GLN
1	A	183	GLN
1	A	207	ASN
1	A	211	HIS
1	A	231	HIS
1	A	234	GLN
1	A	251	GLN
1	A	266	HIS
1	A	297	GLN
1	A	318	GLN
1	A	333	HIS
2	B	30	ASN
2	B	39	HIS
2	B	112	GLN
2	B	160	GLN
2	B	172	GLN
2	B	182	GLN
2	B	186	GLN
2	B	192	ASN
2	B	198	HIS
2	B	260	ASN

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Mol	Chain	Res	Type
2	B	326	GLN
2	B	360	HIS
2	C	21	GLN
2	C	84	GLN
2	C	129	HIS
2	C	134	HIS
2	C	149	HIS
2	C	182	GLN
2	C	198	HIS
2	C	223	GLN
2	C	235	GLN
2	C	260	ASN
2	C	304	ASN
2	C	360	HIS
2	D	13	GLN
2	D	21	GLN
2	D	23	HIS
2	D	38	HIS
2	D	110	ASN
2	D	129	HIS
2	D	198	HIS
2	D	231	GLN
2	D	269	ASN
2	D	296	GLN
2	D	326	GLN
2	D	360	HIS
3	E	19	GLN
3	E	24	HIS
3	E	69	GLN
3	E	101	ASN
3	E	184	GLN
3	E	218	GLN
3	E	237	ASN
3	E	295	HIS
3	E	321	HIS
1	F	14	ASN
1	F	26	ASN
1	F	32	GLN
1	F	35	GLN
1	F	40	GLN
1	F	51	HIS
1	F	96	GLN

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Mol	Chain	Res	Type
1	F	105	HIS
1	F	140	GLN
1	F	168	GLN
1	F	216	HIS
1	F	235	GLN
1	F	259	ASN
1	F	333	HIS
2	G	13	GLN
2	G	21	GLN
2	G	30	ASN
2	G	137	ASN
2	G	182	GLN
2	G	189	HIS
2	G	192	ASN
2	G	198	HIS
2	G	223	GLN
2	G	260	ASN
2	G	326	GLN
2	G	360	HIS
2	H	30	ASN
2	H	172	GLN
2	H	182	GLN
2	H	192	ASN
2	H	198	HIS
2	H	204	GLN
2	H	223	GLN
2	H	326	GLN
2	H	360	HIS
2	I	21	GLN
2	I	160	GLN
2	I	198	HIS
2	I	204	GLN
2	I	223	GLN
2	I	296	GLN
2	I	326	GLN
2	I	360	HIS
3	J	19	GLN
3	J	24	HIS
3	J	73	HIS
3	J	101	ASN
3	J	206	GLN
3	J	218	GLN

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Mol	Chain	Res	Type
3	J	246	HIS
3	J	260	HIS
3	J	307	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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	$\# Z > 2$
5	AGS	B	802	-	32,33,33	1.87	4 (12%)	45,52,52	1.07	4 (8%)
5	AGS	G	804	-	32,33,33	1.88	4 (12%)	45,52,52	1.07	4 (8%)
5	AGS	D	801	-	32,33,33	1.88	4 (12%)	45,52,52	1.06	4 (8%)
6	PO4	H	1400	-	4,4,4	0.40	0	6,6,6	0.38	0
5	AGS	I	803	-	32,33,33	1.88	4 (12%)	45,52,52	1.07	4 (8%)
6	PO4	C	1300	-	4,4,4	1.42	1 (25%)	6,6,6	0.90	0

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
5	AGS	D	801	-	-	5/21/38/38	0/3/3/3
5	AGS	G	804	-	-	5/21/38/38	0/3/3/3
5	AGS	I	803	-	-	5/21/38/38	0/3/3/3
5	AGS	B	802	-	-	5/21/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	803	AGS	PG-S1G	-8.39	1.72	1.90
5	D	801	AGS	PG-S1G	-8.39	1.72	1.90
5	G	804	AGS	PG-S1G	-8.39	1.72	1.90
5	B	802	AGS	PG-S1G	-8.36	1.72	1.90
6	C	1300	PO4	P-O1	2.45	1.56	1.50
5	D	801	AGS	C1'-N9	2.43	1.53	1.46
5	B	802	AGS	C1'-N9	2.40	1.53	1.46
5	G	804	AGS	C1'-N9	2.38	1.52	1.46
5	I	803	AGS	C1'-N9	2.38	1.52	1.46
5	I	803	AGS	C5-C4	2.28	1.43	1.39
5	D	801	AGS	C2-N1	2.28	1.38	1.33
5	B	802	AGS	C5-C4	2.27	1.43	1.39
5	B	802	AGS	C2-N1	2.27	1.38	1.33
5	D	801	AGS	C5-C4	2.27	1.43	1.39
5	G	804	AGS	C2-N1	2.27	1.38	1.33
5	G	804	AGS	C5-C4	2.24	1.43	1.39
5	I	803	AGS	C2-N1	2.21	1.37	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	803	AGS	C4-N9-C1'	3.51	134.84	126.63
5	G	804	AGS	C4-N9-C1'	3.50	134.82	126.63
5	B	802	AGS	C4-N9-C1'	3.49	134.80	126.63
5	D	801	AGS	C4-N9-C1'	3.48	134.78	126.63
5	D	801	AGS	C1'-N9-C8	-2.58	121.36	127.09
5	I	803	AGS	C1'-N9-C8	-2.58	121.38	127.09
5	G	804	AGS	C1'-N9-C8	-2.57	121.39	127.09
5	B	802	AGS	C1'-N9-C8	-2.56	121.42	127.09
5	B	802	AGS	O3G-PG-O3B	2.34	112.46	104.64
5	I	803	AGS	O3G-PG-O3B	2.33	112.42	104.64
5	D	801	AGS	O3G-PG-O3B	2.33	112.42	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	804	AGS	O3G-PG-O3B	2.32	112.39	104.64
5	I	803	AGS	C3'-C2'-C1'	2.11	105.46	101.46
5	G	804	AGS	C3'-C2'-C1'	2.11	105.45	101.46
5	D	801	AGS	C3'-C2'-C1'	2.11	105.45	101.46
5	B	802	AGS	C3'-C2'-C1'	2.08	105.41	101.46

There are no chirality outliers.

All (20) torsion outliers are listed below:

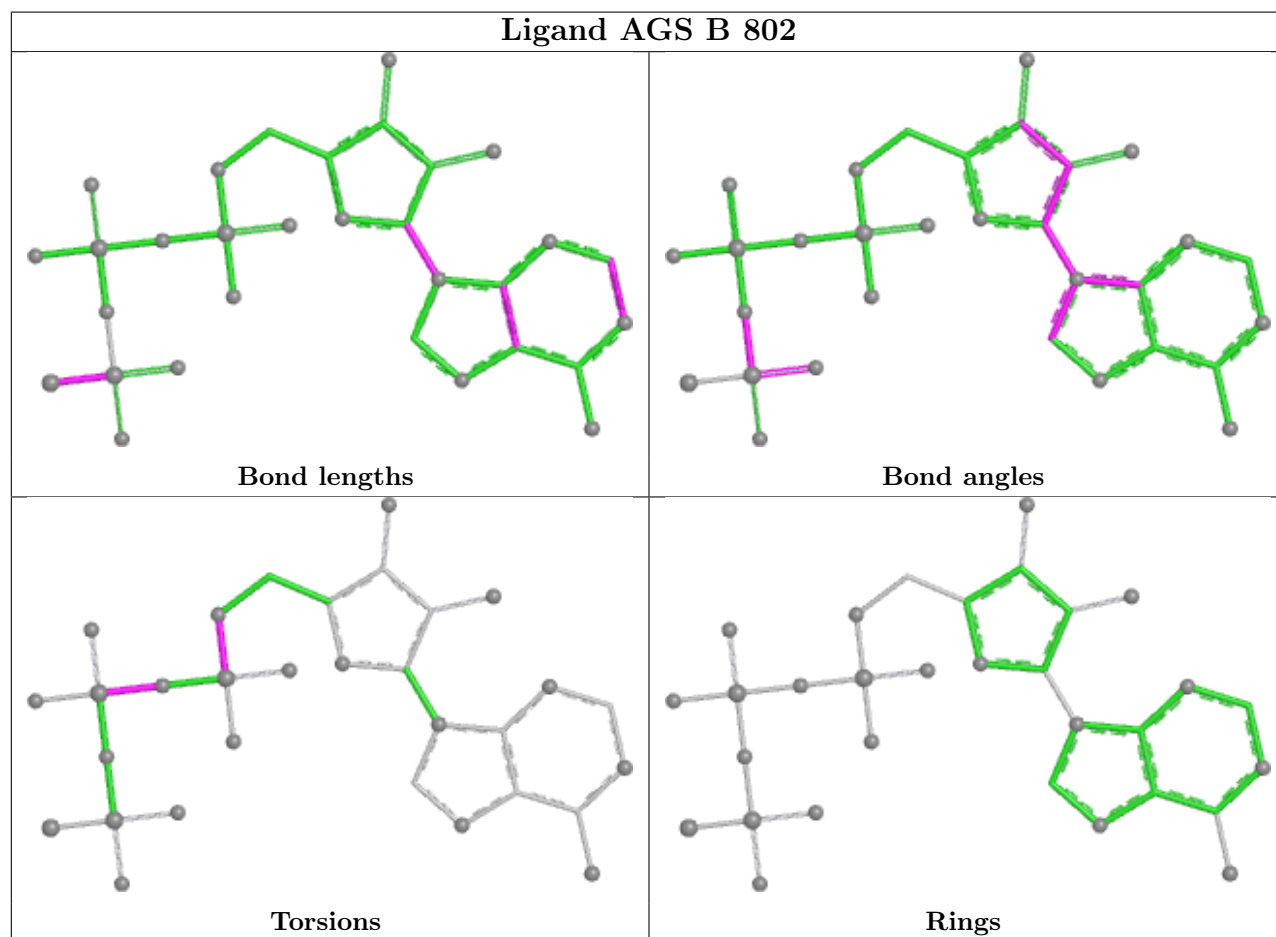
Mol	Chain	Res	Type	Atoms
5	B	802	AGS	C5'-O5'-PA-O2A
5	B	802	AGS	C5'-O5'-PA-O3A
5	D	801	AGS	C5'-O5'-PA-O2A
5	D	801	AGS	C5'-O5'-PA-O3A
5	G	804	AGS	C5'-O5'-PA-O2A
5	G	804	AGS	C5'-O5'-PA-O3A
5	I	803	AGS	C5'-O5'-PA-O2A
5	I	803	AGS	C5'-O5'-PA-O3A
5	B	802	AGS	PA-O3A-PB-O2B
5	D	801	AGS	PA-O3A-PB-O2B
5	G	804	AGS	PA-O3A-PB-O2B
5	I	803	AGS	PA-O3A-PB-O2B
5	B	802	AGS	C5'-O5'-PA-O1A
5	D	801	AGS	C5'-O5'-PA-O1A
5	G	804	AGS	C5'-O5'-PA-O1A
5	I	803	AGS	C5'-O5'-PA-O1A
5	B	802	AGS	PA-O3A-PB-O1B
5	D	801	AGS	PA-O3A-PB-O1B
5	G	804	AGS	PA-O3A-PB-O1B
5	I	803	AGS	PA-O3A-PB-O1B

There are no ring outliers.

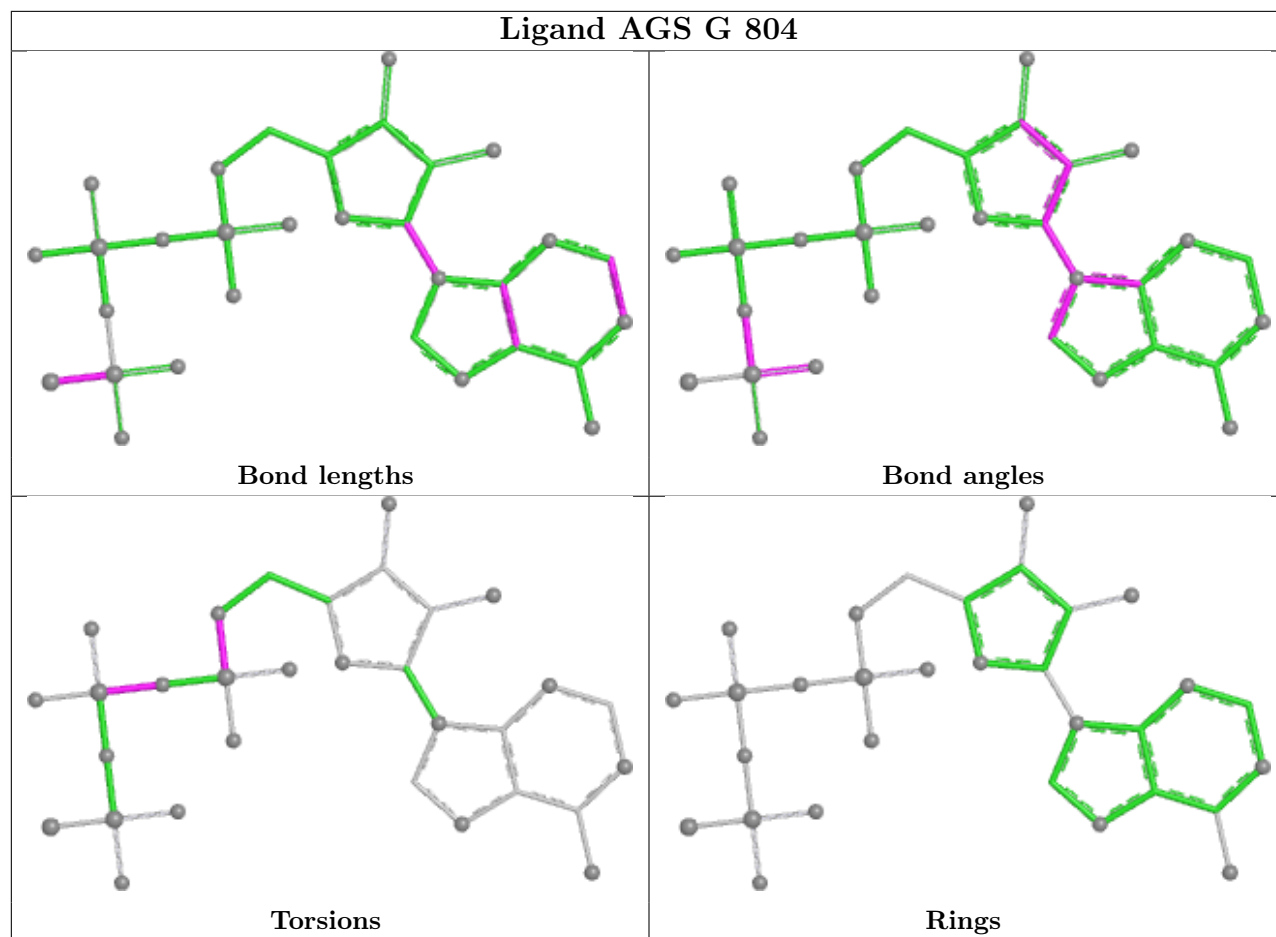
6 monomers are involved in 44 short contacts:

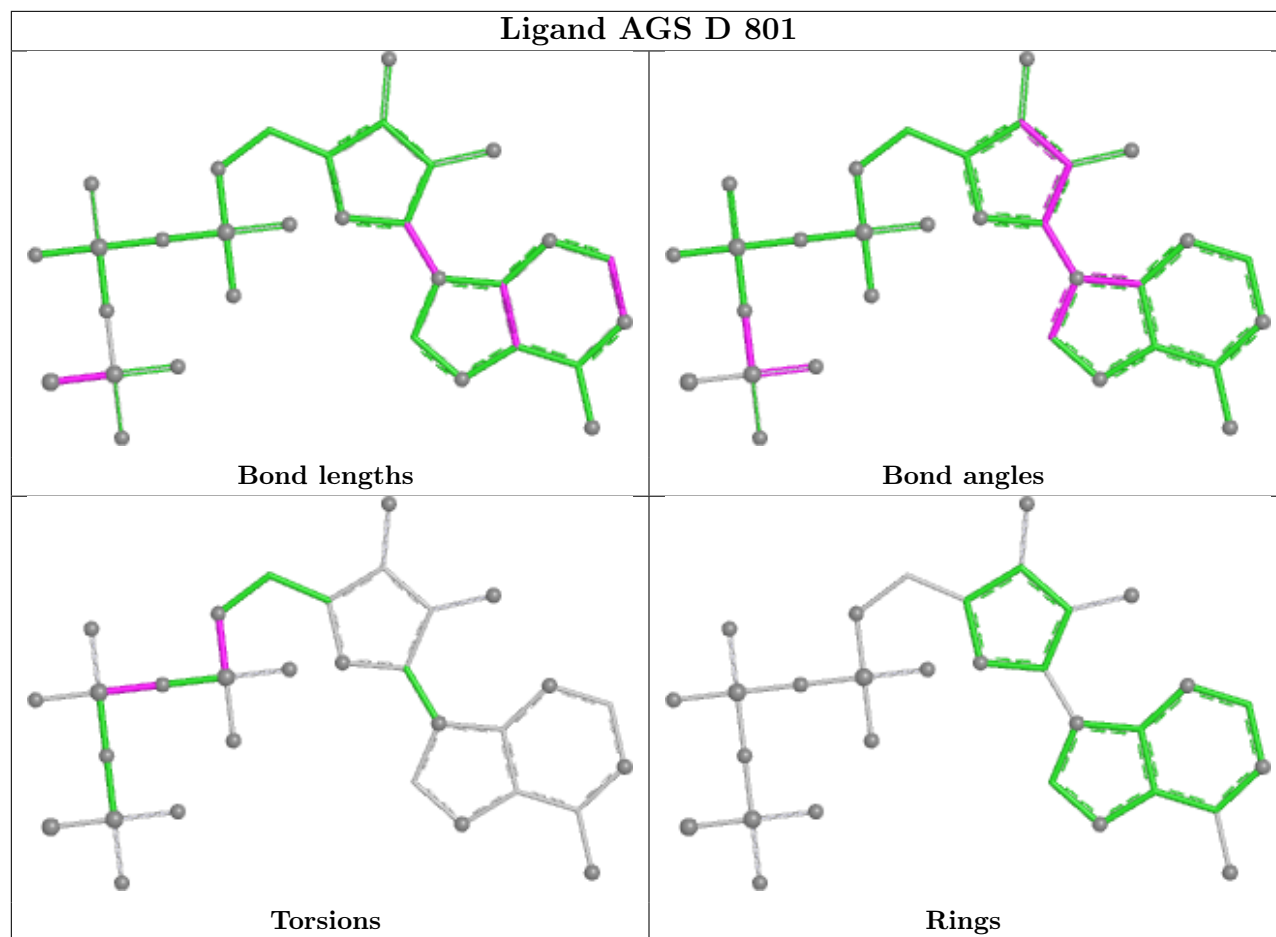
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	802	AGS	4	0
5	G	804	AGS	2	0
5	D	801	AGS	4	0
6	H	1400	PO4	4	0
5	I	803	AGS	27	0
6	C	1300	PO4	3	0

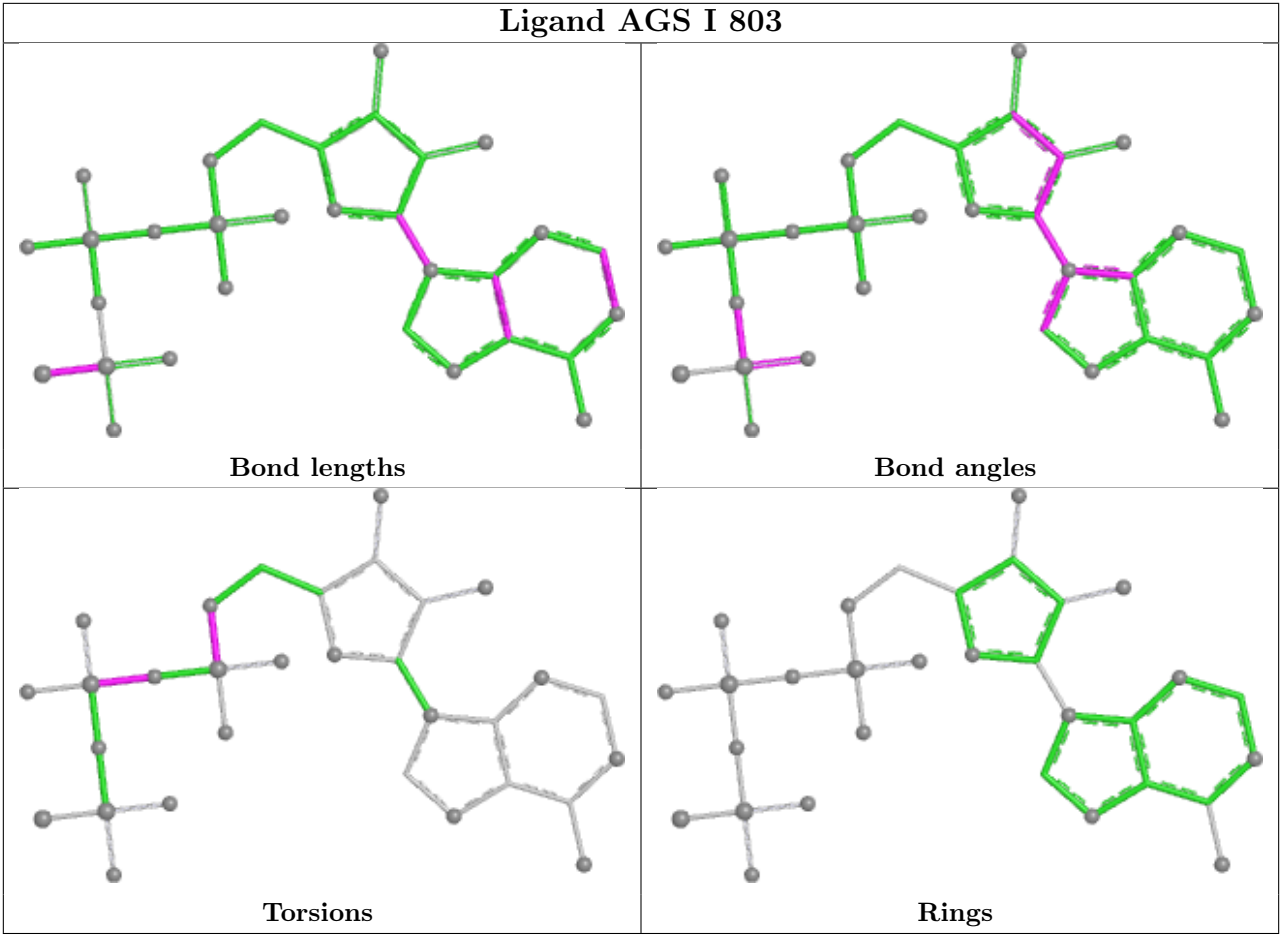
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand AGS G 804







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	285:MSE	C	286:MSE	N	1.06

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	333/343 (97%)	-0.01	6 (1%)	67 43	25, 164, 218, 268	0
1	F	333/343 (97%)	-0.05	4 (1%)	76 53	107, 191, 234, 262	0
2	B	364/373 (97%)	-0.02	9 (2%)	58 35	21, 146, 212, 262	0
2	C	366/373 (98%)	-0.32	3 (0%)	82 61	15, 78, 194, 216	0
2	D	364/373 (97%)	-0.24	7 (1%)	66 42	27, 71, 187, 248	0
2	G	364/373 (97%)	-0.10	9 (2%)	58 35	131, 213, 247, 284	0
2	H	366/373 (98%)	-0.23	5 (1%)	73 49	142, 205, 246, 278	0
2	I	364/373 (97%)	-0.13	6 (1%)	70 46	121, 210, 286, 390	0
3	E	328/334 (98%)	-0.36	1 (0%)	90 77	39, 90, 175, 206	0
3	J	328/334 (98%)	-0.24	3 (0%)	81 58	121, 190, 229, 269	0
All	All	3510/3592 (97%)	-0.17	53 (1%)	72 48	15, 174, 240, 390	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	59	ALA	4.1
2	B	5	VAL	3.4
1	F	338	ASP	3.4
1	A	338	ASP	3.4
1	A	158	LEU	3.3
2	C	124	LEU	3.2
2	B	7	ALA	3.2
2	D	6	LEU	3.2
3	J	143	LEU	3.2
3	J	334	LEU	3.0
2	I	43	PHE	3.0
2	D	305	ASP	2.9
3	E	14	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	54	ILE	2.9
2	C	41	TYR	2.9
1	F	257	LEU	2.8
2	B	159	PRO	2.8
2	H	58	LEU	2.8
2	D	152	PHE	2.7
2	G	164	VAL	2.6
2	G	28	LEU	2.5
2	G	357	LEU	2.5
2	B	82	ILE	2.5
2	B	59	ALA	2.4
2	I	358	ALA	2.4
2	B	62	LEU	2.4
2	C	305	ASP	2.3
2	D	123	TYR	2.3
1	A	100	LEU	2.3
2	I	10	TRP	2.3
2	D	244	LEU	2.3
2	H	244	LEU	2.2
1	F	331	LEU	2.2
2	H	59	ALA	2.2
2	G	24	VAL	2.2
2	B	152	PHE	2.2
2	B	6	LEU	2.2
3	J	154	THR	2.2
1	A	278	VAL	2.2
2	D	20	GLY	2.2
2	D	368	PRO	2.2
1	A	150	TRP	2.2
2	H	104	THR	2.1
2	I	7	ALA	2.1
2	G	15	PHE	2.1
2	G	62	LEU	2.1
2	I	41	TYR	2.1
2	H	55	ALA	2.1
2	G	58	LEU	2.0
2	I	12	PRO	2.0
1	A	82	LEU	2.0
1	F	29	LEU	2.0
2	G	166	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

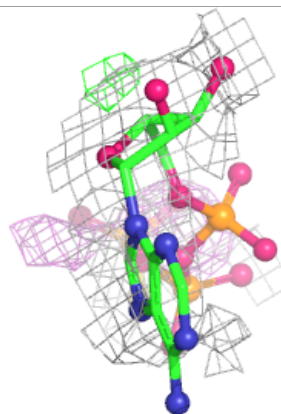
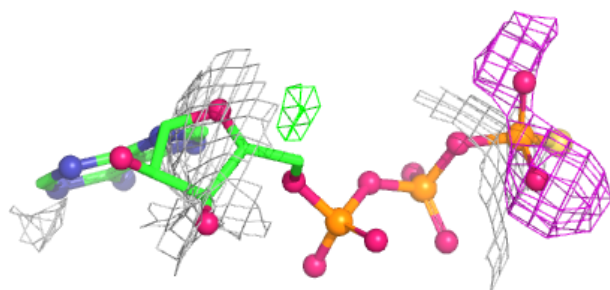
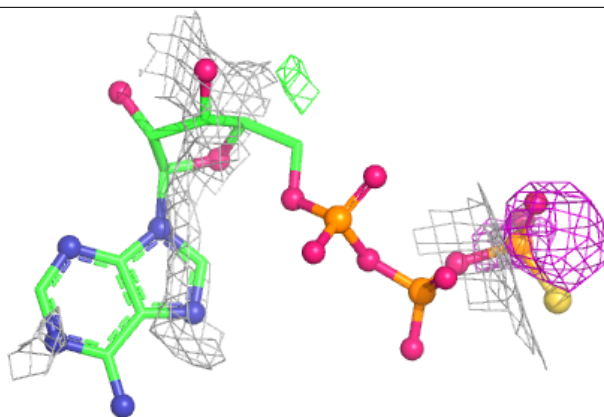
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	AGS	G	804	31/31	0.74	0.11	263,263,263,263	0
5	AGS	I	803	31/31	0.82	0.08	265,265,265,265	0
5	AGS	D	801	31/31	0.88	0.11	132,132,132,132	0
6	PO4	H	1400	5/5	0.90	0.06	180,180,180,180	0
5	AGS	B	802	31/31	0.92	0.10	165,165,165,165	0
6	PO4	C	1300	5/5	0.93	0.07	116,116,116,116	0
4	ZN	G	407	1/1	0.93	0.05	200,200,200,200	0
4	ZN	E	404	1/1	0.97	0.09	175,175,175,175	0
4	ZN	H	405	1/1	0.97	0.04	224,224,224,224	0
4	ZN	I	406	1/1	0.97	0.04	160,160,160,160	0
4	ZN	B	403	1/1	0.98	0.04	173,173,173,173	0
4	ZN	C	401	1/1	0.99	0.04	144,144,144,144	0
4	ZN	D	402	1/1	0.99	0.03	94,94,94,94	0
4	ZN	J	408	1/1	0.99	0.05	169,169,169,169	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

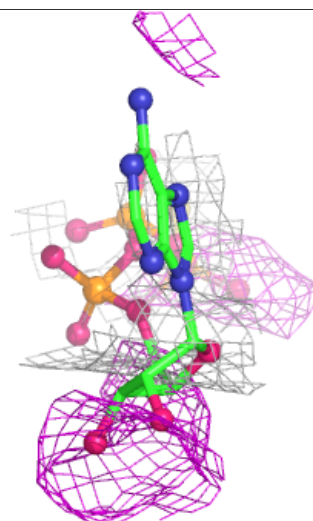
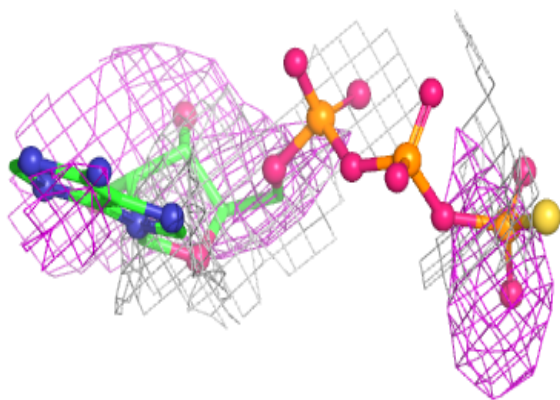
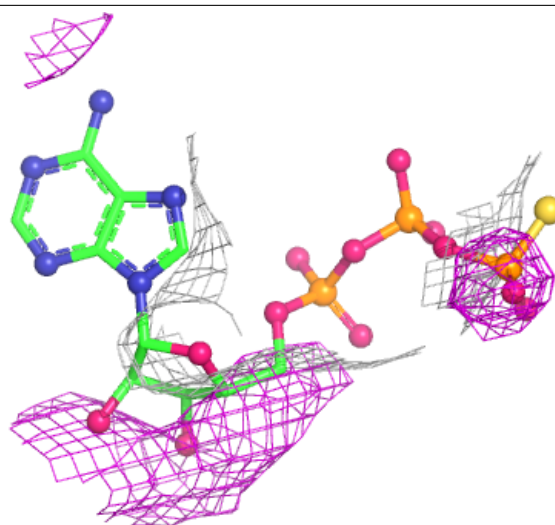
Electron density around AGS G 804:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



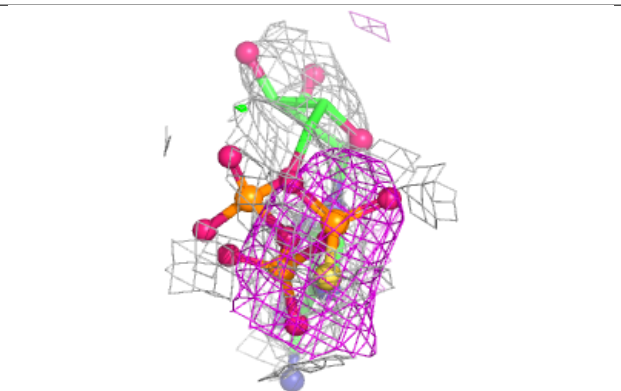
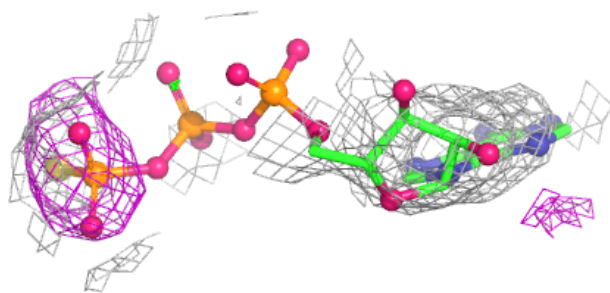
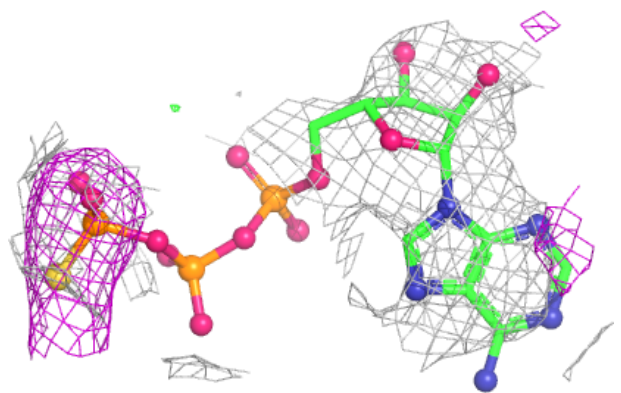
Electron density around AGS I 803:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

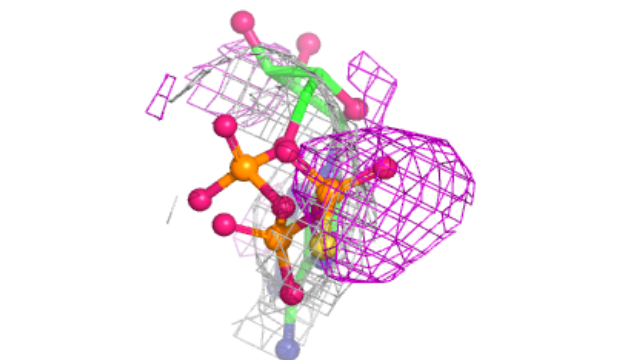
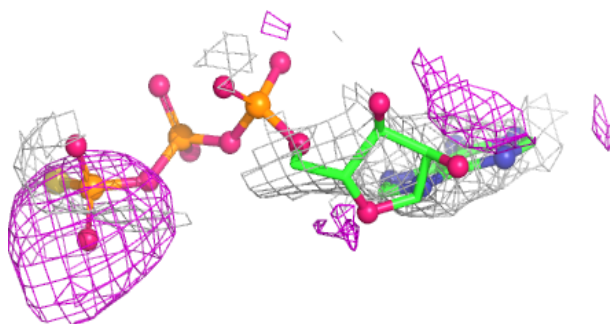
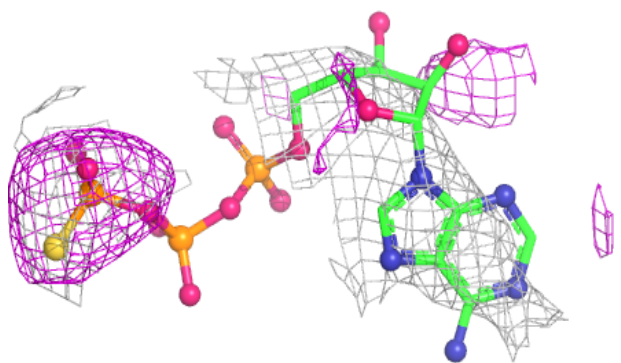


Electron density around AGS D 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around AGS B 802:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.