



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:43 pm BST

PDB ID : 3VXU
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

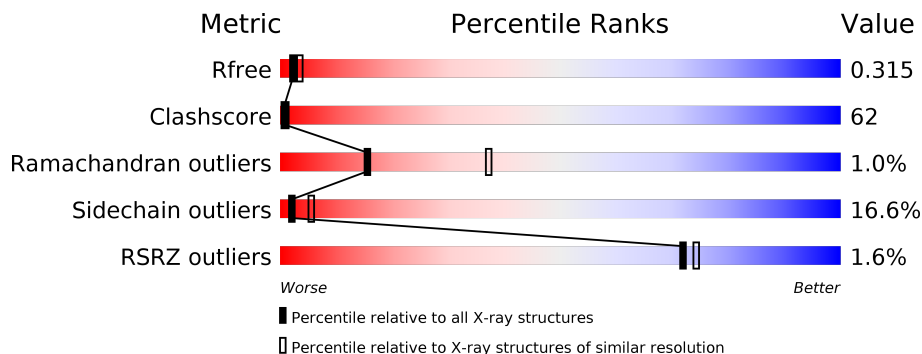
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.





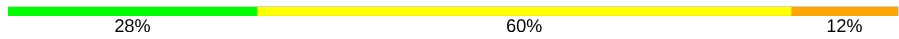
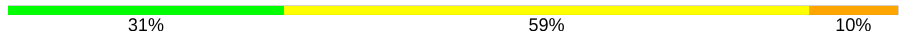
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on 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	
3	H	10	

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Mol	Chain	Length	Quality of chain
4	D	205	 <p>%</p> <p>31% 54% 12%</p>
4	I	205	 <p>2%</p> <p>29% 54% 14%</p>
5	E	242	 <p>28% 60% 12%</p>
5	J	242	 <p>31% 59% 10%</p>

2 Entry composition [i](#)

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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
4	D	199	1553	968	257	321	7	0	0	0
4	I	199	1553	968	257	321	7	0	0	0

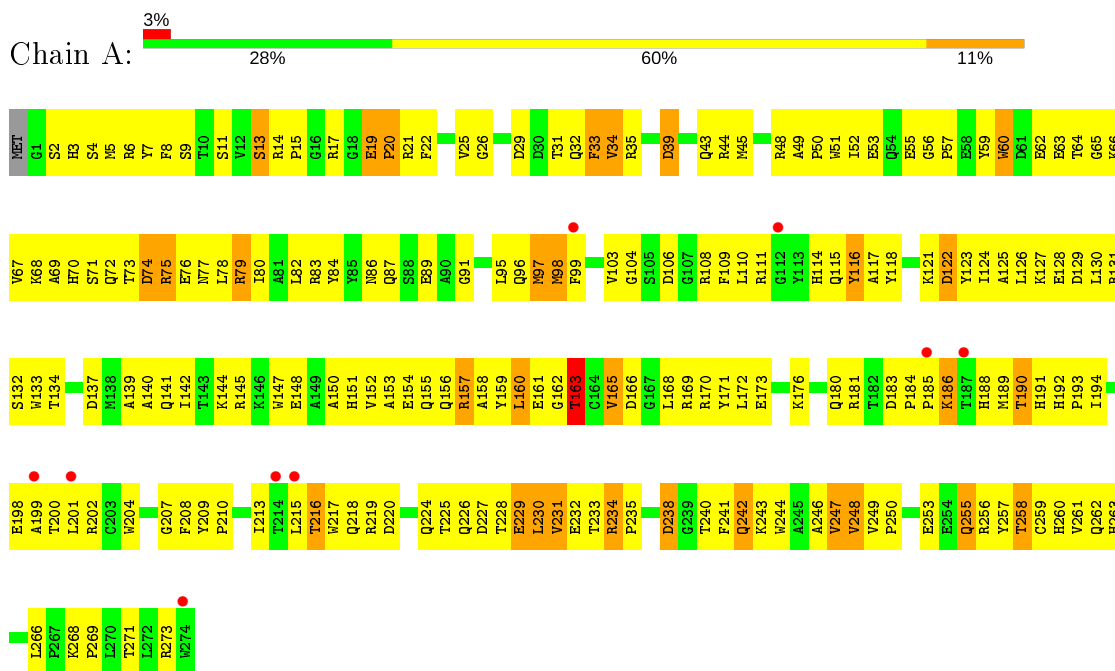
- Molecule 5 is a protein called T36-5 TCR beta chain.

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

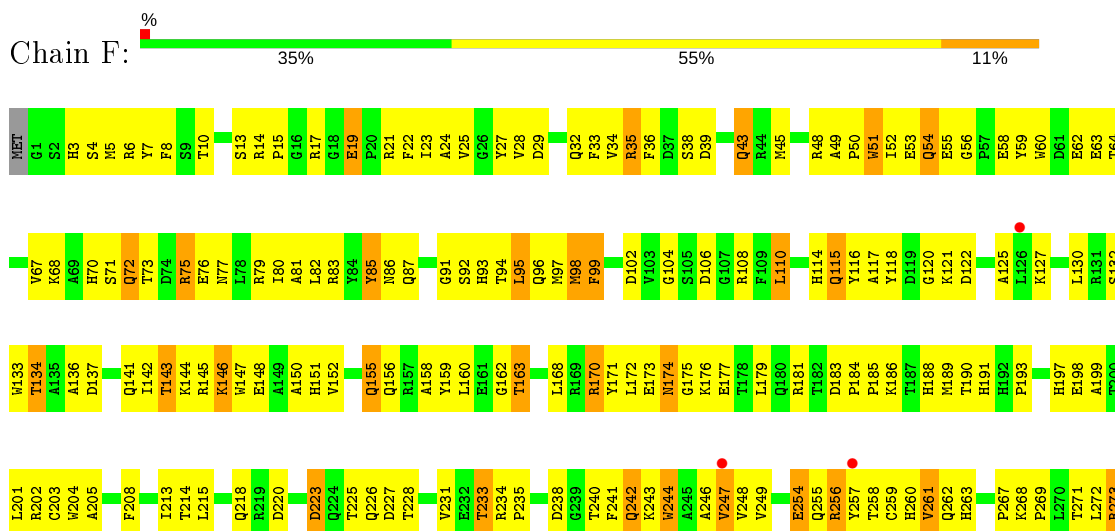
3 Residue-property plots i

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

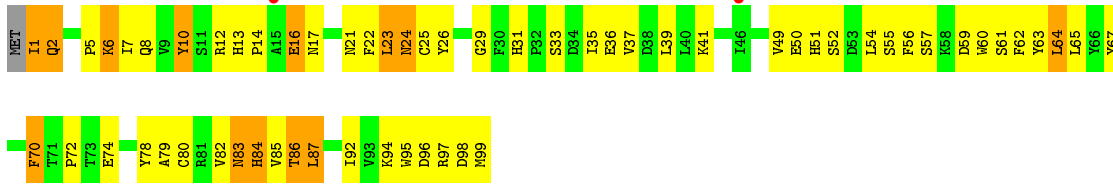


- Molecule 1: HLA class I histocompatibility antigen, A-24 alpha chain

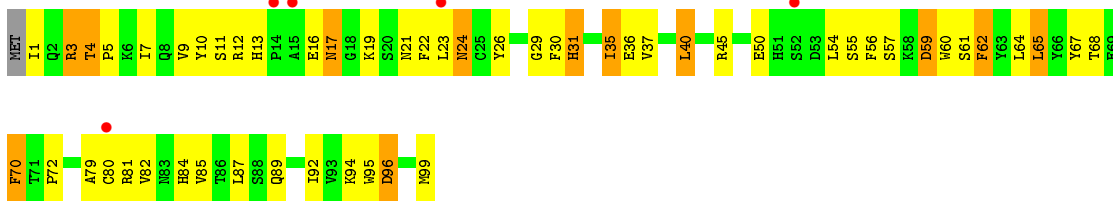
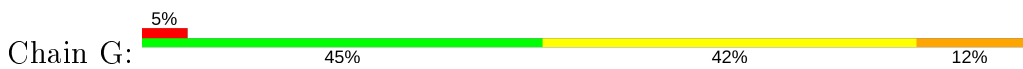


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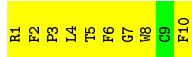
• Molecule 2: Beta-2-microglobulin



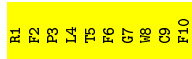
• Molecule 2: Beta-2-microglobulin



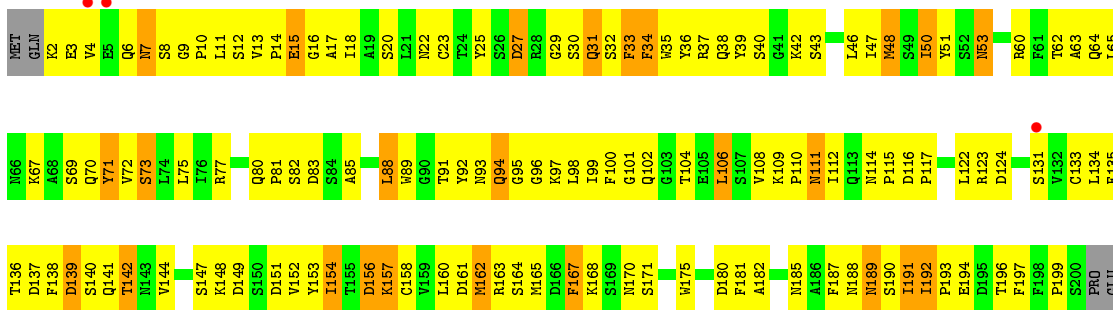
• Molecule 3: 10-mer peptide from Protein Nef



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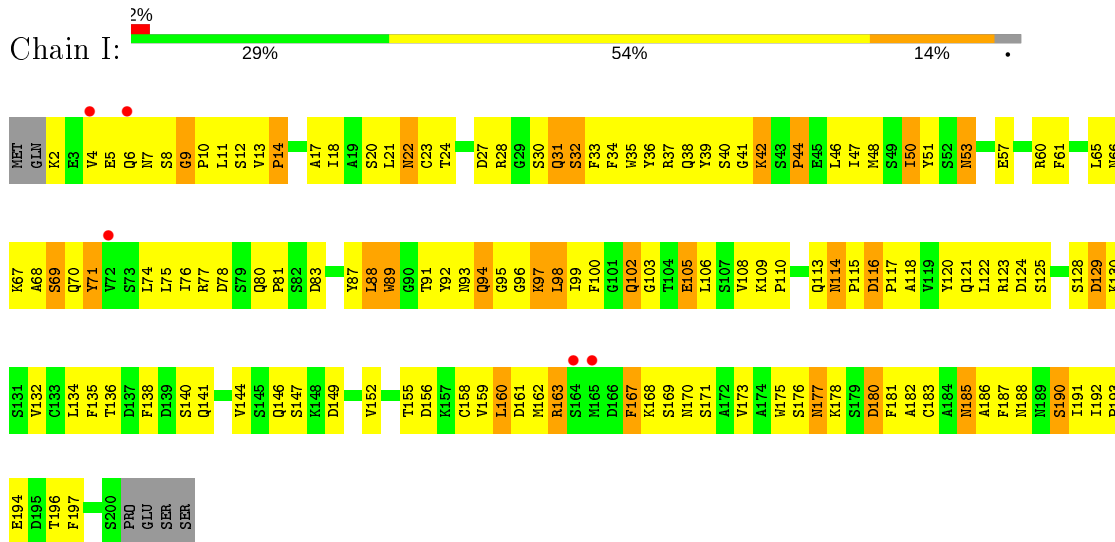


• Molecule 4: T36-5 TCR alpha chain

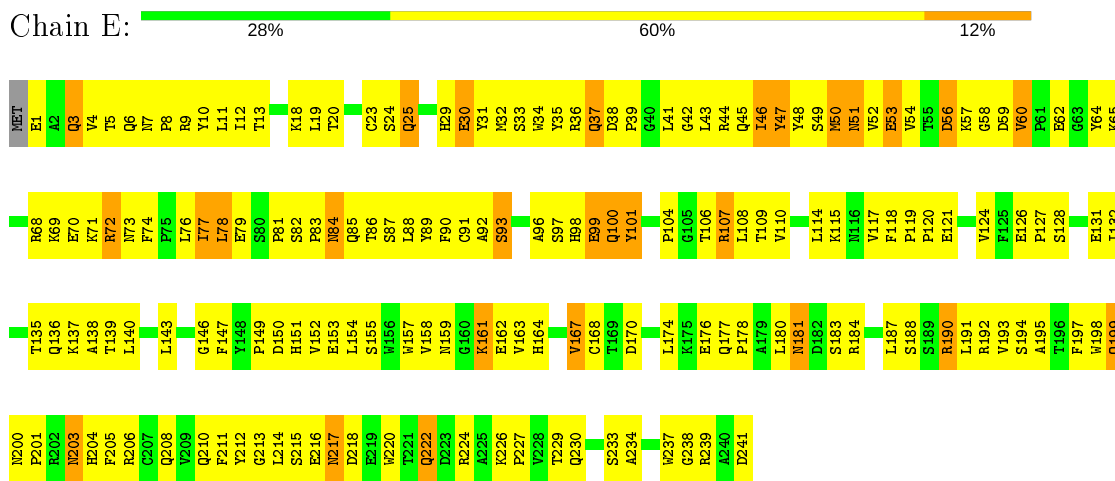


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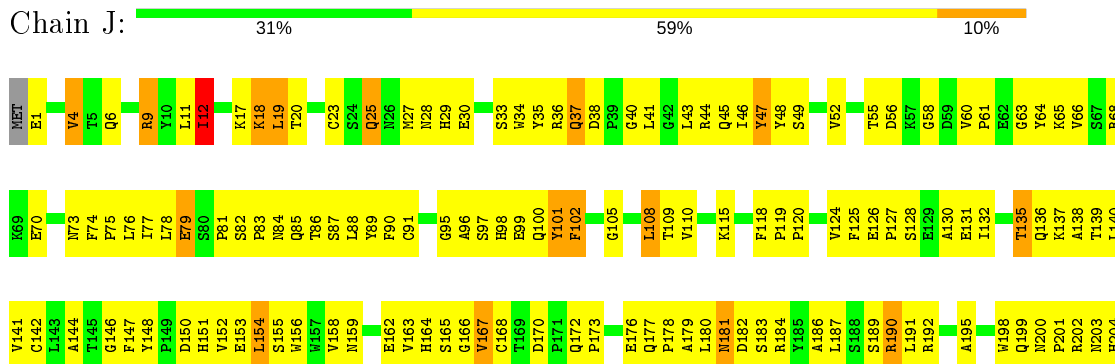
• Molecule 4: T36-5 TCR alpha chain



• Molecule 5: T36-5 TCR beta chain



• Molecule 5: T36-5 TCR beta chain



F205	R206	C207	Q208	V209	Q210	F211	Y212	G213	I214	S215	E216	N217	D218	E219	W220	T221	Q222	I223	R224	A225	K226	P227	Q230	L231	V232	S233	A234	E235	A236	W237	G238	R239	A240	D241
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4 Data and refinement statistics i

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 – 2.60	Depositor EDS
% Data completeness (in resolution range)	92.2 (32.35-2.70) 95.9 (32.35-2.60)	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 0.267 , 0.315	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 , -40.9	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	0.88	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	0.53	0/2282	0.70	0/3092
1	F	0.55	0/2282	0.74	1/3092 (0.0%)
2	B	0.54	0/852	0.71	0/1152
2	G	0.60	0/852	0.71	0/1152
3	C	0.65	0/96	0.83	0/128
3	H	0.65	0/96	0.71	0/128
4	D	0.58	0/1587	0.80	0/2149
4	I	0.59	0/1587	0.80	0/2149
5	E	0.54	0/1986	0.71	0/2705
5	J	0.52	0/1986	0.74	1/2705 (0.0%)
All	All	0.55	0/13606	0.74	2/18452 (0.0%)

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

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	12	ILE	CB-CA-C	-5.57	100.45	111.60
1	F	95	LEU	CA-CB-CG	-5.03	103.74	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	J	101	TYR	Sidechain

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Mol	Chain	Res	Type	Group
5	J	47	TYR	Sidechain

5.2 Too-close contacts [i](#)

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	315	0
1	F	2222	0	2082	278	0
2	B	829	0	794	92	0
2	G	829	0	794	92	0
3	C	91	0	85	24	0
3	H	91	0	85	31	0
4	D	1553	0	1461	212	0
4	I	1553	0	1461	233	0
5	E	1933	0	1845	267	0
5	J	1933	0	1845	282	0
All	All	13256	0	12534	1612	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 62.

All (1612) 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:114:ASN:HA	1:F:108:ARG:NH2	1.66	1.10
4:D:3:GLU:HG3	4:D:4:VAL:H	1.09	1.10
1:A:68:LYS:HZ1	5:E:53:GLU:HB3	1.07	1.09
5:E:107:ARG:HB3	5:E:107:ARG:HH11	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
5:J:181:ASN:ND2	5:J:181:ASN:H	1.52	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:H	5:J:181:ASN:HD22	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:HA	1:F:156:GLN:NE2	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
5:J:36:ARG:HH12	5:J:85:GLN:HA	1.32	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
2:G:24:ASN:HD22	2:G:24:ASN:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:145:ARG:HA	1:A:148:GLU:OE2	1.77	0.85
4:I:159:VAL:HG12	4:I:168:LYS:HZ2	1.42	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
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
1:A:68:LYS:NZ	5:E:53:GLU:HB3	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:SER:CB	1:A:6:ARG:HH12	1.89	0.81
5:E:88:LEU:HD13	5:E:107:ARG:HG2	1.62	0.81
4:D:114:ASN:HB3	1:F:108:ARG:HH12	1.45	0.81
2:G:24:ASN:N	2:G:24:ASN:HD22	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
2:G:24:ASN:N	2:G:24:ASN:ND2	2.25	0.81
4:I:61:PHE:C	4:I:77:ARG:HH22	1.83	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:N	5:E:190:ARG:HD2	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:259:CYS:SG	1:F:272:LEU:HD13	2.22	0.80
1:F:75:ARG:HH11	1:F:75:ARG:HG2	1.46	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:A:19:GLU:OE2	1:A:19:GLU:HA	1.82	0.78
1:F:75:ARG:HG2	1:F:75:ARG:NH1	1.99	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
2:B:21:ASN:CG	2:B:22:PHE:H	1.88	0.77
2:B:56:PHE:HB3	2:B:62:PHE:CD2	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:159:ASN:HD21	5:E:204:HIS:H	1.33	0.77
5:E:52:VAL:HA	5:E:68:ARG:CG	2.14	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:N	5:J:181:ASN:HD22	1.83	0.76
1:A:243:LYS:HD3	1:A:244:TRP:H	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:F:45:MET:N	1:F:64:THR:HG22	1.98	0.76
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:108:ARG:NH2	4:I:114:ASN:HB2	2.01	0.75
1:A:33:PHE:CD1	1:A:34:VAL:N	2.55	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:HD2	4:D:71:TYR:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:MET:CG	1:A:67:VAL:HG11	2.17	0.73
5:E:100:GLN:C	5:E:101:TYR:HD2	1.92	0.73
1:A:80:ILE:HG23	1:A:83:ARG:NH2	2.02	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:161:LYS:NZ	5:E:161:LYS:HB2	2.04	0.73
5:E:119:PRO:HD3	5:E:227:PRO:HB3	1.69	0.73
1:F:121:LYS:HE2	2:G:1:ILE:HG12	1.70	0.73
4:I:160:LEU:HD12	4:I:160:LEU:C	2.08	0.73
5:J:205:PHE:HE2	5:J:238:GLY:N	1.86	0.72
5:J:9:ARG:HB3	5:J:9:ARG:HH11	1.53	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
1:A:137:ASP:O	1:A:141:GLN:HG3	1.90	0.72
5:E:158:VAL:HG23	5:E:163:VAL:HG21	1.70	0.72
4:I:50:ILE:C	4:I:50:ILE:HD12	2.10	0.72
1:F:159:TYR:CD2	1:F:160:LEU:HD23	2.18	0.72
1:F:4:SER:HB2	1:F:102:ASP:OD1	1.89	0.72
4:D:22:ASN:HD22	4:D:71:TYR:HE1	1.38	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
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
4:I:160:LEU:HD13	4:I:162:MET:HE3	1.71	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:OE2	1:A:63:GLU:HA	1.90	0.71
2:G:81:ARG:HA	2:G:92:ILE:HG12	1.72	0.71
1:A:253:GLU:O	1:A:257:TYR:CE2	2.44	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:64:GLN:OE1	4:I:17:ALA:HA	1.92	0.70
4:D:62:THR:HG22	4:D:75:LEU:HD13	1.74	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
4:D:71:TYR:C	4:D:71:TYR:CD2	2.64	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
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:185:ASN:HA	4:D:188:ASN:ND2	2.06	0.69
4:D:94:GLN:HB3	4:D:97:LYS:NZ	2.06	0.69
5:E:77:ILE:N	5:E:77:ILE:HD12	2.07	0.69
2:B:29:GLY:HA2	2:B:61:SER:HB2	1.74	0.69
1:F:185:PRO:HB3	1:F:208:PHE:HB3	1.74	0.69
1:F:35:ARG:HH11	1:F:35:ARG:HG2	1.58	0.69
1:A:200:THR:CG2	1:A:202:ARG:HH12	2.02	0.69
1:A:33:PHE:HD1	1:A:34:VAL:H	1.40	0.69
3:H:4:LEU:HD22	3:H:6:PHE:CE2	2.28	0.69
5:J:108:LEU:C	5:J:108:LEU:HD12	2.12	0.69
1:A:231:VAL:O	1:A:243:LYS:HE3	1.92	0.69
1:A:26:GLY:HA3	1:A:33:PHE:HE1	1.57	0.69
5:E:132:ILE:HG23	5:E:195:ALA:CB	2.23	0.69
4:I:185:ASN:HA	4:I:188:ASN:HD21	1.58	0.69
5:E:132:ILE:HG23	5:E:195:ALA:HB1	1.74	0.69
1:F:202:ARG:HD3	1:F:244:TRP:CD1	2.28	0.69
1:F:28:VAL:HG23	1:F:33:PHE:HD1	1.57	0.69
3:H:4:LEU:HD22	3:H:6:PHE:HE2	1.57	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:HH11	1:F:108:ARG:HG3	1.57	0.69
4:I:97:LYS:HE3	5:J:48:TYR:HE2	1.57	0.69
1:A:209:TYR:HD1	1:A:241:PHE:HE1	1.41	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LYS:HZ1	5:E:53:GLU:CB	1.97	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:N	2:G:7:ILE:HD12	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
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
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
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:19:GLU:CD	1:F:75:ARG:HH21	1.97	0.67
1:F:96:GLN:OE1	2:G:60:TRP:HB3	1.95	0.67
4:D:12:SER:HA	4:D:109:LYS:HZ3	1.60	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
4:I:20:SER:C	4:I:21:LEU:HD23	2.15	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:J:179:ALA:C	5:J:180:LEU:HD12	2.15	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:NZ	1:A:186:LYS:HB2	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
4:I:162:MET:HE3	5:J:166:GLY:HA2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:GLN:OE1	1:A:226:GLN:HA	1.95	0.67
4:D:112:ILE:HG13	4:D:170:ASN:HD21	1.58	0.67
4:D:91:THR:HG23	4:D:91:THR:O	1.95	0.67
1:F:146:LYS:CB	1:F:146:LYS:NZ	2.58	0.66
4:D:89:TRP:HZ3	4:D:91:THR:CG2	2.09	0.66
4:I:159:VAL:CG1	4:I:168:LYS:HZ2	2.07	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
4:D:2:LYS:NZ	5:E:43:LEU:N	2.44	0.66
1:F:234:ARG:HE	1:F:242:GLN:CD	1.98	0.66
5:J:135:THR:O	5:J:137:LYS:NZ	2.29	0.66
4:I:162:MET:CE	5:J:192:ARG:HB3	2.25	0.66
4:I:66:ASN:HB3	4:I:71:TYR:CD2	2.31	0.66
1:A:142:ILE:HA	1:A:145:ARG:HH11	1.60	0.66
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.31	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:J:144:ALA:C	5:J:147:PHE:HE2	1.98	0.66
5:E:9:ARG:NH1	5:E:104:PRO:HB2	2.11	0.66
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:97:MET:HB2	1:F:116:TYR:CE1	2.31	0.66
1:F:70:HIS:HD2	1:F:73:THR:HB	1.58	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
4:D:94:GLN:HG3	4:D:97:LYS:HE2	1.78	0.65
5:E:64:TYR:C	5:E:65:LYS:HD2	2.14	0.65
4:I:20:SER:O	4:I:21:LEU:HD23	1.96	0.65
5:J:79:GLU:HA	5:J:79:GLU:OE1	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
1:F:202:ARG:HH12	1:F:246:ALA:HB2	1.59	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:32:MET:HE1	5:E:71:LYS:O	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:76:GLU:O	1:A:80:ILE:HG13	1.97	0.65
5:E:101:TYR:CD2	5:E:101:TYR:N	2.65	0.65
5:E:23:CYS:HB2	5:E:34:TRP:CZ2	2.31	0.65
4:I:136:THR:HG21	5:J:192:ARG:HH22	1.61	0.65
4:I:38:GLN:HE22	5:J:37:GLN:NE2	1.95	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:CD1	5:J:180:LEU:N	2.59	0.64
2:G:45:ARG:HE	2:G:81:ARG:HH22	1.45	0.64
2:B:24:ASN:N	2:B:24:ASN:ND2	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
4:D:31:GLN:HA	4:D:67:LYS:CE	2.28	0.64
4:D:2:LYS:HZ1	5:E:43:LEU:H	1.44	0.64
4:D:191:ILE:HD12	4:D:191:ILE:N	2.13	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
1:A:69:ALA:CB	5:E:51:ASN:HB2	2.28	0.64
1:A:75:ARG:O	1:A:75:ARG:HD3	1.98	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
2:G:21:ASN:CG	2:G:22:PHE:H	2.01	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:J:206:ARG:HG3	5:J:235:GLU:HB3	1.80	0.63
4:D:191:ILE:CD1	4:D:191:ILE:H	2.10	0.63
5:E:164:HIS:O	5:E:167:VAL:HG13	1.98	0.63
4:D:92:TYR:CE2	5:E:98:HIS:HB3	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HG3	1:F:202:ARG:HH11	1.63	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
5:J:177:GLN:HG3	5:J:180:LEU:HD22	1.81	0.63
4:I:97:LYS:HB3	5:J:48:TYR:CE2	2.34	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
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:111:ARG:NH2	1:A:128:GLU:HA	2.14	0.62
1:A:79:ARG:HH11	1:A:79:ARG:HB2	1.65	0.62
4:D:147:SER:OG	4:D:152:VAL:HG13	1.99	0.62
4:D:48:MET:HE3	4:D:63:ALA:N	2.15	0.62
1:F:127:LYS:CE	1:F:134:THR:HB	2.30	0.62
4:D:182:ALA:HB3	4:D:185:ASN:HD21	1.63	0.62
4:D:31:GLN:HB3	4:D:67:LYS:HZ3	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:HH11	5:E:239:ARG:HG3	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
5:E:150:ASP:OD1	5:E:150:ASP:O	2.17	0.62
1:A:65:GLY:O	5:E:54:VAL:HG11	2.00	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:HG12	4:D:108:VAL:O	1.97	0.62
5:E:4:VAL:HG13	5:E:23:CYS:SG	2.40	0.62
1:F:115:GLN:HG3	2:G:60:TRP:HH2	1.63	0.62
1:F:33:PHE:CD2	1:F:34:VAL:HG13	2.24	0.62
5:J:177:GLN:CB	5:J:180:LEU:HD13	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ARG:NH1	1:A:128:GLU:OE1	2.33	0.62
1:A:99:PHE:CD1	1:A:114:HIS:HD2	2.18	0.62
5:E:128:SER:O	5:E:132:ILE:HD12	1.99	0.62
5:E:48:TYR:HE1	5:E:50:MET:HE2	1.65	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:HD2	5:J:102:PHE:N	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:HB2	1:F:146:LYS:HZ2	1.65	0.61
1:A:111:ARG:HD3	1:A:128:GLU:OE2	1.99	0.61
1:A:7:TYR:CE2	3:C:2:PHE:HA	2.35	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
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: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:168:LEU:O	1:F:172:LEU:HG	2.01	0.61
1:F:63:GLU:O	1:F:67:VAL:HG12	2.00	0.61
4:I:129:ASP:OD1	4:I:130:LYS:HG3	2.01	0.61
2:B:51:HIS:CD2	2:B:64:LEU:HD21	2.33	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
5:J:4:VAL:HG21	5:J:102:PHE:C	2.21	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
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
5:J:163:VAL:O	5:J:164:HIS:ND1	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:TRP:CZ2	1:A:152:VAL:HB	2.36	0.60
2:B:33:SER:HB3	2:B:62:PHE:CD1	2.36	0.60
2:B:23:LEU:HD11	2:B:39:LEU:HD22	1.83	0.60
4:D:18:ILE:HD11	4:D:77:ARG:HG2	1.83	0.60
5:E:19:LEU:HD12	5:E:19:LEU:C	2.22	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:I:41:GLY:C	4:I:42:LYS:HE2	2.21	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:149:ASP:HB3	4:I:152:VAL:HG11	1.81	0.60
4:I:91:THR:OG1	4:I:93:ASN:ND2	2.34	0.60
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:H	5:E:190:ARG:HD2	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:155:GLN:HE22	5:J:98:HIS:CE1	2.19	0.60
1:F:70:HIS:O	1:F:73:THR:HB	2.02	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
1:A:127:LYS:HB2	1:A:129:ASP:OD1	2.01	0.60
1:A:99:PHE:HD1	1:A:114:HIS:HD2	1.49	0.60
4:D:60:ARG:HH22	4:D:83:ASP:CG	2.04	0.60
4:I:158:CYS:HB3	5:J:190:ARG:HH12	1.66	0.60
2:B:7:ILE:N	2:B:7:ILE:HD12	2.16	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:81:ALA:HB1	1:F:118:TYR:CE2	2.37	0.60
1:F:70:HIS:HE1	1:F:97:MET:SD	2.25	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:H	2:B:24:ASN:ND2	1.99	0.59
4:D:71:TYR:C	4:D:71:TYR:HD2	2.04	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:82:SER:O	5:E:110:VAL:HG21	2.02	0.59
5:E:39:PRO:O	5:E:41:LEU:HD22	2.03	0.59
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:152:VAL:HA	1:F:155:GLN:HG3	1.84	0.59
1:F:36:PHE:HB2	1:F:45:MET:CE	2.33	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: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:152:VAL:HG13	4:D:152:VAL:O	2.03	0.58
4:D:148:LYS:CD	4:D:189:ASN:OD1	2.51	0.58
5:E:198:TRP:CZ2	5:E:239:ARG:HB3	2.38	0.58
1:F:181:ARG:NH1	1:F:181:ARG:HG2	2.18	0.58
5:J:138:ALA:O	5:J:192:ARG:HA	2.02	0.58
5:E:154:LEU:HD23	5:E:154:LEU:C	2.23	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:161:ASP:CB	4:I:168:LYS:HE2	2.26	0.58
4:I:74:LEU:HG	4:I:75:LEU:N	2.18	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:132:ILE:HG23	5:J:195:ALA:HB1	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:6:GLN:OE1	5:J:91:CYS:N	2.35	0.58
1:F:244:TRP:C	1:F:244:TRP:HE3	2.07	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
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
4:I:163:ARG:HG2	5:J:165:SER:OG	2.03	0.58
4:I:93:ASN:C	4:I:95:GLY:H	2.07	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:HD22	2:B:24:ASN:H	1.52	0.58
2:B:57:SER:O	2:B:59:ASP:O	2.22	0.58
5:E:20:THR:O	5:E:20:THR:HG23	2.04	0.58
1:A:5:MET:SD	1:A:171:TYR:HE2	2.27	0.58
2:B:1:ILE:HD12	2:B:1:ILE:O	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
4:I:162:MET:HE1	5:J:192:ARG:HB3	1.86	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: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:182:ALA:O	4:I:185:ASN:ND2	2.37	0.57
4:I:97:LYS:HE3	5:J:48:TYR:CE2	2.38	0.57
1:A:200:THR:CG2	1:A:202:ARG:NH1	2.65	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:E:37:GLN:HG2	5:E:42:GLY:C	2.26	0.57
4:I:122:LEU:CD1	5:J:141:VAL:HB	2.33	0.57
3:H:3:PRO:O	3:H:5:THR:HG23	2.04	0.57
4:I:50:ILE:O	4:I:50:ILE:HG13	2.04	0.57
5:J:9:ARG:HH11	5:J:9:ARG:CB	2.18	0.57
4:D:158:CYS:CB	5:E:190:ARG:NH1	2.68	0.57
5:E:135:THR:HG21	5:E:192:ARG:NH1	2.20	0.57
5:E:23:CYS:HB2	5:E:34:TRP:HZ2	1.70	0.57
1:A:68:LYS:HE3	5:E:53:GLU:O	2.05	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
1:F:156:GLN:OE1	3:H:8:TRP:HH2	1.88	0.56
4:I:53:ASN:C	4:I:53:ASN:HD22	2.09	0.56
5:J:206:ARG:NH1	5:J:233:SER:CB	2.64	0.56
1:A:147:TRP:CE3	1:A:152:VAL:HG11	2.40	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:F:143:THR:HA	1:F:146:LYS:HD3	1.88	0.56
4:I:177:ASN:HD22	4:I:178:LYS:N	2.03	0.56
4:I:22:ASN:N	4:I:22:ASN:OD1	2.38	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
1:A:103:VAL:C	1:A:110:LEU:HD22	2.26	0.56
2:B:56:PHE:C	2:B:63:TYR:CE2	2.79	0.56
4:D:48:MET:HE3	4:D:63:ALA:H	1.69	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:141:GLN:O	1:F:145:ARG:HG3	2.04	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
1:F:244:TRP:HE1	2:G:99:MET:CG	2.18	0.56
4:I:167:PHE:C	4:I:167:PHE:CD2	2.79	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
4:D:93:ASN:C	4:D:95:GLY:H	2.10	0.56
5:E:180:LEU:HD12	5:E:180:LEU:N	2.21	0.56
5:E:143:LEU:HD12	5:E:188:SER:HB3	1.87	0.56
2:G:5:PRO:HD3	2:G:84:HIS:HD2	1.71	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
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
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: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
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:HG3	4:I:77:ARG:HH11	1.71	0.55
4:I:123:ARG:HD3	5:J:126:GLU:OE2	2.06	0.55
2:B:10:TYR:N	2:B:10:TYR:CD1	2.75	0.55
1:A:96:GLN:OE1	2:B:60:TRP:HB3	2.06	0.55
5:E:118:PHE:HB3	5:E:184:ARG:NH2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:200:ASN:O	5:J:238:GLY:HA3	2.06	0.55
5:J:36:ARG:NE	5:J:87:SER:CB	2.70	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
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
5:J:27:MET:O	5:J:28:ASN:HB3	2.07	0.55
1:A:224:GLN:O	1:A:228:THR:HG21	2.06	0.55
2:B:21:ASN:CG	2:B:22:PHE:N	2.59	0.55
5:E:124:VAL:HG23	5:E:234:ALA:HB3	1.88	0.55
5:E:77:ILE:C	5:E:78:LEU:HD12	2.27	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
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
5:E:131:GLU:HG2	5:E:137:LYS:O	2.07	0.54
4:D:2:LYS:NZ	5:E:43:LEU:H	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:I:159:VAL:HG12	4:I:168:LYS:HZ1	1.70	0.54
5:J:172:GLN:OE1	5:J:173:PRO:HD2	2.06	0.54
5:J:25:GLN:NE2	5:J:29:HIS:H	2.05	0.54
5:E:211:PHE:HD2	5:E:230:GLN:HG2	1.73	0.54
1:F:35:ARG:C	1:F:35:ARG:HD2	2.28	0.54
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
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:160:LEU:HD11	4:I:167:PHE:CE2	2.35	0.54
4:I:122:LEU:HD11	5:J:141:VAL:HB	1.90	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:133:CYS:SG	4:D:181:PHE:CE1	3.01	0.54
4:D:23:CYS:HB2	4:D:72:VAL:CG1	2.38	0.54
5:E:118:PHE:CE1	5:E:224:ARG:NH2	2.75	0.54
4:I:191:ILE:O	4:I:191:ILE:HG13	2.08	0.54
5:J:153:GLU:HG2	5:J:212:TYR:HE2	1.73	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
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:HH11	1:A:83:ARG:HG2	1.72	0.54
4:D:187:PHE:O	4:D:190:SER:OG	2.26	0.54
4:D:50:ILE:HD11	4:D:65:LEU:CB	2.38	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: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:162:MET:HE2	5:J:192:ARG:HB3	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:178:LYS:HG2	4:I:180:ASP:H	1.73	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
4:D:123:ARG:NH1	5:E:239:ARG:NE	2.57	0.53
1:A:154:GLU:HG3	4:D:51:TYR:CD2	2.43	0.53
4:D:94:GLN:HB3	4:D:97:LYS:HE2	1.88	0.53
1:A:215:LEU:HD12	1:A:243:LYS:CD	2.37	0.53
5:E:117:VAL:HG12	5:E:227:PRO:HB2	1.89	0.53
5:E:35:TYR:HA	5:E:46:ILE:CD1	2.37	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:111:ASN:OD1	4:I:68:ALA:HB3	2.09	0.53
4:D:62:THR:O	4:D:75:LEU:HD12	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:167:VAL:HA	5:E:190:ARG:O	2.09	0.53
5:E:32:MET:SD	5:E:71:LYS:O	2.66	0.53
4:I:178:LYS:HE3	4:I:180:ASP:CB	2.37	0.53
5:E:220:TRP:CH2	5:E:222:GLN:HG3	2.43	0.53
5:E:97:SER:OG	5:E:98:HIS:N	2.33	0.53
1:F:226:GLN:O	1:F:227:ASP:HB2	2.08	0.53
5:J:132:ILE:HG23	5:J:195:ALA:CB	2.38	0.53
5:J:47:TYR:CD1	5:J:66:VAL:HG22	2.43	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
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:H	4:D:88:LEU:HD23	1.73	0.53
4:D:96:GLY:HA3	5:E:50:MET:CE	2.39	0.53
1:F:70:HIS:ND1	3:H:2:PHE:HZ	2.01	0.53
4:I:50:ILE:C	4:I:50:ILE:CD1	2.72	0.52
4:D:182:ALA:HB3	4:D:185:ASN:ND2	2.25	0.52
4:D:114:ASN:CB	1:F:108:ARG:HH22	2.20	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
3:H:9:CYS:SG	5:J:30:GLU:OE1	2.67	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:25:GLN:NE2	5:J:29:HIS:HB2	2.25	0.52
4:I:46:LEU:HD11	5:J:99:GLU:HG2	1.92	0.52
1:A:15:PRO:HG2	1:A:91:GLY:O	2.09	0.52
1:A:8:PHE:HB2	1:A:25:VAL:HG22	1.92	0.52
4:D:123:ARG:CZ	5:E:239:ARG:CZ	2.87	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
1:F:231:VAL:HG22	1:F:244:TRP:O	2.09	0.52
4:I:132:VAL:HG23	5:J:125:PHE:CE1	2.44	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
1:A:130:LEU:CB	1:A:157:ARG:HG3	2.39	0.52
4:D:69:SER:O	4:D:70:GLN:HB2	2.10	0.52
5:E:132:ILE:HD12	5:E:132:ILE:H	1.73	0.52
1:A:66:LYS:HG3	5:E:50:MET:CE	2.40	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: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
1:F:72:GLN:O	1:F:72:GLN:OE1	2.28	0.52
5:J:167:VAL:HA	5:J:190:ARG:O	2.09	0.52
5:J:200:ASN:HD22	5:J:203:ASN:CG	2.13	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
2:B:55:SER:OG	2:B:63:TYR:CE1	2.62	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:O	2:G:1:ILE:HD12	2.10	0.52
4:I:35:TRP:HB2	4:I:48:MET:HB3	1.91	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:E:9:ARG:HH12	5:E:104:PRO:C	2.12	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:206:ARG:HB3	5:J:206:ARG:CZ	2.39	0.52
5:J:41:LEU:CB	5:J:44:ARG:NH1	2.72	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
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:149:ASP:O	4:I:152:VAL:CG1	2.58	0.51
4:I:33:PHE:O	4:I:50:ILE:HG23	2.10	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
2:G:1:ILE:HD12	2:G:1:ILE:C	2.31	0.51
1:F:159:TYR:CZ	3:H:3:PRO:HB3	2.46	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:HA	5:E:136:GLN:OE1	2.10	0.51
5:E:153:GLU:HB2	5:E:210:GLN:HB3	1.92	0.51
5:J:131:GLU:HG2	5:J:137:LYS:O	2.10	0.51
5:J:25:GLN:OE1	5:J:27:MET:N	2.43	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
4:D:131:SER:HB2	4:D:181:PHE:HE2	1.76	0.51
5:E:45:GLN:C	5:E:46:ILE:HD12	2.31	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
1:F:70:HIS:HB2	3:H:2:PHE:HE2	1.76	0.51
4:I:77:ARG:O	4:I:78:ASP:HB3	2.11	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:HG2	5:J:206:ARG:HH11	1.75	0.51
1:A:99:PHE:HD1	1:A:114:HIS:CD2	2.28	0.50
5:E:187:LEU:HG	5:E:188:SER:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:47:TYR:CZ	5:E:57:LYS:HB3	2.45	0.50
5:E:62:GLU:HA	5:E:62:GLU:OE1	2.11	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
5:J:40:GLY:C	5:J:41:LEU:HD22	2.32	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
4:I:160:LEU:CD1	4:I:160:LEU:C	2.79	0.50
5:J:144:ALA:O	5:J:147:PHE:HE2	1.95	0.50
5:J:77:ILE:N	5:J:77:ILE:CD1	2.71	0.50
5:J:36:ARG:HE	5:J:87:SER:CB	2.25	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
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
4:D:147:SER:CB	4:D:152:VAL:HG13	2.41	0.50
5:E:208:GLN:HG2	5:E:233:SER:OG	2.10	0.50
5:E:96:ALA:O	5:E:97:SER:HB3	2.10	0.50
1:F:10:THR:HB	1:F:23:ILE:CG2	2.31	0.50
1:F:7:TYR:HE2	3:H:2:PHE:CA	2.25	0.50
4:I:176:SER:HB3	4:I:181:PHE:CD2	2.46	0.50
4:I:65:LEU:HD21	4:I:67:LYS:HG3	1.93	0.50
5:E:211:PHE:HB3	5:E:230:GLN:O	2.11	0.50
5:E:77:ILE:H	5:E:77:ILE:HD12	1.77	0.50
1:F:244:TRP:C	1:F:244:TRP:CE3	2.85	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
4:D:185:ASN:CA	4:D:188:ASN:ND2	2.75	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
5:J:70:GLU:CD	5:J:73:ASN:HD22	2.15	0.50
4:D:39:TYR:CD1	4:D:85:ALA:HB2	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:99:PHE:HZ	1:F:156:GLN:CD	2.15	0.50
4:I:88:LEU:HB3	4:I:103:GLY:CA	2.41	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:HG13	4:I:152:VAL:O	2.11	0.49
5:J:176:GLU:O	5:J:178:PRO:HD3	2.12	0.49
5:J:96:ALA:O	5:J:97:SER:OG	2.29	0.49
1:A:152:VAL:HG13	1:A:156:GLN:HE21	1.77	0.49
1:A:159:TYR:CE2	1:A:163:THR:HB	2.46	0.49
1:A:3:HIS:HB3	1:A:29:ASP:OD2	2.12	0.49
1:A:75:ARG:C	1:A:75:ARG:HD3	2.32	0.49
1:A:156:GLN:NE2	3:C:8:TRP:CH2	2.79	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:CD1	1:F:147:TRP:N	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
1:A:104:GLY:H	1:A:110:LEU:HD13	1.75	0.49
1:A:9:SER:OG	1:A:97:MET:HB3	2.12	0.49
4:I:136:THR:CG2	5:J:192:ARG:HH22	2.25	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
4:D:133:CYS:SG	4:D:181:PHE:CZ	3.06	0.49
5:E:132:ILE:N	5:E:132:ILE:HD12	2.27	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
1:F:143:THR:HG23	1:F:146:LYS:HD3	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:141:GLN:OE1	4:D:141:GLN:HA	2.13	0.49
4:I:177:ASN:HD22	4:I:177:ASN:C	2.16	0.49
5:J:147:PHE:CZ	5:J:186:ALA:HA	2.47	0.49
1:A:111:ARG:CZ	1:A:128:GLU:HA	2.43	0.49
1:A:55:GLU:OE2	1:A:170:ARG:NH2	2.46	0.49
2:B:92:ILE:N	2:B:92:ILE:HD12	2.28	0.49
1:F:51:TRP:HE1	1:F:179:LEU:HD21	1.78	0.49
4:I:47:ILE:HD12	4:I:47:ILE:C	2.33	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:107:ARG:NH1	5:E:151:HIS:NE2	2.60	0.49
5:E:32:MET:SD	5:E:68:ARG:NH2	2.85	0.49
1:F:272:LEU:H	1:F:272:LEU:HD12	1.77	0.49
1:F:35:ARG:NH1	1:F:35:ARG:HG2	2.26	0.49
1:F:143:THR:HG23	3:H:10:PHE:HA	1.95	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
4:I:4:VAL:HG22	4:I:5:GLU:CD	2.33	0.48
5:J:158:VAL:HG12	5:J:158:VAL:O	2.13	0.48
2:G:12:ARG:HG2	2:G:13:HIS:H	1.78	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
2:B:7:ILE:C	2:B:8:GLN:HE21	2.17	0.48
1:F:202:ARG:HD3	1:F:244:TRP:NE1	2.28	0.48
1:F:51:TRP:CE2	1:F:179:LEU:HD21	2.48	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
4:D:30:SER:C	4:D:31:GLN:HG3	2.32	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
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

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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	0.48
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:A:66:LYS:HG3	5:E:50:MET:HE1	1.95	0.48
1:F:242:GLN:O	1:F:243:LYS:HB2	2.14	0.48
3:H:8:TRP:CD1	3:H:8:TRP:N	2.78	0.48
4:I:167:PHE:CZ	4:I:169:SER:HB3	2.49	0.48
4:I:46:LEU:CD2	5:J:99:GLU:HB3	2.40	0.48
1:F:108:ARG:NH1	1:F:108:ARG:HG3	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:162:MET:HG3	5:J:166:GLY:HA2	1.96	0.48
4:I:160:LEU:C	4:I:168:LYS:HZ3	2.17	0.48
4:I:77:ARG:HG3	4:I:77:ARG:NH1	2.28	0.48
4:I:36:TYR:CE1	5:J:102:PHE:CE2	3.02	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: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
5:J:205:PHE:HE2	5:J:237:TRP:C	2.16	0.48
4:D:192:ILE:HD11	4:D:196:THR:HG21	1.96	0.48
5:E:237:TRP:N	5:E:237:TRP:CD1	2.82	0.48
5:E:19:LEU:HD11	5:E:78:LEU:HD13	1.92	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
5:J:35:TYR:CD1	5:J:45:GLN:HA	2.48	0.48
1:A:242:GLN:O	1:A:243:LYS:HB2	2.13	0.47
2:B:22:PHE:C	2:B:70:PHE:HE1	2.17	0.47
5:E:92:ALA:HB1	5:E:100:GLN:CG	2.30	0.47
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
4:I:114:ASN:HD22	4:I:114:ASN:C	2.18	0.47
1:A:72:GLN:HB2	5:E:51:ASN:CG	2.35	0.47
2:B:41:LYS:HA	2:B:78:TYR:CD2	2.49	0.47
4:D:164:SER:OG	4:D:165:MET:HG2	2.15	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:99:ILE:HD12	4:I:99:ILE:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:108:LEU:C	5:J:108:LEU:CD1	2.82	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
4:I:92:TYR:OH	5:J:98:HIS:O	2.32	0.47
1:A:139:ALA:HA	1:A:142:ILE:CD1	2.44	0.47
5:E:84:ASN:N	5:E:84:ASN:HD22	2.12	0.47
5:J:218:ASP:N	5:J:218:ASP:OD1	2.47	0.47
1:A:194:ILE:HD11	1:A:198:GLU:HB3	1.96	0.47
1:A:229:GLU:O	1:A:230:LEU:HD12	2.14	0.47
1:A:209:TYR:CD1	1:A:241:PHE:HE1	2.27	0.47
4:D:114:ASN:OD1	1:F:108:ARG:NH1	2.47	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
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:81:PRO:HA	4:D:108:VAL:CG1	2.44	0.47
4:D:35:TRP:O	4:D:46:LEU:HD12	2.15	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: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:86:THR:HA	5:J:108:LEU:HD12	1.96	0.47
5:J:204:HIS:NE2	5:J:235:GLU:HB2	2.30	0.47
1:A:185:PRO:HG3	1:A:213:ILE:HD12	1.95	0.47
4:D:80:GLN:C	4:D:108:VAL:HG11	2.35	0.47
4:D:123:ARG:NH1	5:E:239:ARG:CZ	2.78	0.47
5:E:177:GLN:O	5:E:183:SER:HB2	2.14	0.47
5:E:31:TYR:C	5:E:32:MET:HG3	2.34	0.47
1:F:233:THR:CG2	1:F:243:LYS:HD2	2.44	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:49:SER:HB3	5:J:68:ARG:NH1	2.29	0.47
5:J:76:LEU:C	5:J:77:ILE:HD12	2.34	0.47
5:J:97:SER:OG	5:J:98:HIS:N	2.47	0.47
1:A:258:THR:CG2	1:A:271:THR:CG2	2.93	0.47
1:A:26:GLY:CA	1:A:33:PHE:HE1	2.25	0.47
4:D:13:VAL:O	4:D:108:VAL:HA	2.15	0.47
5:E:86:THR:CG2	5:E:109:THR:HA	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:150:ALA:HB3	1:F:152:VAL:HG23	1.95	0.47
1:F:51:TRP:CZ2	1:F:179:LEU:CD2	2.98	0.47
4:I:110:PRO:HD2	4:I:140:SER:OG	2.14	0.47
4:I:50:ILE:HD12	4:I:51:TYR:CA	2.44	0.47
5:J:18:LYS:HB2	5:J:79:GLU:O	2.15	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:135:PHE:CZ	4:I:138:PHE:HB3	2.50	0.47
4:I:4:VAL:HG13	4:I:5:GLU:HG2	1.96	0.47
1:A:130:LEU:HB3	1:A:157:ARG:CG	2.45	0.47
1:A:49:ALA:HB1	1:A:51:TRP:CE2	2.50	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: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
1:F:4:SER:OG	1:F:6:ARG:NE	2.47	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
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
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
1:F:162:GLY:O	1:F:163:THR:C	2.53	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:234:ARG:NH2	2:B:10:TYR:CB	2.78	0.46
2:B:23:LEU:O	2:B:67:TYR:HA	2.15	0.46
1:F:51:TRP:NE1	1:F:179:LEU:HD21	2.29	0.46
1:A:129:ASP:OD2	1:A:131:ARG:HB2	2.15	0.46
1:A:13:SER:HA	1:A:20:PRO:HG3	1.97	0.46
2:B:8:GLN:O	2:B:25:CYS:HA	2.16	0.46
1:F:244:TRP:O	1:F:244:TRP:HE3	1.97	0.46
5:J:215:SER:C	5:J:217:ASN:H	2.18	0.46
5:J:25:GLN:OE1	5:J:28:ASN:N	2.49	0.46
4:D:34:PHE:CD2	4:D:34:PHE:N	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:118:ALA:HB2	4:I:197:PHE:HB3	1.97	0.46
4:I:92:TYR:CE2	5:J:98:HIS:HB3	2.51	0.46
4:D:36:TYR:HD1	4:D:46:LEU:N	2.14	0.46
4:D:23:CYS:HB2	4:D:72:VAL:HG12	1.98	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
5:E:31:TYR:CD2	5:E:100:GLN:NE2	2.84	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:52:VAL:O	5:E:54:VAL:HG23	2.16	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
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
5:E:107:ARG:CZ	5:E:150:ASP:OD1	2.64	0.46
5:E:25:GLN:HB3	5:E:25:GLN:HE21	1.53	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:N	5:J:19:LEU:HD12	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
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
4:D:96:GLY:HA3	5:E:50:MET:HE1	1.96	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
2:B:83:ASN:ND2	2:B:83:ASN:C	2.68	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:117:VAL:HG12	5:E:227:PRO:CB	2.46	0.46
5:E:53:GLU:OE1	5:E:69:LYS:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:SER:O	1:F:92:SER:HB2	2.16	0.46
4:I:160:LEU:CD1	4:I:162:MET:HE3	2.42	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
3:H:6:PHE:CZ	5:J:98:HIS:CD2	3.02	0.46
4:D:156:ASP:OD2	4:D:157:LYS:HD3	2.15	0.46
1:F:120:GLY:CA	2:G:31:HIS:NE2	2.79	0.46
1:F:93:HIS:HB3	1:F:118:TYR:CE1	2.51	0.46
4:D:189:ASN:HD22	4:D:189:ASN:HA	1.66	0.45
4:D:88:LEU:N	4:D:88:LEU:CD2	2.78	0.45
5:E:36:ARG:NH2	5:E:87:SER:HB2	2.23	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
5:J:218:ASP:O	5:J:226:LYS:NZ	2.42	0.45
1:A:152:VAL:HG13	1:A:156:GLN:NE2	2.30	0.45
1:A:190:THR:HG21	2:B:98:ASP:CG	2.36	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
5:J:154:LEU:HD22	5:J:155:SER:H	1.81	0.45
4:I:159:VAL:N	5:J:168:CYS:SG	2.88	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
2:B:5:PRO:O	2:B:7:ILE:HD12	2.17	0.45
1:F:240:THR:C	1:F:241:PHE:CD1	2.90	0.45
2:G:37:VAL:HG13	2:G:80:CYS:SG	2.56	0.45
4:I:135:PHE:HB2	4:I:187:PHE:CE2	2.51	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:62:PHE:N	2:G:62:PHE:CD1	2.84	0.45
2:G:23:LEU:O	2:G:67:TYR:HA	2.17	0.45
2:G:81:ARG:CB	2:G:92:ILE:HG12	2.47	0.45
5:J:154:LEU:HD22	5:J:155:SER:N	2.31	0.45
5:J:82:SER:HB2	5:J:84:ASN:OD1	2.16	0.45
5:J:97:SER:C	5:J:98:HIS:ND1	2.70	0.45
2:B:23:LEU:HG	2:B:23:LEU:O	2.17	0.45
4:D:91:THR:CG2	4:D:91:THR:O	2.63	0.45
5:E:72:ARG:H	5:E:72:ARG:HD2	1.81	0.45
5:E:79:GLU:C	5:E:81:PRO:HD3	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:202:ARG:HD2	1:F:204:TRP:CE2	2.51	0.45
1:F:43:GLN:HE21	1:F:43:GLN:CA	2.28	0.45
2:G:45:ARG:HB2	2:G:81:ARG:NH2	2.30	0.45
2:G:40:LEU:HD11	2:G:81:ARG:HB2	1.99	0.45
5:E:108:LEU:HD12	5:E:109:THR:H	1.82	0.45
5:E:49:SER:CB	5:E:74:PHE:CE1	3.00	0.45
1:F:117:ALA:CB	2:G:60:TRP:CD2	2.99	0.45
1:F:99:PHE:CE2	1:F:159:TYR:CE2	3.03	0.45
1:F:256:ARG:HG2	1:F:256:ARG:HH11	1.82	0.45
4:I:160:LEU:C	4:I:168:LYS:NZ	2.70	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
1:A:186:LYS:HB2	1:A:186:LYS:HZ3	1.80	0.45
5:E:88:LEU:CD1	5:E:107:ARG:HG2	2.41	0.45
5:J:11:LEU:HD12	5:J:12:ILE:H	1.80	0.45
1:A:188:HIS:CE1	1:A:204:TRP:CB	3.00	0.45
1:A:43:GLN:NE2	1:A:43:GLN:HA	2.32	0.45
5:E:124:VAL:HG23	5:E:234:ALA:CB	2.46	0.45
3:C:7:GLY:N	5:E:30:GLU:HG3	2.25	0.45
5:J:20:THR:OG1	5:J:77:ILE:HG13	2.17	0.45
5:J:210:GLN:NE2	5:J:231:ILE:CG1	2.80	0.45
5:J:52:VAL:HG13	5:J:68:ARG:O	2.17	0.45
4:D:154:ILE:O	4:D:154:ILE:HG22	2.17	0.45
4:D:89:TRP:HZ3	4:D:91:THR:HG22	1.77	0.45
1:F:99:PHE:CE1	1:F:114:HIS:CG	3.04	0.45
1:A:200:THR:HG21	1:A:202:ARG:CZ	2.47	0.44
4:D:139:ASP:C	4:D:141:GLN:H	2.20	0.44
5:E:127:PRO:HG3	5:E:139:THR:C	2.38	0.44
5:E:215:SER:C	5:E:217:ASN:H	2.20	0.44
5:E:38:ASP:OD2	5:E:44:ARG:NH2	2.44	0.44
1:F:70:HIS:HD2	1:F:73:THR:CB	2.27	0.44
2:G:21:ASN:CG	2:G:22:PHE:N	2.69	0.44
4:I:102:GLN:OE1	4:I:102:GLN:C	2.56	0.44
4:I:116:ASP:N	4:I:117:PRO:HD3	2.32	0.44
4:I:21:LEU:N	4:I:21:LEU:HD23	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
1:A:97:MET:HE2	1:A:99:PHE:HB2	1.99	0.44
4:D:12:SER:CB	4:D:109:LYS:HZ1	2.30	0.44
4:D:17:ALA:HB2	4:I:71:TYR:OH	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:272:LEU:CD1	1:F:272:LEU:N	2.74	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
4:I:161:ASP:HB2	4:I:168:LYS:HG2	2.00	0.44
4:I:23:CYS:HB3	4:I:89:TRP:CZ2	2.52	0.44
3:H:7:GLY:HA2	5:J:30:GLU:CG	2.48	0.44
1:A:57:PRO:CA	1:A:60:TRP:HD1	2.26	0.44
4:D:136:THR:OG1	4:D:137:ASP:N	2.50	0.44
4:D:15:GLU:HG3	4:D:16:GLY:N	2.33	0.44
1:F:202:ARG:HD3	1:F:244:TRP:CG	2.52	0.44
4:I:87:TYR:C	4:I:88:LEU:HD23	2.37	0.44
1:A:208:PHE:CZ	1:A:241:PHE:HB2	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
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
3:C:4:LEU:O	5:E:98:HIS:NE2	2.50	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: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
1:A:63:GLU:O	1:A:67:VAL:HG12	2.17	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
4:D:75:LEU:N	4:D:75:LEU:HD12	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:189:MET:HB2	1:F:189:MET:HE2	1.82	0.44
1:F:51:TRP:CZ2	1:F:179:LEU:CD1	3.00	0.44
4:I:93:ASN:C	4:I:95:GLY:N	2.70	0.44
5:J:152:VAL:HG12	5:J:210:GLN:O	2.17	0.44
5:J:36:ARG:NH2	5:J:84:ASN:O	2.46	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
4:I:185:ASN:HD22	4:I:185:ASN:C	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:138:PHE:O	4:D:170:ASN:ND2	2.51	0.44
3:C:4:LEU:CD2	4:D:96:GLY:HA2	2.46	0.44
5:E:8:PRO:O	5:E:106:THR:HG23	2.17	0.44
1:F:156:GLN:OE1	3:H:8:TRP:CH2	2.70	0.44
1:F:99:PHE:CE2	3:H:3:PRO:HB3	2.53	0.44
4:I:38:GLN:CG	4:I:44:PRO:HG3	2.48	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:A:68:LYS:NZ	5:E:53:GLU:O	2.51	0.44
1:F:144:LYS:O	1:F:148:GLU:CG	2.65	0.44
1:F:67:VAL:HG13	1:F:68:LYS:N	2.33	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
5:E:70:GLU:HB3	5:E:72:ARG:HD2	2.00	0.44
1:F:106:ASP:CG	1:F:108:ARG:HB2	2.38	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
1:F:51:TRP:C	1:F:51:TRP:HE3	2.22	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
5:E:86:THR:O	5:E:87:SER:HB2	2.18	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:11:SER:OG	1:A:78:LEU:HD11	2.18	0.43
4:D:11:LEU:HG	4:D:12:SER:N	2.31	0.43
1:A:159:TYR:CD1	4:D:31:GLN:OE1	2.70	0.43
1:A:65:GLY:HA2	5:E:54:VAL:CG1	2.48	0.43
1:F:106:ASP:OD2	1:F:108:ARG:CB	2.58	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:41:LEU:N	5:J:41:LEU:HD22	2.33	0.43
5:E:181:ASN:N	5:E:181:ASN:OD1	2.51	0.43
1:A:150:ALA:HB1	5:E:96:ALA:HB1	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:88:LEU:HD12	4:I:100:PHE:CD1	2.53	0.43
1:A:170:ARG:HH11	1:A:170:ARG:HG3	1.84	0.43
1:A:50:PRO:HA	1:A:53:GLU:OE2	2.19	0.43
4:D:53:ASN:HA	4:D:65:LEU:HD23	1.99	0.43
4:I:109:LYS:HD2	4:I:140:SER:OG	2.18	0.43
4:I:38:GLN:CB	4:I:44:PRO:HG3	2.48	0.43
5:J:43:LEU:HD12	5:J:44:ARG:N	2.32	0.43
1:A:19:GLU:CA	1:A:19:GLU:OE2	2.54	0.43
1:A:268:LYS:HG3	1:A:269:PRO:HD2	2.01	0.43
3:C:4:LEU:CD2	3:C:6:PHE:HE2	2.30	0.43
1:F:231:VAL:HG13	1:F:244:TRP:CH2	2.54	0.43
1:F:22:PHE:CE2	1:F:71:SER:HB3	2.52	0.43
4:I:160:LEU:O	4:I:168:LYS:HA	2.19	0.43
5:J:150:ASP:C	5:J:151:HIS:HD2	2.22	0.43
4:D:110:PRO:HG2	4:D:112:ILE:HD11	2.00	0.43
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
1:A:208:PHE:HZ	1:A:233:THR:HG23	1.84	0.43
1:A:33:PHE:CD1	1:A:33:PHE:C	2.91	0.43
1:A:48:ARG:HA	1:A:48:ARG:HD2	1.63	0.43
1:A:44:ARG:HA	1:A:64:THR:HG23	2.00	0.43
2:B:56:PHE:CD2	2:B:62:PHE:HE2	2.36	0.43
1:A:147:TRP:CZ2	3:C:8:TRP:HB3	2.54	0.43
4:D:81:PRO:N	4:D:108:VAL:HG11	2.34	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:205:ALA:O	1:F:208:PHE:HE1	2.02	0.43
5:J:152:VAL:HA	5:J:210:GLN:O	2.19	0.43
5:J:46:ILE:O	5:J:58:GLY:N	2.41	0.43
1:A:162:GLY:O	1:A:163:THR:C	2.57	0.43
1:A:191:HIS:CE1	1:A:193:PRO:HG3	2.54	0.43
1:A:82:LEU:HD22	1:A:87:GLN:HB2	2.01	0.43
4:D:116:ASP:N	4:D:117:PRO:HD3	2.33	0.43
4:D:194:GLU:HA	4:D:194:GLU:OE1	2.19	0.43
1:A:158:ALA:HB1	4:D:31:GLN:CB	2.49	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:127:PRO:HD2	5:J:198:TRP:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:38:ASP:CB	5:J:44:ARG:HH22	2.30	0.43
1:A:130:LEU:O	1:A:157:ARG:HG3	2.18	0.43
1:A:44:ARG:HG2	1:A:64:THR:HG21	2.01	0.43
2:B:23:LEU:HD21	2:B:39:LEU:HD13	2.01	0.43
4:D:111:ASN:HA	4:D:111:ASN:HD22	1.48	0.43
5:E:132:ILE:HG23	5:E:195:ALA:HB2	1.99	0.43
5:E:19:LEU:HD12	5:E:19:LEU:O	2.19	0.43
1:F:104:GLY:CA	1:F:110:LEU:HD23	2.49	0.43
1:F:99:PHE:HE1	1:F:114:HIS:CG	2.37	0.43
1:F:218:GLN:OE1	1:F:223:ASP:N	2.52	0.43
1:F:7:TYR:HE1	1:F:33:PHE:CZ	2.36	0.43
2:G:9:VAL:HA	2:G:24:ASN:O	2.18	0.43
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:111:ARG:HD3	1:A:128:GLU:CD	2.39	0.42
1:A:200:THR:HG21	1:A:202:ARG:NH2	2.34	0.42
1:A:98:MET:SD	1:A:99:PHE:N	2.91	0.42
4:I:193:PRO:HB2	4:I:196:THR:OG1	2.19	0.42
4:I:42:LYS:N	4:I:42:LYS:HE2	2.34	0.42
1:A:150:ALA:HB3	1:A:152:VAL:HG23	2.01	0.42
4:D:112:ILE:HD13	4:D:112:ILE:N	2.34	0.42
4:D:30:SER:HB3	4:D:33:PHE:CE2	2.54	0.42
4:D:32:SER:C	4:D:33:PHE:HD2	2.22	0.42
4:D:43:SER:HA	5:E:90:PHE:CZ	2.55	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
1:F:33:PHE:C	1:F:48:ARG:HB2	2.40	0.42
2:G:12:ARG:HD2	2:G:22:PHE:CB	2.39	0.42
5:J:132:ILE:N	5:J:132:ILE:CD1	2.82	0.42
5:J:64:TYR:CD1	5:J:78:LEU:CD1	3.02	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:HA	1:A:268:LYS:HD2	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:114:LEU:HD13	5:E:214:LEU:HD21	2.02	0.42
5:E:86:THR:OG1	5:E:110:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:125:ALA:O	1:F:134:THR:CG2	2.68	0.42
1:F:137:ASP:OD1	1:F:137:ASP:C	2.56	0.42
1:F:159:TYR:OH	3:H:1:ARG:O	2.31	0.42
4:I:185:ASN:ND2	4:I:185:ASN:C	2.70	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
5:J:79:GLU:C	5:J:81:PRO:HD3	2.40	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:25:TYR:CE2	4:D:33:PHE:CZ	3.07	0.42
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
1:A:44:ARG:HA	1:A:64:THR:CG2	2.50	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:163:ARG:H	4:I:163:ARG:HG2	1.42	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
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
4:D:37:ARG:CB	4:D:47:ILE:HD13	2.49	0.42
5:E:154:LEU:HD23	5:E:155:SER:CA	2.48	0.42
5:E:64:TYR:CD1	5:E:76:LEU:HD21	2.55	0.42
1:F:34:VAL:CG1	1:F:60:TRP:HH2	2.33	0.42
5:J:131:GLU:O	5:J:135:THR:OG1	2.19	0.42
1:A:51:TRP:HZ3	1:A:52:ILE:HD13	1.85	0.42
1:A:98:MET:C	1:A:98:MET:SD	2.98	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:185:ASN:N	4:I:185:ASN:HD22	2.16	0.42
4:I:89:TRP:CD1	4:I:89:TRP:N	2.88	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:60:ARG:NH2	4:D:83:ASP:OD2	2.42	0.42
5:E:239:ARG:NH1	5:E:239:ARG:HG3	2.33	0.42
4:D:2:LYS:NZ	5:E:42:GLY:HA3	2.35	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
1:F:22:PHE:CD2	1:F:71:SER:CB	3.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:134:THR:HG23	1:A:134:THR:O	2.20	0.42
1:A:123:TYR:CE1	1:A:140:ALA:HA	2.55	0.42
2:B:33:SER:HB3	2:B:62:PHE:CE1	2.55	0.42
2:B:22:PHE:C	2:B:70:PHE:CE1	2.93	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:191:HIS:HB2	1:F:274:TRP:CZ3	2.55	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
2:G:35:ILE:HD11	2:G:84:HIS:CG	2.55	0.42
5:J:89:TYR:CE2	5:J:108:LEU:HG	2.55	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
1:A:123:TYR:CE2	3:C:10:PHE:CE2	3.08	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:A:150:ALA:CB	5:E:96:ALA:HB1	2.50	0.42
1:F:82:LEU:HD21	1:F:93:HIS:CE1	2.55	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:N	5:E:3:GLN:OE1	2.53	0.41
1:F:77:ASN:HA	1:F:80:ILE:HD12	2.02	0.41
1:F:8:PHE:HE2	1:F:27:TYR:CD1	2.38	0.41
4:I:98:LEU:HD12	5:J:35:TYR:OH	2.19	0.41
1:A:52:ILE:HA	1:A:52:ILE:HD12	1.88	0.41
1:A:232:GLU:CD	2:B:6:LYS:HE2	2.40	0.41
4:D:93:ASN:C	4:D:95:GLY:N	2.73	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:120:PRO:HG2	5:J:232:VAL:CG2	2.49	0.41
5:J:176:GLU:C	5:J:178:PRO:HD3	2.39	0.41
5:J:29:HIS:CD2	5:J:95:GLY:HA3	2.55	0.41
1:A:173:GLU:OE1	1:A:176:LYS:HD3	2.21	0.41
1:A:244:TRP:C	1:A:244:TRP:CE3	2.93	0.41
1:A:213:ILE:CG1	1:A:262:GLN:O	2.59	0.41
1:A:74:ASP:HB3	1:A:95:LEU:HD23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:ILE:C	2:B:8:GLN:NE2	2.73	0.41
5:E:87:SER:OG	5:E:88:LEU:N	2.52	0.41
1:F:23:ILE:O	1:F:23:ILE:CG2	2.68	0.41
1:F:3:HIS:HB3	1:F:29:ASP:OD2	2.19	0.41
2:G:12:ARG:NH1	2:G:22:PHE:CD1	2.88	0.41
5:J:25:GLN:NE2	5:J:29:HIS:N	2.68	0.41
1:A:14:ARG:HB3	1:A:17:ARG:HB2	2.01	0.41
1:A:255:GLN:HB3	1:A:255:GLN:HE21	1.71	0.41
1:A:70:HIS:HA	1:A:73:THR:OG1	2.21	0.41
5:E:11:LEU:HD21	5:E:19:LEU:HD22	2.02	0.41
5:E:7:ASN:HA	5:E:8:PRO:HA	1.64	0.41
1:F:156:GLN:O	1:F:159:TYR:HB3	2.20	0.41
1:F:204:TRP:HH2	2:G:99:MET:HE2	1.85	0.41
1:F:33:PHE:O	1:F:48:ARG:N	2.47	0.41
4:I:114:ASN:HA	4:I:115:PRO:HD2	1.94	0.41
4:I:13:VAL:O	4:I:108:VAL:HA	2.21	0.41
5:J:132:ILE:CG2	5:J:195:ALA:HB1	2.49	0.41
5:J:19:LEU:HD11	5:J:78:LEU:HB3	2.02	0.41
5:E:220:TRP:NE1	5:E:226:LYS:HA	2.36	0.41
5:E:82:SER:HB2	5:E:85:GLN:CG	2.50	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:158:ALA:HB1	4:D:31:GLN:HB2	2.03	0.41
2:B:23:LEU:C	2:B:23:LEU:HD12	2.41	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: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
5:E:25:GLN:OE1	5:E:29:HIS:HB2	2.19	0.41
5:E:77:ILE:CD1	5:E:77:ILE:N	2.77	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
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
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:HZ3	5:E:161:LYS:HB2	1.83	0.41
1:F:80:ILE:CD1	3:H:10:PHE:H	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:141:GLN:HA	4:I:141:GLN:OE1	2.21	0.41
1:A:5:MET:SD	1:A:171:TYR:CE2	3.10	0.41
1:A:87:GLN:OE1	1:A:118:TYR:OH	2.31	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:J:163:VAL:C	5:J:164:HIS:ND1	2.74	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
5:J:47:TYR:CE2	5:J:61:PRO:HB2	2.56	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
1:F:127:LYS:HG3	1:F:134:THR:HG22	2.02	0.41
5:E:117:VAL:HG12	5:E:227:PRO:CG	2.51	0.41
1:A:68:LYS:CB	5:E:54:VAL:HG22	2.51	0.41
5:E:97:SER:O	5:E:98:HIS:ND1	2.54	0.41
1:F:34:VAL:HG12	1:F:60:TRP:HH2	1.86	0.41
1:F:55:GLU:OE1	1:F:55:GLU:HA	2.21	0.41
2:G:30:PHE:O	2:G:62:PHE:CD1	2.73	0.41
2:G:4:THR:OG1	2:G:87:LEU:HD21	2.20	0.41
1:F:70:HIS:ND1	3:H:2:PHE:CZ	2.70	0.41
4:I:18:ILE:HA	4:I:76:ILE:O	2.20	0.41
1:A:124:ILE:HD11	1:A:144:LYS:HB2	2.03	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
5:E:187:LEU:HG	5:E:188:SER:H	1.85	0.41
5:E:9:ARG:NH1	5:E:104:PRO:CB	2.81	0.41
1:F:183:ASP:HA	1:F:184:PRO:HD3	1.79	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
4:I:134:LEU:CD2	5:J:139:THR:HG21	2.51	0.41
5:J:150:ASP:C	5:J:151:HIS:CD2	2.95	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:217:ASN:ND2	5:E:217:ASN:N	2.68	0.40
5:E:25:GLN:OE1	5:E:29:HIS:N	2.31	0.40
5:E:57:LYS:H	5:E:57:LYS:HG2	1.55	0.40
1:F:143:THR:HA	1:F:146:LYS:CD	2.51	0.40
4:I:114:ASN:ND2	4:I:114:ASN:C	2.74	0.40
5:J:118:PHE:O	5:J:147:PHE:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:154:LEU:CG	5:J:209:VAL:HG22	2.49	0.40
1:A:34:VAL:HG21	1:A:45:MET:HE1	2.03	0.40
4:D:9:GLY:HA2	4:D:10:PRO:HD3	1.73	0.40
5:E:159:ASN:HD22	5:E:204:HIS:HB3	1.87	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
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
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
1:A:33:PHE:C	1:A:48:ARG:HB2	2.42	0.40
4:D:160:LEU:HD12	4:D:160:LEU:O	2.21	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
1:F:115:GLN:CG	2:G:60:TRP:CH2	2.93	0.40
4:I:170:ASN:O	4:I:171:SER:HB3	2.21	0.40
4:I:94:GLN:HB3	4:I:97:LYS:CD	2.30	0.40
5:J:159:ASN:ND2	5:J:204:HIS:N	2.56	0.40
5:J:206:ARG:NH2	5:J:208:GLN:HE21	2.20	0.40
5:J:205:PHE:CD2	5:J:236:ALA:O	2.70	0.40
5:J:47:TYR:HE2	5:J:61:PRO:HB2	1.86	0.40
5:J:33:SER:HA	5:J:74:PHE:HE2	1.86	0.40
5:J:9:ARG:NH1	5:J:9:ARG:CG	2.83	0.40
1:A:181:ARG:HG2	1:A:181:ARG:HH11	1.86	0.40
1:A:191:HIS:HE1	1:A:193:PRO:HG3	1.86	0.40
1:A:31:THR:OG1	1:A:209:TYR:OH	2.36	0.40
2:B:12:ARG:N	2:B:21:ASN:HD21	2.18	0.40
1:F:228:THR:HG22	1:F:247:VAL:CG1	2.46	0.40
2:G:16:GLU:OE2	2:G:19:LYS:NZ	2.47	0.40
5:J:206:ARG:HH11	5:J:206:ARG:CG	2.34	0.40
1:A:234:ARG:CZ	2:B:10:TYR:CG	3.04	0.40
1:A:99:PHE:CD2	3:C:3:PRO:HG3	2.57	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:95:TRP:CD1	2:G:95:TRP:C	2.92	0.40
4:I:122:LEU:HD11	5:J:141:VAL:CB	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:156:TRP:HZ2	5:J:189:SER:O	2.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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%)	34	60
1	F	272/275 (99%)	257 (94%)	14 (5%)	1 (0%)	34	60
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%)	4	10
4	I	197/205 (96%)	169 (86%)	22 (11%)	6 (3%)	4	10
5	E	239/242 (99%)	223 (93%)	15 (6%)	1 (0%)	34	60
5	J	239/242 (99%)	220 (92%)	18 (8%)	1 (0%)	34	60
All	All	1626/1664 (98%)	1497 (92%)	113 (7%)	16 (1%)	15	37

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

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Mol	Chain	Res	Type
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
5	J	222	GLN
4	I	9	GLY

5.3.2 Protein sidechains [i](#)

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	6
1	F	230/231 (100%)	190 (83%)	40 (17%)	2	5
2	B	94/95 (99%)	77 (82%)	17 (18%)	1	4
2	G	94/95 (99%)	78 (83%)	16 (17%)	2	5
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%)	145 (82%)	32 (18%)	1	4
4	I	177/183 (97%)	144 (81%)	33 (19%)	1	4
5	E	214/215 (100%)	176 (82%)	38 (18%)	2	4
5	J	214/215 (100%)	185 (86%)	29 (14%)	3	8
All	All	1448/1466 (99%)	1207 (83%)	241 (17%)	2	5

All (241) 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

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Mol	Chain	Res	Type
1	A	33	PHE
1	A	34	VAL
1	A	39	ASP
1	A	60	TRP
1	A	74	ASP
1	A	75	ARG
1	A	79	ARG
1	A	86	ASN
1	A	89	GLU
1	A	97	MET
1	A	98	MET
1	A	116	TYR
1	A	122	ASP
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	216	THR
1	A	225	THR
1	A	229	GLU
1	A	230	LEU
1	A	231	VAL
1	A	234	ARG
1	A	238	ASP
1	A	242	GLN
1	A	247	VAL
1	A	248	VAL
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

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Mol	Chain	Res	Type
2	B	64	LEU
2	B	70	PHE
2	B	74	GLU
2	B	83	ASN
2	B	84	HIS
2	B	85	VAL
2	B	86	THR
2	B	87	LEU
4	D	6	GLN
4	D	7	ASN
4	D	15	GLU
4	D	20	SER
4	D	31	GLN
4	D	33	PHE
4	D	34	PHE
4	D	48	MET
4	D	50	ILE
4	D	71	TYR
4	D	73	SER
4	D	88	LEU
4	D	98	LEU
4	D	100	PHE
4	D	102	GLN
4	D	104	THR
4	D	106	LEU
4	D	111	ASN
4	D	124	ASP
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	157	LYS
4	D	162	MET
4	D	167	PHE
4	D	180	ASP
4	D	189	ASN
4	D	191	ILE
4	D	192	ILE
5	E	1	GLU
5	E	3	GLN

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Mol	Chain	Res	Type
5	E	13	THR
5	E	18	LYS
5	E	25	GLN
5	E	30	GLU
5	E	33	SER
5	E	37	GLN
5	E	46	ILE
5	E	47	TYR
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	120	PRO
5	E	121	GLU
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	199	GLN
5	E	203	ASN
5	E	216	GLU
5	E	217	ASN
5	E	241	ASP
1	F	19	GLU
1	F	35	ARG
1	F	38	SER
1	F	39	ASP
1	F	43	GLN
1	F	51	TRP

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Mol	Chain	Res	Type
1	F	54	GLN
1	F	72	GLN
1	F	75	ARG
1	F	79	ARG
1	F	85	TYR
1	F	86	ASN
1	F	94	THR
1	F	98	MET
1	F	99	PHE
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	170	ARG
1	F	174	ASN
1	F	177	GLU
1	F	186	LYS
1	F	188	HIS
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	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	17	ASN
2	G	24	ASN
2	G	31	HIS
2	G	35	ILE
2	G	36	GLU
2	G	40	LEU

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Mol	Chain	Res	Type
2	G	50	GLU
2	G	59	ASP
2	G	62	PHE
2	G	65	LEU
2	G	68	THR
2	G	70	PHE
2	G	89	GLN
2	G	96	ASP
4	I	2	LYS
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	50	ILE
4	I	53	ASN
4	I	57	GLU
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	114	ASN
4	I	116	ASP
4	I	128	SER
4	I	129	ASP
4	I	146	GLN
4	I	160	LEU
4	I	163	ARG
4	I	167	PHE
4	I	177	ASN
4	I	180	ASP
4	I	185	ASN
4	I	190	SER
4	I	194	GLU
5	J	1	GLU

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Mol	Chain	Res	Type
5	J	4	VAL
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	37	GLN
5	J	55	THR
5	J	56	ASP
5	J	79	GLU
5	J	101	TYR
5	J	102	PHE
5	J	108	LEU
5	J	115	LYS
5	J	135	THR
5	J	154	LEU
5	J	167	VAL
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	218	ASP
5	J	230	GLN
5	J	232	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	43	GLN
1	A	77	ASN
1	A	86	ASN
1	A	114	HIS
1	A	141	GLN
1	A	155	GLN
1	A	156	GLN
1	A	180	GLN
1	A	188	HIS

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Mol	Chain	Res	Type
1	A	192	HIS
1	A	218	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	64	GLN
4	D	170	ASN
4	D	185	ASN
4	D	188	ASN
5	E	51	ASN
5	E	73	ASN
5	E	84	ASN
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	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	53	ASN
4	I	64	GLN
4	I	70	GLN

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Mol	Chain	Res	Type
4	I	80	GLN
4	I	93	ASN
4	I	113	GLN
4	I	114	ASN
4	I	177	ASN
4	I	185	ASN
4	I	188	ASN
4	I	189	ASN
5	J	37	GLN
5	J	98	HIS
5	J	151	HIS
5	J	159	ASN
5	J	181	ASN
5	J	200	ASN
5	J	208	GLN
5	J	210	GLN
5	J	217	ASN
5	J	230	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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

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%)	0.02	9 (3%) 46 46	36, 69, 105, 120	0
1	F	274/275 (99%)	-0.16	3 (1%) 80 82	33, 67, 86, 91	0
2	B	99/100 (99%)	0.02	2 (2%) 65 67	53, 68, 93, 97	0
2	G	99/100 (99%)	0.25	5 (5%) 28 26	49, 79, 96, 101	0
3	C	10/10 (100%)	-0.46	0 100 100	44, 48, 56, 57	0
3	H	10/10 (100%)	-0.16	0 100 100	34, 40, 59, 64	0
4	D	199/205 (97%)	0.06	3 (1%) 73 76	32, 61, 97, 115	0
4	I	199/205 (97%)	0.09	5 (2%) 57 59	20, 64, 102, 119	0
5	E	241/242 (99%)	-0.27	0 100 100	35, 64, 81, 92	0
5	J	241/242 (99%)	-0.25	0 100 100	29, 62, 84, 94	0
All	All	1646/1664 (98%)	-0.07	27 (1%) 72 74	20, 66, 96, 120	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	I	164	SER	5.2
4	D	131	SER	4.8
4	I	165	MET	4.5
1	A	199	ALA	4.4
1	A	215	LEU	3.9
1	A	185	PRO	3.8
4	D	4	VAL	3.7
1	A	201	LEU	3.3
4	D	5	GLU	3.2
1	A	214	THR	3.0
4	I	4	VAL	2.8
1	F	257	TYR	2.7
1	A	112	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	99	PHE	2.7
2	B	15	ALA	2.6
2	G	23	LEU	2.6
1	A	274	TRP	2.5
2	G	15	ALA	2.4
2	G	80	CYS	2.4
1	F	247	VAL	2.3
1	F	126	LEU	2.2
2	G	52	SER	2.2
4	I	6	GLN	2.1
2	G	14	PRO	2.1
1	A	187	THR	2.0
4	I	72	VAL	2.0
2	B	46	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.