



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:24 PM UTC

PDB ID : 3VXU / pdb_00003vxu
Title : The complex between T36-5 TCR and HLA-A24 bound to HIV-1 Nef134-10(2F) peptide
Authors : Shimizu, A.; Fukai, S.; Yamagata, A.; Iwamoto, A.
Deposited on : 2012-09-20
Resolution : 2.70 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

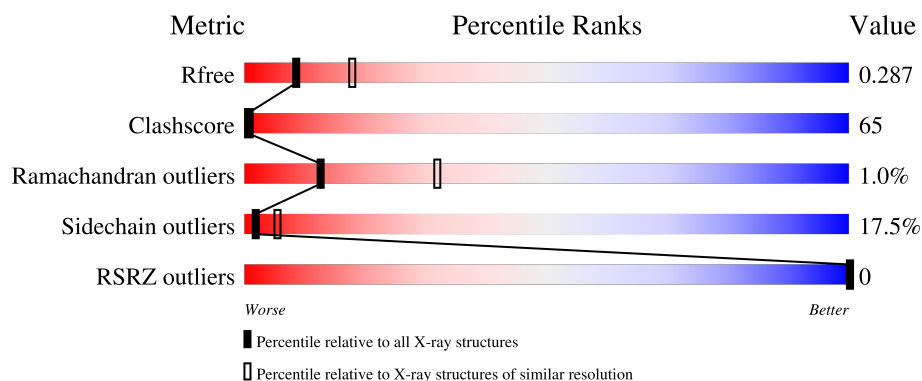
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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.



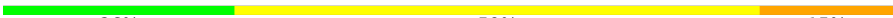
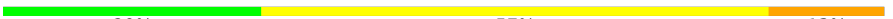
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	275	
1	F	275	
2	B	100	
2	G	100	
3	C	10	

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Mol	Chain	Length	Quality of chain
3	H	10	 100%
4	D	205	 30% 54% 13% •
4	I	205	 24% 56% 16% •
5	E	242	 26% 59% 15%
5	J	242	 29% 57% 13%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13256 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 HLA class I histocompatibility antigen, A-24 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2222	1382	403	427	10			
1	F	274	Total	C	N	O	S	0	0	0
			2222	1382	403	427	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP P05534
F	0	MET	-	expression tag	UNP P05534

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	G	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	expression tag	UNP P61769
G	0	MET	-	expression tag	UNP P61769

- Molecule 3 is a protein called 10-mer peptide from Protein Nef.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	S	0	0	0
			91	64	14	12	1			
3	H	10	Total	C	N	O	S	0	0	0
			91	64	14	12	1			

- Molecule 4 is a protein called T36-5 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	199	Total	C	N	O	S	0	0	0
			1553	968	257	321	7			
4	I	199	Total	C	N	O	S	0	0	0
			1553	968	257	321	7			

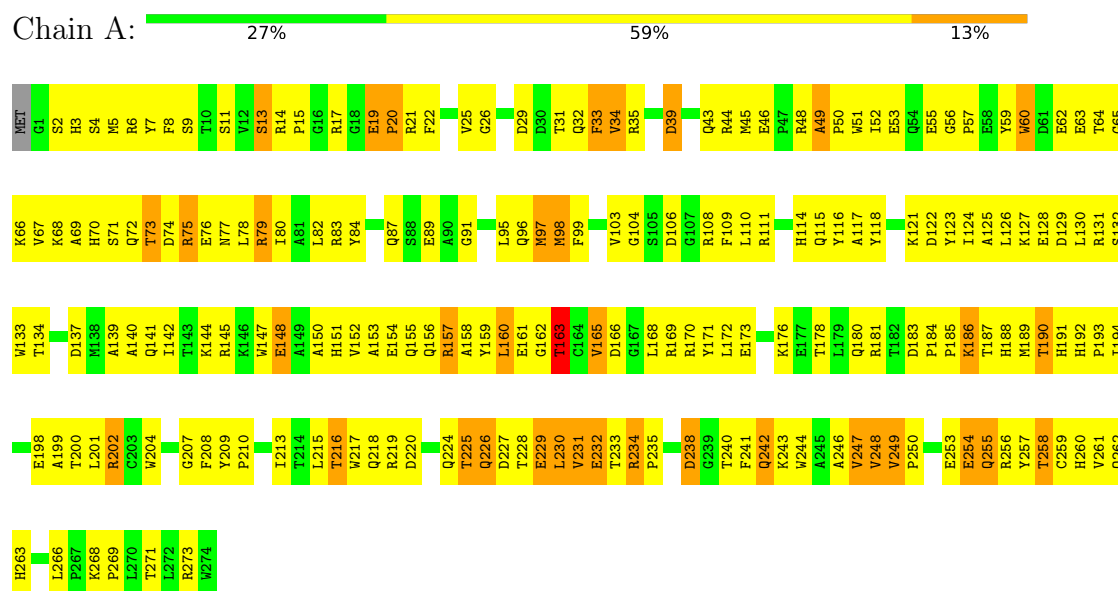
- Molecule 5 is a protein called T36-5 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	241	Total	C	N	O	S	0	0	0
			1933	1217	336	372	8			
5	J	241	Total	C	N	O	S	0	0	0
			1933	1217	336	372	8			

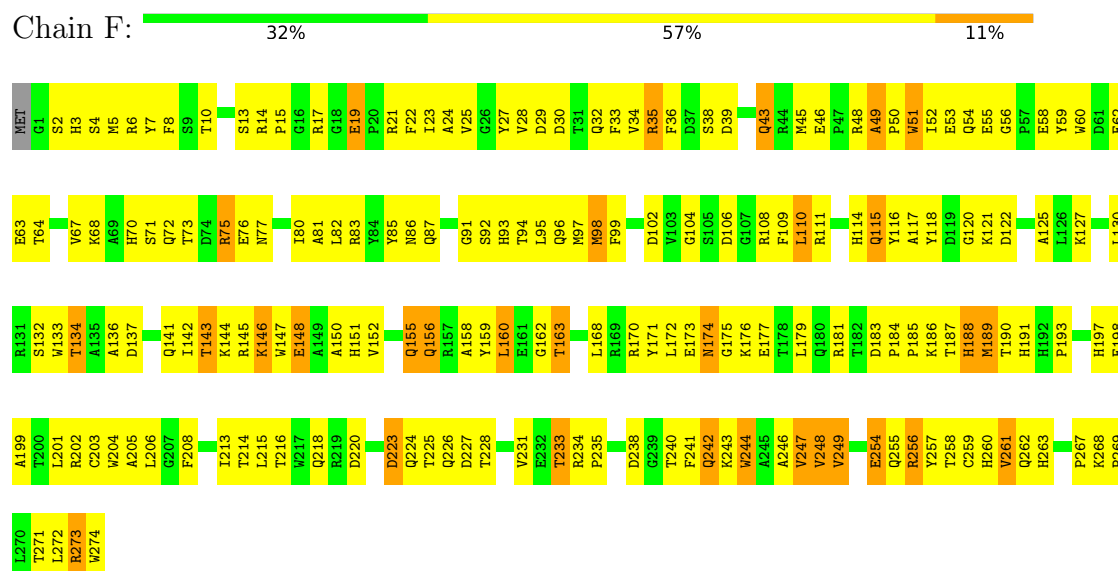
3 Residue-property plots

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.

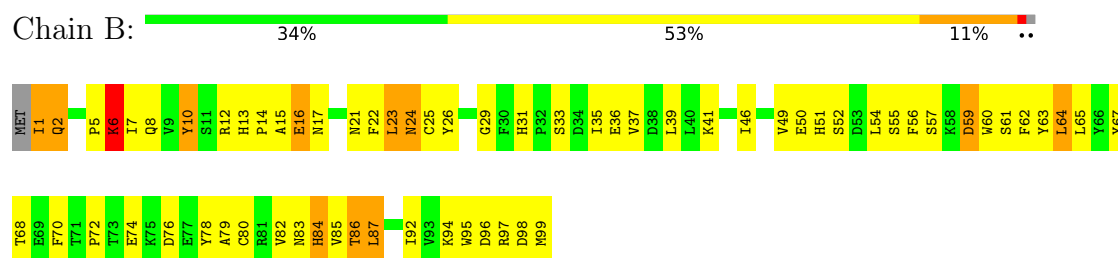
- Molecule 1: HLA class I histocompatibility antigen, A-24 alpha chain



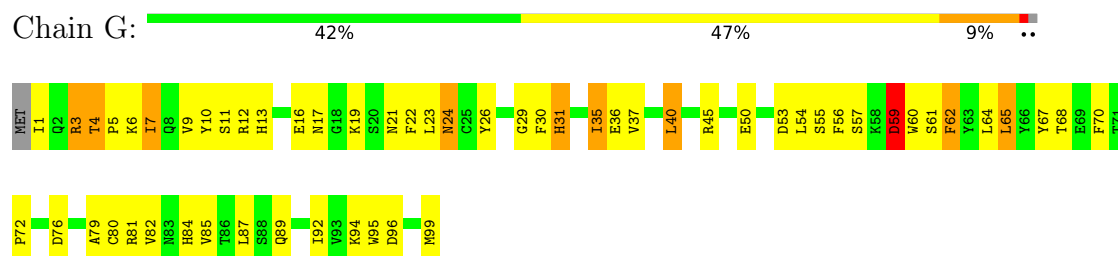
- Molecule 1: HLA class I histocompatibility antigen, A-24 alpha chain



- Molecule 2: Beta-2-microglobulin



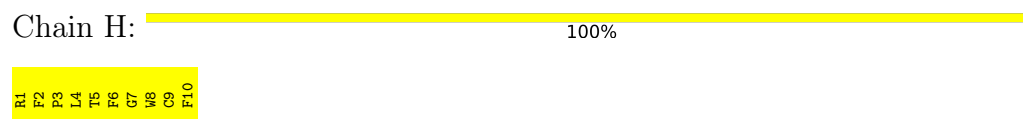
- Molecule 2: Beta-2-microglobulin



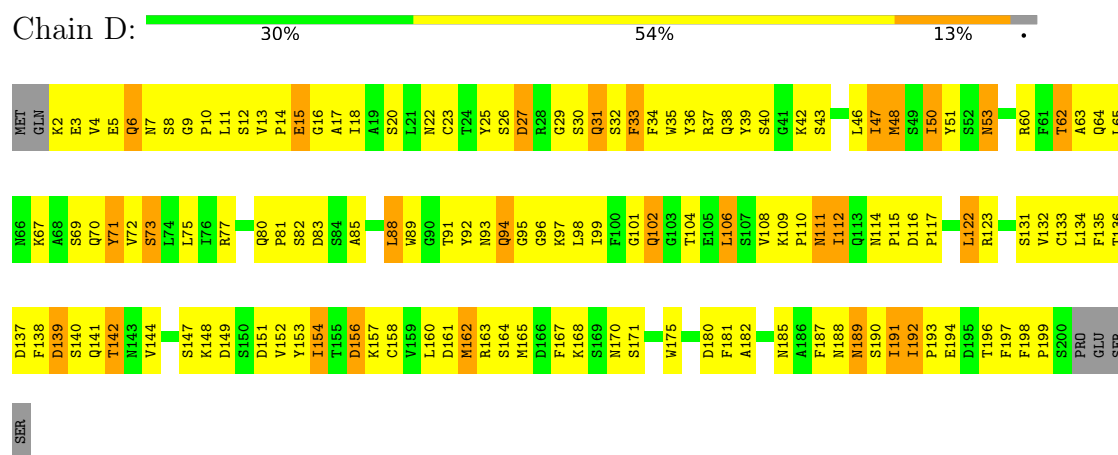
- Molecule 3: 10-mer peptide from Protein Nef



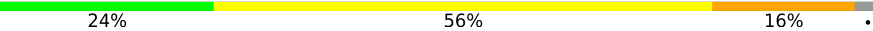
- Molecule 3: 10-mer peptide from Protein Nef



- Molecule 4: T36-5 TCR alpha chain



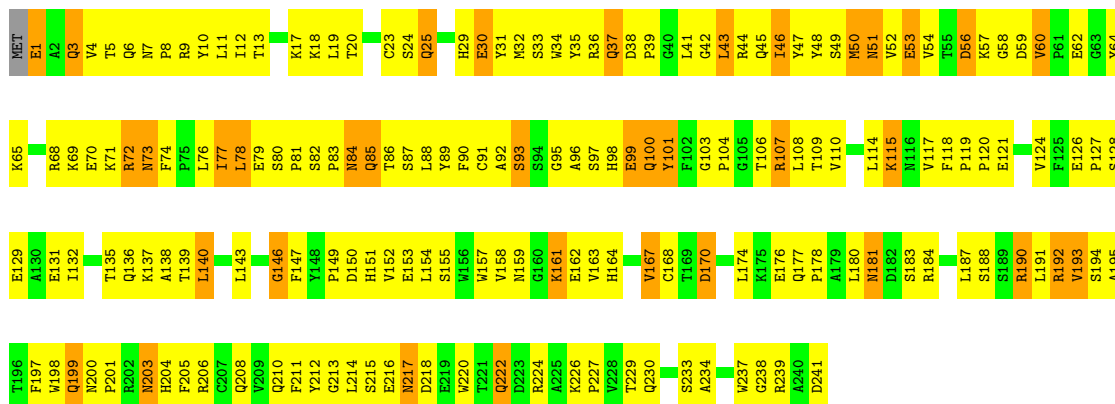
- Molecule 4: T36-5 TCR alpha chain

Chain I:  24% 56% 16%

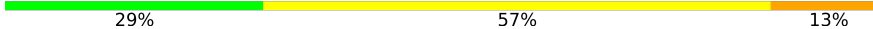


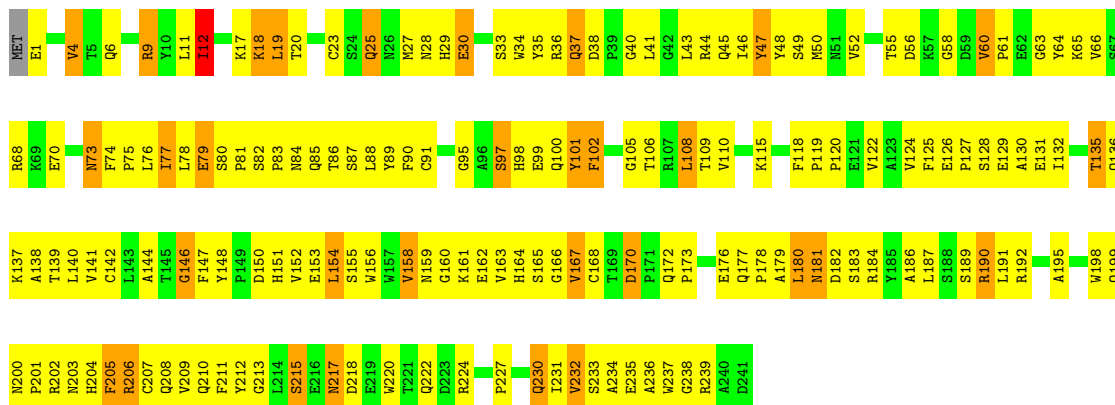
• Molecule 5: T36-5 TCR beta chain

Chain E:  26% 59% 15%



• Molecule 5: T36-5 TCR beta chain

Chain J:  29% 57% 13%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	73.16Å 73.16Å 415.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.35 – 2.70 32.35 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.2 (32.35-2.70) 96.4 (32.35-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.61Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.272 , 0.323 0.262 , 0.287	Depositor DCC
R_{free} test set	3517 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	38.6	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 1.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.069 for -h,-k,l 0.499 for h,-h-k,-l 0.069 for -k,-h,-l	Xtriage
Reported twinning fraction	0.500 for h,k,l 0.500 for h,-h-k,-l	Depositor
Outliers	0 of 73574 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13256	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.64	0/2282	1.06	10/3092 (0.3%)
1	F	0.64	0/2282	1.09	9/3092 (0.3%)
2	B	0.63	0/852	1.00	3/1152 (0.3%)
2	G	0.67	0/852	1.02	3/1152 (0.3%)
3	C	0.63	0/96	0.99	0/128
3	H	0.62	0/96	0.84	0/128
4	D	0.70	0/1587	1.16	5/2149 (0.2%)
4	I	0.71	0/1587	1.17	10/2149 (0.5%)
5	E	0.60	0/1986	1.06	10/2705 (0.4%)
5	J	0.61	0/1986	1.09	11/2705 (0.4%)
All	All	0.65	0/13606	1.09	61/18452 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	J	0	2

There are no bond length outliers.

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	59	ASP	N-CA-C	-8.68	99.05	110.43
1	A	249	VAL	N-CA-C	8.42	117.07	107.89
1	A	46	GLU	CA-C-N	8.39	128.15	119.76
1	A	46	GLU	C-N-CA	8.39	128.15	119.76
2	B	59	ASP	N-CA-C	-8.13	99.80	110.53
4	D	6	GLN	N-CA-C	-7.95	98.51	110.28
1	F	249	VAL	N-CA-C	7.79	116.39	107.89
1	F	46	GLU	CA-C-N	7.59	127.35	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	46	GLU	C-N-CA	7.59	127.35	119.76
4	D	198	PHE	CA-C-N	7.55	127.61	119.90
4	D	198	PHE	C-N-CA	7.55	127.61	119.90
1	F	148	GLU	N-CA-C	-6.86	103.89	111.36
5	J	12	ILE	CB-CA-C	-6.82	100.45	110.62
5	J	80	SER	CA-C-N	6.82	126.85	119.90
5	J	80	SER	C-N-CA	6.82	126.85	119.90
5	E	80	SER	CA-C-N	6.65	126.68	119.90
5	E	80	SER	C-N-CA	6.65	126.68	119.90
4	I	13	VAL	CA-C-N	6.58	126.56	119.78
4	I	13	VAL	C-N-CA	6.58	126.56	119.78
4	I	108	VAL	CB-CA-C	-6.45	103.56	111.88
4	I	6	GLN	N-CA-C	-6.36	100.41	109.96
5	J	129	GLU	N-CA-C	-6.29	104.48	111.71
5	J	170	ASP	CA-C-N	6.21	125.94	119.05
5	J	170	ASP	C-N-CA	6.21	125.94	119.05
5	E	129	GLU	N-CA-C	-6.03	104.78	111.71
4	I	4	VAL	N-CA-C	5.94	117.70	109.80
5	J	60	VAL	CA-C-N	5.86	127.17	119.84
5	J	60	VAL	C-N-CA	5.86	127.17	119.84
1	A	49	ALA	CA-C-N	5.78	125.91	119.32
1	A	49	ALA	C-N-CA	5.78	125.91	119.32
4	I	198	PHE	CA-C-N	5.71	125.64	119.76
4	I	198	PHE	C-N-CA	5.71	125.64	119.76
5	E	103	GLY	CA-C-N	-5.68	113.81	120.12
5	E	103	GLY	C-N-CA	-5.68	113.81	120.12
5	E	73	ASN	N-CA-C	5.68	118.73	109.59
5	J	97	SER	CB-CA-C	-5.64	110.09	116.63
2	G	6	LYS	N-CA-C	-5.58	100.20	109.46
1	A	225	THR	N-CA-C	-5.52	106.68	113.41
1	A	148	GLU	N-CA-C	-5.51	105.19	111.14
2	G	76	ASP	N-CA-C	5.49	118.87	110.20
2	B	76	ASP	N-CA-C	5.41	118.75	110.20
4	D	26	SER	N-CA-C	5.37	119.17	111.02
4	D	5	GLU	N-CA-C	5.31	119.06	112.58
1	A	75	ARG	N-CA-C	-5.24	105.64	111.36
5	J	73	ASN	N-CA-C	5.23	117.92	109.40
1	F	187	THR	N-CA-C	5.19	118.03	109.72
5	J	146	GLY	N-CA-C	5.19	121.05	113.48
2	B	6	LYS	N-CA-C	-5.18	100.86	109.46
4	I	72	VAL	CB-CA-C	-5.16	102.97	110.81
4	I	26	SER	N-CA-C	5.15	118.85	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	170	ASP	CA-C-N	5.13	124.74	119.05
5	E	170	ASP	C-N-CA	5.13	124.74	119.05
4	I	199	PRO	N-CA-C	5.11	119.12	111.14
1	F	49	ALA	CA-C-N	5.10	125.14	119.32
1	F	49	ALA	C-N-CA	5.10	125.14	119.32
1	F	216	THR	N-CA-C	5.08	117.18	108.90
1	A	254	GLU	N-CA-C	5.06	116.80	111.28
1	A	187	THR	N-CA-C	5.06	117.82	109.72
5	E	146	GLY	N-CA-C	5.03	120.83	113.48
5	E	85	GLN	N-CA-C	-5.01	106.76	112.92
1	F	206	LEU	N-CA-C	5.00	117.55	109.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	J	101	TYR	Sidechain
5	J	47	TYR	Sidechain

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	2222	0	2082	322	0
1	F	2222	0	2082	296	0
2	B	829	0	794	95	0
2	G	829	0	794	94	0
3	C	91	0	85	24	0
3	H	91	0	85	34	0
4	D	1553	0	1461	220	0
4	I	1553	0	1461	246	0
5	E	1933	0	1845	283	0
5	J	1933	0	1845	288	0
All	All	13256	0	12534	1674	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 65.

All (1674) 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:69:ALA:HA	5:E:51:ASN:HB2	1.20	1.19
5:J:177:GLN:HB3	5:J:180:LEU:HD13	1.19	1.19
5:J:35:TYR:HB3	5:J:43:LEU:HD11	1.24	1.16
1:A:4:SER:HB2	1:A:6:ARG:HH12	1.08	1.14
4:D:114:ASN:HA	1:F:108:ARG:HH22	0.98	1.11
4:D:3:GLU:HG3	4:D:4:VAL:H	1.09	1.10
4:D:114:ASN:HA	1:F:108:ARG:NH2	1.66	1.10
1:A:68:LYS:HZ1	5:E:53:GLU:HB3	1.07	1.09
5:E:107:ARG:HH11	5:E:107:ARG:HB3	1.16	1.08
4:D:114:ASN:CA	1:F:108:ARG:HH22	1.68	1.05
1:F:45:MET:H	1:F:64:THR:HG22	1.22	1.04
1:A:4:SER:HB2	1:A:6:ARG:NH1	1.72	1.03
4:I:94:GLN:HB3	4:I:97:LYS:HD3	1.42	1.02
5:J:206:ARG:HH22	5:J:208:GLN:HB2	1.24	1.02
4:D:18:ILE:HG12	4:D:77:ARG:HA	1.42	1.01
4:I:66:ASN:HB3	4:I:71:TYR:CE2	1.97	1.00
5:J:52:VAL:HA	5:J:68:ARG:HG3	1.44	0.99
1:A:69:ALA:CA	5:E:51:ASN:HB2	1.93	0.99
1:F:23:ILE:HD13	2:G:54:LEU:HB3	1.42	0.99
4:I:161:ASP:HB2	4:I:168:LYS:HE2	1.40	0.99
4:I:162:MET:HE1	5:J:192:ARG:HB3	1.45	0.98
5:E:86:THR:HG23	5:E:109:THR:HA	1.41	0.98
1:F:10:THR:HB	1:F:23:ILE:HG22	1.44	0.98
1:A:144:LYS:O	1:A:148:GLU:HG3	1.62	0.98
1:A:115:GLN:HG2	1:A:125:ALA:HB1	1.42	0.98
5:E:92:ALA:HB1	5:E:100:GLN:HG2	1.44	0.98
1:F:159:TYR:HD2	1:F:160:LEU:HD23	1.26	0.97
1:A:69:ALA:HA	5:E:51:ASN:CB	1.95	0.97
1:F:49:ALA:O	1:F:52:ILE:HG22	1.64	0.96
5:J:181:ASN:HD22	5:J:181:ASN:H	1.07	0.96
1:A:200:THR:HG21	1:A:202:ARG:HH12	1.27	0.96
1:F:33:PHE:HD2	1:F:34:VAL:HG13	1.31	0.95
4:D:14:PRO:HB2	4:I:71:TYR:CZ	2.01	0.95
4:I:167:PHE:HZ	5:J:192:ARG:HH11	1.03	0.95
1:F:156:GLN:NE2	1:F:156:GLN:HA	1.81	0.95
5:E:177:GLN:HB3	5:E:180:LEU:HD13	1.45	0.95
4:I:185:ASN:HA	4:I:188:ASN:ND2	1.81	0.95
1:A:243:LYS:HD3	1:A:244:TRP:N	1.82	0.94
1:A:76:GLU:HA	1:A:79:ARG:HD3	1.49	0.94
1:A:216:THR:HG23	1:A:260:HIS:HB2	1.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:36:ARG:HH12	5:J:85:GLN:HA	1.32	0.93
5:J:181:ASN:H	5:J:181:ASN:ND2	1.52	0.93
1:A:45:MET:HG3	1:A:67:VAL:HG11	1.47	0.93
4:I:10:PRO:HB3	4:I:105:GLU:HG2	1.47	0.93
4:D:3:GLU:HG3	4:D:4:VAL:N	1.82	0.92
5:J:154:LEU:HD21	5:J:207:CYS:SG	2.10	0.92
4:I:161:ASP:HB2	4:I:168:LYS:CE	1.99	0.91
1:A:156:GLN:O	1:A:160:LEU:HG	1.69	0.91
1:F:234:ARG:HG3	1:F:242:GLN:HG3	1.53	0.91
2:G:12:ARG:HG2	2:G:21:ASN:HD21	1.36	0.90
1:F:156:GLN:HA	1:F:156:GLN:HE21	1.35	0.90
4:D:96:GLY:HA3	5:E:50:MET:HE1	1.53	0.89
2:G:24:ASN:H	2:G:24:ASN:HD22	1.18	0.89
5:J:230:GLN:HE22	5:J:232:VAL:HG13	1.38	0.89
1:A:62:GLU:OE1	4:D:95:GLY:HA3	1.72	0.89
2:G:37:VAL:HG22	2:G:82:VAL:HG22	1.53	0.89
1:A:35:ARG:HH12	1:A:48:ARG:NE	1.70	0.89
5:J:206:ARG:NH1	5:J:233:SER:HB3	1.87	0.88
4:I:66:ASN:HB3	4:I:71:TYR:HE2	1.36	0.88
5:E:212:TYR:HA	5:E:229:THR:HG23	1.56	0.88
1:F:156:GLN:O	1:F:160:LEU:HG	1.74	0.88
1:A:213:ILE:HG13	1:A:262:GLN:O	1.74	0.87
1:F:70:HIS:HD1	3:H:2:PHE:HZ	1.23	0.87
5:J:180:LEU:N	5:J:180:LEU:HD12	1.89	0.87
1:F:234:ARG:CG	1:F:242:GLN:HG3	2.04	0.87
4:I:159:VAL:HG12	4:I:168:LYS:NZ	1.88	0.87
1:F:233:THR:HG23	1:F:243:LYS:HB2	1.57	0.86
4:I:159:VAL:HG12	4:I:168:LYS:HZ2	1.40	0.86
1:A:185:PRO:HB3	1:A:208:PHE:HB3	1.55	0.86
5:J:66:VAL:HG12	5:J:75:PRO:O	1.75	0.86
2:G:12:ARG:HD2	2:G:22:PHE:HB2	1.58	0.86
1:F:106:ASP:OD2	1:F:108:ARG:HB2	1.75	0.86
5:E:64:TYR:O	5:E:65:LYS:HD2	1.75	0.86
4:I:61:PHE:C	4:I:77:ARG:HH22	1.83	0.86
1:A:145:ARG:HA	1:A:148:GLU:OE2	1.77	0.85
1:A:249:VAL:HG13	1:A:257:TYR:HE2	1.41	0.85
4:D:97:LYS:HB2	5:E:45:GLN:OE1	1.77	0.85
1:A:25:VAL:HB	1:A:32:GLN:HE22	1.41	0.85
4:I:88:LEU:N	4:I:88:LEU:HD23	1.91	0.85
5:J:173:PRO:HA	5:J:187:LEU:HD13	1.59	0.85
5:J:159:ASN:HD21	5:J:204:HIS:H	1.22	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLU:OE1	3:C:1:ARG:HG3	1.76	0.84
5:J:35:TYR:CB	5:J:43:LEU:HD11	2.07	0.84
5:E:107:ARG:HB3	5:E:107:ARG:NH1	1.92	0.84
5:E:19:LEU:HD12	5:E:78:LEU:HD13	1.59	0.84
5:E:46:ILE:N	5:E:46:ILE:HD12	1.90	0.84
5:J:142:CYS:HB2	5:J:156:TRP:CH2	2.13	0.83
1:F:19:GLU:HG3	1:F:75:ARG:HE	1.42	0.83
5:E:135:THR:HG22	5:E:137:LYS:HG3	1.59	0.83
5:J:36:ARG:NH1	5:J:85:GLN:HA	1.92	0.83
1:A:69:ALA:HB2	5:E:50:MET:HB2	1.61	0.83
1:F:268:LYS:HD2	1:F:269:PRO:HD2	1.61	0.83
4:I:160:LEU:HD13	4:I:162:MET:HE3	1.59	0.82
1:A:68:LYS:NZ	5:E:53:GLU:HB3	1.92	0.82
2:B:21:ASN:CG	2:B:22:PHE:H	1.88	0.82
5:E:36:ARG:HH21	5:E:87:SER:HB2	1.43	0.82
5:J:159:ASN:ND2	5:J:204:HIS:H	1.77	0.82
1:F:45:MET:H	1:F:64:THR:CG2	1.92	0.82
4:I:120:TYR:CE1	5:J:131:GLU:HA	2.14	0.81
1:A:4:SER:CB	1:A:6:ARG:HH12	1.89	0.81
4:D:114:ASN:HB3	1:F:108:ARG:HH12	1.45	0.81
5:E:88:LEU:HD13	5:E:107:ARG:HG2	1.62	0.81
2:G:24:ASN:HD22	2:G:24:ASN:N	1.72	0.81
4:I:158:CYS:HB3	5:J:190:ARG:NH1	1.95	0.81
1:A:215:LEU:HD12	1:A:243:LYS:HD2	1.62	0.81
2:G:56:PHE:HB2	2:G:61:SER:O	1.81	0.81
4:I:160:LEU:CD1	4:I:162:MET:HE3	2.11	0.81
2:G:24:ASN:N	2:G:24:ASN:ND2	2.25	0.81
1:A:152:VAL:HG12	1:A:156:GLN:HE21	1.45	0.81
4:D:3:GLU:CG	4:D:4:VAL:H	1.90	0.81
4:I:144:VAL:HG21	4:I:156:ASP:HA	1.63	0.81
1:A:249:VAL:HG13	1:A:257:TYR:CE2	2.15	0.81
2:B:51:HIS:HD2	2:B:64:LEU:HD21	1.45	0.81
4:I:78:ASP:OD1	4:I:78:ASP:O	1.99	0.81
5:E:190:ARG:HD2	5:E:190:ARG:N	1.95	0.80
5:E:137:LYS:HB2	5:E:192:ARG:CZ	2.11	0.80
1:A:165:VAL:O	1:A:169:ARG:HG3	1.81	0.80
4:I:160:LEU:HD11	4:I:167:PHE:HE2	1.46	0.80
5:J:38:ASP:H	5:J:44:ARG:NH2	1.79	0.80
1:A:200:THR:HG21	1:A:202:ARG:NH1	1.97	0.80
5:E:19:LEU:CD1	5:E:78:LEU:HD13	2.11	0.80
1:F:75:ARG:HG2	1:F:75:ARG:HH11	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:259:CYS:SG	1:F:272:LEU:HD13	2.22	0.80
5:J:177:GLN:HB3	5:J:180:LEU:CD1	2.09	0.80
1:F:202:ARG:NH1	1:F:246:ALA:HB2	1.95	0.80
5:E:170:ASP:HB2	5:E:187:LEU:HD11	1.62	0.79
1:F:115:GLN:HG3	2:G:60:TRP:CH2	2.16	0.79
5:E:199:GLN:O	5:E:201:PRO:HD3	1.82	0.79
2:G:13:HIS:HB2	2:G:21:ASN:ND2	1.97	0.79
5:E:83:PRO:HA	5:E:110:VAL:HB	1.63	0.79
1:A:141:GLN:O	1:A:145:ARG:HG3	1.82	0.79
4:I:155:THR:HG22	4:I:173:VAL:H	1.46	0.79
2:G:12:ARG:HG2	2:G:21:ASN:ND2	1.97	0.79
1:A:152:VAL:CG1	1:A:156:GLN:HE21	1.96	0.78
1:F:75:ARG:HG2	1:F:75:ARG:NH1	1.99	0.78
5:E:100:GLN:C	5:E:101:TYR:HD2	1.92	0.78
4:I:160:LEU:C	4:I:160:LEU:HD12	2.08	0.78
1:F:58:GLU:O	1:F:62:GLU:HG3	1.84	0.78
1:A:57:PRO:HA	1:A:60:TRP:HD1	1.48	0.78
1:A:19:GLU:HA	1:A:19:GLU:OE2	1.82	0.78
2:B:56:PHE:HB3	2:B:62:PHE:CD2	2.18	0.77
4:D:31:GLN:HB3	4:D:67:LYS:NZ	2.00	0.77
5:J:12:ILE:HD12	5:J:12:ILE:H	1.49	0.77
4:D:153:TYR:HB2	4:D:175:TRP:CZ2	2.20	0.77
4:I:66:ASN:CB	4:I:71:TYR:HE2	1.96	0.77
5:J:86:THR:HG23	5:J:109:THR:HA	1.65	0.77
4:D:31:GLN:HA	4:D:67:LYS:HE2	1.65	0.77
5:E:52:VAL:HA	5:E:68:ARG:CG	2.14	0.77
5:E:159:ASN:HD21	5:E:204:HIS:H	1.33	0.77
4:I:50:ILE:HD12	4:I:50:ILE:C	2.10	0.77
1:A:26:GLY:HA3	1:A:33:PHE:CE1	2.20	0.76
4:I:123:ARG:HB3	5:J:126:GLU:HB2	1.68	0.76
5:J:154:LEU:HD23	5:J:208:GLN:O	1.86	0.76
2:B:56:PHE:HB2	2:B:61:SER:O	1.84	0.76
5:E:154:LEU:HD23	5:E:155:SER:N	2.00	0.76
4:I:47:ILE:HD12	4:I:48:MET:N	2.00	0.76
5:J:181:ASN:HD22	5:J:181:ASN:N	1.83	0.76
1:A:243:LYS:HD3	1:A:244:TRP:H	1.50	0.76
4:D:12:SER:HA	4:D:109:LYS:HZ3	1.50	0.76
4:I:159:VAL:HG22	4:I:170:ASN:OD1	1.86	0.76
5:J:64:TYR:O	5:J:65:LYS:HD2	1.85	0.76
1:A:66:LYS:HG3	5:E:50:MET:HE3	1.68	0.76
1:F:45:MET:N	1:F:64:THR:HG22	1.98	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:25:VAL:HB	1:F:32:GLN:NE2	2.00	0.76
4:I:120:TYR:CZ	5:J:131:GLU:HA	2.20	0.76
4:I:46:LEU:HD22	5:J:99:GLU:HB3	1.67	0.75
1:F:8:PHE:HD2	1:F:25:VAL:HG23	1.50	0.75
1:F:45:MET:HG3	1:F:60:TRP:HZ3	1.49	0.75
1:A:33:PHE:CD1	1:A:34:VAL:N	2.55	0.75
1:A:108:ARG:NH2	4:I:114:ASN:HB2	2.01	0.75
4:D:71:TYR:C	4:D:71:TYR:CD2	2.64	0.75
4:I:122:LEU:HB3	5:J:125:PHE:HB3	1.68	0.75
1:A:35:ARG:NH1	1:A:48:ARG:NE	2.34	0.75
5:E:159:ASN:ND2	5:E:204:HIS:H	1.84	0.75
3:C:7:GLY:H	5:E:30:GLU:HG3	1.51	0.75
5:J:63:GLY:O	5:J:78:LEU:HD12	1.87	0.75
2:B:10:TYR:O	2:B:24:ASN:ND2	2.20	0.74
5:E:52:VAL:HA	5:E:68:ARG:HG2	1.69	0.74
1:A:215:LEU:CD1	1:A:243:LYS:HD2	2.18	0.74
4:D:71:TYR:O	4:D:71:TYR:HD2	1.70	0.74
1:F:59:TYR:O	1:F:63:GLU:HG2	1.87	0.74
5:J:85:GLN:O	5:J:108:LEU:HD11	1.87	0.74
1:A:115:GLN:HG2	1:A:125:ALA:CB	2.18	0.74
4:D:29:GLY:O	4:D:31:GLN:HG3	1.87	0.74
5:J:35:TYR:HB3	5:J:43:LEU:CD1	2.14	0.74
5:J:181:ASN:ND2	5:J:181:ASN:N	2.33	0.74
1:A:45:MET:CG	1:A:67:VAL:HG11	2.17	0.73
1:A:80:ILE:HG23	1:A:83:ARG:NH2	2.02	0.73
4:I:48:MET:HE1	4:I:58:ASP:HB2	1.70	0.73
5:J:108:LEU:C	5:J:108:LEU:HD12	2.12	0.73
1:A:258:THR:HB	1:A:260:HIS:CE1	2.22	0.73
4:D:50:ILE:HD11	4:D:65:LEU:HB3	1.71	0.73
1:F:22:PHE:CD2	1:F:71:SER:HB3	2.22	0.73
1:F:156:GLN:HE21	1:F:156:GLN:CA	2.01	0.73
5:E:119:PRO:HD3	5:E:227:PRO:HB3	1.69	0.73
5:E:161:LYS:HB2	5:E:161:LYS:NZ	2.04	0.73
1:F:121:LYS:HE2	2:G:1:ILE:HG12	1.70	0.73
5:J:9:ARG:HB3	5:J:9:ARG:HH11	1.53	0.72
5:J:205:PHE:HE2	5:J:238:GLY:N	1.86	0.72
1:A:213:ILE:HB	1:A:263:HIS:HD2	1.54	0.72
2:B:35:ILE:HD12	2:B:84:HIS:HD2	1.54	0.72
1:A:157:ARG:HA	1:A:160:LEU:CD1	2.19	0.72
5:J:163:VAL:C	5:J:164:HIS:HD1	1.98	0.72
1:A:137:ASP:O	1:A:141:GLN:HG3	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:158:VAL:HG23	5:E:163:VAL:HG21	1.70	0.72
1:F:4:SER:HB2	1:F:102:ASP:OD1	1.89	0.72
1:F:159:TYR:CD2	1:F:160:LEU:HD23	2.18	0.72
4:I:20:SER:C	4:I:21:LEU:HD23	2.15	0.72
4:D:22:ASN:HD22	4:D:71:TYR:HE1	1.38	0.72
1:F:19:GLU:CD	1:F:75:ARG:HH21	1.97	0.72
5:E:19:LEU:HD11	5:E:78:LEU:HD22	1.71	0.71
5:J:77:ILE:N	5:J:77:ILE:HD12	2.04	0.71
5:J:179:ALA:C	5:J:180:LEU:HD12	2.15	0.71
1:A:258:THR:HG22	1:A:271:THR:HG23	1.70	0.71
1:F:173:GLU:OE2	1:F:176:LYS:NZ	2.22	0.71
1:F:272:LEU:HD12	1:F:272:LEU:N	2.05	0.71
2:G:84:HIS:ND1	2:G:85:VAL:N	2.39	0.71
4:I:160:LEU:HD12	4:I:160:LEU:O	1.90	0.71
1:A:75:ARG:HD3	1:A:79:ARG:HD2	1.72	0.71
4:D:94:GLN:CB	4:D:97:LYS:HE2	2.20	0.71
4:D:122:LEU:HG	5:E:126:GLU:O	1.90	0.71
2:G:31:HIS:HE1	2:G:60:TRP:O	1.72	0.71
5:E:49:SER:OG	5:E:68:ARG:HD3	1.89	0.71
1:F:51:TRP:CZ2	1:F:179:LEU:HD21	2.26	0.71
1:F:234:ARG:HE	1:F:242:GLN:CD	1.98	0.71
1:A:216:THR:CG2	1:A:260:HIS:HB2	2.19	0.71
4:I:149:ASP:HB3	4:I:152:VAL:CG1	2.21	0.71
1:A:63:GLU:HA	1:A:63:GLU:OE2	1.90	0.71
2:G:81:ARG:HA	2:G:92:ILE:HG12	1.72	0.71
5:J:144:ALA:C	5:J:147:PHE:HE2	1.98	0.71
1:A:253:GLU:O	1:A:257:TYR:CE2	2.44	0.70
3:C:4:LEU:HD21	4:D:96:GLY:HA2	1.72	0.70
4:I:18:ILE:HG12	4:I:77:ARG:HA	1.73	0.70
4:D:62:THR:HG22	4:D:75:LEU:HD13	1.74	0.70
4:D:64:GLN:OE1	4:I:17:ALA:HA	1.92	0.70
1:A:190:THR:HG21	2:B:98:ASP:OD1	1.92	0.70
4:D:167:PHE:HD2	4:D:168:LYS:N	1.89	0.70
5:E:64:TYR:C	5:E:65:LYS:HD2	2.14	0.70
1:F:51:TRP:CE2	1:F:179:LEU:HD11	2.27	0.70
1:F:28:VAL:HG23	1:F:33:PHE:CD1	2.26	0.70
5:E:5:THR:HB	5:E:24:SER:OG	1.92	0.70
4:I:100:PHE:CE2	5:J:43:LEU:HD23	2.27	0.70
4:I:178:LYS:HE3	4:I:180:ASP:HB2	1.72	0.70
5:J:102:PHE:N	5:J:102:PHE:CD2	2.59	0.70
5:J:200:ASN:HD21	5:J:202:ARG:HB3	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:71:TYR:CE2	4:D:73:SER:HB3	2.27	0.70
1:A:57:PRO:HA	1:A:60:TRP:CD1	2.26	0.70
1:F:19:GLU:HG3	1:F:75:ARG:NE	2.07	0.70
5:J:119:PRO:HD3	5:J:227:PRO:HB3	1.71	0.70
4:D:94:GLN:HB3	4:D:97:LYS:NZ	2.06	0.69
4:D:185:ASN:HA	4:D:188:ASN:ND2	2.06	0.69
5:E:77:ILE:HD12	5:E:77:ILE:N	2.07	0.69
2:B:29:GLY:HA2	2:B:61:SER:HB2	1.74	0.69
1:F:35:ARG:HG2	1:F:35:ARG:HH11	1.58	0.69
1:F:185:PRO:HB3	1:F:208:PHE:HB3	1.74	0.69
1:A:33:PHE:HD1	1:A:34:VAL:H	1.40	0.69
1:A:200:THR:CG2	1:A:202:ARG:HH12	2.02	0.69
3:H:4:LEU:HD22	3:H:6:PHE:CE2	2.28	0.69
4:I:162:MET:HE1	5:J:192:ARG:CB	2.21	0.69
1:A:26:GLY:HA3	1:A:33:PHE:HE1	1.57	0.69
1:A:231:VAL:O	1:A:243:LYS:HE3	1.92	0.69
5:E:132:ILE:HG23	5:E:195:ALA:CB	2.23	0.69
5:E:132:ILE:HG23	5:E:195:ALA:HB1	1.74	0.69
1:F:28:VAL:HG23	1:F:33:PHE:HD1	1.57	0.69
1:F:202:ARG:HD3	1:F:244:TRP:CD1	2.28	0.69
3:H:4:LEU:HD22	3:H:6:PHE:HE2	1.57	0.69
4:I:185:ASN:HA	4:I:188:ASN:HD21	1.58	0.69
4:D:148:LYS:HD3	4:D:189:ASN:OD1	1.93	0.69
5:E:118:PHE:HB3	5:E:184:ARG:HH21	1.57	0.69
1:F:108:ARG:HG3	1:F:108:ARG:HH11	1.57	0.69
4:I:97:LYS:HE3	5:J:48:TYR:HE2	1.57	0.69
1:A:68:LYS:HZ1	5:E:53:GLU:CB	1.97	0.69
1:A:209:TYR:HD1	1:A:241:PHE:HE1	1.41	0.69
5:E:37:GLN:CG	5:E:43:LEU:HD12	2.23	0.68
5:E:78:LEU:N	5:E:78:LEU:HD12	2.08	0.68
2:G:7:ILE:HD12	2:G:7:ILE:N	2.09	0.68
4:I:34:PHE:HZ	5:J:98:HIS:HB2	1.59	0.68
2:B:23:LEU:HD21	2:B:39:LEU:HD22	1.74	0.68
4:D:2:LYS:HZ1	5:E:43:LEU:H	1.41	0.68
2:G:21:ASN:CG	2:G:22:PHE:H	2.01	0.68
1:A:156:GLN:O	1:A:160:LEU:CG	2.41	0.68
2:B:95:TRP:CZ2	2:B:97:ARG:HG2	2.29	0.68
1:F:51:TRP:CZ2	1:F:179:LEU:HD11	2.28	0.68
2:G:13:HIS:H	2:G:21:ASN:HD21	1.42	0.68
5:J:127:PRO:HD3	5:J:140:LEU:CD2	2.23	0.68
4:I:35:TRP:HB3	4:I:47:ILE:HD11	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:18:LYS:HG3	5:J:79:GLU:OE1	1.94	0.68
4:D:33:PHE:O	4:D:50:ILE:HG23	1.93	0.68
2:G:12:ARG:HG3	2:G:13:HIS:HD2	1.58	0.68
1:A:235:PRO:HG2	2:B:65:LEU:HD13	1.76	0.67
4:I:159:VAL:CG1	4:I:168:LYS:HZ2	2.06	0.67
1:A:75:ARG:NH1	1:A:79:ARG:HE	1.93	0.67
4:I:46:LEU:HD21	5:J:99:GLU:OE2	1.95	0.67
1:F:14:ARG:HB3	1:F:17:ARG:HB2	1.77	0.67
1:F:25:VAL:HB	1:F:32:GLN:HE21	1.57	0.67
2:G:29:GLY:HA2	2:G:61:SER:HB2	1.75	0.67
1:A:49:ALA:O	1:A:52:ILE:HG22	1.93	0.67
1:F:96:GLN:OE1	2:G:60:TRP:HB3	1.95	0.67
4:D:144:VAL:HG21	4:D:156:ASP:HA	1.76	0.67
1:F:27:TYR:CZ	1:F:32:GLN:HB2	2.29	0.67
5:J:87:SER:OG	5:J:88:LEU:N	2.25	0.67
5:J:199:GLN:O	5:J:201:PRO:HD3	1.94	0.67
1:A:69:ALA:O	5:E:51:ASN:ND2	2.28	0.67
4:D:14:PRO:HD2	4:I:71:TYR:CE1	2.29	0.67
5:E:167:VAL:HG12	5:E:191:LEU:HD13	1.76	0.67
1:F:127:LYS:HE2	1:F:134:THR:HB	1.76	0.67
1:F:146:LYS:NZ	1:F:146:LYS:HB3	2.10	0.67
5:J:12:ILE:HD12	5:J:12:ILE:N	2.09	0.67
1:A:186:LYS:HB2	1:A:186:LYS:NZ	2.10	0.67
4:D:191:ILE:H	4:D:191:ILE:HD12	1.60	0.67
1:F:181:ARG:HG2	1:F:181:ARG:HH11	1.60	0.67
1:A:226:GLN:OE1	1:A:226:GLN:HA	1.95	0.67
4:D:91:THR:HG23	4:D:91:THR:O	1.95	0.67
4:D:112:ILE:HG13	4:D:170:ASN:HD21	1.58	0.67
1:F:146:LYS:NZ	1:F:146:LYS:CB	2.58	0.66
4:D:89:TRP:HZ3	4:D:91:THR:CG2	2.09	0.66
4:D:2:LYS:NZ	5:E:43:LEU:N	2.44	0.66
4:D:18:ILE:CD1	4:D:77:ARG:HG2	2.25	0.66
5:E:137:LYS:HB2	5:E:192:ARG:NH2	2.10	0.66
5:J:135:THR:O	5:J:137:LYS:NZ	2.29	0.66
4:I:66:ASN:HB3	4:I:71:TYR:CD2	2.31	0.66
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.31	0.66
1:A:142:ILE:HA	1:A:145:ARG:HH11	1.60	0.66
2:B:96:ASP:HB3	2:B:99:MET:HA	1.77	0.66
1:F:193:PRO:HA	1:F:199:ALA:HA	1.76	0.66
1:F:228:THR:HG22	1:F:247:VAL:HG12	1.78	0.66
5:E:9:ARG:NH1	5:E:104:PRO:HB2	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:120:PRO:HG2	5:J:232:VAL:HG21	1.77	0.66
4:D:83:ASP:O	4:D:106:LEU:HD23	1.96	0.66
1:F:70:HIS:HD2	1:F:73:THR:HB	1.58	0.66
1:F:97:MET:HB2	1:F:116:TYR:CE1	2.31	0.66
4:I:60:ARG:NH2	4:I:80:GLN:HG2	2.10	0.66
3:H:3:PRO:HG2	3:H:5:THR:CG2	2.25	0.66
1:F:76:GLU:HA	1:F:76:GLU:OE2	1.96	0.66
5:J:4:VAL:HG21	5:J:102:PHE:C	2.21	0.66
4:D:94:GLN:HG3	4:D:97:LYS:HE2	1.78	0.65
4:I:20:SER:O	4:I:21:LEU:HD23	1.96	0.65
5:J:79:GLU:OE1	5:J:79:GLU:HA	1.95	0.65
1:F:231:VAL:HG13	1:F:244:TRP:CZ3	2.31	0.65
5:J:127:PRO:HD3	5:J:140:LEU:HD21	1.78	0.65
1:F:213:ILE:HG13	1:F:262:GLN:O	1.97	0.65
4:D:167:PHE:CE1	5:E:137:LYS:HE3	2.32	0.65
5:E:19:LEU:HD12	5:E:19:LEU:C	2.22	0.65
1:F:202:ARG:HH12	1:F:246:ALA:HB2	1.59	0.65
4:I:41:GLY:C	4:I:42:LYS:HE2	2.21	0.65
4:D:142:THR:HG21	4:D:193:PRO:HD3	1.79	0.65
1:A:258:THR:HG22	1:A:271:THR:CG2	2.27	0.65
5:E:46:ILE:N	5:E:46:ILE:CD1	2.59	0.65
4:I:124:ASP:HA	5:J:125:PHE:CZ	2.31	0.65
1:A:33:PHE:HD1	1:A:34:VAL:N	1.94	0.65
1:A:68:LYS:HG2	5:E:54:VAL:HG22	1.79	0.65
4:D:71:TYR:C	4:D:71:TYR:HD2	2.04	0.65
4:I:162:MET:CE	5:J:192:ARG:HB3	2.25	0.65
1:A:76:GLU:O	1:A:80:ILE:HG13	1.97	0.65
4:D:60:ARG:HH22	4:D:83:ASP:CG	2.04	0.65
5:E:23:CYS:HB2	5:E:34:TRP:CZ2	2.31	0.65
5:E:101:TYR:N	5:E:101:TYR:CD2	2.65	0.65
4:I:38:GLN:HE22	5:J:37:GLN:NE2	1.95	0.65
4:I:136:THR:HG21	5:J:192:ARG:HH22	1.61	0.65
1:A:154:GLU:HB2	4:D:51:TYR:HB2	1.78	0.64
5:J:220:TRP:HH2	5:J:224:ARG:HH21	1.42	0.64
4:D:114:ASN:CB	1:F:108:ARG:HH12	2.11	0.64
5:E:146:GLY:O	5:E:184:ARG:NH2	2.30	0.64
5:J:180:LEU:N	5:J:180:LEU:CD1	2.59	0.64
2:G:45:ARG:HE	2:G:81:ARG:HH22	1.45	0.64
2:B:24:ASN:ND2	2:B:24:ASN:N	2.44	0.64
4:D:64:GLN:NE2	4:I:18:ILE:HD12	2.11	0.64
1:A:127:LYS:HD3	1:A:132:SER:OG	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:31:GLN:HA	4:D:67:LYS:CE	2.28	0.64
4:D:191:ILE:HD12	4:D:191:ILE:N	2.13	0.64
1:A:69:ALA:CB	5:E:51:ASN:HB2	2.28	0.64
1:A:75:ARG:HD3	1:A:75:ARG:O	1.98	0.64
1:A:235:PRO:CG	2:B:65:LEU:HD13	2.28	0.64
1:A:242:GLN:OE1	2:B:10:TYR:HE2	1.81	0.64
4:D:92:TYR:HE2	5:E:98:HIS:HB3	1.63	0.64
1:A:13:SER:OG	1:A:15:PRO:HD3	1.97	0.63
1:A:229:GLU:OE2	1:A:230:LEU:N	2.31	0.63
5:E:48:TYR:CE2	5:E:56:ASP:HB2	2.33	0.63
1:A:21:ARG:CZ	1:A:39:ASP:HB2	2.28	0.63
1:A:56:GLY:O	1:A:59:TYR:HB3	1.98	0.63
1:F:159:TYR:O	1:F:163:THR:OG1	2.15	0.63
5:J:159:ASN:HD21	5:J:204:HIS:N	1.94	0.63
1:A:158:ALA:HB1	4:D:67:LYS:HZ1	1.63	0.63
1:A:126:LEU:HD13	1:A:133:TRP:CZ3	2.34	0.63
1:A:228:THR:HG22	1:A:247:VAL:HG12	1.79	0.63
5:E:194:SER:OG	5:E:197:PHE:HB2	1.98	0.63
2:B:10:TYR:OH	2:B:26:TYR:HB2	1.99	0.63
5:E:154:LEU:HD23	5:E:154:LEU:C	2.23	0.63
5:J:206:ARG:HG3	5:J:235:GLU:HB3	1.80	0.63
4:D:92:TYR:CE2	5:E:98:HIS:HB3	2.33	0.63
4:D:191:ILE:H	4:D:191:ILE:CD1	2.10	0.63
5:E:164:HIS:O	5:E:167:VAL:HG13	1.98	0.63
5:J:154:LEU:HG	5:J:209:VAL:HG22	1.81	0.63
1:A:68:LYS:CG	5:E:54:VAL:HG22	2.29	0.63
1:F:146:LYS:CB	1:F:146:LYS:HZ2	2.12	0.63
1:F:244:TRP:HE3	1:F:244:TRP:C	2.07	0.63
4:I:167:PHE:HZ	5:J:192:ARG:NH1	1.85	0.63
1:A:162:GLY:O	1:A:165:VAL:HG23	1.99	0.63
4:D:80:GLN:HB2	4:D:83:ASP:OD2	1.98	0.63
1:F:202:ARG:HH11	1:F:202:ARG:HG3	1.63	0.63
4:I:93:ASN:C	4:I:95:GLY:H	2.07	0.63
4:I:136:THR:HG21	5:J:192:ARG:NH2	2.14	0.63
2:G:12:ARG:HG2	2:G:13:HIS:N	2.14	0.63
4:I:97:LYS:HB3	5:J:48:TYR:CE2	2.34	0.63
5:J:177:GLN:HG3	5:J:180:LEU:HD22	1.81	0.63
1:A:108:ARG:O	1:A:110:LEU:HD13	1.99	0.62
4:D:185:ASN:HA	4:D:188:ASN:HD21	1.64	0.62
4:I:60:ARG:HH21	4:I:80:GLN:HG2	1.62	0.62
2:B:35:ILE:HD11	2:B:82:VAL:HG13	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:4:LEU:HB3	3:C:6:PHE:CE2	2.33	0.62
4:I:92:TYR:HA	4:I:97:LYS:O	1.98	0.62
1:A:79:ARG:HB2	1:A:79:ARG:HH11	1.65	0.62
1:A:111:ARG:NH2	1:A:128:GLU:HA	2.14	0.62
4:D:147:SER:OG	4:D:152:VAL:HG13	1.99	0.62
1:F:127:LYS:CE	1:F:134:THR:HB	2.30	0.62
4:D:31:GLN:HB3	4:D:67:LYS:HZ3	1.63	0.62
4:D:182:ALA:HB3	4:D:185:ASN:HD21	1.63	0.62
4:I:50:ILE:HD12	4:I:51:TYR:N	2.14	0.62
5:J:36:ARG:HG3	5:J:87:SER:OG	2.00	0.62
5:E:239:ARG:HG3	5:E:239:ARG:HH11	1.64	0.62
1:F:150:ALA:O	1:F:151:HIS:HB2	1.99	0.62
1:F:158:ALA:CB	4:I:31:GLN:HB2	2.29	0.62
1:A:65:GLY:O	5:E:54:VAL:HG11	2.00	0.62
5:E:150:ASP:OD1	5:E:150:ASP:O	2.17	0.62
4:I:138:PHE:CZ	4:I:170:ASN:HB3	2.35	0.62
2:B:2:GLN:HG3	2:B:31:HIS:O	1.99	0.62
2:B:33:SER:HB2	2:B:54:LEU:HD11	1.81	0.62
1:F:175:GLY:O	1:F:179:LEU:HG	1.99	0.62
4:I:34:PHE:CZ	5:J:98:HIS:HB2	2.34	0.62
4:D:108:VAL:O	4:D:108:VAL:HG12	1.97	0.62
5:E:4:VAL:HG13	5:E:23:CYS:SG	2.40	0.62
1:F:33:PHE:CD2	1:F:34:VAL:HG13	2.24	0.62
1:F:115:GLN:HG3	2:G:60:TRP:HH2	1.63	0.62
5:J:177:GLN:CB	5:J:180:LEU:HD13	2.12	0.62
1:A:99:PHE:CD1	1:A:114:HIS:HD2	2.18	0.62
1:A:111:ARG:NH1	1:A:128:GLU:OE1	2.33	0.62
5:E:128:SER:O	5:E:132:ILE:HD12	1.99	0.62
1:F:234:ARG:HG2	1:F:242:GLN:HG3	1.82	0.62
2:G:57:SER:O	2:G:59:ASP:O	2.18	0.62
4:I:88:LEU:HB3	4:I:103:GLY:HA2	1.81	0.62
5:J:102:PHE:N	5:J:102:PHE:HD2	1.97	0.62
1:A:193:PRO:HA	1:A:199:ALA:HA	1.81	0.61
4:D:88:LEU:N	4:D:88:LEU:HD23	2.15	0.61
3:H:6:PHE:CZ	5:J:98:HIS:HD2	2.18	0.61
1:A:80:ILE:HG23	1:A:83:ARG:HH22	1.62	0.61
1:F:146:LYS:HZ2	1:F:146:LYS:HB2	1.65	0.61
1:A:7:TYR:CE2	3:C:2:PHE:HA	2.35	0.61
1:A:111:ARG:HD3	1:A:128:GLU:OE2	1.99	0.61
1:A:155:GLN:OE1	3:C:8:TRP:HZ2	1.83	0.61
5:E:168:CYS:O	5:E:190:ARG:HD2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:TRP:HZ2	1:F:179:LEU:HD21	1.65	0.61
2:G:17:ASN:HA	2:G:72:PRO:O	1.99	0.61
3:H:3:PRO:HG2	3:H:5:THR:HG22	1.81	0.61
4:I:38:GLN:HB2	4:I:44:PRO:HG3	1.82	0.61
4:D:112:ILE:CD1	4:D:170:ASN:HD21	2.14	0.61
5:E:37:GLN:HG2	5:E:42:GLY:C	2.26	0.61
5:E:52:VAL:HA	5:E:68:ARG:HG3	1.82	0.61
1:F:158:ALA:HB3	4:I:31:GLN:HB2	1.83	0.61
1:A:34:VAL:HG21	1:A:45:MET:CE	2.30	0.61
4:D:92:TYR:HA	4:D:97:LYS:O	2.00	0.61
1:F:63:GLU:O	1:F:67:VAL:HG12	2.00	0.61
1:F:168:LEU:O	1:F:172:LEU:HG	2.01	0.61
4:I:129:ASP:OD1	4:I:130:LYS:HG3	2.01	0.61
1:A:103:VAL:C	1:A:110:LEU:HD22	2.26	0.61
2:B:51:HIS:CD2	2:B:64:LEU:HD21	2.33	0.61
2:B:56:PHE:C	2:B:63:TYR:CE2	2.79	0.61
5:E:52:VAL:HG13	5:E:68:ARG:O	1.99	0.61
1:F:75:ARG:HH11	1:F:75:ARG:CG	2.11	0.61
1:A:26:GLY:O	1:A:32:GLN:OE1	2.18	0.61
1:F:191:HIS:HE1	1:F:193:PRO:HG3	1.65	0.61
5:E:32:MET:SD	5:E:68:ARG:CZ	2.89	0.61
2:B:21:ASN:CG	2:B:22:PHE:N	2.59	0.60
4:D:135:PHE:HB2	4:D:187:PHE:CE2	2.35	0.60
1:F:99:PHE:HE2	1:F:159:TYR:CE2	2.19	0.60
4:I:167:PHE:C	4:I:167:PHE:CD2	2.79	0.60
1:F:233:THR:HG23	1:F:243:LYS:HD2	1.83	0.60
5:J:230:GLN:HE22	5:J:232:VAL:CG1	2.10	0.60
1:A:133:TRP:CZ2	1:A:152:VAL:HB	2.36	0.60
2:B:23:LEU:HD11	2:B:39:LEU:HD22	1.83	0.60
2:B:33:SER:HB3	2:B:62:PHE:CD1	2.36	0.60
4:D:2:LYS:HZ1	5:E:43:LEU:N	1.98	0.60
4:D:18:ILE:HD11	4:D:77:ARG:HG2	1.83	0.60
4:D:93:ASN:C	4:D:95:GLY:H	2.10	0.60
1:F:5:MET:HE1	3:H:1:ARG:H2	1.65	0.60
1:F:267:PRO:HG2	1:F:268:LYS:H	1.65	0.60
2:G:12:ARG:CD	2:G:22:PHE:HB2	2.31	0.60
4:I:81:PRO:HA	4:I:108:VAL:HB	1.83	0.60
4:D:154:ILE:HD11	4:D:187:PHE:CD1	2.35	0.60
2:G:80:CYS:O	2:G:92:ILE:HA	2.02	0.60
4:I:91:THR:OG1	4:I:93:ASN:ND2	2.34	0.60
4:I:149:ASP:HB3	4:I:152:VAL:HG11	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:38:ASP:H	5:J:44:ARG:HH22	1.47	0.60
1:A:192:HIS:HD2	1:A:202:ARG:HH21	1.50	0.60
5:E:190:ARG:HD2	5:E:190:ARG:H	1.63	0.60
1:F:144:LYS:O	1:F:148:GLU:HG3	2.01	0.60
1:A:250:PRO:O	1:A:253:GLU:HB2	2.01	0.60
1:F:70:HIS:O	1:F:73:THR:HB	2.02	0.60
1:F:155:GLN:HE22	5:J:98:HIS:CE1	2.19	0.60
1:A:238:ASP:OD2	2:B:12:ARG:HD3	2.01	0.60
1:F:249:VAL:HG22	1:F:257:TYR:CE1	2.37	0.60
1:F:260:HIS:CE1	1:F:271:THR:HG23	2.37	0.60
5:J:12:ILE:HD11	5:J:213:GLY:O	2.01	0.60
5:J:163:VAL:O	5:J:164:HIS:ND1	2.34	0.60
1:A:99:PHE:HD1	1:A:114:HIS:HD2	1.49	0.60
1:A:127:LYS:HB2	1:A:129:ASP:OD1	2.01	0.60
4:I:158:CYS:HB3	5:J:190:ARG:HH12	1.66	0.60
2:B:7:ILE:HD12	2:B:7:ILE:N	2.16	0.60
4:D:48:MET:HE3	4:D:63:ALA:N	2.17	0.60
5:E:206:ARG:NH1	5:E:208:GLN:OE1	2.35	0.60
1:F:43:GLN:HA	1:F:43:GLN:HE21	1.67	0.60
1:A:189:MET:SD	1:A:201:LEU:HD22	2.42	0.60
1:A:261:VAL:HG12	1:A:266:LEU:HD11	1.83	0.60
1:F:70:HIS:HE1	1:F:97:MET:SD	2.25	0.60
1:F:81:ALA:HB1	1:F:118:TYR:CE2	2.37	0.60
4:I:190:SER:O	4:I:192:ILE:HG23	2.02	0.60
5:E:49:SER:CB	5:E:68:ARG:HD3	2.32	0.59
2:G:45:ARG:HB2	2:G:81:ARG:HH22	1.66	0.59
1:A:33:PHE:CD1	1:A:34:VAL:HG13	2.37	0.59
2:B:24:ASN:ND2	2:B:24:ASN:H	1.99	0.59
1:F:5:MET:HE1	3:H:1:ARG:N	2.17	0.59
1:F:117:ALA:HB2	2:G:60:TRP:CD2	2.37	0.59
5:J:200:ASN:ND2	5:J:202:ARG:HB3	2.16	0.59
1:A:104:GLY:N	1:A:110:LEU:HD13	2.18	0.59
5:E:77:ILE:C	5:E:78:LEU:HD12	2.27	0.59
5:E:82:SER:HB2	5:E:85:GLN:HG3	1.84	0.59
1:A:25:VAL:HB	1:A:32:GLN:NE2	2.13	0.59
4:D:94:GLN:HB3	4:D:97:LYS:CE	2.32	0.59
4:I:53:ASN:HD22	4:I:53:ASN:C	2.09	0.59
5:J:230:GLN:NE2	5:J:232:VAL:HG22	2.17	0.59
2:B:17:ASN:HA	2:B:72:PRO:O	2.02	0.59
5:E:39:PRO:O	5:E:41:LEU:HD22	2.03	0.59
5:E:82:SER:O	5:E:110:VAL:HG21	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:259:CYS:HB3	1:F:272:LEU:HB2	1.83	0.59
2:G:21:ASN:HB3	2:G:70:PHE:CE1	2.38	0.59
1:F:36:PHE:HB2	1:F:45:MET:CE	2.33	0.59
1:F:152:VAL:HA	1:F:155:GLN:HG3	1.84	0.59
4:I:13:VAL:HG13	4:I:14:PRO:HD2	1.85	0.59
4:I:6:GLN:NE2	4:I:102:GLN:HB2	2.18	0.59
4:I:93:ASN:O	4:I:95:GLY:N	2.35	0.59
5:J:41:LEU:HB3	5:J:44:ARG:CZ	2.32	0.59
3:C:5:THR:HA	3:C:8:TRP:CZ3	2.36	0.59
2:B:39:LEU:HD12	2:B:49:VAL:CG2	2.33	0.59
4:D:14:PRO:HB2	4:I:71:TYR:OH	2.02	0.59
5:E:11:LEU:CD2	5:E:19:LEU:HD22	2.32	0.59
1:F:35:ARG:HD2	1:F:35:ARG:C	2.28	0.59
1:F:273:ARG:HH11	1:F:273:ARG:HG3	1.68	0.59
2:B:21:ASN:ND2	2:B:22:PHE:H	2.01	0.59
4:D:89:TRP:HZ3	4:D:91:THR:HG21	1.67	0.59
1:A:152:VAL:CG1	1:A:156:GLN:NE2	2.66	0.58
1:F:268:LYS:HD2	1:F:269:PRO:CD	2.31	0.58
5:J:230:GLN:HE21	5:J:232:VAL:HG22	1.67	0.58
4:D:48:MET:HE3	4:D:63:ALA:H	1.68	0.58
4:D:148:LYS:CD	4:D:189:ASN:OD1	2.51	0.58
4:D:152:VAL:HG13	4:D:152:VAL:O	2.03	0.58
5:E:198:TRP:CZ2	5:E:239:ARG:HB3	2.38	0.58
1:F:181:ARG:HG2	1:F:181:ARG:NH1	2.18	0.58
5:J:138:ALA:O	5:J:192:ARG:HA	2.02	0.58
5:E:138:ALA:O	5:E:192:ARG:HA	2.03	0.58
1:F:54:GLN:OE1	1:F:174:ASN:ND2	2.36	0.58
4:I:74:LEU:HG	4:I:75:LEU:N	2.18	0.58
4:I:161:ASP:CB	4:I:168:LYS:HE2	2.26	0.58
1:A:97:MET:HE2	1:A:99:PHE:HB2	1.85	0.58
1:A:242:GLN:HE22	2:B:10:TYR:HD2	1.51	0.58
5:E:217:ASN:HD22	5:E:217:ASN:N	1.99	0.58
5:J:6:GLN:OE1	5:J:91:CYS:N	2.35	0.58
5:J:132:ILE:HG23	5:J:195:ALA:HB1	1.86	0.58
1:F:5:MET:O	1:F:6:ARG:HD3	2.03	0.58
2:G:23:LEU:HG	2:G:70:PHE:CE1	2.39	0.58
4:I:155:THR:CG2	4:I:173:VAL:H	2.16	0.58
1:A:98:MET:O	1:A:114:HIS:HA	2.03	0.58
5:E:25:GLN:HE21	5:E:32:MET:HE3	1.67	0.58
1:A:231:VAL:O	1:A:243:LYS:CE	2.52	0.58
5:E:101:TYR:HD2	5:E:101:TYR:N	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:163:ARG:HG2	5:J:165:SER:OG	2.03	0.58
5:J:132:ILE:HD12	5:J:132:ILE:N	2.18	0.58
4:D:94:GLN:HB2	4:D:97:LYS:HG3	1.85	0.58
1:A:157:ARG:HA	1:A:160:LEU:HD12	1.86	0.58
2:B:24:ASN:H	2:B:24:ASN:HD22	1.52	0.58
2:B:57:SER:O	2:B:59:ASP:O	2.22	0.58
5:E:20:THR:HG23	5:E:20:THR:O	2.04	0.58
1:A:5:MET:SD	1:A:171:TYR:HE2	2.27	0.58
2:B:1:ILE:O	2:B:1:ILE:HD12	2.03	0.58
4:D:93:ASN:O	4:D:95:GLY:N	2.36	0.58
1:F:142:ILE:O	1:F:146:LYS:HG3	2.04	0.58
2:G:11:SER:HB2	2:G:21:ASN:OD1	2.03	0.58
4:I:121:GLN:HB2	4:I:183:CYS:SG	2.43	0.58
5:J:126:GLU:HA	5:J:140:LEU:HD23	1.84	0.58
3:H:2:PHE:CG	3:H:3:PRO:HD2	2.39	0.57
1:A:6:ARG:HG2	1:A:6:ARG:HH11	1.70	0.57
5:E:37:GLN:HG3	5:E:43:LEU:CD1	2.34	0.57
1:F:233:THR:OG1	1:F:243:LYS:HD2	2.04	0.57
1:A:117:ALA:HB2	2:B:60:TRP:CD2	2.39	0.57
1:A:255:GLN:O	1:A:273:ARG:HD3	2.03	0.57
4:D:31:GLN:HB3	4:D:67:LYS:HZ1	1.67	0.57
2:B:83:ASN:HD22	2:B:84:HIS:N	2.02	0.57
4:D:149:ASP:HB3	4:D:152:VAL:CG1	2.35	0.57
5:E:118:PHE:CE1	5:E:224:ARG:CZ	2.87	0.57
4:I:94:GLN:HB2	4:I:99:ILE:HD11	1.87	0.57
5:J:108:LEU:HD12	5:J:108:LEU:O	2.05	0.57
1:A:51:TRP:CD1	1:A:178:THR:HG1	2.22	0.57
1:A:227:ASP:O	1:A:248:VAL:HG23	2.03	0.57
4:I:11:LEU:HD12	4:I:12:SER:H	1.69	0.57
4:I:50:ILE:C	4:I:50:ILE:CD1	2.72	0.57
4:I:97:LYS:HE3	5:J:48:TYR:CE2	2.38	0.57
4:I:182:ALA:O	4:I:185:ASN:ND2	2.37	0.57
1:A:186:LYS:HB2	1:A:186:LYS:HZ2	1.69	0.57
1:A:200:THR:CG2	1:A:202:ARG:NH1	2.65	0.57
4:D:131:SER:HB2	4:D:181:PHE:CE2	2.40	0.57
4:D:158:CYS:HB3	5:E:190:ARG:NH1	2.19	0.57
5:E:118:PHE:HE1	5:E:224:ARG:CZ	2.17	0.57
5:J:135:THR:O	5:J:136:GLN:HB2	2.04	0.57
5:J:206:ARG:HH11	5:J:233:SER:HB3	1.70	0.57
2:B:23:LEU:HD11	2:B:39:LEU:CD2	2.34	0.57
4:I:122:LEU:CD1	5:J:141:VAL:HB	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:3:PRO:O	3:H:5:THR:HG23	2.04	0.57
4:I:50:ILE:HG13	4:I:50:ILE:O	2.04	0.57
5:J:9:ARG:HH11	5:J:9:ARG:CB	2.18	0.57
5:J:131:GLU:O	5:J:135:THR:OG1	2.19	0.57
1:A:68:LYS:HE3	5:E:53:GLU:O	2.05	0.57
4:D:158:CYS:CB	5:E:190:ARG:NH1	2.68	0.57
5:E:23:CYS:HB2	5:E:34:TRP:HZ2	1.70	0.57
5:E:135:THR:HG21	5:E:192:ARG:NH1	2.20	0.57
1:F:130:LEU:HD13	1:F:160:LEU:HD12	1.87	0.57
4:I:11:LEU:HD12	4:I:12:SER:N	2.19	0.57
4:D:123:ARG:HB3	5:E:126:GLU:HB2	1.87	0.56
4:I:78:ASP:OD1	4:I:80:GLN:NE2	2.38	0.56
5:E:9:ARG:HH12	5:E:104:PRO:C	2.12	0.56
1:F:156:GLN:OE1	3:H:8:TRP:HH2	1.88	0.56
5:J:206:ARG:NH1	5:J:233:SER:CB	2.64	0.56
1:A:33:PHE:CE1	1:A:34:VAL:HG22	2.40	0.56
1:A:35:ARG:HH12	1:A:48:ARG:CZ	2.18	0.56
1:A:147:TRP:CE3	1:A:152:VAL:HG11	2.40	0.56
4:D:94:GLN:CG	4:D:97:LYS:HE2	2.34	0.56
5:E:30:GLU:O	5:E:68:ARG:NH2	2.38	0.56
1:F:143:THR:HA	1:F:146:LYS:HD3	1.88	0.56
4:I:22:ASN:OD1	4:I:22:ASN:N	2.38	0.56
4:I:177:ASN:HD22	4:I:178:LYS:N	2.03	0.56
5:J:154:LEU:CD2	5:J:155:SER:H	2.18	0.56
5:J:170:ASP:OD1	5:J:190:ARG:NH2	2.39	0.56
5:J:200:ASN:HD22	5:J:203:ASN:CG	2.13	0.56
1:A:234:ARG:HG3	1:A:242:GLN:HG3	1.87	0.56
1:F:120:GLY:HA3	2:G:31:HIS:NE2	2.20	0.56
4:I:122:LEU:HD12	4:I:132:VAL:HB	1.87	0.56
1:A:209:TYR:HD1	1:A:241:PHE:CE1	2.22	0.56
2:B:57:SER:N	2:B:63:TYR:HE2	2.02	0.56
4:D:167:PHE:HD2	4:D:168:LYS:H	1.52	0.56
1:F:7:TYR:HE2	3:H:2:PHE:N	2.04	0.56
4:I:35:TRP:CB	4:I:47:ILE:HD11	2.35	0.56
5:J:230:GLN:NE2	5:J:232:VAL:HG13	2.16	0.56
1:F:254:GLU:OE2	1:F:274:TRP:HD1	1.89	0.56
4:I:149:ASP:HB3	4:I:152:VAL:HG12	1.86	0.56
4:I:176:SER:HB3	4:I:181:PHE:CG	2.41	0.56
1:A:108:ARG:HH22	4:I:114:ASN:HB2	1.70	0.56
1:F:33:PHE:CE2	1:F:34:VAL:HG22	2.40	0.56
1:F:117:ALA:HB2	2:G:60:TRP:CE2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:141:GLN:O	1:F:145:ARG:HG3	2.04	0.56
1:F:244:TRP:HE1	2:G:99:MET:CG	2.18	0.56
2:G:1:ILE:C	2:G:1:ILE:HD12	2.31	0.56
4:D:89:TRP:CZ2	4:D:101:GLY:HA3	2.40	0.56
4:D:197:PHE:CZ	4:D:199:PRO:HA	2.40	0.56
1:F:233:THR:HG23	1:F:243:LYS:CB	2.34	0.56
5:E:143:LEU:HD12	5:E:188:SER:HB3	1.87	0.56
5:E:180:LEU:N	5:E:180:LEU:HD12	2.21	0.56
2:G:5:PRO:HD3	2:G:84:HIS:HD2	1.71	0.56
4:I:38:GLN:HE22	5:J:37:GLN:HE21	1.52	0.56
5:J:38:ASP:HB2	5:J:44:ARG:HH22	1.71	0.56
5:J:49:SER:OG	5:J:68:ARG:HG2	2.06	0.56
5:J:120:PRO:HB3	5:J:147:PHE:CD2	2.41	0.56
5:J:127:PRO:HD2	5:J:198:TRP:CZ2	2.41	0.56
1:A:235:PRO:HG2	2:B:65:LEU:CD1	2.35	0.56
2:B:80:CYS:O	2:B:92:ILE:HA	2.06	0.56
1:F:97:MET:HE3	1:F:99:PHE:CD1	2.41	0.56
1:F:249:VAL:HG22	1:F:257:TYR:CD1	2.40	0.56
5:J:64:TYR:HB3	5:J:76:LEU:HD11	1.88	0.56
5:E:45:GLN:C	5:E:46:ILE:HD12	2.31	0.55
1:A:202:ARG:HG3	1:A:246:ALA:HB2	1.88	0.55
5:E:48:TYR:CZ	5:E:56:ASP:HB2	2.42	0.55
1:F:14:ARG:CZ	1:F:21:ARG:HB2	2.37	0.55
5:J:211:PHE:CE2	5:J:213:GLY:HA3	2.41	0.55
1:A:14:ARG:NH2	1:A:19:GLU:O	2.37	0.55
1:A:97:MET:CE	1:A:99:PHE:HB2	2.36	0.55
4:D:91:THR:HG23	4:D:93:ASN:ND2	2.21	0.55
1:F:244:TRP:HE1	2:G:99:MET:HG3	1.72	0.55
4:I:77:ARG:HH11	4:I:77:ARG:HG3	1.71	0.55
4:I:123:ARG:HD3	5:J:126:GLU:OE2	2.06	0.55
4:I:160:LEU:CD1	4:I:160:LEU:C	2.79	0.55
1:A:96:GLN:OE1	2:B:60:TRP:HB3	2.06	0.55
2:B:10:TYR:N	2:B:10:TYR:CD1	2.75	0.55
5:E:118:PHE:HB3	5:E:184:ARG:NH2	2.21	0.55
5:E:132:ILE:HG21	5:E:199:GLN:HE22	1.72	0.55
1:F:227:ASP:O	1:F:248:VAL:HG23	2.07	0.55
5:J:36:ARG:NE	5:J:87:SER:CB	2.70	0.55
5:J:200:ASN:O	5:J:238:GLY:HA3	2.06	0.55
4:D:38:GLN:NE2	4:D:42:LYS:O	2.39	0.55
1:F:115:GLN:CG	2:G:60:TRP:HH2	2.19	0.55
1:F:218:GLN:HB2	1:F:258:THR:OG1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:160:LEU:HB3	5:J:168:CYS:HB2	1.89	0.55
1:A:55:GLU:O	1:A:60:TRP:CZ2	2.60	0.55
4:I:50:ILE:CD1	4:I:65:LEU:HD22	2.36	0.55
1:A:123:TYR:CZ	1:A:140:ALA:HA	2.41	0.55
4:D:112:ILE:CG1	4:D:170:ASN:HD21	2.18	0.55
1:F:19:GLU:CG	1:F:75:ARG:HE	2.15	0.55
1:A:156:GLN:O	1:A:160:LEU:CD2	2.54	0.55
4:D:39:TYR:CE1	4:D:85:ALA:HB2	2.41	0.55
5:J:126:GLU:HA	5:J:140:LEU:CD2	2.36	0.55
5:J:205:PHE:HD2	5:J:236:ALA:O	1.88	0.55
1:A:224:GLN:O	1:A:228:THR:HG21	2.06	0.55
5:E:124:VAL:HG23	5:E:234:ALA:HB3	1.88	0.55
1:F:244:TRP:C	1:F:244:TRP:CE3	2.85	0.55
4:D:167:PHE:CD1	5:E:137:LYS:HE3	2.41	0.55
1:F:168:LEU:O	1:F:168:LEU:HD12	2.06	0.55
1:F:215:LEU:HD21	1:F:261:VAL:HG13	1.88	0.55
1:F:259:CYS:O	1:F:272:LEU:HD12	2.07	0.55
2:G:5:PRO:HD3	2:G:84:HIS:CD2	2.42	0.55
4:I:30:SER:HA	4:I:93:ASN:OD1	2.07	0.55
4:I:50:ILE:HD13	4:I:65:LEU:HD22	1.89	0.55
5:J:70:GLU:CD	5:J:73:ASN:HD22	2.15	0.55
1:A:75:ARG:HD3	1:A:75:ARG:C	2.32	0.54
1:A:83:ARG:NH1	1:A:84:TYR:CE1	2.74	0.54
2:B:23:LEU:HD12	2:B:24:ASN:N	2.22	0.54
4:D:27:ASP:O	4:D:30:SER:OG	2.14	0.54
5:E:127:PRO:HG3	5:E:139:THR:O	2.07	0.54
5:E:170:ASP:HB2	5:E:187:LEU:CD1	2.35	0.54
4:D:2:LYS:NZ	5:E:43:LEU:H	2.04	0.54
5:E:131:GLU:HG2	5:E:137:LYS:O	2.07	0.54
1:F:99:PHE:HZ	1:F:156:GLN:CD	2.15	0.54
2:G:10:TYR:CD1	2:G:10:TYR:N	2.75	0.54
1:A:231:VAL:O	1:A:243:LYS:NZ	2.40	0.54
5:E:49:SER:HB3	5:E:68:ARG:HH11	1.72	0.54
1:F:115:GLN:HG3	2:G:60:TRP:CZ2	2.42	0.54
4:I:36:TYR:OH	5:J:100:GLN:HB2	2.08	0.54
1:A:152:VAL:HG12	1:A:156:GLN:NE2	2.20	0.54
2:G:79:ALA:HB2	2:G:94:LYS:HA	1.89	0.54
1:A:157:ARG:HA	1:A:160:LEU:HD11	1.88	0.54
5:J:25:GLN:NE2	5:J:29:HIS:H	2.05	0.54
5:J:172:GLN:OE1	5:J:173:PRO:HD2	2.06	0.54
5:E:211:PHE:HD2	5:E:230:GLN:HG2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:31:HIS:CE1	2:G:60:TRP:O	2.59	0.54
4:I:185:ASN:HD22	4:I:186:ALA:N	2.05	0.54
5:J:40:GLY:C	5:J:41:LEU:HD22	2.32	0.54
3:C:4:LEU:HB3	3:C:6:PHE:HE2	1.71	0.54
1:F:45:MET:HG3	1:F:60:TRP:CZ3	2.38	0.54
4:I:122:LEU:HD11	5:J:141:VAL:HB	1.90	0.54
4:I:160:LEU:HD11	4:I:167:PHE:CE2	2.35	0.54
5:J:38:ASP:N	5:J:44:ARG:HH22	2.05	0.54
1:A:108:ARG:NH2	4:I:114:ASN:CB	2.70	0.54
2:B:56:PHE:CB	2:B:61:SER:O	2.56	0.54
4:D:23:CYS:HB2	4:D:72:VAL:CG1	2.38	0.54
4:D:133:CYS:SG	4:D:181:PHE:CE1	3.01	0.54
5:E:118:PHE:CE1	5:E:224:ARG:NH2	2.75	0.54
4:I:191:ILE:HG13	4:I:191:ILE:O	2.08	0.54
5:J:41:LEU:CB	5:J:44:ARG:CZ	2.86	0.54
5:J:49:SER:OG	5:J:68:ARG:NH1	2.40	0.54
5:J:153:GLU:HG2	5:J:212:TYR:HE2	1.73	0.54
4:D:149:ASP:HB3	4:D:152:VAL:HG11	1.90	0.54
5:E:168:CYS:O	5:E:190:ARG:CD	2.56	0.54
1:F:235:PRO:HG2	2:G:65:LEU:HD13	1.89	0.54
2:G:45:ARG:HH21	2:G:81:ARG:HH12	1.55	0.54
4:I:32:SER:HG	4:I:51:TYR:HE1	1.55	0.54
1:A:83:ARG:HG2	1:A:83:ARG:HH11	1.72	0.54
4:D:50:ILE:HD11	4:D:65:LEU:CB	2.38	0.54
4:D:187:PHE:O	4:D:190:SER:OG	2.26	0.54
4:I:177:ASN:HD22	4:I:177:ASN:C	2.16	0.54
1:A:68:LYS:CE	5:E:53:GLU:O	2.56	0.53
2:B:35:ILE:HG12	2:B:37:VAL:HG23	1.89	0.53
4:I:47:ILE:HD12	4:I:47:ILE:C	2.33	0.53
4:I:178:LYS:HG2	4:I:180:ASP:HB2	1.88	0.53
1:A:75:ARG:HH11	1:A:79:ARG:HE	1.56	0.53
4:D:89:TRP:CE2	4:D:101:GLY:HA3	2.44	0.53
1:F:191:HIS:HB3	1:F:274:TRP:CH2	2.43	0.53
4:I:80:GLN:HB2	4:I:83:ASP:OD2	2.07	0.53
3:C:3:PRO:HG2	3:C:5:THR:HG23	1.90	0.53
4:I:4:VAL:HG22	4:I:5:GLU:CD	2.33	0.53
4:I:178:LYS:HG2	4:I:180:ASP:H	1.73	0.53
5:J:27:MET:O	5:J:28:ASN:HB3	2.07	0.53
5:J:38:ASP:N	5:J:44:ARG:NH2	2.53	0.53
1:A:26:GLY:CA	1:A:33:PHE:CE1	2.89	0.53
1:A:154:GLU:HG3	4:D:51:TYR:CD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:ASN:HD22	2:B:83:ASN:C	2.15	0.53
4:D:94:GLN:HB3	4:D:97:LYS:HE2	1.88	0.53
4:D:123:ARG:NH1	5:E:239:ARG:NE	2.57	0.53
1:F:36:PHE:HB2	1:F:45:MET:HE1	1.89	0.53
1:A:215:LEU:HD12	1:A:243:LYS:CD	2.37	0.53
2:B:7:ILE:C	2:B:8:GLN:HE21	2.17	0.53
5:E:35:TYR:HA	5:E:46:ILE:CD1	2.37	0.53
5:E:117:VAL:HG12	5:E:227:PRO:HB2	1.89	0.53
1:F:99:PHE:CE2	3:H:3:PRO:HG3	2.43	0.53
1:A:123:TYR:CD2	1:A:124:ILE:HG22	2.44	0.53
1:A:176:LYS:HD2	1:A:180:GLN:NE2	2.23	0.53
2:B:39:LEU:HD12	2:B:49:VAL:HG21	1.91	0.53
2:B:41:LYS:HA	2:B:78:TYR:HD2	1.74	0.53
4:D:30:SER:C	4:D:31:GLN:HG3	2.32	0.53
4:D:62:THR:O	4:D:75:LEU:HD12	2.09	0.53
4:D:111:ASN:OD1	4:I:68:ALA:HB3	2.09	0.53
5:E:11:LEU:HD23	5:E:19:LEU:HD22	1.91	0.53
4:I:66:ASN:OD1	4:I:69:SER:N	2.31	0.53
1:A:208:PHE:CE2	1:A:241:PHE:HB2	2.44	0.53
2:B:56:PHE:CD2	2:B:62:PHE:CE2	2.97	0.53
5:E:32:MET:SD	5:E:71:LYS:O	2.66	0.53
5:E:167:VAL:HA	5:E:190:ARG:O	2.09	0.53
4:I:178:LYS:HE3	4:I:180:ASP:CB	2.37	0.53
5:E:97:SER:OG	5:E:98:HIS:N	2.33	0.53
5:E:220:TRP:CH2	5:E:222:GLN:HG3	2.43	0.53
1:F:226:GLN:O	1:F:227:ASP:HB2	2.08	0.53
5:J:47:TYR:CD1	5:J:66:VAL:HG22	2.43	0.53
5:J:132:ILE:HG23	5:J:195:ALA:CB	2.38	0.53
5:E:31:TYR:C	5:E:32:MET:HG3	2.34	0.53
5:E:37:GLN:HB2	5:E:43:LEU:HD12	1.90	0.53
1:F:98:MET:O	1:F:114:HIS:HA	2.08	0.53
4:I:159:VAL:HG12	4:I:168:LYS:HZ1	1.72	0.53
5:J:64:TYR:CD1	5:J:78:LEU:HD13	2.44	0.53
1:A:242:GLN:OE1	2:B:10:TYR:CE2	2.61	0.53
4:D:88:LEU:HD23	4:D:88:LEU:H	1.73	0.53
1:F:70:HIS:ND1	3:H:2:PHE:HZ	2.01	0.53
5:J:205:PHE:HE2	5:J:237:TRP:C	2.16	0.52
4:D:114:ASN:CB	1:F:108:ARG:HH22	2.20	0.52
4:D:182:ALA:HB3	4:D:185:ASN:ND2	2.25	0.52
1:F:35:ARG:HD2	1:F:36:PHE:N	2.24	0.52
1:F:96:GLN:NE2	2:G:56:PHE:CD2	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:9:CYS:SG	5:J:30:GLU:OE1	2.67	0.52
4:I:46:LEU:HD11	5:J:99:GLU:HG2	1.92	0.52
5:J:25:GLN:NE2	5:J:29:HIS:HB2	2.25	0.52
1:A:8:PHE:HB2	1:A:25:VAL:HG22	1.92	0.52
1:A:15:PRO:HG2	1:A:91:GLY:O	2.09	0.52
4:D:72:VAL:O	4:D:72:VAL:HG13	2.08	0.52
4:D:94:GLN:HB2	4:D:99:ILE:HD11	1.92	0.52
4:D:123:ARG:CZ	5:E:239:ARG:CZ	2.87	0.52
1:F:231:VAL:HG22	1:F:244:TRP:O	2.09	0.52
4:I:88:LEU:N	4:I:88:LEU:CD2	2.63	0.52
4:I:120:TYR:CE1	5:J:131:GLU:CA	2.90	0.52
4:I:132:VAL:HG23	5:J:125:PHE:CE1	2.44	0.52
1:A:72:GLN:HB2	5:E:51:ASN:CG	2.35	0.52
1:A:130:LEU:CB	1:A:157:ARG:HG3	2.39	0.52
2:B:22:PHE:C	2:B:70:PHE:HE1	2.17	0.52
5:E:132:ILE:HD12	5:E:132:ILE:H	1.73	0.52
4:I:114:ASN:C	4:I:114:ASN:HD22	2.18	0.52
5:J:41:LEU:HB3	5:J:44:ARG:NH1	2.24	0.52
1:A:55:GLU:CB	1:A:59:TYR:CD2	2.93	0.52
4:D:153:TYR:HB2	4:D:175:TRP:CE2	2.45	0.52
1:F:72:GLN:OE1	1:F:72:GLN:O	2.28	0.52
1:F:155:GLN:O	4:I:31:GLN:NE2	2.42	0.52
1:F:190:THR:O	1:F:201:LEU:HD23	2.09	0.52
5:J:167:VAL:HA	5:J:190:ARG:O	2.09	0.52
1:A:133:TRP:HZ2	1:A:152:VAL:HB	1.74	0.52
3:C:6:PHE:CD1	5:E:31:TYR:HB2	2.45	0.52
5:E:37:GLN:CB	5:E:43:LEU:HD12	2.39	0.52
2:G:96:ASP:HB3	2:G:99:MET:HA	1.91	0.52
4:D:69:SER:O	4:D:70:GLN:HB2	2.10	0.52
5:E:135:THR:HG22	5:E:137:LYS:CG	2.35	0.52
5:E:135:THR:HG21	5:E:192:ARG:HH12	1.74	0.52
2:G:1:ILE:HD12	2:G:1:ILE:O	2.10	0.52
4:I:35:TRP:HB2	4:I:48:MET:HB3	1.91	0.52
4:I:160:LEU:C	4:I:168:LYS:HZ3	2.18	0.52
1:A:123:TYR:HD2	1:A:124:ILE:HG22	1.75	0.52
1:A:130:LEU:HB3	1:A:157:ARG:HG3	1.91	0.52
4:D:39:TYR:OH	4:D:82:SER:O	2.18	0.52
5:J:76:LEU:C	5:J:77:ILE:HD12	2.34	0.52
5:J:83:PRO:HA	5:J:110:VAL:HB	1.92	0.52
1:A:160:LEU:O	1:A:165:VAL:HG22	2.09	0.52
4:D:80:GLN:C	4:D:108:VAL:HG11	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:37:GLN:HG2	5:E:42:GLY:O	2.10	0.52
1:F:95:LEU:HD12	1:F:117:ALA:O	2.10	0.52
4:I:53:ASN:ND2	4:I:65:LEU:O	2.43	0.52
5:J:41:LEU:CB	5:J:44:ARG:NH1	2.72	0.52
5:J:206:ARG:HB3	5:J:206:ARG:CZ	2.39	0.52
2:B:57:SER:N	2:B:63:TYR:CE2	2.78	0.52
4:D:53:ASN:HD21	4:D:67:LYS:HB2	1.74	0.52
2:G:13:HIS:N	2:G:21:ASN:HD21	2.08	0.52
2:G:19:LYS:O	2:G:72:PRO:HD2	2.09	0.52
4:D:96:GLY:CA	5:E:50:MET:HE1	2.35	0.51
5:E:32:MET:HE1	5:E:71:LYS:O	2.11	0.51
4:I:160:LEU:HD11	4:I:162:MET:HE3	1.90	0.51
5:J:70:GLU:HG3	5:J:73:ASN:H	1.74	0.51
1:A:209:TYR:CD1	1:A:210:PRO:HA	2.44	0.51
1:A:242:GLN:NE2	2:B:10:TYR:CD2	2.78	0.51
4:D:3:GLU:HG3	4:D:4:VAL:HG12	1.91	0.51
5:E:161:LYS:HB2	5:E:161:LYS:HZ2	1.75	0.51
4:I:33:PHE:O	4:I:50:ILE:HG23	2.10	0.51
4:I:149:ASP:O	4:I:152:VAL:CG1	2.58	0.51
1:F:104:GLY:N	1:F:110:LEU:HD23	2.24	0.51
4:I:124:ASP:HA	5:J:125:PHE:CE1	2.45	0.51
5:E:37:GLN:HG3	5:E:43:LEU:HD12	1.90	0.51
1:F:5:MET:SD	1:F:171:TYR:HE2	2.33	0.51
1:F:159:TYR:CZ	3:H:3:PRO:HB3	2.46	0.51
1:F:162:GLY:O	1:F:163:THR:C	2.53	0.51
5:E:158:VAL:CG2	5:E:163:VAL:HG21	2.38	0.51
5:J:19:LEU:H	5:J:19:LEU:HD12	1.76	0.51
5:J:220:TRP:HH2	5:J:224:ARG:NH2	2.08	0.51
4:D:157:LYS:H	4:D:157:LYS:CD	2.23	0.51
5:E:136:GLN:OE1	5:E:136:GLN:HA	2.10	0.51
5:E:153:GLU:HB2	5:E:210:GLN:HB3	1.92	0.51
5:J:25:GLN:OE1	5:J:27:MET:N	2.43	0.51
5:J:131:GLU:HG2	5:J:137:LYS:O	2.10	0.51
1:F:261:VAL:CG2	1:F:272:LEU:HD11	2.41	0.51
4:I:14:PRO:HA	4:I:109:LYS:HB2	1.93	0.51
5:J:49:SER:CB	5:J:68:ARG:HH11	2.24	0.51
5:J:215:SER:C	5:J:217:ASN:H	2.18	0.51
4:D:131:SER:HB2	4:D:181:PHE:HE2	1.76	0.51
1:F:70:HIS:HB2	3:H:2:PHE:HE2	1.76	0.51
1:F:191:HIS:CE1	1:F:193:PRO:HG3	2.45	0.51
2:G:4:THR:OG1	2:G:5:PRO:HD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LYS:HG3	5:E:50:MET:CE	2.40	0.51
5:E:12:ILE:HD11	5:E:213:GLY:HA2	1.93	0.51
5:E:200:ASN:O	5:E:238:GLY:HA3	2.11	0.51
5:J:206:ARG:HH11	5:J:206:ARG:HG2	1.75	0.51
1:A:99:PHE:HD1	1:A:114:HIS:CD2	2.28	0.50
5:E:47:TYR:CZ	5:E:57:LYS:HB3	2.45	0.50
5:E:62:GLU:OE1	5:E:62:GLU:HA	2.11	0.50
5:E:187:LEU:HG	5:E:188:SER:N	2.26	0.50
2:G:23:LEU:HG	2:G:70:PHE:CZ	2.46	0.50
4:I:173:VAL:HG12	4:I:175:TRP:CE3	2.45	0.50
1:A:22:PHE:CE1	1:A:71:SER:HA	2.46	0.50
5:E:4:VAL:HG11	5:E:91:CYS:O	2.11	0.50
5:E:78:LEU:N	5:E:78:LEU:CD1	2.73	0.50
1:F:27:TYR:CE2	1:F:32:GLN:N	2.79	0.50
1:F:80:ILE:HG23	1:F:83:ARG:NH2	2.26	0.50
2:G:21:ASN:CG	2:G:22:PHE:N	2.69	0.50
4:I:77:ARG:O	4:I:78:ASP:HB3	2.11	0.50
5:J:36:ARG:HE	5:J:87:SER:CB	2.25	0.50
5:J:77:ILE:N	5:J:77:ILE:CD1	2.71	0.50
5:J:144:ALA:O	5:J:147:PHE:HE2	1.95	0.50
4:D:37:ARG:HB2	4:D:47:ILE:HD13	1.93	0.50
4:I:50:ILE:O	4:I:50:ILE:CG1	2.59	0.50
5:J:23:CYS:HB2	5:J:34:TRP:CZ2	2.46	0.50
5:J:47:TYR:CD1	5:J:66:VAL:CG2	2.95	0.50
4:D:94:GLN:HB3	4:D:97:LYS:HZ3	1.77	0.50
5:E:46:ILE:HG23	5:E:60:VAL:O	2.11	0.50
2:G:40:LEU:HD21	2:G:81:ARG:HE	1.76	0.50
1:A:75:ARG:CD	1:A:79:ARG:HD2	2.42	0.50
2:B:83:ASN:C	2:B:83:ASN:ND2	2.68	0.50
4:D:147:SER:CB	4:D:152:VAL:HG13	2.41	0.50
5:E:96:ALA:O	5:E:97:SER:HB3	2.10	0.50
5:E:208:GLN:HG2	5:E:233:SER:OG	2.10	0.50
1:F:7:TYR:HE2	3:H:2:PHE:CA	2.25	0.50
1:F:10:THR:HB	1:F:23:ILE:CG2	2.31	0.50
4:I:65:LEU:HD21	4:I:67:LYS:HG3	1.93	0.50
4:I:176:SER:HB3	4:I:181:PHE:CD2	2.46	0.50
1:A:190:THR:HG21	2:B:98:ASP:CG	2.36	0.50
5:E:77:ILE:HD12	5:E:77:ILE:H	1.77	0.50
5:E:211:PHE:HB3	5:E:230:GLN:O	2.11	0.50
2:G:40:LEU:HD21	2:G:81:ARG:NE	2.27	0.50
2:B:84:HIS:HB3	2:B:86:THR:HG23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:185:ASN:CA	4:D:188:ASN:ND2	2.75	0.50
1:F:240:THR:C	1:F:241:PHE:CD1	2.90	0.50
5:J:128:SER:OG	5:J:130:ALA:HB3	2.12	0.50
5:J:139:THR:OG1	5:J:192:ARG:HB2	2.12	0.50
4:D:39:TYR:CD1	4:D:85:ALA:HB2	2.46	0.50
5:E:79:GLU:C	5:E:81:PRO:HD3	2.37	0.50
1:F:220:ASP:OD2	1:F:256:ARG:HD3	2.11	0.50
4:I:30:SER:O	4:I:67:LYS:NZ	2.41	0.50
4:I:33:PHE:H	4:I:50:ILE:HG13	1.76	0.50
5:J:97:SER:C	5:J:98:HIS:ND1	2.70	0.50
5:J:173:PRO:CA	5:J:187:LEU:HD13	2.36	0.50
1:A:45:MET:SD	1:A:63:GLU:HB3	2.52	0.50
4:D:139:ASP:C	4:D:141:GLN:H	2.20	0.50
4:I:88:LEU:HB3	4:I:103:GLY:CA	2.41	0.50
4:I:160:LEU:C	4:I:168:LYS:NZ	2.70	0.50
5:J:164:HIS:O	5:J:167:VAL:HG13	2.12	0.50
5:J:200:ASN:HB3	5:J:203:ASN:OD1	2.12	0.50
1:A:68:LYS:HD3	5:E:54:VAL:HA	1.93	0.49
2:B:79:ALA:HB2	2:B:94:LYS:HA	1.94	0.49
3:C:2:PHE:CG	3:C:3:PRO:HD2	2.46	0.49
4:I:152:VAL:O	4:I:152:VAL:HG13	2.11	0.49
5:J:176:GLU:O	5:J:178:PRO:HD3	2.12	0.49
1:A:3:HIS:HB3	1:A:29:ASP:OD2	2.12	0.49
1:A:152:VAL:HG13	1:A:156:GLN:HE21	1.77	0.49
1:A:156:GLN:NE2	3:C:8:TRP:CH2	2.79	0.49
1:A:159:TYR:CE2	1:A:163:THR:HB	2.46	0.49
5:E:132:ILE:CG2	5:E:195:ALA:HB1	2.40	0.49
5:E:140:LEU:HD12	5:E:140:LEU:N	2.27	0.49
2:G:23:LEU:HD21	2:G:95:TRP:CE3	2.47	0.49
5:J:36:ARG:HE	5:J:87:SER:HB2	1.77	0.49
1:A:2:SER:O	1:A:3:HIS:ND1	2.45	0.49
2:B:41:LYS:HG3	2:B:78:TYR:HE2	1.77	0.49
4:D:12:SER:HB2	4:D:109:LYS:CE	2.41	0.49
1:F:147:TRP:N	1:F:147:TRP:CD1	2.74	0.49
1:A:130:LEU:HD13	1:A:160:LEU:HD12	1.92	0.49
5:E:157:TRP:CE3	5:E:162:GLU:N	2.80	0.49
5:J:156:TRP:NE1	5:J:189:SER:OG	2.44	0.49
4:I:102:GLN:C	4:I:102:GLN:OE1	2.56	0.49
1:A:9:SER:OG	1:A:97:MET:HB3	2.12	0.49
1:A:104:GLY:H	1:A:110:LEU:HD13	1.75	0.49
1:A:189:MET:HE1	1:A:217:TRP:HH2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:215:SER:C	5:E:217:ASN:H	2.20	0.49
4:I:136:THR:CG2	5:J:192:ARG:HH22	2.25	0.49
4:D:133:CYS:SG	4:D:181:PHE:CZ	3.06	0.49
4:D:139:ASP:O	4:D:142:THR:OG1	2.30	0.49
4:D:149:ASP:O	4:D:152:VAL:HG12	2.13	0.49
5:E:36:ARG:NE	5:E:38:ASP:OD2	2.46	0.49
5:E:72:ARG:HB2	5:E:73:ASN:HD22	1.76	0.49
5:E:132:ILE:HD12	5:E:132:ILE:N	2.27	0.49
1:F:143:THR:HG23	1:F:146:LYS:HD3	1.93	0.49
4:I:87:TYR:C	4:I:88:LEU:HD23	2.37	0.49
4:I:134:LEU:HD21	5:J:139:THR:HG21	1.94	0.49
4:I:161:ASP:HB2	4:I:168:LYS:NZ	2.28	0.49
5:J:90:PHE:CE1	5:J:105:GLY:HA3	2.48	0.49
4:D:12:SER:CA	4:D:109:LYS:HZ3	2.24	0.49
4:D:141:GLN:OE1	4:D:141:GLN:HA	2.13	0.49
5:J:147:PHE:CZ	5:J:186:ALA:HA	2.47	0.49
1:A:55:GLU:OE2	1:A:170:ARG:NH2	2.46	0.49
1:A:111:ARG:CZ	1:A:128:GLU:HA	2.43	0.49
2:B:92:ILE:HD12	2:B:92:ILE:N	2.28	0.49
1:F:51:TRP:HE1	1:F:179:LEU:HD21	1.78	0.49
4:I:91:THR:O	4:I:91:THR:HG23	2.13	0.49
4:I:171:SER:OG	5:J:190:ARG:NH1	2.46	0.49
5:J:97:SER:O	5:J:98:HIS:ND1	2.46	0.49
4:D:89:TRP:CZ3	4:D:91:THR:HG22	2.48	0.49
5:E:32:MET:SD	5:E:68:ARG:NH2	2.85	0.49
5:E:107:ARG:NH1	5:E:151:HIS:NE2	2.60	0.49
1:F:35:ARG:HG2	1:F:35:ARG:NH1	2.26	0.49
1:F:143:THR:HG23	3:H:10:PHE:HA	1.95	0.49
1:F:272:LEU:HD12	1:F:272:LEU:H	1.77	0.49
3:H:4:LEU:HD21	4:I:96:GLY:HA2	1.95	0.49
1:A:26:GLY:O	1:A:33:PHE:CD1	2.66	0.48
4:D:192:ILE:HG13	4:D:193:PRO:N	2.28	0.48
5:E:51:ASN:O	5:E:68:ARG:HG2	2.13	0.48
2:G:54:LEU:HD12	2:G:55:SER:N	2.27	0.48
5:J:158:VAL:O	5:J:158:VAL:HG12	2.13	0.48
5:E:127:PRO:HG3	5:E:139:THR:C	2.38	0.48
1:F:106:ASP:CG	1:F:108:ARG:HB2	2.38	0.48
2:G:12:ARG:HG2	2:G:13:HIS:H	1.78	0.48
4:I:48:MET:HE1	4:I:58:ASP:CB	2.40	0.48
4:I:147:SER:OG	4:I:152:VAL:O	2.21	0.48
1:A:106:ASP:OD1	1:A:108:ARG:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:TRP:CE2	1:F:179:LEU:HD21	2.48	0.48
1:F:51:TRP:HE3	1:F:51:TRP:C	2.22	0.48
1:F:202:ARG:HD3	1:F:244:TRP:NE1	2.28	0.48
4:I:47:ILE:HD12	4:I:48:MET:CB	2.43	0.48
4:I:122:LEU:HD11	5:J:141:VAL:CG2	2.42	0.48
5:J:78:LEU:HD11	5:J:85:GLN:NE2	2.28	0.48
5:E:7:ASN:OD1	5:E:8:PRO:HA	2.13	0.48
4:D:36:TYR:CD1	4:D:46:LEU:HA	2.49	0.48
5:E:143:LEU:CD1	5:E:188:SER:HB3	2.43	0.48
2:G:10:TYR:O	2:G:24:ASN:ND2	2.46	0.48
2:G:81:ARG:CA	2:G:92:ILE:HG12	2.41	0.48
4:I:185:ASN:HD22	4:I:185:ASN:C	2.20	0.48
1:A:35:ARG:NH1	1:A:48:ARG:CD	2.77	0.48
1:A:55:GLU:HB2	1:A:59:TYR:CD2	2.49	0.48
4:D:134:LEU:HD11	4:D:171:SER:HB2	1.96	0.48
4:D:192:ILE:HD11	4:D:196:THR:HB	1.96	0.48
1:F:242:GLN:O	1:F:243:LYS:HB2	2.14	0.48
3:H:8:TRP:N	3:H:8:TRP:CD1	2.78	0.48
4:I:46:LEU:CD2	5:J:99:GLU:HB3	2.40	0.48
4:I:167:PHE:CZ	4:I:169:SER:HB3	2.49	0.48
1:F:108:ARG:HG3	1:F:108:ARG:NH1	2.27	0.48
1:F:213:ILE:HG13	1:F:263:HIS:HB2	1.94	0.48
2:G:30:PHE:O	2:G:62:PHE:HD1	1.96	0.48
4:I:36:TYR:CE1	5:J:102:PHE:CE2	3.02	0.48
4:I:77:ARG:HG3	4:I:77:ARG:NH1	2.28	0.48
4:I:162:MET:HG3	5:J:166:GLY:HA2	1.96	0.48
5:J:177:GLN:HB2	5:J:183:SER:HB2	1.95	0.48
1:A:73:THR:HG23	5:E:30:GLU:OE1	2.12	0.48
2:G:3:ARG:HD2	2:G:29:GLY:O	2.13	0.48
5:J:150:ASP:C	5:J:151:HIS:HD2	2.22	0.48
5:E:152:VAL:HA	5:E:210:GLN:O	2.14	0.48
1:F:231:VAL:CG2	1:F:244:TRP:H	2.27	0.48
4:D:192:ILE:HD11	4:D:196:THR:HG21	1.96	0.48
5:E:19:LEU:HD11	5:E:78:LEU:HD13	1.92	0.48
5:E:237:TRP:CD1	5:E:237:TRP:N	2.82	0.48
5:J:35:TYR:CD1	5:J:45:GLN:HA	2.48	0.48
5:J:125:PHE:O	5:J:140:LEU:HD23	2.14	0.48
5:J:205:PHE:CE2	5:J:238:GLY:N	2.75	0.48
1:A:33:PHE:CD1	1:A:33:PHE:C	2.91	0.47
1:A:242:GLN:O	1:A:243:LYS:HB2	2.13	0.47
5:E:92:ALA:HB1	5:E:100:GLN:CG	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:133:TRP:HB2	1:F:144:LYS:HG3	1.95	0.47
2:B:26:TYR:HD1	2:B:64:LEU:O	1.97	0.47
4:D:192:ILE:CD1	4:D:196:THR:HG21	2.44	0.47
2:B:41:LYS:HA	2:B:78:TYR:CD2	2.49	0.47
2:B:55:SER:OG	2:B:63:TYR:CE1	2.62	0.47
4:D:164:SER:OG	4:D:165:MET:HG2	2.15	0.47
5:E:25:GLN:NE2	5:E:32:MET:HE3	2.29	0.47
5:E:49:SER:HB2	5:E:74:PHE:CE1	2.49	0.47
1:F:15:PRO:HG2	1:F:91:GLY:O	2.14	0.47
1:F:51:TRP:CD1	1:F:175:GLY:CA	2.97	0.47
4:I:92:TYR:OH	5:J:98:HIS:O	2.32	0.47
4:I:99:ILE:HD12	4:I:99:ILE:N	2.30	0.47
4:I:132:VAL:HG23	5:J:125:PHE:CD1	2.49	0.47
5:J:162:GLU:CG	5:J:164:HIS:CE1	2.98	0.47
1:A:111:ARG:HD3	1:A:128:GLU:CD	2.39	0.47
1:A:139:ALA:HA	1:A:142:ILE:CD1	2.44	0.47
4:D:32:SER:C	4:D:33:PHE:HD2	2.22	0.47
5:E:84:ASN:N	5:E:84:ASN:HD22	2.12	0.47
1:F:33:PHE:C	1:F:48:ARG:HB2	2.40	0.47
2:G:16:GLU:OE2	2:G:19:LYS:NZ	2.47	0.47
5:J:218:ASP:OD1	5:J:218:ASP:N	2.47	0.47
1:A:194:ILE:HD11	1:A:198:GLU:HB3	1.96	0.47
1:A:209:TYR:CD1	1:A:241:PHE:HE1	2.27	0.47
1:A:229:GLU:O	1:A:230:LEU:HD12	2.14	0.47
4:D:48:MET:CE	4:D:63:ALA:N	2.77	0.47
4:D:94:GLN:CB	4:D:97:LYS:CE	2.89	0.47
4:D:114:ASN:OD1	1:F:108:ARG:NH1	2.47	0.47
5:E:32:MET:CE	5:E:71:LYS:O	2.62	0.47
1:F:202:ARG:NH1	1:F:244:TRP:CZ3	2.82	0.47
2:G:13:HIS:HB2	2:G:21:ASN:HD21	1.76	0.47
1:A:87:GLN:NE2	1:A:118:TYR:OH	2.47	0.47
1:A:200:THR:HG21	1:A:202:ARG:HH22	1.79	0.47
4:D:35:TRP:O	4:D:46:LEU:HD12	2.15	0.47
4:D:81:PRO:HA	4:D:108:VAL:CG1	2.44	0.47
5:E:36:ARG:HB2	5:E:89:TYR:CE1	2.49	0.47
1:F:99:PHE:HZ	1:F:156:GLN:OE1	1.98	0.47
1:F:137:ASP:C	1:F:137:ASP:OD1	2.56	0.47
1:F:168:LEU:HD11	1:F:172:LEU:HD21	1.96	0.47
3:H:2:PHE:CD1	3:H:3:PRO:HD2	2.50	0.47
5:J:79:GLU:C	5:J:81:PRO:HD3	2.40	0.47
5:J:86:THR:HA	5:J:108:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:204:HIS:NE2	5:J:235:GLU:HB2	2.30	0.47
1:A:26:GLY:CA	1:A:33:PHE:HE1	2.25	0.47
1:A:185:PRO:HG3	1:A:213:ILE:HD12	1.95	0.47
1:A:258:THR:CG2	1:A:271:THR:CG2	2.93	0.47
4:D:13:VAL:O	4:D:108:VAL:HA	2.15	0.47
4:D:123:ARG:NH1	5:E:239:ARG:CZ	2.78	0.47
5:E:86:THR:CG2	5:E:109:THR:HA	2.29	0.47
5:E:177:GLN:O	5:E:183:SER:HB2	2.14	0.47
1:F:51:TRP:CZ2	1:F:179:LEU:CD2	2.98	0.47
1:F:150:ALA:HB3	1:F:152:VAL:HG23	1.95	0.47
1:F:233:THR:CG2	1:F:243:LYS:HD2	2.44	0.47
4:I:50:ILE:HD12	4:I:51:TYR:CA	2.44	0.47
4:I:110:PRO:HD2	4:I:140:SER:OG	2.14	0.47
4:I:135:PHE:CE1	4:I:138:PHE:HB3	2.49	0.47
4:I:162:MET:HG3	5:J:166:GLY:CA	2.45	0.47
5:J:18:LYS:HB2	5:J:79:GLU:O	2.15	0.47
5:J:49:SER:HB3	5:J:68:ARG:NH1	2.29	0.47
5:J:97:SER:OG	5:J:98:HIS:N	2.47	0.47
2:B:12:ARG:H	2:B:21:ASN:HD21	1.63	0.47
4:D:12:SER:HA	4:D:109:LYS:NZ	2.27	0.47
4:D:162:MET:CE	5:E:192:ARG:HG2	2.45	0.47
5:E:19:LEU:HD11	5:E:78:LEU:CD2	2.42	0.47
5:E:199:GLN:HA	5:E:239:ARG:O	2.14	0.47
1:F:33:PHE:CD2	1:F:34:VAL:HG22	2.50	0.47
4:I:4:VAL:HG13	4:I:5:GLU:HG2	1.96	0.47
4:I:135:PHE:CZ	4:I:138:PHE:HB3	2.50	0.47
1:A:49:ALA:HB1	1:A:51:TRP:CE2	2.50	0.47
1:A:98:MET:SD	1:A:98:MET:C	2.98	0.47
1:A:130:LEU:HB3	1:A:157:ARG:CG	2.45	0.47
4:D:154:ILE:HD11	4:D:187:PHE:HD1	1.77	0.47
5:E:11:LEU:O	5:E:108:LEU:HD12	2.15	0.47
4:D:25:TYR:CD2	4:D:33:PHE:CE1	3.03	0.47
4:D:36:TYR:CE1	4:D:46:LEU:HB2	2.50	0.47
1:F:4:SER:OG	1:F:6:ARG:NE	2.47	0.47
1:F:202:ARG:NH1	1:F:202:ARG:HG3	2.27	0.47
1:F:203:CYS:SG	1:F:272:LEU:HD22	2.55	0.47
2:G:12:ARG:CG	2:G:13:HIS:N	2.78	0.47
4:I:6:GLN:HE21	4:I:102:GLN:HB2	1.77	0.47
4:I:185:ASN:ND2	4:I:185:ASN:C	2.70	0.47
5:J:9:ARG:HH11	5:J:9:ARG:CG	2.28	0.47
1:A:83:ARG:HH12	1:A:84:TYR:HE1	1.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:GLU:HB3	2:B:67:TYR:CE1	2.50	0.46
5:E:128:SER:O	5:E:132:ILE:CD1	2.63	0.46
5:J:86:THR:HA	5:J:108:LEU:CD1	2.45	0.46
1:A:159:TYR:CD1	4:D:31:GLN:NE2	2.83	0.46
1:A:162:GLY:O	1:A:163:THR:C	2.57	0.46
1:A:234:ARG:NH2	2:B:10:TYR:CB	2.78	0.46
2:B:22:PHE:C	2:B:70:PHE:CE1	2.93	0.46
2:B:23:LEU:O	2:B:67:TYR:HA	2.15	0.46
4:D:2:LYS:HZ1	5:E:42:GLY:HA3	1.81	0.46
1:F:51:TRP:NE1	1:F:179:LEU:HD21	2.29	0.46
5:J:176:GLU:C	5:J:178:PRO:HD3	2.39	0.46
1:A:13:SER:HA	1:A:20:PRO:HG3	1.97	0.46
1:A:129:ASP:OD2	1:A:131:ARG:HB2	2.15	0.46
2:B:8:GLN:O	2:B:25:CYS:HA	2.16	0.46
1:F:244:TRP:HE3	1:F:244:TRP:O	1.97	0.46
5:J:25:GLN:OE1	5:J:28:ASN:N	2.49	0.46
1:A:232:GLU:CD	2:B:6:LYS:HE2	2.40	0.46
4:D:34:PHE:CD2	4:D:34:PHE:N	2.83	0.46
4:D:48:MET:HG2	4:D:63:ALA:HB2	1.97	0.46
1:F:7:TYR:CD2	3:H:2:PHE:HD1	2.33	0.46
4:I:9:GLY:HA2	4:I:10:PRO:HD3	1.68	0.46
4:I:92:TYR:CE2	5:J:98:HIS:HB3	2.51	0.46
4:I:118:ALA:HB2	4:I:197:PHE:HB3	1.97	0.46
1:A:244:TRP:CE3	1:A:244:TRP:C	2.93	0.46
2:B:7:ILE:C	2:B:8:GLN:NE2	2.73	0.46
4:D:23:CYS:HB2	4:D:72:VAL:HG12	1.98	0.46
4:D:36:TYR:HD1	4:D:46:LEU:N	2.14	0.46
5:E:31:TYR:CD2	5:E:100:GLN:NE2	2.84	0.46
5:E:115:LYS:NZ	5:E:118:PHE:HZ	2.13	0.46
5:E:135:THR:O	5:E:136:GLN:HB2	2.15	0.46
1:F:51:TRP:HZ2	1:F:179:LEU:CD2	2.26	0.46
1:F:158:ALA:HB1	4:I:31:GLN:HB2	1.98	0.46
5:J:154:LEU:CD2	5:J:209:VAL:HG22	2.46	0.46
1:A:33:PHE:CG	1:A:34:VAL:HG13	2.50	0.46
4:D:89:TRP:CZ3	4:D:91:THR:CG2	2.94	0.46
5:E:6:GLN:NE2	5:E:34:TRP:CZ3	2.84	0.46
5:E:32:MET:HG2	5:E:93:SER:OG	2.15	0.46
5:E:52:VAL:O	5:E:54:VAL:HG23	2.16	0.46
4:I:123:ARG:CB	5:J:126:GLU:HB2	2.41	0.46
1:A:55:GLU:O	1:A:60:TRP:HZ2	1.98	0.46
2:B:52:SER:O	2:B:64:LEU:HD21	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:25:GLN:HE21	5:E:25:GLN:HB3	1.53	0.46
5:E:107:ARG:CZ	5:E:150:ASP:OD1	2.64	0.46
1:F:122:ASP:O	1:F:136:ALA:CB	2.64	0.46
2:G:56:PHE:CB	2:G:61:SER:O	2.58	0.46
5:J:19:LEU:HD12	5:J:19:LEU:N	2.30	0.46
5:J:60:VAL:HG23	5:J:60:VAL:O	2.16	0.46
1:A:4:SER:N	1:A:29:ASP:OD1	2.49	0.46
2:B:23:LEU:HD12	2:B:23:LEU:C	2.41	0.46
4:D:14:PRO:HB2	4:I:71:TYR:CE1	2.48	0.46
4:D:133:CYS:SG	4:D:181:PHE:HE1	2.39	0.46
5:E:32:MET:HB2	5:E:68:ARG:NH1	2.31	0.46
1:F:51:TRP:CD1	1:F:175:GLY:HA3	2.51	0.46
1:F:76:GLU:O	1:F:80:ILE:HG13	2.15	0.46
4:I:192:ILE:HG13	4:I:193:PRO:O	2.16	0.46
5:J:49:SER:CB	5:J:68:ARG:NH1	2.79	0.46
4:D:114:ASN:HB3	1:F:108:ARG:NH1	2.23	0.46
4:D:187:PHE:HB3	4:D:190:SER:OG	2.16	0.46
5:E:53:GLU:OE1	5:E:69:LYS:HA	2.16	0.46
5:E:117:VAL:HG12	5:E:227:PRO:CB	2.46	0.46
1:F:13:SER:O	1:F:92:SER:HB2	2.16	0.46
3:H:6:PHE:CZ	5:J:98:HIS:CD2	3.02	0.46
4:I:28:ARG:HA	4:I:70:GLN:NE2	2.30	0.46
5:J:124:VAL:HG23	5:J:234:ALA:HB3	1.98	0.46
4:D:156:ASP:OD2	4:D:157:LYS:HD3	2.15	0.46
1:F:93:HIS:HB3	1:F:118:TYR:CE1	2.51	0.46
1:F:120:GLY:CA	2:G:31:HIS:NE2	2.79	0.46
4:D:88:LEU:N	4:D:88:LEU:CD2	2.78	0.45
4:D:189:ASN:HD22	4:D:189:ASN:HA	1.66	0.45
5:E:36:ARG:NH2	5:E:87:SER:HB2	2.23	0.45
1:A:87:GLN:CD	1:A:118:TYR:HH	2.22	0.45
1:F:35:ARG:O	1:F:45:MET:SD	2.74	0.45
4:I:69:SER:O	4:I:70:GLN:HB2	2.16	0.45
1:A:152:VAL:HG13	1:A:156:GLN:NE2	2.30	0.45
4:D:192:ILE:HD11	4:D:196:THR:CB	2.46	0.45
1:F:98:MET:HB3	1:F:115:GLN:HG2	1.98	0.45
4:I:159:VAL:N	5:J:168:CYS:SG	2.88	0.45
5:J:150:ASP:C	5:J:151:HIS:CD2	2.95	0.45
5:J:154:LEU:HD22	5:J:155:SER:H	1.81	0.45
5:J:199:GLN:HA	5:J:239:ARG:O	2.15	0.45
1:A:185:PRO:HG3	1:A:213:ILE:CD1	2.46	0.45
1:A:219:ARG:HG3	1:A:257:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:PRO:O	2:B:7:ILE:HD12	2.17	0.45
2:G:37:VAL:HG13	2:G:80:CYS:SG	2.56	0.45
4:I:114:ASN:C	4:I:114:ASN:ND2	2.74	0.45
4:I:135:PHE:HB2	4:I:187:PHE:CE2	2.51	0.45
1:A:33:PHE:C	1:A:48:ARG:HB2	2.42	0.45
1:A:51:TRP:CZ3	1:A:52:ILE:HD13	2.52	0.45
1:A:53:GLU:HA	1:A:60:TRP:HH2	1.81	0.45
3:C:3:PRO:HG2	3:C:5:THR:CG2	2.46	0.45
1:F:50:PRO:HA	1:F:53:GLU:OE1	2.15	0.45
2:G:23:LEU:O	2:G:67:TYR:HA	2.17	0.45
2:G:62:PHE:CD1	2:G:62:PHE:N	2.84	0.45
2:G:81:ARG:CB	2:G:92:ILE:HG12	2.47	0.45
5:J:82:SER:HB2	5:J:84:ASN:OD1	2.16	0.45
5:J:154:LEU:HD22	5:J:155:SER:N	2.31	0.45
2:B:23:LEU:O	2:B:23:LEU:HG	2.17	0.45
4:D:91:THR:O	4:D:91:THR:CG2	2.63	0.45
5:E:72:ARG:H	5:E:72:ARG:HD2	1.81	0.45
1:F:43:GLN:HE21	1:F:43:GLN:CA	2.28	0.45
1:F:202:ARG:HD2	1:F:204:TRP:CE2	2.51	0.45
2:G:40:LEU:HD11	2:G:81:ARG:HB2	1.99	0.45
2:G:45:ARG:HB2	2:G:81:ARG:NH2	2.30	0.45
5:E:49:SER:CB	5:E:74:PHE:CE1	3.00	0.45
5:E:108:LEU:HD12	5:E:109:THR:H	1.82	0.45
1:F:99:PHE:CE2	1:F:159:TYR:CE2	3.03	0.45
1:F:117:ALA:CB	2:G:60:TRP:CD2	2.99	0.45
1:F:256:ARG:HH11	1:F:256:ARG:HG2	1.82	0.45
4:I:33:PHE:HB2	4:I:50:ILE:HG12	1.99	0.45
5:J:210:GLN:HE21	5:J:231:ILE:HG12	1.81	0.45
1:A:145:ARG:O	1:A:148:GLU:HB2	2.17	0.45
5:E:88:LEU:CD1	5:E:107:ARG:HG2	2.41	0.45
1:F:159:TYR:OH	3:H:1:ARG:O	2.31	0.45
2:G:95:TRP:CD1	2:G:95:TRP:C	2.92	0.45
5:J:11:LEU:HD12	5:J:12:ILE:H	1.80	0.45
1:A:43:GLN:NE2	1:A:43:GLN:HA	2.32	0.45
1:A:188:HIS:CE1	1:A:204:TRP:CB	3.00	0.45
3:C:7:GLY:N	5:E:30:GLU:HG3	2.25	0.45
5:E:124:VAL:HG23	5:E:234:ALA:CB	2.46	0.45
5:J:20:THR:OG1	5:J:77:ILE:HG13	2.17	0.45
5:J:52:VAL:HG13	5:J:68:ARG:O	2.17	0.45
5:J:210:GLN:NE2	5:J:231:ILE:CG1	2.80	0.45
4:D:89:TRP:HZ3	4:D:91:THR:HG22	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:154:ILE:O	4:D:154:ILE:HG22	2.17	0.45
1:F:99:PHE:CE1	1:F:114:HIS:CG	3.04	0.45
1:A:60:TRP:CD1	1:A:60:TRP:H	2.33	0.44
1:A:200:THR:HG21	1:A:202:ARG:CZ	2.47	0.44
4:D:101:GLY:O	4:D:102:GLN:C	2.59	0.44
4:D:114:ASN:CG	1:F:108:ARG:HH12	2.24	0.44
5:E:38:ASP:OD2	5:E:44:ARG:NH2	2.44	0.44
1:F:48:ARG:HH21	2:G:53:ASP:CG	2.24	0.44
1:F:70:HIS:HD2	1:F:73:THR:CB	2.27	0.44
4:I:116:ASP:N	4:I:117:PRO:HD3	2.32	0.44
5:J:154:LEU:HD23	5:J:155:SER:H	1.81	0.44
5:J:210:GLN:HG2	5:J:212:TYR:CE2	2.52	0.44
4:D:17:ALA:HB2	4:I:71:TYR:OH	2.18	0.44
1:F:56:GLY:O	1:F:59:TYR:HB3	2.17	0.44
1:F:82:LEU:HD23	1:F:87:GLN:HB2	2.00	0.44
1:F:272:LEU:N	1:F:272:LEU:CD1	2.74	0.44
3:H:7:GLY:HA2	5:J:30:GLU:CG	2.48	0.44
4:I:23:CYS:HB3	4:I:89:TRP:CZ2	2.52	0.44
4:I:161:ASP:HB2	4:I:168:LYS:HG2	2.00	0.44
4:I:163:ARG:HH21	5:J:164:HIS:C	2.25	0.44
1:A:57:PRO:CA	1:A:60:TRP:HD1	2.26	0.44
4:D:15:GLU:HG3	4:D:16:GLY:N	2.33	0.44
4:D:136:THR:OG1	4:D:137:ASP:N	2.50	0.44
5:E:100:GLN:C	5:E:101:TYR:CD2	2.82	0.44
1:F:202:ARG:HD3	1:F:244:TRP:CG	2.52	0.44
1:A:68:LYS:HB3	5:E:54:VAL:HG22	1.99	0.44
1:A:75:ARG:NH1	1:A:79:ARG:NE	2.62	0.44
1:A:208:PHE:CZ	1:A:241:PHE:HB2	2.52	0.44
3:C:4:LEU:O	5:E:98:HIS:NE2	2.50	0.44
4:D:32:SER:C	4:D:33:PHE:CD2	2.96	0.44
4:D:192:ILE:HD11	4:D:196:THR:CG2	2.47	0.44
5:E:159:ASN:OD1	5:E:203:ASN:ND2	2.50	0.44
5:E:218:ASP:O	5:E:226:LYS:NZ	2.43	0.44
1:F:146:LYS:HB3	1:F:146:LYS:HZ3	1.82	0.44
4:I:182:ALA:H	4:I:185:ASN:HD21	1.66	0.44
5:J:18:LYS:HG2	5:J:19:LEU:N	2.32	0.44
1:A:63:GLU:O	1:A:67:VAL:HG12	2.17	0.44
1:A:234:ARG:O	1:A:242:GLN:HG3	2.17	0.44
1:A:249:VAL:CG1	1:A:257:TYR:CE2	2.95	0.44
2:B:14:PRO:O	2:B:16:GLU:HG2	2.18	0.44
2:B:56:PHE:HD2	2:B:62:PHE:CE2	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:75:LEU:HD12	4:D:75:LEU:N	2.32	0.44
4:D:158:CYS:HB2	5:E:190:ARG:NH1	2.32	0.44
5:E:85:GLN:O	5:E:89:TYR:OH	2.23	0.44
1:F:51:TRP:CZ2	1:F:179:LEU:CD1	3.00	0.44
5:J:36:ARG:NH2	5:J:84:ASN:O	2.46	0.44
5:J:152:VAL:HG12	5:J:210:GLN:O	2.17	0.44
1:A:66:LYS:HB2	1:A:66:LYS:HE3	1.74	0.44
5:E:203:ASN:HB3	5:E:205:PHE:CZ	2.53	0.44
1:F:204:TRP:HH2	2:G:99:MET:CE	2.31	0.44
1:F:260:HIS:CE1	1:F:271:THR:CG2	3.00	0.44
5:J:162:GLU:CG	5:J:164:HIS:HE1	2.30	0.44
1:A:200:THR:CG2	1:A:202:ARG:HH22	2.31	0.44
3:C:4:LEU:CD2	4:D:96:GLY:HA2	2.46	0.44
4:D:138:PHE:O	4:D:170:ASN:ND2	2.51	0.44
5:E:8:PRO:O	5:E:106:THR:HG23	2.17	0.44
5:E:82:SER:C	5:E:110:VAL:HG11	2.42	0.44
1:F:99:PHE:CE2	3:H:3:PRO:HB3	2.53	0.44
1:F:156:GLN:OE1	3:H:8:TRP:CH2	2.70	0.44
4:I:38:GLN:CG	4:I:44:PRO:HG3	2.48	0.44
1:A:68:LYS:NZ	5:E:53:GLU:O	2.51	0.44
1:A:111:ARG:NH2	1:A:128:GLU:CA	2.79	0.44
1:A:202:ARG:HH11	1:A:246:ALA:HB2	1.83	0.44
1:A:219:ARG:HG3	1:A:257:TYR:HE1	1.83	0.44
1:F:67:VAL:HG13	1:F:68:LYS:N	2.33	0.44
1:F:144:LYS:O	1:F:148:GLU:CG	2.65	0.44
5:J:154:LEU:CD2	5:J:155:SER:N	2.81	0.44
1:A:207:GLY:HA2	1:A:240:THR:HB	2.00	0.44
2:B:23:LEU:N	2:B:70:PHE:CE1	2.85	0.44
3:C:4:LEU:HD22	3:C:6:PHE:HE2	1.83	0.44
4:D:115:PRO:HD2	1:F:108:ARG:NH2	2.32	0.44
4:D:164:SER:OG	4:D:165:MET:HE2	2.18	0.44
5:E:9:ARG:NH1	5:E:104:PRO:C	2.76	0.44
5:E:70:GLU:HB3	5:E:72:ARG:HD2	2.00	0.44
1:F:202:ARG:HD3	1:F:244:TRP:CE2	2.52	0.44
1:F:244:TRP:CE3	1:F:244:TRP:O	2.71	0.44
5:J:148:TYR:HB2	5:J:184:ARG:HG3	2.00	0.44
1:A:126:LEU:HD13	1:A:133:TRP:CE3	2.52	0.43
1:A:145:ARG:HA	1:A:148:GLU:CD	2.41	0.43
5:E:86:THR:O	5:E:87:SER:HB2	2.18	0.43
1:F:77:ASN:CG	3:H:10:PHE:CE1	2.96	0.43
4:I:139:ASP:C	4:I:141:GLN:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:SER:OG	1:A:78:LEU:HD11	2.18	0.43
1:A:65:GLY:HA2	5:E:54:VAL:CG1	2.48	0.43
1:A:109:PHE:O	1:A:110:LEU:HD12	2.17	0.43
1:A:121:LYS:HD3	1:A:122:ASP:H	1.84	0.43
1:A:159:TYR:CD1	4:D:31:GLN:OE1	2.70	0.43
4:D:11:LEU:HG	4:D:12:SER:N	2.31	0.43
1:F:106:ASP:OD2	1:F:108:ARG:CB	2.58	0.43
1:F:168:LEU:HD12	1:F:168:LEU:C	2.43	0.43
1:F:189:MET:HE3	1:F:189:MET:HB2	1.77	0.43
1:F:189:MET:HE2	1:F:272:LEU:HB3	2.00	0.43
2:G:22:PHE:HD2	2:G:67:TYR:HD2	1.64	0.43
2:G:54:LEU:HA	2:G:64:LEU:HD21	2.00	0.43
4:I:4:VAL:HG22	4:I:5:GLU:N	2.33	0.43
5:J:4:VAL:CG2	5:J:102:PHE:C	2.89	0.43
5:J:41:LEU:HD22	5:J:41:LEU:N	2.33	0.43
1:A:68:LYS:NZ	5:E:53:GLU:C	2.76	0.43
1:A:150:ALA:HB1	5:E:96:ALA:HB1	1.99	0.43
5:E:181:ASN:OD1	5:E:181:ASN:N	2.51	0.43
1:F:8:PHE:CD2	1:F:25:VAL:HG23	2.40	0.43
4:I:37:ARG:CZ	4:I:39:TYR:OH	2.66	0.43
4:I:87:TYR:CE2	4:I:106:LEU:HB3	2.53	0.43
4:I:88:LEU:HD12	4:I:100:PHE:CD1	2.53	0.43
1:A:50:PRO:HA	1:A:53:GLU:OE2	2.19	0.43
1:A:170:ARG:HH11	1:A:170:ARG:HG3	1.84	0.43
4:D:53:ASN:HA	4:D:65:LEU:HD23	1.99	0.43
1:F:188:HIS:CD2	1:F:188:HIS:C	2.96	0.43
1:F:204:TRP:HH2	2:G:99:MET:HE3	1.83	0.43
4:I:38:GLN:CB	4:I:44:PRO:HG3	2.48	0.43
4:I:60:ARG:C	4:I:77:ARG:NH2	2.76	0.43
4:I:109:LYS:HD2	4:I:140:SER:OG	2.18	0.43
5:J:43:LEU:HD12	5:J:44:ARG:N	2.32	0.43
5:J:108:LEU:C	5:J:108:LEU:CD1	2.82	0.43
1:A:19:GLU:OE2	1:A:19:GLU:CA	2.54	0.43
1:A:268:LYS:HG3	1:A:269:PRO:HD2	2.01	0.43
2:B:21:ASN:C	2:B:22:PHE:CD1	2.96	0.43
3:C:4:LEU:CD2	3:C:6:PHE:HE2	2.30	0.43
1:F:22:PHE:CE2	1:F:71:SER:HB3	2.52	0.43
1:F:231:VAL:HG13	1:F:244:TRP:CH2	2.54	0.43
4:I:160:LEU:O	4:I:168:LYS:HA	2.19	0.43
5:J:9:ARG:C	5:J:106:THR:HG23	2.44	0.43
4:D:110:PRO:HG2	4:D:112:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:157:LYS:CD	4:D:157:LYS:N	2.82	0.43
4:I:124:ASP:OD2	5:J:125:PHE:CZ	2.72	0.43
1:A:133:TRP:HB2	1:A:144:LYS:HG3	2.00	0.43
5:E:6:GLN:OE1	5:E:91:CYS:N	2.46	0.43
4:I:10:PRO:O	4:I:11:LEU:C	2.62	0.43
1:A:44:ARG:HA	1:A:64:THR:HG23	2.00	0.43
1:A:48:ARG:HD2	1:A:48:ARG:HA	1.63	0.43
1:A:147:TRP:CZ2	3:C:8:TRP:HB3	2.54	0.43
1:A:208:PHE:HZ	1:A:233:THR:HG23	1.84	0.43
2:B:15:ALA:C	2:B:16:GLU:HG2	2.43	0.43
2:B:56:PHE:CD2	2:B:62:PHE:HE2	2.36	0.43
4:D:81:PRO:N	4:D:108:VAL:HG11	2.34	0.43
4:D:139:ASP:C	4:D:141:GLN:N	2.75	0.43
4:D:161:ASP:OD2	4:D:163:ARG:HG2	2.19	0.43
5:E:9:ARG:HB3	5:E:10:TYR:CD2	2.54	0.43
1:F:51:TRP:C	1:F:51:TRP:CE3	2.97	0.43
1:F:205:ALA:O	1:F:208:PHE:HE1	2.02	0.43
5:J:46:ILE:O	5:J:58:GLY:N	2.41	0.43
5:J:152:VAL:HA	5:J:210:GLN:O	2.19	0.43
1:A:82:LEU:HD22	1:A:87:GLN:HB2	2.01	0.43
1:A:158:ALA:HB1	4:D:31:GLN:CB	2.49	0.43
1:A:191:HIS:CE1	1:A:193:PRO:HG3	2.54	0.43
4:D:116:ASP:N	4:D:117:PRO:HD3	2.33	0.43
4:D:194:GLU:OE1	4:D:194:GLU:HA	2.19	0.43
5:E:176:GLU:O	5:E:178:PRO:HD3	2.18	0.43
1:F:201:LEU:HD23	1:F:201:LEU:HA	1.94	0.43
1:F:234:ARG:HG3	1:F:242:GLN:CG	2.38	0.43
5:J:38:ASP:CB	5:J:44:ARG:HH22	2.30	0.43
5:J:127:PRO:HD2	5:J:198:TRP:CE2	2.54	0.43
1:A:44:ARG:HG2	1:A:64:THR:HG21	2.01	0.43
1:A:130:LEU:O	1:A:157:ARG:HG3	2.18	0.43
2:B:23:LEU:HD21	2:B:39:LEU:HD13	2.01	0.43
4:D:111:ASN:HD22	4:D:111:ASN:HA	1.48	0.43
5:E:1:GLU:OE2	5:E:1:GLU:C	2.61	0.43
5:E:19:LEU:HD12	5:E:19:LEU:O	2.19	0.43
5:E:132:ILE:HG23	5:E:195:ALA:HB2	1.99	0.43
1:F:7:TYR:HE1	1:F:33:PHE:CZ	2.36	0.43
1:F:99:PHE:HE1	1:F:114:HIS:CG	2.37	0.43
1:F:104:GLY:CA	1:F:110:LEU:HD23	2.49	0.43
1:F:218:GLN:OE1	1:F:223:ASP:N	2.52	0.43
2:G:9:VAL:HA	2:G:24:ASN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:36:TYR:CD1	4:I:46:LEU:N	2.87	0.43
4:I:94:GLN:CB	4:I:97:LYS:HD3	2.30	0.43
5:J:203:ASN:O	5:J:205:PHE:CE2	2.72	0.43
1:A:11:SER:HA	1:A:21:ARG:O	2.19	0.42
1:A:98:MET:SD	1:A:99:PHE:N	2.91	0.42
1:A:200:THR:HG21	1:A:202:ARG:NH2	2.34	0.42
2:B:1:ILE:CD1	2:B:1:ILE:C	2.92	0.42
1:F:54:GLN:CD	1:F:174:ASN:HD21	2.26	0.42
4:I:42:LYS:HE2	4:I:42:LYS:N	2.34	0.42
4:I:101:GLY:O	4:I:102:GLN:C	2.61	0.42
4:I:193:PRO:HB2	4:I:196:THR:OG1	2.19	0.42
1:A:150:ALA:HB3	1:A:152:VAL:HG23	2.01	0.42
4:D:30:SER:HB3	4:D:33:PHE:CE2	2.54	0.42
4:D:43:SER:HA	5:E:90:PHE:CZ	2.55	0.42
4:D:112:ILE:HD13	4:D:112:ILE:N	2.34	0.42
5:E:79:GLU:O	5:E:81:PRO:HD3	2.18	0.42
1:F:185:PRO:HB3	1:F:208:PHE:CD1	2.54	0.42
2:G:12:ARG:HD2	2:G:22:PHE:CB	2.39	0.42
5:J:64:TYR:CD1	5:J:78:LEU:CD1	3.02	0.42
5:J:132:ILE:N	5:J:132:ILE:CD1	2.82	0.42
1:A:108:ARG:O	1:A:110:LEU:CD1	2.64	0.42
1:A:161:GLU:O	1:A:165:VAL:HG21	2.20	0.42
1:A:188:HIS:CE1	1:A:204:TRP:HB2	2.54	0.42
1:A:213:ILE:CD1	1:A:263:HIS:HB2	2.49	0.42
1:A:268:LYS:HD2	1:A:268:LYS:HA	1.85	0.42
2:B:23:LEU:CD2	2:B:39:LEU:HD13	2.50	0.42
4:D:12:SER:CB	4:D:109:LYS:NZ	2.82	0.42
5:E:86:THR:OG1	5:E:110:VAL:HG23	2.19	0.42
5:E:93:SER:C	5:E:100:GLN:HG3	2.43	0.42
5:E:114:LEU:HD13	5:E:214:LEU:HD21	2.02	0.42
1:F:125:ALA:O	1:F:134:THR:CG2	2.68	0.42
4:I:35:TRP:O	4:I:47:ILE:HG13	2.18	0.42
5:J:146:GLY:HA2	5:J:176:GLU:OE2	2.20	0.42
1:A:68:LYS:HZ2	5:E:53:GLU:C	2.27	0.42
1:A:220:ASP:OD1	1:A:256:ARG:HD3	2.19	0.42
1:A:235:PRO:HG2	2:B:65:LEU:HD22	2.01	0.42
4:D:10:PRO:O	4:D:11:LEU:C	2.63	0.42
4:D:25:TYR:CE2	4:D:33:PHE:CZ	3.07	0.42
1:F:109:PHE:HE1	1:F:111:ARG:C	2.28	0.42
4:I:159:VAL:C	5:J:168:CYS:SG	3.03	0.42
1:A:44:ARG:HA	1:A:64:THR:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ARG:CZ	1:A:161:GLU:OE1	2.67	0.42
1:A:183:ASP:HA	1:A:184:PRO:HD3	1.79	0.42
2:B:41:LYS:HG3	2:B:78:TYR:CE2	2.55	0.42
1:F:127:LYS:HE3	1:F:133:TRP:O	2.19	0.42
4:I:14:PRO:HG2	4:I:17:ALA:CB	2.49	0.42
4:I:36:TYR:CE1	5:J:102:PHE:HE2	2.35	0.42
4:I:124:ASP:OD2	5:J:125:PHE:HZ	2.02	0.42
4:I:163:ARG:HG2	4:I:163:ARG:H	1.42	0.42
5:J:177:GLN:O	5:J:183:SER:HB2	2.20	0.42
1:A:63:GLU:OE2	1:A:63:GLU:CA	2.64	0.42
1:A:69:ALA:C	5:E:51:ASN:HD22	2.27	0.42
4:D:37:ARG:CB	4:D:47:ILE:HD13	2.49	0.42
5:E:64:TYR:CD1	5:E:76:LEU:HD21	2.55	0.42
5:E:154:LEU:HD23	5:E:155:SER:CA	2.48	0.42
1:F:34:VAL:CG1	1:F:60:TRP:HH2	2.33	0.42
1:A:51:TRP:HZ3	1:A:52:ILE:HD13	1.85	0.42
4:D:122:LEU:HD12	5:E:128:SER:N	2.35	0.42
1:F:8:PHE:O	1:F:24:ALA:HA	2.20	0.42
4:I:89:TRP:CD1	4:I:89:TRP:N	2.88	0.42
4:I:185:ASN:HD22	4:I:185:ASN:N	2.16	0.42
5:J:68:ARG:HG2	5:J:68:ARG:HH11	1.84	0.42
1:A:244:TRP:HE1	2:B:99:MET:HG3	1.84	0.42
2:B:35:ILE:HD11	2:B:82:VAL:CG1	2.48	0.42
4:D:2:LYS:NZ	5:E:42:GLY:HA3	2.35	0.42
4:D:60:ARG:NH2	4:D:83:ASP:OD2	2.42	0.42
5:E:239:ARG:HG3	5:E:239:ARG:NH1	2.33	0.42
1:F:22:PHE:CD2	1:F:71:SER:CB	3.00	0.42
1:F:27:TYR:CD2	1:F:30:ASP:C	2.97	0.42
1:F:115:GLN:HE21	1:F:115:GLN:HB3	1.55	0.42
1:F:202:ARG:NH1	1:F:244:TRP:CH2	2.88	0.42
2:G:10:TYR:OH	2:G:26:TYR:HB2	2.20	0.42
2:G:35:ILE:HD11	2:G:84:HIS:CD2	2.55	0.42
4:I:162:MET:HE1	5:J:192:ARG:CG	2.49	0.42
1:A:123:TYR:CE1	1:A:140:ALA:HA	2.55	0.42
1:A:134:THR:HG23	1:A:134:THR:O	2.20	0.42
2:B:33:SER:HB3	2:B:62:PHE:CE1	2.55	0.42
4:D:34:PHE:HB3	4:D:46:LEU:CD1	2.50	0.42
4:D:122:LEU:HG	5:E:127:PRO:HA	2.01	0.42
5:E:20:THR:O	5:E:20:THR:CG2	2.67	0.42
1:F:71:SER:O	1:F:75:ARG:HB2	2.20	0.42
1:F:96:GLN:HB3	2:G:56:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:191:HIS:HB2	1:F:274:TRP:CZ3	2.55	0.42
2:G:35:ILE:HD11	2:G:84:HIS:CG	2.55	0.42
4:I:4:VAL:C	4:I:5:GLU:HG2	2.44	0.42
4:I:162:MET:HE2	5:J:166:GLY:CA	2.50	0.42
5:J:25:GLN:HE22	5:J:29:HIS:N	2.17	0.42
5:J:36:ARG:NH2	5:J:86:THR:O	2.53	0.42
5:J:89:TYR:CE2	5:J:108:LEU:HG	2.55	0.42
1:A:123:TYR:CE2	3:C:10:PHE:CE2	3.08	0.42
1:A:150:ALA:CB	5:E:96:ALA:HB1	2.50	0.42
3:C:5:THR:HG22	3:C:8:TRP:HZ3	1.84	0.42
4:D:94:GLN:HB2	4:D:97:LYS:CG	2.48	0.42
1:F:82:LEU:HD21	1:F:93:HIS:CE1	2.55	0.42
1:F:224:GLN:CD	1:F:226:GLN:O	2.62	0.42
4:I:47:ILE:HD12	4:I:48:MET:HB2	2.01	0.42
5:J:172:GLN:HA	5:J:173:PRO:HD3	1.94	0.42
1:A:217:TRP:CD1	1:A:247:VAL:HG13	2.54	0.41
5:E:3:GLN:OE1	5:E:3:GLN:N	2.53	0.41
1:F:8:PHE:HE2	1:F:27:TYR:CD1	2.38	0.41
1:F:77:ASN:HA	1:F:80:ILE:HD12	2.02	0.41
4:I:98:LEU:HD12	5:J:35:TYR:OH	2.19	0.41
1:A:52:ILE:HD12	1:A:52:ILE:HA	1.88	0.41
5:E:19:LEU:CD1	5:E:19:LEU:C	2.90	0.41
5:E:46:ILE:O	5:E:58:GLY:N	2.45	0.41
1:F:85:TYR:HB3	1:F:87:GLN:HG3	2.01	0.41
4:I:160:LEU:O	4:I:168:LYS:NZ	2.52	0.41
5:J:29:HIS:CD2	5:J:95:GLY:HA3	2.55	0.41
5:J:120:PRO:HG2	5:J:232:VAL:CG2	2.49	0.41
1:A:74:ASP:HB3	1:A:95:LEU:HD23	2.01	0.41
1:A:173:GLU:OE1	1:A:176:LYS:HD3	2.21	0.41
1:A:213:ILE:CG1	1:A:262:GLN:O	2.59	0.41
5:E:87:SER:OG	5:E:88:LEU:N	2.52	0.41
5:E:151:HIS:C	5:E:152:VAL:HG13	2.45	0.41
1:F:3:HIS:HB3	1:F:29:ASP:OD2	2.19	0.41
1:F:23:ILE:CG2	1:F:23:ILE:O	2.68	0.41
2:G:12:ARG:NH1	2:G:22:PHE:CD1	2.88	0.41
4:I:93:ASN:C	4:I:95:GLY:N	2.70	0.41
5:J:25:GLN:NE2	5:J:29:HIS:N	2.68	0.41
5:J:160:GLY:C	5:J:161:LYS:HG3	2.44	0.41
1:A:14:ARG:HB3	1:A:17:ARG:HB2	2.01	0.41
1:A:70:HIS:HA	1:A:73:THR:OG1	2.21	0.41
1:A:255:GLN:HE21	1:A:255:GLN:HB3	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:7:ASN:HA	5:E:8:PRO:HA	1.64	0.41
5:E:11:LEU:HD21	5:E:19:LEU:HD22	2.02	0.41
1:F:33:PHE:O	1:F:48:ARG:N	2.47	0.41
1:F:156:GLN:O	1:F:159:TYR:HB3	2.20	0.41
4:I:13:VAL:O	4:I:108:VAL:HA	2.21	0.41
4:I:78:ASP:OD1	4:I:78:ASP:C	2.62	0.41
4:I:114:ASN:HA	4:I:115:PRO:HD2	1.94	0.41
5:J:19:LEU:HD11	5:J:78:LEU:HB3	2.02	0.41
5:J:132:ILE:CG2	5:J:195:ALA:HB1	2.49	0.41
5:E:82:SER:HB2	5:E:85:GLN:CG	2.50	0.41
5:E:220:TRP:NE1	5:E:226:LYS:HA	2.36	0.41
1:F:241:PHE:CD1	1:F:241:PHE:N	2.88	0.41
5:J:144:ALA:O	5:J:147:PHE:CE2	2.73	0.41
5:J:191:LEU:HD12	5:J:192:ARG:N	2.35	0.41
5:J:204:HIS:HD2	5:J:236:ALA:O	2.03	0.41
1:A:133:TRP:CZ2	1:A:153:ALA:N	2.88	0.41
1:A:156:GLN:O	1:A:157:ARG:C	2.63	0.41
1:A:158:ALA:HB1	4:D:31:GLN:HB2	2.03	0.41
3:C:2:PHE:CD2	3:C:3:PRO:O	2.74	0.41
4:D:14:PRO:HD2	4:I:71:TYR:HE1	1.82	0.41
5:E:25:GLN:OE1	5:E:29:HIS:HB2	2.19	0.41
5:E:77:ILE:N	5:E:77:ILE:CD1	2.77	0.41
5:E:118:PHE:O	5:E:147:PHE:HA	2.21	0.41
5:E:193:VAL:HG23	5:E:194:SER:O	2.20	0.41
1:A:95:LEU:HD11	1:A:116:TYR:CD1	2.54	0.41
1:A:99:PHE:CE2	3:C:3:PRO:HG3	2.55	0.41
1:A:218:GLN:HB2	1:A:260:HIS:NE2	2.36	0.41
1:A:259:CYS:O	1:A:271:THR:HA	2.19	0.41
2:B:84:HIS:CB	2:B:87:LEU:HD12	2.51	0.41
4:D:138:PHE:HE2	4:D:171:SER:HA	1.85	0.41
5:E:161:LYS:HB2	5:E:161:LYS:HZ3	1.83	0.41
1:F:80:ILE:CD1	3:H:10:PHE:H	2.33	0.41
4:I:141:GLN:OE1	4:I:141:GLN:HA	2.21	0.41
1:A:5:MET:SD	1:A:171:TYR:CE2	3.10	0.41
2:B:35:ILE:HD12	2:B:84:HIS:CD2	2.44	0.41
4:D:50:ILE:CD1	4:D:65:LEU:HB3	2.46	0.41
4:D:99:ILE:N	4:D:99:ILE:HD12	2.36	0.41
4:D:123:ARG:NH1	5:E:239:ARG:HD3	2.35	0.41
5:E:215:SER:C	5:E:217:ASN:N	2.77	0.41
5:J:36:ARG:NE	5:J:87:SER:HB3	2.34	0.41
5:J:41:LEU:HB2	5:J:44:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:47:TYR:CE2	5:J:61:PRO:HB2	2.56	0.41
1:A:68:LYS:CB	5:E:54:VAL:HG22	2.51	0.41
1:A:95:LEU:HD11	1:A:116:TYR:CE1	2.55	0.41
1:A:217:TRP:CH2	1:A:259:CYS:HB2	2.55	0.41
5:E:97:SER:O	5:E:98:HIS:ND1	2.54	0.41
5:E:117:VAL:HG12	5:E:227:PRO:CG	2.51	0.41
1:F:34:VAL:HG12	1:F:60:TRP:HH2	1.86	0.41
1:F:55:GLU:HA	1:F:55:GLU:OE1	2.21	0.41
1:F:70:HIS:ND1	3:H:2:PHE:CZ	2.70	0.41
1:F:127:LYS:HG3	1:F:134:THR:HG22	2.02	0.41
2:G:4:THR:OG1	2:G:87:LEU:HD21	2.20	0.41
2:G:30:PHE:O	2:G:62:PHE:CD1	2.73	0.41
4:I:18:ILE:HA	4:I:76:ILE:O	2.20	0.41
5:J:200:ASN:ND2	5:J:203:ASN:CG	2.77	0.41
1:A:5:MET:HB2	1:A:168:LEU:HD13	2.03	0.41
1:A:74:ASP:HA	1:A:77:ASN:ND2	2.35	0.41
1:A:124:ILE:HD11	1:A:144:LYS:HB2	2.03	0.41
5:E:9:ARG:NH1	5:E:104:PRO:CB	2.81	0.41
5:E:187:LEU:HG	5:E:188:SER:H	1.85	0.41
1:F:51:TRP:CD1	1:F:175:GLY:HA2	2.56	0.41
1:F:80:ILE:HD13	3:H:10:PHE:H	1.85	0.41
1:F:183:ASP:HA	1:F:184:PRO:HD3	1.79	0.41
4:I:134:LEU:CD2	5:J:139:THR:HG21	2.51	0.41
5:J:49:SER:HB3	5:J:68:ARG:HH11	1.86	0.41
1:A:151:HIS:O	1:A:154:GLU:HG2	2.20	0.40
5:E:25:GLN:OE1	5:E:29:HIS:N	2.31	0.40
5:E:30:GLU:C	5:E:68:ARG:HH22	2.28	0.40
5:E:57:LYS:H	5:E:57:LYS:HG2	1.55	0.40
5:E:217:ASN:N	5:E:217:ASN:ND2	2.68	0.40
1:F:143:THR:HA	1:F:146:LYS:CD	2.51	0.40
5:J:118:PHE:O	5:J:147:PHE:HA	2.21	0.40
5:J:154:LEU:CG	5:J:209:VAL:HG22	2.49	0.40
4:D:9:GLY:HA2	4:D:10:PRO:HD3	1.73	0.40
5:E:30:GLU:HB3	5:E:51:ASN:ND2	2.36	0.40
5:E:97:SER:HB3	5:E:99:GLU:OE1	2.21	0.40
5:E:159:ASN:HD22	5:E:204:HIS:HB3	1.87	0.40
1:F:55:GLU:OE2	1:F:170:ARG:NE	2.54	0.40
1:F:197:HIS:CE1	1:F:198:GLU:HG3	2.56	0.40
4:I:28:ARG:HA	4:I:70:GLN:HE21	1.84	0.40
4:I:125:SER:N	5:J:125:PHE:CE2	2.89	0.40
5:J:41:LEU:HB2	5:J:44:ARG:CZ	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:43:LEU:HD12	5:J:44:ARG:H	1.86	0.40
1:A:185:PRO:CB	1:A:208:PHE:HB3	2.38	0.40
1:A:234:ARG:NH2	2:B:10:TYR:CG	2.89	0.40
4:D:160:LEU:HD12	4:D:160:LEU:O	2.21	0.40
1:F:115:GLN:CG	2:G:60:TRP:CH2	2.93	0.40
1:F:267:PRO:CG	1:F:268:LYS:H	2.33	0.40
2:G:12:ARG:HD2	2:G:22:PHE:N	2.37	0.40
4:I:94:GLN:HB3	4:I:97:LYS:CD	2.30	0.40
4:I:170:ASN:O	4:I:171:SER:HB3	2.21	0.40
5:J:9:ARG:CG	5:J:9:ARG:NH1	2.83	0.40
5:J:33:SER:HA	5:J:74:PHE:HE2	1.86	0.40
5:J:47:TYR:HE2	5:J:61:PRO:HB2	1.86	0.40
5:J:159:ASN:ND2	5:J:204:HIS:N	2.56	0.40
5:J:205:PHE:CD2	5:J:236:ALA:O	2.70	0.40
5:J:206:ARG:NH2	5:J:208:GLN:HE21	2.20	0.40
1:A:31:THR:OG1	1:A:209:TYR:OH	2.36	0.40
1:A:181:ARG:HH11	1:A:181:ARG:HG2	1.86	0.40
1:A:191:HIS:HE1	1:A:193:PRO:HG3	1.86	0.40
2:B:12:ARG:N	2:B:21:ASN:HD21	2.18	0.40
1:F:54:GLN:CD	1:F:174:ASN:ND2	2.80	0.40
1:F:155:GLN:C	4:I:31:GLN:NE2	2.79	0.40
1:F:220:ASP:CG	1:F:256:ARG:HD3	2.46	0.40
1:F:228:THR:HG22	1:F:247:VAL:CG1	2.46	0.40
4:I:139:ASP:C	4:I:141:GLN:N	2.80	0.40
5:J:206:ARG:HH11	5:J:206:ARG:CG	2.34	0.40
5:J:215:SER:C	5:J:217:ASN:N	2.77	0.40
1:A:99:PHE:CD2	3:C:3:PRO:HG3	2.57	0.40
1:A:234:ARG:CZ	2:B:10:TYR:CG	3.04	0.40
5:E:95:GLY:O	5:E:96:ALA:C	2.65	0.40
5:E:99:GLU:H	5:E:99:GLU:HG2	1.59	0.40
1:F:7:TYR:HE2	3:H:2:PHE:HA	1.86	0.40
1:F:80:ILE:HG21	3:H:10:PHE:HB2	2.04	0.40
2:G:56:PHE:CD1	2:G:56:PHE:C	2.99	0.40
4:I:122:LEU:HD11	5:J:141:VAL:CB	2.50	0.40
5:J:156:TRP:HZ2	5:J:189:SER:O	2.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	272/275 (99%)	259 (95%)	12 (4%)	1 (0%)	30	54
1	F	272/275 (99%)	257 (94%)	14 (5%)	1 (0%)	30	54
2	B	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
2	G	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
3	C	8/10 (80%)	8 (100%)	0	0	100	100
3	H	8/10 (80%)	8 (100%)	0	0	100	100
4	D	197/205 (96%)	167 (85%)	24 (12%)	6 (3%)	3	8
4	I	197/205 (96%)	169 (86%)	22 (11%)	6 (3%)	3	8
5	E	239/242 (99%)	223 (93%)	15 (6%)	1 (0%)	30	54
5	J	239/242 (99%)	220 (92%)	18 (8%)	1 (0%)	30	54
All	All	1626/1664 (98%)	1497 (92%)	113 (7%)	16 (1%)	12	32

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	94	GLN
4	D	8	SER
4	D	40	SER
4	I	7	ASN
4	I	40	SER
4	I	94	GLN
4	D	7	ASN
4	I	8	SER
1	F	163	THR
1	A	163	THR
4	D	27	ASP
4	D	53	ASN
5	E	222	GLN
4	I	27	ASP

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Mol	Chain	Res	Type
5	J	222	GLN
4	I	9	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	230/231 (100%)	194 (84%)	36 (16%)	2	7
1	F	230/231 (100%)	191 (83%)	39 (17%)	2	6
2	B	94/95 (99%)	77 (82%)	17 (18%)	2	5
2	G	94/95 (99%)	80 (85%)	14 (15%)	3	8
3	C	9/9 (100%)	9 (100%)	0	100	100
3	H	9/9 (100%)	9 (100%)	0	100	100
4	D	177/183 (97%)	146 (82%)	31 (18%)	2	5
4	I	177/183 (97%)	138 (78%)	39 (22%)	1	3
5	E	214/215 (100%)	171 (80%)	43 (20%)	1	4
5	J	214/215 (100%)	180 (84%)	34 (16%)	2	7
All	All	1448/1466 (99%)	1195 (82%)	253 (18%)	2	5

All (253) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	19	GLU
1	A	20	PRO
1	A	33	PHE
1	A	34	VAL
1	A	39	ASP
1	A	60	TRP
1	A	73	THR
1	A	79	ARG
1	A	89	GLU
1	A	97	MET

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Mol	Chain	Res	Type
1	A	98	MET
1	A	157	ARG
1	A	160	LEU
1	A	163	THR
1	A	165	VAL
1	A	166	ASP
1	A	172	LEU
1	A	186	LYS
1	A	190	THR
1	A	202	ARG
1	A	216	THR
1	A	225	THR
1	A	226	GLN
1	A	229	GLU
1	A	230	LEU
1	A	231	VAL
1	A	232	GLU
1	A	234	ARG
1	A	238	ASP
1	A	242	GLN
1	A	247	VAL
1	A	248	VAL
1	A	254	GLU
1	A	255	GLN
1	A	258	THR
2	B	1	ILE
2	B	2	GLN
2	B	6	LYS
2	B	10	TYR
2	B	13	HIS
2	B	16	GLU
2	B	23	LEU
2	B	24	ASN
2	B	36	GLU
2	B	46	ILE
2	B	64	LEU
2	B	68	THR
2	B	74	GLU
2	B	84	HIS
2	B	85	VAL
2	B	86	THR
2	B	87	LEU

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Mol	Chain	Res	Type
4	D	6	GLN
4	D	15	GLU
4	D	20	SER
4	D	31	GLN
4	D	33	PHE
4	D	47	ILE
4	D	48	MET
4	D	50	ILE
4	D	62	THR
4	D	71	TYR
4	D	73	SER
4	D	88	LEU
4	D	98	LEU
4	D	102	GLN
4	D	104	THR
4	D	106	LEU
4	D	111	ASN
4	D	112	ILE
4	D	122	LEU
4	D	132	VAL
4	D	139	ASP
4	D	140	SER
4	D	142	THR
4	D	151	ASP
4	D	154	ILE
4	D	156	ASP
4	D	162	MET
4	D	180	ASP
4	D	189	ASN
4	D	191	ILE
4	D	192	ILE
5	E	1	GLU
5	E	3	GLN
5	E	13	THR
5	E	17	LYS
5	E	18	LYS
5	E	25	GLN
5	E	30	GLU
5	E	33	SER
5	E	37	GLN
5	E	43	LEU
5	E	46	ILE

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Mol	Chain	Res	Type
5	E	50	MET
5	E	51	ASN
5	E	53	GLU
5	E	56	ASP
5	E	59	ASP
5	E	60	VAL
5	E	72	ARG
5	E	77	ILE
5	E	78	LEU
5	E	84	ASN
5	E	93	SER
5	E	99	GLU
5	E	100	GLN
5	E	101	TYR
5	E	107	ARG
5	E	115	LYS
5	E	120	PRO
5	E	121	GLU
5	E	140	LEU
5	E	149	PRO
5	E	161	LYS
5	E	167	VAL
5	E	174	LEU
5	E	181	ASN
5	E	190	ARG
5	E	192	ARG
5	E	193	VAL
5	E	199	GLN
5	E	203	ASN
5	E	216	GLU
5	E	217	ASN
5	E	241	ASP
1	F	2	SER
1	F	19	GLU
1	F	35	ARG
1	F	38	SER
1	F	39	ASP
1	F	43	GLN
1	F	51	TRP
1	F	75	ARG
1	F	86	ASN
1	F	94	THR

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Mol	Chain	Res	Type
1	F	98	MET
1	F	110	LEU
1	F	115	GLN
1	F	132	SER
1	F	134	THR
1	F	143	THR
1	F	146	LYS
1	F	155	GLN
1	F	156	GLN
1	F	160	LEU
1	F	174	ASN
1	F	177	GLU
1	F	186	LYS
1	F	188	HIS
1	F	189	MET
1	F	214	THR
1	F	223	ASP
1	F	225	THR
1	F	233	THR
1	F	238	ASP
1	F	242	GLN
1	F	244	TRP
1	F	247	VAL
1	F	248	VAL
1	F	254	GLU
1	F	255	GLN
1	F	256	ARG
1	F	261	VAL
1	F	273	ARG
2	G	3	ARG
2	G	4	THR
2	G	7	ILE
2	G	24	ASN
2	G	31	HIS
2	G	35	ILE
2	G	36	GLU
2	G	40	LEU
2	G	50	GLU
2	G	59	ASP
2	G	62	PHE
2	G	65	LEU
2	G	68	THR

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Mol	Chain	Res	Type
2	G	89	GLN
4	I	2	LYS
4	I	3	GLU
4	I	13	VAL
4	I	14	PRO
4	I	22	ASN
4	I	24	THR
4	I	31	GLN
4	I	32	SER
4	I	42	LYS
4	I	44	PRO
4	I	46	LEU
4	I	50	ILE
4	I	57	GLU
4	I	64	GLN
4	I	69	SER
4	I	71	TYR
4	I	88	LEU
4	I	89	TRP
4	I	97	LYS
4	I	98	LEU
4	I	102	GLN
4	I	105	GLU
4	I	113	GLN
4	I	116	ASP
4	I	128	SER
4	I	144	VAL
4	I	146	GLN
4	I	148	LYS
4	I	152	VAL
4	I	160	LEU
4	I	163	ARG
4	I	167	PHE
4	I	168	LYS
4	I	177	ASN
4	I	180	ASP
4	I	185	ASN
4	I	190	SER
4	I	192	ILE
4	I	194	GLU
5	J	1	GLU
5	J	4	VAL

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Mol	Chain	Res	Type
5	J	9	ARG
5	J	12	ILE
5	J	17	LYS
5	J	18	LYS
5	J	19	LEU
5	J	25	GLN
5	J	30	GLU
5	J	37	GLN
5	J	50	MET
5	J	55	THR
5	J	56	ASP
5	J	77	ILE
5	J	79	GLU
5	J	101	TYR
5	J	102	PHE
5	J	108	LEU
5	J	115	LYS
5	J	122	VAL
5	J	135	THR
5	J	154	LEU
5	J	158	VAL
5	J	167	VAL
5	J	180	LEU
5	J	181	ASN
5	J	182	ASP
5	J	190	ARG
5	J	205	PHE
5	J	206	ARG
5	J	215	SER
5	J	217	ASN
5	J	230	GLN
5	J	232	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	43	GLN
1	A	70	HIS
1	A	86	ASN
1	A	114	HIS
1	A	141	GLN

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Mol	Chain	Res	Type
1	A	155	GLN
1	A	156	GLN
1	A	180	GLN
1	A	188	HIS
1	A	192	HIS
1	A	218	GLN
1	A	224	GLN
1	A	255	GLN
2	B	8	GLN
2	B	24	ASN
2	B	51	HIS
2	B	83	ASN
2	B	84	HIS
4	D	6	GLN
4	D	22	ASN
4	D	64	GLN
4	D	146	GLN
4	D	170	ASN
4	D	185	ASN
4	D	188	ASN
5	E	37	GLN
5	E	51	ASN
5	E	73	ASN
5	E	84	ASN
5	E	100	GLN
5	E	159	ASN
5	E	199	GLN
5	E	203	ASN
5	E	208	GLN
5	E	217	ASN
1	F	32	GLN
1	F	43	GLN
1	F	86	ASN
1	F	115	GLN
1	F	141	GLN
1	F	155	GLN
1	F	156	GLN
1	F	174	ASN
1	F	188	HIS
1	F	191	HIS
1	F	192	HIS
1	F	242	GLN

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Mol	Chain	Res	Type
1	F	255	GLN
1	F	260	HIS
2	G	2	GLN
2	G	13	HIS
2	G	21	ASN
2	G	24	ASN
2	G	31	HIS
4	I	6	GLN
4	I	38	GLN
4	I	53	ASN
4	I	64	GLN
4	I	70	GLN
4	I	80	GLN
4	I	93	ASN
4	I	94	GLN
4	I	113	GLN
4	I	114	ASN
4	I	143	ASN
4	I	177	ASN
4	I	185	ASN
4	I	188	ASN
4	I	189	ASN
5	J	29	HIS
5	J	37	GLN
5	J	73	ASN
5	J	98	HIS
5	J	134	HIS
5	J	151	HIS
5	J	159	ASN
5	J	181	ASN
5	J	200	ASN
5	J	204	HIS
5	J	208	GLN
5	J	210	GLN
5	J	217	ASN
5	J	222	GLN
5	J	230	GLN

5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	274/275 (99%)	-1.21	0 100 100	36, 69, 105, 120	0
1	F	274/275 (99%)	-1.26	0 100 100	33, 67, 86, 91	0
2	B	99/100 (99%)	-1.24	0 100 100	53, 68, 93, 97	0
2	G	99/100 (99%)	-1.19	0 100 100	49, 79, 96, 101	0
3	C	10/10 (100%)	-1.28	0 100 100	44, 48, 56, 57	0
3	H	10/10 (100%)	-1.25	0 100 100	34, 40, 59, 64	0
4	D	199/205 (97%)	-1.20	0 100 100	32, 61, 97, 115	0
4	I	199/205 (97%)	-1.25	0 100 100	20, 64, 102, 119	0
5	E	241/242 (99%)	-1.28	0 100 100	35, 64, 81, 92	0
5	J	241/242 (99%)	-1.31	0 100 100	29, 62, 84, 94	0
All	All	1646/1664 (98%)	-1.25	0 100 100	20, 66, 96, 120	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.