



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 08:50 am BST

PDB ID : 5W1T
Title : X-ray crystal structure of Escherichia coli RNA polymerase and DksA complex
Authors : Murakami, K.S.; Molodtsov, V.
Deposited on : 2017-06-04
Resolution : 4.50 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

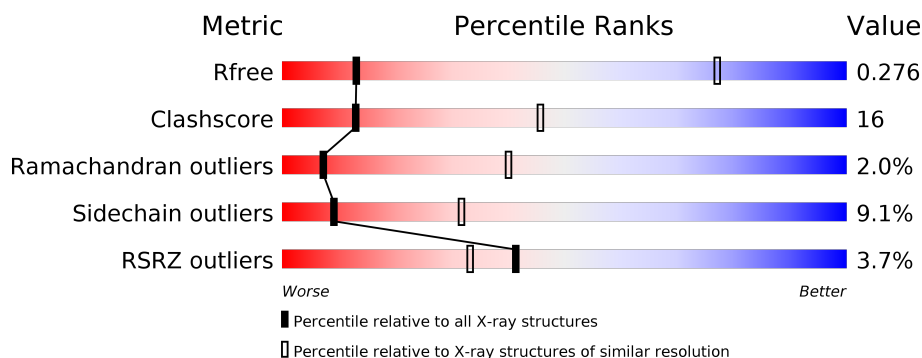
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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	1055 (5.20-3.80)
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)
RSRZ outliers	127900	1101 (5.30-3.70)

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	329	<div> <div>6%</div> <div> <div>45%</div> <div>41%</div> <div>10%</div> </div> </div>
1	B	329	<div> <div>%</div> <div> <div>42%</div> <div>22%</div> <div>34%</div> </div> </div>
1	G	329	<div> <div>%</div> <div> <div>41%</div> <div>24%</div> <div>31%</div> </div> </div>
1	H	329	<div> <div>6%</div> <div> <div>43%</div> <div>21%</div> <div>34%</div> </div> </div>
2	C	1342	<div> <div>2%</div> <div> <div>59%</div> <div>37%</div> </div> </div>
2	I	1342	<div> <div>4%</div> <div> <div>60%</div> <div>36%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	D	1407	<div><div>%</div><div><div></div><div>48%</div><div>31%</div><div>•</div><div>17%</div></div></div>
3	J	1407	<div><div>2%</div><div><div></div><div>47%</div><div>31%</div><div>•</div><div>18%</div></div></div>
4	E	91	<div><div></div><div><div></div><div>65%</div><div>26%</div><div>7%</div><div>•</div></div></div>
4	K	91	<div><div>14%</div><div><div></div><div>62%</div><div>20%</div><div>5%</div><div>13%</div></div></div>
5	F	613	<div><div>3%</div><div><div></div><div>49%</div><div>24%</div><div>•</div><div>24%</div></div></div>
5	L	613	<div><div>4%</div><div><div></div><div>48%</div><div>26%</div><div>•</div><div>23%</div></div></div>
6	M	151	<div><div>19%</div><div><div></div><div>62%</div><div>29%</div><div>•</div><div>7%</div></div></div>
6	N	151	<div><div>21%</div><div><div></div><div>58%</div><div>30%</div><div>•</div><div>7%</div></div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 58066 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2490	1557	439	486	8			
1	B	217	Total	C	N	O	S	0	0	0
			1677	1047	295	329	6			
1	G	227	Total	C	N	O	S	0	0	0
			1755	1093	311	345	6			
1	H	216	Total	C	N	O	S	0	0	0
			1662	1038	292	326	6			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0	0
			10570	6631	1841	2055	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10566	6629	1840	2054	43			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1171	Total	C	N	O	S	0	0	0
			9085	5712	1626	1701	46			
3	J	1159	Total	C	N	O	S	0	0	0
			9021	5671	1616	1688	46			

- Molecule 4 is a protein called RpoZ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	468	Total	C	N	O	S	0	0	0
			3813	2389	678	723	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

- Molecule 6 is a protein called RNA polymerase-binding transcription factor DksA.

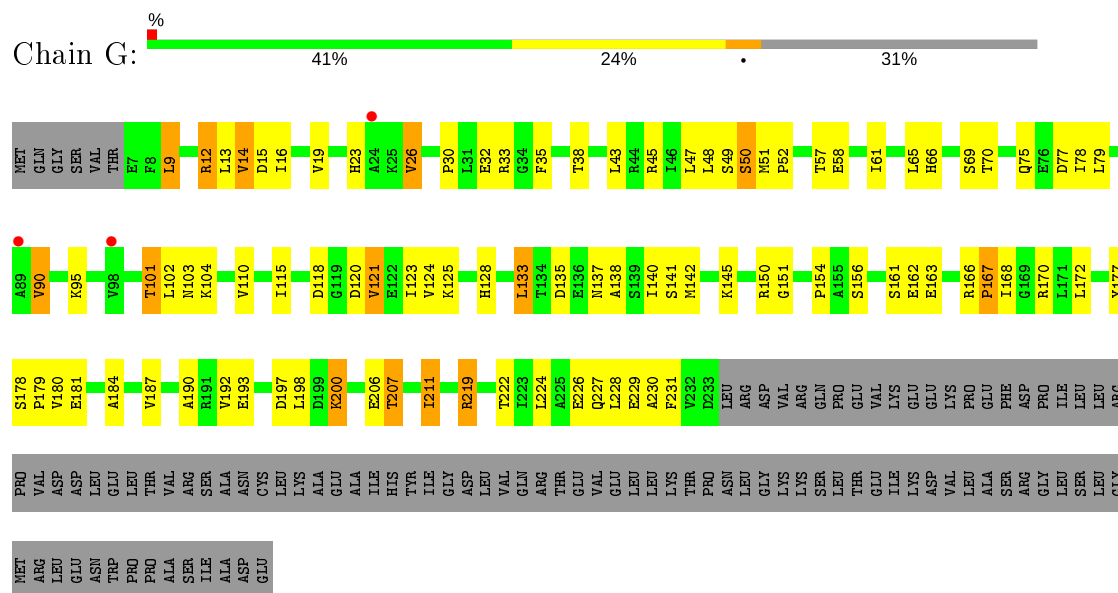
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	M	140	Total	C	N	O	S	0	0	0
			1140	703	206	224	7			
6	N	140	Total	C	N	O	S	0	0	0
			1140	703	206	224	7			

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

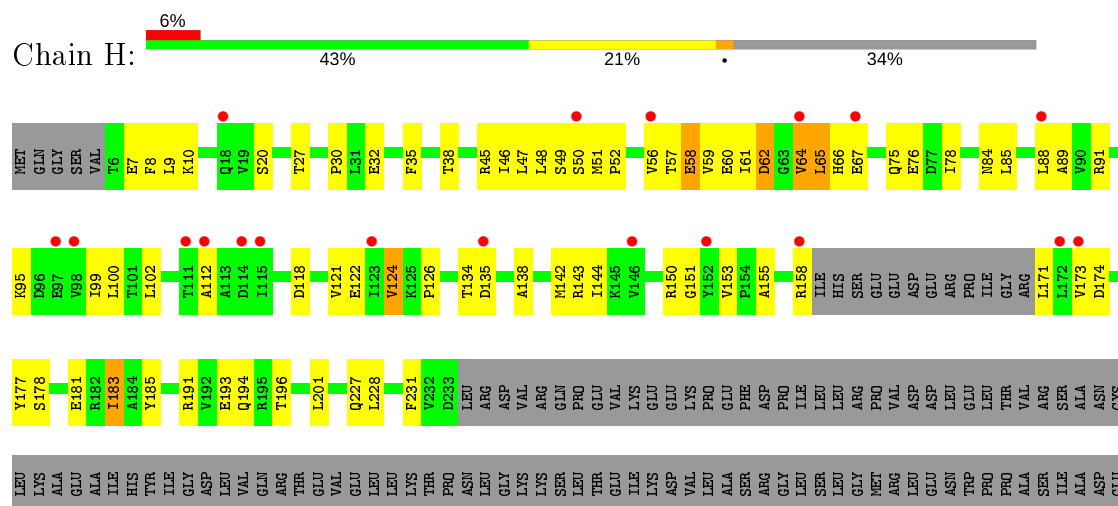
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

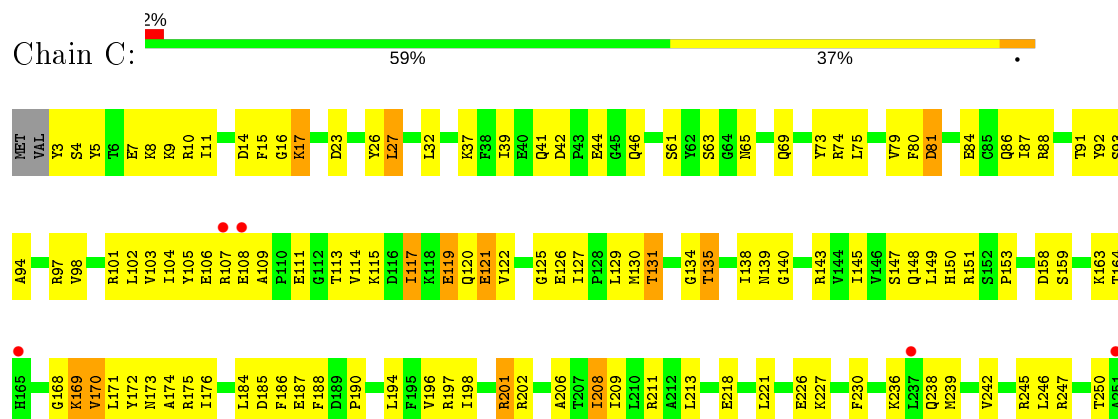
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	2	Total	Zn	0	0
			2	2		
8	D	2	Total	Zn	0	0
			2	2		
8	N	1	Total	Zn	0	0
			1	1		
8	M	1	Total	Zn	0	0
			1	1		

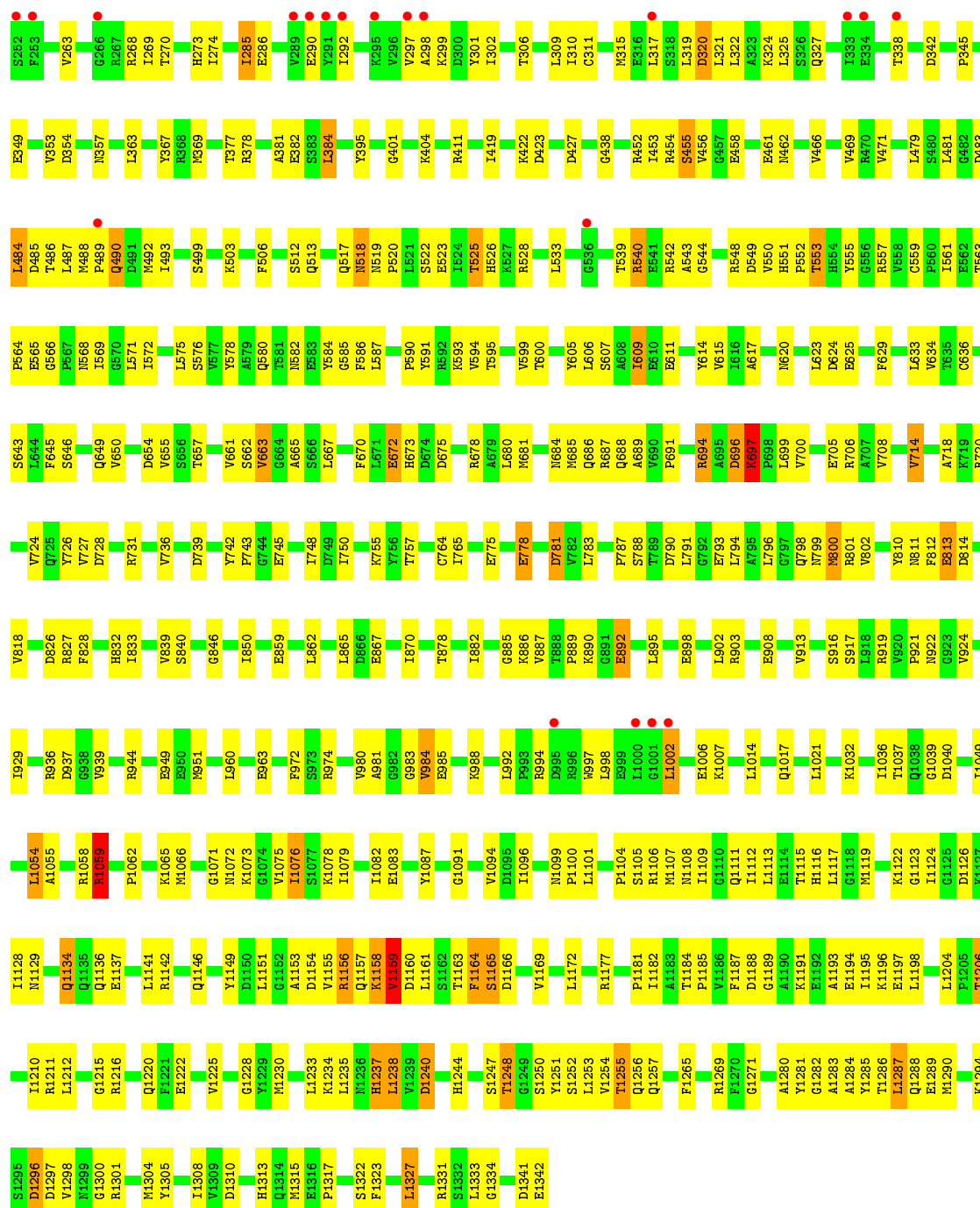


• Molecule 1: DNA-directed RNA polymerase subunit alpha

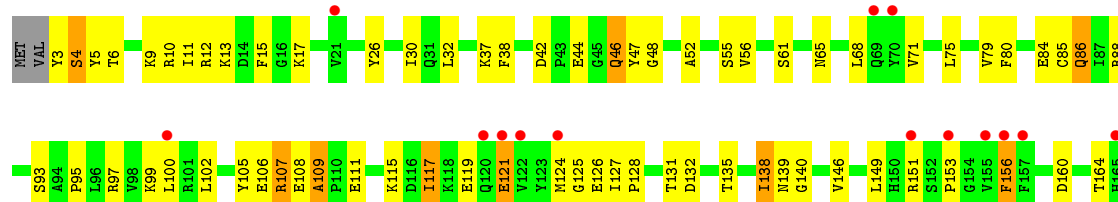


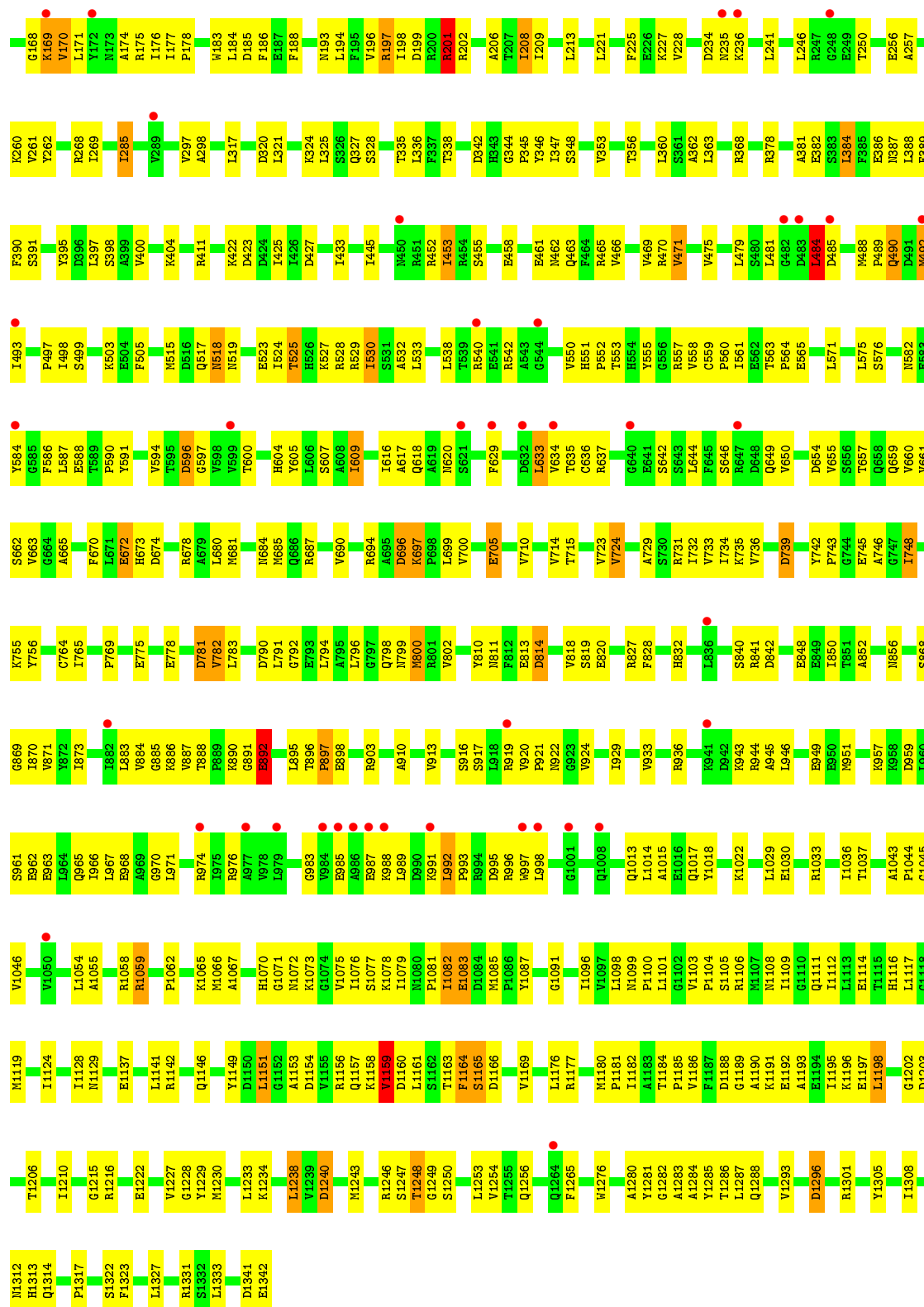
• Molecule 2: DNA-directed RNA polymerase subunit beta





• Molecule 2: DNA-directed RNA polymerase subunit beta



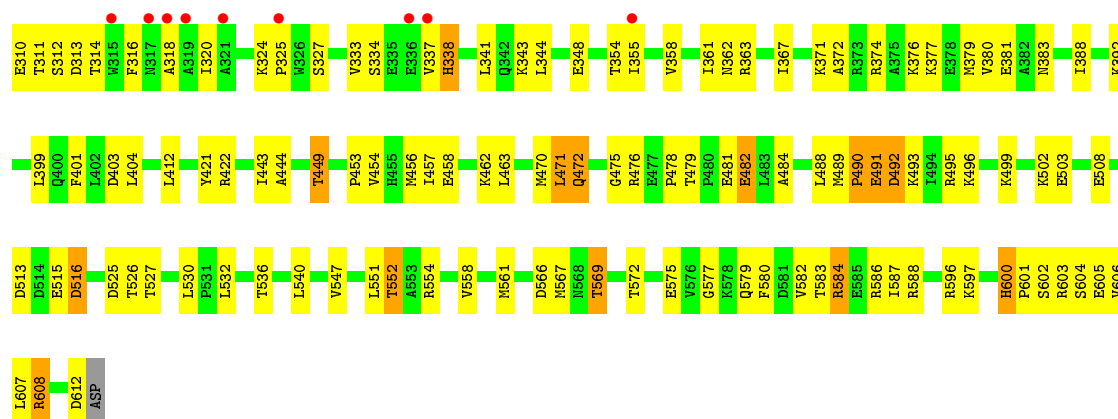


• Molecule 3: DNA-directed RNA polymerase subunit beta'

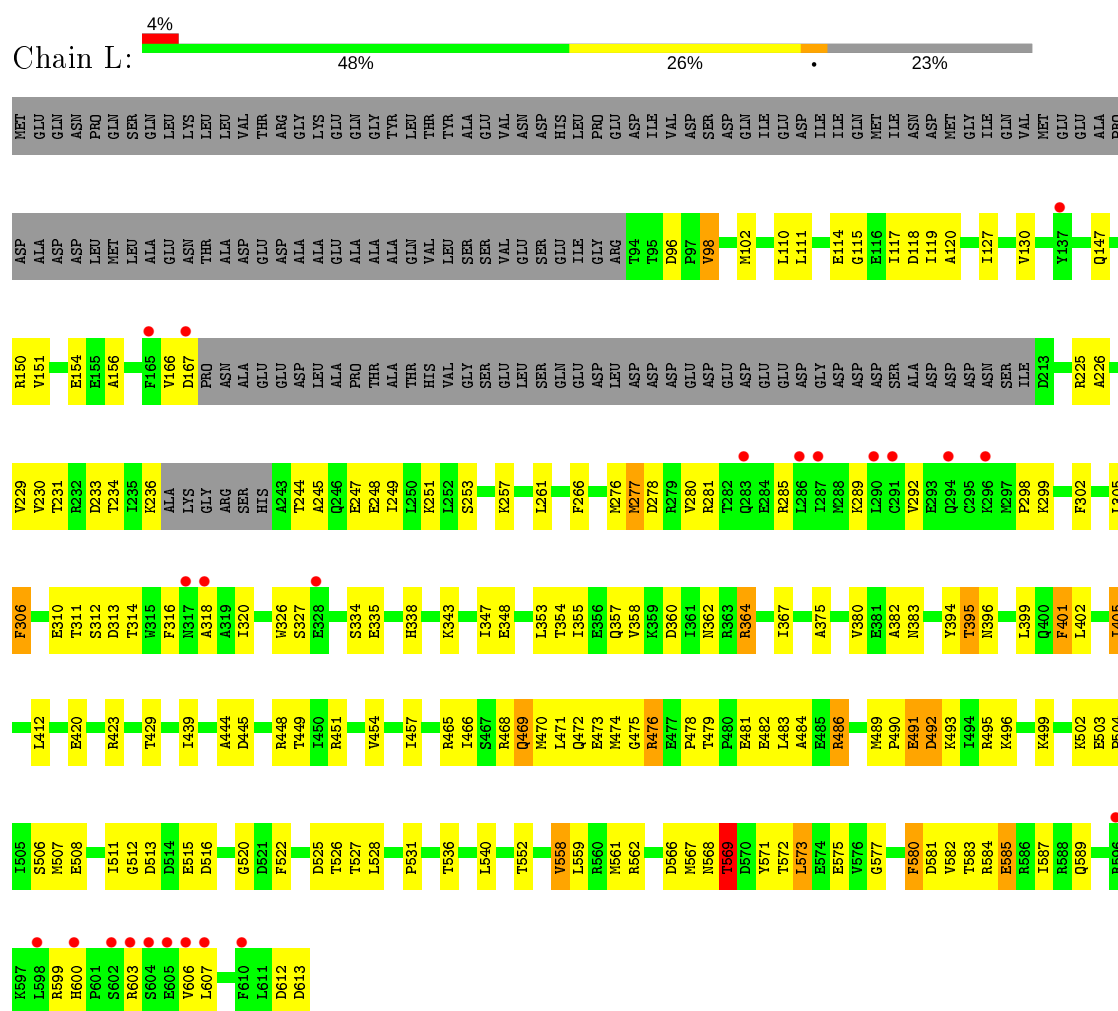




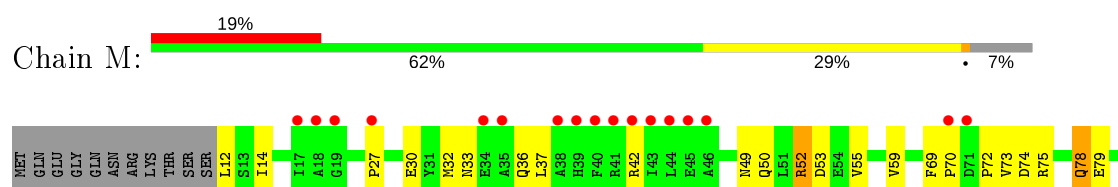


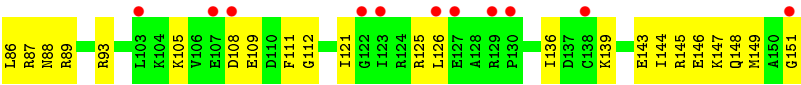


• Molecule 5: RNA polymerase sigma factor RpoD

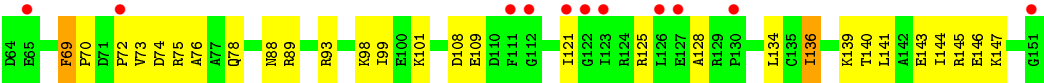
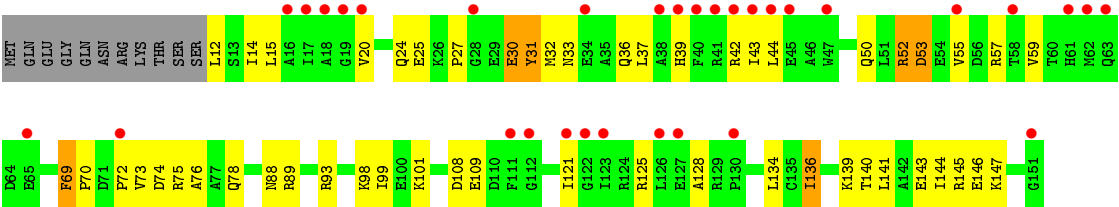


• Molecule 6: RNA polymerase-binding transcription factor DksA





● Molecule 6: RNA polymerase-binding transcription factor DksA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	184.00Å 204.89Å 314.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.08 – 4.50 49.64 – 4.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.08-4.50) 88.6 (49.64-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.95 (at 4.45Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.220 , 0.276 0.220 , 0.276	Depositor DCC
R_{free} test set	1995 reflections (2.83%)	wwPDB-VP
Wilson B-factor (Å ²)	198.5	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 232.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	58066	wwPDB-VP
Average B, all atoms (Å ²)	291.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.34	0/2524	0.67	1/3421 (0.0%)
1	B	0.33	0/1697	0.64	1/2300 (0.0%)
1	G	0.32	0/1777	0.61	0/2408
1	H	0.29	0/1681	0.62	1/2278 (0.0%)
2	C	0.36	0/10739	0.61	1/14489 (0.0%)
2	I	0.32	0/10735	0.57	1/14484 (0.0%)
3	D	0.37	0/9225	0.66	1/12458 (0.0%)
3	J	0.35	0/9160	0.63	3/12369 (0.0%)
4	E	0.34	0/693	0.57	0/935
4	K	0.27	0/629	0.54	0/847
5	F	0.32	0/3864	0.58	0/5194
5	L	0.31	0/3872	0.54	0/5205
6	M	0.31	0/1155	0.66	0/1549
6	N	0.33	0/1155	0.70	0/1549
All	All	0.34	0/58906	0.61	9/79486 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1
2	C	0	2
2	I	0	2
3	D	0	2
3	J	0	2
4	K	0	1
All	All	0	10

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	LEU	CA-CB-CG	6.76	130.84	115.30
3	J	857	LEU	CA-CB-CG	6.38	129.96	115.30
3	D	239	LEU	CA-CB-CG	-6.19	101.06	115.30
1	H	65	LEU	CA-CB-CG	6.01	129.11	115.30
1	A	318	LEU	CA-CB-CG	5.91	128.90	115.30
3	J	120	LEU	CA-CB-CG	5.74	128.51	115.30
3	J	1221	LEU	CA-CB-CG	5.51	127.97	115.30
2	I	484	LEU	CA-CB-CG	5.15	127.14	115.30
2	C	27	LEU	CA-CB-CG	-5.04	103.71	115.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	109	ALA	Peptide
2	C	236	LYS	Peptide
3	D	1184	ASP	Peptide
3	D	901	ARG	Peptide
1	H	171	LEU	Peptide
2	I	109	ALA	Peptide
2	I	236	LYS	Peptide
3	J	1184	ASP	Peptide
3	J	853	THR	Peptide
4	K	3	ARG	Peptide

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	2490	0	2542	120	0
1	B	1677	0	1703	53	1
1	G	1755	0	1773	61	1
1	H	1662	0	1687	49	0
2	C	10570	0	10582	391	2
2	I	10566	0	10576	366	0
3	D	9085	0	9218	384	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	9021	0	9175	375	0
4	E	691	0	695	21	0
4	K	627	0	634	15	0
5	F	3813	0	3880	112	1
5	L	3821	0	3884	109	0
6	M	1140	0	1119	33	0
6	N	1140	0	1119	50	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0
8	D	2	0	0	0	0
8	J	2	0	0	0	0
8	M	1	0	0	0	0
8	N	1	0	0	0	0
All	All	58066	0	58587	1914	3

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 16.

All (1914) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.39	1.04
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.45	0.98
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.43	0.97
1:A:45:ARG:HG2	1:B:38:THR:HB	1.48	0.95
2:C:1073:LYS:HE3	3:D:462:ASP:HB2	1.49	0.94
6:N:30:GLU:HG3	6:N:31:TYR:H	1.31	0.93
2:C:202:ARG:HD3	2:C:369:MET:HG2	1.51	0.92
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.17	0.91
2:C:700:VAL:HG13	2:C:1117:LEU:HD22	1.52	0.91
3:J:325:LYS:HD3	5:L:508:GLU:HG2	1.52	0.90
3:D:35:PHE:HD1	3:D:101:ARG:HD3	1.38	0.89
3:J:905:ARG:HH21	3:J:907:HIS:HB2	1.39	0.86
2:I:873:ILE:HG13	2:I:944:ARG:HH22	1.35	0.86
2:C:1101:LEU:HB3	3:D:731:ARG:HD3	1.56	0.85
2:I:1073:LYS:HE3	3:J:462:ASP:HB2	1.58	0.85
5:L:277:MET:HG3	5:L:362:ASN:HD21	1.39	0.85
2:I:1105:SER:OG	6:N:74:ASP:OD2	1.93	0.85
3:D:126:LEU:HD13	3:D:223:LEU:HD21	1.59	0.84
3:D:362:ARG:H	3:D:365:GLN:HE21	1.25	0.84
3:J:746:LEU:HD22	3:J:754:ILE:HD11	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:324:LYS:O	2:C:327:GLN:NE2	2.11	0.83
3:J:418:GLU:HG3	4:K:45:LYS:H	1.43	0.83
6:N:33:ASN:ND2	6:N:36:GLN:OE1	2.11	0.83
1:G:12:ARG:H	1:G:30:PRO:HD2	1.41	0.83
3:J:430:HIS:CD2	3:J:432:LEU:HB2	2.14	0.83
3:J:430:HIS:HD2	3:J:432:LEU:HB2	1.44	0.83
3:J:258:GLY:HA3	5:L:499:LYS:HE2	1.62	0.82
6:N:20:VAL:HG21	6:N:43:ILE:HG12	1.62	0.82
5:L:484:ALA:HB1	5:L:491:GLU:HB2	1.61	0.81
3:J:1291:GLU:HG2	3:J:1297:LYS:HD2	1.63	0.81
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.62	0.81
2:I:811:ASN:O	2:I:1099:ASN:ND2	2.14	0.81
3:D:668:PHE:HB2	3:D:678:ARG:HG3	1.63	0.81
1:A:296:GLY:H	1:A:299:SER:HB2	1.44	0.81
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.63	0.80
3:D:460:ASP:OD1	3:D:462:ASP:OD1	1.98	0.80
3:D:660:GLU:HB3	3:D:685:ILE:HD13	1.61	0.80
2:I:196:VAL:HG12	2:I:206:ALA:HA	1.61	0.80
2:I:1256:GLN:HB3	2:I:1301:ARG:HH22	1.45	0.80
3:D:72:CYS:HB3	3:D:88:CYS:SG	2.22	0.80
3:J:126:LEU:HD13	3:J:223:LEU:HD21	1.64	0.79
1:A:191:ARG:NH1	1:A:198:LEU:O	2.15	0.79
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.62	0.79
3:D:17:PHE:O	3:D:1355:ARG:NH2	2.16	0.79
3:D:1238:GLN:NE2	3:D:1248:ILE:O	2.15	0.79
1:G:226:GLU:HB3	1:H:10:LYS:HE3	1.64	0.79
2:I:987:GLU:HG2	2:I:991:LYS:HE3	1.64	0.79
3:J:114:ILE:HD12	3:J:304:ASP:HB3	1.65	0.78
5:F:444:ALA:HB1	5:F:457:ILE:HD13	1.65	0.78
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.65	0.78
4:K:14:GLY:O	4:K:16:ARG:N	2.15	0.78
3:D:746:LEU:HD22	3:D:754:ILE:HD11	1.66	0.78
3:D:844:THR:HG21	3:D:858:VAL:HG21	1.66	0.78
3:J:892:PHE:H	3:J:1281:GLU:HG2	1.49	0.78
5:L:573:LEU:H	5:L:573:LEU:HD23	1.49	0.78
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.66	0.78
2:C:1160:ASP:HB2	2:C:1161:LEU:HA	1.65	0.77
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.17	0.77
3:J:137:ARG:HG2	3:J:142:GLU:HB2	1.65	0.77
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.48	0.77
3:D:746:LEU:HG	3:D:758:PRO:HB3	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:118:ASP:HB3	1:G:121:VAL:HB	1.65	0.77
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.65	0.77
5:L:111:LEU:HD11	5:L:119:ILE:HD12	1.67	0.76
3:J:259:ARG:HD3	5:L:502:LYS:HD2	1.68	0.76
2:I:1160:ASP:HB2	2:I:1161:LEU:HA	1.66	0.75
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.68	0.75
3:J:885:VAL:HG12	3:J:894:VAL:HG11	1.67	0.75
3:D:905:ARG:HH21	3:D:907:HIS:HB2	1.51	0.75
2:I:557:ARG:HB3	2:I:587:LEU:HD13	1.69	0.75
2:I:1101:LEU:HB3	3:J:731:ARG:HD3	1.66	0.75
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.66	0.75
2:C:678:ARG:CZ	2:C:1106:ARG:HG2	2.17	0.75
2:I:814:ASP:OD2	2:I:1106:ARG:NH1	2.20	0.75
2:C:1256:GLN:HB3	2:C:1301:ARG:HH22	1.51	0.75
2:C:974:ARG:HD2	2:C:1014:LEU:HD21	1.70	0.74
2:C:814:ASP:OD2	2:C:1106:ARG:NH1	2.20	0.74
2:C:4:SER:HB3	2:C:7:GLU:HG3	1.67	0.74
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.20	0.74
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.69	0.74
3:J:79:LYS:HB2	5:L:569:THR:H	1.51	0.74
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.70	0.73
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.69	0.73
2:C:1100:PRO:HB3	3:D:639:VAL:HG12	1.70	0.73
3:D:490:ILE:HD13	3:D:490:ILE:H	1.52	0.73
2:C:168:GLY:O	2:C:170:VAL:N	2.17	0.73
3:D:885:VAL:HG12	3:D:894:VAL:HG11	1.70	0.73
5:F:292:VAL:HG11	5:F:299:LYS:HG3	1.69	0.73
3:J:808:VAL:HG13	3:J:914:ALA:HA	1.70	0.73
6:M:121:ILE:HG23	6:M:125:ARG:HH11	1.53	0.73
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.20	0.73
2:C:898:GLU:HB3	5:F:540:LEU:HD22	1.71	0.73
2:I:6:THR:OG1	2:I:781:ASP:OD2	2.05	0.73
3:J:48:THR:O	3:J:50:LYS:N	2.21	0.73
2:I:550:VAL:HG11	3:J:776:THR:HG22	1.71	0.73
6:N:20:VAL:HG11	6:N:43:ILE:HD11	1.71	0.73
3:D:1163:VAL:HG23	3:D:1177:ILE:HG23	1.70	0.73
2:C:594:VAL:HG11	2:C:650:VAL:HG23	1.71	0.72
3:D:848:VAL:HG12	3:D:858:VAL:HG22	1.71	0.72
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.53	0.72
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.71	0.72
3:D:664:ILE:HD11	3:D:685:ILE:HD12	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.70	0.72
3:D:609:TYR:HE2	3:D:614:LEU:HD12	1.54	0.72
2:I:674:ASP:OD2	2:I:1070:HIS:ND1	2.20	0.72
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.70	0.72
3:D:664:ILE:HD13	3:D:681:LYS:HG2	1.72	0.72
2:I:528:ARG:NH2	2:I:576:SER:O	2.22	0.72
2:I:1062:PRO:HA	2:I:1076:ILE:HG23	1.71	0.72
1:G:45:ARG:HH21	2:I:1216:ARG:HA	1.55	0.72
2:I:30:ILE:HD12	2:I:30:ILE:H	1.53	0.72
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.72	0.72
6:N:121:ILE:HG23	6:N:125:ARG:HH11	1.53	0.71
2:C:810:TYR:CE2	3:D:359:PRO:HD2	2.24	0.71
3:D:473:THR:HG23	3:D:476:ALA:H	1.55	0.71
2:I:176:ILE:HB	2:I:184:LEU:HB3	1.70	0.71
2:I:724:VAL:HG23	2:I:775:GLU:H	1.54	0.71
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.26	0.71
2:I:892:GLU:OE2	3:J:66:LYS:NZ	2.24	0.71
2:I:1240:ASP:N	2:I:1240:ASP:OD1	2.23	0.71
3:D:1181:ASP:HA	3:J:202:ARG:HD3	1.73	0.71
2:I:1106:ARG:HH21	6:N:73:VAL:HG21	1.56	0.71
3:D:310:GLY:HA2	3:D:314:ARG:HD2	1.73	0.70
2:C:1087:TYR:HE1	2:C:1215:GLY:HA2	1.57	0.70
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.74	0.70
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	1.71	0.70
3:D:495:ASN:O	3:D:497:GLU:N	2.25	0.70
5:F:277:MET:HG3	5:F:362:ASN:HD21	1.56	0.70
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.74	0.70
3:D:430:HIS:CD2	3:D:432:LEU:HB2	2.26	0.70
2:I:475:VAL:HG22	2:I:492:MET:HB2	1.72	0.70
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.73	0.70
3:J:42:GLU:OE2	5:L:451:ARG:NE	2.22	0.70
3:J:495:ASN:O	3:J:497:GLU:N	2.24	0.70
1:H:134:THR:HG23	1:H:135:ASP:H	1.56	0.69
3:J:536:LEU:HD12	3:J:542:ALA:HB2	1.73	0.69
3:J:709:ARG:O	3:J:711:GLY:N	2.24	0.69
1:H:118:ASP:HB2	1:H:121:VAL:HB	1.73	0.69
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.75	0.69
5:L:479:THR:HG22	5:L:482:GLU:HB2	1.73	0.69
2:I:97:ARG:HB3	2:I:121:GLU:HB3	1.75	0.69
2:I:168:GLY:O	2:I:170:VAL:N	2.26	0.69
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:674:THR:HG21	6:M:139:LYS:HG3	1.75	0.68
3:D:709:ARG:O	3:D:711:GLY:N	2.25	0.68
3:J:107:LEU:HD11	3:J:242:LEU:HB2	1.74	0.68
3:J:473:THR:HG23	3:J:476:ALA:H	1.58	0.68
2:C:175:ARG:HG3	2:C:185:ASP:OD1	1.93	0.68
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.76	0.68
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.75	0.68
5:F:479:THR:HG23	5:F:481:GLU:H	1.59	0.68
2:I:810:TYR:HE1	2:I:1078:LYS:HD2	1.59	0.68
3:J:1280:VAL:HG11	3:J:1304:ARG:HE	1.59	0.68
3:D:1159:ILE:HG22	3:D:1177:ILE:HD12	1.75	0.68
3:D:1298:VAL:H	3:D:1299:GLY:HA3	1.57	0.68
5:F:278:ASP:OD1	5:F:281:ARG:NH1	2.27	0.68
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.76	0.68
2:C:1160:ASP:CB	2:C:1161:LEU:HA	2.22	0.68
2:C:724:VAL:HG11	2:C:727:VAL:HG22	1.76	0.68
3:D:536:LEU:HD12	3:D:542:ALA:HB2	1.75	0.68
3:D:935:PHE:O	6:M:87:ARG:NH2	2.28	0.68
1:A:47:LEU:O	1:A:180:VAL:HG21	1.94	0.67
1:A:77:ASP:N	1:A:77:ASP:OD1	2.27	0.67
2:C:617:ALA:HA	2:C:636:CYS:SG	2.34	0.67
4:E:32:VAL:O	4:E:34:GLY:N	2.26	0.67
4:E:4:VAL:HG13	4:E:5:THR:H	1.59	0.67
1:G:45:ARG:HG2	1:H:38:THR:HB	1.76	0.67
2:I:1160:ASP:CB	2:I:1161:LEU:HA	2.24	0.67
1:A:100:LEU:HD23	1:A:115:ILE:HG21	1.76	0.67
1:A:14:VAL:HG22	1:A:15:ASP:H	1.59	0.67
3:D:1181:ASP:HB3	3:J:202:ARG:HH11	1.59	0.67
2:C:697:LYS:HD2	2:C:1181:PRO:HG3	1.75	0.67
3:D:1167:LYS:NZ	3:D:1168:GLU:O	2.28	0.67
3:D:48:THR:O	3:D:50:LYS:N	2.28	0.67
2:I:324:LYS:O	2:I:327:GLN:NE2	2.28	0.67
3:J:1167:LYS:NZ	3:J:1168:GLU:O	2.27	0.67
1:H:52:PRO:HG3	1:H:150:ARG:HG2	1.77	0.66
3:J:746:LEU:HG	3:J:758:PRO:HB3	1.76	0.66
3:J:460:ASP:OD1	3:J:462:ASP:OD1	2.13	0.66
6:M:121:ILE:HG23	6:M:125:ARG:NH1	2.10	0.66
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.78	0.66
6:N:139:LYS:NZ	6:N:143:GLU:OE2	2.28	0.66
3:J:700:ASN:O	3:J:704:GLU:HB2	1.95	0.66
3:D:1160:SER:HB2	3:D:1206:ARG:HG2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:242:VAL:HB	2:C:245:ARG:HD2	1.77	0.66
2:C:519:ASN:HB3	2:C:522:SER:HB2	1.78	0.66
2:I:723:VAL:O	2:I:735:LYS:N	2.25	0.66
3:J:661:VAL:HG13	3:J:682:VAL:HG11	1.78	0.66
2:C:138:ILE:HD11	2:C:506:PHE:HB3	1.78	0.66
3:D:140:TYR:OH	3:D:312:ARG:NH1	2.28	0.66
3:J:357:VAL:HG22	3:J:461:PHE:HE1	1.60	0.66
3:J:367:GLY:HA3	3:J:448:GLN:HB2	1.78	0.66
6:M:105:LYS:HB3	6:M:111:PHE:HB2	1.78	0.66
3:D:258:GLY:HA3	5:F:499:LYS:HE2	1.77	0.65
3:J:839:VAL:HG12	3:J:864:LEU:HD12	1.77	0.65
5:L:454:VAL:HA	5:L:457:ILE:HD12	1.79	0.65
1:G:38:THR:OG1	1:H:45:ARG:NH1	2.28	0.65
3:J:526:VAL:HG12	3:J:549:LYS:HB2	1.78	0.65
4:K:32:VAL:O	4:K:34:GLY:N	2.29	0.65
4:K:25:ARG:HD3	4:K:64:LEU:HD13	1.76	0.65
1:B:118:ASP:HB2	1:B:121:VAL:HB	1.76	0.65
2:C:675:ASP:HB2	2:C:1107:MET:HB2	1.78	0.65
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.26	0.65
3:D:378:LYS:NZ	3:D:382:TYR:OH	2.27	0.65
1:H:181:GLU:HA	3:J:535:ARG:HH21	1.61	0.65
3:J:705:THR:HG21	3:J:719:PHE:H	1.61	0.65
3:J:72:CYS:HB3	3:J:88:CYS:SG	2.36	0.65
3:D:491:LEU:HD22	3:D:496:GLY:O	1.96	0.65
2:C:1065:LYS:HD3	2:C:1235:LEU:HD12	1.78	0.65
3:D:793:SER:O	3:D:797:THR:HG23	1.97	0.65
1:A:236:ASP:HA	1:B:14:VAL:O	1.96	0.65
2:C:1066:MET:HG2	2:C:1234:LYS:HA	1.77	0.65
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.77	0.65
3:D:515:ARG:O	3:D:545:HIS:HB3	1.97	0.65
1:G:48:LEU:HA	1:G:180:VAL:HG21	1.79	0.65
3:D:1159:ILE:HD12	3:D:1206:ARG:HD2	1.78	0.65
2:I:976:ARG:HD2	2:I:989:LEU:HD23	1.79	0.65
3:J:430:HIS:ND1	3:J:925:GLU:HG3	2.11	0.65
5:F:316:PHE:HE1	5:F:337:VAL:HB	1.62	0.64
2:I:745:GLU:HG3	2:I:1017:GLN:HB3	1.79	0.64
2:I:206:ALA:O	2:I:209:ILE:HG22	1.97	0.64
3:J:786:THR:HG21	6:N:76:ALA:HB2	1.79	0.64
2:I:697:LYS:HD2	2:I:1181:PRO:HG3	1.79	0.64
2:I:1248:THR:HG21	5:L:531:PRO:HG3	1.78	0.64
2:I:102:LEU:HB2	2:I:489:PRO:HG3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1179:PRO:HD2	3:J:1184:ASP:HA	1.79	0.64
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.79	0.64
2:I:870:ILE:HG13	2:I:884:VAL:HG22	1.78	0.64
5:L:470:MET:HB2	5:L:478:PRO:HG3	1.77	0.64
2:C:1142:ARG:HH12	2:C:1169:VAL:HG21	1.62	0.64
3:D:114:ILE:HD12	3:D:304:ASP:HB3	1.78	0.64
3:D:202:ARG:HD3	3:J:1181:ASP:HA	1.80	0.64
3:J:1239:ASP:OD1	3:J:1242:ARG:NH2	2.26	0.64
3:J:902:ASP:HB2	3:J:1251:LYS:HE3	1.78	0.64
2:I:1331:ARG:HG2	3:J:33:TRP:CZ3	2.32	0.64
3:J:491:LEU:HB2	3:J:904:ALA:HA	1.80	0.64
2:I:1100:PRO:HB3	3:J:639:VAL:HG12	1.78	0.64
2:C:591:TYR:OH	2:C:611:GLU:OE1	2.07	0.64
3:J:425:ARG:HG2	3:J:426:ALA:H	1.63	0.64
3:D:731:ARG:HH22	6:M:73:VAL:HG11	1.63	0.64
2:C:657:THR:HG21	2:C:1188:ASP:HB2	1.80	0.64
3:J:702:GLN:HA	3:J:723:TYR:CE2	2.33	0.63
2:I:30:ILE:HD11	2:I:575:LEU:HD22	1.80	0.63
6:N:20:VAL:HG21	6:N:43:ILE:CG1	2.28	0.63
2:C:1269:ARG:HG3	3:D:346:ARG:HG2	1.81	0.63
2:C:93:SER:OG	2:C:126:GLU:OE1	2.15	0.63
3:D:161:THR:HG22	3:D:164:GLN:HB2	1.79	0.63
3:J:35:PHE:HD1	3:J:101:ARG:HD3	1.63	0.63
2:I:1247:SER:HB3	3:J:375:GLU:O	1.96	0.63
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.64	0.63
2:C:802:VAL:HG11	2:C:1230:MET:HB3	1.80	0.63
2:I:117:ILE:HD12	2:I:488:MET:HG2	1.81	0.63
2:I:9:LYS:HD2	2:I:791:LEU:HD21	1.80	0.63
3:J:650:LYS:NZ	3:J:762:ASN:HD22	1.97	0.63
2:C:810:TYR:HE1	2:C:1078:LYS:HD2	1.64	0.63
2:C:1297:ASP:OD1	2:C:1300:GLY:N	2.28	0.62
2:I:596:ASP:CG	2:I:597:GLY:H	2.02	0.62
1:A:22:THR:O	1:A:207:THR:N	2.30	0.62
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.00	0.62
3:D:430:HIS:HD2	3:D:432:LEU:HB2	1.63	0.62
2:I:1082:ILE:H	2:I:1082:ILE:HD12	1.64	0.62
2:I:37:LYS:HD2	2:I:46:GLN:HE21	1.65	0.62
2:I:949:GLU:HG2	2:I:1036:ILE:HG22	1.80	0.62
3:J:31:ARG:NH2	3:J:106:GLU:OE2	2.28	0.62
3:J:357:VAL:HG22	3:J:461:PHE:CE1	2.34	0.62
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.80	0.62
1:G:90:VAL:HG23	1:G:123:ILE:HD13	1.82	0.62
2:I:810:TYR:CE1	2:I:1078:LYS:HD2	2.34	0.62
2:I:1283:ALA:HB1	2:I:1286:THR:HB	1.80	0.62
2:I:149:LEU:HB2	2:I:530:ILE:HG22	1.80	0.62
2:C:27:LEU:HD13	2:C:663:VAL:HG11	1.81	0.62
3:D:128:LEU:HB3	3:D:157:GLN:HE22	1.65	0.62
2:I:386:GLU:HA	2:I:390:PHE:HD2	1.63	0.62
2:I:739:ASP:N	2:I:739:ASP:OD1	2.28	0.62
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.82	0.62
2:C:594:VAL:HG22	2:C:599:VAL:HG22	1.81	0.62
2:I:119:GLU:HG3	2:I:489:PRO:HD2	1.81	0.62
5:F:111:LEU:HD11	5:F:119:ILE:HD12	1.80	0.62
2:I:61:SER:HB3	2:I:479:LEU:HB3	1.82	0.62
5:L:484:ALA:HB1	5:L:491:GLU:CB	2.28	0.62
1:H:51:MET:HB3	1:H:178:SER:HB2	1.82	0.62
2:I:852:ALA:HB2	2:I:869:GLY:HA2	1.80	0.62
5:L:277:MET:HG3	5:L:362:ASN:ND2	2.12	0.62
1:B:102:LEU:O	1:B:141:SER:HA	2.00	0.62
3:J:767:LEU:HD23	3:J:771:GLN:HB3	1.81	0.62
2:C:239:MET:N	2:C:285:ILE:O	2.28	0.61
1:G:102:LEU:HD23	1:G:115:ILE:HG12	1.80	0.61
2:C:1282:GLY:O	2:C:1284:ALA:N	2.33	0.61
2:C:269:ILE:HA	2:C:273:HIS:ND1	2.14	0.61
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.82	0.61
2:I:885:GLY:HA2	2:I:917:SER:HB3	1.82	0.61
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.15	0.61
3:D:189:LEU:HB3	3:D:234:PRO:HB2	1.81	0.61
5:F:600:HIS:CD2	5:F:601:PRO:HD3	2.35	0.61
2:C:1240:ASP:HB3	3:D:445:LYS:HD2	1.83	0.61
3:J:663:GLU:HB3	6:N:12:LEU:HD22	1.81	0.61
2:C:949:GLU:HG2	2:C:1036:ILE:HG22	1.81	0.61
2:C:125:GLY:HA3	2:C:499:SER:HB2	1.81	0.61
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.83	0.61
3:J:702:GLN:HA	3:J:723:TYR:HE2	1.64	0.61
5:F:231:THR:HG23	5:F:249:ILE:HG12	1.83	0.61
1:G:14:VAL:HG13	1:G:15:ASP:H	1.64	0.61
2:C:1073:LYS:CE	3:D:462:ASP:HB2	2.26	0.61
5:L:278:ASP:OD1	5:L:281:ARG:NH1	2.34	0.61
2:C:1122:LYS:NZ	2:C:1126:ASP:OD1	2.32	0.61
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:550:VAL:HG11	3:D:776:THR:HG22	1.83	0.61
1:A:44:ARG:HB2	1:A:183:ILE:HG21	1.83	0.60
5:F:492:ASP:HB2	5:F:495:ARG:HH12	1.64	0.60
6:M:32:MET:SD	6:M:37:LEU:HD21	2.41	0.60
2:C:1002:LEU:HD22	2:C:1007:LYS:HB2	1.82	0.60
2:C:411:ARG:NH2	2:C:427:ASP:OD2	2.22	0.60
3:D:1178:THR:HG23	3:D:1184:ASP:HB3	1.84	0.60
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.83	0.60
2:I:1176:LEU:HD13	2:I:1180:MET:HG3	1.84	0.60
2:C:1256:GLN:HB3	2:C:1301:ARG:NH2	2.15	0.60
3:J:378:LYS:NZ	3:J:382:TYR:OH	2.29	0.60
2:C:670:PHE:CD2	2:C:1113:LEU:HB3	2.37	0.60
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.83	0.60
2:I:86:GLN:HA	2:I:140:GLY:HA2	1.82	0.60
1:A:66:HIS:CE1	1:A:69:SER:HB3	2.37	0.60
2:I:183:TRP:HB2	2:I:199:ASP:HA	1.83	0.60
3:J:844:THR:OG1	3:J:860:ARG:O	2.14	0.60
2:C:292:ILE:HB	2:C:322:LEU:HD11	1.83	0.60
3:D:504:GLN:HG3	3:D:505:ASP:H	1.67	0.60
5:F:493:LYS:HG2	5:F:496:LYS:HE2	1.82	0.60
2:I:1256:GLN:HB3	2:I:1301:ARG:NH2	2.17	0.60
2:I:873:ILE:HG13	2:I:944:ARG:NH2	2.13	0.60
6:N:59:VAL:HG22	6:N:89:ARG:HD2	1.83	0.60
2:C:196:VAL:HG12	2:C:206:ALA:HA	1.84	0.60
2:C:557:ARG:HB3	2:C:587:LEU:HD13	1.84	0.60
3:D:418:GLU:HG3	4:E:45:LYS:H	1.67	0.60
3:D:325:LYS:HD3	5:F:508:GLU:HG2	1.83	0.60
6:N:30:GLU:HG3	6:N:31:TYR:N	2.12	0.60
1:B:37:HIS:CE1	2:C:1216:ARG:HD2	2.37	0.60
3:D:510:LEU:HA	3:D:513:MET:HE2	1.84	0.60
1:G:135:ASP:HB3	1:G:138:ALA:HB2	1.82	0.60
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.66	0.60
2:I:71:VAL:HB	2:I:99:LYS:HB2	1.84	0.60
1:B:14:VAL:HB	1:B:28:LEU:HD13	1.84	0.59
2:C:102:LEU:HB2	2:C:489:PRO:HG3	1.84	0.59
4:E:71:GLU:HA	4:E:74:GLU:HG3	1.84	0.59
5:F:470:MET:HB2	5:F:478:PRO:HG3	1.83	0.59
2:I:856:ASN:HB3	5:L:613:ASP:HA	1.83	0.59
1:B:29:GLU:HB3	1:B:200:LYS:HG3	1.84	0.59
2:C:97:ARG:HB3	2:C:121:GLU:HB3	1.82	0.59
1:H:151:GLY:O	1:H:177:TYR:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1106:ARG:NH2	6:N:73:VAL:HG21	2.16	0.59
3:J:1143:ASP:HA	3:J:1148:ARG:HH11	1.67	0.59
6:M:52:ARG:HB2	6:M:52:ARG:HH11	1.67	0.59
3:D:252:LEU:HD23	3:D:262:THR:HB	1.85	0.59
3:D:849:LEU:HD22	3:D:849:LEU:H	1.66	0.59
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.85	0.59
3:J:793:SER:O	3:J:797:THR:HG23	2.01	0.59
3:J:436:ALA:HB3	3:J:485:MET:HA	1.83	0.59
3:J:863:LEU:HD11	3:J:901:ARG:HB3	1.84	0.59
1:B:62:ASP:OD1	1:B:62:ASP:N	2.29	0.59
2:C:16:GLY:O	2:C:1156:ARG:HG2	2.03	0.59
2:I:814:ASP:CG	2:I:1106:ARG:HH12	2.06	0.59
3:J:16:GLU:HG3	3:J:17:PHE:H	1.66	0.59
3:J:287:ALA:HB3	3:J:292:VAL:HG12	1.83	0.59
3:D:1289:ASN:O	3:D:1289:ASN:ND2	2.35	0.59
1:G:161:SER:O	1:G:163:GLU:N	2.35	0.59
2:I:929:ILE:HD13	2:I:1055:ALA:HB2	1.85	0.59
3:J:128:LEU:HB3	3:J:157:GLN:HE22	1.66	0.59
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.83	0.59
2:C:563:THR:HG22	2:C:680:LEU:HD11	1.84	0.59
3:D:1157:ALA:HB3	3:D:1207:GLY:H	1.67	0.59
4:E:4:VAL:HG13	4:E:5:THR:HG23	1.84	0.59
2:C:661:VAL:HB	2:C:665:ALA:HB3	1.85	0.59
2:I:633:LEU:HB2	2:I:644:LEU:HD12	1.84	0.59
3:J:190:LYS:HD3	3:J:235:GLU:HG2	1.84	0.59
1:H:48:LEU:HD21	3:J:535:ARG:HG3	1.84	0.59
2:C:1289:GLU:OE2	3:D:473:THR:HG22	2.03	0.59
2:C:149:LEU:HD13	2:C:453:ILE:HG13	1.84	0.59
2:C:488:MET:O	2:C:490:GLN:N	2.30	0.59
4:E:39:VAL:HG22	4:E:40:PRO:HD2	1.85	0.59
2:I:38:PHE:HA	2:I:48:GLY:HA2	1.85	0.59
2:I:471:VAL:HG21	2:I:498:ILE:HD11	1.85	0.59
3:J:609:TYR:HE2	3:J:614:LEU:HD12	1.68	0.59
4:E:49:ILE:O	4:E:53:GLU:HG3	2.02	0.58
2:I:1106:ARG:HD2	2:I:1106:ARG:H	1.68	0.58
2:I:4:SER:OG	2:I:5:TYR:N	2.34	0.58
5:L:364:ARG:HA	5:L:367:ILE:HD12	1.85	0.58
1:A:135:ASP:O	1:A:137:ASN:N	2.36	0.58
2:C:557:ARG:HD3	2:C:587:LEU:HB3	1.84	0.58
2:I:452:ARG:NH1	2:I:584:TYR:O	2.36	0.58
3:J:35:PHE:CD1	3:J:101:ARG:HD3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:720:ASN:OD1	3:J:722:ILE:HG22	2.03	0.58
1:B:41:ASN:OD1	1:B:44:ARG:NH1	2.37	0.58
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.85	0.58
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.85	0.58
3:D:650:LYS:NZ	3:D:762:ASN:HD22	2.01	0.58
3:D:708:ASN:N	3:D:708:ASN:OD1	2.36	0.58
2:C:1282:GLY:HA3	4:E:17:PHE:CE1	2.38	0.58
2:C:122:VAL:HG23	5:F:472:GLN:HG3	1.86	0.58
5:F:561:MET:HA	5:F:567:MET:HE1	1.85	0.58
3:J:50:LYS:HD3	3:J:71:LEU:HD21	1.84	0.58
3:J:598:LYS:O	3:J:601:ILE:HG22	2.03	0.58
5:L:231:THR:HG23	5:L:249:ILE:HG12	1.84	0.58
2:C:86:GLN:HA	2:C:140:GLY:HA2	1.85	0.58
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.69	0.58
3:D:905:ARG:HH21	3:D:907:HIS:CB	2.16	0.58
2:C:395:TYR:HD2	2:C:419:ILE:HG22	1.68	0.58
2:C:810:TYR:HE2	3:D:359:PRO:HD2	1.68	0.58
5:F:299:LYS:HA	5:F:302:PHE:HB3	1.84	0.58
2:C:268:ARG:HH21	2:C:270:THR:HG21	1.68	0.58
2:C:80:PHE:HB3	2:C:84:GLU:HB2	1.84	0.58
3:D:731:ARG:NH1	6:M:73:VAL:HG21	2.17	0.58
1:A:266:SER:HB3	1:A:303:ILE:HD11	1.85	0.58
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.38	0.58
2:C:936:ARG:HD2	2:C:939:VAL:HG23	1.86	0.58
5:F:348:GLU:HG2	5:F:354:THR:HA	1.84	0.58
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.84	0.58
2:I:138:ILE:O	2:I:139:ASN:ND2	2.37	0.58
2:I:168:GLY:C	2:I:170:VAL:H	2.07	0.58
3:J:83:VAL:O	3:J:91:GLU:HA	2.04	0.58
1:B:19:VAL:HB	1:B:23:HIS:HD2	1.66	0.58
3:D:1165:PHE:HE1	3:D:1200:GLU:HB2	1.68	0.58
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.04	0.58
3:J:789:LYS:NZ	3:J:932:MET:H	2.02	0.58
2:I:1117:LEU:HD12	2:I:1195:ILE:HG12	1.86	0.57
3:D:926:PRO:HB3	3:D:1246:VAL:HG11	1.86	0.57
2:I:1276:TRP:HH2	3:J:798:ARG:HG3	1.69	0.57
3:J:211:GLU:OE2	3:J:214:ARG:NH1	2.37	0.57
1:A:159:ILE:HG13	1:A:162:GLU:HG3	1.84	0.57
3:D:676:GLY:HA2	3:D:679:TYR:HD2	1.69	0.57
3:D:866:GLU:OE2	3:D:901:ARG:NH2	2.28	0.57
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:672:GLU:HG2	2:C:1187:PHE:HD2	1.70	0.57
3:J:268:LEU:HB3	3:J:306:LEU:HD23	1.86	0.57
3:J:747:MET:HB2	3:J:774:ILE:HG22	1.86	0.57
1:A:112:ALA:HB3	1:A:126:PRO:HA	1.86	0.57
3:J:304:ASP:OD2	3:J:312:ARG:NH2	2.37	0.57
5:L:380:VAL:HG13	5:L:412:LEU:HD23	1.86	0.57
2:C:718:ALA:HB2	2:C:783:LEU:HD23	1.86	0.57
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.86	0.57
3:J:1252:HIS:O	3:J:1255:VAL:HG13	2.05	0.57
3:J:664:ILE:HG12	6:N:12:LEU:HD11	1.87	0.57
1:A:318:LEU:O	1:A:320:ASN:N	2.36	0.57
3:D:357:VAL:HG22	3:D:461:PHE:CE1	2.39	0.57
2:I:1013:GLN:O	2:I:1017:GLN:HG2	2.05	0.57
2:I:961:SER:O	2:I:965:GLN:N	2.36	0.57
3:J:1266:ILE:HD12	3:J:1273:ASP:O	2.03	0.57
2:C:1164:PHE:O	2:C:1166:ASP:N	2.38	0.57
3:D:128:LEU:HD21	3:D:189:LEU:HD23	1.87	0.57
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.53	0.57
2:I:1281:TYR:CD1	3:J:484:MET:HG2	2.40	0.57
1:A:102:LEU:HD23	1:A:115:ILE:HG12	1.87	0.56
1:A:11:PRO:HA	1:A:30:PRO:HG2	1.86	0.56
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.86	0.56
2:C:41:GLN:NE2	2:C:73:TYR:O	2.38	0.56
3:D:357:VAL:HG22	3:D:461:PHE:HE1	1.70	0.56
2:I:347:ILE:HD11	2:I:433:ILE:HD11	1.86	0.56
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.70	0.56
2:C:490:GLN:HG3	5:F:472:GLN:CD	2.25	0.56
2:I:119:GLU:HG3	2:I:488:MET:HB3	1.87	0.56
3:J:1280:VAL:HG11	3:J:1304:ARG:NE	2.20	0.56
2:C:1244:HIS:HD2	2:C:1265:PHE:HB2	1.70	0.56
1:H:185:TYR:HB2	1:H:201:LEU:HD11	1.87	0.56
1:A:115:ILE:HG22	1:A:116:THR:H	1.70	0.56
2:C:811:ASN:O	2:C:1099:ASN:ND2	2.34	0.56
2:I:670:PHE:CD1	2:I:1184:THR:HG21	2.39	0.56
2:I:52:ALA:HB2	2:I:461:GLU:HG3	1.87	0.56
3:J:849:LEU:HB3	3:J:853:THR:HG23	1.87	0.56
3:J:908:ILE:HG12	3:J:909:ILE:N	2.20	0.56
1:A:39:LEU:HD21	1:B:224:LEU:HD11	1.87	0.56
2:C:452:ARG:NH1	2:C:584:TYR:O	2.37	0.56
3:D:513:MET:HE1	3:D:579:LEU:HD13	1.87	0.56
1:H:191:ARG:NH1	3:J:413:ASP:OD2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:582:ASN:HB3	2:I:586:PHE:H	1.71	0.56
3:J:1287:ILE:O	3:J:1291:GLU:HG3	2.04	0.56
2:I:1333:LEU:HD23	3:J:307:LEU:HD22	1.87	0.56
3:J:842:ARG:NH2	3:J:1254:GLU:OE1	2.36	0.56
6:N:44:LEU:HD22	6:N:99:ILE:HG23	1.87	0.56
1:A:270:LEU:HD11	1:A:281:LEU:HD22	1.88	0.56
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.87	0.56
2:C:1247:SER:HB3	3:D:375:GLU:O	2.05	0.56
3:D:202:ARG:NH2	3:D:225:GLU:OE1	2.38	0.56
2:I:588:GLU:HB3	2:I:607:SER:HA	1.85	0.56
1:A:12:ARG:H	1:A:30:PRO:HD2	1.70	0.56
1:A:98:VAL:HG22	1:A:100:LEU:HD12	1.88	0.56
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.88	0.56
2:I:175:ARG:HG3	2:I:185:ASP:OD1	2.05	0.56
3:J:708:ASN:N	3:J:708:ASN:OD1	2.36	0.56
3:J:750:PRO:HA	3:J:777:HIS:CE1	2.41	0.56
1:A:137:ASN:OD1	1:A:137:ASN:N	2.37	0.56
3:D:322:ARG:HB2	3:D:322:ARG:NH1	2.21	0.56
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.87	0.56
2:I:968:GLU:HG3	2:I:1018:TYR:HE1	1.70	0.56
3:J:1158:GLU:HA	3:J:1223:LEU:HD11	1.87	0.56
3:J:1344:LEU:O	3:J:1346:GLY:N	2.36	0.56
5:L:316:PHE:HZ	5:L:334:SER:HA	1.71	0.56
3:D:672:LEU:O	3:D:673:VAL:HG22	2.05	0.56
3:D:460:ASP:CG	3:D:462:ASP:OD1	2.45	0.56
2:I:842:ASP:N	2:I:1045:GLY:O	2.39	0.56
2:I:515:MET:HG2	2:I:517:GLN:HB2	1.88	0.56
2:I:810:TYR:CE2	3:J:359:PRO:HD2	2.41	0.56
6:N:52:ARG:HB2	6:N:52:ARG:HH11	1.71	0.56
3:J:786:THR:HG21	6:N:76:ALA:CB	2.35	0.56
1:A:192:VAL:HG12	1:A:195:ARG:HB2	1.88	0.56
3:D:227:PHE:O	3:D:230:SER:HB3	2.04	0.56
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.88	0.56
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.71	0.56
3:D:674:THR:HB	6:M:139:LYS:HD2	1.88	0.56
2:C:629:PHE:CE2	2:C:650:VAL:HG21	2.41	0.55
2:C:9:LYS:NZ	2:C:775:GLU:OE2	2.38	0.55
2:C:1285:TYR:CZ	3:D:1356:LEU:HD11	2.41	0.55
2:I:590:PRO:HG3	2:I:605:TYR:CZ	2.40	0.55
3:J:632:ALA:O	3:J:635:SER:OG	2.21	0.55
3:J:430:HIS:CE1	3:J:925:GLU:HG3	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:559:ALA:HB3	3:D:562:GLU:HB3	1.87	0.55
2:I:560:PRO:O	3:J:780:ARG:NH2	2.35	0.55
1:G:103:ASN:OD1	1:G:141:SER:HB2	2.05	0.55
1:G:227:GLN:NE2	1:H:9:LEU:O	2.34	0.55
6:N:59:VAL:HG22	6:N:89:ARG:HH11	1.71	0.55
2:I:378:ARG:NH1	2:I:382:GLU:OE2	2.40	0.55
2:I:898:GLU:HB3	5:L:540:LEU:HD22	1.88	0.55
1:A:289:LEU:HD13	1:A:300:LEU:HD21	1.89	0.55
2:C:1123:GLY:HA3	2:C:1204:LEU:HD11	1.87	0.55
2:C:187:GLU:OE2	2:C:197:ARG:NH2	2.40	0.55
2:C:73:TYR:HB2	2:C:98:VAL:HG22	1.87	0.55
3:D:811:GLU:OE1	3:D:890:THR:OG1	2.24	0.55
2:I:10:ARG:NH2	2:I:790:ASP:OD2	2.37	0.55
1:A:44:ARG:HB2	1:A:183:ILE:CG2	2.37	0.55
2:C:1283:ALA:HB1	2:C:1286:THR:HB	1.89	0.55
3:J:786:THR:HA	3:J:789:LYS:HG3	1.87	0.55
2:C:1149:TYR:HD1	2:C:1159:VAL:HG11	1.70	0.55
2:C:629:PHE:CE2	2:C:634:VAL:HG11	2.42	0.55
3:D:518:VAL:CG1	3:D:707:ILE:HD13	2.37	0.55
1:A:257:VAL:HG13	1:A:276:HIS:O	2.06	0.55
2:C:1269:ARG:HB3	3:D:343:LEU:HG	1.89	0.55
1:A:86:LYS:NZ	2:C:826:ASP:OD2	2.36	0.55
3:D:425:ARG:HG2	3:D:426:ALA:H	1.71	0.55
5:F:601:PRO:HA	5:F:604:SER:HB3	1.89	0.55
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.89	0.55
3:J:425:ARG:HG2	3:J:426:ALA:N	2.22	0.55
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.88	0.55
2:C:1017:GLN:O	2:C:1021:LEU:HG	2.07	0.55
2:I:974:ARG:HD2	2:I:1014:LEU:HD21	1.89	0.55
4:K:40:PRO:O	4:K:52:ARG:NH2	2.39	0.55
1:A:310:ARG:O	5:F:608:ARG:NH2	2.40	0.55
1:A:45:ARG:HG3	1:A:46:ILE:HD13	1.89	0.55
2:C:1158:LYS:O	2:C:1159:VAL:HG13	2.07	0.55
2:C:564:PRO:HG3	2:C:572:ILE:HG13	1.89	0.55
3:J:24:LEU:HD23	3:J:232:ASN:ND2	2.21	0.55
1:B:104:LYS:HG2	1:B:110:VAL:HG13	1.88	0.54
2:C:1334:GLY:H	3:D:113:HIS:HE2	1.54	0.54
2:I:213:LEU:HD13	2:I:422:LYS:HG2	1.89	0.54
3:J:664:ILE:CG1	6:N:12:LEU:HD11	2.37	0.54
3:J:770:LEU:HD22	3:J:770:LEU:H	1.71	0.54
3:J:785:ASP:HB3	3:J:789:LYS:HE2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1284:ALA:N	3:D:479:GLU:OE1	2.40	0.54
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	1.88	0.54
3:D:68:TYR:HA	3:D:92:VAL:HG23	1.88	0.54
2:I:852:ALA:HB2	2:I:869:GLY:CA	2.37	0.54
3:J:362:ARG:H	3:J:365:GLN:HE21	1.54	0.54
5:L:292:VAL:HG11	5:L:299:LYS:HE3	1.89	0.54
6:M:108:ASP:CG	6:M:109:GLU:H	2.10	0.54
2:C:798:GLN:OE1	2:C:827:ARG:HB2	2.07	0.54
5:F:312:SER:OG	5:F:313:ASP:N	2.41	0.54
2:I:106:GLU:O	2:I:109:ALA:HB2	2.06	0.54
5:L:562:ARG:NH2	5:L:573:LEU:HD22	2.22	0.54
2:C:1282:GLY:H	3:D:483:LEU:HD13	1.71	0.54
3:D:1160:SER:N	3:D:1206:ARG:HB3	2.23	0.54
3:D:201:LEU:HB2	3:D:221:ILE:HD13	1.88	0.54
3:D:426:ALA:CB	3:D:427:PRO:HD3	2.38	0.54
2:I:185:ASP:HB2	2:I:197:ARG:HG3	1.90	0.54
3:J:438:GLU:OE1	4:K:3:ARG:NH2	2.41	0.54
2:I:174:ALA:N	2:I:186:PHE:O	2.40	0.54
2:I:618:GLN:HG3	3:J:770:LEU:HD21	1.90	0.54
5:L:312:SER:OG	5:L:313:ASP:N	2.41	0.54
2:C:1248:THR:HG22	2:C:1251:TYR:OH	2.07	0.54
3:D:1181:ASP:HB3	3:J:202:ARG:NH1	2.22	0.54
3:J:789:LYS:HZ2	3:J:932:MET:H	1.55	0.54
2:C:188:PHE:CE1	2:C:194:LEU:HD13	2.43	0.54
3:D:425:ARG:NH1	3:D:459:ALA:HA	2.22	0.54
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.88	0.54
2:I:963:GLU:O	2:I:967:LEU:HB2	2.07	0.54
1:B:182:ARG:NH1	3:D:534:GLU:OE1	2.41	0.54
2:C:1288:GLN:HG2	2:C:1315:MET:HE1	1.90	0.54
2:C:174:ALA:N	2:C:186:PHE:O	2.36	0.54
2:C:708:VAL:HG11	2:C:794:LEU:HD22	1.89	0.54
2:C:778:GLU:O	2:C:781:ASP:HB2	2.08	0.54
5:F:261:LEU:H	5:F:261:LEU:HD12	1.72	0.54
2:I:736:VAL:HG23	2:I:748:ILE:HA	1.90	0.54
2:I:1305:TYR:CE1	3:J:379:PRO:HG3	2.43	0.54
3:J:797:THR:O	3:J:801:VAL:HG12	2.08	0.54
1:A:49:SER:O	1:A:51:MET:N	2.39	0.54
2:C:686:GLN:HG2	2:C:796:LEU:HD22	1.89	0.54
2:I:1081:PRO:HB3	2:I:1083:GLU:OE2	2.08	0.54
2:I:563:THR:HG22	2:I:680:LEU:HD11	1.90	0.54
2:I:798:GLN:OE1	2:I:827:ARG:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:56:LEU:H	3:J:56:LEU:HD12	1.73	0.54
2:C:130:MET:SD	2:C:134:GLY:HA2	2.48	0.54
2:C:250:THR:HA	2:C:268:ARG:HA	1.90	0.54
2:C:582:ASN:HB3	2:C:586:PHE:H	1.73	0.54
2:C:88:ARG:NH2	2:C:1040:ASP:OD1	2.40	0.54
3:D:1181:ASP:OD1	3:D:1182:GLY:N	2.41	0.54
2:C:810:TYR:CD2	3:D:359:PRO:HD2	2.42	0.54
3:D:596:LEU:HD12	3:D:601:ILE:HG13	1.89	0.54
5:F:371:LYS:HA	5:F:374:ARG:NH1	2.23	0.54
2:I:411:ARG:NH2	2:I:427:ASP:OD2	2.41	0.54
2:I:75:LEU:HD11	2:I:127:ILE:HD11	1.89	0.54
3:J:612:LEU:HB3	3:J:616:PRO:HG2	1.90	0.54
3:J:650:LYS:HZ3	3:J:762:ASN:HD22	1.54	0.54
1:H:76:GLU:N	1:H:76:GLU:OE1	2.40	0.53
3:J:1239:ASP:O	3:J:1243:LEU:HB2	2.07	0.53
2:C:452:ARG:NH2	2:C:458:GLU:OE2	2.40	0.53
3:D:1280:VAL:HG21	3:D:1304:ARG:HH21	1.72	0.53
3:J:64:PRO:O	3:J:95:THR:OG1	2.22	0.53
1:A:241:GLU:HG3	1:A:242:VAL:H	1.72	0.53
2:C:1296:ASP:OD2	2:C:1322:SER:HB3	2.08	0.53
3:D:1309:ILE:HG13	3:D:1310:THR:N	2.24	0.53
2:I:260:LYS:HE3	2:I:262:TYR:CE1	2.43	0.53
2:I:395:TYR:HE2	2:I:397:LEU:HD12	1.72	0.53
2:I:868:SER:HB2	2:I:943:LYS:HB3	1.91	0.53
3:J:930:LEU:HD23	3:J:1244:GLN:HG3	1.89	0.53
3:J:355:ILE:HG21	3:J:466:MET:HG3	1.90	0.53
3:D:24:LEU:HD11	3:D:116:PHE:CZ	2.44	0.53
1:G:102:LEU:HD11	1:G:110:VAL:HG11	1.89	0.53
2:I:1149:TYR:CD1	2:I:1159:VAL:HG11	2.43	0.53
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.90	0.53
1:A:154:PRO:HB2	2:C:1059:ARG:NH2	2.23	0.53
1:G:184:ALA:HB2	2:I:1091:GLY:CA	2.39	0.53
1:H:89:ALA:HB3	1:H:124:VAL:HG12	1.89	0.53
2:I:820:GLU:HA	2:I:1079:ILE:HD11	1.89	0.53
3:J:674:THR:HG22	6:N:136:ILE:HD12	1.91	0.53
2:C:1142:ARG:HH12	2:C:1165:SER:HA	1.73	0.53
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.91	0.53
3:D:22:ILE:HG23	3:D:1336:ALA:HA	1.91	0.53
3:D:848:VAL:HG13	3:D:857:LEU:HB2	1.90	0.53
3:D:43:THR:OG1	5:F:449:THR:O	2.15	0.53
5:L:561:MET:HA	5:L:567:MET:HE1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:885:GLY:HA2	2:C:917:SER:HB3	1.90	0.53
3:D:659:ALA:O	3:D:663:GLU:HG2	2.09	0.53
3:D:81:ARG:C	3:D:83:VAL:H	2.12	0.53
1:G:35:PHE:HE1	1:H:46:ILE:HG12	1.73	0.53
3:J:99:ARG:HG3	3:J:249:LEU:HD21	1.90	0.53
3:D:1183:SER:C	3:D:1185:PRO:HD3	2.29	0.53
3:D:137:ARG:HG2	3:D:142:GLU:HB2	1.90	0.53
5:L:343:LYS:O	5:L:347:ILE:HG13	2.08	0.53
1:A:211:ILE:HG21	1:A:216:ALA:HB2	1.91	0.53
2:C:218:GLU:HG3	2:C:299:LYS:HA	1.91	0.53
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.91	0.53
3:D:54:ASP:N	3:D:54:ASP:OD1	2.41	0.53
5:F:127:ILE:O	5:F:130:VAL:HG22	2.09	0.53
5:F:612:ASP:OD1	5:F:612:ASP:N	2.42	0.53
2:I:387:ASN:HA	2:I:391:SER:HB2	1.90	0.53
2:I:518:ASN:N	2:I:518:ASN:OD1	2.41	0.53
3:J:128:LEU:HD23	3:J:192:MET:HE3	1.91	0.53
3:J:504:GLN:HG3	3:J:505:ASP:H	1.73	0.53
5:L:245:ALA:O	5:L:249:ILE:HG13	2.08	0.53
3:D:424:ASN:HB2	3:D:434:ILE:HG12	1.91	0.53
3:D:349:TYR:CD1	3:D:472:LEU:HD11	2.44	0.53
3:D:666:GLU:O	3:D:669:GLN:HG3	2.09	0.53
5:F:281:ARG:O	5:F:285:ARG:HG3	2.09	0.53
5:F:380:VAL:HG13	5:F:412:LEU:HD23	1.90	0.53
5:F:582:VAL:HG12	5:F:586:ARG:HG2	1.91	0.53
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.90	0.53
3:J:705:THR:OG1	3:J:718:SER:HA	2.08	0.53
2:C:813:GLU:HG3	3:D:460:ASP:HA	1.91	0.52
2:I:871:VAL:O	2:I:944:ARG:NH1	2.42	0.52
3:J:405:GLU:O	3:J:408:VAL:HG22	2.09	0.52
3:D:1174:ARG:NE	3:D:1187:GLU:OE2	2.39	0.52
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.91	0.52
3:D:362:ARG:H	3:D:365:GLN:NE2	2.00	0.52
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.45	0.52
2:I:800:MET:O	2:I:1229:TYR:HA	2.08	0.52
6:N:108:ASP:OD1	6:N:109:GLU:N	2.33	0.52
1:B:192:VAL:O	1:B:194:GLN:N	2.43	0.52
2:C:519:ASN:HB3	2:C:522:SER:CB	2.39	0.52
3:D:930:LEU:HB2	3:D:1138:LEU:HB2	1.91	0.52
3:D:98:ARG:HB3	3:D:248:ASP:OD2	2.09	0.52
5:F:316:PHE:CZ	5:F:338:HIS:HB2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:670:PHE:HZ	2:I:1117:LEU:HD13	1.73	0.52
2:I:1284:ALA:HB3	3:J:1361:THR:HB	1.90	0.52
5:L:127:ILE:O	5:L:130:VAL:HG22	2.09	0.52
5:L:479:THR:HG23	5:L:481:GLU:H	1.74	0.52
3:J:79:LYS:HD3	5:L:568:ASN:HB3	1.90	0.52
6:N:141:LEU:O	6:N:145:ARG:HG3	2.09	0.52
2:C:540:ARG:HH11	2:C:540:ARG:HB2	1.75	0.52
2:C:705:GLU:HB2	2:C:794:LEU:H	1.75	0.52
5:F:245:ALA:O	5:F:249:ILE:HG13	2.10	0.52
1:G:104:LYS:HG2	1:G:110:VAL:HG22	1.92	0.52
5:L:449:THR:OG1	5:L:503:GLU:OE1	2.25	0.52
2:C:1211:ARG:HE	2:C:1220:GLN:NE2	2.07	0.52
2:I:12:ARG:NH1	2:I:1182:ILE:O	2.39	0.52
4:K:31:GLN:HB2	4:K:46:THR:HG21	1.91	0.52
2:C:1165:SER:HA	2:C:1169:VAL:HG21	1.91	0.52
3:D:317:THR:HG22	3:D:322:ARG:O	2.08	0.52
3:D:664:ILE:HG12	3:D:681:LYS:HE2	1.91	0.52
1:B:98:VAL:O	1:B:146:VAL:HG13	2.09	0.52
1:B:35:PHE:HA	1:B:38:THR:HG22	1.91	0.52
3:D:667:GLN:O	3:D:672:LEU:HB2	2.08	0.52
5:F:148:TYR:OH	5:F:218:ARG:HA	2.10	0.52
1:G:133:LEU:HD21	1:G:140:ILE:HG12	1.91	0.52
1:G:66:HIS:CE1	1:G:69:SER:HB3	2.45	0.52
2:I:594:VAL:HG11	2:I:650:VAL:HG23	1.91	0.52
6:N:20:VAL:HG13	6:N:39:HIS:NE2	2.24	0.52
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	1.91	0.52
3:D:190:LYS:HD3	3:D:235:GLU:HG2	1.90	0.52
1:G:32:GLU:HA	1:G:198:LEU:HD22	1.91	0.52
1:G:50:SER:HG	1:H:35:PHE:HE1	1.56	0.52
2:I:1164:PHE:O	2:I:1166:ASP:N	2.43	0.52
3:J:755:ILE:HD12	3:J:774:ILE:HG23	1.90	0.52
2:C:1062:PRO:HA	2:C:1076:ILE:HG13	1.91	0.52
2:C:1296:ASP:CG	2:C:1322:SER:HB3	2.30	0.52
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.92	0.52
3:D:214:ARG:HA	3:D:217:LEU:HB3	1.92	0.52
3:D:813:ASP:OD1	3:D:883:ARG:NH2	2.42	0.52
5:F:584:ARG:HH11	5:F:584:ARG:HA	1.75	0.52
1:G:140:ILE:O	1:G:140:ILE:HG13	2.10	0.52
2:I:178:PRO:HB3	2:I:395:TYR:CZ	2.45	0.52
2:I:1116:HIS:CE1	3:J:641:ILE:H	2.10	0.52
5:L:466:ILE:HB	5:L:483:LEU:HD23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:PHE:HE1	1:B:46:ILE:HG12	1.75	0.52
1:H:112:ALA:HB3	1:H:126:PRO:HA	1.92	0.52
2:I:169:LYS:O	2:I:170:VAL:HG22	2.10	0.52
3:J:845:ALA:HB3	3:J:881:LYS:HB3	1.92	0.52
5:L:470:MET:O	5:L:478:PRO:HD3	2.10	0.52
1:A:51:MET:HE2	1:A:220:ALA:HB2	1.93	0.51
3:D:1198:VAL:HB	3:D:1210:ILE:HG23	1.91	0.51
1:G:166:ARG:O	1:G:168:ILE:N	2.43	0.51
1:A:211:ILE:HD12	1:A:215:GLU:HG2	1.92	0.51
1:A:252:ILE:HG21	1:A:312:LEU:HD11	1.92	0.51
2:C:238:GLN:HA	2:C:286:GLU:HA	1.91	0.51
2:C:1323:PHE:CE1	3:D:1353:VAL:HG23	2.45	0.51
5:F:292:VAL:HG13	5:F:297:MET:O	2.10	0.51
1:G:58:GLU:OE2	1:G:170:ARG:HD3	2.09	0.51
6:N:121:ILE:HG23	6:N:125:ARG:NH1	2.24	0.51
1:B:82:LEU:HD22	1:B:173:VAL:HG22	1.93	0.51
1:A:261:GLU:CD	2:C:859:GLU:HB2	2.30	0.51
3:D:1273:ASP:HB2	3:D:1276:GLU:HB3	1.91	0.51
3:D:709:ARG:HD2	3:D:710:ASP:H	1.74	0.51
1:G:61:ILE:HG23	1:G:142:MET:HB3	1.91	0.51
2:I:1116:HIS:CE1	3:J:641:ILE:HB	2.46	0.51
2:I:1066:MET:HG2	2:I:1234:LYS:HA	1.92	0.51
3:J:1183:SER:C	3:J:1185:PRO:HD3	2.31	0.51
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.46	0.51
5:L:612:ASP:OD1	5:L:612:ASP:N	2.43	0.51
3:D:133:ARG:O	3:D:137:ARG:HB2	2.11	0.51
5:F:311:THR:HG21	5:F:348:GLU:OE2	2.11	0.51
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.75	0.51
3:J:37:GLU:HG3	3:J:105:ILE:HA	1.91	0.51
1:A:57:THR:HG22	1:A:58:GLU:HG3	1.93	0.51
2:C:452:ARG:NH1	2:C:585:GLY:HA3	2.25	0.51
5:L:244:THR:O	5:L:247:GLU:HG2	2.09	0.51
5:L:281:ARG:O	5:L:285:ARG:HG3	2.10	0.51
2:C:818:VAL:O	2:C:1079:ILE:HD12	2.10	0.51
2:C:1107:MET:HG2	3:D:740:LEU:HD11	1.93	0.51
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.91	0.51
3:J:218:THR:HG21	3:J:1275:LEU:HD21	1.93	0.51
3:J:460:ASP:CG	3:J:462:ASP:OD1	2.48	0.51
3:J:760:THR:H	3:J:771:GLN:HE21	1.58	0.51
3:J:883:ARG:HB3	3:J:898:CYS:SG	2.51	0.51
2:C:74:ARG:NH1	2:C:121:GLU:OE1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.92	0.51
3:D:83:VAL:HG13	3:D:92:VAL:HG13	1.91	0.51
4:E:2:ALA:HB2	4:E:55:GLU:CD	2.31	0.51
1:G:47:LEU:O	1:G:51:MET:HG3	2.11	0.51
2:I:998:LEU:HD23	2:I:1015:ALA:HA	1.93	0.51
2:C:555:TYR:OH	2:C:654:ASP:OD1	2.20	0.51
3:D:1292:LEU:HA	3:J:1226:VAL:HG21	1.93	0.51
2:I:68:LEU:HD11	2:I:100:LEU:HB3	1.93	0.51
5:L:253:SER:O	5:L:257:LYS:HG3	2.11	0.51
5:L:306:PHE:CZ	5:L:310:GLU:HG3	2.46	0.51
1:A:316:MET:SD	5:F:600:HIS:CE1	3.04	0.51
1:A:56:VAL:HG11	1:A:85:LEU:HB3	1.93	0.51
2:C:17:LYS:NZ	2:C:1194:GLU:OE1	2.44	0.51
3:D:205:LEU:HD22	3:D:214:ARG:HB2	1.92	0.51
2:I:88:ARG:HH11	2:I:88:ARG:HB2	1.75	0.51
3:D:1181:ASP:CA	3:J:202:ARG:HD3	2.41	0.51
3:D:1356:LEU:HD13	3:D:1362:GLY:HA2	1.93	0.51
3:J:322:ARG:NH1	3:J:322:ARG:HB2	2.26	0.51
1:H:194:GLN:NE2	3:J:406:ALA:HB2	2.26	0.51
3:J:673:VAL:HG13	6:N:128:ALA:HB1	1.93	0.51
2:C:801:ARG:HG2	2:C:1094:VAL:HG23	1.92	0.50
2:C:1134:GLN:HB3	2:C:1136:GLN:HG2	1.93	0.50
3:D:107:LEU:HD11	3:D:242:LEU:HB2	1.92	0.50
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.92	0.50
3:J:709:ARG:HD2	3:J:710:ASP:H	1.75	0.50
5:L:316:PHE:CZ	5:L:334:SER:HA	2.45	0.50
2:C:198:ILE:O	2:C:201:ARG:HB2	2.11	0.50
5:F:552:THR:OG1	5:F:554:ARG:HG2	2.12	0.50
2:I:125:GLY:HA3	2:I:499:SER:HB2	1.93	0.50
2:I:338:THR:HG22	2:I:345:PRO:HB3	1.93	0.50
5:L:465:ARG:HD2	5:L:468:ARG:HH22	1.76	0.50
2:C:624:ASP:OD1	2:C:625:GLU:N	2.42	0.50
3:D:268:LEU:HD11	3:D:324:LEU:HD13	1.93	0.50
3:D:421:VAL:HG13	3:D:439:PRO:HG3	1.92	0.50
5:F:117:ILE:HA	5:F:120:ALA:HB3	1.93	0.50
5:F:575:GLU:O	5:F:579:GLN:HG2	2.11	0.50
1:G:166:ARG:N	1:G:167:PRO:HD2	2.26	0.50
3:J:1156:LEU:HA	3:J:1208:ASP:O	2.11	0.50
6:M:112:GLY:HA2	6:M:126:LEU:HD11	1.92	0.50
2:C:1101:LEU:HB3	3:D:731:ARG:CD	2.38	0.50
2:C:1255:THR:O	2:C:1257:GLN:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:425:ARG:HG2	3:D:426:ALA:N	2.27	0.50
1:H:51:MET:HB3	1:H:178:SER:CB	2.41	0.50
2:I:499:SER:O	2:I:503:LYS:HB2	2.12	0.50
3:J:1307:LEU:HD23	3:J:1312:ALA:HA	1.94	0.50
3:J:1309:ILE:HG13	3:J:1310:THR:N	2.26	0.50
3:J:709:ARG:HD2	3:J:710:ASP:N	2.26	0.50
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.39	0.50
2:C:172:TYR:OH	6:M:148:GLN:O	2.30	0.50
3:D:833:GLU:OE1	3:D:1242:ARG:HD3	2.11	0.50
3:D:30:ILE:HD13	3:D:243:PRO:HG3	1.92	0.50
2:I:1158:LYS:O	2:I:1159:VAL:HG13	2.11	0.50
2:I:1323:PHE:CE1	3:J:1353:VAL:HG23	2.45	0.50
3:J:494:ALA:HB2	3:J:922:SER:HB3	1.93	0.50
2:C:119:GLU:OE2	2:C:490:GLN:HB3	2.12	0.50
2:C:593:LYS:HG3	2:C:595:THR:HG23	1.92	0.50
3:D:709:ARG:HD2	3:D:710:ASP:N	2.25	0.50
5:F:493:LYS:HA	5:F:496:LYS:HG3	1.94	0.50
2:I:519:ASN:HD21	2:I:796:LEU:HD23	1.76	0.50
3:J:930:LEU:HB2	3:J:1138:LEU:HB2	1.92	0.50
5:L:117:ILE:HA	5:L:120:ALA:HB3	1.93	0.50
6:N:93:ARG:HG2	6:N:93:ARG:HH11	1.77	0.50
1:A:54:CYS:HB3	1:A:148:ARG:HB2	1.93	0.50
1:A:61:ILE:HB	1:A:64:VAL:CG2	2.42	0.50
3:D:1264:ALA:O	3:D:1277:GLY:HA2	2.11	0.50
3:D:1298:VAL:N	3:D:1299:GLY:HA3	2.21	0.50
3:D:1347:LEU:HD12	3:D:1358:PRO:HG2	1.92	0.50
3:D:903:LEU:HD21	3:D:913:GLU:OE1	2.12	0.50
1:G:197:ASP:O	1:G:198:LEU:HD23	2.12	0.50
2:I:109:ALA:HB1	2:I:111:GLU:HA	1.92	0.50
2:I:1103:VAL:HG11	2:I:1112:ILE:HG13	1.94	0.50
2:I:1124:ILE:O	2:I:1128:ILE:HG13	2.11	0.50
3:J:268:LEU:HD11	3:J:324:LEU:HD13	1.93	0.50
6:N:53:ASP:O	6:N:57:ARG:HG3	2.11	0.50
1:A:45:ARG:HG2	1:B:38:THR:CB	2.33	0.50
1:A:134:THR:HG21	2:C:727:VAL:O	2.11	0.50
3:D:37:GLU:HB2	3:D:104:HIS:CE1	2.47	0.50
3:D:56:LEU:H	3:D:56:LEU:HD12	1.77	0.50
5:F:489:MET:O	5:F:491:GLU:N	2.44	0.50
2:I:213:LEU:HB3	2:I:422:LYS:HD2	1.93	0.50
2:C:138:ILE:O	2:C:139:ASN:ND2	2.44	0.50
3:D:609:TYR:CE2	3:D:614:LEU:HD12	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:62:PHE:CD1	3:D:247:PRO:HD3	2.47	0.50
1:G:167:PRO:HB2	1:G:170:ARG:HB2	1.93	0.50
2:I:13:LYS:HD2	2:I:1157:GLN:OE1	2.12	0.50
3:J:122:SER:O	3:J:126:LEU:HG	2.11	0.50
2:C:1032:LYS:O	2:C:1036:ILE:HG13	2.12	0.49
2:C:1333:LEU:HD23	3:D:307:LEU:HD22	1.94	0.49
3:D:48:THR:C	3:D:50:LYS:H	2.15	0.49
3:D:615:LYS:HB2	3:D:616:PRO:HD3	1.94	0.49
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.94	0.49
2:I:297:VAL:HB	2:I:317:LEU:HD21	1.94	0.49
3:J:664:ILE:HD12	3:J:682:VAL:HG22	1.94	0.49
6:M:59:VAL:HG22	6:M:89:ARG:HD2	1.94	0.49
2:C:1087:TYR:CE1	2:C:1215:GLY:HA2	2.41	0.49
3:D:1221:LEU:HB2	3:D:1229:VAL:HG11	1.94	0.49
3:D:615:LYS:HE2	3:D:616:PRO:HD3	1.95	0.49
5:F:372:ALA:O	5:F:376:LYS:HG3	2.11	0.49
2:I:209:ILE:HD11	2:I:425:ILE:HD13	1.93	0.49
3:J:362:ARG:H	3:J:365:GLN:NE2	2.10	0.49
2:I:1281:TYR:CE1	3:J:484:MET:HE3	2.46	0.49
3:J:598:LYS:N	3:J:728:SER:O	2.30	0.49
2:C:1142:ARG:HD3	2:C:1161:LEU:HD22	1.93	0.49
2:C:980:VAL:HG13	2:C:984:VAL:HB	1.94	0.49
3:D:88:CYS:O	3:D:90:VAL:N	2.44	0.49
2:I:802:VAL:HG11	2:I:1230:MET:HB3	1.95	0.49
2:I:887:VAL:HB	2:I:913:VAL:CG2	2.42	0.49
3:J:820:ILE:HG22	3:J:1227:HIS:ND1	2.27	0.49
6:M:93:ARG:HH11	6:M:93:ARG:HG2	1.77	0.49
2:C:833:ILE:HA	2:C:1054:LEU:O	2.12	0.49
2:C:812:PHE:CZ	3:D:503:SER:HB2	2.48	0.49
1:G:13:LEU:HD23	1:G:13:LEU:H	1.77	0.49
2:I:802:VAL:HG21	2:I:1098:LEU:HD22	1.94	0.49
2:I:800:MET:SD	2:I:1096:ILE:HD11	2.52	0.49
2:I:924:VAL:HG12	2:I:1058:ARG:HH21	1.78	0.49
3:J:1350:ASN:OD1	3:J:1355:ARG:HD2	2.13	0.49
3:J:18:ASP:HB2	3:J:1373:ARG:NH2	2.27	0.49
3:J:650:LYS:HZ2	3:J:742:GLY:HA2	1.77	0.49
3:J:833:GLU:OE2	3:J:1247:LYS:NZ	2.44	0.49
2:C:61:SER:O	2:C:63:SER:N	2.46	0.49
3:D:292:VAL:O	3:D:296:LYS:HG3	2.11	0.49
2:C:1107:MET:HG2	3:D:740:LEU:CD1	2.42	0.49
1:G:95:LYS:HE3	1:G:120:ASP:OD1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:198:ILE:O	2:I:201:ARG:HB2	2.12	0.49
2:I:257:ALA:HB2	2:I:285:ILE:HA	1.94	0.49
3:J:859:PRO:HG2	3:J:862:THR:HG21	1.94	0.49
1:B:215:GLU:HA	1:B:218:ARG:HG3	1.95	0.49
1:A:83:LEU:HB3	2:C:694:ARG:HH21	1.78	0.49
3:D:363:LEU:HA	3:D:450:HIS:CD2	2.47	0.49
2:I:149:LEU:O	2:I:532:ALA:HA	2.13	0.49
2:I:617:ALA:HA	2:I:636:CYS:SG	2.51	0.49
3:J:513:MET:HE1	3:J:579:LEU:HD13	1.95	0.49
5:L:483:LEU:H	5:L:483:LEU:HD12	1.78	0.49
3:D:322:ARG:HB2	3:D:322:ARG:HH11	1.78	0.49
2:C:1271:GLY:HA2	3:D:344:GLY:HA3	1.95	0.49
3:D:405:GLU:O	3:D:408:VAL:HG22	2.12	0.49
2:C:549:ASP:OD1	3:D:750:PRO:HG3	2.12	0.49
5:F:343:LYS:H	5:F:343:LYS:HD2	1.76	0.49
1:G:150:ARG:NH2	1:H:32:GLU:OE1	2.45	0.49
2:I:672:GLU:HG2	2:I:1186:VAL:O	2.12	0.49
2:I:564:PRO:HA	2:I:684:ASN:HD21	1.77	0.49
2:I:93:SER:HA	2:I:128:PRO:HA	1.95	0.49
5:L:511:ILE:HG21	5:L:522:PHE:HE2	1.77	0.49
1:B:73:GLY:HA2	1:B:134:THR:HG22	1.93	0.49
2:I:462:ASN:O	2:I:466:VAL:HG23	2.13	0.49
2:I:745:GLU:N	2:I:1017:GLN:HG3	2.27	0.49
3:J:258:GLY:HA3	5:L:499:LYS:CE	2.38	0.49
3:J:278:ARG:HD2	3:J:295:GLU:CD	2.33	0.49
5:L:476:ARG:HB3	5:L:476:ARG:NH1	2.28	0.49
5:L:507:MET:HE3	5:L:520:GLY:HA3	1.94	0.49
1:B:6:THR:OG1	1:B:7:GLU:N	2.44	0.49
3:D:1232:TYR:HD2	3:D:1233:ILE:HD12	1.77	0.49
3:D:667:GLN:OE1	3:D:681:LYS:NZ	2.23	0.49
3:D:901:ARG:HA	3:D:908:ILE:HA	1.94	0.49
2:I:746:ALA:HB2	2:I:974:ARG:HE	1.78	0.49
2:I:778:GLU:O	2:I:781:ASP:HB2	2.13	0.49
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.78	0.49
1:A:195:ARG:HD2	1:A:196:THR:H	1.78	0.49
1:A:285:THR:OG1	1:A:286:GLU:N	2.46	0.49
3:D:749:LYS:HB2	3:D:750:PRO:HD2	1.95	0.49
1:H:91:ARG:HG3	1:H:122:GLU:HB3	1.95	0.49
2:I:517:GLN:HG3	2:I:523:GLU:OE2	2.12	0.49
2:I:732:ILE:HD11	2:I:769:PRO:HB3	1.95	0.49
2:I:976:ARG:HB2	2:I:997:TRP:CZ3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:3:ARG:HG3	4:K:3:ARG:O	2.12	0.49
2:C:395:TYR:CD2	2:C:419:ILE:HG22	2.48	0.48
2:C:145:ILE:HG21	2:C:456:VAL:HG13	1.95	0.48
5:F:314:THR:O	5:F:318:ALA:HB3	2.13	0.48
1:G:219:ARG:HB2	1:G:219:ARG:HE	1.34	0.48
3:J:161:THR:H	3:J:164:GLN:HB2	1.77	0.48
2:C:629:PHE:CD2	2:C:634:VAL:HG11	2.48	0.48
3:D:1257:VAL:HA	3:D:1260:MET:HG3	1.95	0.48
3:D:861:ASN:HD22	3:D:883:ARG:NH1	2.11	0.48
3:J:279:LEU:HD11	3:J:296:LYS:HG2	1.95	0.48
1:A:265:ARG:O	1:A:269:CYS:HB2	2.14	0.48
3:D:53:ARG:HA	3:D:54:ASP:HA	1.60	0.48
3:D:842:ARG:HB3	3:D:882:VAL:HG11	1.94	0.48
2:I:700:VAL:HG21	2:I:1114:GLU:HG2	1.94	0.48
2:I:700:VAL:HG13	2:I:1117:LEU:HD22	1.95	0.48
2:I:42:ASP:O	2:I:44:GLU:N	2.42	0.48
2:I:620:ASN:ND2	2:I:620:ASN:O	2.46	0.48
3:J:88:CYS:O	3:J:90:VAL:N	2.46	0.48
4:K:15:ASN:ND2	4:K:18:ASP:OD2	2.37	0.48
5:L:515:GLU:HG2	5:L:516:ASP:N	2.28	0.48
6:M:139:LYS:NZ	6:M:143:GLU:OE2	2.45	0.48
2:C:670:PHE:CD1	2:C:1184:THR:HG21	2.49	0.48
2:C:796:LEU:H	2:C:796:LEU:HD12	1.78	0.48
3:D:650:LYS:HZ3	3:D:762:ASN:HD22	1.61	0.48
2:I:15:PHE:CD2	2:I:1190:ALA:HB2	2.48	0.48
2:I:80:PHE:HB2	2:I:85:CYS:SG	2.54	0.48
3:J:674:THR:CG2	6:N:125:ARG:HH21	2.27	0.48
1:A:289:LEU:HD11	1:A:314:LEU:HD21	1.95	0.48
2:C:520:PRO:HG3	2:C:714:VAL:HG21	1.95	0.48
3:D:797:THR:O	3:D:801:VAL:HG12	2.13	0.48
3:D:83:VAL:O	3:D:91:GLU:HA	2.13	0.48
5:F:288:MET:HG2	5:F:299:LYS:HE2	1.94	0.48
5:F:453:PRO:O	5:F:456:MET:HB2	2.13	0.48
1:G:13:LEU:HD22	1:H:231:PHE:CD1	2.48	0.48
2:I:156:PHE:CE1	2:I:445:ILE:HG13	2.49	0.48
5:L:444:ALA:HB1	5:L:457:ILE:HD13	1.95	0.48
1:B:97:GLU:OE1	1:B:147:GLN:NE2	2.47	0.48
2:C:105:TYR:CD1	2:C:111:GLU:HB3	2.49	0.48
5:F:484:ALA:HB1	5:F:491:GLU:HB2	1.96	0.48
2:I:1296:ASP:CG	2:I:1322:SER:HB3	2.34	0.48
2:I:117:ILE:HD12	2:I:488:MET:CG	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:515:ARG:NH2	3:J:717:VAL:O	2.47	0.48
5:L:226:ALA:O	5:L:229:VAL:HG22	2.13	0.48
3:D:197:GLU:O	3:D:201:LEU:HG	2.14	0.48
2:I:241:LEU:HD11	2:I:246:LEU:HD11	1.96	0.48
3:J:365:GLN:O	3:J:437:PHE:HD1	1.97	0.48
3:J:48:THR:C	3:J:50:LYS:H	2.15	0.48
3:J:572:THR:OG1	3:J:576:ARG:HB2	2.13	0.48
5:L:230:VAL:O	5:L:234:THR:HG23	2.14	0.48
5:L:383:ASN:HB2	5:L:412:LEU:HD21	1.95	0.48
2:C:1106:ARG:O	2:C:1108:ASN:N	2.45	0.48
2:C:862:LEU:HA	2:C:865:LEU:HB2	1.96	0.48
2:I:470:ARG:HE	2:I:497:PRO:HB3	1.79	0.48
3:J:1270:GLY:HA3	3:J:1298:VAL:O	2.13	0.48
3:J:363:LEU:HA	3:J:450:HIS:CD2	2.49	0.48
5:L:314:THR:O	5:L:318:ALA:HB3	2.14	0.48
6:N:20:VAL:HG13	6:N:39:HIS:CE1	2.49	0.48
3:D:827:GLU:O	3:D:829:GLY:N	2.45	0.48
1:G:32:GLU:HB2	1:G:35:PHE:CD2	2.48	0.48
2:I:1065:LYS:HE2	3:J:462:ASP:O	2.14	0.48
2:I:993:PRO:HB2	2:I:995:ASP:OD2	2.14	0.48
3:J:317:THR:HG22	3:J:322:ARG:O	2.14	0.48
3:J:929:GLN:HA	6:N:75:ARG:HD2	1.96	0.48
2:C:213:LEU:HD13	2:C:422:LYS:HG2	1.96	0.48
2:C:691:PRO:HA	2:C:788:SER:OG	2.14	0.48
3:D:850:LYS:HE2	3:D:855:ASP:HB3	1.95	0.48
4:E:4:VAL:HG13	4:E:5:THR:N	2.28	0.48
5:F:151:VAL:HG22	5:F:156:ALA:HB3	1.95	0.48
1:G:172:LEU:HD12	1:G:172:LEU:H	1.79	0.48
5:L:573:LEU:H	5:L:573:LEU:CD2	2.21	0.48
1:H:62:ASP:N	1:H:62:ASP:OD1	2.33	0.47
3:J:925:GLU:HB3	3:J:926:PRO:HD3	1.95	0.47
1:A:166:ARG:O	1:A:168:ILE:N	2.47	0.47
3:D:824:PRO:HD3	3:D:835:LEU:HB2	1.96	0.47
2:C:902:LEU:HD12	5:F:607:LEU:HD23	1.95	0.47
1:G:137:ASN:N	1:G:137:ASN:OD1	2.47	0.47
1:G:228:LEU:O	1:G:230:ALA:N	2.47	0.47
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.62	0.47
2:I:1280:ALA:HB3	3:J:431:ARG:HB3	1.95	0.47
3:J:665:GLN:CG	3:J:678:ARG:HH21	2.27	0.47
1:A:233:ASP:HA	1:B:218:ARG:NH1	2.29	0.47
2:C:678:ARG:HG3	2:C:1108:ASN:HD22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1304:MET:O	2:C:1308:ILE:HG12	2.14	0.47
2:C:490:GLN:HG3	5:F:472:GLN:OE1	2.14	0.47
1:G:125:LYS:HG3	1:G:128:HIS:HB2	1.96	0.47
2:I:616:ILE:HG22	2:I:617:ALA:O	2.14	0.47
3:J:1184:ASP:O	3:J:1186:TYR:N	2.48	0.47
3:J:210:SER:HB2	3:J:213:LYS:HB2	1.96	0.47
5:L:478:PRO:HG2	5:L:483:LEU:HD11	1.96	0.47
6:M:55:VAL:O	6:M:59:VAL:HG23	2.13	0.47
1:A:14:VAL:HG22	1:A:15:ASP:N	2.26	0.47
1:A:323:PRO:CB	1:A:324:ALA:HB2	2.44	0.47
1:A:223:ILE:HD13	1:B:8:PHE:CZ	2.48	0.47
3:D:1199:PHE:HB2	3:D:1202:GLU:CB	2.42	0.47
3:D:518:VAL:N	3:D:716:GLN:HE22	2.13	0.47
3:D:690:ASN:ND2	3:D:745:GLY:HA2	2.29	0.47
5:F:515:GLU:HG2	5:F:516:ASP:N	2.29	0.47
2:I:733:VAL:HG21	2:I:966:ILE:HD13	1.95	0.47
3:J:186:GLN:HG3	3:J:238:ILE:HB	1.96	0.47
3:J:361:LEU:HD22	3:J:365:GLN:HG3	1.97	0.47
5:L:298:PRO:HD2	5:L:326:TRP:CD1	2.49	0.47
5:L:395:THR:OG1	5:L:396:ASN:N	2.45	0.47
1:A:145:LYS:NZ	1:A:147:GLN:OE1	2.47	0.47
3:D:701:LEU:CD1	3:D:723:TYR:HB2	2.44	0.47
5:F:276:MET:SD	5:F:279:ARG:NH1	2.87	0.47
2:I:1087:TYR:CE1	2:I:1215:GLY:HA2	2.48	0.47
2:I:1238:LEU:H	2:I:1238:LEU:HD12	1.79	0.47
3:J:901:ARG:HA	3:J:908:ILE:HA	1.95	0.47
4:K:15:ASN:HB3	4:K:18:ASP:H	1.80	0.47
2:C:681:MET:O	2:C:685:MET:HE2	2.14	0.47
2:C:981:ALA:HB1	2:C:1007:LYS:NZ	2.30	0.47
3:D:1215:GLU:HG3	3:D:1220:ILE:HD11	1.96	0.47
3:D:1273:ASP:O	3:D:1275:LEU:N	2.41	0.47
3:D:210:SER:HB2	3:D:213:LYS:HB2	1.96	0.47
3:D:748:ALA:O	3:D:777:HIS:CD2	2.68	0.47
5:F:399:LEU:HA	5:F:399:LEU:HD12	1.60	0.47
2:I:1246:ARG:NH2	2:I:1249:GLY:H	2.13	0.47
2:I:463:GLN:HG3	2:I:505:PHE:HB2	1.95	0.47
3:J:161:THR:HG22	3:J:164:GLN:HB2	1.96	0.47
4:K:15:ASN:C	4:K:17:PHE:H	2.18	0.47
5:L:489:MET:O	5:L:491:GLU:N	2.47	0.47
1:A:73:GLY:O	1:A:134:THR:HG22	2.15	0.47
1:B:89:ALA:HB3	1:B:124:VAL:CG1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:263:VAL:HG21	2:C:273:HIS:CG	2.50	0.47
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.97	0.47
2:C:728:ASP:HB3	2:C:731:ARG:H	1.79	0.47
3:D:770:LEU:H	3:D:770:LEU:HD22	1.79	0.47
5:F:399:LEU:HG	5:F:403:ASP:HB3	1.97	0.47
2:I:1149:TYR:HD1	2:I:1159:VAL:HG11	1.80	0.47
2:I:124:MET:HB3	2:I:493:ILE:HD11	1.96	0.47
2:I:782:VAL:HG11	2:I:792:GLY:HA2	1.96	0.47
3:J:198:CYS:O	3:J:202:ARG:HG3	2.14	0.47
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.95	0.47
2:C:268:ARG:NH2	2:C:270:THR:HG21	2.30	0.47
2:C:607:SER:OG	2:C:609:ILE:HG13	2.15	0.47
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.97	0.47
2:I:710:VAL:HA	2:I:715:THR:HG21	1.95	0.47
3:J:849:LEU:H	3:J:849:LEU:HD22	1.80	0.47
5:L:571:TYR:HD1	5:L:575:GLU:HG2	1.79	0.47
2:C:551:HIS:ND1	2:C:553:THR:OG1	2.47	0.47
5:F:454:VAL:HA	5:F:457:ILE:HD12	1.97	0.47
2:I:1022:LYS:HD2	2:I:1022:LYS:HA	1.73	0.47
2:I:1281:TYR:HE1	3:J:484:MET:HE3	1.78	0.47
2:I:596:ASP:CG	2:I:597:GLY:N	2.68	0.47
2:I:661:VAL:HB	2:I:665:ALA:HB3	1.96	0.47
3:J:292:VAL:O	3:J:296:LYS:HG3	2.15	0.47
2:I:1243:MET:SD	3:J:445:LYS:HD3	2.54	0.47
3:J:825:VAL:C	3:J:826:ILE:HG13	2.35	0.47
6:N:108:ASP:CG	6:N:109:GLU:H	2.13	0.47
1:A:32:GLU:HB2	1:A:35:PHE:CD2	2.50	0.47
1:A:261:GLU:OE2	2:C:859:GLU:HB2	2.15	0.47
3:D:489:ASN:HA	3:D:904:ALA:CB	2.45	0.47
5:F:379:MET:O	5:F:383:ASN:ND2	2.48	0.47
2:I:1030:GLU:OE1	2:I:1033:ARG:NH2	2.48	0.47
2:I:959:ASP:O	2:I:963:GLU:HG2	2.14	0.47
3:J:1350:ASN:HA	3:J:1353:VAL:HG12	1.97	0.47
1:B:89:ALA:HB3	1:B:124:VAL:HG12	1.97	0.47
2:C:487:LEU:H	2:C:487:LEU:HD23	1.80	0.47
2:C:593:LYS:HE3	2:C:595:THR:HG22	1.97	0.47
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.80	0.47
5:F:226:ALA:O	5:F:229:VAL:HG22	2.15	0.47
2:I:17:LYS:NZ	2:I:1154:ASP:OD1	2.38	0.47
2:I:1288:GLN:HE21	3:J:1355:ARG:HA	1.80	0.47
3:J:1154:ALA:HB3	3:J:1215:GLU:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:587:LEU:HD23	3:J:591:ILE:HG21	1.95	0.47
2:C:104:ILE:O	2:C:113:THR:HA	2.14	0.46
2:C:1305:TYR:OH	5:F:532:LEU:HG	2.15	0.46
2:C:176:ILE:HB	2:C:184:LEU:HB3	1.97	0.46
2:C:301:TYR:HB2	2:C:311:CYS:SG	2.55	0.46
2:C:566:GLY:O	2:C:569:ILE:HG13	2.14	0.46
2:C:887:VAL:HB	2:C:913:VAL:HG22	1.96	0.46
5:F:551:LEU:CD2	5:F:597:LYS:HD2	2.44	0.46
2:I:1282:GLY:O	2:I:1284:ALA:N	2.48	0.46
2:I:557:ARG:HD3	2:I:587:LEU:HB3	1.97	0.46
2:I:565:GLU:O	2:I:565:GLU:HG2	2.15	0.46
3:J:900:GLY:HA3	3:J:1251:LYS:HD3	1.98	0.46
3:J:17:PHE:O	3:J:1355:ARG:NH2	2.47	0.46
1:A:115:ILE:HG22	1:A:116:THR:N	2.30	0.46
1:A:233:ASP:HA	1:B:218:ARG:HH11	1.79	0.46
1:B:44:ARG:HG3	1:B:183:ILE:HD13	1.98	0.46
2:C:1234:LYS:HE2	2:C:1238:LEU:HD23	1.97	0.46
2:C:147:SER:OG	2:C:455:SER:HB3	2.16	0.46
2:C:26:TYR:HE2	2:C:32:LEU:HD12	1.80	0.46
2:C:1253:LEU:HD11	3:D:253:VAL:HG11	1.97	0.46
3:D:277:ASN:HA	3:D:280:LYS:HG3	1.96	0.46
3:D:45:ASN:HB3	3:D:48:THR:O	2.15	0.46
3:D:863:LEU:HD11	3:D:901:ARG:HB3	1.96	0.46
2:I:384:LEU:O	2:I:388:LEU:HG	2.15	0.46
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.98	0.46
1:H:59:VAL:HG22	1:H:144:ILE:HG13	1.98	0.46
2:I:1151:LEU:HD23	2:I:1151:LEU:HA	1.82	0.46
2:I:1308:ILE:HD12	3:J:380:PHE:CZ	2.50	0.46
3:J:1181:ASP:OD1	3:J:1182:GLY:N	2.47	0.46
3:J:522:GLY:O	3:J:525:MET:HG2	2.14	0.46
3:J:665:GLN:HG3	3:J:678:ARG:HH21	1.80	0.46
5:L:320:ILE:HG23	5:L:327:SER:O	2.15	0.46
6:N:140:THR:O	6:N:144:ILE:HG12	2.15	0.46
3:D:510:LEU:O	3:D:514:THR:HG22	2.15	0.46
3:D:430:HIS:ND1	3:D:925:GLU:HG3	2.30	0.46
5:F:130:VAL:HA	5:F:133:SER:HB2	1.96	0.46
2:I:998:LEU:HD12	2:I:998:LEU:H	1.80	0.46
3:J:1238:GLN:NE2	3:J:1248:ILE:O	2.44	0.46
3:J:559:ALA:HB3	3:J:562:GLU:HB3	1.97	0.46
3:J:664:ILE:HD11	3:J:685:ILE:HD12	1.96	0.46
3:J:504:GLN:OE1	3:J:731:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ASP:H	1:A:121:VAL:HB	1.80	0.46
1:A:195:ARG:HD2	1:A:196:THR:N	2.31	0.46
2:C:886:LYS:NZ	2:C:916:SER:HB3	2.30	0.46
2:C:9:LYS:O	2:C:1172:LEU:HD23	2.15	0.46
3:D:510:LEU:HD22	3:D:601:ILE:HD11	1.97	0.46
3:D:733:SER:O	3:D:736:GLN:N	2.48	0.46
3:D:850:LYS:HB2	3:D:852:GLY:O	2.15	0.46
2:I:832:HIS:CE1	2:I:1058:ARG:HD2	2.51	0.46
3:J:57:PHE:HB3	3:J:98:ARG:HH22	1.80	0.46
1:A:163:GLU:O	1:A:164:ASP:HB2	2.14	0.46
2:C:14:ASP:OD2	2:C:1156:ARG:NE	2.49	0.46
2:C:171:LEU:HA	2:C:171:LEU:HD23	1.73	0.46
2:C:338:THR:HG22	2:C:345:PRO:HB3	1.98	0.46
2:C:998:LEU:HD12	2:C:998:LEU:H	1.80	0.46
3:D:365:GLN:O	3:D:437:PHE:HD1	1.98	0.46
3:D:518:VAL:HG22	3:D:709:ARG:HB2	1.96	0.46
3:D:395:LYS:NZ	5:F:612:ASP:HB3	2.31	0.46
2:I:678:ARG:HD3	2:I:678:ARG:HA	1.79	0.46
2:I:897:PRO:HB2	2:I:898:GLU:OE1	2.16	0.46
2:I:957:LYS:HG3	2:I:1029:LEU:HD11	1.97	0.46
3:J:827:GLU:O	3:J:829:GLY:N	2.44	0.46
2:C:1124:ILE:O	2:C:1128:ILE:HG13	2.15	0.46
2:C:1129:ASN:OD1	2:C:1177:ARG:NH2	2.35	0.46
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.49	0.46
2:C:1327:LEU:O	2:C:1331:ARG:HB2	2.16	0.46
2:C:563:THR:OG1	2:C:564:PRO:HD2	2.16	0.46
2:C:684:ASN:HA	2:C:687:ARG:NH1	2.31	0.46
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.81	0.46
2:I:176:ILE:HD12	2:I:184:LEU:HD23	1.97	0.46
2:I:208:ILE:HG12	2:I:362:ALA:CB	2.46	0.46
2:I:246:LEU:HB2	2:I:269:ILE:HG21	1.97	0.46
2:I:819:SER:HB2	2:I:1085:MET:HG3	1.97	0.46
3:J:495:ASN:C	3:J:497:GLU:H	2.17	0.46
3:J:53:ARG:HA	3:J:54:ASP:HA	1.56	0.46
3:J:599:LYS:CE	6:N:69:PHE:HE1	2.29	0.46
2:C:119:GLU:HG3	2:C:488:MET:HB3	1.97	0.46
2:C:936:ARG:HD2	2:C:939:VAL:CG2	2.44	0.46
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.51	0.46
3:D:825:VAL:C	3:D:826:ILE:HG13	2.36	0.46
1:A:49:SER:HB3	2:C:1083:GLU:CD	2.37	0.46
2:C:151:ARG:HH12	2:C:175:ARG:HH11	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:483:ASP:HB2	2:C:486:THR:CG2	2.45	0.46
2:C:517:GLN:HG3	2:C:523:GLU:OE2	2.16	0.46
2:C:972:PHE:CB	2:C:994:ARG:HH21	2.28	0.46
3:D:120:LEU:HG	3:D:1330:ARG:HH21	1.81	0.46
3:D:500:ILE:O	3:D:500:ILE:HG22	2.16	0.46
3:D:659:ALA:O	3:D:663:GLU:N	2.49	0.46
3:D:1361:THR:HG22	4:E:21:LEU:HD22	1.97	0.46
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.27	0.46
3:J:227:PHE:O	3:J:230:SER:HB3	2.16	0.46
5:L:166:VAL:O	5:L:167:ASP:HB2	2.15	0.46
6:N:25:GLU:HG2	6:N:25:GLU:H	1.44	0.46
1:A:11:PRO:HA	1:A:30:PRO:CG	2.46	0.46
1:A:211:ILE:HD13	1:A:211:ILE:HA	1.63	0.46
2:C:667:LEU:HA	2:C:667:LEU:HD23	1.69	0.46
5:F:309:ASN:HD21	5:F:312:SER:HB3	1.80	0.46
2:I:533:LEU:HD21	2:I:571:LEU:HD13	1.98	0.46
3:J:197:GLU:O	3:J:201:LEU:HG	2.16	0.46
3:J:24:LEU:HD11	3:J:116:PHE:CZ	2.51	0.46
3:J:395:LYS:HG2	5:L:536:THR:HG21	1.98	0.46
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.81	0.45
2:C:1238:LEU:H	2:C:1238:LEU:HD12	1.80	0.45
2:C:27:LEU:HD23	2:C:27:LEU:HA	1.68	0.45
1:A:70:THR:HG21	2:C:755:LYS:HE2	1.97	0.45
3:D:1301:THR:HG21	3:J:1299:GLY:O	2.16	0.45
3:D:268:LEU:HD23	3:D:268:LEU:HA	1.62	0.45
3:D:536:LEU:HD13	3:D:541:LEU:HB2	1.98	0.45
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.97	0.45
5:F:354:THR:O	5:F:358:VAL:HG23	2.16	0.45
5:F:377:LYS:O	5:F:381:GLU:HG3	2.16	0.45
2:I:1142:ARG:HD3	2:I:1161:LEU:HD13	1.98	0.45
2:I:555:TYR:OH	2:I:654:ASP:OD1	2.22	0.45
2:I:742:TYR:HD2	2:I:743:PRO:HD2	1.80	0.45
3:J:123:ARG:NH2	3:J:1334:GLU:HG3	2.31	0.45
3:J:644:MET:HB2	3:J:764:ARG:HG3	1.97	0.45
3:J:789:LYS:HZ2	3:J:932:MET:N	2.13	0.45
3:J:915:ILE:HA	3:J:918:ILE:HG23	1.98	0.45
5:L:420:GLU:OE1	5:L:423:ARG:NH2	2.46	0.45
2:C:169:LYS:O	2:C:170:VAL:HG22	2.17	0.45
3:D:1176:VAL:HG22	3:D:1187:GLU:HB3	1.98	0.45
3:D:418:GLU:OE1	4:E:3:ARG:NH2	2.49	0.45
3:D:79:LYS:HG3	3:D:80:HIS:ND1	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:817:HIS:CE1	3:D:860:ARG:HE	2.35	0.45
3:D:929:GLN:HG2	6:M:75:ARG:HD2	1.98	0.45
5:F:310:GLU:O	5:F:344:LEU:HD21	2.16	0.45
5:F:484:ALA:HB1	5:F:491:GLU:CB	2.46	0.45
2:I:840:SER:HB2	2:I:850:ILE:HD11	1.98	0.45
3:J:358:GLY:N	3:J:359:PRO:HD3	2.31	0.45
3:J:418:GLU:HB2	4:K:45:LYS:HB2	1.98	0.45
2:I:1286:THR:N	3:J:479:GLU:OE2	2.44	0.45
3:J:826:ILE:HD12	3:J:826:ILE:O	2.16	0.45
1:A:11:PRO:HD3	1:B:227:GLN:OE1	2.17	0.45
2:C:1065:LYS:CD	2:C:1235:LEU:HD12	2.45	0.45
2:C:438:GLY:O	6:M:148:GLN:NE2	2.49	0.45
2:C:718:ALA:HB2	2:C:783:LEU:CD2	2.45	0.45
2:C:929:ILE:HD13	2:C:1055:ALA:HB2	1.97	0.45
2:C:1280:ALA:HB3	3:D:431:ARG:HB3	1.98	0.45
3:D:555:TYR:HB2	3:D:586:GLY:HA2	1.98	0.45
3:D:638:SER:OG	3:D:639:VAL:N	2.50	0.45
5:F:363:ARG:O	5:F:367:ILE:HG13	2.16	0.45
1:H:57:THR:HG22	1:H:58:GLU:OE1	2.16	0.45
2:I:250:THR:HA	2:I:268:ARG:HA	1.98	0.45
3:J:482:ALA:HA	4:K:6:VAL:HG11	1.97	0.45
2:C:1105:SER:OG	6:M:74:ASP:OD1	2.25	0.45
2:C:297:VAL:HG12	2:C:315:MET:O	2.15	0.45
3:D:1344:LEU:O	3:D:1346:GLY:N	2.46	0.45
1:H:7:GLU:HG2	1:H:8:PHE:H	1.82	0.45
2:I:188:PHE:CE1	2:I:194:LEU:HD13	2.50	0.45
3:J:1290:ARG:HD2	3:J:1298:VAL:HG12	1.96	0.45
3:J:422:LEU:HD13	3:J:471:PRO:HG3	1.98	0.45
5:L:310:GLU:OE2	5:L:355:ILE:HG21	2.16	0.45
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.46	0.45
2:C:206:ALA:O	2:C:209:ILE:HG22	2.17	0.45
2:C:670:PHE:CZ	2:C:1195:ILE:HD11	2.51	0.45
3:D:1287:ILE:HG22	3:D:1300:ALA:H	1.81	0.45
3:D:13:LYS:HD3	3:D:13:LYS:HA	1.78	0.45
3:D:81:ARG:O	3:D:83:VAL:N	2.50	0.45
5:F:532:LEU:O	5:F:536:THR:HG23	2.16	0.45
2:I:678:ARG:NH1	2:I:1071:GLY:O	2.35	0.45
2:I:618:GLN:CG	3:J:770:LEU:HD21	2.46	0.45
3:J:599:LYS:HE2	6:N:69:PHE:HE1	1.81	0.45
3:J:848:VAL:HB	3:J:858:VAL:HG22	1.97	0.45
5:L:98:VAL:HB	5:L:402:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:525:ASP:CG	5:L:528:LEU:HG	2.36	0.45
1:G:224:LEU:HD13	1:H:228:LEU:HD11	1.97	0.45
1:G:65:LEU:HA	1:G:65:LEU:HD13	1.82	0.45
3:J:246:PRO:HA	3:J:247:PRO:HD3	1.88	0.45
3:J:316:ILE:HA	3:J:323:PRO:HA	1.99	0.45
3:J:615:LYS:HB2	3:J:616:PRO:HD3	1.98	0.45
3:J:843:VAL:HG13	3:J:883:ARG:HD3	1.99	0.45
3:J:866:GLU:OE2	3:J:901:ARG:NH2	2.49	0.45
1:A:89:ALA:O	1:A:124:VAL:HG12	2.17	0.45
2:C:151:ARG:HH12	2:C:175:ARG:NH1	2.15	0.45
2:C:587:LEU:HD23	2:C:587:LEU:HA	1.53	0.45
3:D:1332:LEU:O	3:D:1336:ALA:N	2.44	0.45
3:D:664:ILE:CD1	3:D:681:LYS:HG2	2.44	0.45
3:J:1156:LEU:HB3	3:J:1207:GLY:HA2	1.99	0.45
3:J:1280:VAL:HG11	3:J:1304:ARG:NH2	2.32	0.45
3:J:1292:LEU:O	3:J:1293:GLU:HB2	2.17	0.45
3:J:749:LYS:HB3	3:J:755:ILE:HD11	1.99	0.45
3:J:923:ILE:O	3:J:926:PRO:HD2	2.17	0.45
6:M:145:ARG:O	6:M:149:MET:N	2.32	0.45
2:C:1111:GLN:HB2	2:C:1230:MET:CE	2.47	0.45
2:C:518:ASN:N	2:C:518:ASN:OD1	2.50	0.45
2:C:699:LEU:HA	2:C:699:LEU:HD23	1.75	0.45
3:D:161:THR:HG23	3:D:164:GLN:H	1.82	0.45
5:F:166:VAL:O	5:F:167:ASP:HB2	2.17	0.45
1:H:196:THR:HG23	3:J:443:GLU:HG3	1.98	0.45
2:I:1106:ARG:O	2:I:1108:ASN:N	2.46	0.45
3:J:1365:TYR:OH	3:J:1369:ARG:NH1	2.49	0.45
3:J:156:ARG:NH1	3:J:157:GLN:HE21	2.14	0.45
3:J:342:LEU:HA	3:J:343:LEU:HA	1.69	0.45
1:A:178:SER:OG	1:A:180:VAL:HG23	2.17	0.45
1:A:224:LEU:HG	1:A:228:LEU:HD12	1.98	0.45
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.47	0.45
2:C:1331:ARG:HG2	3:D:33:TRP:CZ3	2.51	0.45
1:A:135:ASP:HB2	2:C:726:TYR:HE1	1.82	0.45
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.47	0.45
2:C:88:ARG:HH11	2:C:88:ARG:HB2	1.81	0.45
3:D:1297:LYS:N	3:D:1298:VAL:HA	2.32	0.45
3:D:739:GLN:OE1	3:D:744:ARG:HB2	2.17	0.45
5:F:94:THR:HG21	5:F:99:ARG:HG2	1.99	0.45
1:H:99:ILE:HD11	1:H:143:ARG:HB3	1.99	0.45
2:I:655:VAL:N	2:I:659:GLN:OE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:205:LEU:HD23	3:J:217:LEU:HG	1.99	0.45
3:J:657:ALA:O	3:J:661:VAL:HG23	2.16	0.45
5:L:233:ASP:O	5:L:236:LYS:HE2	2.16	0.45
1:B:69:SER:H	1:B:78:ILE:HD12	1.82	0.45
2:C:1156:ARG:HH11	2:C:1156:ARG:HB2	1.82	0.45
2:C:290:GLU:HG2	2:C:319:LEU:CD1	2.47	0.45
2:C:568:ASN:HB2	2:C:571:LEU:HB2	1.99	0.45
1:H:49:SER:O	1:H:151:GLY:HA2	2.17	0.45
1:H:59:VAL:HG23	1:H:173:VAL:HG21	1.98	0.45
2:I:1253:LEU:HA	5:L:525:ASP:HB2	1.99	0.45
2:I:1285:TYR:CZ	3:J:1356:LEU:HD11	2.52	0.45
3:J:494:ALA:CB	3:J:922:SER:HB3	2.46	0.45
5:L:225:ARG:O	5:L:229:VAL:HG13	2.17	0.45
5:L:493:LYS:HG2	5:L:496:LYS:HE2	1.99	0.45
1:A:31:LEU:HD23	1:A:31:LEU:HA	1.66	0.44
2:C:42:ASP:OD1	2:C:44:GLU:HG2	2.17	0.44
2:C:565:GLU:HG2	2:C:565:GLU:O	2.17	0.44
3:D:372:MET:O	3:D:376:LEU:HD12	2.17	0.44
3:D:73:GLY:O	3:D:76:LYS:HG3	2.17	0.44
1:G:69:SER:O	1:G:78:ILE:HG12	2.18	0.44
2:I:153:PRO:HA	2:I:177:ILE:O	2.18	0.44
2:I:637:ARG:HA	2:I:642:SER:HA	1.98	0.44
2:I:891:GLY:O	2:I:892:GLU:HG3	2.17	0.44
3:J:599:LYS:HD3	3:J:599:LYS:HA	1.49	0.44
5:L:276:MET:O	5:L:280:VAL:HG23	2.17	0.44
1:A:169:GLY:O	1:A:171:LEU:HD22	2.17	0.44
1:A:249:PHE:HE2	1:A:254:LEU:HG	1.81	0.44
2:C:395:TYR:HB3	2:C:419:ILE:HG22	1.97	0.44
2:C:800:MET:SD	2:C:1096:ILE:HD11	2.57	0.44
3:D:599:LYS:HA	3:D:599:LYS:HD3	1.56	0.44
3:D:678:ARG:O	3:D:682:VAL:HG23	2.17	0.44
5:F:490:PRO:HB2	5:F:493:LYS:HG3	1.99	0.44
2:I:705:GLU:HB2	2:I:794:LEU:H	1.81	0.44
2:I:810:TYR:HE2	3:J:359:PRO:HD2	1.81	0.44
2:I:887:VAL:HB	2:I:913:VAL:HG21	1.98	0.44
3:J:268:LEU:HD23	3:J:268:LEU:HA	1.71	0.44
2:C:1164:PHE:HD1	2:C:1164:PHE:HA	1.67	0.44
2:C:1240:ASP:N	2:C:1240:ASP:OD1	2.45	0.44
2:C:221:LEU:HD12	2:C:298:ALA:O	2.18	0.44
2:C:620:ASN:ND2	2:C:620:ASN:O	2.50	0.44
2:C:92:TYR:CD2	2:C:129:LEU:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:310:GLU:OE2	5:F:355:ILE:HG21	2.17	0.44
2:I:227:LYS:NZ	2:I:298:ALA:HB1	2.31	0.44
3:J:1221:LEU:HD11	3:J:1304:ARG:O	2.18	0.44
5:L:448:ARG:HB3	5:L:448:ARG:HE	1.61	0.44
6:N:98:LYS:NZ	6:N:101:LYS:HD3	2.32	0.44
1:A:175:ALA:HB1	1:A:177:TYR:CE1	2.53	0.44
1:A:239:GLN:HG3	1:A:240:PRO:HD2	2.00	0.44
1:A:253:LEU:HA	1:A:278:ILE:HD11	1.99	0.44
2:C:870:ILE:HG22	2:C:944:ARG:NH1	2.33	0.44
1:B:48:LEU:HD21	3:D:535:ARG:HG3	1.99	0.44
3:D:744:ARG:O	3:D:744:ARG:HG3	2.18	0.44
2:C:367:TYR:HA	2:C:384:LEU:HD22	2.00	0.44
3:D:37:GLU:HA	3:D:104:HIS:O	2.18	0.44
3:D:707:ILE:H	3:D:707:ILE:HD12	1.82	0.44
1:G:181:GLU:HB3	1:G:206:GLU:HG2	1.99	0.44
2:I:202:ARG:NH2	2:I:368:ARG:HH12	2.16	0.44
2:I:356:THR:HG21	2:I:362:ALA:HA	2.00	0.44
2:I:724:VAL:HG23	2:I:775:GLU:N	2.28	0.44
2:I:996:ARG:HA	2:I:996:ARG:HD3	1.57	0.44
5:L:281:ARG:HG3	5:L:285:ARG:HH11	1.82	0.44
5:L:357:GLN:HA	5:L:360:ASP:HB2	2.00	0.44
6:M:139:LYS:HZ2	6:M:143:GLU:CD	2.20	0.44
1:A:67:GLU:HG2	1:A:171:LEU:HD12	1.98	0.44
2:C:320:ASP:OD1	2:C:324:LYS:HE3	2.17	0.44
2:C:148:GLN:OE1	2:C:454:ARG:NH2	2.51	0.44
3:D:259:ARG:NH1	5:F:502:LYS:HB3	2.31	0.44
5:F:388:ILE:HG22	5:F:392:LYS:HE3	1.98	0.44
1:G:9:LEU:O	1:H:227:GLN:NE2	2.51	0.44
2:I:107:ARG:HA	2:I:108:GLU:HA	1.61	0.44
2:I:151:ARG:CZ	2:I:445:ILE:HD11	2.48	0.44
2:I:681:MET:O	2:I:685:MET:HE2	2.17	0.44
3:J:1179:PRO:CD	3:J:1184:ASP:HA	2.47	0.44
3:J:331:ILE:O	3:J:337:ARG:HA	2.18	0.44
3:J:435:GLN:HE21	3:J:486:SER:HA	1.83	0.44
3:J:594:GLN:HB2	3:J:595:ALA:H	1.59	0.44
1:A:162:GLU:HB3	1:A:163:GLU:H	1.62	0.44
1:B:64:VAL:HG11	1:B:69:SER:CB	2.48	0.44
2:C:1287:LEU:HD22	3:D:1357:ILE:CG1	2.48	0.44
2:C:739:ASP:OD1	2:C:739:ASP:N	2.49	0.44
2:C:812:PHE:HZ	3:D:503:SER:HB2	1.82	0.44
5:F:316:PHE:CZ	5:F:334:SER:HA	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1067:ALA:HB2	2:I:1073:LYS:HA	1.99	0.44
3:J:528:THR:O	3:J:551:ARG:HB3	2.17	0.44
3:J:748:ALA:O	3:J:777:HIS:HD2	2.00	0.44
1:A:29:GLU:HB3	1:A:30:PRO:HD3	1.99	0.44
1:B:22:THR:O	1:B:213:PRO:HG3	2.18	0.44
1:B:41:ASN:O	1:B:45:ARG:HG3	2.18	0.44
2:C:1164:PHE:C	2:C:1166:ASP:H	2.21	0.44
2:C:688:GLN:OE1	2:C:1237:HIS:HE1	2.01	0.44
3:D:239:LEU:HA	3:D:239:LEU:HD23	1.49	0.44
4:E:15:ASN:C	4:E:17:PHE:H	2.21	0.44
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.18	0.44
2:I:800:MET:HG3	2:I:1096:ILE:HD11	2.00	0.44
5:L:559:LEU:HA	5:L:559:LEU:HD12	1.75	0.44
6:N:69:PHE:HA	6:N:70:PRO:HD3	1.85	0.44
1:B:31:LEU:HA	1:B:31:LEU:HD13	1.85	0.44
2:C:551:HIS:CG	2:C:552:PRO:HD2	2.53	0.44
3:D:1166:GLY:O	3:D:1174:ARG:HB2	2.18	0.44
3:D:358:GLY:N	3:D:359:PRO:HD3	2.33	0.44
3:D:789:LYS:HZ1	3:D:932:MET:N	2.16	0.44
4:E:50:ALA:O	4:E:54:ILE:HG12	2.17	0.44
5:F:584:ARG:HA	5:F:584:ARG:HD2	1.66	0.44
1:H:67:GLU:HA	1:H:78:ILE:HG21	2.00	0.44
1:H:88:LEU:HD12	1:H:89:ALA:H	1.83	0.44
2:I:550:VAL:HB	3:J:780:ARG:CZ	2.48	0.44
3:D:1227:HIS:CD2	3:J:1293:GLU:HG2	2.53	0.44
3:J:617:THR:O	3:J:620:PHE:HB3	2.18	0.44
5:L:115:GLY:HA2	5:L:118:ASP:HB2	2.00	0.44
1:B:44:ARG:CG	1:B:183:ILE:HD13	2.48	0.43
2:C:750:ILE:HD13	2:C:963:GLU:OE2	2.18	0.43
3:D:1284:ARG:HE	3:D:1304:ARG:NH2	2.16	0.43
3:D:528:THR:O	3:D:551:ARG:HB3	2.17	0.43
5:F:421:TYR:CE2	5:F:422:ARG:HG3	2.53	0.43
5:F:608:ARG:HH11	5:F:608:ARG:CG	2.30	0.43
2:I:1193:ALA:O	2:I:1197:GLU:HB2	2.18	0.43
2:I:13:LYS:HD3	2:I:1149:TYR:HA	1.99	0.43
3:J:364:HIS:CG	4:K:4:VAL:HG23	2.52	0.43
1:B:211:ILE:HD11	1:B:215:GLU:CD	2.39	0.43
3:D:309:ASN:HD21	3:D:315:ALA:N	2.15	0.43
3:D:317:THR:HA	3:D:324:LEU:HD23	2.00	0.43
1:H:153:VAL:HG11	1:H:158:ARG:HH11	1.83	0.43
2:I:1072:ASN:OD1	2:I:1072:ASN:N	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:147:GLN:HE22	5:L:150:ARG:HH11	1.66	0.43
2:C:1142:ARG:NH2	2:C:1165:SER:HB2	2.32	0.43
2:C:1290:MET:SD	2:C:1294:LYS:HE3	2.58	0.43
2:C:149:LEU:HD12	2:C:452:ARG:O	2.17	0.43
3:D:159:ILE:HG13	3:D:159:ILE:O	2.18	0.43
3:D:705:THR:OG1	3:D:718:SER:HA	2.18	0.43
5:F:111:LEU:HD13	5:F:116:GLU:HA	2.00	0.43
1:G:16:ILE:HG23	1:G:26:VAL:HG12	2.00	0.43
2:I:119:GLU:CG	2:I:488:MET:HB3	2.49	0.43
2:I:225:PHE:HZ	2:I:348:SER:H	1.65	0.43
2:I:65:ASN:HB3	2:I:105:TYR:HB2	2.00	0.43
3:J:288:PRO:O	3:J:292:VAL:HG13	2.18	0.43
2:C:15:PHE:HE2	2:C:1182:ILE:HG21	1.84	0.43
2:C:37:LYS:HD3	2:C:37:LYS:HA	1.81	0.43
2:C:533:LEU:HD11	2:C:540:ARG:HD2	2.00	0.43
2:C:1269:ARG:HD3	3:D:343:LEU:HB2	2.00	0.43
3:D:513:MET:HE2	3:D:513:MET:HB3	1.80	0.43
2:C:1101:LEU:CB	3:D:731:ARG:HD3	2.39	0.43
2:I:841:ARG:HA	2:I:1046:VAL:HA	2.00	0.43
2:I:1151:LEU:HD11	2:I:1198:LEU:HB2	1.99	0.43
2:I:814:ASP:HB3	2:I:1073:LYS:O	2.19	0.43
3:J:1170:LYS:C	3:J:1172:LYS:H	2.22	0.43
3:J:275:ARG:HD3	3:J:298:MET:HB3	2.00	0.43
1:A:125:LYS:HE3	1:A:128:HIS:HB2	2.01	0.43
3:D:1219:ASP:O	3:D:1222:ARG:N	2.50	0.43
3:D:22:ILE:O	3:D:1339:GLY:HA2	2.18	0.43
3:D:518:VAL:HG11	3:D:707:ILE:HD13	2.01	0.43
4:E:38:LEU:HB2	4:E:53:GLU:OE1	2.18	0.43
2:I:1184:THR:HG23	2:I:1189:GLY:CA	2.48	0.43
2:I:234:ASP:OD1	2:I:235:ASN:N	2.51	0.43
2:I:75:LEU:HD13	2:I:75:LEU:HA	1.85	0.43
2:I:933:VAL:HG11	2:I:945:ALA:HB2	2.00	0.43
2:I:748:ILE:HD13	2:I:970:GLY:HA3	2.01	0.43
6:N:32:MET:SD	6:N:37:LEU:HD11	2.58	0.43
1:A:321:TRP:HA	1:A:322:PRO:HA	1.86	0.43
1:A:77:ASP:OD2	2:C:755:LYS:NZ	2.48	0.43
1:B:190:ALA:O	1:B:198:LEU:HB2	2.19	0.43
4:E:56:GLU:HB2	4:E:58:LEU:HD11	2.01	0.43
1:G:207:THR:HG21	1:G:211:ILE:HG22	2.00	0.43
2:I:1075:VAL:HG21	3:J:463:GLY:HA2	2.00	0.43
2:I:778:GLU:HB3	2:I:781:ASP:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1267:VAL:HB	3:J:1301:THR:OG1	2.19	0.43
3:J:382:TYR:HE1	3:J:401:VAL:HG21	1.84	0.43
3:J:706:VAL:HG12	3:J:715:LYS:HB3	2.01	0.43
2:C:1161:LEU:HD21	2:C:1165:SER:HB3	2.01	0.43
2:C:513:GLN:HG3	2:C:526:HIS:CE1	2.53	0.43
3:D:1292:LEU:HA	3:J:1226:VAL:CG2	2.49	0.43
3:D:809:VAL:HA	3:D:894:VAL:O	2.18	0.43
3:D:835:LEU:O	3:D:839:VAL:HG23	2.19	0.43
3:D:902:ASP:OD1	3:D:903:LEU:N	2.52	0.43
3:D:929:GLN:HG2	6:M:75:ARG:CD	2.49	0.43
5:F:141:ILE:HG21	5:F:228:TYR:CD1	2.54	0.43
5:F:584:ARG:O	5:F:588:ARG:HG3	2.19	0.43
2:I:587:LEU:HD23	2:I:587:LEU:HA	1.87	0.43
3:J:1344:LEU:HB3	3:J:1350:ASN:ND2	2.34	0.43
3:J:1356:LEU:HA	3:J:1356:LEU:HD23	1.82	0.43
3:J:421:VAL:HG22	3:J:439:PRO:HG3	2.00	0.43
3:J:363:LEU:HD11	3:J:500:ILE:HG21	1.99	0.43
3:J:825:VAL:HG22	3:J:833:GLU:H	1.83	0.43
3:J:872:LEU:HD23	3:J:872:LEU:HA	1.77	0.43
2:I:936:ARG:NH1	5:L:495:ARG:HE	2.15	0.43
1:B:73:GLY:HA2	1:B:134:THR:CG2	2.49	0.43
2:C:246:LEU:HB2	2:C:269:ILE:HG21	2.01	0.43
2:C:349:GLU:O	2:C:353:VAL:HG23	2.17	0.43
2:C:994:ARG:HD2	2:C:997:TRP:CH2	2.54	0.43
3:D:103:GLY:C	3:D:244:VAL:HG22	2.39	0.43
3:D:1183:SER:CB	3:J:206:ASN:HD21	2.31	0.43
3:D:416:ILE:HA	3:D:416:ILE:HD13	1.72	0.43
3:D:525:MET:O	3:D:548:VAL:HG13	2.19	0.43
3:D:872:LEU:HD23	3:D:872:LEU:HA	1.77	0.43
1:G:219:ARG:HA	1:G:222:THR:HB	2.01	0.43
2:I:678:ARG:NH2	6:N:73:VAL:HG11	2.33	0.43
2:I:886:LYS:NZ	2:I:916:SER:HB3	2.34	0.43
3:J:1143:ASP:HA	3:J:1148:ARG:NH1	2.33	0.43
3:D:1292:LEU:O	3:J:1227:HIS:HD2	2.01	0.43
3:J:716:GLN:HG3	3:J:717:VAL:O	2.19	0.43
2:I:1192:GLU:OE1	3:J:764:ARG:NH1	2.50	0.43
5:L:580:PHE:HD1	5:L:580:PHE:HA	1.65	0.43
2:C:106:GLU:OE1	2:C:114:VAL:HG22	2.18	0.43
2:C:131:THR:OG1	2:C:135:THR:O	2.37	0.43
2:C:153:PRO:HB2	2:C:401:GLY:HA2	2.00	0.43
2:C:742:TYR:HD2	2:C:743:PRO:HD2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:316:ILE:HA	3:D:323:PRO:HA	2.00	0.43
2:C:1112:ILE:HD11	3:D:639:VAL:HG22	2.01	0.43
3:D:929:GLN:O	6:M:79:GLU:OE2	2.36	0.43
1:G:49:SER:HB3	2:I:1083:GLU:CD	2.39	0.43
1:H:47:LEU:HD13	1:H:183:ILE:HG21	2.01	0.43
2:I:47:TYR:OH	2:I:398:SER:HB2	2.18	0.43
2:I:921:PRO:O	2:I:924:VAL:HG22	2.18	0.43
3:J:28:ASP:OD1	3:J:31:ARG:NH1	2.52	0.43
3:J:338:PHE:O	3:J:340:GLN:N	2.52	0.43
1:A:104:LYS:HD3	1:A:114:ASP:OD2	2.19	0.43
2:C:143:ARG:NH2	2:C:512:SER:O	2.52	0.43
3:D:218:THR:HA	3:D:221:ILE:HG22	2.01	0.43
3:D:810:THR:CG2	3:D:893:GLY:HA3	2.49	0.43
5:F:316:PHE:HZ	5:F:334:SER:O	2.01	0.43
1:H:155:ALA:HB2	1:H:174:ASP:N	2.34	0.43
2:I:678:ARG:CG	2:I:1108:ASN:HD22	2.29	0.43
2:I:168:GLY:C	2:I:170:VAL:N	2.72	0.43
2:I:227:LYS:HA	2:I:335:THR:O	2.18	0.43
2:I:228:VAL:HB	2:I:335:THR:OG1	2.18	0.43
2:I:149:LEU:HD13	2:I:453:ILE:HG13	2.00	0.43
3:J:1157:ALA:HB3	3:J:1206:ARG:HA	2.00	0.43
3:J:1147:ALA:O	3:J:1218:HIS:NE2	2.52	0.43
5:L:558:VAL:HG23	5:L:580:PHE:CE2	2.54	0.43
3:D:731:ARG:NH2	6:M:73:VAL:HG11	2.31	0.43
1:A:76:GLU:N	1:A:76:GLU:OE2	2.52	0.42
2:C:185:ASP:HB2	2:C:197:ARG:HG3	2.00	0.42
2:C:800:MET:HE3	2:C:800:MET:HB3	1.83	0.42
3:D:357:VAL:HB	3:D:358:GLY:H	1.69	0.42
5:F:341:LEU:CD2	5:F:344:LEU:HD23	2.49	0.42
1:G:154:PRO:HB2	2:I:1059:ARG:HH21	1.84	0.42
2:I:802:VAL:HA	2:I:1096:ILE:O	2.19	0.42
2:I:629:PHE:CD2	2:I:634:VAL:HG11	2.54	0.42
5:L:499:LYS:HB2	5:L:499:LYS:HE3	1.76	0.42
6:M:144:ILE:HG23	6:M:147:LYS:HE2	2.01	0.42
6:N:144:ILE:HG23	6:N:147:LYS:HE2	2.01	0.42
6:N:24:GLN:HG3	6:N:24:GLN:O	2.19	0.42
1:A:220:ALA:O	1:A:223:ILE:HG13	2.18	0.42
2:C:517:GLN:HG2	2:C:517:GLN:O	2.19	0.42
2:C:39:ILE:HD11	2:C:75:LEU:HG	2.00	0.42
3:D:1136:GLY:HA2	3:D:1140:ARG:HG2	2.00	0.42
3:D:337:ARG:NH2	3:D:1323:ALA:HB3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:356:THR:OG1	3:D:357:VAL:N	2.52	0.42
4:E:2:ALA:HB2	4:E:55:GLU:OE2	2.19	0.42
5:F:458:GLU:O	5:F:462:LYS:HG3	2.19	0.42
3:J:195:GLU:H	3:J:195:GLU:HG3	1.65	0.42
3:J:24:LEU:HB2	3:J:232:ASN:OD1	2.20	0.42
3:J:426:ALA:CB	3:J:427:PRO:HD3	2.44	0.42
5:L:482:GLU:HG3	5:L:486:ARG:HH22	1.84	0.42
6:M:33:ASN:OD1	6:M:36:GLN:HB2	2.18	0.42
2:C:107:ARG:HA	2:C:108:GLU:HA	1.28	0.42
2:C:1115:THR:HG22	2:C:1228:GLY:HA3	2.00	0.42
2:C:1222:GLU:HG3	3:D:634:ARG:O	2.19	0.42
2:C:1308:ILE:HD12	3:D:380:PHE:CZ	2.54	0.42
2:C:543:ALA:HA	2:C:544:GLY:HA3	1.75	0.42
3:D:16:GLU:O	3:D:1369:ARG:NH2	2.46	0.42
3:D:194:LEU:HD13	3:D:228:VAL:HG22	2.01	0.42
3:D:903:LEU:HD23	3:D:905:ARG:HD3	2.01	0.42
2:I:678:ARG:HH21	6:N:73:VAL:HG11	1.84	0.42
3:J:1372:ARG:HB2	3:J:1372:ARG:HE	1.64	0.42
3:J:268:LEU:CB	3:J:306:LEU:HD23	2.49	0.42
3:J:650:LYS:O	3:J:654:ILE:HG13	2.19	0.42
3:J:809:VAL:HA	3:J:894:VAL:O	2.20	0.42
6:N:55:VAL:O	6:N:59:VAL:HG23	2.18	0.42
1:A:142:MET:HG3	1:A:144:ILE:HG13	2.01	0.42
2:C:1111:GLN:HB2	2:C:1230:MET:HE2	2.00	0.42
2:C:117:ILE:H	2:C:117:ILE:HG12	1.66	0.42
2:C:230:PHE:CE1	2:C:239:MET:HB2	2.53	0.42
2:C:297:VAL:HB	2:C:317:LEU:HD21	2.01	0.42
2:C:153:PRO:HB2	2:C:401:GLY:CA	2.49	0.42
2:C:466:VAL:HA	2:C:469:VAL:HG22	2.01	0.42
2:C:606:LEU:HD21	2:C:614:TYR:HD1	1.84	0.42
2:C:882:ILE:H	2:C:882:ILE:HD12	1.83	0.42
2:C:846:GLY:C	2:C:889:PRO:HG3	2.40	0.42
3:D:342:LEU:HA	3:D:343:LEU:HA	1.66	0.42
3:D:478:LEU:HG	4:E:47:THR:HG23	2.00	0.42
3:D:529:GLY:HA2	3:D:551:ARG:O	2.19	0.42
3:D:826:ILE:HD12	3:D:826:ILE:O	2.18	0.42
2:C:1298:VAL:HG11	3:D:96:LYS:HZ1	1.83	0.42
5:F:277:MET:HG3	5:F:362:ASN:ND2	2.27	0.42
2:I:194:LEU:HA	2:I:194:LEU:HD12	1.78	0.42
2:I:452:ARG:HH21	2:I:458:GLU:CD	2.23	0.42
2:I:490:GLN:CG	5:L:472:GLN:HG3	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:490:GLN:HG2	5:L:472:GLN:HG3	2.00	0.42
2:I:992:LEU:HD12	2:I:996:ARG:HB3	2.00	0.42
5:L:476:ARG:HH11	5:L:476:ARG:HB3	1.84	0.42
6:N:30:GLU:HG3	6:N:32:MET:H	1.85	0.42
1:A:153:VAL:O	1:A:175:ALA:HB3	2.20	0.42
1:A:272:ALA:C	1:A:274:ALA:H	2.23	0.42
1:A:285:THR:O	1:A:289:LEU:HG	2.20	0.42
2:C:1159:VAL:HB	2:C:1160:ASP:H	1.62	0.42
2:C:1252:SER:HB3	2:C:1255:THR:O	2.20	0.42
3:D:1319:PHE:CE2	3:D:1342:ASP:HB2	2.55	0.42
3:D:548:VAL:HG12	3:D:550:VAL:HG13	2.01	0.42
1:A:251:PRO:HD2	5:F:605:GLU:HG3	2.00	0.42
1:H:60:GLU:O	1:H:142:MET:HB2	2.20	0.42
2:I:1142:ARG:NH1	2:I:1161:LEU:HD11	2.34	0.42
2:I:690:VAL:HG12	2:I:1234:LYS:O	2.20	0.42
3:J:1167:LYS:NZ	3:J:1170:LYS:HB2	2.33	0.42
3:J:322:ARG:HG3	3:J:323:PRO:HD2	2.01	0.42
3:J:773:PHE:O	3:J:776:THR:HB	2.19	0.42
6:N:125:ARG:NH2	6:N:134:LEU:O	2.39	0.42
2:C:832:HIS:CE1	2:C:1058:ARG:HD2	2.53	0.42
2:C:580:GLN:HB2	2:C:605:TYR:HE1	1.83	0.42
3:D:266:ASN:O	3:D:270:ARG:HB2	2.19	0.42
3:D:511:TYR:CD2	3:D:728:SER:HB3	2.54	0.42
3:D:511:TYR:HE1	3:D:724:MET:HG2	1.85	0.42
2:I:559:CYS:HA	2:I:560:PRO:HD3	1.90	0.42
2:I:629:PHE:CE2	2:I:650:VAL:HG21	2.55	0.42
2:I:810:TYR:O	2:I:1077:SER:OG	2.31	0.42
3:J:1156:LEU:HD22	3:J:1156:LEU:N	2.35	0.42
3:J:474:LEU:HD12	3:J:474:LEU:HA	1.96	0.42
3:J:491:LEU:HA	3:J:491:LEU:HD23	1.87	0.42
3:J:491:LEU:HD22	3:J:496:GLY:O	2.20	0.42
3:J:514:THR:O	3:J:514:THR:OG1	2.32	0.42
2:C:672:GLU:HG2	2:C:1187:PHE:HA	2.01	0.42
2:C:685:MET:HE1	2:C:1071:GLY:HA2	2.02	0.42
2:C:706:ARG:HG3	2:C:793:GLU:HG2	2.00	0.42
2:C:87:ILE:H	2:C:87:ILE:HG13	1.65	0.42
2:C:5:TYR:O	2:C:8:LYS:HG2	2.20	0.42
2:C:886:LYS:H	2:C:917:SER:HB3	1.84	0.42
3:D:1221:LEU:HD11	3:D:1304:ARG:O	2.19	0.42
3:D:436:ALA:HB3	3:D:485:MET:HA	2.01	0.42
3:D:442:ILE:HD13	3:D:442:ILE:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:461:PHE:C	3:D:463:GLY:H	2.22	0.42
2:I:1293:VAL:HG13	2:I:1301:ARG:HA	2.00	0.42
2:I:465:ARG:O	2:I:469:VAL:HG13	2.19	0.42
3:J:239:LEU:HA	3:J:239:LEU:HD23	1.78	0.42
5:L:394:TYR:CD2	5:L:439:ILE:HG21	2.55	0.42
2:C:145:ILE:HG22	2:C:456:VAL:HG22	2.00	0.42
2:C:208:ILE:HG13	2:C:354:ASP:OD1	2.19	0.42
2:C:678:ARG:HG3	2:C:1106:ARG:HB3	2.01	0.42
3:D:1138:LEU:HB3	3:D:1139:PRO:HD3	2.01	0.42
3:D:1170:LYS:C	3:D:1172:LYS:H	2.22	0.42
3:D:1262:ARG:HD2	3:D:1279:GLN:OE1	2.20	0.42
3:D:789:LYS:HZ1	3:D:932:MET:H	1.68	0.42
3:D:614:LEU:HD23	4:E:5:THR:HB	2.01	0.42
1:H:52:PRO:CG	1:H:150:ARG:HG2	2.49	0.42
2:I:1142:ARG:HH12	2:I:1165:SER:HA	1.85	0.42
3:J:1167:LYS:HE3	3:J:1174:ARG:HD2	2.00	0.42
3:J:118:LYS:HE2	3:J:118:LYS:HB3	1.93	0.42
3:J:30:ILE:HD13	3:J:243:PRO:HG3	2.00	0.42
3:J:264:ASP:OD2	5:L:506:SER:OG	2.22	0.42
3:J:824:PRO:HD3	3:J:835:LEU:HB2	2.02	0.42
3:J:832:LYS:HD3	3:J:1242:ARG:NH1	2.34	0.42
1:A:12:ARG:H	1:A:30:PRO:CD	2.33	0.42
1:A:224:LEU:HD23	1:B:228:LEU:HD11	2.02	0.42
2:C:91:THR:HB	2:C:138:ILE:O	2.20	0.42
3:D:114:ILE:HD11	3:D:311:ARG:HB2	2.01	0.42
3:D:493:PRO:O	3:D:1252:HIS:NE2	2.36	0.42
5:F:306:PHE:CE1	5:F:310:GLU:HG3	2.54	0.42
5:F:513:ASP:C	5:F:515:GLU:H	2.23	0.42
2:I:551:HIS:CG	2:I:552:PRO:HD2	2.54	0.42
3:J:45:ASN:HB3	3:J:48:THR:O	2.19	0.42
3:J:646:ILE:HG22	3:J:650:LYS:HD2	2.02	0.42
3:J:903:LEU:HD21	3:J:913:GLU:OE1	2.20	0.42
5:L:577:GLY:O	5:L:581:ASP:N	2.49	0.42
6:N:31:TYR:O	6:N:31:TYR:CG	2.73	0.42
1:A:187:VAL:HG23	1:A:187:VAL:O	2.20	0.42
2:C:211:ARG:NH1	2:C:357:ASN:O	2.53	0.42
2:C:363:LEU:HB3	2:C:381:ALA:HB1	2.02	0.42
2:C:42:ASP:O	2:C:44:GLU:N	2.52	0.42
2:C:519:ASN:ND2	2:C:689:ALA:HB3	2.35	0.42
3:D:1281:GLU:O	3:D:1285:VAL:HG13	2.19	0.42
3:D:279:LEU:HD12	3:D:295:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1308:ILE:HG23	3:D:380:PHE:CE2	2.55	0.42
3:D:527:LEU:HD21	3:D:536:LEU:HG	2.01	0.42
5:F:276:MET:O	5:F:280:VAL:HG23	2.20	0.42
5:F:471:LEU:HD23	5:F:476:ARG:O	2.20	0.42
5:F:580:PHE:C	5:F:582:VAL:H	2.23	0.42
1:G:151:GLY:O	1:G:177:TYR:HB2	2.19	0.42
1:H:56:VAL:HG11	1:H:144:ILE:HD11	2.02	0.42
3:J:591:ILE:HD11	3:J:603:LYS:HE3	2.00	0.42
2:I:1276:TRP:CH2	3:J:798:ARG:HG3	2.53	0.42
5:L:289:LYS:HE2	5:L:289:LYS:HB3	1.85	0.42
5:L:401:PHE:O	5:L:405:ILE:HG23	2.19	0.42
1:A:66:HIS:HE1	1:A:69:SER:HB3	1.83	0.41
2:C:143:ARG:HH21	2:C:513:GLN:HA	1.85	0.41
3:D:215:LYS:HE2	3:D:215:LYS:HB3	1.93	0.41
3:D:748:ALA:HA	3:D:754:ILE:HA	2.02	0.41
5:F:561:MET:HA	5:F:567:MET:CE	2.48	0.41
1:G:57:THR:HG22	1:G:58:GLU:HG3	2.02	0.41
1:H:64:VAL:HG12	1:H:66:HIS:H	1.85	0.41
1:H:59:VAL:HG21	1:H:85:LEU:HD13	2.02	0.41
2:I:731:ARG:NH1	2:I:962:GLU:OE1	2.53	0.41
3:J:442:ILE:HA	3:J:442:ILE:HD13	1.92	0.41
3:J:850:LYS:HG2	3:J:857:LEU:CD2	2.50	0.41
5:L:399:LEU:HA	5:L:399:LEU:HD12	1.79	0.41
1:A:290:LEU:HB3	1:A:291:LYS:HE2	2.02	0.41
1:A:226:GLU:HB3	1:B:10:LYS:HE2	2.03	0.41
2:C:158:ASP:HB3	2:C:173:ASN:OD1	2.20	0.41
2:C:458:GLU:O	2:C:461:GLU:HB3	2.21	0.41
2:C:643:SER:HG	2:C:645:PHE:HE1	1.66	0.41
2:C:714:VAL:HB	2:C:787:PRO:HD2	2.01	0.41
2:C:80:PHE:HB3	2:C:84:GLU:CB	2.50	0.41
2:C:937:ASP:CB	2:C:1039:GLY:HA3	2.50	0.41
4:E:15:ASN:ND2	4:E:18:ASP:OD2	2.53	0.41
2:I:1159:VAL:HB	2:I:1160:ASP:H	1.48	0.41
2:I:1191:LYS:HD3	2:I:1192:GLU:N	2.35	0.41
2:I:79:VAL:HG23	2:I:80:PHE:H	1.85	0.41
2:I:870:ILE:CG2	2:I:944:ARG:HD3	2.50	0.41
2:I:903:ARG:HE	2:I:910:ALA:HB2	1.85	0.41
1:H:48:LEU:CD2	3:J:535:ARG:HG3	2.50	0.41
3:J:594:GLN:HG3	3:J:596:LEU:HD22	2.02	0.41
5:L:354:THR:O	5:L:358:VAL:HG23	2.19	0.41
5:L:511:ILE:HA	5:L:511:ILE:HD12	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:12:LEU:C	6:M:14:ILE:H	2.23	0.41
1:A:323:PRO:HB2	1:A:324:ALA:HB2	2.02	0.41
1:B:51:MET:HB3	1:B:178:SER:HB2	2.01	0.41
2:C:1193:ALA:O	2:C:1197:GLU:HB2	2.20	0.41
2:C:247:ARG:NH2	2:C:274:ILE:HD12	2.36	0.41
3:D:133:ARG:HA	3:D:133:ARG:HD2	1.90	0.41
3:D:544:LEU:HD12	3:D:544:LEU:HA	1.80	0.41
5:F:324:LYS:HB3	5:F:325:PRO:HD2	2.02	0.41
1:G:51:MET:HA	1:G:52:PRO:HD3	1.91	0.41
3:J:647:PRO:CG	3:J:697:MET:HB3	2.50	0.41
5:L:151:VAL:HG22	5:L:156:ALA:HB3	2.02	0.41
5:L:492:ASP:HB2	5:L:495:ARG:HH12	1.86	0.41
1:A:249:PHE:CE2	1:A:254:LEU:HG	2.54	0.41
2:C:227:LYS:NZ	2:C:298:ALA:HB1	2.35	0.41
2:C:697:LYS:HB3	2:C:697:LYS:HE2	1.79	0.41
2:C:79:VAL:HG23	2:C:80:PHE:H	1.84	0.41
3:D:305:ALA:O	3:D:309:ASN:HB2	2.19	0.41
2:I:646:SER:HB3	2:I:649:GLN:HG3	2.02	0.41
2:I:814:ASP:N	2:I:814:ASP:OD1	2.53	0.41
2:I:946:LEU:HD23	2:I:946:LEU:HA	1.90	0.41
3:J:123:ARG:HH22	3:J:1334:GLU:HG3	1.84	0.41
3:J:324:LEU:HD12	3:J:324:LEU:O	2.20	0.41
3:J:343:LEU:HG	3:J:343:LEU:H	1.72	0.41
5:L:474:MET:O	5:L:476:ARG:N	2.49	0.41
6:M:70:PRO:HG2	6:M:78:GLN:HG3	2.01	0.41
2:C:1101:LEU:O	2:C:1104:PRO:HD2	2.21	0.41
2:C:42:ASP:C	2:C:44:GLU:H	2.24	0.41
2:C:903:ARG:HD2	2:C:908:GLU:HB3	2.02	0.41
3:D:403:ARG:HB3	3:D:405:GLU:HG3	2.02	0.41
1:B:181:GLU:HA	3:D:535:ARG:HH21	1.85	0.41
3:D:710:ASP:OD1	3:D:711:GLY:N	2.53	0.41
1:G:77:ASP:OD2	2:I:755:LYS:NZ	2.47	0.41
1:H:35:PHE:HA	1:H:38:THR:HG22	2.01	0.41
2:I:325:LEU:HA	2:I:328:SER:OG	2.20	0.41
3:J:1192:LYS:HB2	3:J:1192:LYS:HE3	1.83	0.41
3:J:320:ASN:OD1	3:J:322:ARG:HB3	2.20	0.41
3:J:902:ASP:OD1	3:J:903:LEU:N	2.53	0.41
1:A:106:GLY:HA2	1:A:136:GLU:O	2.20	0.41
1:A:112:ALA:O	1:A:115:ILE:HG13	2.20	0.41
1:A:105:SER:HB3	1:A:139:SER:OG	2.20	0.41
1:A:92:VAL:HA	1:A:120:ASP:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:LEU:HD11	1:B:140:ILE:HG21	2.02	0.41
2:C:1212:LEU:HD22	2:C:1225:VAL:HG21	2.02	0.41
2:C:159:SER:HB2	6:M:151:GLY:O	2.20	0.41
2:C:404:LYS:HA	2:C:404:LYS:HD2	1.78	0.41
2:C:81:ASP:HA	2:C:92:TYR:HE1	1.86	0.41
2:C:960:LEU:O	2:C:963:GLU:HB2	2.21	0.41
3:D:27:PRO:HB3	3:D:241:VAL:HG23	2.03	0.41
3:D:259:ARG:NH1	5:F:503:GLU:O	2.53	0.41
1:G:179:PRO:O	1:G:207:THR:HA	2.21	0.41
1:H:7:GLU:HG2	1:H:8:PHE:N	2.36	0.41
2:I:404:LYS:HA	2:I:404:LYS:HD2	1.80	0.41
2:I:850:ILE:O	2:I:850:ILE:HG22	2.20	0.41
3:J:500:ILE:O	3:J:500:ILE:HG22	2.21	0.41
3:J:865:HIS:HE1	3:J:867:GLN:HB2	1.85	0.41
3:J:901:ARG:HD2	3:J:906:GLY:O	2.20	0.41
5:L:248:GLU:HG2	5:L:251:LYS:NZ	2.35	0.41
1:A:262:LEU:HD12	1:A:262:LEU:H	1.86	0.41
1:B:99:ILE:HD12	1:B:145:LYS:HB2	2.02	0.41
1:B:178:SER:HA	1:B:179:PRO:HD3	1.85	0.41
2:C:75:LEU:HD11	2:C:127:ILE:HD11	2.03	0.41
3:D:833:GLU:OE2	3:D:1247:LYS:NZ	2.49	0.41
5:F:292:VAL:HG21	5:F:299:LYS:HG2	2.02	0.41
5:F:309:ASN:HB3	5:F:310:GLU:H	1.69	0.41
5:F:489:MET:HB2	5:F:490:PRO:HD2	2.02	0.41
2:C:1253:LEU:HA	5:F:525:ASP:HB2	2.01	0.41
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	2.01	0.41
2:I:146:VAL:HG13	2:I:529:ARG:HB3	2.02	0.41
2:I:344:GLY:O	2:I:346:TYR:N	2.53	0.41
2:I:55:SER:OG	2:I:56:VAL:N	2.54	0.41
3:J:511:TYR:HE1	3:J:724:MET:HG2	1.85	0.41
3:J:525:MET:O	3:J:548:VAL:HG13	2.20	0.41
3:J:81:ARG:C	3:J:83:VAL:H	2.23	0.41
5:L:110:LEU:HD23	5:L:382:ALA:O	2.21	0.41
5:L:511:ILE:HG21	5:L:522:PHE:CE2	2.55	0.41
1:A:284:ARG:HG3	1:A:288:GLU:HG3	2.03	0.41
1:A:315:GLY:C	1:A:316:MET:HG3	2.40	0.41
2:C:1083:GLU:HG3	2:C:1083:GLU:H	1.54	0.41
2:C:528:ARG:NH2	2:C:576:SER:O	2.54	0.41
2:C:578:TYR:HB3	2:C:590:PRO:HG2	2.03	0.41
3:D:412:LEU:O	3:D:415:VAL:HG22	2.20	0.41
3:D:580:TRP:HH2	3:D:587:LEU:O	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:130:VAL:O	5:F:134:VAL:N	2.49	0.41
2:I:171:LEU:HD23	2:I:171:LEU:HA	1.95	0.41
2:I:400:VAL:HG22	2:I:584:TYR:HD1	1.86	0.41
3:J:381:ILE:O	3:J:385:LEU:HB2	2.20	0.41
3:J:418:GLU:H	4:K:45:LYS:NZ	2.19	0.41
2:I:1222:GLU:O	3:J:636:GLY:HA3	2.21	0.41
5:L:299:LYS:HA	5:L:302:PHE:HB3	2.03	0.41
1:A:70:THR:CG2	2:C:755:LYS:HE2	2.51	0.41
2:C:678:ARG:NH2	2:C:1106:ARG:HG2	2.36	0.41
2:C:921:PRO:O	2:C:924:VAL:HG22	2.20	0.41
3:D:1168:GLU:O	3:D:1170:LYS:N	2.54	0.41
3:D:123:ARG:HH12	3:D:1334:GLU:HG3	1.85	0.41
3:D:110:PRO:HD2	3:D:183:GLU:HG2	2.02	0.41
3:D:275:ARG:HD3	3:D:298:MET:HB3	2.02	0.41
4:E:26:ARG:NH2	4:E:38:LEU:HD13	2.35	0.41
5:F:274:ARG:HA	5:F:277:MET:HB2	2.03	0.41
5:F:479:THR:HG22	5:F:482:GLU:HB2	2.02	0.41
1:G:75:GLN:HA	2:I:729:ALA:N	2.36	0.41
2:I:1142:ARG:HH12	2:I:1169:VAL:HG21	1.86	0.41
2:I:135:THR:HG22	2:I:527:LYS:HE2	2.03	0.41
2:I:389:PHE:HD1	2:I:395:TYR:CE1	2.39	0.41
2:I:848:GLU:HG2	2:I:888:THR:HG22	2.02	0.41
2:I:985:GLU:HG2	2:I:988:LYS:HD2	2.02	0.41
3:J:833:GLU:HA	3:J:834:PRO:HD3	1.89	0.41
5:L:311:THR:HG21	5:L:348:GLU:CD	2.41	0.41
5:L:503:GLU:OE1	5:L:504:PRO:HD2	2.20	0.41
1:A:185:TYR:HA	1:A:202:VAL:O	2.20	0.41
1:A:289:LEU:CD1	1:A:314:LEU:HD21	2.51	0.41
2:C:673:HIS:O	2:C:1109:ILE:HG22	2.20	0.41
3:D:304:ASP:OD2	3:D:312:ARG:NH2	2.54	0.41
5:F:404:LEU:HD22	5:F:443:ILE:HD11	2.02	0.41
2:I:1103:VAL:HB	2:I:1104:PRO:HD3	2.03	0.41
2:I:591:TYR:HA	2:I:655:VAL:HG23	2.03	0.41
2:I:796:LEU:H	2:I:796:LEU:HD12	1.86	0.41
2:I:886:LYS:H	2:I:917:SER:HB3	1.85	0.41
2:I:745:GLU:HA	2:I:971:LEU:HD12	2.03	0.41
6:M:49:ASN:HA	6:M:52:ARG:NH1	2.35	0.41
6:N:12:LEU:C	6:N:14:ILE:N	2.74	0.41
1:B:197:ASP:OD1	1:B:197:ASP:N	2.54	0.41
2:C:226:GLU:HB2	2:C:245:ARG:HH22	1.86	0.41
2:C:548:ARG:HG2	2:C:571:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:126:LEU:H	3:D:126:LEU:HG	1.70	0.41
3:D:205:LEU:CD2	3:D:214:ARG:HB2	2.51	0.41
3:D:474:LEU:HD12	3:D:474:LEU:HA	1.78	0.41
1:H:50:SER:HA	1:H:150:ARG:O	2.21	0.41
2:I:37:LYS:HD3	2:I:37:LYS:HA	1.95	0.41
2:I:88:ARG:NH1	2:I:88:ARG:HB2	2.36	0.41
2:I:896:THR:HB	2:I:897:PRO:HD2	2.03	0.41
3:J:548:VAL:HG12	3:J:550:VAL:HG13	2.02	0.41
3:J:596:LEU:HD11	3:J:604:MET:CE	2.51	0.41
3:J:674:THR:HG22	6:N:136:ILE:CD1	2.50	0.41
3:J:796:LEU:HD12	3:J:796:LEU:HA	1.79	0.41
3:J:850:LYS:HB2	3:J:852:GLY:O	2.20	0.41
5:L:513:ASP:C	5:L:515:GLU:H	2.25	0.41
2:C:169:LYS:HE2	2:C:190:PRO:O	2.21	0.40
2:C:503:LYS:HA	2:C:503:LYS:HD2	1.91	0.40
2:C:720:ARG:HE	2:C:736:VAL:HG11	1.85	0.40
3:D:580:TRP:CZ3	3:D:589:TYR:HA	2.56	0.40
3:D:762:ASN:OD1	3:D:764:ARG:N	2.54	0.40
3:D:860:ARG:HD2	3:D:860:ARG:HA	1.81	0.40
5:F:100:MET:HG2	5:F:100:MET:H	1.65	0.40
2:I:818:VAL:HB	2:I:1076:ILE:HD11	2.04	0.40
2:I:1109:ILE:HA	2:I:1109:ILE:HD12	1.93	0.40
2:I:221:LEU:HB3	2:I:336:LEU:HD21	2.03	0.40
3:J:1344:LEU:HB3	3:J:1350:ASN:HD21	1.85	0.40
1:H:84:ASN:CG	3:J:551:ARG:HH22	2.24	0.40
3:J:638:SER:OG	3:J:639:VAL:N	2.52	0.40
3:J:517:CYS:HA	3:J:716:GLN:HE22	1.86	0.40
1:B:62:ASP:OD2	1:B:140:ILE:HD12	2.20	0.40
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	2.03	0.40
2:C:378:ARG:NH1	2:C:382:GLU:OE2	2.54	0.40
3:D:19:ALA:HB2	3:D:1373:ARG:NH2	2.36	0.40
3:D:347:VAL:HG12	3:D:348:ASP:O	2.21	0.40
1:B:196:THR:OG1	3:D:443:GLU:HG3	2.21	0.40
3:D:84:ILE:HG13	3:D:84:ILE:H	1.70	0.40
5:F:383:ASN:HB2	5:F:412:LEU:HD21	2.03	0.40
5:F:463:LEU:HA	5:F:463:LEU:HD23	1.93	0.40
1:G:133:LEU:HD12	1:G:138:ALA:HB3	2.03	0.40
1:G:43:LEU:HD23	1:G:43:LEU:HA	1.78	0.40
2:I:1043:ALA:HB1	2:I:1044:PRO:HD2	2.03	0.40
2:I:607:SER:OG	2:I:609:ILE:HG13	2.21	0.40
2:I:699:LEU:HD23	2:I:699:LEU:HA	1.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:502:PRO:HB2	3:J:507:VAL:HG12	2.03	0.40
5:L:348:GLU:HA	5:L:353:LEU:O	2.21	0.40
3:D:935:PHE:C	6:M:86:LEU:HD21	2.42	0.40
6:N:15:LEU:HA	6:N:15:LEU:HD23	1.97	0.40
1:A:59:VAL:HG22	1:A:144:ILE:HA	2.03	0.40
3:D:1143:ASP:HA	3:D:1148:ARG:HH11	1.86	0.40
3:D:1186:TYR:HE2	3:D:1188:GLU:HB2	1.85	0.40
3:D:1280:VAL:HG11	3:D:1304:ARG:NH2	2.36	0.40
3:D:224:LEU:O	3:D:227:PHE:N	2.54	0.40
3:D:28:ASP:OD1	3:D:31:ARG:NH1	2.54	0.40
3:D:860:ARG:HB3	3:D:861:ASN:H	1.72	0.40
5:F:320:ILE:HG23	5:F:327:SER:O	2.22	0.40
2:I:193:ASN:ND2	2:I:353:VAL:HG21	2.36	0.40
2:I:503:LYS:HA	2:I:503:LYS:HD2	1.80	0.40
2:I:697:LYS:HE2	2:I:697:LYS:HB3	1.83	0.40
2:I:883:LEU:HG	2:I:920:VAL:HG23	2.03	0.40
3:J:1259:GLN:NE2	3:J:1262:ARG:NH1	2.70	0.40
3:J:1262:ARG:O	3:J:1280:VAL:HG23	2.21	0.40
3:J:45:ASN:O	3:J:46:TYR:HB3	2.21	0.40
3:J:517:CYS:HA	3:J:716:GLN:OE1	2.21	0.40
5:L:119:ILE:HG23	5:L:375:ALA:HB1	2.04	0.40
1:A:166:ARG:N	1:A:167:PRO:HD2	2.36	0.40
1:B:88:LEU:HD12	1:B:89:ALA:H	1.86	0.40
2:C:1211:ARG:HE	2:C:1220:GLN:HE21	1.70	0.40
2:C:462:ASN:O	2:C:466:VAL:HG23	2.21	0.40
3:D:117:LEU:HG	3:D:117:LEU:O	2.20	0.40
3:D:310:GLY:HA2	3:D:314:ARG:CD	2.48	0.40
3:D:363:LEU:HG	3:D:363:LEU:O	2.21	0.40
3:D:429:LEU:HA	3:D:429:LEU:HD13	1.73	0.40
3:D:786:THR:HA	3:D:789:LYS:HG3	2.03	0.40
2:I:1129:ASN:HB2	2:I:1177:ARG:HB2	2.03	0.40
2:I:1184:THR:HG23	2:I:1189:GLY:HA2	2.01	0.40
2:I:80:PHE:HB3	2:I:84:GLU:HB2	2.04	0.40
3:J:201:LEU:HD11	3:J:220:ARG:NH1	2.36	0.40
3:J:750:PRO:HA	3:J:777:HIS:NE2	2.35	0.40
5:L:585:GLU:O	5:L:589:GLN:HG3	2.22	0.40
6:M:144:ILE:HD12	6:M:147:LYS:HE2	2.03	0.40
1:B:152:TYR:CE2	3:D:536:LEU:HD21	2.56	0.40
2:C:1075:VAL:HG23	3:D:461:PHE:O	2.22	0.40
2:C:139:ASN:HA	2:C:139:ASN:HD22	1.61	0.40
3:D:1227:HIS:HA	3:D:1230:THR:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1298:VAL:N	3:D:1299:GLY:CA	2.84	0.40
5:F:111:LEU:HA	5:F:111:LEU:HD23	1.93	0.40
5:F:484:ALA:HB1	5:F:491:GLU:CG	2.52	0.40
2:I:745:GLU:H	2:I:1017:GLN:HG3	1.85	0.40
2:I:256:GLU:HB3	2:I:261:VAL:HG22	2.04	0.40
3:J:679:TYR:O	3:J:683:ILE:HG13	2.22	0.40
5:L:469:GLN:O	5:L:473:GLU:HB2	2.21	0.40
5:L:511:ILE:HG13	5:L:512:GLY:H	1.86	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ASP:O	1:G:101:THR:OG1[4_545]	1.98	0.22
2:C:1006:GLU:OE1	3:D:68:TYR:OH[4_555]	2.17	0.03
2:C:44:GLU:OE2	5:F:596:ARG:NH1[4_555]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	317/329 (96%)	248 (78%)	52 (16%)	17 (5%)	2	22
1	B	213/329 (65%)	195 (92%)	14 (7%)	4 (2%)	8	41
1	G	225/329 (68%)	202 (90%)	18 (8%)	5 (2%)	6	38
1	H	212/329 (64%)	197 (93%)	11 (5%)	4 (2%)	8	41
2	C	1338/1342 (100%)	1202 (90%)	118 (9%)	18 (1%)	12	48
2	I	1338/1342 (100%)	1197 (90%)	120 (9%)	21 (2%)	9	45
3	D	1167/1407 (83%)	1037 (89%)	103 (9%)	27 (2%)	6	37
3	J	1155/1407 (82%)	1029 (89%)	100 (9%)	26 (2%)	6	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	87/91 (96%)	80 (92%)	5 (6%)	2 (2%)	6	37
4	K	77/91 (85%)	69 (90%)	4 (5%)	4 (5%)	2	22
5	F	462/613 (75%)	426 (92%)	28 (6%)	8 (2%)	9	43
5	L	463/613 (76%)	425 (92%)	31 (7%)	7 (2%)	10	46
6	M	138/151 (91%)	128 (93%)	8 (6%)	2 (1%)	11	47
6	N	138/151 (91%)	129 (94%)	6 (4%)	3 (2%)	6	38
All	All	7330/8524 (86%)	6564 (90%)	618 (8%)	148 (2%)	7	40

All (148) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	107	ILE
1	A	136	GLU
1	A	162	GLU
1	A	167	PRO
1	A	242	VAL
1	B	193	GLU
2	C	169	LYS
2	C	170	VAL
2	C	484	LEU
2	C	697	LYS
2	C	1137	GLU
2	C	1153	ALA
2	C	1154	ASP
2	C	1159	VAL
2	C	1165	SER
3	D	10	ALA
3	D	49	PHE
3	D	426	ALA
3	D	496	GLY
3	D	669	GLN
3	D	673	VAL
3	D	710	ASP
3	D	712	GLN
3	D	745	GLY
3	D	1169	THR
3	D	1294	ALA
4	E	33	GLY
5	F	490	PRO

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Mol	Chain	Res	Type
5	F	569	THR
1	G	193	GLU
2	I	121	GLU
2	I	169	LYS
2	I	170	VAL
2	I	484	LEU
2	I	697	LYS
2	I	897	PRO
2	I	1137	GLU
2	I	1153	ALA
2	I	1159	VAL
2	I	1203	ASP
3	J	49	PHE
3	J	341	ASN
3	J	426	ALA
3	J	496	GLY
3	J	710	ASP
3	J	712	GLN
3	J	805	GLN
3	J	850	LYS
3	J	1294	ALA
4	K	4	VAL
4	K	15	ASN
4	K	33	GLY
5	L	584	ARG
6	M	30	GLU
6	N	30	GLU
6	N	31	TYR
1	A	50	SER
1	A	119	GLY
1	A	164	ASP
1	A	232	VAL
1	A	315	GLY
1	A	320	ASN
1	B	13	LEU
2	C	121	GLU
3	D	89	GLY
3	D	805	GLN
3	D	1274	PHE
5	F	566	ASP
5	F	584	ARG
1	G	162	GLU

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Mol	Chain	Res	Type
1	G	167	PRO
1	H	138	ALA
1	H	193	GLU
2	I	1059	ARG
2	I	1165	SER
3	J	314	ARG
3	J	339	ARG
3	J	745	GLY
3	J	826	ILE
3	J	1169	THR
3	J	1297	LYS
5	L	96	ASP
5	L	490	PRO
5	L	566	ASP
5	L	569	THR
1	A	62	ASP
1	B	136	GLU
2	C	163	LYS
2	C	696	ASP
2	C	892	GLU
2	C	1317	PRO
3	D	173	GLY
3	D	314	ARG
3	D	417	ARG
3	D	1344	LEU
1	G	229	GLU
2	I	892	GLU
2	I	983	GLY
2	I	1317	PRO
3	J	89	GLY
3	J	417	ARG
4	K	14	GLY
1	A	324	ALA
1	B	138	ALA
2	C	813	GLU
2	C	1059	ARG
3	D	1297	LYS
1	H	20	SER
2	I	696	ASP
2	I	813	GLU
3	J	332	LYS
3	J	344	GLY

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Mol	Chain	Res	Type
3	J	1344	LEU
1	A	318	LEU
1	A	319	GLU
2	C	983	GLY
2	C	1158	LYS
3	D	46	TYR
5	F	602	SER
2	I	160	ASP
3	J	338	PHE
3	J	357	VAL
6	N	27	PRO
1	A	19	VAL
3	D	345	LYS
3	D	357	VAL
2	I	201	ARG
2	I	756	TYR
3	J	333	GLY
5	L	585	GLU
6	M	27	PRO
3	D	826	ILE
3	D	828	GLY
5	F	96	ASP
3	J	173	GLY
3	J	336	GLY
3	D	82	GLY
3	D	120	LEU
3	D	831	VAL
5	F	361	ILE
3	J	639	VAL
5	L	475	GLY
1	G	14	VAL
2	I	1202	GLY
4	E	86	ILE
5	F	475	GLY
1	H	30	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	278/286 (97%)	228 (82%)	50 (18%)	1	11
1	B	186/286 (65%)	171 (92%)	15 (8%)	11	37
1	G	193/286 (68%)	169 (88%)	24 (12%)	4	22
1	H	183/286 (64%)	172 (94%)	11 (6%)	19	46
2	C	1155/1157 (100%)	1051 (91%)	104 (9%)	9	32
2	I	1154/1157 (100%)	1056 (92%)	98 (8%)	10	36
3	D	962/1168 (82%)	878 (91%)	84 (9%)	10	34
3	J	960/1168 (82%)	877 (91%)	83 (9%)	10	35
4	E	72/75 (96%)	63 (88%)	9 (12%)	4	21
4	K	67/75 (89%)	61 (91%)	6 (9%)	9	32
5	F	417/540 (77%)	386 (93%)	31 (7%)	13	40
5	L	418/540 (77%)	380 (91%)	38 (9%)	9	32
6	M	121/131 (92%)	111 (92%)	10 (8%)	11	36
6	N	121/131 (92%)	111 (92%)	10 (8%)	11	36
All	All	6287/7286 (86%)	5714 (91%)	573 (9%)	9	32

All (573) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	8	PHE
1	A	18	GLN
1	A	26	VAL
1	A	29	GLU
1	A	44	ARG
1	A	50	SER
1	A	56	VAL
1	A	66	HIS
1	A	70	THR
1	A	71	LYS
1	A	72	GLU
1	A	74	VAL
1	A	77	ASP
1	A	83	LEU
1	A	90	VAL
1	A	98	VAL

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Mol	Chain	Res	Type
1	A	99	ILE
1	A	105	SER
1	A	116	THR
1	A	125	LYS
1	A	133	LEU
1	A	139	SER
1	A	159	ILE
1	A	164	ASP
1	A	165	GLU
1	A	180	VAL
1	A	183	ILE
1	A	186	ASN
1	A	192	VAL
1	A	195	ARG
1	A	207	THR
1	A	211	ILE
1	A	223	ILE
1	A	231	PHE
1	A	243	LYS
1	A	245	GLU
1	A	246	LYS
1	A	258	ASP
1	A	262	LEU
1	A	280	ASP
1	A	282	VAL
1	A	284	ARG
1	A	285	THR
1	A	300	LEU
1	A	302	GLU
1	A	306	VAL
1	A	316	MET
1	A	318	LEU
1	A	320	ASN
1	B	9	LEU
1	B	16	ILE
1	B	27	THR
1	B	60	GLU
1	B	62	ASP
1	B	64	VAL
1	B	79	LEU
1	B	95	LYS
1	B	102	LEU

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Mol	Chain	Res	Type
1	B	124	VAL
1	B	139	SER
1	B	183	ILE
1	B	191	ARG
1	B	196	THR
1	B	233	ASP
2	C	3	TYR
2	C	11	ILE
2	C	17	LYS
2	C	23	ASP
2	C	46	GLN
2	C	81	ASP
2	C	103	VAL
2	C	115	LYS
2	C	117	ILE
2	C	119	GLU
2	C	120	GLN
2	C	131	THR
2	C	135	THR
2	C	150	HIS
2	C	164	THR
2	C	201	ARG
2	C	208	ILE
2	C	285	ILE
2	C	306	THR
2	C	320	ASP
2	C	321	LEU
2	C	342	ASP
2	C	377	THR
2	C	384	LEU
2	C	423	ASP
2	C	455	SER
2	C	471	VAL
2	C	481	LEU
2	C	484	LEU
2	C	485	ASP
2	C	490	GLN
2	C	492	MET
2	C	493	ILE
2	C	518	ASN
2	C	525	THR
2	C	539	THR

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Mol	Chain	Res	Type
2	C	540	ARG
2	C	542	ARG
2	C	553	THR
2	C	561	ILE
2	C	575	LEU
2	C	600	THR
2	C	609	ILE
2	C	615	VAL
2	C	623	LEU
2	C	633	LEU
2	C	663	VAL
2	C	672	GLU
2	C	694	ARG
2	C	697	LYS
2	C	714	VAL
2	C	748	ILE
2	C	757	THR
2	C	764	CYS
2	C	765	ILE
2	C	778	GLU
2	C	781	ASP
2	C	791	LEU
2	C	799	ASN
2	C	800	MET
2	C	828	PHE
2	C	867	GLU
2	C	878	THR
2	C	890	LYS
2	C	892	GLU
2	C	895	LEU
2	C	919	ARG
2	C	922	ASN
2	C	951	MET
2	C	984	VAL
2	C	992	LEU
2	C	1002	LEU
2	C	1037	THR
2	C	1054	LEU
2	C	1059	ARG
2	C	1076	ILE
2	C	1082	ILE
2	C	1134	GLN

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Mol	Chain	Res	Type
2	C	1141	LEU
2	C	1146	GLN
2	C	1151	LEU
2	C	1155	VAL
2	C	1156	ARG
2	C	1159	VAL
2	C	1163	THR
2	C	1164	PHE
2	C	1198	LEU
2	C	1206	THR
2	C	1210	ILE
2	C	1233	LEU
2	C	1237	HIS
2	C	1238	LEU
2	C	1240	ASP
2	C	1248	THR
2	C	1250	SER
2	C	1254	VAL
2	C	1255	THR
2	C	1287	LEU
2	C	1296	ASP
2	C	1310	ASP
2	C	1313	HIS
2	C	1327	LEU
2	C	1341	ASP
2	C	1342	GLU
3	D	8	LEU
3	D	11	GLN
3	D	12	THR
3	D	46	TYR
3	D	47	ARG
3	D	54	ASP
3	D	79	LYS
3	D	93	THR
3	D	95	THR
3	D	97	VAL
3	D	172	PHE
3	D	175	GLU
3	D	176	PHE
3	D	206	ASN
3	D	248	ASP
3	D	252	LEU

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Mol	Chain	Res	Type
3	D	259	ARG
3	D	292	VAL
3	D	324	LEU
3	D	330	MET
3	D	335	GLN
3	D	343	LEU
3	D	376	LEU
3	D	386	GLU
3	D	392	THR
3	D	394	ILE
3	D	413	ASP
3	D	416	ILE
3	D	425	ARG
3	D	429	LEU
3	D	490	ILE
3	D	505	ASP
3	D	514	THR
3	D	536	LEU
3	D	545	HIS
3	D	560	ASN
3	D	569	LEU
3	D	571	ASP
3	D	573	THR
3	D	639	VAL
3	D	641	ILE
3	D	678	ARG
3	D	701	LEU
3	D	707	ILE
3	D	708	ASN
3	D	717	VAL
3	D	753	SER
3	D	754	ILE
3	D	764	ARG
3	D	772	TYR
3	D	797	THR
3	D	801	VAL
3	D	810	THR
3	D	847	ASP
3	D	849	LEU
3	D	853	THR
3	D	858	VAL
3	D	860	ARG

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Mol	Chain	Res	Type
3	D	890	THR
3	D	897	HIS
3	D	903	LEU
3	D	908	ILE
3	D	910	ASN
3	D	918	ILE
3	D	1135	THR
3	D	1155	ILE
3	D	1162	ILE
3	D	1169	THR
3	D	1177	ILE
3	D	1186	TYR
3	D	1194	ARG
3	D	1199	PHE
3	D	1221	LEU
3	D	1251	LYS
3	D	1261	LEU
3	D	1266	ILE
3	D	1272	SER
3	D	1279	GLN
3	D	1289	ASN
3	D	1310	THR
3	D	1332	LEU
3	D	1333	THR
3	D	1343	GLU
3	D	1366	HIS
4	E	3	ARG
4	E	5	THR
4	E	13	ILE
4	E	18	ASP
4	E	21	LEU
4	E	36	ASP
4	E	39	VAL
4	E	58	LEU
4	E	62	GLN
5	F	98	VAL
5	F	114	GLU
5	F	154	GLU
5	F	163	THR
5	F	261	LEU
5	F	277	MET
5	F	305	LEU

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Mol	Chain	Res	Type
5	F	306	PHE
5	F	338	HIS
5	F	401	PHE
5	F	449	THR
5	F	471	LEU
5	F	472	GLN
5	F	482	GLU
5	F	488	LEU
5	F	491	GLU
5	F	492	ASP
5	F	516	ASP
5	F	526	THR
5	F	527	THR
5	F	530	LEU
5	F	547	VAL
5	F	552	THR
5	F	558	VAL
5	F	569	THR
5	F	572	THR
5	F	587	ILE
5	F	600	HIS
5	F	603	ARG
5	F	606	VAL
5	F	608	ARG
1	G	9	LEU
1	G	12	ARG
1	G	19	VAL
1	G	23	HIS
1	G	26	VAL
1	G	33	ARG
1	G	50	SER
1	G	70	THR
1	G	79	LEU
1	G	90	VAL
1	G	101	THR
1	G	121	VAL
1	G	124	VAL
1	G	133	LEU
1	G	145	LYS
1	G	156	SER
1	G	178	SER
1	G	187	VAL

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Mol	Chain	Res	Type
1	G	192	VAL
1	G	200	LYS
1	G	207	THR
1	G	211	ILE
1	G	219	ARG
1	G	231	PHE
1	H	27	THR
1	H	58	GLU
1	H	61	ILE
1	H	62	ASP
1	H	64	VAL
1	H	65	LEU
1	H	75	GLN
1	H	95	LYS
1	H	102	LEU
1	H	124	VAL
1	H	183	ILE
2	I	3	TYR
2	I	4	SER
2	I	11	ILE
2	I	46	GLN
2	I	86	GLN
2	I	107	ARG
2	I	115	LYS
2	I	117	ILE
2	I	131	THR
2	I	132	ASP
2	I	138	ILE
2	I	156	PHE
2	I	164	THR
2	I	197	ARG
2	I	201	ARG
2	I	208	ILE
2	I	285	ILE
2	I	320	ASP
2	I	321	LEU
2	I	342	ASP
2	I	360	LEU
2	I	384	LEU
2	I	423	ASP
2	I	453	ILE
2	I	455	SER

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Mol	Chain	Res	Type
2	I	471	VAL
2	I	481	LEU
2	I	484	LEU
2	I	485	ASP
2	I	490	GLN
2	I	492	MET
2	I	518	ASN
2	I	524	ILE
2	I	525	THR
2	I	530	ILE
2	I	538	LEU
2	I	540	ARG
2	I	542	ARG
2	I	553	THR
2	I	558	VAL
2	I	561	ILE
2	I	596	ASP
2	I	600	THR
2	I	604	HIS
2	I	609	ILE
2	I	633	LEU
2	I	635	THR
2	I	660	VAL
2	I	663	VAL
2	I	672	GLU
2	I	694	ARG
2	I	705	GLU
2	I	714	VAL
2	I	724	VAL
2	I	739	ASP
2	I	748	ILE
2	I	764	CYS
2	I	765	ILE
2	I	781	ASP
2	I	782	VAL
2	I	799	ASN
2	I	800	MET
2	I	814	ASP
2	I	828	PHE
2	I	890	LYS
2	I	892	GLU
2	I	895	LEU

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Mol	Chain	Res	Type
2	I	919	ARG
2	I	922	ASN
2	I	951	MET
2	I	992	LEU
2	I	1037	THR
2	I	1054	LEU
2	I	1082	ILE
2	I	1083	GLU
2	I	1141	LEU
2	I	1146	GLN
2	I	1151	LEU
2	I	1156	ARG
2	I	1159	VAL
2	I	1163	THR
2	I	1164	PHE
2	I	1198	LEU
2	I	1210	ILE
2	I	1227	VAL
2	I	1233	LEU
2	I	1238	LEU
2	I	1240	ASP
2	I	1248	THR
2	I	1250	SER
2	I	1254	VAL
2	I	1265	PHE
2	I	1287	LEU
2	I	1296	ASP
2	I	1313	HIS
2	I	1327	LEU
2	I	1341	ASP
2	I	1342	GLU
3	J	20	ILE
3	J	46	TYR
3	J	47	ARG
3	J	54	ASP
3	J	79	LYS
3	J	92	VAL
3	J	93	THR
3	J	95	THR
3	J	97	VAL
3	J	98	ARG
3	J	172	PHE

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Mol	Chain	Res	Type
3	J	175	GLU
3	J	176	PHE
3	J	206	ASN
3	J	218	THR
3	J	235	GLU
3	J	244	VAL
3	J	248	ASP
3	J	252	LEU
3	J	259	ARG
3	J	292	VAL
3	J	324	LEU
3	J	343	LEU
3	J	363	LEU
3	J	374	LEU
3	J	376	LEU
3	J	386	GLU
3	J	392	THR
3	J	394	ILE
3	J	413	ASP
3	J	416	ILE
3	J	423	LEU
3	J	425	ARG
3	J	429	LEU
3	J	505	ASP
3	J	510	LEU
3	J	514	THR
3	J	536	LEU
3	J	545	HIS
3	J	560	ASN
3	J	567	THR
3	J	569	LEU
3	J	571	ASP
3	J	573	THR
3	J	641	ILE
3	J	701	LEU
3	J	707	ILE
3	J	708	ASN
3	J	717	VAL
3	J	754	ILE
3	J	764	ARG
3	J	772	TYR
3	J	797	THR

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Mol	Chain	Res	Type
3	J	801	VAL
3	J	810	THR
3	J	827	GLU
3	J	847	ASP
3	J	849	LEU
3	J	853	THR
3	J	857	LEU
3	J	897	HIS
3	J	898	CYS
3	J	908	ILE
3	J	910	ASN
3	J	918	ILE
3	J	1155	ILE
3	J	1162	ILE
3	J	1163	VAL
3	J	1169	THR
3	J	1186	TYR
3	J	1194	ARG
3	J	1199	PHE
3	J	1221	LEU
3	J	1251	LYS
3	J	1261	LEU
3	J	1266	ILE
3	J	1273	ASP
3	J	1282	TYR
3	J	1285	VAL
3	J	1289	ASN
3	J	1292	LEU
3	J	1333	THR
3	J	1366	HIS
4	K	13	ILE
4	K	18	ASP
4	K	21	LEU
4	K	36	ASP
4	K	39	VAL
4	K	58	LEU
5	L	98	VAL
5	L	102	MET
5	L	114	GLU
5	L	154	GLU
5	L	261	LEU
5	L	266	PHE

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Mol	Chain	Res	Type
5	L	277	MET
5	L	305	LEU
5	L	306	PHE
5	L	335	GLU
5	L	338	HIS
5	L	364	ARG
5	L	395	THR
5	L	401	PHE
5	L	405	ILE
5	L	429	THR
5	L	445	ASP
5	L	469	GLN
5	L	471	LEU
5	L	476	ARG
5	L	486	ARG
5	L	491	GLU
5	L	492	ASP
5	L	526	THR
5	L	527	THR
5	L	552	THR
5	L	558	VAL
5	L	569	THR
5	L	572	THR
5	L	573	LEU
5	L	580	PHE
5	L	582	VAL
5	L	587	ILE
5	L	599	ARG
5	L	600	HIS
5	L	603	ARG
5	L	606	VAL
5	L	607	LEU
6	M	42	ARG
6	M	50	GLN
6	M	52	ARG
6	M	53	ASP
6	M	69	PHE
6	M	72	PRO
6	M	78	GLN
6	M	88	ASN
6	M	136	ILE
6	M	146	GLU

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Mol	Chain	Res	Type
6	N	42	ARG
6	N	50	GLN
6	N	52	ARG
6	N	53	ASP
6	N	69	PHE
6	N	72	PRO
6	N	78	GLN
6	N	88	ASN
6	N	136	ILE
6	N	146	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	320	ASN
1	B	23	HIS
1	B	132	HIS
2	C	133	ASN
2	C	139	ASN
2	C	343	HIS
2	C	513	GLN
2	C	620	ASN
2	C	760	ASN
2	C	1108	ASN
2	C	1111	GLN
2	C	1116	HIS
2	C	1220	GLN
2	C	1237	HIS
2	C	1288	GLN
2	C	1314	GLN
3	D	200	GLN
3	D	320	ASN
3	D	365	GLN
3	D	702	GLN
3	D	716	GLN
3	D	777	HIS
3	D	861	ASN
3	D	929	GLN
3	D	1227	HIS
5	F	131	GLN
5	F	258	GLN

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Mol	Chain	Res	Type
5	F	383	ASN
5	F	446	GLN
5	F	579	GLN
5	F	600	HIS
1	G	66	HIS
1	G	132	HIS
2	I	46	GLN
2	I	139	ASN
2	I	327	GLN
2	I	490	GLN
2	I	673	HIS
2	I	1038	GLN
2	I	1108	ASN
2	I	1111	GLN
2	I	1116	HIS
2	I	1146	GLN
2	I	1220	GLN
2	I	1288	GLN
2	I	1314	GLN
3	J	157	GLN
3	J	200	GLN
3	J	206	ASN
3	J	294	ASN
3	J	365	GLN
3	J	430	HIS
3	J	465	GLN
3	J	594	GLN
3	J	1295	ASN
5	L	301	ASN
5	L	362	ASN
5	L	406	GLN
5	L	446	GLN
5	L	469	GLN
5	L	579	GLN
6	M	78	GLN
6	N	50	GLN
6	N	78	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	319/329 (96%)	0.26	20 (6%) 20 16	230, 295, 400, 420	0
1	B	217/329 (65%)	-0.13	2 (0%) 84 77	243, 301, 356, 388	0
1	G	227/329 (68%)	-0.01	3 (1%) 77 68	270, 312, 357, 389	0
1	H	216/329 (65%)	0.41	19 (8%) 10 9	287, 356, 409, 427	0
2	C	1340/1342 (99%)	-0.07	25 (1%) 66 58	166, 255, 352, 403	0
2	I	1340/1342 (99%)	0.12	55 (4%) 37 30	203, 303, 382, 423	0
3	D	1171/1407 (83%)	-0.10	12 (1%) 82 74	169, 238, 355, 404	0
3	J	1159/1407 (82%)	-0.07	22 (1%) 66 58	183, 262, 356, 405	0
4	E	89/91 (97%)	-0.06	0 100 100	225, 281, 318, 330	0
4	K	79/91 (86%)	0.86	13 (16%) 1 2	320, 426, 502, 516	0
5	F	468/613 (76%)	-0.01	18 (3%) 40 32	199, 288, 436, 472	0
5	L	469/613 (76%)	0.19	23 (4%) 29 25	212, 309, 420, 437	0
6	M	140/151 (92%)	0.71	28 (20%) 1 1	374, 435, 492, 503	0
6	N	140/151 (92%)	0.99	32 (22%) 0 1	417, 439, 458, 465	0
All	All	7374/8524 (86%)	0.05	272 (3%) 41 33	166, 283, 416, 516	0

All (272) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	1001	GLY	7.6
2	I	482	GLY	6.8
6	N	41	ARG	6.7
1	A	303	ILE	5.9
3	J	1375	ALA	5.8
6	N	39	HIS	5.8
6	N	38	ALA	5.7
6	N	42	ARG	5.5

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Mol	Chain	Res	Type	RSRZ
6	N	62	MET	5.3
2	C	252	SER	5.3
3	J	1198	VAL	5.2
3	D	677	GLU	5.2
6	M	39	HIS	5.1
1	H	172	LEU	5.0
5	L	603	ARG	4.9
2	C	1000	LEU	4.9
2	C	291	TYR	4.8
4	K	33	GLY	4.7
6	N	45	GLU	4.7
2	I	236	LYS	4.7
5	L	287	ILE	4.7
6	N	17	ILE	4.7
6	M	127	GLU	4.5
6	N	20	VAL	4.4
2	C	333	ILE	4.3
5	L	604	SER	4.3
2	C	251	ALA	4.3
5	F	165	PHE	4.2
1	H	146	VAL	4.1
5	L	598	LEU	4.1
6	M	123	ILE	4.1
1	H	135	ASP	4.0
5	L	317	ASN	4.0
6	N	151	GLY	4.0
1	H	158	ARG	4.0
1	A	280	ASP	4.0
6	N	16	ALA	3.9
6	M	70	PRO	3.9
2	I	155	VAL	3.9
6	N	34	GLU	3.8
6	N	43	ILE	3.7
2	I	124	MET	3.7
5	L	605	GLU	3.7
5	L	318	ALA	3.7
4	K	34	GLY	3.6
4	K	23	ALA	3.6
6	M	129	ARG	3.5
2	I	235	ASN	3.4
1	H	67	GLU	3.4
6	M	18	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	262	LEU	3.4
3	J	1204	VAL	3.4
5	F	337	VAL	3.4
1	H	56	VAL	3.4
6	M	34	GLU	3.3
2	C	334	GLU	3.3
6	N	19	GLY	3.3
2	I	998	LEU	3.3
1	H	173	VAL	3.3
1	A	281	LEU	3.3
5	F	259	PHE	3.3
1	A	284	ARG	3.3
3	D	1134	ILE	3.3
6	N	111	PHE	3.3
6	N	58	THR	3.2
6	N	127	GLU	3.2
6	M	45	GLU	3.2
2	I	1001	GLY	3.2
1	G	89	ALA	3.2
3	J	16	GLU	3.2
1	A	304	LYS	3.2
3	J	1161	GLY	3.2
2	C	292	ILE	3.2
3	J	311	ARG	3.1
5	F	319	ALA	3.1
2	C	289	VAL	3.1
6	M	27	PRO	3.1
6	N	65	GLU	3.1
2	C	165	HIS	3.1
5	F	336	GLU	3.0
5	L	602	SER	3.0
1	A	294	ASN	3.0
2	I	540	ARG	3.0
6	N	18	ALA	3.0
1	A	249	PHE	3.0
3	J	1215	GLU	3.0
4	K	31	GLN	2.9
2	I	599	VAL	2.9
2	C	253	PHE	2.9
5	L	606	VAL	2.9
2	I	634	VAL	2.9
6	N	55	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
5	F	317	ASN	2.9
1	A	321	TRP	2.9
2	I	120	GLN	2.9
2	I	493	ILE	2.9
2	I	21	VAL	2.9
6	M	40	PHE	2.9
4	K	46	THR	2.9
5	L	283	GLN	2.9
1	H	112	ALA	2.9
2	C	108	GLU	2.8
6	N	126	LEU	2.8
2	I	151	ARG	2.8
5	L	290	LEU	2.8
4	K	35	LYS	2.8
3	D	1172	LYS	2.8
3	D	878	ASP	2.8
3	J	1160	SER	2.8
6	M	41	ARG	2.8
1	A	293	PRO	2.8
1	A	292	THR	2.8
6	M	17	ILE	2.7
2	I	987	GLU	2.7
5	L	596	ARG	2.7
5	F	286	LEU	2.7
2	C	295	LYS	2.7
2	I	974	ARG	2.7
1	H	123	ILE	2.7
6	M	107	GLU	2.7
3	D	877	VAL	2.7
1	A	253	LEU	2.7
3	J	1203	ARG	2.7
5	L	286	LEU	2.7
1	A	323	PRO	2.7
3	J	392	THR	2.7
1	H	98	VAL	2.7
2	I	584	TYR	2.7
5	L	607	LEU	2.7
6	M	108	ASP	2.6
4	K	66	VAL	2.6
5	F	301	ASN	2.6
6	N	123	ILE	2.6
2	C	297	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	I	882	ILE	2.6
2	I	153	PRO	2.6
2	I	121	GLU	2.6
2	I	122	VAL	2.6
3	D	830	ASP	2.6
3	D	1215	GLU	2.6
2	I	69	GLN	2.6
1	A	260	LEU	2.6
6	N	112	GLY	2.6
3	J	1168	GLU	2.6
6	M	42	ARG	2.5
2	I	632	ASP	2.5
5	F	321	ALA	2.5
2	C	317	LEU	2.5
2	I	169	LYS	2.5
2	I	991	LYS	2.5
6	N	122	GLY	2.5
5	F	325	PRO	2.5
3	J	1165	PHE	2.5
6	M	44	LEU	2.5
1	G	98	VAL	2.5
2	I	640	GLY	2.5
5	L	328	GLU	2.5
2	I	985	GLU	2.5
2	I	156	PHE	2.5
4	K	26	ARG	2.5
1	H	50	SER	2.5
2	I	485	ASP	2.5
3	D	713	GLU	2.5
2	I	919	ARG	2.5
6	M	122	GLY	2.5
6	N	47	TRP	2.5
2	C	290	GLU	2.4
3	J	715	LYS	2.4
2	I	172	TYR	2.4
5	L	610	PHE	2.4
1	A	255	ARG	2.4
3	D	1151	LYS	2.4
6	M	138	CYS	2.4
3	D	1212	ASP	2.4
1	G	24	ALA	2.4
2	I	492	MET	2.4

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Mol	Chain	Res	Type	RSRZ
3	J	516	ASP	2.4
2	I	621	SER	2.4
2	I	988	LYS	2.4
2	I	979	LEU	2.4
2	I	997	TRP	2.4
2	C	1002	LEU	2.4
1	H	97	GLU	2.4
1	H	114	ASP	2.4
1	H	64	VAL	2.4
5	L	137	TYR	2.4
2	C	298	ALA	2.3
6	N	72	PRO	2.3
3	D	1152	GLU	2.3
2	I	629	PHE	2.3
5	F	355	ILE	2.3
6	N	130	PRO	2.3
2	I	941	LYS	2.3
1	A	275	ILE	2.3
2	I	450	ASN	2.3
4	K	30	MET	2.3
2	I	1008	GLN	2.3
2	I	977	ALA	2.3
6	M	43	ILE	2.3
6	M	71	ASP	2.3
1	A	302	GLU	2.3
1	H	18	GLN	2.3
2	I	157	PHE	2.3
1	H	115	ILE	2.3
2	I	70	TYR	2.3
6	M	130	PRO	2.3
5	F	158	LEU	2.3
1	H	88	LEU	2.2
4	K	29	GLN	2.2
1	A	306	VAL	2.2
6	N	28	GLY	2.2
2	C	237	LEU	2.2
6	N	61	HIS	2.2
2	C	266	GLY	2.2
2	C	995	ASP	2.2
2	I	984	VAL	2.2
3	J	77	ARG	2.2
6	M	151	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
5	F	318	ALA	2.2
5	L	294	GLN	2.2
5	L	165	PHE	2.2
6	M	19	GLY	2.2
5	L	291	CYS	2.2
3	J	1374	ALA	2.2
2	I	248	GLY	2.2
5	F	162	ILE	2.2
6	N	63	GLN	2.2
2	I	483	ASP	2.2
2	I	289	VAL	2.2
2	I	544	GLY	2.1
2	I	1050	VAL	2.1
2	I	647	ARG	2.1
1	B	233	ASP	2.1
1	A	320	ASN	2.1
5	F	167	ASP	2.1
5	F	283	GLN	2.1
1	B	136	GLU	2.1
2	I	165	HIS	2.1
6	M	103	LEU	2.1
6	N	40	PHE	2.1
3	D	1149	ARG	2.1
4	K	36	ASP	2.1
4	K	69	ARG	2.1
6	M	35	ALA	2.1
6	M	126	LEU	2.1
5	F	315	TRP	2.1
3	J	713	GLU	2.1
5	L	600	HIS	2.1
3	J	1190	ILE	2.1
1	H	111	THR	2.1
2	C	489	PRO	2.1
2	C	536	GLY	2.1
2	I	986	ALA	2.1
6	M	46	ALA	2.1
5	L	296	LYS	2.1
3	J	512	TYR	2.1
1	A	256	PRO	2.0
4	K	78	ALA	2.0
2	I	100	LEU	2.0
3	J	1177	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
5	F	287	ILE	2.0
6	N	121	ILE	2.0
2	C	338	THR	2.0
5	L	167	ASP	2.0
2	I	836	LEU	2.0
3	J	91	GLU	2.0
6	M	38	ALA	2.0
2	C	107	ARG	2.0
3	J	1296	GLY	2.0
6	N	44	LEU	2.0
2	I	1264	GLN	2.0
1	H	152	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	ZN	N	200	1/1	0.68	0.07	506,506,506,506	0
8	ZN	M	200	1/1	0.92	0.17	512,512,512,512	0
7	MG	J	2001	1/1	0.93	0.39	335,335,335,335	0
8	ZN	J	2002	1/1	0.97	0.09	269,269,269,269	0
7	MG	D	2001	1/1	0.97	0.47	268,268,268,268	0
8	ZN	D	2003	1/1	0.98	0.26	245,245,245,245	0
8	ZN	D	2002	1/1	0.98	0.14	271,271,271,271	0
8	ZN	J	2003	1/1	0.99	0.23	211,211,211,211	0

6.5 Other polymers [i](#)

There are no such residues in this entry.