



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2017 – 11:11 AM EST

PDB ID : 4XLR
Title : Crystal structure of T.aquaticus transcription initiation complex with CarD containing bubble promoter and RNA
Authors : Bae, B.; Darst, S.A.
Deposited on : unknown
Resolution : 4.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

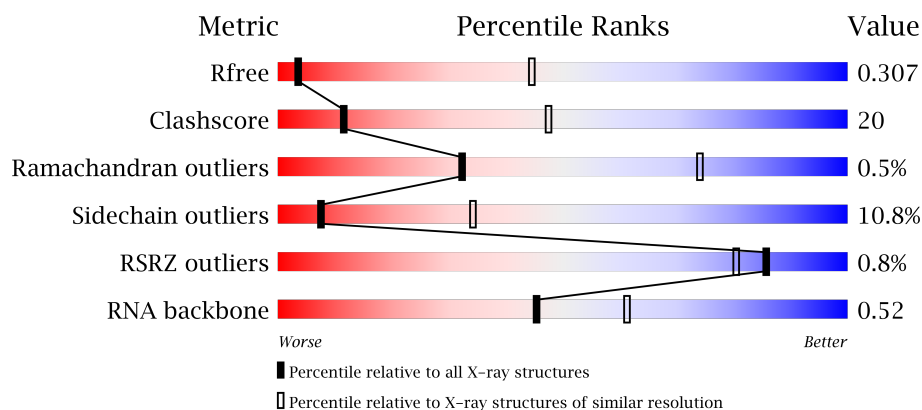
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 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.









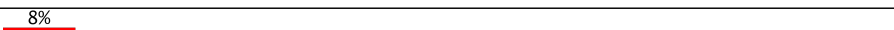
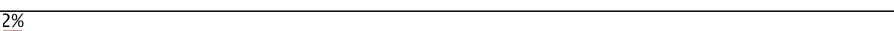
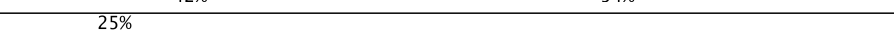

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1002 (4.92-3.62)
Clashscore	112137	1001 (4.92-3.68)
Ramachandran outliers	110173	1012 (4.92-3.64)
Sidechain outliers	110143	1021 (4.92-3.62)
RSRZ outliers	101464	1009 (4.92-3.62)
RNA backbone	2435	1034 (5.60-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	314	
1	B	314	
1	G	314	
1	H	314	

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Mol	Chain	Length	Quality of chain
2	C	1119	
2	I	1119	
3	D	1524	
3	J	1524	
4	E	99	
4	K	99	
5	F	347	
5	L	347	
6	M	164	
6	N	164	
7	O	48	
7	R	48	
8	P	48	
8	S	48	
9	Q	4	
9	T	4	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 60854 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	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	B	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	G	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	H	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1117	Total	C	N	O	S	0	0	0
			8762	5544	1558	1637	23			
2	I	1117	Total	C	N	O	S	0	0	0
			8762	5544	1558	1637	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1490	Total	C	N	O	S	0	0	0
			11761	7439	2088	2196	38			
3	J	1367	Total	C	N	O	S	0	0	0
			10779	6810	1923	2010	36			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	93	Total	C	N	O	S	0	0	0
			768	490	136	138	4			
4	K	93	Total	C	N	O	S	0	0	0
			768	490	136	138	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2787	1758	502	523	4			
5	L	345	Total	C	N	O	S	0	0	0
			2787	1758	502	523	4			

- Molecule 6 is a protein called CarD-like transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	M	158	Total	C	N	O	S	0	0	0
			1239	787	229	221	2			
6	N	158	Total	C	N	O	S	0	0	0
			1239	787	229	221	2			

- Molecule 7 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	O	48	Total	C	N	O	P	0	0	0
			988	472	182	287	47			
7	R	48	Total	C	N	O	P	0	0	0
			988	472	182	287	47			

- Molecule 8 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	P	48	Total	C	N	O	P	0	0	0
			985	471	183	284	47			
8	S	48	Total	C	N	O	P	0	0	0
			985	471	183	284	47			

- Molecule 9 is a RNA chain called RNA (5'-R(P*UP*CP*GP*A)-3').

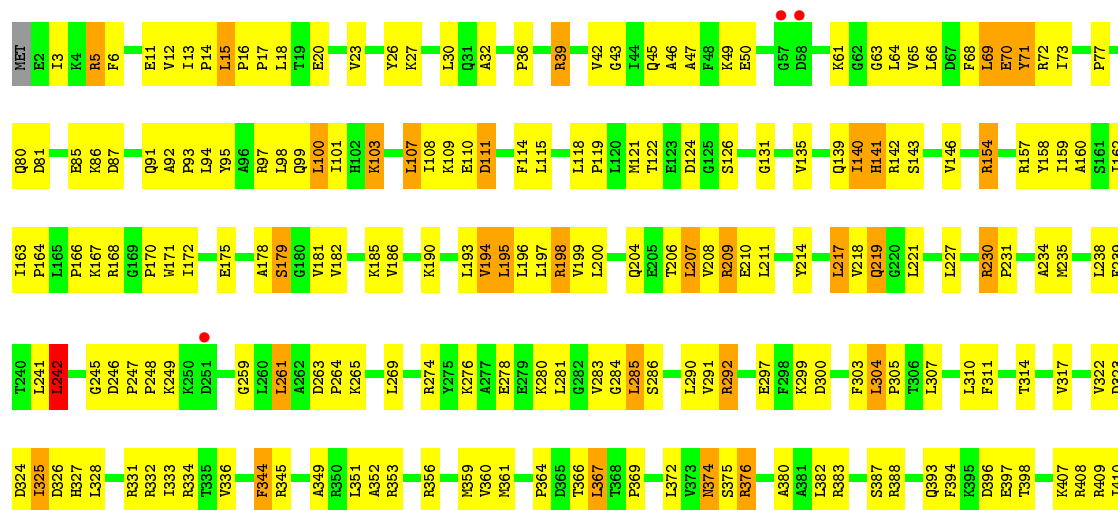
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	Q	4	Total	C	N	O	P	0	0	0
			85	38	15	28	4			
9	T	4	Total	C	N	O	P	0	0	0
			85	38	15	28	4			

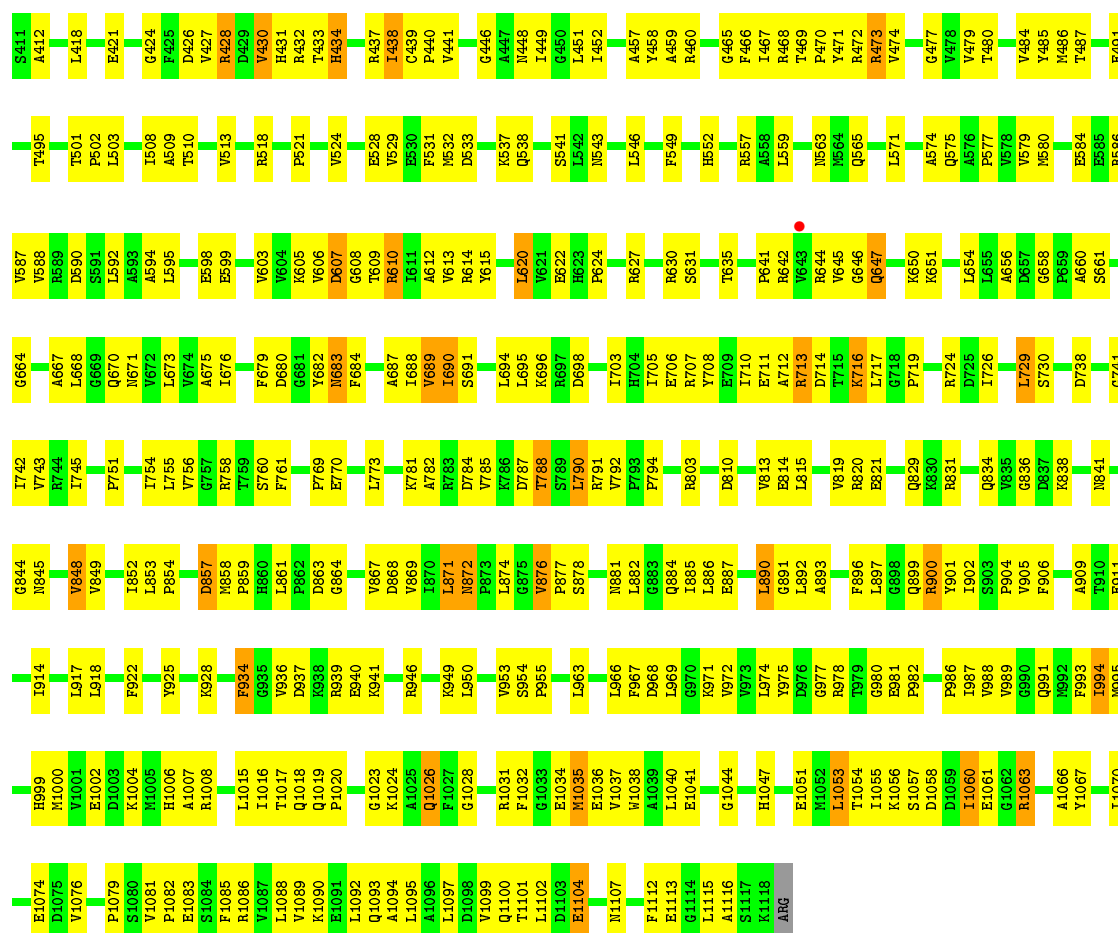
- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	J	2	Total 2	Zn 2	0	0
10	D	2	Total 2	Zn 2	0	0

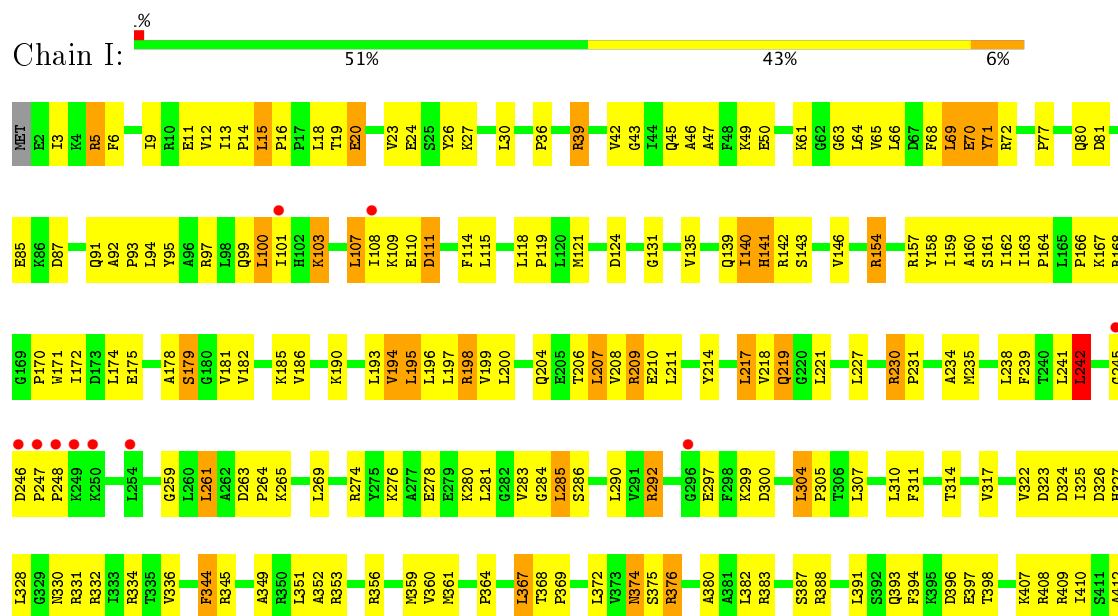
- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

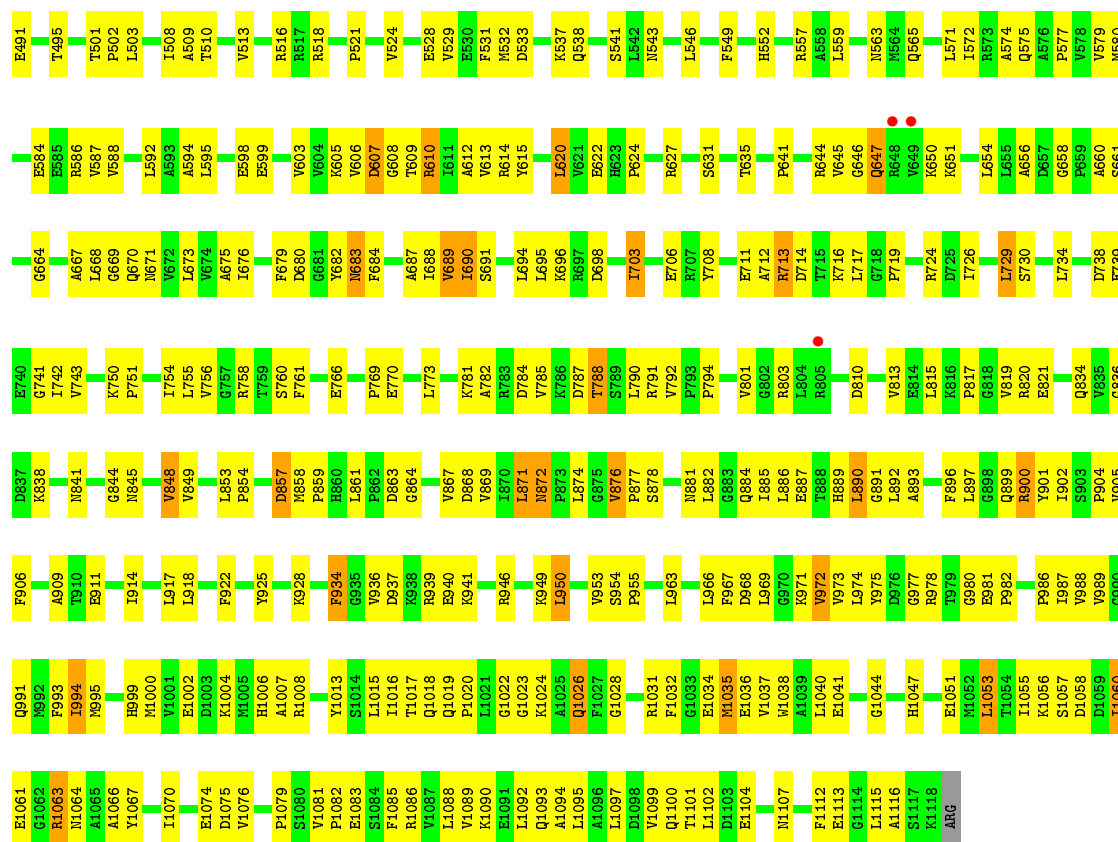
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	J	1	Total 1	Mg 1	0	0
11	D	1	Total 1	Mg 1	0	0



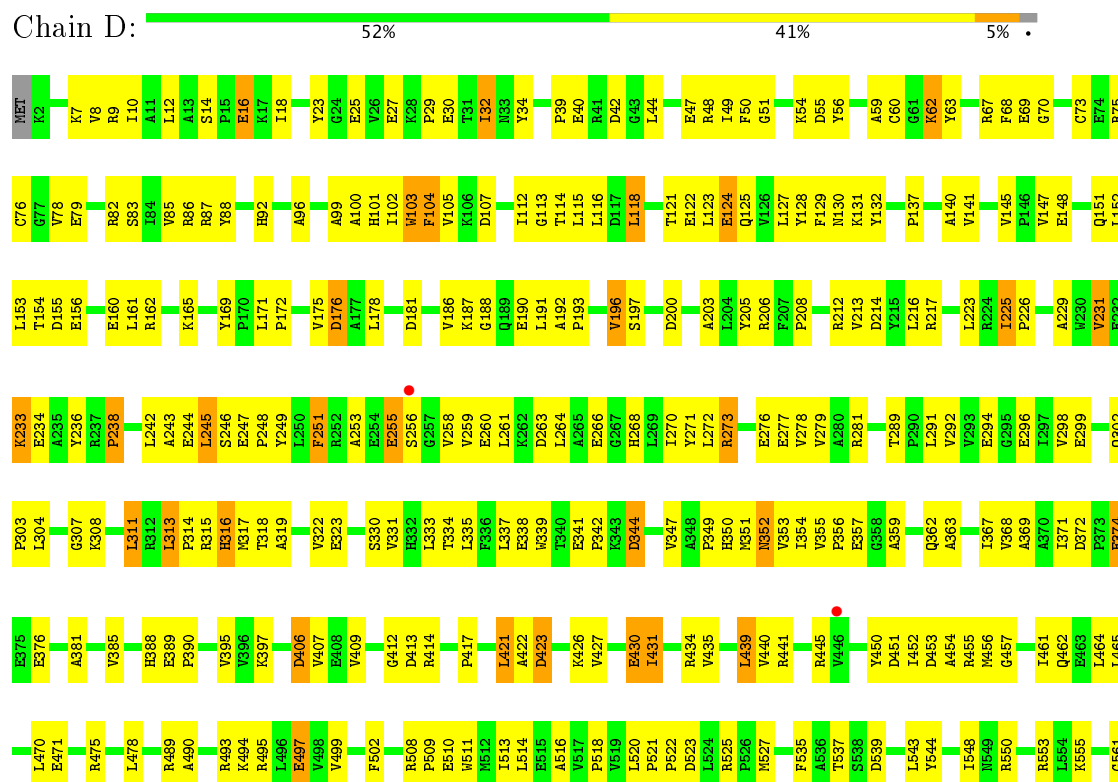


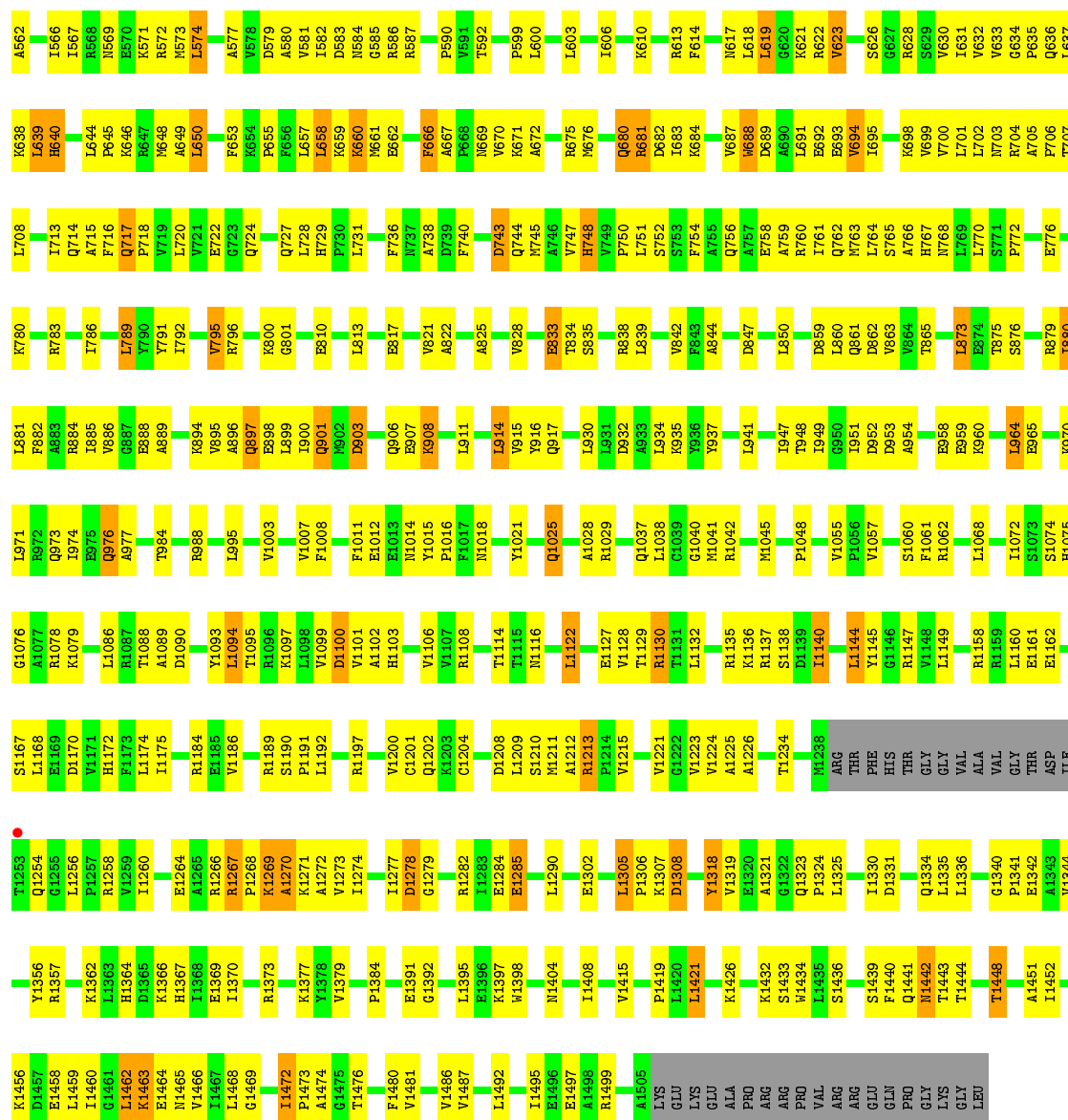
- Molecule 2: DNA-directed RNA polymerase subunit beta





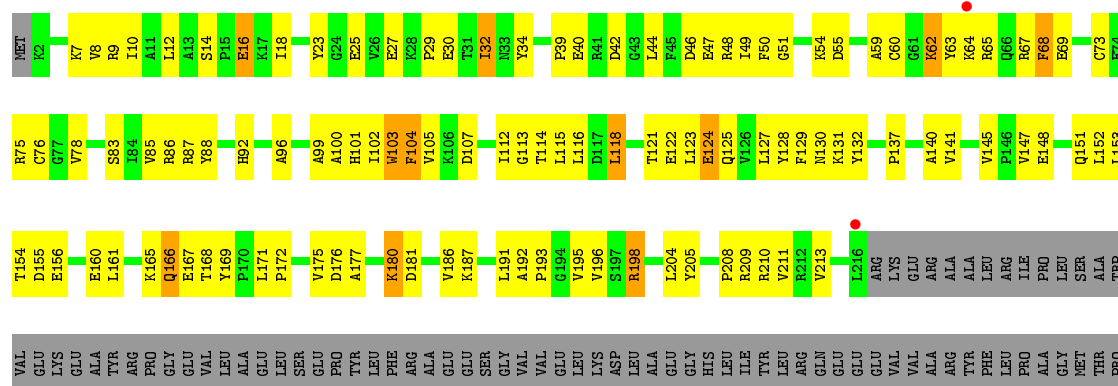
• Molecule 3: DNA-directed RNA polymerase subunit beta'

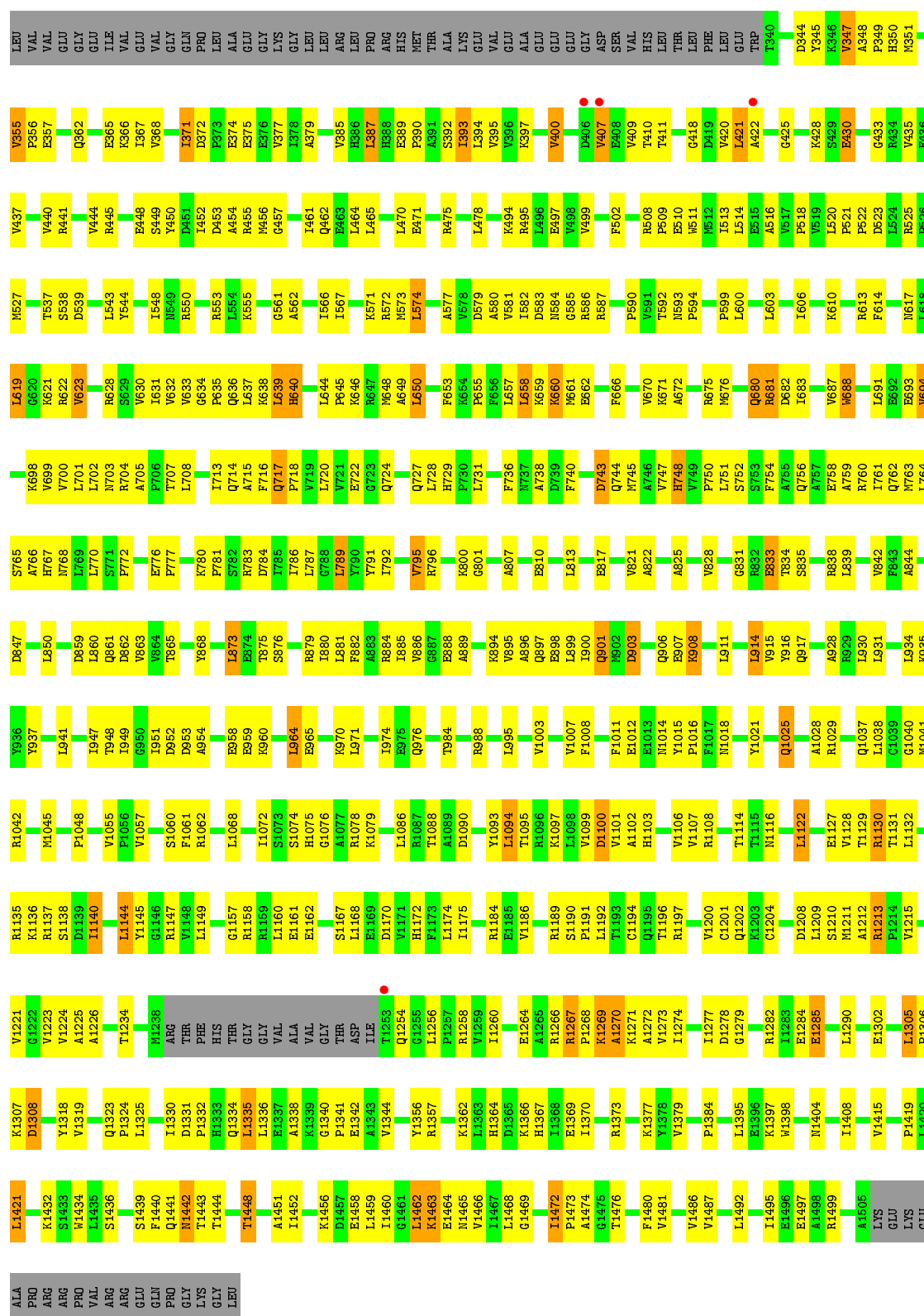


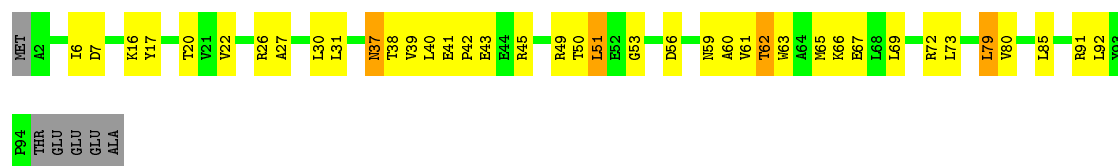


• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain J: 49% 37% 10%

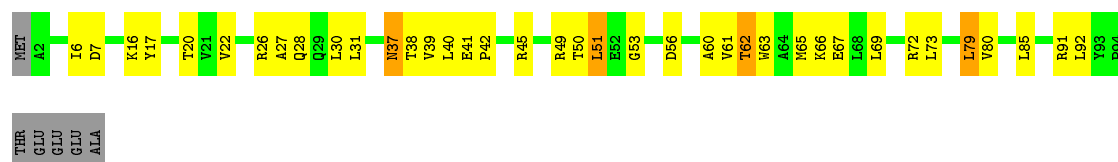






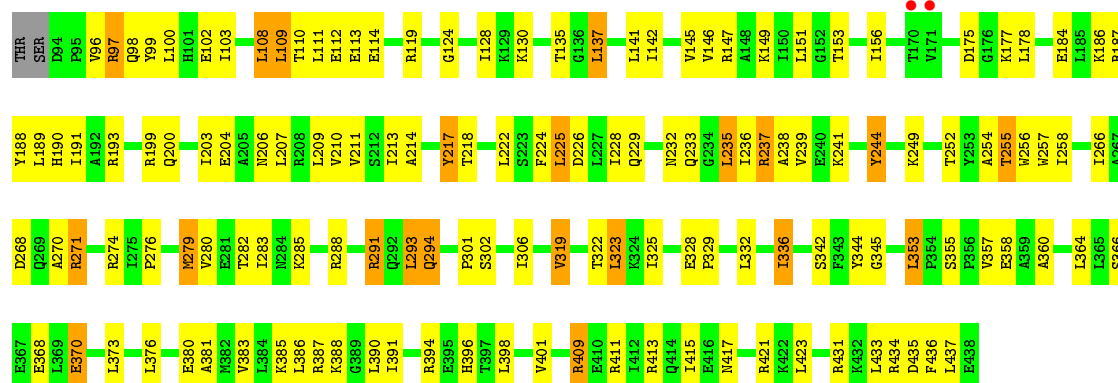
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain K: 56% 34% 6%



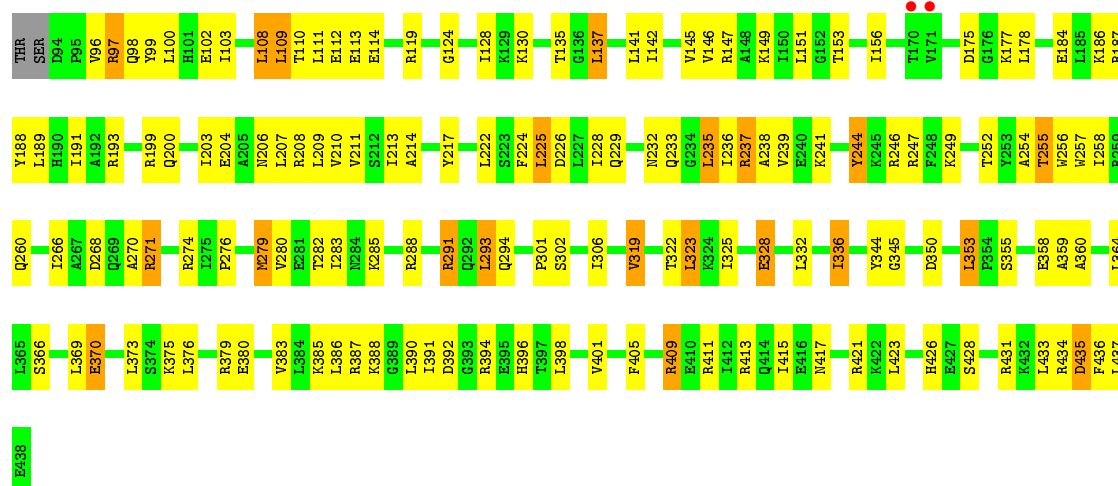
- Molecule 5: RNA polymerase sigma factor SigA

Chain F: 59% 35% 6%

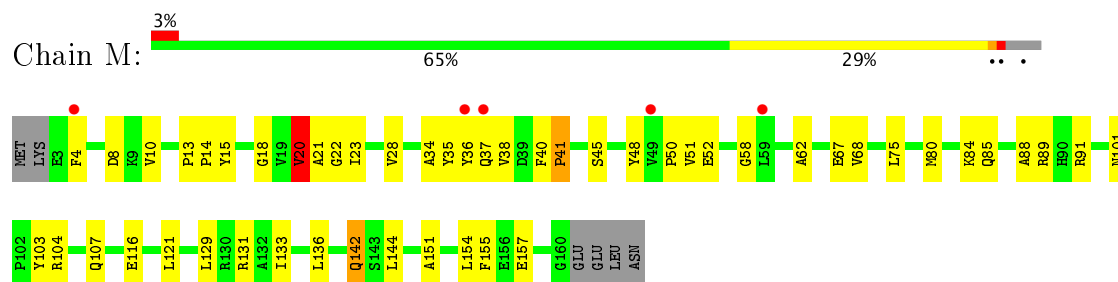


- Molecule 5: RNA polymerase sigma factor SigA

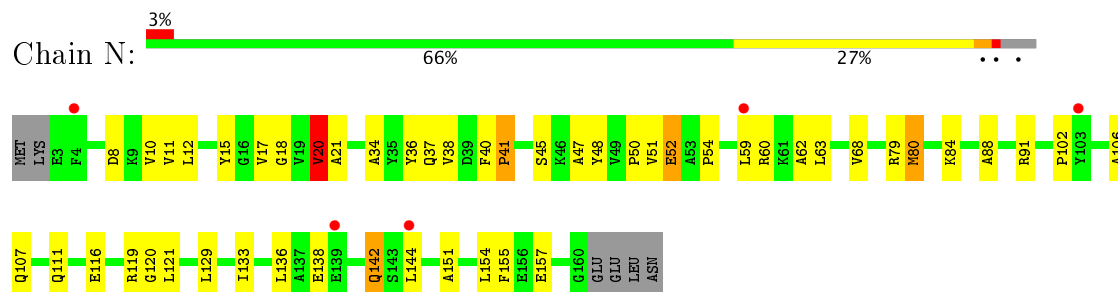
Chain L: 57% 36% 6%



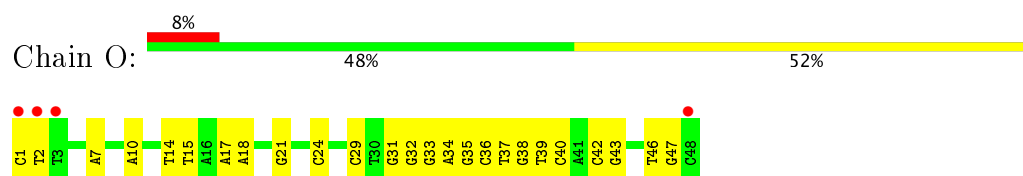
- Molecule 6: CarD-like transcriptional regulator



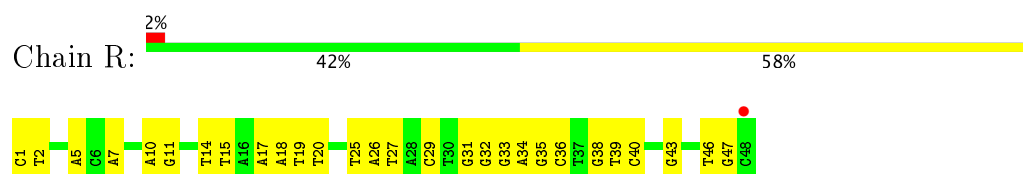
- Molecule 6: CarD-like transcriptional regulator



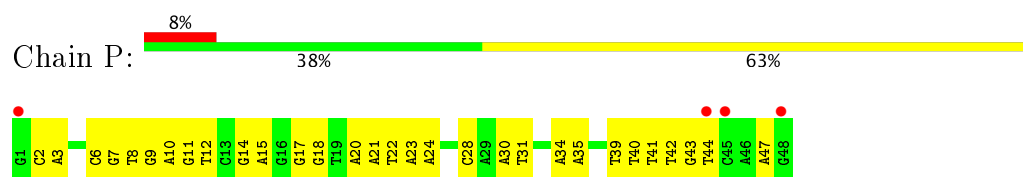
- Molecule 7: DNA (48-MER)



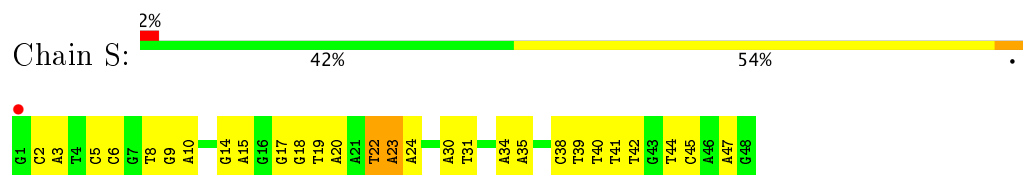
- Molecule 7: DNA (48-MER)



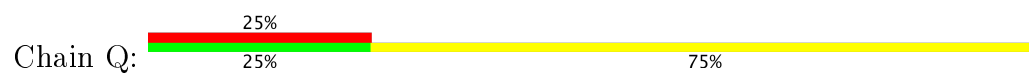
- Molecule 8: DNA (48-MER)



- Molecule 8: DNA (48-MER)



- Molecule 9: RNA (5'-R(P*UP*CP*GP*A)-3')



- Molecule 9: RNA (5'-R(P*UP*CP*GP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	289.84Å 289.84Å 536.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.56 – 4.30 39.56 – 4.30	Depositor EDS
% Data completeness (in resolution range)	94.8 (39.56-4.30) 94.8 (39.56-4.30)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 4.28Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, R_{free}	0.275 , 0.310 0.268 , 0.307	Depositor DCC
R_{free} test set	7326 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	165.1	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 123.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	60854	wwPDB-VP
Average B, all atoms (Å ²)	179.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.29	0/1804	0.52	0/2455
1	B	0.27	0/1804	0.49	0/2455
1	G	0.30	0/1804	0.52	0/2455
1	H	0.27	0/1804	0.49	0/2455
2	C	0.29	0/8929	0.51	1/12074 (0.0%)
2	I	0.29	0/8929	0.51	1/12074 (0.0%)
3	D	0.29	0/11963	0.50	0/16165
3	J	0.28	0/10959	0.49	0/14802
4	E	0.27	0/783	0.53	0/1054
4	K	0.27	0/783	0.53	0/1054
5	F	0.34	0/2829	0.54	0/3804
5	L	0.33	0/2829	0.54	0/3804
6	M	0.35	0/1267	0.55	0/1719
6	N	0.35	0/1267	0.55	0/1719
7	O	0.59	0/1109	0.92	0/1712
7	R	0.56	0/1109	0.92	0/1712
8	P	0.64	0/1106	0.88	0/1706
8	S	0.61	0/1106	0.90	2/1706 (0.1%)
9	Q	0.24	0/94	0.71	0/144
9	T	0.24	0/94	0.76	0/144
All	All	0.33	0/62372	0.55	4/85213 (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
2	C	0	2
2	I	0	2
3	D	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	J	0	1
6	M	0	2
6	N	0	2
All	All	0	10

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	23	DA	O5'-P-OP1	-6.61	99.75	105.70
2	C	242	LEU	CA-CB-CG	5.68	128.36	115.30
2	I	242	LEU	CA-CB-CG	5.57	128.10	115.30
8	S	22	DT	OP1-P-O3'	5.13	116.48	105.20

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	360	VAL	Peptide
2	C	71	TYR	Mainchain
3	D	1270	ALA	Peptide
2	I	360	VAL	Peptide
2	I	71	TYR	Mainchain
3	J	1270	ALA	Peptide
6	M	20	VAL	Mainchain,Peptide
6	N	20	VAL	Mainchain,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	1770	0	1799	87	0
1	B	1770	0	1799	66	0
1	G	1770	0	1799	88	0
1	H	1770	0	1799	65	0
2	C	8762	0	8854	435	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	8762	0	8854	436	0
3	D	11761	0	11976	537	0
3	J	10779	0	10993	490	0
4	E	768	0	784	38	0
4	K	768	0	784	36	0
5	F	2787	0	2866	122	0
5	L	2787	0	2866	127	0
6	M	1239	0	1259	38	0
6	N	1239	0	1259	39	0
7	O	988	0	544	30	0
7	R	988	0	544	38	0
8	P	985	0	543	36	0
8	S	985	0	543	30	0
9	Q	85	0	43	1	0
9	T	85	0	43	2	0
10	D	2	0	0	0	0
10	J	2	0	0	0	0
11	D	1	0	0	0	0
11	J	1	0	0	0	0
All	All	60854	0	59951	2363	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (2363) 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)
3:D:73:CYS:HB3	3:D:76:CYS:SG	1.97	1.04
3:J:73:CYS:HB3	3:J:76:CYS:SG	1.97	1.04
3:D:105:VAL:HA	3:D:112:ILE:HD11	1.55	0.89
3:D:412:GLY:HA2	3:D:434:ARG:HD3	1.55	0.89
3:J:105:VAL:HA	3:J:112:ILE:HD11	1.55	0.88
1:A:42:ARG:HH12	2:C:857:ASP:HB3	1.38	0.86
3:D:208:PRO:HA	3:D:390:PRO:HA	1.56	0.85
1:G:42:ARG:HH12	2:I:857:ASP:HB3	1.38	0.85
3:J:210:ARG:HG2	3:J:389:GLU:HB3	1.58	0.85
2:I:679:PHE:H	2:I:683:ASN:HD21	1.25	0.85
2:C:858:MET:H	2:C:977:GLY:HA3	1.40	0.84
2:I:374:ASN:HD21	5:L:291:ARG:HE	1.22	0.84
2:I:858:MET:H	2:I:977:GLY:HA3	1.42	0.84
5:L:203:ILE:HG12	5:L:239:VAL:HG21	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:55:SER:HB3	1:G:143:ARG:HB2	1.61	0.83
2:C:679:PHE:H	2:C:683:ASN:HD21	1.26	0.82
5:F:203:ILE:HG12	5:F:239:VAL:HG21	1.61	0.82
2:C:374:ASN:HD21	5:F:291:ARG:HE	1.26	0.82
2:I:364:PRO:HA	2:I:367:LEU:HD12	1.61	0.82
2:C:364:PRO:HA	2:C:367:LEU:HD12	1.61	0.82
6:N:20:VAL:HA	6:N:38:VAL:HA	1.60	0.81
2:C:836:GLY:H	2:C:849:VAL:HB	1.44	0.81
3:D:954:ALA:O	3:D:1062:ARG:NH1	2.12	0.81
3:J:208:PRO:HB3	3:J:387:LEU:HD21	1.60	0.81
2:I:836:GLY:H	2:I:849:VAL:HB	1.45	0.80
1:A:55:SER:HB3	1:A:143:ARG:HB2	1.61	0.80
2:C:603:VAL:HB	2:C:646:GLY:HA2	1.63	0.80
2:I:292:ARG:HH11	2:I:292:ARG:H	1.29	0.80
2:I:603:VAL:HA	2:I:613:VAL:HG12	1.63	0.80
6:M:20:VAL:HA	6:M:38:VAL:HA	1.63	0.80
2:C:71:TYR:HA	2:C:95:TYR:O	1.81	0.80
2:C:712:ALA:HB3	2:C:821:GLU:H	1.47	0.80
2:C:603:VAL:HA	2:C:613:VAL:HG12	1.64	0.80
3:D:73:CYS:CB	3:D:76:CYS:SG	2.65	0.80
8:P:30:DA:H2"	8:P:31:DT:H5"	1.64	0.80
2:C:292:ARG:H	2:C:292:ARG:HH11	1.30	0.80
3:D:1103:HIS:HB2	3:D:1462:LEU:HD11	1.64	0.79
2:C:1102:LEU:HB2	3:D:7:LYS:HB2	1.63	0.79
3:J:73:CYS:CB	3:J:76:CYS:SG	2.64	0.79
2:I:71:TYR:HA	2:I:95:TYR:O	1.83	0.79
3:J:954:ALA:O	3:J:1062:ARG:NH1	2.15	0.79
2:I:603:VAL:HB	2:I:646:GLY:HA2	1.63	0.79
2:I:1102:LEU:HB2	3:J:7:LYS:HB2	1.63	0.78
3:D:1189:ARG:NH2	3:D:1204:CYS:SG	2.55	0.78
7:R:7:DA:H61	8:S:42:DT:H3	1.30	0.78
3:D:130:ASN:HD22	5:F:98:GLN:HE22	1.31	0.78
3:J:1103:HIS:HB2	3:J:1462:LEU:HD11	1.66	0.78
2:I:63:GLY:HA3	2:I:103:LYS:HB2	1.67	0.77
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.65	0.77
2:C:374:ASN:HD21	5:F:291:ARG:NE	1.83	0.77
2:I:154:ARG:HD3	2:I:178:ALA:HB2	1.65	0.77
2:I:1063:ARG:HH22	5:L:353:LEU:HD11	1.49	0.77
2:I:712:ALA:HB3	2:I:821:GLU:H	1.48	0.77
3:D:953:ASP:O	3:D:1018:ASN:ND2	2.17	0.77
8:S:30:DA:H2"	8:S:31:DT:H5"	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:367:ILE:HG22	3:D:368:VAL:HG23	1.67	0.77
3:J:953:ASP:O	3:J:1018:ASN:ND2	2.16	0.77
2:C:63:GLY:HA3	2:C:103:LYS:HB2	1.67	0.77
3:J:951:ILE:O	3:J:1062:ARG:NH1	2.18	0.76
3:D:323:GLU:HB3	3:D:334:THR:H	1.49	0.76
2:C:154:ARG:HD3	2:C:178:ALA:HB2	1.66	0.76
5:F:218:THR:O	8:P:23:DA:N6	2.19	0.76
3:D:462:GLN:HB2	3:D:513:ILE:HG21	1.68	0.76
2:I:427:VAL:HG22	7:R:38:DG:H21	1.51	0.76
2:I:537:LYS:HZ3	2:I:905:VAL:H	1.32	0.76
3:J:48:ARG:HA	3:J:78:VAL:HG22	1.68	0.75
3:J:1189:ARG:NH2	3:J:1204:CYS:SG	2.56	0.75
3:J:462:GLN:HB2	3:J:513:ILE:HG21	1.67	0.75
3:D:423:ASP:HB3	3:D:426:LYS:HB3	1.69	0.75
3:J:130:ASN:HD22	5:L:98:GLN:HE22	1.31	0.75
3:D:951:ILE:O	3:D:1062:ARG:NH1	2.19	0.75
4:K:79:LEU:HG	4:K:80:VAL:HG22	1.69	0.75
3:D:48:ARG:HA	3:D:78:VAL:HG22	1.69	0.75
2:I:911:GLU:OE1	3:J:1062:ARG:NH2	2.20	0.75
1:G:53:VAL:HG23	1:G:144:VAL:HG22	1.69	0.74
3:J:715:ALA:HB3	3:J:764:LEU:HA	1.67	0.74
5:F:398:LEU:HB3	5:F:409:ARG:HB2	1.67	0.74
2:I:694:LEU:HD11	2:I:868:ASP:HB3	1.68	0.74
2:C:876:VAL:HG11	2:C:885:ILE:HD11	1.70	0.74
4:E:79:LEU:HG	4:E:80:VAL:HG22	1.69	0.74
2:I:167:LYS:HD3	7:R:35:DG:H5'	1.69	0.74
5:L:428:SER:HA	5:L:434:ARG:HH22	1.52	0.74
3:D:1379:VAL:HG12	3:D:1419:PRO:HA	1.69	0.74
5:L:332:LEU:HD22	5:L:345:GLY:HA2	1.70	0.74
3:J:67:ARG:HD2	5:L:394:ARG:HD3	1.67	0.74
3:D:760:ARG:HH22	4:E:62:THR:HG23	1.50	0.74
2:I:876:VAL:HG11	2:I:885:ILE:HD11	1.70	0.74
2:C:694:LEU:HD11	2:C:868:ASP:HB3	1.69	0.74
1:A:53:VAL:HG23	1:A:144:VAL:HG22	1.68	0.74
3:D:188:GLY:N	3:D:197:SER:O	2.20	0.74
3:J:760:ARG:HH22	4:K:62:THR:HG23	1.51	0.74
3:D:214:ASP:HA	3:D:342:PRO:HA	1.69	0.74
2:I:3:ILE:HG23	2:I:900:ARG:HB2	1.70	0.73
2:I:108:ILE:HB	6:N:48:TYR:HB2	1.70	0.73
3:D:792:ILE:HG21	3:D:941:LEU:HD22	1.70	0.73
3:J:1254:GLN:HB2	3:J:1258:ARG:HB2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:786:ILE:HD13	3:J:908:LYS:HG2	1.69	0.73
5:L:398:LEU:HB3	5:L:409:ARG:HB2	1.69	0.73
3:J:1379:VAL:HG12	3:J:1419:PRO:HA	1.71	0.73
2:C:3:ILE:HG23	2:C:900:ARG:HB2	1.71	0.73
3:J:792:ILE:HG21	3:J:941:LEU:HD22	1.71	0.72
5:L:235:LEU:HB2	5:L:258:ILE:HD11	1.70	0.72
2:C:427:VAL:HG22	7:O:38:DG:H21	1.55	0.72
3:D:786:ILE:HD13	3:D:908:LYS:HG2	1.69	0.72
3:J:670:VAL:HB	5:L:364:LEU:HD11	1.70	0.72
5:F:235:LEU:HB2	5:F:258:ILE:HD11	1.70	0.72
2:C:911:GLU:OE1	3:D:1062:ARG:NH2	2.23	0.71
2:I:72:ARG:HB2	2:I:95:TYR:HB2	1.71	0.71
2:I:1019:GLN:HG3	3:J:617:ASN:HD22	1.54	0.71
3:J:18:ILE:HG12	3:J:518:PRO:HG3	1.72	0.71
2:C:366:THR:HA	6:M:14:PRO:HG3	1.72	0.71
2:C:72:ARG:HB2	2:C:95:TYR:HB2	1.72	0.71
1:A:179:PHE:HB3	1:A:197:LEU:HD12	1.73	0.71
3:D:1436:SER:HB2	3:D:1464:GLU:HG2	1.72	0.71
2:C:971:LYS:HB2	2:C:986:PRO:HB2	1.72	0.71
3:D:917:GLN:HE22	3:D:1168:LEU:HD11	1.57	0.70
3:D:1254:GLN:HB2	3:D:1258:ARG:HB2	1.71	0.70
3:D:1135:ARG:HH21	3:D:1357:ARG:HH12	1.39	0.70
2:I:14:PRO:HB3	2:I:586:ARG:HH22	1.57	0.70
2:C:537:LYS:HZ3	2:C:905:VAL:H	1.37	0.70
3:D:226:PRO:HA	3:D:330:SER:HA	1.73	0.70
1:A:175:ARG:N	1:A:200:TRP:O	2.25	0.70
1:G:175:ARG:N	1:G:200:TRP:O	2.24	0.70
2:I:214:TYR:HB2	2:I:217:LEU:HD11	1.74	0.70
3:D:165:LYS:HB3	3:D:397:LYS:HE2	1.72	0.70
5:F:293:LEU:HD11	5:F:306:ILE:HD13	1.74	0.70
2:C:217:LEU:HD13	2:C:311:PHE:HD2	1.57	0.69
3:D:1472:ILE:HG13	3:D:1474:ALA:H	1.56	0.69
2:I:971:LYS:HB2	2:I:986:PRO:HB2	1.72	0.69
2:C:214:TYR:HB2	2:C:217:LEU:HD11	1.74	0.69
1:B:175:ARG:HB3	3:D:847:ASP:HB3	1.73	0.69
2:C:472:ARG:HD3	2:C:479:VAL:HG13	1.74	0.69
2:I:230:ARG:HH21	2:I:231:PRO:HD2	1.57	0.69
3:D:18:ILE:HG12	3:D:518:PRO:HG3	1.74	0.69
1:H:175:ARG:HB3	3:J:847:ASP:HB3	1.74	0.69
3:J:1135:ARG:HH21	3:J:1357:ARG:HH12	1.40	0.69
2:I:472:ARG:HD3	2:I:479:VAL:HG13	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:293:LEU:HD11	5:L:306:ILE:HD13	1.74	0.69
2:C:230:ARG:HH21	2:C:231:PRO:HD2	1.57	0.69
1:A:34:VAL:HG11	2:C:981:GLU:HG2	1.74	0.69
3:D:628:ARG:NH2	3:D:744:GLN:OE1	2.24	0.69
1:G:179:PHE:HB3	1:G:197:LEU:HD12	1.74	0.69
3:J:658:LEU:HD22	3:J:670:VAL:HG13	1.74	0.69
2:C:872:ASN:HD21	2:C:874:LEU:HG	1.57	0.69
2:I:324:ASP:HB3	2:I:327:HIS:HB2	1.75	0.69
2:I:484:VAL:HG21	2:I:531:PHE:HE1	1.57	0.69
2:I:872:ASN:HD21	2:I:874:LEU:HG	1.58	0.69
5:F:411:ARG:HD3	7:O:1:DC:H2'	1.75	0.69
3:J:1472:ILE:HG13	3:J:1474:ALA:H	1.57	0.69
2:C:304:LEU:HB3	2:C:305:PRO:HD3	1.74	0.69
2:C:484:VAL:HG21	2:C:531:PHE:HE1	1.56	0.69
3:D:835:SER:HB3	3:D:838:ARG:HG3	1.75	0.69
2:C:502:PRO:HB2	2:C:509:ALA:HB3	1.74	0.69
3:D:704:ARG:HG2	3:D:738:ALA:HB2	1.75	0.69
2:I:304:LEU:HB3	2:I:305:PRO:HD3	1.75	0.69
3:J:917:GLN:HE22	3:J:1168:LEU:HD11	1.57	0.69
3:D:9:ARG:HG3	3:D:1456:LYS:HB3	1.75	0.68
1:A:41:ARG:HG3	1:A:177:VAL:HB	1.76	0.68
3:J:1122:LEU:HD23	3:J:1140:ILE:HG21	1.75	0.68
6:M:88:ALA:HA	6:M:91:ARG:HD2	1.76	0.68
5:F:288:ARG:NH1	8:P:24:DA:OP1	2.26	0.68
1:G:41:ARG:HG3	1:G:177:VAL:HB	1.75	0.68
1:G:34:VAL:HG11	2:I:981:GLU:HG2	1.74	0.68
3:J:356:PRO:HB3	3:J:441:ARG:HA	1.75	0.68
3:J:628:ARG:NH2	3:J:744:GLN:OE1	2.25	0.68
3:J:835:SER:HB3	3:J:838:ARG:HG3	1.75	0.68
7:O:7:DA:H61	8:P:42:DT:H3	1.39	0.68
2:C:1063:ARG:HH22	5:F:353:LEU:HD11	1.59	0.68
3:J:704:ARG:HG2	3:J:738:ALA:HB2	1.75	0.68
2:C:264:PRO:HG2	2:C:265:LYS:HE2	1.75	0.68
3:D:1122:LEU:HD23	3:D:1140:ILE:HG21	1.75	0.68
2:I:502:PRO:HB2	2:I:509:ALA:HB3	1.74	0.68
3:J:572:ARG:NH1	5:L:98:GLN:HE21	1.92	0.68
5:L:124:GLY:HA2	5:L:191:ILE:HG22	1.76	0.68
7:R:2:DT:H3	8:S:47:DA:H2	1.40	0.68
2:C:6:PHE:HE1	2:C:901:TYR:HD1	1.42	0.68
3:D:743:ASP:HA	9:Q:4:A:H4'	1.75	0.68
2:I:217:LEU:HD13	2:I:311:PHE:HD2	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:902:ILE:HG22	2:C:904:PRO:HD3	1.75	0.67
2:I:711:GLU:O	2:I:758:ARG:NH1	2.27	0.67
2:C:108:ILE:HB	6:M:48:TYR:HB2	1.76	0.67
2:I:6:PHE:HE1	2:I:901:TYR:HD1	1.42	0.67
2:C:328:LEU:HD22	2:C:437:ARG:HD2	1.75	0.67
2:C:711:GLU:O	2:C:758:ARG:NH1	2.27	0.67
5:F:103:ILE:HG21	5:F:211:VAL:HG21	1.76	0.67
3:J:67:ARG:HG3	5:L:392:ASP:HB2	1.77	0.67
2:C:1008:ARG:HH11	2:C:1028:GLY:HA2	1.59	0.67
2:C:14:PRO:HB3	2:C:586:ARG:HH22	1.58	0.67
3:D:102:ILE:HD11	3:D:587:ARG:HG3	1.77	0.67
2:I:12:VAL:HG11	2:I:472:ARG:HH12	1.59	0.67
3:J:12:LEU:HD11	3:J:1452:ILE:HA	1.77	0.67
3:J:9:ARG:HG3	3:J:1456:LYS:HB3	1.77	0.67
2:C:487:THR:O	2:C:491:GLU:N	2.28	0.66
3:D:572:ARG:NH1	5:F:98:GLN:HE21	1.92	0.66
2:I:902:ILE:HG22	2:I:904:PRO:HD3	1.75	0.66
2:I:487:THR:O	2:I:491:GLU:N	2.28	0.66
3:J:743:ASP:HA	9:T:4:A:H4'	1.77	0.66
2:I:211:LEU:HD11	2:I:221:LEU:HB3	1.78	0.66
2:I:770:GLU:HG2	5:L:366:SER:HA	1.76	0.66
7:R:10:DA:H2	8:S:39:DT:H3	1.43	0.66
2:C:770:GLU:HG2	5:F:366:SER:HA	1.76	0.66
5:F:383:VAL:HG13	5:F:401:VAL:HG11	1.78	0.66
2:C:12:VAL:HG11	2:C:472:ARG:HH12	1.60	0.66
3:D:543:LEU:HG	3:D:600:LEU:HD23	1.78	0.66
5:F:124:GLY:HA2	5:F:191:ILE:HG22	1.76	0.66
2:I:1008:ARG:HH11	2:I:1028:GLY:HA2	1.59	0.66
2:I:328:LEU:HD22	2:I:437:ARG:HD2	1.76	0.66
2:I:468:ARG:HB3	2:I:485:TYR:O	1.96	0.66
3:D:191:LEU:HD11	3:D:197:SER:HB2	1.76	0.66
3:D:349:PRO:HB3	5:F:112:GLU:HG2	1.77	0.66
2:I:264:PRO:HG2	2:I:265:LYS:HE2	1.76	0.66
3:D:12:LEU:HD11	3:D:1452:ILE:HA	1.78	0.66
5:F:332:LEU:HD22	5:F:345:GLY:HA2	1.75	0.66
2:I:859:PRO:HB2	2:I:974:LEU:HD23	1.76	0.66
6:M:21:ALA:O	6:M:37:GLN:HB3	1.96	0.66
3:D:178:LEU:HD21	3:D:190:GLU:HB3	1.78	0.66
1:B:176:ARG:HD2	3:D:884:ARG:HH22	1.61	0.66
4:E:30:LEU:HA	4:E:37:ASN:HD21	1.60	0.66
2:I:100:LEU:HB2	2:I:369:PRO:HD3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:199:VAL:HA	2:C:231:PRO:HB3	1.77	0.66
3:J:543:LEU:HG	3:J:600:LEU:HD23	1.76	0.66
1:H:55:SER:HB2	1:H:166:PRO:HA	1.78	0.65
2:I:199:VAL:HA	2:I:231:PRO:HB3	1.77	0.65
2:I:595:LEU:HB2	2:I:656:ALA:HB3	1.76	0.65
5:L:103:ILE:HG21	5:L:211:VAL:HG21	1.77	0.65
2:C:100:LEU:HB2	2:C:369:PRO:HD3	1.77	0.65
2:C:630:ARG:HA	2:C:705:ILE:HD13	1.77	0.65
3:D:1331:ASP:HB3	3:D:1334:GLN:HB2	1.78	0.65
3:J:102:ILE:HD11	3:J:587:ARG:HG3	1.77	0.65
2:I:1095:LEU:HD11	3:J:603:LEU:HB3	1.77	0.65
2:C:468:ARG:HB3	2:C:485:TYR:O	1.96	0.65
5:F:222:LEU:HB3	5:F:226:ASP:HB3	1.78	0.65
7:R:39:DT:H2''	7:R:40:DC:H5'	1.77	0.65
2:C:859:PRO:HB2	2:C:974:LEU:HD23	1.78	0.65
3:D:561:GLY:HA3	5:F:147:ARG:HD3	1.77	0.65
2:I:458:TYR:HB3	2:I:470:PRO:HG2	1.78	0.65
4:K:30:LEU:HA	4:K:37:ASN:HD21	1.61	0.65
1:B:55:SER:HB2	1:B:166:PRO:HA	1.78	0.65
3:D:973:GLN:HG2	3:J:831:GLY:HA2	1.78	0.65
3:J:1331:ASP:HB3	3:J:1334:GLN:HB2	1.79	0.65
8:P:17:DG:H2''	8:P:18:DG:O4'	1.97	0.65
7:O:39:DT:H2''	7:O:40:DC:H5'	1.77	0.65
2:C:211:LEU:HD11	2:C:221:LEU:HB3	1.77	0.65
3:J:411:THR:HG22	3:J:437:VAL:H	1.62	0.65
3:D:1088:THR:HG22	3:D:1234:THR:HG23	1.78	0.65
2:I:158:TYR:HB2	2:I:314:THR:HG22	1.79	0.65
1:A:53:VAL:HG22	1:A:54:THR:H	1.61	0.65
2:C:595:LEU:HB2	2:C:656:ALA:HB3	1.78	0.65
3:D:759:ALA:HA	3:D:763:MET:HB3	1.78	0.65
2:I:751:PRO:HD2	3:J:681:ARG:HD2	1.78	0.64
1:H:176:ARG:HD2	3:J:884:ARG:HH22	1.62	0.64
5:L:222:LEU:HB3	5:L:226:ASP:HB3	1.78	0.64
2:C:143:SER:H	2:C:331:ARG:HA	1.63	0.64
3:J:561:GLY:HA3	5:L:147:ARG:HD3	1.79	0.64
7:R:46:DT:H3	8:S:3:DA:H61	1.45	0.64
2:C:374:ASN:ND2	5:F:291:ARG:HE	1.94	0.64
2:I:36:PRO:HB2	2:I:70:GLU:HG2	1.79	0.64
1:A:73:GLU:HB3	1:A:77:GLU:HB3	1.80	0.64
3:D:1138:SER:HB3	3:D:1362:LYS:HD3	1.80	0.64
3:D:1486:VAL:HG11	4:E:22:VAL:HG13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.80	0.64
3:D:32:ILE:HG22	3:D:39:PRO:HA	1.80	0.64
2:I:374:ASN:HD21	5:L:291:ARG:NE	1.95	0.64
1:A:219:LYS:HB2	1:B:222:LEU:HD22	1.79	0.64
2:I:966:LEU:HD11	2:I:986:PRO:HG3	1.80	0.64
2:I:874:LEU:HD13	3:J:783:ARG:HB3	1.80	0.64
2:C:36:PRO:HB2	2:C:70:GLU:HG2	1.80	0.64
3:J:1486:VAL:HG11	4:K:22:VAL:HG13	1.80	0.64
5:L:383:VAL:HG13	5:L:401:VAL:HG11	1.79	0.64
2:C:157:ARG:HH22	2:C:314:THR:HB	1.62	0.63
2:C:1095:LEU:HD11	3:D:603:LEU:HB3	1.79	0.63
3:J:759:ALA:HA	3:J:763:MET:HB3	1.78	0.63
3:D:229:ALA:HA	3:D:245:LEU:H	1.63	0.63
6:N:18:GLY:HA2	6:N:41:PRO:HD3	1.78	0.63
8:S:14:DG:H1	9:T:2:C:H42	1.46	0.63
2:C:458:TYR:HB3	2:C:470:PRO:HG2	1.78	0.63
1:G:219:LYS:HB2	1:H:222:LEU:HD22	1.79	0.63
3:J:168:THR:HA	3:J:394:LEU:HG	1.81	0.63
1:B:184:THR:HG23	1:B:192:LEU:HB2	1.81	0.63
3:D:1459:LEU:HD21	3:D:1468:LEU:HG	1.80	0.63
3:D:637:LEU:O	3:D:935:LYS:NZ	2.32	0.63
1:G:53:VAL:HG22	1:G:54:THR:H	1.63	0.63
2:I:42:VAL:HA	2:I:46:ALA:HB2	1.81	0.63
2:I:914:ILE:HA	2:I:917:LEU:HD12	1.81	0.63
3:D:1432:LYS:HG3	3:D:1460:ILE:HD11	1.81	0.63
3:J:1138:SER:HB3	3:J:1362:LYS:HD3	1.80	0.63
3:D:1038:LEU:O	3:D:1060:SER:OG	2.17	0.63
1:G:73:GLU:HB3	1:G:77:GLU:HB3	1.79	0.63
3:J:192:ALA:HB1	3:J:193:PRO:HD2	1.81	0.63
2:C:158:TYR:HB2	2:C:314:THR:HG22	1.80	0.63
4:E:41:GLU:HB3	4:E:42:PRO:HD2	1.81	0.63
2:I:157:ARG:HH22	2:I:314:THR:HB	1.63	0.63
3:J:1432:LYS:HG3	3:J:1460:ILE:HD11	1.80	0.63
5:L:409:ARG:NH2	7:R:5:DA:H61	1.95	0.63
3:D:291:LEU:HD23	3:D:303:PRO:HB2	1.80	0.63
1:H:184:THR:HG23	1:H:192:LEU:HB2	1.81	0.63
2:I:437:ARG:NH1	2:I:467:ILE:O	2.32	0.63
7:O:47:DG:N2	8:P:2:DC:N3	2.46	0.63
3:D:675:ARG:HH12	5:F:437:LEU:HG	1.64	0.63
2:I:675:ALA:HA	2:I:989:VAL:HG12	1.81	0.63
1:B:186:LEU:HD13	4:E:51:LEU:HD13	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1064:ASN:HD22	5:L:359:ALA:HB2	1.64	0.62
3:J:1038:LEU:O	3:J:1060:SER:OG	2.17	0.62
5:L:431:ARG:HG3	5:L:434:ARG:HE	1.64	0.62
2:C:42:VAL:HA	2:C:46:ALA:HB2	1.81	0.62
3:D:1323:GLN:HG2	3:D:1324:PRO:HD2	1.81	0.62
2:C:1034:GLU:HG2	3:D:619:LEU:HB3	1.82	0.62
3:D:658:LEU:HD22	3:D:670:VAL:HG13	1.81	0.62
2:I:245:GLY:HA2	5:L:97:ARG:HD2	1.81	0.62
6:N:20:VAL:HA	6:N:38:VAL:CA	2.29	0.62
3:J:1323:GLN:HG2	3:J:1324:PRO:HD2	1.81	0.62
3:D:264:LEU:HG	3:D:316:HIS:HE2	1.63	0.62
2:I:876:VAL:HG13	2:I:884:GLN:HE21	1.65	0.62
3:J:1088:THR:HG22	3:J:1234:THR:HG23	1.80	0.62
2:C:1055:ILE:HD11	2:C:1079:PRO:HD3	1.82	0.62
2:C:914:ILE:HA	2:C:917:LEU:HD12	1.81	0.62
3:J:1201:CYS:SG	3:J:1204:CYS:HB2	2.40	0.62
3:J:32:ILE:HG22	3:J:39:PRO:HA	1.81	0.62
2:C:118:LEU:HD12	2:C:119:PRO:HD2	1.82	0.62
3:D:30:GLU:HB2	5:F:274:ARG:HB2	1.82	0.62
2:C:874:LEU:HD13	3:D:783:ARG:HB3	1.81	0.62
3:J:680:GLN:O	3:J:682:ASP:N	2.29	0.62
4:K:41:GLU:HB3	4:K:42:PRO:HD2	1.81	0.62
3:D:1201:CYS:SG	3:D:1204:CYS:HB2	2.39	0.62
3:J:125:GLN:NE2	3:J:130:ASN:OD1	2.33	0.62
3:J:462:GLN:HA	3:J:513:ILE:HG13	1.82	0.62
2:C:876:VAL:HG13	2:C:884:GLN:HE21	1.65	0.62
1:H:186:LEU:HD13	4:K:51:LEU:HD13	1.80	0.62
2:I:143:SER:H	2:I:331:ARG:HA	1.64	0.61
2:I:124:ASP:O	2:I:407:LYS:NZ	2.31	0.61
2:C:164:PRO:HB3	2:C:269:LEU:HG	1.82	0.61
2:C:437:ARG:NH1	2:C:467:ILE:O	2.33	0.61
7:R:11:DG:N2	8:S:38:DC:O2	2.32	0.61
1:A:14:THR:HG1	1:B:231:SER:HG	1.46	0.61
3:D:8:VAL:HG21	3:D:1468:LEU:HD21	1.82	0.61
3:J:30:GLU:HB2	5:L:274:ARG:HB2	1.80	0.61
2:C:1060:ILE:HG13	2:C:1061:GLU:H	1.65	0.61
3:J:1436:SER:HB2	3:J:1464:GLU:HG2	1.82	0.61
3:J:700:VAL:HG22	3:J:718:PRO:HG3	1.82	0.61
3:D:770:LEU:HB2	3:D:1210:SER:HA	1.81	0.61
3:J:1106:VAL:HB	3:J:1108:ARG:HH22	1.66	0.61
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1100:GLN:HB2	3:J:9:ARG:HB3	1.82	0.61
2:C:966:LEU:HD11	2:C:986:PRO:HG3	1.82	0.61
3:D:417:PRO:HA	3:D:430:GLU:HA	1.82	0.61
3:D:661:MET:HG2	3:D:666:PHE:CZ	2.35	0.61
6:N:21:ALA:O	6:N:37:GLN:HB3	2.00	0.61
3:D:700:VAL:HG22	3:D:718:PRO:HG3	1.82	0.61
1:G:175:ARG:HB3	1:G:200:TRP:HB3	1.83	0.61
2:I:15:LEU:HD21	2:I:457:ALA:HB1	1.83	0.61
2:C:197:LEU:HD23	2:C:200:LEU:HD23	1.81	0.61
3:J:770:LEU:HB2	3:J:1210:SER:HA	1.83	0.61
3:J:1384:PRO:HA	3:J:1415:VAL:HG13	1.83	0.61
3:J:1459:LEU:HD21	3:J:1468:LEU:HG	1.83	0.61
2:I:383:ARG:HH21	2:I:388:ARG:NH2	1.99	0.61
2:C:15:LEU:HD21	2:C:457:ALA:HB1	1.83	0.60
2:C:383:ARG:HH21	2:C:388:ARG:NH2	1.99	0.60
3:D:125:GLN:NE2	3:D:130:ASN:OD1	2.33	0.60
2:I:1060:ILE:HG13	2:I:1061:GLU:H	1.65	0.60
3:J:191:LEU:HB2	3:J:195:VAL:HG11	1.81	0.60
3:J:1465:ASN:O	3:J:1468:LEU:N	2.34	0.60
3:D:101:HIS:NE2	3:D:582:ILE:HG21	2.17	0.60
2:I:139:GLN:HB3	2:I:334:ARG:HB2	1.83	0.60
3:J:1149:LEU:HB3	3:J:1162:GLU:HA	1.83	0.60
1:A:175:ARG:HB3	1:A:200:TRP:HB3	1.84	0.60
3:D:462:GLN:HA	3:D:513:ILE:HG13	1.82	0.60
3:D:699:VAL:HG13	3:D:760:ARG:HD3	1.83	0.60
3:J:100:ALA:HA	3:J:513:ILE:HA	1.83	0.60
3:J:637:LEU:O	3:J:935:LYS:NZ	2.34	0.60
4:K:37:ASN:N	4:K:37:ASN:OD1	2.34	0.60
2:C:994:ILE:HG22	2:C:995:MET:H	1.65	0.60
3:D:1106:VAL:HB	3:D:1108:ARG:HH22	1.66	0.60
3:D:1149:LEU:HB3	3:D:1162:GLU:HA	1.83	0.60
3:D:260:GLU:HB3	3:D:271:TYR:HB2	1.84	0.60
4:E:37:ASN:N	4:E:37:ASN:OD1	2.34	0.60
1:A:40:LEU:O	1:A:44:LEU:HB2	2.02	0.60
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.82	0.60
2:I:276:LYS:HD3	2:I:466:PHE:HZ	1.67	0.60
3:D:162:ARG:HG2	3:D:414:ARG:HH22	1.67	0.60
3:D:960:LYS:O	3:D:964:LEU:HB3	2.02	0.60
2:I:714:ASP:HA	2:I:719:PRO:HA	1.84	0.60
3:D:100:ALA:HA	3:D:513:ILE:HA	1.84	0.60
2:I:549:PHE:HZ	2:I:890:LEU:HD12	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:729:HIS:HE1	3:J:731:LEU:HD23	1.66	0.60
3:D:1465:ASN:O	3:D:1468:LEU:N	2.34	0.60
3:D:213:VAL:HG22	3:D:385:VAL:HG12	1.82	0.60
3:J:433:GLY:HA2	3:J:449:SER:H	1.67	0.60
3:J:644:LEU:HD12	3:J:645:PRO:HD2	1.83	0.60
7:O:32:DG:H2'	7:O:33:DG:C8	2.37	0.60
1:A:32:PHE:O	1:A:35:THR:OG1	2.16	0.59
2:C:139:GLN:HB3	2:C:334:ARG:HB2	1.82	0.59
4:K:67:GLU:HB3	4:K:73:LEU:HD11	1.84	0.59
6:M:18:GLY:HA2	6:M:41:PRO:HD3	1.84	0.59
2:C:532:MET:HG2	2:C:533:ASP:H	1.68	0.59
2:C:675:ALA:HA	2:C:989:VAL:HG12	1.83	0.59
3:D:1384:PRO:HA	3:D:1415:VAL:HG13	1.84	0.59
1:H:18:ASP:O	1:H:201:THR:OG1	2.11	0.59
1:G:215:VAL:HG13	1:H:222:LEU:HD23	1.84	0.59
2:I:994:ILE:HG22	2:I:995:MET:H	1.66	0.59
3:J:699:VAL:HG13	3:J:760:ARG:HD3	1.83	0.59
4:E:38:THR:HG21	4:E:63:TRP:HZ3	1.67	0.59
1:G:14:THR:OG1	1:H:231:SER:OG	2.20	0.59
2:I:197:LEU:HD23	2:I:200:LEU:HD23	1.83	0.59
3:J:729:HIS:CE1	3:J:731:LEU:HD23	2.37	0.59
3:J:960:LYS:O	3:J:964:LEU:HB3	2.01	0.59
5:L:210:VAL:HA	5:L:213:ILE:HD12	1.85	0.59
2:C:15:LEU:HD13	2:C:16:PRO:HD2	1.84	0.59
2:C:182:VAL:HG21	2:C:193:LEU:HD12	1.85	0.59
2:C:238:LEU:HD23	2:C:241:LEU:HD12	1.84	0.59
2:C:575:GLN:HB3	2:C:670:GLN:HG3	1.84	0.59
3:D:729:HIS:HE1	3:D:731:LEU:HD23	1.66	0.59
2:C:1100:GLN:HB2	3:D:9:ARG:HB3	1.82	0.59
2:I:163:ILE:HD13	2:I:171:TRP:CD1	2.37	0.59
2:I:193:LEU:HD21	2:I:307:LEU:HD11	1.84	0.59
3:J:421:LEU:H	3:J:428:LYS:HA	1.67	0.59
3:J:1197:ARG:HE	3:J:1398:TRP:HB3	1.66	0.59
3:J:127:LEU:HG	3:J:461:ILE:HG13	1.85	0.59
6:N:106:ALA:HA	6:N:136:LEU:HD11	1.85	0.59
1:A:215:VAL:HG13	1:B:222:LEU:HD23	1.84	0.59
2:C:1019:GLN:HG3	3:D:617:ASN:HD22	1.67	0.59
2:C:1056:LYS:HE2	3:D:751:LEU:HG	1.84	0.59
2:C:886:LEU:HD21	3:D:951:ILE:HD13	1.84	0.59
1:G:40:LEU:O	1:G:44:LEU:HB2	2.02	0.59
2:I:238:LEU:HD23	2:I:241:LEU:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:575:GLN:HB3	2:I:670:GLN:HG3	1.83	0.59
3:J:101:HIS:NE2	3:J:582:ILE:HG21	2.17	0.59
2:C:714:ASP:HA	2:C:719:PRO:HA	1.85	0.59
2:I:754:ILE:HG12	2:I:791:ARG:HD3	1.85	0.59
2:I:886:LEU:HD21	3:J:951:ILE:HD13	1.85	0.59
6:N:88:ALA:HA	6:N:91:ARG:HD2	1.84	0.59
2:C:261:LEU:HB3	2:C:290:LEU:HD12	1.85	0.59
3:D:181:ASP:HB3	3:D:357:GLU:HG2	1.85	0.59
3:J:186:VAL:HG12	3:J:187:LYS:H	1.67	0.59
2:I:1034:GLU:HG2	3:J:619:LEU:HB3	1.85	0.59
2:I:1056:LYS:HE2	3:J:751:LEU:HG	1.84	0.58
2:I:118:LEU:HD12	2:I:119:PRO:HD2	1.84	0.58
3:J:355:VAL:HG12	3:J:356:PRO:HD2	1.85	0.58
4:K:38:THR:HG21	4:K:63:TRP:HZ3	1.68	0.58
2:C:14:PRO:HB3	2:C:586:ARG:NH2	2.18	0.58
3:D:1201:CYS:SG	3:D:1204:CYS:CB	2.91	0.58
3:D:977:ALA:HB2	3:J:831:GLY:HA3	1.85	0.58
1:B:18:ASP:O	1:B:201:THR:OG1	2.11	0.58
2:C:163:ILE:HD13	2:C:171:TRP:CD1	2.37	0.58
3:D:729:HIS:CE1	3:D:731:LEU:HD23	2.37	0.58
2:I:164:PRO:HB3	2:I:269:LEU:HG	1.83	0.58
7:O:10:DA:H2	8:P:39:DT:H3	1.51	0.58
2:I:532:MET:HG2	2:I:533:ASP:H	1.68	0.58
3:D:1197:ARG:HE	3:D:1398:TRP:HB3	1.66	0.58
3:J:1336:LEU:HD22	3:J:1421:LEU:HB3	1.86	0.58
5:L:364:LEU:HD22	5:L:436:PHE:HZ	1.68	0.58
1:A:53:VAL:HA	1:A:144:VAL:HG13	1.85	0.58
3:D:1045:MET:HE2	3:D:1057:VAL:HG11	1.86	0.58
3:D:245:LEU:HD11	3:D:249:TYR:HB3	1.85	0.58
2:I:1082:PRO:HG3	3:J:1469:GLY:HA3	1.86	0.58
2:I:15:LEU:HD13	2:I:16:PRO:HD2	1.84	0.58
2:I:182:VAL:HG21	2:I:193:LEU:HD12	1.86	0.58
2:I:261:LEU:HB3	2:I:290:LEU:HD12	1.85	0.58
4:K:91:ARG:HH21	4:K:92:LEU:HG	1.68	0.58
6:M:151:ALA:HA	6:M:154:LEU:HD12	1.86	0.58
7:O:32:DG:H2''	7:O:33:DG:H5'	1.86	0.58
2:C:239:PHE:HA	2:C:242:LEU:HD12	1.85	0.58
3:D:127:LEU:HG	3:D:461:ILE:HG13	1.85	0.58
4:E:67:GLU:HB3	4:E:73:LEU:HD11	1.84	0.58
3:J:1201:CYS:SG	3:J:1204:CYS:CB	2.91	0.58
6:M:20:VAL:HA	6:M:38:VAL:CA	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:549:PHE:HZ	2:C:890:LEU:HD12	1.68	0.58
5:F:210:VAL:HA	5:F:213:ILE:HD12	1.85	0.58
2:C:773:LEU:HD13	5:F:388:LYS:HG3	1.86	0.58
5:L:417:ASN:HD22	5:L:421:ARG:HH12	1.52	0.58
2:C:432:ARG:HH12	2:C:518:ARG:HH21	1.52	0.58
3:D:1336:LEU:HD22	3:D:1421:LEU:HB3	1.86	0.58
2:I:14:PRO:HB3	2:I:586:ARG:NH2	2.17	0.58
3:J:371:ILE:HD12	5:L:247:ARG:HE	1.68	0.58
6:M:116:GLU:HB2	6:M:121:LEU:HD22	1.84	0.58
7:O:2:DT:H3	8:P:47:DA:H2	1.52	0.58
2:C:1047:HIS:O	2:C:1051:GLU:HG2	2.04	0.58
2:C:754:ILE:HG12	2:C:791:ARG:HD3	1.86	0.58
2:I:949:LYS:HD2	3:J:796:ARG:HH11	1.69	0.58
5:F:252:THR:HA	7:O:29:DC:H5	1.69	0.58
2:C:1057:SER:HB3	3:D:623:VAL:HG13	1.86	0.57
2:I:239:PHE:HA	2:I:242:LEU:HD12	1.85	0.57
3:J:1045:MET:HE2	3:J:1057:VAL:HG11	1.86	0.57
2:I:1017:THR:HG21	3:J:617:ASN:ND2	2.18	0.57
5:L:151:LEU:HD23	5:L:156:ILE:HD12	1.86	0.57
1:A:36:LEU:HB2	1:A:195:LEU:HD12	1.86	0.57
2:C:86:LYS:HE2	2:C:814:GLU:H	1.68	0.57
3:D:672:ALA:O	3:D:676:MET:HB2	2.04	0.57
3:D:520:LEU:HB3	3:D:525:ARG:HD3	1.86	0.57
3:D:527:MET:HG3	3:D:537:THR:HB	1.86	0.57
3:D:60:CYS:SG	3:D:76:CYS:HB3	2.44	0.57
5:F:100:LEU:HD13	7:O:31:DG:H21	1.69	0.57
3:D:44:LEU:HB3	3:D:525:ARG:HH22	1.70	0.57
1:G:53:VAL:HA	1:G:144:VAL:HG13	1.87	0.57
1:A:224:TYR:CE1	1:B:9:PRO:HG2	2.39	0.57
3:D:1462:LEU:HD12	3:D:1463:LYS:H	1.69	0.57
3:J:527:MET:HG3	3:J:537:THR:HB	1.87	0.57
3:J:661:MET:HG2	3:J:666:PHE:CZ	2.39	0.57
1:B:72:LYS:HG3	1:B:131:THR:HB	1.86	0.57
3:D:236:TYR:HB2	3:D:319:ALA:HB3	1.85	0.57
4:E:91:ARG:HH21	4:E:92:LEU:HG	1.69	0.57
3:J:60:CYS:SG	3:J:76:CYS:HB3	2.45	0.57
2:I:1057:SER:HB3	3:J:623:VAL:HG13	1.87	0.57
3:J:1097:LYS:HE2	3:J:1440:PHE:HZ	1.69	0.57
2:C:167:LYS:HD3	7:O:35:DG:H5'	1.86	0.57
2:C:690:ILE:HD11	2:C:849:VAL:HG22	1.87	0.57
1:H:72:LYS:HG3	1:H:131:THR:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:773:LEU:HD13	5:L:388:LYS:HG3	1.85	0.57
2:C:163:ILE:HD13	2:C:171:TRP:HD1	1.69	0.57
3:D:229:ALA:HB1	3:D:243:ALA:HB1	1.86	0.57
3:D:703:ASN:HB2	3:D:713:ILE:HG12	1.87	0.57
2:C:949:LYS:HD2	3:D:796:ARG:HH11	1.69	0.57
2:I:285:LEU:HD23	2:I:286:SER:H	1.70	0.57
2:I:660:ALA:HB1	2:I:667:ALA:O	2.05	0.57
3:J:1462:LEU:HD12	3:J:1463:LYS:H	1.69	0.57
3:J:141:VAL:HG12	3:J:450:TYR:HE2	1.69	0.57
2:C:193:LEU:HD21	2:C:307:LEU:HD11	1.86	0.57
1:G:178:ALA:HB2	2:I:864:GLY:HA3	1.87	0.57
3:J:1045:MET:HB2	3:J:1072:ILE:HG22	1.86	0.57
2:C:93:PRO:HB3	2:C:114:PHE:HE1	1.69	0.56
2:C:439:CYS:HB2	2:C:541:SER:HB3	1.87	0.56
5:F:252:THR:HA	7:O:29:DC:C5	2.40	0.56
2:I:432:ARG:HH12	2:I:518:ARG:HH21	1.53	0.56
3:J:672:ALA:O	3:J:676:MET:HB2	2.04	0.56
3:J:703:ASN:HB2	3:J:713:ILE:HG12	1.87	0.56
3:J:828:VAL:HA	3:J:833:GLU:HA	1.87	0.56
1:A:153:ALA:HB1	1:A:166:PRO:HB2	1.86	0.56
2:C:194:VAL:HA	2:C:197:LEU:HD12	1.88	0.56
1:G:36:LEU:HB2	1:G:195:LEU:HD12	1.86	0.56
1:G:224:TYR:CE1	1:H:9:PRO:HG2	2.40	0.56
2:I:194:VAL:HA	2:I:197:LEU:HD12	1.87	0.56
2:I:93:PRO:HB3	2:I:114:PHE:HE1	1.70	0.56
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.87	0.56
3:D:1045:MET:HB2	3:D:1072:ILE:HG22	1.86	0.56
4:E:38:THR:HG21	4:E:63:TRP:CZ3	2.40	0.56
5:F:151:LEU:HD23	5:F:156:ILE:HD12	1.87	0.56
3:J:1042:ARG:HE	3:J:1061:PHE:HE2	1.53	0.56
3:J:1377:LYS:O	3:J:1397:LYS:N	2.38	0.56
3:J:613:ARG:HD3	3:J:617:ASN:OD1	2.05	0.56
3:J:628:ARG:HH12	8:S:14:DG:H2"	1.69	0.56
3:J:886:VAL:HG11	3:J:900:ILE:HD11	1.86	0.56
1:A:67:THR:HG21	2:C:627:ARG:HG3	1.87	0.56
2:C:71:TYR:HA	2:C:95:TYR:C	2.26	0.56
3:D:886:VAL:HG11	3:D:900:ILE:HD11	1.86	0.56
2:C:376:ARG:HH22	5:F:294:GLN:HG3	1.70	0.56
2:I:163:ILE:HD13	2:I:171:TRP:HD1	1.69	0.56
2:I:26:TYR:HB2	2:I:336:VAL:HB	1.87	0.56
2:I:69:LEU:HB2	2:I:97:ARG:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:349:PRO:HB3	5:L:112:GLU:HG2	1.85	0.56
3:J:901:GLN:HG2	3:J:906:GLN:HE22	1.70	0.56
1:A:62:LEU:HD13	2:C:745:ILE:HG21	1.88	0.56
2:I:853:LEU:HD12	2:I:854:PRO:HD2	1.86	0.56
3:J:86:ARG:O	3:J:521:PRO:HB3	2.06	0.56
5:L:252:THR:HA	7:R:29:DC:C5	2.41	0.56
7:R:47:DG:N2	8:S:2:DC:N3	2.54	0.56
2:C:437:ARG:HB3	2:C:467:ILE:HG21	1.88	0.56
2:I:606:VAL:HG23	2:I:645:VAL:HA	1.87	0.56
2:I:690:ILE:HD11	2:I:849:VAL:HG22	1.87	0.56
3:J:1068:LEU:HD12	3:J:1068:LEU:H	1.70	0.56
3:J:916:TYR:HE2	3:J:1168:LEU:HD22	1.71	0.56
3:D:1042:ARG:HE	3:D:1061:PHE:HE2	1.54	0.56
2:C:1066:ALA:HA	2:C:1076:VAL:HG12	1.87	0.56
2:C:473:ARG:O	2:C:480:THR:OG1	2.17	0.56
2:C:606:VAL:HG23	2:C:645:VAL:HA	1.87	0.56
3:D:439:LEU:HD22	3:D:439:LEU:H	1.70	0.56
2:I:458:TYR:HD1	2:I:538:GLN:HB3	1.70	0.56
1:G:67:THR:HG21	2:I:627:ARG:HG3	1.87	0.56
3:J:208:PRO:HA	3:J:390:PRO:HA	1.88	0.56
2:C:146:VAL:HG21	2:C:281:LEU:HD11	1.88	0.56
2:C:374:ASN:ND2	2:C:375:SER:H	2.04	0.56
3:D:613:ARG:HD3	3:D:617:ASN:OD1	2.06	0.56
5:F:417:ASN:HD22	5:F:421:ARG:HH12	1.53	0.56
1:G:153:ALA:HB1	1:G:166:PRO:HB2	1.87	0.56
1:G:32:PHE:O	1:G:35:THR:OG1	2.18	0.56
2:I:1047:HIS:O	2:I:1051:GLU:HG2	2.05	0.56
2:I:473:ARG:O	2:I:480:THR:OG1	2.19	0.56
3:J:470:LEU:HD22	3:J:499:VAL:HG13	1.88	0.56
3:J:572:ARG:HH12	5:L:98:GLN:HE21	1.54	0.56
5:L:252:THR:HG23	7:R:29:DC:H41	1.71	0.56
2:C:571:LEU:HB2	2:C:574:ALA:HB2	1.88	0.56
2:C:660:ALA:HB1	2:C:667:ALA:O	2.05	0.56
1:A:178:ALA:HB2	2:C:864:GLY:HA3	1.86	0.56
3:D:317:MET:HB3	3:D:337:LEU:HD21	1.86	0.56
3:D:800:LYS:HB3	3:D:822:ALA:HB2	1.88	0.56
2:I:146:VAL:HG21	2:I:281:LEU:HD11	1.88	0.56
3:J:44:LEU:HB3	3:J:525:ARG:HH22	1.71	0.56
2:C:546:LEU:HB2	2:C:565:GLN:HE22	1.71	0.56
3:D:638:LYS:HG2	3:D:639:LEU:H	1.70	0.56
2:I:71:TYR:HA	2:I:95:TYR:C	2.27	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:99:TYR:HA	5:L:102:GLU:HB2	1.88	0.56
2:C:245:GLY:HA2	5:F:97:ARG:HD2	1.88	0.55
2:C:328:LEU:HD21	2:C:438:ILE:HD11	1.88	0.55
2:C:605:LYS:HG2	2:C:612:ALA:HB3	1.88	0.55
2:C:853:LEU:HD12	2:C:854:PRO:HD2	1.87	0.55
3:D:203:ALA:HB2	3:D:395:VAL:HB	1.87	0.55
3:D:470:LEU:HD22	3:D:499:VAL:HG13	1.88	0.55
3:D:828:VAL:HA	3:D:833:GLU:HA	1.88	0.55
3:D:901:GLN:HG2	3:D:906:GLN:HE22	1.70	0.55
2:I:1066:ALA:HA	2:I:1076:VAL:HG12	1.88	0.55
3:J:758:GLU:HG2	3:J:1476:THR:HG21	1.87	0.55
3:J:171:LEU:HD12	3:J:393:ILE:HD11	1.88	0.55
2:C:428:ARG:HH11	2:C:451:LEU:HD21	1.71	0.55
2:C:69:LEU:HB2	2:C:97:ARG:O	2.06	0.55
3:D:234:GLU:HA	3:D:322:VAL:HB	1.88	0.55
3:D:453:ASP:OD2	3:D:455:ARG:NE	2.37	0.55
2:I:23:VAL:HA	2:I:121:MET:SD	2.47	0.55
3:J:407:VAL:HA	3:J:422:ALA:HB1	1.87	0.55
3:J:800:LYS:HB3	3:J:822:ALA:HB2	1.87	0.55
6:N:151:ALA:HA	6:N:154:LEU:HD12	1.88	0.55
2:C:124:ASP:O	2:C:407:LYS:NZ	2.38	0.55
3:D:1458:GLU:HB2	3:D:1460:ILE:HG23	1.89	0.55
3:J:1272:ALA:HB3	3:J:1330:ILE:HD13	1.88	0.55
2:C:26:TYR:HB2	2:C:336:VAL:HB	1.88	0.55
3:D:1444:THR:O	3:D:1448:THR:OG1	2.24	0.55
3:D:758:GLU:HG2	3:D:1476:THR:HG21	1.88	0.55
2:I:328:LEU:HD12	2:I:328:LEU:H	1.72	0.55
3:J:1404:ASN:O	3:J:1408:ILE:HG12	2.06	0.55
3:J:371:ILE:HG23	3:J:372:ASP:H	1.72	0.55
3:J:520:LEU:HB3	3:J:525:ARG:HD3	1.87	0.55
4:K:38:THR:HG21	4:K:63:TRP:CZ3	2.41	0.55
2:C:278:GLU:HG3	2:C:284:GLY:HA2	1.89	0.55
2:C:458:TYR:HD1	2:C:538:GLN:HB3	1.69	0.55
3:D:421:LEU:H	3:D:421:LEU:HD12	1.71	0.55
5:F:99:TYR:HA	5:F:102:GLU:HB2	1.88	0.55
2:I:344:PHE:HA	2:I:382:LEU:HD21	1.89	0.55
3:J:140:ALA:HB1	3:J:161:LEU:HD21	1.88	0.55
2:C:172:ILE:HA	2:C:186:VAL:HG22	1.89	0.55
2:C:71:TYR:HD1	2:C:94:LEU:HD11	1.71	0.55
5:F:235:LEU:HD12	5:F:254:ALA:HB1	1.89	0.55
2:I:428:ARG:HH11	2:I:451:LEU:HD21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:897:LEU:HB3	2:I:899:GLN:HE21	1.72	0.55
3:J:633:VAL:HG13	3:J:635:PRO:HD3	1.87	0.55
3:J:699:VAL:HA	3:J:718:PRO:HD3	1.89	0.55
2:I:439:CYS:HB2	2:I:541:SER:HB3	1.88	0.55
3:J:1444:THR:O	3:J:1448:THR:OG1	2.25	0.55
3:J:176:ASP:OD1	3:J:177:ALA:N	2.40	0.55
5:L:235:LEU:HD12	5:L:254:ALA:HB1	1.88	0.55
7:R:46:DT:H2"	7:R:47:DG:C8	2.41	0.55
2:C:897:LEU:HB3	2:C:899:GLN:HE21	1.71	0.55
2:I:259:GLY:HA2	2:I:263:ASP:HB2	1.89	0.55
2:I:605:LYS:HG2	2:I:612:ALA:HB3	1.89	0.55
3:J:1011:PHE:HD1	3:J:1021:TYR:HB2	1.71	0.55
3:J:130:ASN:HD22	5:L:98:GLN:NE2	2.04	0.55
2:C:328:LEU:H	2:C:328:LEU:HD12	1.72	0.55
2:C:344:PHE:HA	2:C:382:LEU:HD21	1.89	0.55
3:D:1404:ASN:O	3:D:1408:ILE:HG12	2.07	0.55
3:D:792:ILE:HG12	3:D:941:LEU:HD13	1.88	0.55
3:J:1273:VAL:HG23	3:J:1325:LEU:HB2	1.89	0.55
3:D:1377:LYS:O	3:D:1397:LYS:N	2.37	0.55
3:D:258:VAL:HG22	3:D:273:ARG:HG2	1.88	0.55
3:D:976:GLN:HG2	3:J:807:ALA:HB1	1.87	0.55
2:I:546:LEU:HB2	2:I:565:GLN:HE22	1.72	0.55
2:I:571:LEU:HB2	2:I:574:ALA:HB2	1.89	0.55
2:C:1067:TYR:CZ	5:F:357:VAL:HG12	2.41	0.54
2:C:988:VAL:H	3:D:948:THR:HG21	1.73	0.54
3:D:1042:ARG:HD3	3:D:1045:MET:HE3	1.89	0.54
3:D:1068:LEU:HD12	3:D:1068:LEU:H	1.71	0.54
2:I:328:LEU:HD21	2:I:438:ILE:HD11	1.88	0.54
2:I:584:GLU:HA	2:I:587:VAL:HB	1.89	0.54
3:J:792:ILE:HG12	3:J:941:LEU:HD13	1.89	0.54
2:C:50:GLU:HG2	2:C:265:LYS:HZ2	1.73	0.54
2:C:607:ASP:OD2	2:C:610:ARG:NH1	2.40	0.54
3:D:1011:PHE:HD1	3:D:1021:TYR:HB2	1.72	0.54
3:D:680:GLN:C	3:D:682:ASP:H	2.10	0.54
5:F:302:SER:O	5:F:306:ILE:HG22	2.08	0.54
1:G:221:HIS:HA	1:G:224:TYR:CD1	2.42	0.54
3:J:453:ASP:OD2	3:J:455:ARG:NE	2.38	0.54
2:C:584:GLU:HA	2:C:587:VAL:HB	1.89	0.54
3:D:1290:LEU:HD12	3:D:1307:LYS:HG2	1.90	0.54
3:D:535:PHE:O	5:F:329:PRO:HA	2.06	0.54
3:D:634:GLY:O	3:D:637:LEU:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:78:ILE:HA	1:H:81:ASN:HD22	1.72	0.54
2:I:195:LEU:HD12	2:I:198:ARG:HH11	1.71	0.54
3:J:418:GLY:H	3:J:430:GLU:HA	1.72	0.54
7:R:14:DT:H1'	7:R:15:DT:H5''	1.89	0.54
1:A:184:THR:HB	1:A:194:LYS:HB3	1.90	0.54
3:D:1209:LEU:O	3:D:1212:ALA:N	2.36	0.54
3:D:1272:ALA:HB3	3:D:1330:ILE:HD13	1.88	0.54
1:G:44:LEU:O	1:G:174:VAL:HG11	2.06	0.54
3:J:573:MET:SD	5:L:229:GLN:HG3	2.47	0.54
3:J:8:VAL:HG23	3:J:1459:LEU:HD11	1.89	0.54
5:L:204:GLU:O	5:L:207:LEU:HB3	2.07	0.54
3:D:1256:LEU:O	3:D:1260:ILE:HG13	2.08	0.54
3:D:8:VAL:HG23	3:D:1459:LEU:HD11	1.89	0.54
3:D:1472:ILE:HD12	3:D:1473:PRO:HD2	1.90	0.54
3:D:29:PRO:HB3	3:D:548:ILE:HB	1.90	0.54
3:D:573:MET:SD	5:F:229:GLN:HG3	2.47	0.54
2:I:278:GLU:HG3	2:I:284:GLY:HA2	1.89	0.54
2:I:437:ARG:HB3	2:I:467:ILE:HG21	1.89	0.54
7:O:43:DG:H1	8:P:6:DC:H42	1.55	0.54
3:J:1093:TYR:HD1	8:S:10:DA:H5''	1.71	0.54
3:D:916:TYR:HE2	3:D:1168:LEU:HD22	1.72	0.54
2:I:172:ILE:HA	2:I:186:VAL:HG22	1.88	0.54
2:I:71:TYR:HD1	2:I:94:LEU:HD11	1.71	0.54
3:J:147:VAL:HG21	3:J:153:LEU:HD21	1.89	0.54
2:C:969:LEU:HG	3:D:952:ASP:HB2	1.90	0.54
3:D:1048:PRO:HD3	3:D:1075:HIS:HB3	1.90	0.54
3:D:140:ALA:HB1	3:D:161:LEU:HD21	1.89	0.54
3:D:414:ARG:HG3	3:D:451:ASP:HB2	1.89	0.54
3:D:572:ARG:HH12	5:F:98:GLN:HE21	1.54	0.54
3:D:699:VAL:HA	3:D:718:PRO:HD3	1.89	0.54
1:G:38:ASN:HB2	2:I:980:GLY:HA3	1.90	0.54
3:J:1202:GLN:NE2	3:J:1215:VAL:O	2.32	0.54
3:J:704:ARG:NE	3:J:705:ALA:O	2.41	0.54
5:L:100:LEU:HD13	7:R:31:DG:H21	1.73	0.54
1:B:58:ILE:HB	1:B:61:VAL:HB	1.90	0.54
2:C:276:LYS:HD3	2:C:466:PHE:HZ	1.73	0.54
2:C:283:VAL:HG11	2:C:305:PRO:HG3	1.90	0.54
1:A:38:ASN:HB2	2:C:980:GLY:HA3	1.90	0.54
1:G:184:THR:HB	1:G:194:LYS:HB3	1.90	0.54
2:I:1035:MET:HG3	3:J:707:THR:HB	1.89	0.54
3:J:101:HIS:HB3	3:J:104:PHE:CE2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1290:LEU:HD12	3:J:1307:LYS:HG2	1.89	0.54
3:J:881:LEU:O	3:J:885:ILE:HG13	2.08	0.54
1:A:44:LEU:O	1:A:174:VAL:HG11	2.07	0.54
1:B:151:VAL:HG13	1:B:155:ARG:HB2	1.89	0.54
3:D:1273:VAL:HG23	3:D:1325:LEU:HB2	1.89	0.54
5:F:204:GLU:O	5:F:207:LEU:HB3	2.06	0.54
1:H:58:ILE:HB	1:H:61:VAL:HB	1.90	0.54
2:I:936:VAL:HB	2:I:941:LYS:HE2	1.90	0.54
3:J:8:VAL:HG21	3:J:1468:LEU:HD21	1.89	0.54
2:C:195:LEU:HD12	2:C:198:ARG:HH11	1.73	0.54
3:D:633:VAL:HG13	3:D:635:PRO:HD3	1.88	0.54
1:G:35:THR:HG22	1:H:39:PRO:HA	1.89	0.54
2:I:47:ALA:HA	2:I:345:ARG:HG2	1.90	0.54
3:J:1042:ARG:HD3	3:J:1045:MET:HE3	1.90	0.54
2:I:111:ASP:HA	6:N:45:SER:HB2	1.89	0.54
3:J:610:LYS:NZ	8:S:10:DA:OP2	2.37	0.54
2:C:285:LEU:HD23	2:C:286:SER:H	1.71	0.53
3:D:1147:ARG:HH12	3:D:1190:SER:HA	1.73	0.53
3:D:225:ILE:O	3:D:331:VAL:HG12	2.08	0.53
1:H:151:VAL:HG13	1:H:155:ARG:HB2	1.90	0.53
3:D:977:ALA:HB2	3:J:831:GLY:N	2.24	0.53
4:K:27:ALA:HB1	4:K:60:ALA:HB1	1.90	0.53
3:D:628:ARG:HH22	8:P:14:DG:H2"	1.73	0.53
2:C:1023:GLY:HA2	8:P:15:DA:OP2	2.08	0.53
2:C:829:GLN:HE21	2:C:831:ARG:HH21	1.57	0.53
3:D:1202:GLN:NE2	3:D:1215:VAL:O	2.32	0.53
3:D:147:VAL:HG21	3:D:153:LEU:HD21	1.90	0.53
3:D:192:ALA:HB1	3:D:193:PRO:HD2	1.89	0.53
3:D:245:LEU:HB2	3:D:311:LEU:HD21	1.90	0.53
3:D:810:GLU:HA	3:D:813:LEU:HD12	1.89	0.53
4:E:27:ALA:HB1	4:E:60:ALA:HB1	1.89	0.53
6:N:119:ARG:HG3	6:N:120:GLY:H	1.72	0.53
5:F:217:TYR:O	8:P:23:DA:N6	2.41	0.53
1:A:79:ILE:HA	1:A:82:LEU:HD12	1.90	0.53
3:D:407:VAL:HG22	3:D:409:VAL:H	1.73	0.53
2:I:142:ARG:HG3	2:I:331:ARG:HG2	1.89	0.53
3:J:1256:LEU:O	3:J:1260:ILE:HG13	2.08	0.53
3:J:1274:ILE:HD11	3:J:1334:GLN:HG2	1.90	0.53
3:J:211:VAL:HG12	3:J:345:TYR:HB2	1.89	0.53
2:C:1017:THR:HG21	3:D:617:ASN:ND2	2.24	0.53
2:C:1035:MET:HG3	3:D:707:THR:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:110:THR:HG23	5:F:113:GLU:H	1.74	0.53
2:I:124:ASP:HA	2:I:592:LEU:HD12	1.90	0.53
2:I:988:VAL:HG22	3:J:948:THR:OG1	2.09	0.53
5:L:302:SER:O	5:L:306:ILE:HG22	2.07	0.53
2:C:1037:VAL:O	2:C:1041:GLU:HG3	2.07	0.53
2:C:259:GLY:HA2	2:C:263:ASP:HB2	1.90	0.53
3:D:223:LEU:HB2	3:D:251:PHE:HZ	1.74	0.53
2:I:742:ILE:HD12	2:I:803:ARG:HD2	1.91	0.53
3:J:357:GLU:HG2	3:J:387:LEU:HB2	1.91	0.53
2:C:47:ALA:HA	2:C:345:ARG:HG2	1.90	0.53
2:C:668:LEU:HB2	2:C:993:PHE:HZ	1.73	0.53
3:D:231:VAL:HB	3:D:243:ALA:H	1.73	0.53
3:D:371:ILE:HG23	3:D:372:ASP:H	1.73	0.53
2:I:502:PRO:HG3	2:I:510:THR:HG22	1.89	0.53
2:I:552:HIS:HB3	2:I:882:LEU:HB2	1.91	0.53
2:I:668:LEU:HB2	2:I:993:PHE:HZ	1.74	0.53
2:I:969:LEU:HG	3:J:952:ASP:HB2	1.90	0.53
1:A:221:HIS:HA	1:A:224:TYR:CD1	2.43	0.53
1:B:78:ILE:HA	1:B:81:ASN:HD22	1.72	0.53
2:C:878:SER:HB3	3:D:1029:ARG:HG3	1.91	0.53
3:D:1269:LYS:HD3	3:D:1269:LYS:H	1.74	0.53
3:D:801:GLY:HA2	3:D:821:VAL:HA	1.90	0.53
5:F:210:VAL:HG11	5:F:232:ASN:HA	1.91	0.53
1:G:58:ILE:HG22	1:G:60:ASP:H	1.74	0.53
2:I:1037:VAL:O	2:I:1041:GLU:HG3	2.09	0.53
3:J:1209:LEU:O	3:J:1212:ALA:N	2.37	0.53
3:J:638:LYS:HG2	3:J:639:LEU:H	1.72	0.53
3:D:101:HIS:HB3	3:D:104:PHE:CE2	2.44	0.53
2:I:374:ASN:ND2	2:I:375:SER:H	2.07	0.53
2:I:577:PRO:HG2	2:I:580:MET:HB3	1.90	0.53
2:I:607:ASP:OD2	2:I:610:ARG:NH1	2.41	0.53
3:J:421:LEU:HD21	3:J:444:VAL:HG11	1.90	0.53
1:B:118:ALA:O	1:B:120:VAL:N	2.42	0.53
1:B:68:ILE:HG23	1:B:71:VAL:HB	1.91	0.53
2:C:388:ARG:NH2	8:P:20:DA:O5'	2.42	0.53
2:C:859:PRO:HA	2:C:975:TYR:O	2.09	0.53
2:C:552:HIS:HB3	2:C:882:LEU:HB2	1.90	0.53
2:C:936:VAL:HB	2:C:941:LYS:HE2	1.91	0.53
3:D:881:LEU:O	3:D:885:ILE:HG13	2.09	0.53
2:I:878:SER:HB3	3:J:1029:ARG:HG3	1.90	0.53
2:I:374:ASN:ND2	5:L:291:ARG:HE	2.00	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:17:DG:H2"	8:S:18:DG:O4'	2.08	0.53
2:C:142:ARG:HG3	2:C:331:ARG:HG2	1.90	0.53
2:C:502:PRO:HG3	2:C:510:THR:HG22	1.90	0.53
3:D:313:LEU:HG	3:D:314:PRO:HD2	1.91	0.53
2:C:684:PHE:HE1	3:D:783:ARG:HB2	1.74	0.53
2:I:352:ALA:HB1	2:I:356:ARG:NH1	2.23	0.53
2:I:971:LYS:HA	2:I:988:VAL:HA	1.91	0.53
3:J:49:ILE:HG13	3:J:50:PHE:H	1.72	0.53
3:J:99:ALA:HB2	3:J:574:LEU:HD21	1.91	0.53
3:J:577:ALA:O	3:J:581:VAL:HG23	2.09	0.53
3:J:810:GLU:HA	3:J:813:LEU:HD12	1.90	0.53
6:N:80:MET:HB3	6:N:107:GLN:HG2	1.90	0.53
2:C:23:VAL:HA	2:C:121:MET:SD	2.49	0.52
2:C:988:VAL:HG21	3:D:949:ILE:O	2.09	0.52
3:D:1145:TYR:O	3:D:1364:HIS:NE2	2.37	0.52
3:D:49:ILE:HG13	3:D:50:PHE:H	1.73	0.52
3:D:704:ARG:NE	3:D:705:ALA:O	2.42	0.52
2:C:988:VAL:HG22	3:D:948:THR:OG1	2.08	0.52
2:I:1013:TYR:O	5:L:350:ASP:N	2.42	0.52
2:I:204:GLN:HB2	2:I:227:LEU:HD21	1.92	0.52
2:I:577:PRO:HA	2:I:671:ASN:HD21	1.74	0.52
3:J:1145:TYR:O	3:J:1364:HIS:NE2	2.37	0.52
3:J:801:GLY:HA2	3:J:821:VAL:HA	1.90	0.52
6:N:20:VAL:CA	6:N:38:VAL:HA	2.35	0.52
8:S:22:DT:H2"	8:S:23:DA:C8	2.44	0.52
2:C:577:PRO:HG2	2:C:580:MET:HB3	1.90	0.52
3:D:1060:SER:OG	3:D:1061:PHE:N	2.42	0.52
3:D:99:ALA:HB2	3:D:574:LEU:HD21	1.92	0.52
2:I:87:ASP:HA	2:I:131:GLY:HA3	1.92	0.52
3:J:180:LYS:HA	3:J:205:TYR:CZ	2.45	0.52
5:L:398:LEU:HD21	5:L:413:ARG:HB2	1.91	0.52
8:P:8:DT:H1'	8:P:9:DG:H5"	1.89	0.52
2:C:742:ILE:HD12	2:C:803:ARG:HD2	1.91	0.52
1:H:118:ALA:O	1:H:120:VAL:N	2.43	0.52
3:J:29:PRO:HB3	3:J:548:ILE:HB	1.92	0.52
1:A:104:GLU:HG3	1:A:137:LYS:HG2	1.91	0.52
2:I:457:ALA:HB3	2:I:538:GLN:HA	1.92	0.52
2:I:644:ARG:HG2	2:I:647:GLN:HG2	1.92	0.52
2:I:988:VAL:H	3:J:948:THR:HG21	1.73	0.52
3:J:1060:SER:OG	3:J:1061:PHE:N	2.42	0.52
3:J:1273:VAL:HG21	3:J:1305:LEU:HD22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:699:VAL:HG22	3:J:760:ARG:HG2	1.92	0.52
2:C:374:ASN:HD22	2:C:375:SER:H	1.58	0.52
2:C:457:ALA:HB3	2:C:538:GLN:HA	1.92	0.52
2:C:694:LEU:O	2:C:698:ASP:N	2.42	0.52
2:C:971:LYS:HA	2:C:988:VAL:HA	1.91	0.52
3:D:10:ILE:HG23	3:D:1451:ALA:HA	1.92	0.52
3:D:577:ALA:O	3:D:581:VAL:HG23	2.09	0.52
5:L:210:VAL:HG11	5:L:232:ASN:HA	1.92	0.52
6:M:68:VAL:HG21	6:M:144:LEU:HD21	1.92	0.52
1:G:104:GLU:HG3	1:G:137:LYS:HG2	1.90	0.52
1:G:79:ILE:HA	1:G:82:LEU:HD12	1.92	0.52
1:H:68:ILE:HG23	1:H:71:VAL:HB	1.91	0.52
2:I:283:VAL:HG11	2:I:305:PRO:HG3	1.92	0.52
3:J:1269:LYS:H	3:J:1269:LYS:HD3	1.75	0.52
3:J:367:ILE:HD11	3:J:379:ALA:HB2	1.92	0.52
2:I:988:VAL:HG21	3:J:949:ILE:O	2.10	0.52
3:D:27:GLU:H	3:D:42:ASP:HB3	1.75	0.52
3:D:650:LEU:HD12	3:D:688:TRP:HZ3	1.74	0.52
5:F:398:LEU:HD21	5:F:413:ARG:HB2	1.90	0.52
2:C:352:ALA:HB1	2:C:356:ARG:NH1	2.24	0.52
5:F:285:LYS:O	5:F:288:ARG:HB3	2.10	0.52
5:F:385:LYS:HA	5:F:390:LEU:HD12	1.91	0.52
2:I:332:ARG:HB2	2:I:465:GLY:HA3	1.91	0.52
3:J:1048:PRO:HD3	3:J:1075:HIS:HB3	1.90	0.52
3:J:1436:SER:O	3:J:1439:SER:OG	2.23	0.52
3:D:977:ALA:HB2	3:J:831:GLY:CA	2.39	0.52
7:O:46:DT:H2"	7:O:47:DG:C8	2.44	0.52
5:L:411:ARG:HD3	7:R:1:DC:C6	2.45	0.52
3:D:1021:TYR:O	3:D:1025:GLN:HB2	2.10	0.52
1:G:16:GLN:HB3	1:G:20:TYR:O	2.10	0.52
1:G:42:ARG:NH1	2:I:978:ARG:HA	2.25	0.52
2:I:431:HIS:H	2:I:434:HIS:CE1	2.28	0.52
2:I:448:ASN:HA	2:I:451:LEU:HD23	1.92	0.52
2:I:694:LEU:O	2:I:698:ASP:N	2.43	0.52
2:C:292:ARG:H	2:C:292:ARG:NH1	2.04	0.52
2:C:448:ASN:HA	2:C:451:LEU:HD23	1.92	0.52
3:D:1426:LYS:HE3	7:O:43:DG:H5"	1.91	0.52
3:D:86:ARG:O	3:D:521:PRO:HB3	2.10	0.52
2:I:859:PRO:HA	2:I:975:TYR:O	2.09	0.52
2:I:974:LEU:HD13	2:I:987:ILE:HB	1.92	0.52
1:A:35:THR:HG22	1:B:39:PRO:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:204:GLN:HB2	2:C:227:LEU:HD21	1.92	0.51
2:C:966:LEU:HD21	2:C:986:PRO:HB3	1.92	0.51
3:D:699:VAL:HG22	3:D:760:ARG:HG2	1.92	0.51
3:J:96:ALA:HB2	3:J:555:LYS:HG2	1.92	0.51
8:S:34:DA:H1'	8:S:35:DA:H5'	1.92	0.51
1:B:161:ARG:HG2	1:B:162:ILE:H	1.76	0.51
2:C:27:LYS:HA	2:C:30:LEU:HD22	1.92	0.51
2:C:644:ARG:HG2	2:C:647:GLN:HG2	1.92	0.51
3:D:1273:VAL:HG21	3:D:1305:LEU:HD22	1.91	0.51
5:F:130:LYS:HD3	5:F:188:TYR:CZ	2.45	0.51
3:J:1147:ARG:HH12	3:J:1190:SER:HA	1.74	0.51
2:I:376:ARG:HD2	5:L:291:ARG:CZ	2.40	0.51
5:L:336:ILE:HB	8:S:17:DG:H21	1.75	0.51
3:D:96:ALA:HB2	3:D:555:LYS:HG2	1.93	0.51
4:E:26:ARG:HH22	4:E:37:ASN:HB2	1.76	0.51
1:G:9:PRO:HB2	1:G:25:LEU:HD21	1.91	0.51
3:J:27:GLU:H	3:J:42:ASP:HB3	1.75	0.51
3:J:650:LEU:HD12	3:J:688:TRP:HZ3	1.76	0.51
4:K:26:ARG:HH22	4:K:37:ASN:HB2	1.76	0.51
5:L:130:LYS:HD3	5:L:188:TYR:CZ	2.45	0.51
6:N:62:ALA:HB1	6:N:142:GLN:HE22	1.75	0.51
3:D:260:GLU:HA	3:D:294:GLU:HG3	1.92	0.51
2:I:65:VAL:HG13	2:I:101:ILE:HB	1.92	0.51
2:I:557:ARG:O	2:I:844:GLY:HA3	2.10	0.51
3:J:1458:GLU:HB2	3:J:1460:ILE:HG23	1.92	0.51
3:J:175:VAL:HG11	3:J:193:PRO:HG3	1.92	0.51
3:J:640:HIS:O	3:J:717:GLN:HB2	2.09	0.51
2:I:684:PHE:HE1	3:J:783:ARG:HB2	1.76	0.51
5:L:206:ASN:HB3	5:L:235:LEU:HD11	1.92	0.51
2:C:937:ASP:HB3	2:C:940:GLU:HG3	1.92	0.51
1:A:42:ARG:NH1	2:C:978:ARG:HA	2.26	0.51
3:D:1100:ASP:CG	3:D:1440:PHE:HB2	2.31	0.51
5:F:186:LYS:O	5:F:189:LEU:HB3	2.10	0.51
5:F:387:ARG:HD3	5:F:398:LEU:HD12	1.93	0.51
3:D:675:ARG:HH22	5:F:437:LEU:HG	1.76	0.51
3:J:1021:TYR:O	3:J:1025:GLN:HB2	2.11	0.51
3:J:628:ARG:NH1	8:S:14:DG:H2''	2.26	0.51
5:L:285:LYS:O	5:L:288:ARG:HB3	2.10	0.51
5:L:387:ARG:HD3	5:L:398:LEU:HD12	1.93	0.51
6:M:62:ALA:HB1	6:M:142:GLN:HE22	1.76	0.51
1:B:153:ALA:HA	1:B:156:HIS:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:LEU:HB3	1:B:222:LEU:HD21	1.93	0.51
2:C:332:ARG:HB2	2:C:465:GLY:HA3	1.93	0.51
3:D:465:LEU:HD22	3:D:509:PRO:HB2	1.93	0.51
3:D:592:THR:HG22	3:D:599:PRO:HA	1.93	0.51
5:L:110:THR:HG23	5:L:113:GLU:H	1.75	0.51
6:N:37:GLN:HA	6:N:47:ALA:O	2.10	0.51
1:A:16:GLN:HB3	1:A:20:TYR:O	2.10	0.51
1:A:32:PHE:O	1:A:36:LEU:HG	2.11	0.51
1:B:184:THR:OG1	1:B:185:ARG:N	2.44	0.51
2:C:65:VAL:HG13	2:C:101:ILE:HB	1.92	0.51
2:C:124:ASP:HA	2:C:592:LEU:HD12	1.92	0.51
3:D:493:ARG:HD3	3:D:1392:GLY:O	2.11	0.51
4:E:40:LEU:HD21	4:E:67:GLU:HA	1.93	0.51
1:H:48:ILE:HA	1:H:213:GLN:HE22	1.76	0.51
3:J:137:PRO:HA	3:J:452:ILE:HG13	1.92	0.51
5:F:413:ARG:HD2	8:P:44:DT:H72	1.92	0.51
2:C:577:PRO:HA	2:C:671:ASN:HD21	1.75	0.51
3:D:699:VAL:HG12	3:D:717:GLN:HG2	1.92	0.51
3:D:67:ARG:HD2	5:F:394:ARG:HD3	1.92	0.51
1:G:63:HIS:HE2	2:I:801:VAL:HG13	1.76	0.51
3:J:367:ILE:HG22	3:J:368:VAL:HG23	1.91	0.51
5:L:252:THR:O	5:L:255:THR:OG1	2.26	0.51
7:O:46:DT:H3	8:P:3:DA:H61	1.58	0.51
1:B:177:VAL:HG12	1:B:197:LEU:HD11	1.92	0.51
2:C:471:TYR:N	2:C:484:VAL:O	2.37	0.51
2:C:974:LEU:HD13	2:C:987:ILE:HB	1.92	0.51
3:D:680:GLN:O	3:D:682:ASP:N	2.31	0.51
5:F:199:ARG:O	5:F:203:ILE:HG13	2.11	0.51
2:I:292:ARG:NH1	2:I:292:ARG:H	2.04	0.51
2:I:966:LEU:HD21	2:I:986:PRO:HB3	1.92	0.51
3:J:1472:ILE:HD12	3:J:1473:PRO:HD2	1.92	0.51
6:M:20:VAL:CA	6:M:38:VAL:HA	2.36	0.51
3:D:1442:ASN:N	8:P:9:DG:OP1	2.42	0.51
3:D:1274:ILE:HD11	3:D:1334:GLN:HG2	1.92	0.51
3:D:750:PRO:HG2	3:D:756:GLN:NE2	2.26	0.51
1:G:218:LEU:HB3	1:H:222:LEU:HD21	1.93	0.51
1:H:153:ALA:HA	1:H:156:HIS:CE1	2.46	0.51
3:J:1003:VAL:O	3:J:1007:VAL:HG23	2.11	0.51
5:L:385:LYS:HA	5:L:390:LEU:HD12	1.93	0.51
2:C:431:HIS:H	2:C:434:HIS:CE1	2.28	0.50
3:D:188:GLY:HA2	3:D:196:VAL:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:137:PRO:HA	3:D:452:ILE:HG13	1.92	0.50
1:B:198:ARG:NH1	3:D:937:TYR:OH	2.42	0.50
1:H:184:THR:OG1	1:H:185:ARG:N	2.44	0.50
2:I:1032:PHE:HZ	2:I:1040:LEU:HD13	1.76	0.50
3:J:1279:GLY:H	3:J:1319:VAL:HG23	1.75	0.50
3:J:592:THR:HG22	3:J:599:PRO:HA	1.92	0.50
5:L:214:ALA:HB3	5:L:228:ILE:HG13	1.91	0.50
1:G:232:LEU:HD23	1:H:16:GLN:HG3	1.93	0.50
2:I:27:LYS:HA	2:I:30:LEU:HD22	1.93	0.50
3:J:1042:ARG:HB3	3:J:1057:VAL:HG21	1.93	0.50
3:J:121:THR:HA	3:J:124:GLU:HB3	1.93	0.50
3:J:636:GLN:HG2	3:J:637:LEU:HD12	1.93	0.50
3:J:680:GLN:C	3:J:682:ASP:H	2.12	0.50
3:J:699:VAL:HG12	3:J:717:GLN:HG2	1.92	0.50
1:A:151:VAL:HG22	1:A:156:HIS:HD2	1.77	0.50
2:C:688:ILE:HG22	2:C:689:VAL:H	1.76	0.50
3:D:1003:VAL:O	3:D:1007:VAL:HG23	2.11	0.50
3:D:272:LEU:O	3:D:279:VAL:N	2.42	0.50
3:D:636:GLN:HG2	3:D:637:LEU:HD12	1.94	0.50
2:I:18:LEU:HD12	2:I:408:ARG:NE	2.26	0.50
2:I:758:ARG:HB3	2:I:788:THR:HB	1.93	0.50
1:A:232:LEU:HD23	1:B:16:GLN:HG3	1.92	0.50
3:D:1042:ARG:HB3	3:D:1057:VAL:HG21	1.94	0.50
3:J:420:VAL:HG21	3:J:425:GLY:HA2	1.94	0.50
3:J:634:GLY:O	3:J:637:LEU:N	2.41	0.50
2:C:758:ARG:HB3	2:C:788:THR:HB	1.93	0.50
3:D:121:THR:HA	3:D:124:GLU:HB3	1.94	0.50
3:D:791:TYR:CD1	3:D:947:ILE:HD11	2.46	0.50
1:G:32:PHE:O	1:G:36:LEU:HG	2.12	0.50
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.94	0.50
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.93	0.50
2:C:1082:PRO:HG3	3:D:1469:GLY:HA3	1.94	0.50
2:C:18:LEU:HD12	2:C:408:ARG:NE	2.26	0.50
2:C:690:ILE:HG22	2:C:691:SER:H	1.76	0.50
3:D:1279:GLY:H	3:D:1319:VAL:HG23	1.76	0.50
3:D:537:THR:O	5:F:332:LEU:N	2.43	0.50
3:D:645:PRO:HB2	3:D:648:MET:HB3	1.93	0.50
3:D:628:ARG:HB2	3:D:745:MET:O	2.12	0.50
5:F:206:ASN:HB3	5:F:235:LEU:HD11	1.92	0.50
2:I:743:VAL:HG11	2:I:755:LEU:HD22	1.94	0.50
2:I:937:ASP:HB3	2:I:940:GLU:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:10:ILE:HG23	3:J:1451:ALA:HA	1.94	0.50
3:J:660:LYS:HD3	3:J:693:GLU:HB3	1.93	0.50
5:L:319:VAL:O	5:L:323:LEU:HB2	2.11	0.50
2:I:110:GLU:O	6:N:45:SER:HB2	2.12	0.50
7:O:34:DA:H2''	7:O:35:DG:O4'	2.12	0.50
1:B:48:ILE:HA	1:B:213:GLN:HE22	1.76	0.50
2:C:1032:PHE:HZ	2:C:1040:LEU:HD13	1.76	0.50
2:C:714:ASP:OD1	2:C:820:ARG:HB2	2.12	0.50
3:D:714:GLN:HB2	3:D:736:PHE:HZ	1.76	0.50
1:G:68:ILE:HG21	1:G:138:LEU:HD13	1.93	0.50
2:I:162:ILE:HB	2:I:172:ILE:HB	1.94	0.50
3:J:1037:GLN:HB3	3:J:1042:ARG:HG3	1.93	0.50
3:J:1201:CYS:SG	3:J:1204:CYS:N	2.84	0.50
4:K:40:LEU:HD21	4:K:67:GLU:HA	1.93	0.50
1:A:63:HIS:CE1	1:A:65:PHE:HB2	2.47	0.50
1:A:68:ILE:HG21	1:A:138:LEU:HD13	1.93	0.50
1:B:185:ARG:NH1	1:B:187:GLY:O	2.45	0.50
3:D:413:ASP:O	3:D:435:VAL:HG22	2.11	0.50
1:H:80:LEU:HD11	3:J:842:VAL:HG12	1.94	0.50
2:I:1060:ILE:HG23	2:I:1083:GLU:HB2	1.93	0.50
3:J:87:ARG:HG2	3:J:523:ASP:HB3	1.94	0.50
3:J:750:PRO:HG2	3:J:756:GLN:NE2	2.26	0.50
1:B:80:LEU:HD11	3:D:842:VAL:HG12	1.93	0.50
3:D:1018:ASN:HB3	3:D:1021:TYR:HB3	1.94	0.50
3:D:1436:SER:O	3:D:1439:SER:OG	2.24	0.50
5:F:206:ASN:O	5:F:210:VAL:HG23	2.12	0.50
2:I:766:GLU:OE2	3:J:64:LYS:HB3	2.12	0.50
3:J:1285:GLU:HB3	3:J:1290:LEU:HG	1.94	0.50
3:J:137:PRO:HG3	3:J:148:GLU:HA	1.93	0.50
6:N:12:LEU:HB3	6:N:40:PHE:HE1	1.76	0.50
6:N:12:LEU:HD13	6:N:59:LEU:HD13	1.93	0.50
2:C:841:ASN:HD21	2:C:845:ASN:HB3	1.77	0.49
3:D:1037:GLN:HB3	3:D:1042:ARG:HG3	1.93	0.49
3:D:137:PRO:HG3	3:D:148:GLU:HA	1.93	0.49
3:J:1462:LEU:HD12	3:J:1463:LYS:N	2.26	0.49
3:J:465:LEU:HD22	3:J:509:PRO:HB2	1.92	0.49
2:I:750:LYS:HD3	3:J:681:ARG:HG3	1.93	0.49
1:A:101:LEU:HB3	1:A:140:MET:HB3	1.94	0.49
3:D:1462:LEU:HD12	3:D:1463:LYS:N	2.26	0.49
2:C:1031:ARG:HB3	3:D:622:ARG:HD3	1.93	0.49
1:G:151:VAL:HG22	1:G:156:HIS:HD2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:167:LYS:HD3	7:R:35:DG:C5'	2.42	0.49
2:I:369:PRO:HA	2:I:372:LEU:HB3	1.94	0.49
3:J:789:LEU:O	3:J:792:ILE:HG13	2.13	0.49
1:H:198:ARG:NH1	3:J:937:TYR:OH	2.41	0.49
5:L:186:LYS:O	5:L:189:LEU:HB3	2.11	0.49
2:C:162:ILE:HB	2:C:172:ILE:HB	1.93	0.49
2:C:557:ARG:O	2:C:844:GLY:HA3	2.12	0.49
3:D:1094:LEU:HD21	3:D:1260:ILE:HG12	1.93	0.49
1:H:161:ARG:HG2	1:H:162:ILE:H	1.77	0.49
3:J:1099:VAL:HG22	3:J:1226:ALA:HB1	1.94	0.49
3:J:1264:GLU:HB3	3:J:1266:ARG:HG3	1.93	0.49
3:J:1448:THR:O	3:J:1452:ILE:HG12	2.12	0.49
3:J:461:ILE:HG22	3:J:465:LEU:HD12	1.95	0.49
6:N:18:GLY:HA3	6:N:40:PHE:HA	1.94	0.49
8:S:19:DT:H4'	8:S:19:DT:OP1	2.12	0.49
1:A:70:GLY:HA2	1:A:133:GLU:HG2	1.94	0.49
2:C:94:LEU:HD23	2:C:115:LEU:HD12	1.93	0.49
3:D:900:ILE:HG12	3:D:914:LEU:HD11	1.94	0.49
5:F:214:ALA:HB3	5:F:228:ILE:HG13	1.93	0.49
1:H:185:ARG:NH1	1:H:187:GLY:O	2.45	0.49
3:J:1094:LEU:HD21	3:J:1260:ILE:HG12	1.94	0.49
3:J:348:ALA:HB1	3:J:350:HIS:ND1	2.28	0.49
5:L:199:ARG:O	5:L:203:ILE:HG13	2.12	0.49
8:S:8:DT:H1'	8:S:9:DG:H5''	1.93	0.49
2:C:1115:LEU:HD13	3:D:88:TYR:CG	2.48	0.49
1:G:218:LEU:HD23	1:H:222:LEU:HD21	1.93	0.49
1:G:39:PRO:HG3	1:H:39:PRO:HG3	1.93	0.49
1:G:63:HIS:CE1	1:G:65:PHE:HB2	2.47	0.49
1:H:177:VAL:HG12	1:H:197:LEU:HD11	1.94	0.49
6:M:101:ASN:HD22	6:M:104:ARG:H	1.57	0.49
1:A:88:ARG:HB2	1:A:204:SER:HA	1.94	0.49
2:C:170:PRO:HB3	7:O:36:DC:H42	1.76	0.49
2:C:610:ARG:HA	2:C:624:PRO:HA	1.94	0.49
2:C:743:VAL:HG11	2:C:755:LEU:HD22	1.94	0.49
2:C:874:LEU:O	2:C:877:PRO:HD2	2.12	0.49
3:D:562:ALA:HB3	3:D:567:ILE:HD11	1.94	0.49
5:F:319:VAL:O	5:F:323:LEU:HB2	2.12	0.49
1:H:78:ILE:O	1:H:82:LEU:HG	2.12	0.49
2:I:1075:ASP:OD1	4:K:28:GLN:NE2	2.45	0.49
2:I:217:LEU:HD13	2:I:311:PHE:CD2	2.43	0.49
2:I:231:PRO:O	2:I:235:MET:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:791:TYR:CD1	3:J:947:ILE:HD11	2.47	0.49
5:L:254:ALA:O	5:L:258:ILE:HG12	2.13	0.49
1:A:90:LEU:HB2	1:A:119:ASP:HA	1.94	0.49
2:C:387:SER:HB2	2:C:388:ARG:HH11	1.77	0.49
3:D:1099:VAL:HG22	3:D:1226:ALA:HB1	1.94	0.49
3:D:347:VAL:HG23	3:D:368:VAL:HG11	1.94	0.49
2:I:207:LEU:HD21	2:I:221:LEU:O	2.13	0.49
2:I:714:ASP:OD1	2:I:820:ARG:HB2	2.13	0.49
2:I:874:LEU:O	2:I:877:PRO:HD2	2.13	0.49
2:I:1053:LEU:HG	3:J:621:LYS:HD3	1.94	0.49
5:L:224:PHE:HZ	7:R:33:DG:H5'	1.76	0.49
1:A:133:GLU:OE1	2:C:606:VAL:N	2.46	0.49
1:A:58:ILE:HG22	1:A:60:ASP:H	1.76	0.49
5:F:235:LEU:O	5:F:239:VAL:HG23	2.13	0.49
1:G:101:LEU:HB3	1:G:140:MET:HB3	1.94	0.49
1:G:70:GLY:HA2	1:G:133:GLU:HG2	1.94	0.49
2:I:437:ARG:HA	2:I:459:ALA:HB2	1.95	0.49
2:I:688:ILE:HG22	2:I:689:VAL:H	1.77	0.49
3:J:1225:ALA:HB2	3:J:1370:ILE:HD12	1.94	0.49
3:J:907:GLU:O	3:J:911:LEU:HG	2.13	0.49
5:L:280:VAL:HA	5:L:283:ILE:HD12	1.95	0.49
5:F:224:PHE:HE1	7:O:32:DG:H21	1.59	0.49
2:C:369:PRO:HA	2:C:372:LEU:HB3	1.94	0.49
3:D:1225:ALA:HB2	3:D:1370:ILE:HD12	1.95	0.49
3:D:489:ARG:HD3	3:D:1391:GLU:OE2	2.12	0.49
3:D:660:LYS:HD3	3:D:693:GLU:HB3	1.93	0.49
2:C:684:PHE:CE1	3:D:783:ARG:HB2	2.47	0.49
3:D:761:ILE:HD13	4:E:20:THR:HA	1.95	0.49
2:I:387:SER:HB2	2:I:388:ARG:HH11	1.77	0.49
2:I:690:ILE:HG22	2:I:691:SER:H	1.77	0.49
2:I:742:ILE:HG22	2:I:756:VAL:HG13	1.95	0.49
3:J:1011:PHE:CD1	3:J:1021:TYR:HB2	2.48	0.49
3:J:628:ARG:HB2	3:J:745:MET:O	2.12	0.49
3:J:761:ILE:HD13	4:K:20:THR:HA	1.94	0.49
2:C:1060:ILE:HG23	2:C:1083:GLU:HB2	1.94	0.49
2:C:434:HIS:CD2	2:C:438:ILE:HD13	2.48	0.49
2:C:437:ARG:HA	2:C:459:ALA:HB2	1.95	0.49
3:D:671:LYS:HG3	5:F:436:PHE:CE2	2.47	0.49
1:G:57:TYR:HD1	1:G:163:ASN:O	1.96	0.49
1:G:133:GLU:OE1	2:I:606:VAL:N	2.46	0.49
2:I:610:ARG:HA	2:I:624:PRO:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:129:PHE:O	3:J:572:ARG:NH2	2.46	0.49
3:D:130:ASN:HD22	5:F:98:GLN:NE2	2.04	0.48
3:D:1495:ILE:HD12	4:E:85:LEU:HA	1.94	0.48
3:D:423:ASP:HB2	3:D:427:VAL:HG12	1.93	0.48
2:I:135:VAL:HG21	2:I:407:LYS:HG2	1.95	0.48
3:J:1018:ASN:HB3	3:J:1021:TYR:HB3	1.93	0.48
3:J:645:PRO:HB2	3:J:648:MET:HB3	1.94	0.48
4:K:61:VAL:O	4:K:65:MET:HG2	2.12	0.48
6:M:34:ALA:HB3	6:M:51:VAL:HG21	1.94	0.48
1:A:9:PRO:HB2	1:A:25:LEU:HD21	1.94	0.48
1:B:78:ILE:O	1:B:82:LEU:HG	2.12	0.48
2:C:231:PRO:O	2:C:235:MET:HB2	2.13	0.48
3:D:129:PHE:O	3:D:572:ARG:NH2	2.46	0.48
3:D:706:PRO:HG3	8:P:11:DG:N2	2.27	0.48
3:D:789:LEU:O	3:D:792:ILE:HG13	2.13	0.48
4:E:61:VAL:O	4:E:65:MET:HG2	2.11	0.48
1:G:218:LEU:HG	1:H:222:LEU:HD11	1.95	0.48
2:I:434:HIS:CD2	2:I:438:ILE:HD13	2.48	0.48
2:I:471:TYR:N	2:I:484:VAL:O	2.37	0.48
3:J:1495:ILE:HD12	4:K:85:LEU:HA	1.94	0.48
4:K:26:ARG:HH12	4:K:37:ASN:HD22	1.60	0.48
1:A:72:LYS:HG3	2:C:606:VAL:HG11	1.96	0.48
2:C:571:LEU:HD23	2:C:668:LEU:O	2.14	0.48
5:F:280:VAL:HA	5:F:283:ILE:HD12	1.95	0.48
2:I:280:LYS:HD3	2:I:323:ASP:OD2	2.13	0.48
2:I:352:ALA:HB1	2:I:356:ARG:HH12	1.78	0.48
1:G:72:LYS:HG3	2:I:606:VAL:HG11	1.96	0.48
2:I:607:ASP:O	2:I:609:THR:N	2.47	0.48
2:I:1097:LEU:HB3	3:J:10:ILE:HD11	1.95	0.48
3:J:1462:LEU:O	3:J:1466:VAL:HG23	2.13	0.48
3:J:900:ILE:HG12	3:J:914:LEU:HD11	1.94	0.48
3:J:970:LYS:O	3:J:974:ILE:HG13	2.14	0.48
2:C:437:ARG:HH11	2:C:467:ILE:HG22	1.79	0.48
2:C:607:ASP:O	2:C:609:THR:N	2.46	0.48
3:D:1448:THR:O	3:D:1452:ILE:HG12	2.13	0.48
3:D:1462:LEU:O	3:D:1466:VAL:HG23	2.14	0.48
3:D:203:ALA:HA	3:D:395:VAL:HA	1.95	0.48
3:D:238:PRO:HB3	3:D:315:ARG:O	2.13	0.48
5:F:142:ILE:O	5:F:146:VAL:HG23	2.13	0.48
2:I:1115:LEU:HD13	3:J:88:TYR:CG	2.47	0.48
3:J:14:SER:HB3	3:J:511:TRP:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:357:GLU:HG2	3:J:387:LEU:CB	2.43	0.48
3:J:822:ALA:HB3	3:J:825:ALA:HB2	1.96	0.48
1:A:176:ARG:HG3	1:A:200:TRP:CE3	2.49	0.48
1:A:173:PRO:HB3	1:A:204:SER:HB2	1.96	0.48
2:C:110:GLU:O	6:M:45:SER:HB2	2.14	0.48
2:C:280:LYS:HD3	2:C:323:ASP:OD2	2.13	0.48
2:C:397:GLU:HB3	2:C:631:SER:HB2	1.94	0.48
2:C:742:ILE:HG22	2:C:756:VAL:HG13	1.96	0.48
3:D:1285:GLU:HB3	3:D:1290:LEU:HG	1.94	0.48
3:D:1440:PHE:CE1	3:D:1441:GLN:HG2	2.49	0.48
3:D:1487:VAL:HG21	3:D:1492:LEU:HD23	1.95	0.48
3:D:699:VAL:HB	3:D:716:PHE:O	2.13	0.48
2:I:94:LEU:HD23	2:I:115:LEU:HD12	1.94	0.48
2:I:397:GLU:HB3	2:I:631:SER:HB2	1.95	0.48
2:I:706:GLU:HB3	2:I:708:TYR:HE1	1.78	0.48
3:J:1442:ASN:N	8:S:9:DG:OP1	2.45	0.48
5:L:235:LEU:O	5:L:239:VAL:HG23	2.13	0.48
3:D:1201:CYS:SG	3:D:1204:CYS:N	2.85	0.48
3:D:1476:THR:HA	4:E:17:TYR:HB3	1.95	0.48
3:D:253:ALA:HB2	3:D:304:LEU:HG	1.95	0.48
3:D:255:GLU:OE2	3:D:256:SER:N	2.45	0.48
3:D:761:ILE:O	3:D:767:HIS:ND1	2.47	0.48
4:E:39:VAL:HB	4:E:72:ARG:HD2	1.95	0.48
2:I:684:PHE:CE1	3:J:783:ARG:HB2	2.48	0.48
3:J:714:GLN:HB2	3:J:736:PHE:HZ	1.78	0.48
3:J:714:GLN:HB3	3:J:765:SER:HB3	1.96	0.48
3:D:714:GLN:HB3	3:D:765:SER:HB3	1.96	0.48
3:D:764:LEU:HB3	3:D:767:HIS:CD2	2.49	0.48
5:F:199:ARG:HE	5:F:200:GLN:NE2	2.12	0.48
2:I:1035:MET:HA	2:I:1038:TRP:CE3	2.49	0.48
2:I:1094:ALA:HB2	3:J:520:LEU:HD13	1.96	0.48
2:I:706:GLU:HB3	2:I:708:TYR:CE1	2.49	0.48
6:N:91:ARG:NH1	7:R:27:DT:OP1	2.46	0.48
7:R:32:DG:H2'	7:R:33:DG:C8	2.48	0.48
2:C:706:GLU:HB3	2:C:708:TYR:HE1	1.79	0.48
3:D:1095:THR:O	3:D:1099:VAL:HG23	2.14	0.48
3:D:907:GLU:O	3:D:911:LEU:HG	2.14	0.48
1:G:173:PRO:HB3	1:G:204:SER:HB2	1.96	0.48
2:I:1008:ARG:NH2	2:I:1020:PRO:HB3	2.29	0.48
2:I:374:ASN:HD22	2:I:375:SER:H	1.61	0.48
2:I:857:ASP:N	2:I:857:ASP:OD1	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1487:VAL:HG21	3:J:1492:LEU:HD23	1.94	0.48
3:J:900:ILE:HA	3:J:914:LEU:HD21	1.96	0.48
8:P:34:DA:H1'	8:P:35:DA:H5'	1.96	0.48
1:B:156:HIS:O	1:B:156:HIS:ND1	2.47	0.48
2:C:1035:MET:HA	2:C:1038:TRP:CE3	2.48	0.48
2:C:658:GLY:H	2:C:661:SER:HB3	1.79	0.48
3:D:263:ASP:HB3	3:D:268:HIS:CD2	2.49	0.48
3:D:461:ILE:HG22	3:D:465:LEU:HD12	1.95	0.48
1:G:88:ARG:HB2	1:G:204:SER:HA	1.94	0.48
2:I:299:LYS:HG3	2:I:300:ASP:H	1.79	0.48
4:K:39:VAL:HB	4:K:72:ARG:HD2	1.95	0.48
5:F:398:LEU:HD13	8:P:43:DG:OP2	2.13	0.48
2:C:409:ARG:HG2	2:C:452:ILE:HG22	1.96	0.48
2:C:430:VAL:HG12	2:C:434:HIS:CD2	2.49	0.48
2:C:892:LEU:HD23	2:C:918:LEU:HD11	1.96	0.48
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.49	0.48
3:D:87:ARG:HG2	3:D:523:ASP:HB3	1.94	0.48
2:I:658:GLY:H	2:I:661:SER:HB3	1.77	0.48
3:J:1364:HIS:CE1	3:J:1366:LYS:HG3	2.48	0.48
3:J:622:ARG:HH12	8:S:14:DG:H5'	1.79	0.48
7:O:14:DT:H1'	7:O:15:DT:H5''	1.96	0.48
2:C:430:VAL:HG12	2:C:434:HIS:HD2	1.79	0.47
3:D:1341:PRO:O	3:D:1344:VAL:HB	2.14	0.47
3:D:1364:HIS:CE1	3:D:1366:LYS:HG3	2.49	0.47
3:D:900:ILE:HA	3:D:914:LEU:HD21	1.97	0.47
1:G:90:LEU:HB2	1:G:119:ASP:HA	1.96	0.47
2:I:430:VAL:HG12	2:I:434:HIS:CD2	2.49	0.47
3:J:131:LYS:HG2	3:J:153:LEU:O	2.14	0.47
3:J:63:TYR:HE2	3:J:73:CYS:HA	1.79	0.47
3:J:761:ILE:O	3:J:767:HIS:ND1	2.47	0.47
5:L:252:THR:HA	7:R:29:DC:H5	1.78	0.47
1:A:218:LEU:HG	1:B:222:LEU:HD11	1.96	0.47
2:C:49:LYS:NZ	2:C:50:GLU:HG3	2.29	0.47
2:C:726:ILE:HB	2:C:729:LEU:HB2	1.96	0.47
3:D:1144:LEU:HD21	3:D:1186:VAL:HG11	1.96	0.47
3:D:1264:GLU:HB3	3:D:1266:ARG:HG3	1.94	0.47
2:C:1053:LEU:HG	3:D:621:LYS:HD3	1.94	0.47
3:D:762:GLN:HB3	4:E:16:LYS:HE2	1.96	0.47
3:D:822:ALA:HB3	3:D:825:ALA:HB2	1.97	0.47
1:B:186:LEU:HD22	4:E:51:LEU:HD22	1.96	0.47
1:G:65:PHE:CE1	2:I:703:ILE:HG21	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1067:TYR:CE1	3:J:655:PRO:HG3	2.49	0.47
2:I:521:PRO:HG2	3:J:1055:VAL:HG21	1.96	0.47
2:I:892:LEU:HD23	2:I:918:LEU:HD11	1.95	0.47
3:J:762:GLN:HB3	4:K:16:LYS:HE2	1.97	0.47
3:J:1476:THR:HA	4:K:17:TYR:HB3	1.96	0.47
5:L:137:LEU:HB3	5:L:141:LEU:HD23	1.96	0.47
5:L:206:ASN:O	5:L:210:VAL:HG23	2.13	0.47
1:A:26:GLU:HG3	1:A:186:LEU:HD12	1.96	0.47
2:C:1097:LEU:HB3	3:D:10:ILE:HD11	1.96	0.47
2:C:508:ILE:HD11	2:C:529:VAL:HG11	1.96	0.47
3:D:1097:LYS:HE2	3:D:1440:PHE:HZ	1.79	0.47
1:G:26:GLU:HG3	1:G:186:LEU:HD12	1.96	0.47
3:J:10:ILE:HB	3:J:1434:TRP:CH2	2.50	0.47
3:J:743:ASP:OD1	3:J:743:ASP:N	2.47	0.47
3:J:764:LEU:HB3	3:J:767:HIS:CD2	2.48	0.47
4:K:65:MET:O	4:K:69:LEU:HG	2.13	0.47
5:L:119:ARG:HA	5:L:244:TYR:CE1	2.49	0.47
6:M:75:LEU:HD11	6:M:136:LEU:HD13	1.96	0.47
1:A:17:GLY:HA3	1:A:19:HIS:CE1	2.49	0.47
1:A:198:ARG:HD2	2:C:934:PHE:CE1	2.49	0.47
2:C:18:LEU:HD12	2:C:408:ARG:HE	1.80	0.47
3:D:1042:ARG:HD3	3:D:1045:MET:CE	2.45	0.47
3:D:585:GLY:HA2	3:D:590:PRO:HG3	1.96	0.47
3:D:646:LYS:HA	3:D:720:LEU:HD22	1.96	0.47
2:I:430:VAL:HG12	2:I:434:HIS:HD2	1.79	0.47
2:I:437:ARG:HH11	2:I:467:ILE:HG22	1.80	0.47
2:I:971:LYS:HD2	2:I:986:PRO:HG2	1.96	0.47
3:J:165:LYS:H	3:J:397:LYS:HE2	1.79	0.47
2:I:1031:ARG:HB3	3:J:622:ARG:HD3	1.95	0.47
5:L:271:ARG:HG2	5:L:328:GLU:HB3	1.96	0.47
1:A:57:TYR:HD1	1:A:163:ASN:O	1.97	0.47
2:C:352:ALA:HB1	2:C:356:ARG:HH12	1.79	0.47
2:C:706:GLU:HB3	2:C:708:TYR:CE1	2.49	0.47
4:E:26:ARG:HH12	4:E:37:ASN:HD22	1.61	0.47
2:I:140:ILE:HG12	2:I:141:HIS:N	2.30	0.47
2:I:185:LYS:HD3	2:I:190:LYS:HB3	1.96	0.47
2:I:817:PRO:HB3	5:L:323:LEU:HB3	1.96	0.47
3:J:140:ALA:HA	3:J:450:TYR:CD2	2.50	0.47
2:C:682:TYR:HA	3:D:633:VAL:HG11	1.95	0.47
3:D:131:LYS:HG2	3:D:153:LEU:O	2.15	0.47
3:D:141:VAL:HG12	3:D:450:TYR:HE2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:639:LEU:HD22	3:D:766:ALA:HA	1.97	0.47
2:I:1112:PHE:HB3	2:I:1115:LEU:HB2	1.97	0.47
3:J:630:VAL:HG22	3:J:631:ILE:H	1.79	0.47
1:H:186:LEU:HD22	4:K:51:LEU:HD22	1.97	0.47
8:P:9:DG:H2''	8:P:10:DA:H5'	1.97	0.47
2:C:1026:GLN:HB2	2:C:1026:GLN:HE21	1.50	0.47
3:D:273:ARG:HB3	3:D:278:VAL:HG12	1.95	0.47
3:D:471:GLU:O	3:D:475:ARG:HG2	2.15	0.47
3:D:630:VAL:HG22	3:D:631:ILE:H	1.79	0.47
1:H:52:ALA:HB3	1:H:145:ASP:O	2.15	0.47
2:I:163:ILE:HD12	2:I:164:PRO:HD2	1.96	0.47
2:I:18:LEU:HD12	2:I:408:ARG:HE	1.80	0.47
2:I:424:GLY:H	2:I:427:VAL:CG2	2.28	0.47
3:J:367:ILE:HB	3:J:377:VAL:HB	1.97	0.47
3:D:772:PRO:O	3:D:1209:LEU:HD12	2.14	0.47
5:F:137:LEU:HB3	5:F:141:LEU:HD23	1.97	0.47
5:F:368:GLU:HB3	5:F:433:LEU:HD21	1.97	0.47
2:I:36:PRO:CB	2:I:70:GLU:HG2	2.45	0.47
2:I:508:ILE:HD11	2:I:529:VAL:HG11	1.96	0.47
3:J:1341:PRO:O	3:J:1344:VAL:HB	2.15	0.47
6:M:136:LEU:HB3	6:M:155:PHE:CZ	2.50	0.47
6:N:68:VAL:HG21	6:N:144:LEU:HD21	1.96	0.47
1:A:53:VAL:HA	1:A:144:VAL:HA	1.97	0.47
2:C:135:VAL:HG21	2:C:407:LYS:HG2	1.95	0.47
2:C:398:THR:HA	2:C:635:THR:HG21	1.97	0.47
2:I:409:ARG:HG2	2:I:452:ILE:HG22	1.97	0.47
2:I:68:PHE:O	2:I:69:LEU:HD13	2.14	0.47
2:I:708:TYR:HE2	2:I:792:VAL:HG23	1.79	0.47
2:I:922:PHE:HB2	2:I:967:PHE:CD2	2.50	0.47
3:J:1267:ARG:NE	3:J:1267:ARG:H	2.13	0.47
3:J:646:LYS:HA	3:J:720:LEU:HD22	1.96	0.47
2:C:1112:PHE:HB3	2:C:1115:LEU:HB2	1.97	0.47
3:D:1089:ALA:O	8:P:11:DG:H5'	2.15	0.47
3:D:151:GLN:HG2	3:D:152:LEU:H	1.80	0.47
3:D:704:ARG:HB2	3:D:745:MET:HG2	1.97	0.47
1:G:176:ARG:HG3	1:G:200:TRP:CE3	2.50	0.47
1:G:198:ARG:HD2	2:I:934:PHE:CE1	2.49	0.47
1:H:156:HIS:ND1	1:H:156:HIS:O	2.48	0.47
1:H:30:ARG:HB3	1:H:191:ASP:O	2.15	0.47
3:J:167:GLU:OE2	3:J:198:ARG:NH2	2.48	0.47
3:J:699:VAL:HB	3:J:716:PHE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:207:LEU:HD21	2:C:221:LEU:O	2.15	0.47
2:C:68:PHE:O	2:C:69:LEU:HD13	2.15	0.47
3:D:83:SER:O	3:D:86:ARG:HB2	2.15	0.47
3:D:970:LYS:O	3:D:974:ILE:HG13	2.15	0.47
2:I:101:ILE:HG12	2:I:108:ILE:HG23	1.95	0.47
2:I:549:PHE:HE1	2:I:909:ALA:HB3	1.80	0.47
2:I:726:ILE:HB	2:I:729:LEU:HB2	1.96	0.47
3:J:112:ILE:HD12	3:J:113:GLY:N	2.29	0.47
3:J:1364:HIS:CD2	3:J:1366:LYS:HE2	2.49	0.47
3:J:538:SER:HA	5:L:332:LEU:HB2	1.97	0.47
6:N:34:ALA:HB3	6:N:51:VAL:HG21	1.96	0.47
2:C:922:PHE:HB2	2:C:967:PHE:CD2	2.50	0.46
3:D:10:ILE:HB	3:D:1434:TRP:CH2	2.50	0.46
3:D:1364:HIS:CD2	3:D:1366:LYS:HE2	2.49	0.46
3:D:339:TRP:HE1	3:D:341:GLU:HG3	1.79	0.46
3:D:881:LEU:HG	3:D:885:ILE:HD11	1.96	0.46
5:F:276:PRO:O	5:F:280:VAL:HG23	2.15	0.46
5:F:342:SER:OG	8:P:17:DG:N2	2.48	0.46
5:F:386:LEU:HB3	5:F:396:HIS:HB2	1.98	0.46
1:G:94:MET:O	1:G:146:ARG:HD3	2.16	0.46
2:I:42:VAL:HG12	2:I:43:GLY:H	1.79	0.46
2:I:841:ASN:HD21	2:I:845:ASN:HB3	1.78	0.46
3:J:1042:ARG:HD3	3:J:1045:MET:CE	2.45	0.46
3:J:585:GLY:HA2	3:J:590:PRO:HG3	1.96	0.46
3:J:896:ALA:O	3:J:900:ILE:HG13	2.15	0.46
5:L:142:ILE:O	5:L:146:VAL:HG23	2.15	0.46
5:L:413:ARG:HE	8:S:44:DT:H2'	1.80	0.46
3:D:628:ARG:NH2	8:P:14:DG:H2''	2.30	0.46
5:L:411:ARG:HD3	7:R:1:DC:H6	1.78	0.46
2:C:1094:ALA:HB2	3:D:520:LEU:HD13	1.96	0.46
2:C:470:PRO:HG3	2:C:485:TYR:CZ	2.50	0.46
2:C:874:LEU:O	3:D:1029:ARG:HG2	2.15	0.46
2:C:893:ALA:HB2	2:C:918:LEU:HD22	1.97	0.46
2:I:893:ALA:HB2	2:I:918:LEU:HD22	1.97	0.46
3:J:1144:LEU:HD21	3:J:1186:VAL:HG11	1.98	0.46
3:J:1440:PHE:CE1	3:J:1441:GLN:HG2	2.50	0.46
3:J:166:GLN:HE21	3:J:166:GLN:HB2	1.52	0.46
3:J:657:LEU:HB2	3:J:691:LEU:HD13	1.97	0.46
5:L:187:ARG:O	5:L:191:ILE:HG13	2.15	0.46
3:J:34:TYR:HD1	5:L:325:ILE:HG21	1.80	0.46
2:C:971:LYS:HD2	2:C:986:PRO:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:63:TYR:HE2	3:D:73:CYS:HA	1.80	0.46
5:F:254:ALA:O	5:F:258:ILE:HG12	2.15	0.46
3:D:34:TYR:HD1	5:F:325:ILE:HG21	1.80	0.46
1:G:133:GLU:OE1	2:I:607:ASP:HB2	2.15	0.46
1:G:9:PRO:HG3	1:H:224:TYR:CZ	2.50	0.46
3:J:881:LEU:HG	3:J:885:ILE:HD11	1.96	0.46
2:C:1008:ARG:NH2	2:C:1020:PRO:HB3	2.30	0.46
2:C:101:ILE:HG12	2:C:108:ILE:HG23	1.97	0.46
2:C:140:ILE:HG12	2:C:141:HIS:N	2.30	0.46
2:C:163:ILE:HD12	2:C:164:PRO:HD2	1.97	0.46
2:C:708:TYR:HE2	2:C:792:VAL:HG23	1.80	0.46
2:C:882:LEU:HD21	3:D:1038:LEU:HD22	1.97	0.46
3:D:169:TYR:CZ	3:D:197:SER:HA	2.50	0.46
3:D:229:ALA:HA	3:D:244:GLU:HB2	1.97	0.46
3:D:259:VAL:HG23	3:D:294:GLU:HA	1.98	0.46
3:D:363:ALA:HA	3:D:381:ALA:O	2.16	0.46
3:D:671:LYS:H	5:F:364:LEU:HD11	1.81	0.46
1:H:78:ILE:HD12	1:H:130:ALA:HB2	1.97	0.46
1:H:80:LEU:HD12	3:J:844:ALA:HB2	1.98	0.46
2:I:438:ILE:H	2:I:438:ILE:HD12	1.80	0.46
2:I:874:LEU:O	3:J:1029:ARG:HG2	2.14	0.46
3:J:772:PRO:O	3:J:1209:LEU:HD12	2.15	0.46
5:L:369:LEU:HD23	5:L:433:LEU:HD13	1.96	0.46
1:B:52:ALA:HB3	1:B:145:ASP:O	2.16	0.46
2:C:185:LYS:HD3	2:C:190:LYS:HB3	1.97	0.46
2:C:521:PRO:HG2	3:D:1055:VAL:HG21	1.98	0.46
3:D:729:HIS:CE1	3:D:935:LYS:HD3	2.50	0.46
3:D:889:ALA:HB1	3:D:930:LEU:HA	1.97	0.46
1:H:74:ASP:O	1:H:78:ILE:HG12	2.15	0.46
2:I:107:LEU:HD12	6:N:50:PRO:HD2	1.98	0.46
3:J:562:ALA:HB3	3:J:567:ILE:HD11	1.96	0.46
3:J:606:ILE:HG22	3:J:613:ARG:HB2	1.98	0.46
5:L:199:ARG:HE	5:L:200:GLN:NE2	2.13	0.46
5:L:355:SER:HB3	5:L:358:GLU:HG3	1.97	0.46
5:L:360:ALA:O	5:L:364:LEU:HB2	2.16	0.46
2:C:1083:GLU:HA	2:C:1086:ARG:HG3	1.98	0.46
2:C:418:LEU:HD11	7:O:38:DG:C4	2.50	0.46
2:C:42:VAL:HG12	2:C:43:GLY:H	1.79	0.46
2:C:472:ARG:HB3	2:C:532:MET:HB3	1.97	0.46
3:D:1267:ARG:H	3:D:1267:ARG:NE	2.13	0.46
4:E:65:MET:O	4:E:69:LEU:HG	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:149:LYS:HB3	5:F:193:ARG:HH12	1.81	0.46
1:G:83:LYS:H	1:G:83:LYS:HD3	1.81	0.46
2:I:49:LYS:NZ	2:I:50:GLU:HG3	2.29	0.46
2:I:571:LEU:HD23	2:I:668:LEU:O	2.15	0.46
2:I:607:ASP:O	2:I:610:ARG:N	2.49	0.46
5:L:411:ARG:HB2	7:R:1:DC:H2'	1.97	0.46
1:B:20:TYR:HD1	1:B:21:GLY:H	1.64	0.46
2:C:1104:GLU:HG2	2:C:1104:GLU:H	1.52	0.46
2:C:588:VAL:HG21	2:C:664:GLY:HA2	1.98	0.46
3:D:1011:PHE:CD1	3:D:1021:TYR:HB2	2.49	0.46
5:F:364:LEU:HD22	5:F:436:PHE:HZ	1.81	0.46
2:I:140:ILE:HG23	2:I:412:ALA:HA	1.98	0.46
3:J:1282:ARG:NH1	3:J:1284:GLU:OE2	2.49	0.46
3:J:1192:LEU:HD23	3:J:1373:ARG:HB2	1.98	0.46
3:J:440:VAL:HG13	3:J:441:ARG:HD2	1.98	0.46
3:J:580:ALA:O	3:J:584:ASN:HB2	2.16	0.46
3:J:639:LEU:HD22	3:J:766:ALA:HA	1.98	0.46
6:N:20:VAL:HG22	6:N:38:VAL:HG22	1.96	0.46
2:C:1038:TRP:O	3:D:1223:VAL:HG11	2.16	0.46
2:C:86:LYS:HE2	2:C:813:VAL:HA	1.97	0.46
3:D:1192:LEU:HD23	3:D:1373:ARG:HB2	1.98	0.46
3:D:233:LYS:HB3	3:D:236:TYR:CZ	2.51	0.46
3:D:263:ASP:HA	3:D:268:HIS:HA	1.97	0.46
3:D:539:ASP:HB3	3:D:600:LEU:HG	1.97	0.46
3:D:606:ILE:HG22	3:D:613:ARG:HB2	1.98	0.46
3:D:657:LEU:HB2	3:D:691:LEU:HD13	1.98	0.46
3:D:896:ALA:O	3:D:900:ILE:HG13	2.16	0.46
5:F:119:ARG:HA	5:F:244:TYR:CE1	2.50	0.46
1:G:17:GLY:HA3	1:G:19:HIS:CE1	2.50	0.46
2:I:163:ILE:HA	2:I:164:PRO:HD2	1.75	0.46
2:I:398:THR:HA	2:I:635:THR:HG21	1.97	0.46
3:J:1095:THR:O	3:J:1099:VAL:HG23	2.15	0.46
3:J:151:GLN:HG2	3:J:152:LEU:H	1.80	0.46
2:I:682:TYR:HA	3:J:633:VAL:HG11	1.96	0.46
1:B:64:GLU:HG3	1:B:165:ILE:HG21	1.98	0.46
2:C:332:ARG:HH11	2:C:334:ARG:HD2	1.81	0.46
2:C:438:ILE:H	2:C:438:ILE:HD12	1.81	0.46
5:F:431:ARG:HG3	5:F:434:ARG:CZ	2.46	0.46
2:I:472:ARG:HB3	2:I:532:MET:HB3	1.98	0.46
3:J:729:HIS:CE1	3:J:935:LYS:HD3	2.51	0.46
6:N:10:VAL:HB	6:N:60:ARG:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:34:DA:H2"	7:R:35:DG:O4'	2.16	0.46
5:L:413:ARG:NH2	8:S:45:DC:OP2	2.48	0.46
2:C:15:LEU:HD11	2:C:457:ALA:O	2.16	0.46
2:C:424:GLY:H	2:C:427:VAL:CG2	2.29	0.46
2:C:607:ASP:O	2:C:610:ARG:N	2.49	0.46
2:C:620:LEU:H	2:C:620:LEU:HD12	1.81	0.46
3:D:783:ARG:HD3	3:D:1028:ALA:O	2.16	0.46
3:D:834:THR:HG21	3:D:839:LEU:HD21	1.98	0.46
2:C:1102:LEU:HD21	3:D:9:ARG:HB2	1.97	0.46
5:F:244:TYR:N	5:F:244:TYR:CD2	2.84	0.46
1:H:20:TYR:HD1	1:H:21:GLY:H	1.64	0.46
1:H:20:TYR:HD1	1:H:21:GLY:N	2.14	0.46
2:I:676:ILE:HA	2:I:871:LEU:O	2.16	0.46
5:L:276:PRO:O	5:L:280:VAL:HG23	2.16	0.46
5:L:386:LEU:HB3	5:L:396:HIS:HB2	1.98	0.46
8:P:6:DC:H2"	8:P:7:DG:H5'	1.98	0.46
1:A:185:ARG:O	1:A:185:ARG:HG2	2.16	0.45
2:C:409:ARG:NH2	2:C:563:ASN:OD1	2.49	0.45
1:A:133:GLU:OE1	2:C:607:ASP:HB2	2.15	0.45
2:C:939:ARG:HB3	2:C:982:PRO:HG3	1.98	0.45
2:I:1083:GLU:HA	2:I:1086:ARG:HG3	1.98	0.45
3:J:862:ASP:O	3:J:876:SER:HA	2.16	0.45
3:J:889:ALA:HB1	3:J:930:LEU:HA	1.98	0.45
2:I:1102:LEU:HD21	3:J:9:ARG:HB2	1.97	0.45
6:M:23:ILE:HA	6:M:35:TYR:O	2.16	0.45
2:C:954:SER:HA	2:C:955:PRO:HD3	1.85	0.45
3:D:112:ILE:HD12	3:D:113:GLY:N	2.30	0.45
3:D:1318:TYR:N	3:J:1157:GLY:O	2.49	0.45
3:D:156:GLU:O	3:D:160:GLU:HB2	2.16	0.45
3:D:406:ASP:HB3	3:D:407:VAL:H	1.50	0.45
5:F:252:THR:O	5:F:255:THR:OG1	2.25	0.45
1:G:53:VAL:HA	1:G:144:VAL:HA	1.97	0.45
1:H:138:LEU:HD22	1:H:139:TYR:N	2.31	0.45
2:I:167:LYS:HD2	2:I:167:LYS:O	2.15	0.45
2:I:620:LEU:H	2:I:620:LEU:HD12	1.80	0.45
2:C:1016:ILE:HG13	2:C:1017:THR:H	1.82	0.45
2:C:204:GLN:HA	2:C:227:LEU:HD11	1.98	0.45
3:D:1040:GLY:O	3:D:1060:SER:HB2	2.16	0.45
3:D:859:ASP:HB2	3:D:862:ASP:OD2	2.17	0.45
2:I:109:LYS:HG2	6:N:15:TYR:OH	2.16	0.45
2:I:276:LYS:HD3	2:I:466:PHE:CZ	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1100:ASP:CG	3:J:1440:PHE:HB2	2.37	0.45
3:J:521:PRO:HA	3:J:522:PRO:HD3	1.77	0.45
3:J:539:ASP:HB3	3:J:600:LEU:HG	1.97	0.45
3:J:783:ARG:HD3	3:J:1028:ALA:O	2.15	0.45
1:A:71:VAL:HG11	1:A:78:ILE:HD11	1.99	0.45
1:B:214:ALA:O	1:B:218:LEU:HD13	2.16	0.45
1:B:20:TYR:HD1	1:B:21:GLY:N	2.13	0.45
2:C:676:ILE:HA	2:C:871:LEU:O	2.15	0.45
3:D:1197:ARG:NE	3:D:1398:TRP:HB3	2.32	0.45
3:D:743:ASP:N	3:D:743:ASP:OD1	2.48	0.45
2:C:1083:GLU:OE1	3:D:88:TYR:OH	2.34	0.45
2:I:1086:ARG:HD2	2:I:1112:PHE:CD2	2.52	0.45
2:I:204:GLN:HA	2:I:227:LEU:HD11	1.96	0.45
2:I:769:PRO:HB3	5:L:390:LEU:HA	1.98	0.45
3:J:1269:LYS:HG2	3:J:1270:ALA:N	2.31	0.45
3:J:169:TYR:O	3:J:392:SER:OG	2.34	0.45
3:J:675:ARG:HH12	5:L:437:LEU:HB3	1.80	0.45
3:J:699:VAL:HG21	3:J:764:LEU:HD13	1.99	0.45
7:R:15:DT:H5'	7:R:15:DT:H6	1.81	0.45
1:B:138:LEU:HD22	1:B:139:TYR:N	2.32	0.45
1:B:30:ARG:HB3	1:B:191:ASP:O	2.16	0.45
1:A:9:PRO:HG3	1:B:224:TYR:CZ	2.51	0.45
2:C:167:LYS:HD2	2:C:167:LYS:O	2.17	0.45
2:C:729:LEU:HD13	2:C:730:SER:O	2.16	0.45
3:D:1282:ARG:NH1	3:D:1284:GLU:OE2	2.49	0.45
3:D:16:GLU:CD	3:D:16:GLU:H	2.20	0.45
3:D:59:ALA:HB2	3:D:78:VAL:HG21	1.99	0.45
2:I:1026:GLN:HB2	2:I:1026:GLN:HE21	1.51	0.45
2:I:332:ARG:HH11	2:I:334:ARG:HD2	1.81	0.45
2:I:470:PRO:HG3	2:I:485:TYR:CZ	2.51	0.45
2:I:588:VAL:HG21	2:I:664:GLY:HA2	1.98	0.45
2:I:939:ARG:HB3	2:I:982:PRO:HG3	1.97	0.45
3:J:1040:GLY:O	3:J:1060:SER:HB2	2.16	0.45
3:J:859:ASP:HB2	3:J:862:ASP:OD2	2.17	0.45
6:M:4:PHE:HE1	6:M:10:VAL:HG11	1.82	0.45
7:R:32:DG:H2''	7:R:33:DG:O4'	2.17	0.45
1:B:63:HIS:CD2	1:B:64:GLU:H	2.35	0.45
2:C:549:PHE:HE1	2:C:909:ALA:HB3	1.81	0.45
2:C:724:ARG:HD3	2:C:741:GLY:N	2.32	0.45
3:D:1072:ILE:O	3:D:1075:HIS:HB2	2.17	0.45
3:D:186:VAL:HG13	3:D:200:ASP:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:217:ARG:HH12	3:D:381:ALA:CB	2.29	0.45
3:D:580:ALA:O	3:D:584:ASN:HB2	2.16	0.45
3:D:699:VAL:HG21	3:D:764:LEU:HD13	1.99	0.45
5:F:355:SER:HB3	5:F:358:GLU:HG3	1.99	0.45
2:I:1089:VAL:HG13	2:I:1099:VAL:HG11	1.98	0.45
2:I:15:LEU:HD11	2:I:457:ALA:O	2.16	0.45
2:I:521:PRO:HB2	3:J:1055:VAL:HG11	1.98	0.45
3:J:704:ARG:HB2	3:J:745:MET:HG2	1.97	0.45
3:D:973:GLN:CG	3:J:831:GLY:HA2	2.46	0.45
3:J:83:SER:O	3:J:86:ARG:HB2	2.17	0.45
3:J:903:ASP:N	3:J:903:ASP:OD1	2.49	0.45
7:R:39:DT:C2'	7:R:40:DC:H5'	2.43	0.45
2:C:1089:VAL:O	2:C:1093:GLN:HG2	2.16	0.45
2:C:299:LYS:HG3	2:C:300:ASP:H	1.81	0.45
2:C:642:ARG:HA	2:C:642:ARG:HD3	1.55	0.45
2:C:751:PRO:HA	2:C:792:VAL:HG13	1.99	0.45
3:D:102:ILE:HB	3:D:579:ASP:HB3	1.99	0.45
3:D:101:HIS:CE1	3:D:103:TRP:HB2	2.52	0.45
3:D:764:LEU:HD23	3:D:767:HIS:CD2	2.52	0.45
5:F:124:GLY:O	5:F:128:ILE:HG13	2.17	0.45
5:F:96:VAL:HA	5:F:225:LEU:HD11	1.97	0.45
2:I:409:ARG:NH2	2:I:563:ASN:OD1	2.49	0.45
2:I:658:GLY:N	2:I:661:SER:HB3	2.32	0.45
3:J:118:LEU:HD12	3:J:123:LEU:HB2	1.99	0.45
3:J:351:MET:HE3	3:J:375:GLU:O	2.17	0.45
8:S:19:DT:H5'	8:S:20:DA:OP1	2.16	0.45
1:B:78:ILE:HD12	1:B:130:ALA:HB2	1.98	0.45
1:B:80:LEU:HD12	3:D:844:ALA:HB2	1.99	0.45
2:C:1086:ARG:HD2	2:C:1112:PHE:CD2	2.52	0.45
2:C:521:PRO:HB2	3:D:1055:VAL:HG11	1.99	0.45
2:C:905:VAL:HG12	2:C:906:PHE:CD2	2.52	0.45
3:D:862:ASP:O	3:D:876:SER:HA	2.16	0.45
2:I:882:LEU:HD21	3:J:1038:LEU:HD22	1.97	0.45
3:J:101:HIS:CE1	3:J:103:TRP:HB2	2.52	0.45
2:I:1083:GLU:OE1	3:J:88:TYR:OH	2.34	0.45
4:K:31:LEU:HG	4:K:60:ALA:HB2	1.98	0.45
5:L:96:VAL:HA	5:L:225:LEU:HD11	1.97	0.45
6:M:20:VAL:HG22	6:M:38:VAL:HG22	1.98	0.45
6:N:84:LYS:HE2	6:N:84:LYS:HB2	1.75	0.45
1:A:158:ILE:HG13	1:A:166:PRO:HG3	1.99	0.45
1:A:53:VAL:HG22	1:A:54:THR:N	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ASP:O	1:B:78:ILE:HG12	2.17	0.45
2:C:217:LEU:HD13	2:C:311:PHE:CD2	2.43	0.45
3:D:1208:ASP:N	3:D:1213:ARG:O	2.47	0.45
3:D:1269:LYS:HG2	3:D:1270:ALA:N	2.32	0.45
3:D:880:ILE:HG12	3:D:880:ILE:H	1.42	0.45
1:H:211:LEU:O	1:H:215:VAL:HG13	2.16	0.45
2:I:211:LEU:HD22	2:I:218:VAL:HA	1.99	0.45
2:I:729:LEU:HD13	2:I:730:SER:O	2.16	0.45
3:J:123:LEU:HG	3:J:127:LEU:HD12	1.98	0.45
3:J:550:ARG:HG3	3:J:553:ARG:HH21	1.82	0.45
3:J:764:LEU:HD23	3:J:767:HIS:CD2	2.52	0.45
5:L:244:TYR:N	5:L:244:TYR:CD2	2.83	0.45
1:A:83:LYS:HD3	1:A:83:LYS:H	1.82	0.45
2:C:1054:THR:OG1	2:C:1079:PRO:HG3	2.17	0.45
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.76	0.45
2:C:726:ILE:HG23	2:C:787:ASP:HB2	1.99	0.45
2:C:829:GLN:NE2	2:C:831:ARG:HH21	2.14	0.45
3:D:245:LEU:HA	3:D:245:LEU:HD23	1.66	0.45
3:D:369:ALA:HA	3:D:376:GLU:HG2	1.99	0.45
2:I:160:ALA:HB2	2:I:310:LEU:HD13	1.99	0.45
3:J:156:GLU:O	3:J:160:GLU:HB2	2.16	0.45
3:J:102:ILE:HB	3:J:579:ASP:HB3	1.99	0.45
2:I:368:THR:HB	6:N:15:TYR:HE2	1.82	0.45
1:A:28:LEU:HD13	1:A:36:LEU:HD11	1.99	0.44
1:A:56:VAL:HG22	1:A:142:VAL:HG12	1.99	0.44
2:C:209:ARG:HG3	2:C:210:GLU:N	2.32	0.44
2:C:891:GLY:HA3	2:C:991:GLN:O	2.17	0.44
3:D:1340:GLY:O	3:D:1344:VAL:HG23	2.17	0.44
3:D:521:PRO:HA	3:D:522:PRO:HD3	1.78	0.44
1:G:71:VAL:HG11	1:G:78:ILE:HD11	1.98	0.44
1:H:214:ALA:O	1:H:218:LEU:HD13	2.16	0.44
2:I:1102:LEU:HA	2:I:1107:ASN:O	2.17	0.44
3:J:16:GLU:H	3:J:16:GLU:CD	2.19	0.44
3:J:365:GLU:HG2	3:J:366:LYS:H	1.82	0.44
7:O:39:DT:C2'	7:O:40:DC:H5'	2.44	0.44
3:D:1170:ASP:O	3:D:1174:LEU:HG	2.18	0.44
5:F:187:ARG:O	5:F:191:ILE:HG13	2.16	0.44
1:G:56:VAL:HG22	1:G:142:VAL:HG12	1.99	0.44
1:H:63:HIS:CD2	1:H:64:GLU:H	2.35	0.44
1:H:73:GLU:HB2	1:H:78:ILE:HD11	1.99	0.44
2:I:1008:ARG:NH1	2:I:1028:GLY:HA2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1089:VAL:O	2:I:1093:GLN:HG2	2.16	0.44
2:I:111:ASP:HA	6:N:45:SER:CB	2.47	0.44
2:I:446:GLY:O	2:I:449:ILE:HG13	2.18	0.44
5:L:336:ILE:HD11	5:L:344:TYR:HD2	1.82	0.44
6:M:18:GLY:HA3	6:M:40:PHE:HA	1.99	0.44
2:C:327:HIS:O	2:C:331:ARG:HG3	2.17	0.44
2:C:36:PRO:CB	2:C:70:GLU:HG2	2.46	0.44
2:C:838:LYS:HD3	2:C:999:HIS:HB2	1.99	0.44
3:D:1221:VAL:HA	3:D:1224:VAL:HB	2.00	0.44
3:D:248:PRO:HA	3:D:307:GLY:O	2.17	0.44
5:F:360:ALA:O	5:F:364:LEU:HB2	2.17	0.44
1:G:28:LEU:HD13	1:G:36:LEU:HD11	2.00	0.44
2:I:1066:ALA:O	2:I:1070:ILE:HD12	2.17	0.44
2:I:64:LEU:HD11	2:I:100:LEU:HD11	2.00	0.44
5:L:149:LYS:HB3	5:L:193:ARG:HH12	1.81	0.44
1:B:211:LEU:O	1:B:215:VAL:HG13	2.17	0.44
1:B:36:LEU:C	1:B:39:PRO:HD2	2.37	0.44
2:C:1019:GLN:OE1	3:D:621:LYS:HE3	2.18	0.44
2:C:1035:MET:SD	8:P:12:DT:H4'	2.57	0.44
2:C:484:VAL:HG12	2:C:486:MET:H	1.82	0.44
3:D:470:LEU:HD11	3:D:502:PHE:HB3	2.00	0.44
3:D:550:ARG:HG3	3:D:553:ARG:HH21	1.82	0.44
3:D:566:ILE:HG23	5:F:229:GLN:HE22	1.83	0.44
4:E:41:GLU:O	4:E:45:ARG:HG2	2.18	0.44
1:H:101:LEU:HD22	1:H:102:ARG:H	1.82	0.44
2:I:708:TYR:CE2	2:I:792:VAL:HG23	2.52	0.44
3:J:1003:VAL:HG21	3:J:1041:MET:HB3	1.99	0.44
3:J:1170:ASP:O	3:J:1174:LEU:HG	2.17	0.44
2:I:1038:TRP:O	3:J:1223:VAL:HG11	2.17	0.44
3:J:702:LEU:HG	3:J:747:VAL:HG22	1.99	0.44
6:N:17:VAL:HG13	6:N:138:GLU:HB3	1.98	0.44
1:B:87:VAL:HG12	1:B:122:ILE:HG12	2.00	0.44
1:A:133:GLU:OE1	2:C:605:LYS:HB2	2.17	0.44
2:C:658:GLY:N	2:C:661:SER:HB3	2.33	0.44
3:D:1003:VAL:HG21	3:D:1041:MET:HB3	1.99	0.44
3:D:1209:LEU:HA	3:D:1209:LEU:HD23	1.73	0.44
3:D:1190:SER:HB2	3:D:1369:GLU:OE1	2.18	0.44
3:D:32:ILE:HA	3:D:40:GLU:HG2	2.00	0.44
3:D:894:LYS:H	3:D:894:LYS:HG2	1.53	0.44
2:I:484:VAL:HG12	2:I:486:MET:H	1.83	0.44
3:J:1172:HIS:O	3:J:1175:ILE:HB	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:205:TYR:CD2	3:J:387:LEU:HD22	2.53	0.44
3:J:59:ALA:HB2	3:J:78:VAL:HG21	1.98	0.44
2:I:946:ARG:HH12	3:J:860:LEU:HD13	1.82	0.44
3:J:566:ILE:HG23	5:L:229:GLN:HE22	1.82	0.44
6:N:11:VAL:HG22	6:N:17:VAL:HG12	1.98	0.44
7:O:17:DA:H1'	7:O:18:DA:H5''	1.98	0.44
7:O:21:DG:N2	8:P:28:DC:O2	2.51	0.44
1:A:94:MET:O	1:A:146:ARG:HD3	2.17	0.44
2:C:683:ASN:HB2	2:C:872:ASN:HB3	1.99	0.44
3:D:314:PRO:HB2	3:D:317:MET:HG3	2.00	0.44
2:I:166:PRO:C	2:I:168:ARG:H	2.21	0.44
2:I:773:LEU:HD22	5:L:390:LEU:HD11	1.99	0.44
2:I:838:LYS:HD3	2:I:999:HIS:HB2	2.00	0.44
2:I:549:PHE:CE1	2:I:909:ALA:HB3	2.53	0.44
3:J:101:HIS:HB3	3:J:104:PHE:CZ	2.52	0.44
3:J:130:ASN:O	3:J:456:MET:HE1	2.18	0.44
3:J:1197:ARG:NE	3:J:1398:TRP:HB3	2.32	0.44
3:J:1495:ILE:HD13	4:K:80:VAL:HG21	1.99	0.44
5:L:252:THR:O	5:L:256:TRP:HD1	2.01	0.44
5:L:266:ILE:O	5:L:270:ALA:HB2	2.18	0.44
8:P:40:DT:H1'	8:P:41:DT:H5'	1.99	0.44
2:C:154:ARG:HB2	2:C:157:ARG:HB2	1.99	0.44
2:C:200:LEU:HA	2:C:200:LEU:HD12	1.82	0.44
3:D:1122:LEU:H	3:D:1122:LEU:HD12	1.82	0.44
3:D:353:VAL:HG22	3:D:355:VAL:H	1.82	0.44
3:J:471:GLU:O	3:J:475:ARG:HG2	2.17	0.44
3:J:465:LEU:HD12	3:J:513:ILE:HD11	1.99	0.44
3:J:911:LEU:O	3:J:915:VAL:HG23	2.17	0.44
6:M:84:LYS:HE2	6:M:84:LYS:HB2	1.79	0.44
2:C:650:LYS:HG2	2:C:651:LYS:H	1.82	0.44
2:C:708:TYR:CE2	2:C:792:VAL:HG23	2.53	0.44
3:D:1093:TYR:HD1	8:P:10:DA:H5''	1.82	0.44
3:D:130:ASN:O	3:D:456:MET:HE1	2.18	0.44
3:D:520:LEU:HD12	3:D:521:PRO:HD2	1.99	0.44
3:D:675:ARG:HH12	5:F:437:LEU:H	1.65	0.44
1:H:156:HIS:NE2	1:H:167:VAL:O	2.51	0.44
2:I:324:ASP:O	2:I:330:ASN:ND2	2.51	0.44
2:I:724:ARG:HD3	2:I:741:GLY:N	2.33	0.44
2:I:440:PRO:HB2	3:J:1074:SER:OG	2.18	0.44
3:J:834:THR:HG21	3:J:839:LEU:HD21	1.98	0.44
1:A:82:LEU:O	1:A:85:LEU:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1102:LEU:CD2	3:D:9:ARG:HB2	2.48	0.44
2:C:1116:ALA:HA	3:D:23:TYR:OH	2.18	0.44
2:C:166:PRO:C	2:C:168:ARG:H	2.22	0.44
2:C:716:LYS:H	2:C:716:LYS:HG2	1.59	0.44
2:C:72:ARG:N	2:C:95:TYR:O	2.49	0.44
3:D:1090:ASP:O	3:D:1093:TYR:HB3	2.18	0.44
3:D:1495:ILE:HD13	4:E:80:VAL:HG21	1.99	0.44
3:D:895:VAL:O	3:D:898:GLU:HB3	2.18	0.44
5:F:336:ILE:HD11	5:F:344:TYR:HD2	1.81	0.44
1:G:209:GLU:HA	1:G:212:ASN:HB2	2.00	0.44
2:I:1019:GLN:OE1	3:J:621:LYS:HE3	2.18	0.44
2:I:46:ALA:O	2:I:50:GLU:HB2	2.18	0.44
2:I:501:THR:O	2:I:503:LEU:HG	2.18	0.44
1:G:133:GLU:OE1	2:I:605:LYS:HB2	2.18	0.44
5:L:375:LYS:HD2	5:L:426:HIS:ND1	2.32	0.44
2:C:211:LEU:HD22	2:C:218:VAL:HA	2.00	0.43
2:C:328:LEU:HD21	2:C:434:HIS:HA	2.00	0.43
2:C:446:GLY:O	2:C:449:ILE:HG13	2.17	0.43
2:C:673:LEU:HD12	2:C:673:LEU:H	1.83	0.43
3:D:171:LEU:HD21	3:D:175:VAL:O	2.17	0.43
2:C:1067:TYR:CE2	5:F:357:VAL:HA	2.53	0.43
3:D:670:VAL:HB	5:F:364:LEU:HD11	2.00	0.43
2:I:230:ARG:NH2	2:I:231:PRO:HD2	2.28	0.43
2:I:874:LEU:HD22	3:J:1029:ARG:HB2	2.00	0.43
2:I:72:ARG:N	2:I:95:TYR:O	2.49	0.43
3:J:1267:ARG:HE	3:J:1267:ARG:HB2	1.63	0.43
3:J:129:PHE:CE1	3:J:457:GLY:HA3	2.53	0.43
3:J:400:VAL:HG12	3:J:445:ARG:HG2	1.99	0.43
3:D:622:ARG:NH1	8:P:14:DG:OP2	2.51	0.43
1:A:206:THR:HG23	1:A:209:GLU:OE2	2.17	0.43
2:C:160:ALA:HB2	2:C:310:LEU:HD13	1.99	0.43
2:C:751:PRO:HD2	3:D:681:ARG:HD2	2.00	0.43
3:D:1172:HIS:O	3:D:1175:ILE:HB	2.18	0.43
3:D:1433:SER:HB3	3:D:1464:GLU:CD	2.39	0.43
2:C:946:ARG:HH12	3:D:860:LEU:HD13	1.83	0.43
3:D:762:GLN:CB	4:E:16:LYS:HE2	2.48	0.43
3:D:439:LEU:HD11	5:F:190:HIS:CB	2.48	0.43
5:F:266:ILE:O	5:F:270:ALA:HB2	2.18	0.43
2:I:1081:VAL:HG21	2:I:1086:ARG:CZ	2.48	0.43
2:I:19:THR:HG22	2:I:407:LYS:HZ1	1.82	0.43
2:I:3:ILE:HG13	2:I:900:ARG:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:905:VAL:HG12	2:I:906:PHE:CD2	2.53	0.43
2:I:892:LEU:HD13	2:I:989:VAL:HG23	2.00	0.43
3:J:1072:ILE:O	3:J:1075:HIS:HB2	2.18	0.43
3:J:1208:ASP:HB3	3:J:1211:MET:HB2	2.00	0.43
4:K:42:PRO:HA	4:K:45:ARG:HG3	1.99	0.43
4:K:30:LEU:HD11	4:K:67:GLU:OE2	2.17	0.43
5:L:124:GLY:O	5:L:128:ILE:HG13	2.18	0.43
1:A:179:PHE:HD1	1:A:195:LEU:HD21	1.84	0.43
2:C:1006:HIS:HB2	2:C:1024:LYS:HG3	2.00	0.43
2:C:1066:ALA:O	2:C:1070:ILE:HD12	2.18	0.43
2:C:683:ASN:C	2:C:687:ALA:HB3	2.39	0.43
2:C:769:PRO:HB3	5:F:390:LEU:HA	1.99	0.43
2:C:773:LEU:HD22	5:F:390:LEU:HD11	2.01	0.43
3:D:123:LEU:HG	3:D:127:LEU:HD12	1.99	0.43
3:D:1225:ALA:HA	3:D:1367:HIS:HB3	2.00	0.43
3:D:716:PHE:CZ	3:D:728:LEU:HD11	2.54	0.43
1:G:206:THR:HG23	1:G:209:GLU:OE2	2.19	0.43
1:H:87:VAL:HG12	1:H:122:ILE:HG12	2.00	0.43
2:I:327:HIS:O	2:I:331:ARG:HG3	2.17	0.43
2:I:351:LEU:HD11	2:I:374:ASN:H	1.84	0.43
2:I:376:ARG:O	2:I:380:ALA:HB3	2.19	0.43
3:J:1225:ALA:HA	3:J:1367:HIS:HB3	2.00	0.43
3:J:675:ARG:HD3	5:L:435:ASP:OD2	2.18	0.43
4:K:45:ARG:HD2	4:K:63:TRP:CH2	2.54	0.43
6:M:67:GLU:OE2	6:M:103:TYR:OH	2.36	0.43
1:A:63:HIS:CE1	1:A:66:SER:HB2	2.53	0.43
2:C:166:PRO:HA	7:O:37:DT:H71	2.01	0.43
2:C:440:PRO:HB2	3:D:1074:SER:OG	2.18	0.43
3:D:1127:GLU:C	3:D:1129:THR:H	2.22	0.43
3:D:475:ARG:O	3:D:478:LEU:HB2	2.19	0.43
3:D:465:LEU:HD12	3:D:513:ILE:HD11	2.00	0.43
3:D:702:LEU:HG	3:D:747:VAL:HG22	1.99	0.43
4:E:31:LEU:HG	4:E:60:ALA:HB2	2.00	0.43
4:E:42:PRO:HA	4:E:45:ARG:HG3	1.99	0.43
1:G:158:ILE:HG13	1:G:166:PRO:HG3	2.00	0.43
1:G:71:VAL:HG21	1:G:138:LEU:HD22	2.01	0.43
2:I:181:VAL:HG22	2:I:182:VAL:H	1.83	0.43
2:I:20:GLU:O	2:I:24:GLU:N	2.44	0.43
2:I:683:ASN:HB2	2:I:872:ASN:HB3	1.99	0.43
3:J:1090:ASP:O	3:J:1093:TYR:HB3	2.19	0.43
3:J:1208:ASP:N	3:J:1213:ARG:O	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:895:VAL:O	3:J:898:GLU:HB3	2.18	0.43
1:B:101:LEU:HD22	1:B:102:ARG:N	2.33	0.43
2:C:1008:ARG:NH1	2:C:1028:GLY:HA2	2.31	0.43
2:C:1067:TYR:CE1	3:D:655:PRO:HG3	2.53	0.43
2:C:219:GLN:H	2:C:219:GLN:HG3	1.60	0.43
3:D:107:ASP:HA	3:D:586:ARG:HH21	1.84	0.43
3:D:1167:SER:H	3:D:1170:ASP:HB2	1.83	0.43
1:G:110:ARG:HA	1:G:129:ILE:HG12	2.00	0.43
1:G:53:VAL:HG22	1:G:54:THR:N	2.31	0.43
1:G:63:HIS:CE1	1:G:66:SER:HB2	2.53	0.43
2:I:1044:GLY:HA3	4:K:17:TYR:CE1	2.53	0.43
2:I:427:VAL:HG22	7:R:38:DG:N2	2.26	0.43
2:I:650:LYS:HG2	2:I:651:LYS:H	1.83	0.43
2:I:781:LYS:HE2	2:I:782:ALA:O	2.19	0.43
5:L:238:ALA:HB2	5:L:257:TRP:CG	2.54	0.43
8:P:24:DA:P	8:P:24:DA:H3'	2.58	0.43
1:B:174:VAL:HA	1:B:200:TRP:O	2.19	0.43
2:C:140:ILE:HG23	2:C:412:ALA:HA	1.99	0.43
2:C:501:THR:O	2:C:503:LEU:HG	2.19	0.43
2:C:781:LYS:HE2	2:C:782:ALA:O	2.18	0.43
2:C:5:ARG:HB2	2:C:902:ILE:HB	2.01	0.43
3:D:132:TYR:HB3	3:D:454:ALA:HB1	2.00	0.43
3:D:897:GLN:HE21	3:D:897:GLN:HB3	1.66	0.43
3:D:439:LEU:HD11	5:F:190:HIS:HB3	2.01	0.43
1:G:58:ILE:HG22	1:G:60:ASP:N	2.33	0.43
1:H:101:LEU:HD22	1:H:102:ARG:N	2.32	0.43
1:H:64:GLU:HG3	1:H:165:ILE:HG21	1.98	0.43
2:I:1055:ILE:HD11	2:I:1079:PRO:HD3	2.01	0.43
2:I:754:ILE:HA	2:I:791:ARG:HA	2.01	0.43
3:J:362:GLN:HB2	3:J:365:GLU:HB2	2.00	0.43
3:J:44:LEU:HD21	3:J:544:TYR:HB3	2.01	0.43
3:J:561:GLY:HA2	5:L:151:LEU:HD22	2.00	0.43
3:J:762:GLN:CB	4:K:16:LYS:HE2	2.49	0.43
6:M:22:GLY:O	6:M:36:TYR:HA	2.19	0.43
5:F:241:LYS:HE2	7:O:24:DC:H3'	1.99	0.43
2:I:1023:GLY:HA2	8:S:15:DA:P	2.58	0.43
2:C:46:ALA:O	2:C:50:GLU:HB2	2.18	0.43
2:C:760:SER:O	2:C:785:VAL:HA	2.19	0.43
3:D:372:ASP:HB3	3:D:374:GLU:HG3	2.00	0.43
3:D:475:ARG:HG2	3:D:475:ARG:H	1.67	0.43
3:D:930:LEU:O	3:D:934:LEU:HD12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:999:HIS:CD2	2:I:1004:LYS:HE3	2.54	0.43
2:I:1102:LEU:CD2	3:J:9:ARG:HB2	2.49	0.43
3:J:508:ARG:HB2	3:J:511:TRP:CE2	2.53	0.43
6:M:80:MET:HB3	6:M:107:GLN:HG2	1.99	0.43
6:M:85:GLN:HG2	6:M:85:GLN:H	1.58	0.43
1:A:110:ARG:HA	1:A:129:ILE:HG12	2.00	0.43
2:C:1102:LEU:HA	2:C:1107:ASN:O	2.17	0.43
2:C:276:LYS:HD3	2:C:466:PHE:CZ	2.54	0.43
2:C:537:LYS:HZ3	2:C:905:VAL:N	2.12	0.43
2:C:549:PHE:HB3	2:C:552:HIS:CD2	2.53	0.43
2:C:946:ARG:NH2	3:D:860:LEU:H	2.17	0.43
3:D:1191:PRO:O	3:D:1373:ARG:HD3	2.19	0.43
3:D:129:PHE:CE1	3:D:457:GLY:HA3	2.54	0.43
3:D:51:GLY:HA3	3:D:85:VAL:HG23	2.00	0.43
3:D:54:LYS:HD3	3:D:55:ASP:N	2.34	0.43
3:D:646:LYS:HD2	3:D:722:GLU:OE1	2.18	0.43
3:D:911:LEU:O	3:D:915:VAL:HG23	2.18	0.43
2:C:1044:GLY:HA3	4:E:17:TYR:CE1	2.53	0.43
2:I:1007:ALA:HB2	3:J:648:MET:HG3	2.01	0.43
2:I:1016:ILE:HG13	2:I:1017:THR:H	1.83	0.43
2:I:751:PRO:HA	2:I:792:VAL:HG13	2.00	0.43
3:J:537:THR:C	5:L:332:LEU:HG	2.39	0.43
4:K:41:GLU:O	4:K:45:ARG:HG2	2.18	0.43
6:M:18:GLY:CA	6:M:41:PRO:HD3	2.47	0.43
7:R:43:DG:H1	8:S:6:DC:H42	1.67	0.43
2:C:1018:GLN:HB2	2:C:1058:ASP:HB2	2.00	0.43
2:C:1081:VAL:HG21	2:C:1086:ARG:CZ	2.49	0.43
2:C:1092:LEU:HD22	2:C:1097:LEU:HD13	2.00	0.43
3:D:248:PRO:HG3	3:D:308:LYS:HD3	2.00	0.43
3:D:632:VAL:O	3:D:727:GLN:HA	2.19	0.43
1:G:179:PHE:HD1	1:G:195:LEU:HD21	1.83	0.43
2:I:1090:LYS:HD2	2:I:1090:LYS:HA	1.72	0.43
2:I:208:VAL:HA	2:I:211:LEU:HB2	2.00	0.43
2:I:64:LEU:HD22	2:I:359:MET:SD	2.59	0.43
2:I:726:ILE:HG23	2:I:787:ASP:HB2	2.00	0.43
2:I:874:LEU:HA	2:I:874:LEU:HD23	1.91	0.43
3:J:409:VAL:HG23	3:J:437:VAL:HG22	2.01	0.43
3:J:587:ARG:HB3	3:J:587:ARG:HE	1.62	0.43
5:L:137:LEU:HD11	5:L:178:LEU:HD11	2.00	0.43
2:C:351:LEU:HD11	2:C:374:ASN:H	1.84	0.43
2:C:874:LEU:HD22	3:D:1029:ARG:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:892:LEU:HD13	2:C:989:VAL:HG23	2.01	0.43
3:D:101:HIS:HB3	3:D:104:PHE:CZ	2.54	0.43
3:D:1480:PHE:CD2	3:D:1481:VAL:HG13	2.54	0.43
3:D:903:ASP:OD1	3:D:903:ASP:N	2.51	0.43
5:F:238:ALA:HB2	5:F:257:TRP:CG	2.54	0.43
1:H:109:VAL:HG12	1:H:129:ILE:HB	2.01	0.43
1:H:36:LEU:C	1:H:39:PRO:HD2	2.38	0.43
2:I:1082:PRO:O	2:I:1083:GLU:HB3	2.19	0.43
2:I:1081:VAL:HG21	2:I:1086:ARG:NE	2.34	0.43
2:I:159:ILE:HG13	2:I:175:GLU:HA	2.01	0.43
2:I:328:LEU:HD21	2:I:434:HIS:HA	2.01	0.43
3:J:1127:GLU:C	3:J:1129:THR:H	2.22	0.43
3:J:1167:SER:H	3:J:1170:ASP:HB2	1.84	0.43
3:J:1221:VAL:HA	3:J:1224:VAL:HB	2.01	0.43
3:J:583:ASP:OD1	3:J:586:ARG:HB2	2.18	0.43
3:J:671:LYS:HG3	5:L:436:PHE:CE2	2.54	0.43
6:N:52:GLU:HG2	6:N:52:GLU:H	1.52	0.43
6:N:36:TYR:HE2	6:N:54:PRO:HG3	1.83	0.43
2:C:1089:VAL:HG13	2:C:1099:VAL:HG11	2.00	0.42
2:C:109:LYS:HE2	6:M:40:PHE:CZ	2.53	0.42
2:C:376:ARG:O	2:C:380:ALA:HB3	2.19	0.42
1:A:42:ARG:NH1	2:C:857:ASP:HB3	2.19	0.42
3:D:1267:ARG:HB2	3:D:1267:ARG:HE	1.62	0.42
3:D:698:LYS:HB3	3:D:756:GLN:NE2	2.34	0.42
1:H:182:GLU:HG3	1:H:194:LYS:HB3	2.01	0.42
2:I:1038:TRP:CE3	3:J:1099:VAL:HG21	2.54	0.42
2:I:418:LEU:HD11	7:R:38:DG:C4	2.54	0.42
2:I:572:ILE:HD11	2:I:703:ILE:HD11	2.00	0.42
2:I:925:TYR:O	2:I:928:LYS:HB3	2.19	0.42
3:J:1122:LEU:HD12	3:J:1122:LEU:H	1.84	0.42
3:J:470:LEU:HD11	3:J:502:PHE:HB3	2.01	0.42
3:J:716:PHE:CZ	3:J:728:LEU:HD11	2.53	0.42
3:J:51:GLY:HA3	3:J:85:VAL:HG23	1.99	0.42
7:R:32:DG:H2''	7:R:33:DG:H5'	2.01	0.42
3:J:1093:TYR:CD1	8:S:10:DA:H5''	2.52	0.42
1:A:209:GLU:HA	1:A:212:ASN:HB2	2.02	0.42
1:A:48:ILE:HA	1:A:49:PRO:HD3	1.91	0.42
2:C:159:ILE:HG13	2:C:175:GLU:HA	2.01	0.42
2:C:64:LEU:HD11	2:C:100:LEU:HD11	2.01	0.42
3:D:212:ARG:HG2	3:D:344:ASP:HB3	2.01	0.42
3:D:561:GLY:HA2	5:F:151:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:691:LEU:HA	3:D:694:VAL:HG23	2.01	0.42
5:F:279:MET:O	5:F:283:ILE:HG13	2.19	0.42
5:F:431:ARG:HG3	5:F:434:ARG:NE	2.34	0.42
1:G:185:ARG:O	1:G:185:ARG:HG2	2.18	0.42
1:G:23:PHE:HE2	1:G:199:ILE:HD12	1.85	0.42
2:I:1006:HIS:HB2	2:I:1024:LYS:HG3	2.00	0.42
2:I:1116:ALA:HA	3:J:23:TYR:OH	2.19	0.42
2:I:549:PHE:HB3	2:I:552:HIS:CD2	2.54	0.42
2:I:760:SER:O	2:I:785:VAL:HA	2.20	0.42
3:J:107:ASP:HA	3:J:586:ARG:HH21	1.84	0.42
3:J:1099:VAL:O	3:J:1103:HIS:HB3	2.19	0.42
3:J:103:TRP:CH2	3:J:1444:THR:HA	2.54	0.42
3:J:209:ARG:H	3:J:390:PRO:HA	1.83	0.42
2:I:946:ARG:NH2	3:J:860:LEU:H	2.17	0.42
1:B:101:LEU:HD22	1:B:102:ARG:H	1.84	0.42
2:C:1038:TRP:CE3	3:D:1099:VAL:HG21	2.54	0.42
2:C:477:GLY:HA2	2:C:508:ILE:HG13	2.02	0.42
3:D:583:ASP:OD1	3:D:586:ARG:HB2	2.18	0.42
5:F:137:LEU:HD11	5:F:178:LEU:HD11	2.00	0.42
2:I:1090:LYS:HD2	2:I:1093:GLN:HG3	2.01	0.42
2:I:647:GLN:HE21	2:I:647:GLN:HB2	1.52	0.42
3:J:1340:GLY:O	3:J:1344:VAL:HG23	2.18	0.42
3:J:68:PHE:CZ	5:L:394:ARG:HD2	2.54	0.42
3:J:752:SER:O	3:J:756:GLN:N	2.50	0.42
3:J:789:LEU:HD23	3:J:882:PHE:HE1	1.84	0.42
3:J:914:LEU:HD13	3:J:914:LEU:HA	1.84	0.42
5:L:108:LEU:O	5:L:109:LEU:HB3	2.19	0.42
5:L:199:ARG:HG3	5:L:239:VAL:HG11	2.02	0.42
3:D:706:PRO:HG3	8:P:11:DG:H21	1.83	0.42
8:S:40:DT:H1'	8:S:41:DT:H5'	2.02	0.42
1:A:54:THR:O	1:A:167:VAL:HG22	2.19	0.42
1:B:109:VAL:HG12	1:B:129:ILE:HB	2.01	0.42
1:B:176:ARG:HG2	1:B:177:VAL:N	2.34	0.42
2:C:1007:ALA:HB2	3:D:648:MET:HG3	2.02	0.42
2:C:1081:VAL:HG21	2:C:1086:ARG:NE	2.35	0.42
2:C:111:ASP:HA	6:M:45:SER:HB2	2.00	0.42
2:C:208:VAL:HA	2:C:211:LEU:HB2	2.00	0.42
2:C:374:ASN:HD22	2:C:375:SER:N	2.17	0.42
2:C:16:PRO:HB2	2:C:460:ARG:NH2	2.34	0.42
2:C:614:ARG:HH21	2:C:620:LEU:HD23	1.84	0.42
2:C:881:ASN:OD1	2:C:884:GLN:NE2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1208:ASP:HB3	3:D:1211:MET:HB2	2.00	0.42
3:D:407:VAL:HG23	3:D:422:ALA:HB2	2.00	0.42
3:D:508:ARG:HB2	3:D:511:TRP:CE2	2.54	0.42
3:D:752:SER:O	3:D:756:GLN:N	2.49	0.42
3:D:795:VAL:HG13	3:D:879:ARG:NH2	2.34	0.42
3:D:970:LYS:O	3:D:973:GLN:HB3	2.20	0.42
4:E:30:LEU:HD11	4:E:67:GLU:OE2	2.18	0.42
5:F:135:THR:HG21	5:F:177:LYS:HG2	2.01	0.42
1:G:99:LEU:HB2	1:G:142:VAL:HG23	2.02	0.42
1:G:54:THR:O	1:G:167:VAL:HG22	2.19	0.42
1:G:36:LEU:HD12	1:G:195:LEU:HD12	2.01	0.42
2:I:477:GLY:HA2	2:I:508:ILE:HG13	2.01	0.42
3:J:1191:PRO:O	3:J:1373:ARG:HD3	2.20	0.42
3:J:141:VAL:HG12	3:J:450:TYR:CE2	2.52	0.42
3:J:32:ILE:HA	3:J:40:GLU:HG2	2.01	0.42
3:J:132:TYR:HB3	3:J:454:ALA:HB1	2.00	0.42
3:J:475:ARG:O	3:J:478:LEU:HB2	2.19	0.42
3:J:658:LEU:HD21	3:J:670:VAL:O	2.20	0.42
3:J:691:LEU:HA	3:J:694:VAL:HG23	2.01	0.42
3:J:698:LYS:HB3	3:J:756:GLN:NE2	2.34	0.42
3:J:795:VAL:HG13	3:J:879:ARG:NH2	2.34	0.42
3:J:884:ARG:NE	3:J:888:GLU:OE2	2.52	0.42
5:L:135:THR:HG21	5:L:177:LYS:HG2	2.02	0.42
1:B:73:GLU:HB2	1:B:78:ILE:HD11	2.02	0.42
2:C:1082:PRO:O	2:C:1083:GLU:HB3	2.18	0.42
2:C:198:ARG:HG2	2:C:234:ALA:HB3	2.02	0.42
2:C:549:PHE:CE1	2:C:909:ALA:HB3	2.54	0.42
2:C:999:HIS:CD2	2:C:1004:LYS:HE3	2.54	0.42
3:D:1114:THR:OG1	3:D:1116:ASN:ND2	2.48	0.42
3:D:118:LEU:HD12	3:D:123:LEU:HB2	2.01	0.42
3:D:44:LEU:HD21	3:D:544:TYR:HB3	2.01	0.42
3:D:720:LEU:HD23	3:D:720:LEU:HA	1.90	0.42
3:D:638:LYS:C	3:D:729:HIS:HD2	2.22	0.42
5:F:380:GLU:HB2	5:F:415:ILE:HG23	2.02	0.42
2:I:1092:LEU:HD22	2:I:1097:LEU:HD13	2.00	0.42
2:I:683:ASN:C	2:I:687:ALA:HB3	2.40	0.42
2:I:688:ILE:HG23	2:I:871:LEU:HD23	2.02	0.42
2:I:77:PRO:HD3	2:I:92:ALA:HA	2.00	0.42
2:I:810:ASP:O	2:I:813:VAL:HG12	2.19	0.42
3:J:1190:SER:HB2	3:J:1369:GLU:OE1	2.20	0.42
3:J:1480:PHE:CD2	3:J:1481:VAL:HG13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:421:LEU:CD2	3:J:422:ALA:H	2.32	0.42
3:J:649:ALA:HB3	3:J:720:LEU:HD21	2.00	0.42
6:N:129:LEU:O	6:N:133:ILE:HG12	2.19	0.42
1:A:71:VAL:HG21	1:A:138:LEU:HD22	2.01	0.42
1:B:100:ILE:HG22	1:B:141:GLU:HB3	2.02	0.42
2:C:1017:THR:OG1	2:C:1019:GLN:HG2	2.20	0.42
2:C:1056:LYS:HG3	3:D:751:LEU:HD11	2.02	0.42
2:C:179:SER:OG	2:C:181:VAL:HG12	2.20	0.42
2:C:39:ARG:HD3	2:C:45:GLN:OE1	2.20	0.42
2:C:925:TYR:O	2:C:928:LYS:HB3	2.19	0.42
3:D:171:LEU:HD23	3:D:172:PRO:O	2.19	0.42
3:D:181:ASP:HB2	3:D:205:TYR:CE2	2.54	0.42
5:F:199:ARG:HG3	5:F:239:VAL:HG11	2.02	0.42
2:I:99:GLN:HB3	2:I:110:GLU:HG3	2.01	0.42
2:I:247:PRO:HA	2:I:248:PRO:HD3	1.76	0.42
2:I:891:GLY:HA3	2:I:991:GLN:O	2.19	0.42
3:J:167:GLU:HB3	3:J:395:VAL:HG12	2.01	0.42
3:J:632:VAL:O	3:J:727:GLN:HA	2.19	0.42
4:K:50:THR:HB	4:K:53:GLY:O	2.20	0.42
3:J:553:ARG:NH2	5:L:226:ASP:OD1	2.47	0.42
1:B:182:GLU:HG3	1:B:194:LYS:HB3	2.01	0.42
2:C:181:VAL:HG22	2:C:182:VAL:H	1.84	0.42
2:C:524:VAL:HB	2:C:528:GLU:HG3	2.01	0.42
2:C:77:PRO:HD3	2:C:92:ALA:HA	2.01	0.42
3:D:176:ASP:OD2	3:D:388:HIS:HB3	2.19	0.42
2:C:1031:ARG:HA	3:D:622:ARG:HA	2.02	0.42
5:F:252:THR:O	5:F:256:TRP:HD1	2.03	0.42
1:G:180:GLN:HB3	2:I:934:PHE:CZ	2.54	0.42
2:I:524:VAL:HB	2:I:528:GLU:HG3	2.00	0.42
2:I:441:VAL:O	2:I:559:LEU:HD12	2.20	0.42
2:I:946:ARG:HH22	3:J:860:LEU:HD13	1.84	0.42
2:I:954:SER:HA	2:I:955:PRO:HD3	1.85	0.42
3:J:1008:PHE:O	3:J:1012:GLU:HG3	2.20	0.42
3:J:1103:HIS:HE1	3:J:1464:GLU:HG3	1.84	0.42
3:J:397:LYS:HE3	3:J:448:GLU:O	2.19	0.42
3:J:520:LEU:HD12	3:J:521:PRO:HD2	2.01	0.42
3:J:593:ASN:HA	3:J:594:PRO:HD3	1.91	0.42
3:D:610:LYS:NZ	8:P:10:DA:OP2	2.28	0.42
1:A:180:GLN:HB3	2:C:934:PHE:CZ	2.55	0.42
2:C:122:THR:OG1	2:C:126:SER:O	2.35	0.42
3:D:514:LEU:HD11	3:D:516:ALA:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:914:LEU:HA	3:D:914:LEU:HD13	1.84	0.42
5:F:114:GLU:OE1	5:F:249:LYS:HD2	2.20	0.42
2:I:848:VAL:HG22	3:J:740:PHE:O	2.20	0.42
3:J:1268:PRO:HB2	3:J:1271:LYS:HB2	2.02	0.42
3:J:930:LEU:O	3:J:934:LEU:HD12	2.19	0.42
5:L:370:GLU:O	5:L:373:LEU:HB3	2.20	0.42
6:M:131:ARG:HA	6:M:131:ARG:HD2	1.89	0.42
1:B:76:VAL:O	1:B:80:LEU:HD22	2.20	0.42
2:C:1056:LYS:HE3	2:C:1056:LYS:HB2	1.84	0.42
2:C:109:LYS:HG2	6:M:15:TYR:OH	2.20	0.42
2:C:946:ARG:HH22	3:D:860:LEU:HD13	1.85	0.42
2:C:99:GLN:HB3	2:C:110:GLU:HG3	2.00	0.42
3:D:1462:LEU:HG	3:D:1462:LEU:H	1.71	0.42
3:D:789:LEU:HD23	3:D:882:PHE:HE1	1.84	0.42
4:E:45:ARG:HD2	4:E:63:TRP:CH2	2.55	0.42
1:H:174:VAL:HA	1:H:200:TRP:O	2.19	0.42
1:H:58:ILE:HG23	1:H:140:MET:HB3	2.02	0.42
2:I:1019:GLN:HE21	3:J:617:ASN:HB3	1.85	0.42
2:I:179:SER:OG	2:I:181:VAL:HG12	2.20	0.42
2:I:1031:ARG:HA	3:J:622:ARG:HA	2.02	0.42
3:J:720:LEU:HD23	3:J:720:LEU:HA	1.90	0.42
5:L:376:LEU:HD21	5:L:423:LEU:HG	2.02	0.42
8:S:24:DA:OP1	8:S:24:DA:H3'	2.20	0.42
1:A:58:ILE:HG22	1:A:60:ASP:N	2.34	0.42
2:C:1090:LYS:HD2	2:C:1093:GLN:HG3	2.00	0.42
2:C:91:GLN:HA	2:C:119:PRO:HA	2.02	0.42
2:C:349:ALA:O	2:C:353:ARG:HG2	2.19	0.42
2:C:72:ARG:CB	2:C:95:TYR:HB2	2.46	0.42
3:D:494:LYS:O	3:D:497:GLU:HB3	2.19	0.42
3:D:658:LEU:HD21	3:D:670:VAL:O	2.20	0.42
2:C:848:VAL:HG22	3:D:740:PHE:O	2.20	0.42
4:E:50:THR:HB	4:E:53:GLY:O	2.20	0.42
2:I:200:LEU:HA	2:I:200:LEU:HD12	1.83	0.42
2:I:16:PRO:HB2	2:I:460:ARG:NH2	2.34	0.42
2:I:934:PHE:HD2	2:I:934:PHE:HA	1.62	0.42
2:I:552:HIS:ND1	3:J:1061:PHE:O	2.50	0.42
3:J:161:LEU:HA	3:J:161:LEU:HD12	1.78	0.42
3:J:508:ARG:HB3	3:J:510:GLU:CD	2.40	0.42
3:J:62:LYS:HD2	3:J:75:ARG:HD2	2.02	0.42
3:J:623:VAL:HB	3:J:748:HIS:CE1	2.55	0.42
4:K:39:VAL:HG21	4:K:72:ARG:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:111:LEU:HD22	5:L:111:LEU:H	1.85	0.42
5:L:206:ASN:O	5:L:209:LEU:HB3	2.20	0.42
6:N:116:GLU:HB2	6:N:121:LEU:HD22	2.02	0.42
8:P:22:DT:H4'	8:P:23:DA:OP1	2.19	0.42
1:B:85:LEU:HD12	1:B:124:ASN:HB3	2.01	0.41
2:C:441:VAL:O	2:C:559:LEU:HD12	2.20	0.41
3:D:585:GLY:CA	3:D:590:PRO:HG3	2.50	0.41
3:D:640:HIS:H	3:D:640:HIS:CD2	2.38	0.41
3:D:660:LYS:HD2	3:D:694:VAL:HG22	2.02	0.41
3:D:682:ASP:C	3:D:684:LYS:H	2.24	0.41
2:C:1115:LEU:HD23	3:D:85:VAL:HG12	2.01	0.41
5:F:388:LYS:HA	5:F:388:LYS:HD3	1.73	0.41
2:I:91:GLN:HA	2:I:119:PRO:HA	2.02	0.41
2:I:39:ARG:HD3	2:I:45:GLN:OE1	2.20	0.41
3:J:1014:ASN:O	3:J:1016:PRO:HD3	2.20	0.41
3:J:103:TRP:CE2	3:J:1444:THR:HG23	2.55	0.41
3:J:1331:ASP:HA	3:J:1332:PRO:HD3	1.90	0.41
6:N:12:LEU:HD23	6:N:40:PHE:CZ	2.55	0.41
6:N:136:LEU:HB3	6:N:155:PHE:CZ	2.55	0.41
2:I:1023:GLY:HA2	8:S:15:DA:OP2	2.20	0.41
1:A:23:PHE:HE2	1:A:199:ILE:HD12	1.85	0.41
1:A:36:LEU:HD12	1:A:195:LEU:HD12	2.01	0.41
1:B:115:THR:HA	1:B:116:PRO:HD3	1.90	0.41
1:B:176:ARG:HD2	3:D:884:ARG:NH2	2.30	0.41
2:C:594:ALA:HB1	2:C:654:LEU:HD11	2.01	0.41
2:C:688:ILE:HG23	2:C:871:LEU:HD23	2.02	0.41
3:D:1008:PHE:O	3:D:1012:GLU:HG3	2.20	0.41
3:D:1099:VAL:O	3:D:1103:HIS:HB3	2.20	0.41
3:D:1268:PRO:HB2	3:D:1271:LYS:HB2	2.03	0.41
3:D:260:GLU:O	3:D:270:ILE:HA	2.20	0.41
3:D:313:LEU:HG	3:D:314:PRO:CD	2.50	0.41
3:D:659:LYS:O	3:D:662:GLU:HB3	2.20	0.41
3:D:884:ARG:NE	3:D:888:GLU:OE2	2.53	0.41
3:D:976:GLN:HG2	3:J:807:ALA:CB	2.50	0.41
1:H:176:ARG:HG3	3:J:850:LEU:HD22	2.02	0.41
2:I:198:ARG:HG2	2:I:234:ALA:HB3	2.02	0.41
2:I:724:ARG:NE	2:I:739:GLU:O	2.51	0.41
2:I:751:PRO:HB2	2:I:794:PRO:HA	2.02	0.41
2:I:5:ARG:HB2	2:I:902:ILE:HB	2.02	0.41
3:J:1194:CYS:SG	3:J:1196:THR:OG1	2.69	0.41
5:L:380:GLU:HB2	5:L:415:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ASP:O	1:A:61:VAL:HB	2.20	0.41
2:C:108:ILE:HD11	6:M:28:VAL:HG21	2.02	0.41
2:C:3:ILE:HG13	2:C:900:ARG:HG3	2.02	0.41
3:D:103:TRP:CH2	3:D:1444:THR:HA	2.55	0.41
3:D:225:ILE:HG23	3:D:229:ALA:HB3	2.02	0.41
3:D:351:MET:HB3	3:D:368:VAL:HG12	2.02	0.41
2:I:325:ILE:HG23	2:I:326:ASP:H	1.84	0.41
2:I:376:ARG:HG2	2:I:376:ARG:H	1.58	0.41
2:I:599:GLU:HA	2:I:651:LYS:HB3	2.03	0.41
2:I:614:ARG:HH21	2:I:620:LEU:HD23	1.84	0.41
3:J:1042:ARG:NE	3:J:1061:PHE:HE2	2.18	0.41
3:J:1209:LEU:HA	3:J:1209:LEU:HD23	1.72	0.41
3:J:585:GLY:CA	3:J:590:PRO:HG3	2.50	0.41
3:J:653:PHE:HB2	3:J:691:LEU:HD11	2.02	0.41
4:K:66:LYS:HA	4:K:69:LEU:HB2	2.02	0.41
5:L:249:LYS:HG2	7:R:29:DC:OP2	2.19	0.41
1:B:176:ARG:HG3	3:D:850:LEU:HD22	2.02	0.41
1:B:48:ILE:HA	1:B:49:PRO:HD2	1.94	0.41
3:D:1306:PRO:HB2	3:D:1308:ASP:OD1	2.21	0.41
5:F:108:LEU:O	5:F:109:LEU:HB3	2.19	0.41
3:D:675:ARG:NH1	5:F:437:LEU:H	2.19	0.41
1:G:63:HIS:CE1	1:G:66:SER:H	2.38	0.41
2:I:209:ARG:HG3	2:I:210:GLU:N	2.33	0.41
2:I:513:VAL:O	2:I:524:VAL:HG22	2.20	0.41
2:I:881:ASN:OD1	2:I:884:GLN:NE2	2.53	0.41
3:J:213:VAL:HG13	3:J:385:VAL:HG12	2.02	0.41
3:J:660:LYS:HD2	3:J:694:VAL:HG22	2.01	0.41
3:J:638:LYS:C	3:J:729:HIS:HD2	2.22	0.41
1:B:156:HIS:NE2	1:B:167:VAL:O	2.52	0.41
2:C:107:LEU:HA	6:M:50:PRO:HD3	2.03	0.41
2:C:513:VAL:O	2:C:524:VAL:HG22	2.20	0.41
3:D:1076:GLY:O	3:D:1079:LYS:HB3	2.21	0.41
3:D:186:VAL:HG12	3:D:187:LYS:N	2.36	0.41
3:D:298:VAL:HB	3:D:302:GLN:HG2	2.03	0.41
3:D:129:PHE:CE1	3:D:571:LYS:HE2	2.56	0.41
3:D:618:LEU:HD13	3:D:618:LEU:HA	1.87	0.41
3:D:623:VAL:HB	3:D:748:HIS:CE1	2.55	0.41
3:D:62:LYS:HD2	3:D:75:ARG:HD2	2.03	0.41
3:D:984:THR:O	3:D:988:ARG:HB2	2.20	0.41
4:E:39:VAL:HG21	4:E:72:ARG:HB2	2.02	0.41
1:H:100:ILE:HG22	1:H:141:GLU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1002:GLU:HA	3:J:724:GLN:OE1	2.20	0.41
1:G:170:ILE:HG23	2:I:696:LYS:HD3	2.02	0.41
5:L:279:MET:O	5:L:283:ILE:HG13	2.20	0.41
7:R:19:DT:H1'	7:R:20:DT:H5'	2.03	0.41
1:A:63:HIS:CE1	1:A:66:SER:H	2.37	0.41
2:C:1002:GLU:HA	3:D:724:GLN:OE1	2.21	0.41
2:C:872:ASN:OD1	2:C:874:LEU:HB2	2.20	0.41
3:D:314:PRO:HG3	3:D:317:MET:HE3	2.02	0.41
3:D:508:ARG:HB3	3:D:510:GLU:CD	2.41	0.41
3:D:638:LYS:HA	3:D:932:ASP:OD1	2.20	0.41
3:D:649:ALA:HB3	3:D:720:LEU:HD21	2.02	0.41
3:D:669:ASN:HD22	5:F:364:LEU:HD21	1.85	0.41
3:D:873:LEU:HD22	3:D:875:THR:HG23	2.02	0.41
5:F:370:GLU:O	5:F:373:LEU:HB3	2.21	0.41
5:F:381:ALA:O	5:F:385:LYS:HG3	2.20	0.41
1:G:82:LEU:O	1:G:85:LEU:HB3	2.20	0.41
1:H:85:LEU:HD12	1:H:124:ASN:HB3	2.02	0.41
1:H:76:VAL:O	1:H:80:LEU:HD22	2.21	0.41
2:I:1022:GLY:HA3	3:J:622:ARG:CZ	2.50	0.41
2:I:349:ALA:O	2:I:353:ARG:HG2	2.20	0.41
2:I:594:ALA:HB1	2:I:654:LEU:HD11	2.01	0.41
3:J:781:PRO:O	3:J:908:LYS:NZ	2.50	0.41
3:J:886:VAL:HG12	3:J:896:ALA:HB1	2.03	0.41
5:L:141:LEU:O	5:L:145:VAL:HG23	2.21	0.41
6:N:79:ARG:HB3	6:N:111:GLN:OE1	2.20	0.41
1:A:36:LEU:O	1:A:39:PRO:HD2	2.20	0.41
1:B:212:ASN:O	1:B:215:VAL:HG22	2.21	0.41
2:C:1085:PHE:O	2:C:1089:VAL:HG23	2.21	0.41
2:C:325:ILE:HG23	2:C:326:ASP:H	1.86	0.41
2:C:140:ILE:HB	2:C:333:ILE:HD13	2.03	0.41
2:C:64:LEU:HD22	2:C:359:MET:SD	2.60	0.41
2:C:754:ILE:HA	2:C:791:ARG:HA	2.02	0.41
3:D:1014:ASN:O	3:D:1016:PRO:HD3	2.20	0.41
5:F:206:ASN:O	5:F:209:LEU:HB3	2.21	0.41
2:I:1017:THR:OG1	2:I:1019:GLN:HG2	2.20	0.41
2:I:1018:GLN:HB2	2:I:1058:ASP:HB2	2.01	0.41
2:I:1085:PHE:O	2:I:1089:VAL:HG23	2.20	0.41
2:I:161:SER:HA	2:I:172:ILE:O	2.21	0.41
3:J:1335:LEU:HA	3:J:1338:ALA:HB3	2.03	0.41
3:J:171:LEU:HD23	3:J:172:PRO:O	2.21	0.41
3:J:129:PHE:CE1	3:J:571:LYS:HE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:646:LYS:HE3	3:J:688:TRP:HZ2	1.86	0.41
5:L:233:GLN:HG3	5:L:236:ILE:HD12	2.03	0.41
6:M:129:LEU:O	6:M:133:ILE:HG12	2.21	0.41
6:M:142:GLN:HB3	6:M:142:GLN:HE21	1.66	0.41
6:M:21:ALA:N	6:M:37:GLN:O	2.54	0.41
6:M:13:PRO:HD2	6:M:58:GLY:O	2.20	0.41
2:C:1037:VAL:HG12	2:C:1041:GLU:OE2	2.20	0.41
2:C:230:ARG:NH2	2:C:231:PRO:HD2	2.29	0.41
2:C:598:GLU:HG2	2:C:615:TYR:CE2	2.56	0.41
3:D:1278:ASP:OD2	3:D:1321:ALA:N	2.54	0.41
3:D:354:ILE:HD11	3:D:369:ALA:HB2	2.02	0.41
3:D:430:GLU:O	3:D:431:ILE:HB	2.20	0.41
4:E:66:LYS:HA	4:E:69:LEU:HB2	2.02	0.41
4:E:6:ILE:HG23	4:E:7:ASP:H	1.85	0.41
1:G:150:TYR:HE1	1:G:168:ASP:HB3	1.86	0.41
2:I:66:LEU:HD11	2:I:372:LEU:HD23	2.03	0.41
2:I:872:ASN:OD1	2:I:874:LEU:HB2	2.21	0.41
3:J:1076:GLY:O	3:J:1079:LYS:HB3	2.21	0.41
3:J:181:ASP:HB3	3:J:357:GLU:HG3	2.02	0.41
3:J:494:LYS:O	3:J:497:GLU:HB3	2.19	0.41
3:J:514:LEU:HD11	3:J:516:ALA:O	2.21	0.41
3:J:659:LYS:O	3:J:662:GLU:HB3	2.20	0.41
3:J:894:LYS:HG2	3:J:894:LYS:H	1.54	0.41
5:L:208:ARG:HH21	7:R:31:DG:H8	1.69	0.41
1:A:122:ILE:HG13	1:A:124:ASN:H	1.86	0.41
2:C:1035:MET:HG2	2:C:1036:GLU:N	2.36	0.41
2:C:206:THR:HG22	2:C:209:ARG:NH2	2.36	0.41
3:D:103:TRP:CE2	3:D:1444:THR:HG23	2.56	0.41
3:D:1072:ILE:HG13	3:D:1072:ILE:H	1.69	0.41
3:D:1130:ARG:CZ	3:D:1130:ARG:HB3	2.51	0.41
3:D:653:PHE:HB2	3:D:691:LEU:HD11	2.02	0.41
3:D:553:ARG:NH2	5:F:226:ASP:OD1	2.47	0.41
5:F:233:GLN:HG3	5:F:236:ILE:HD12	2.03	0.41
5:F:376:LEU:HD21	5:F:423:LEU:HG	2.02	0.41
1:G:36:LEU:O	1:G:39:PRO:HD2	2.20	0.41
2:I:608:GLY:HA2	2:I:641:PRO:HG2	2.03	0.41
2:I:1082:PRO:CG	3:J:1469:GLY:HA3	2.50	0.41
3:J:39:PRO:HB3	3:J:46:ASP:HA	2.03	0.41
3:J:54:LYS:HD3	3:J:55:ASP:N	2.35	0.41
8:S:5:DC:H2'	8:S:6:DC:C5	2.56	0.41
2:C:1051:GLU:OE1	2:C:1055:ILE:HD12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:249:LYS:HE2	2:C:249:LYS:HB3	1.88	0.41
2:C:437:ARG:NH2	2:C:469:THR:HG22	2.36	0.41
2:C:751:PRO:HB2	2:C:794:PRO:HA	2.03	0.41
3:D:122:GLU:HG2	3:D:152:LEU:HD21	2.03	0.41
3:D:206:ARG:HD3	3:D:206:ARG:HA	1.76	0.41
3:D:299:GLU:O	3:D:302:GLN:HB3	2.21	0.41
3:D:352:ASN:O	3:D:368:VAL:HG13	2.21	0.41
3:D:490:ALA:O	3:D:493:ARG:HB3	2.21	0.41
3:D:569:ASN:O	3:D:572:ARG:HB3	2.21	0.41
3:D:7:LYS:HE3	3:D:1458:GLU:OE1	2.21	0.41
3:D:56:TYR:HE2	3:D:82:ARG:HE	1.69	0.41
1:G:99:LEU:HD13	1:G:144:VAL:HG23	2.03	0.41
2:I:1115:LEU:HD23	3:J:85:VAL:HG12	2.02	0.41
2:I:217:LEU:H	2:I:217:LEU:HG	1.58	0.41
2:I:537:LYS:HZ3	2:I:905:VAL:N	2.08	0.41
2:I:673:LEU:HD12	2:I:673:LEU:H	1.85	0.41
2:I:885:ILE:HG22	2:I:889:HIS:NE2	2.36	0.41
3:J:1101:VAL:HG13	3:J:1102:ALA:H	1.86	0.41
3:J:770:LEU:HD23	3:J:777:PRO:HA	2.03	0.41
3:J:873:LEU:HD22	3:J:875:THR:HG23	2.01	0.41
3:J:984:THR:O	3:J:988:ARG:HB2	2.20	0.41
5:L:237:ARG:NH1	5:L:241:LYS:HD2	2.36	0.41
5:L:114:GLU:OE1	5:L:249:LYS:HD2	2.21	0.41
5:L:293:LEU:HD13	5:L:301:PRO:HG3	2.02	0.41
5:F:252:THR:HG23	7:O:29:DC:H41	1.86	0.41
8:P:21:DA:H4'	8:P:22:DT:OP1	2.21	0.41
2:C:1044:GLY:O	3:D:1476:THR:HG23	2.21	0.41
2:C:6:PHE:HE1	2:C:901:TYR:CD1	2.30	0.41
2:C:552:HIS:ND1	3:D:1061:PHE:O	2.49	0.41
3:D:1101:VAL:HG13	3:D:1102:ALA:H	1.85	0.41
3:D:440:VAL:HG13	3:D:441:ARG:H	1.85	0.41
3:D:114:THR:O	3:D:495:ARG:HG3	2.20	0.41
3:D:970:LYS:HG2	3:D:995:LEU:HD13	2.03	0.41
5:F:293:LEU:HD13	5:F:301:PRO:HG3	2.02	0.41
1:H:176:ARG:HD2	3:J:884:ARG:NH2	2.32	0.41
2:I:893:ALA:HB2	2:I:918:LEU:HD13	2.03	0.41
2:I:9:ILE:HG13	2:I:9:ILE:H	1.70	0.41
3:J:1306:PRO:HB2	3:J:1308:ASP:OD1	2.20	0.41
3:J:122:GLU:HG2	3:J:152:LEU:HD21	2.03	0.41
3:J:114:THR:O	3:J:495:ARG:HG3	2.21	0.41
3:J:646:LYS:HD2	3:J:722:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:970:LYS:HG2	3:J:995:LEU:HD13	2.03	0.41
3:J:67:ARG:HH11	5:L:394:ARG:NH1	2.19	0.41
8:P:42:DT:H2"	8:P:43:DG:C8	2.56	0.41
5:L:246:ARG:HG3	7:R:26:DA:N1	2.35	0.41
1:B:58:ILE:HG23	1:B:140:MET:HB3	2.03	0.40
2:C:32:ALA:HB1	2:C:73:ILE:HD13	2.03	0.40
2:C:599:GLU:HA	2:C:651:LYS:HB3	2.03	0.40
2:C:537:LYS:NZ	2:C:905:VAL:H	2.13	0.40
2:C:66:LEU:HD22	2:C:98:LEU:HD12	2.03	0.40
3:D:236:TYR:HB3	3:D:313:LEU:HD13	2.03	0.40
3:D:273:ARG:HE	3:D:278:VAL:HG12	1.86	0.40
1:H:212:ASN:O	1:H:215:VAL:HG22	2.22	0.40
2:I:1035:MET:HG2	2:I:1036:GLU:N	2.37	0.40
3:J:1130:ARG:CZ	3:J:1130:ARG:HB3	2.51	0.40
3:J:176:ASP:HA	3:J:389:GLU:HA	2.03	0.40
3:J:683:ILE:H	3:J:683:ILE:HG12	1.67	0.40
5:L:379:ARG:HG3	5:L:405:PHE:CE2	2.56	0.40
7:R:17:DA:H1'	7:R:18:DA:H5"	2.03	0.40
1:A:99:LEU:HB2	1:A:142:VAL:HG23	2.03	0.40
2:C:690:ILE:HB	2:C:852:ILE:HG23	2.03	0.40
3:D:118:LEU:HD13	3:D:122:GLU:OE2	2.21	0.40
3:D:1266:ARG:CD	7:O:42:DC:H5"	2.51	0.40
3:D:276:GLU:HG2	3:D:277:GLU:H	1.86	0.40
3:D:691:LEU:O	3:D:695:ILE:HG13	2.20	0.40
3:D:689:ASP:O	3:D:692:GLU:HB2	2.20	0.40
5:F:111:LEU:H	5:F:111:LEU:HD22	1.86	0.40
1:G:60:ASP:O	1:G:61:VAL:HB	2.21	0.40
2:I:170:PRO:HB3	7:R:36:DC:H42	1.86	0.40
2:I:598:GLU:HG2	2:I:615:TYR:CE2	2.57	0.40
2:I:950:LEU:H	2:I:950:LEU:HD23	1.86	0.40
2:I:972:VAL:HG12	2:I:973:VAL:H	1.86	0.40
3:J:1129:THR:C	3:J:1131:THR:H	2.25	0.40
2:I:769:PRO:HD3	3:J:65:ARG:HH12	1.86	0.40
5:L:257:TRP:O	5:L:260:GLN:HB3	2.22	0.40
5:L:388:LYS:HA	5:L:388:LYS:HD3	1.73	0.40
2:I:109:LYS:HE2	6:N:40:PHE:CZ	2.57	0.40
5:L:260:GLN:HB2	7:R:25:DT:O4	2.22	0.40
1:A:170:ILE:HG23	2:C:696:LYS:HD3	2.03	0.40
2:C:608:GLY:HA2	2:C:641:PRO:HG2	2.03	0.40
2:C:710:ILE:HB	2:C:790:LEU:HD13	2.03	0.40
2:C:810:ASP:O	2:C:813:VAL:HG12	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:161:LEU:HD12	3:D:161:LEU:HA	1.78	0.40
3:D:116:LEU:HD21	3:D:465:LEU:HG	2.03	0.40
3:D:646:LYS:HE3	3:D:688:TRP:HZ2	1.86	0.40
3:D:731:LEU:HD13	3:D:731:LEU:HA	1.93	0.40
3:D:70:GLY:HA2	3:D:79:GLU:HG3	2.03	0.40
1:H:176:ARG:HG2	1:H:177:VAL:N	2.36	0.40
2:I:724:ARG:O	2:I:734:LEU:HD11	2.21	0.40
3:J:124:GLU:HG3	3:J:125:GLN:N	2.37	0.40
3:J:213:VAL:HG22	3:J:385:VAL:HG12	2.03	0.40
3:J:537:THR:O	5:L:332:LEU:N	2.54	0.40
6:N:63:LEU:HD11	6:N:102:PRO:HB2	2.04	0.40
1:B:44:LEU:HA	1:B:48:ILE:HD13	2.04	0.40
2:C:17:PRO:HA	2:C:590:ASP:OD1	2.21	0.40
2:C:630:ARG:HE	2:C:707:ARG:HH11	1.70	0.40
3:D:247:GLU:O	3:D:249:TYR:N	2.51	0.40
3:D:786:ILE:H	3:D:786:ILE:HG13	1.70	0.40
4:E:27:ALA:HB1	4:E:60:ALA:CB	2.51	0.40
4:E:41:GLU:HB2	4:E:43:GLU:OE2	2.22	0.40
5:F:141:LEU:O	5:F:145:VAL:HG23	2.21	0.40
5:F:237:ARG:NH1	5:F:241:LYS:HD2	2.37	0.40
1:G:58:ILE:HG23	1:G:139:TYR:O	2.21	0.40
1:H:115:THR:HA	1:H:116:PRO:HD3	1.90	0.40
2:I:219:GLN:H	2:I:219:GLN:HG3	1.60	0.40
2:I:391:LEU:CD2	2:I:415:PRO:HD2	2.50	0.40
2:I:72:ARG:CB	2:I:95:TYR:HB2	2.44	0.40
3:J:116:LEU:HD21	3:J:465:LEU:HG	2.03	0.40
3:J:928:ALA:HA	3:J:931:LEU:HD12	2.03	0.40
1:A:40:LEU:HD23	1:A:40:LEU:HA	1.91	0.40
2:C:185:LYS:HG2	2:C:190:LYS:HA	2.04	0.40
2:C:291:VAL:HG13	2:C:303:PHE:HE1	1.87	0.40
2:C:64:LEU:HD13	2:C:359:MET:HB2	2.04	0.40
2:C:713:ARG:HA	2:C:819:VAL:HA	2.03	0.40
3:D:1135:ARG:O	3:D:1140:ILE:HD11	2.21	0.40
3:D:318:THR:O	3:D:337:LEU:HG	2.22	0.40
3:D:626:SER:HB3	3:D:748:HIS:CE1	2.56	0.40
4:E:59:ASN:HD21	4:E:61:VAL:HG23	1.86	0.40
5:F:271:ARG:H	5:F:271:ARG:HE	1.69	0.40
1:G:122:ILE:HG13	1:G:124:ASN:H	1.86	0.40
1:H:44:LEU:HA	1:H:48:ILE:HD13	2.04	0.40
2:I:174:LEU:HA	2:I:174:LEU:HD23	1.84	0.40
2:I:206:THR:HG22	2:I:209:ARG:NH2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:669:GLY:HA3	2:I:994:ILE:O	2.22	0.40
2:I:6:PHE:HE1	2:I:901:TYR:CD1	2.31	0.40
2:I:713:ARG:HA	2:I:819:VAL:HA	2.03	0.40
3:J:1107:VAL:HG23	3:J:1221:VAL:HG11	2.03	0.40
3:J:1114:THR:OG1	3:J:1116:ASN:ND2	2.47	0.40
3:J:1135:ARG:O	3:J:1140:ILE:HD11	2.21	0.40
3:J:209:ARG:HA	3:J:347:VAL:CG1	2.51	0.40
3:J:374:GLU:HG3	3:J:375:GLU:N	2.36	0.40
3:J:784:ASP:O	3:J:787:LEU:HB3	2.22	0.40
4:K:6:ILE:HG23	4:K:7:ASP:H	1.87	0.40
6:M:75:LEU:HA	6:M:75:LEU:HD23	1.92	0.40
7:O:18:DA:H5'	7:O:18:DA:C8	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	225/314 (72%)	191 (85%)	32 (14%)	2 (1%)	20	63
1	B	225/314 (72%)	196 (87%)	27 (12%)	2 (1%)	20	63
1	G	225/314 (72%)	190 (84%)	33 (15%)	2 (1%)	20	63
1	H	225/314 (72%)	196 (87%)	27 (12%)	2 (1%)	20	63
2	C	1115/1119 (100%)	974 (87%)	137 (12%)	4 (0%)	38	77
2	I	1115/1119 (100%)	974 (87%)	137 (12%)	4 (0%)	38	77
3	D	1486/1524 (98%)	1306 (88%)	171 (12%)	9 (1%)	28	71
3	J	1361/1524 (89%)	1200 (88%)	156 (12%)	5 (0%)	38	77
4	E	91/99 (92%)	82 (90%)	9 (10%)	0	100	100
4	K	91/99 (92%)	82 (90%)	9 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	343/347 (99%)	301 (88%)	41 (12%)	1 (0%)	44	81
5	L	343/347 (99%)	300 (88%)	42 (12%)	1 (0%)	44	81
6	M	156/164 (95%)	143 (92%)	11 (7%)	2 (1%)	14	56
6	N	156/164 (95%)	142 (91%)	12 (8%)	2 (1%)	14	56
All	All	7157/7762 (92%)	6277 (88%)	844 (12%)	36 (0%)	32	74

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	VAL
3	D	681	ARG
3	D	683	ILE
3	D	1128	VAL
1	G	53	VAL
3	J	681	ARG
3	J	1128	VAL
2	C	738	ASP
3	D	431	ILE
3	D	666	PHE
2	I	738	ASP
6	M	20	VAL
6	N	20	VAL
2	C	61	LYS
2	I	61	LYS
1	B	118	ALA
1	B	119	ASP
2	C	607	ASP
3	D	680	GLN
1	H	118	ALA
2	I	607	ASP
3	J	680	GLN
5	F	391	ILE
1	H	119	ASP
3	J	868	TYR
5	L	391	ILE
1	A	61	VAL
2	C	1060	ILE
3	D	667	ALA
1	G	61	VAL
2	I	1060	ILE
6	M	41	PRO

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Mol	Chain	Res	Type
6	N	41	PRO
3	D	1277	ILE
3	J	1277	ILE
3	D	238	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	194/270 (72%)	171 (88%)	23 (12%)	6	30
1	B	194/270 (72%)	167 (86%)	27 (14%)	4	26
1	G	194/270 (72%)	171 (88%)	23 (12%)	6	30
1	H	194/270 (72%)	167 (86%)	27 (14%)	4	26
2	C	931/936 (100%)	820 (88%)	111 (12%)	6	30
2	I	931/936 (100%)	820 (88%)	111 (12%)	6	30
3	D	1252/1281 (98%)	1115 (89%)	137 (11%)	7	33
3	J	1150/1281 (90%)	1033 (90%)	117 (10%)	8	36
4	E	83/88 (94%)	77 (93%)	6 (7%)	17	51
4	K	83/88 (94%)	77 (93%)	6 (7%)	17	51
5	F	296/299 (99%)	267 (90%)	29 (10%)	9	37
5	L	296/299 (99%)	267 (90%)	29 (10%)	9	37
6	M	127/133 (96%)	122 (96%)	5 (4%)	37	68
6	N	127/133 (96%)	122 (96%)	5 (4%)	37	68
All	All	6052/6554 (92%)	5396 (89%)	656 (11%)	7	34

All (656) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	28	LEU
1	A	32	PHE

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Mol	Chain	Res	Type
1	A	36	LEU
1	A	44	LEU
1	A	51	THR
1	A	54	THR
1	A	61	VAL
1	A	80	LEU
1	A	83	LYS
1	A	85	LEU
1	A	86	VAL
1	A	87	VAL
1	A	113	ASP
1	A	114	PHE
1	A	161	ARG
1	A	186	LEU
1	A	195	LEU
1	A	200	TRP
1	A	206	THR
1	A	209	GLU
1	A	213	GLN
1	A	227	ASN
1	B	19	HIS
1	B	20	TYR
1	B	23	PHE
1	B	30	ARG
1	B	36	LEU
1	B	41	ARG
1	B	51	THR
1	B	54	THR
1	B	58	ILE
1	B	62	LEU
1	B	68	ILE
1	B	74	ASP
1	B	75	VAL
1	B	80	LEU
1	B	100	ILE
1	B	110	ARG
1	B	114	PHE
1	B	162	ILE
1	B	170	ILE
1	B	177	VAL
1	B	186	LEU
1	B	193	ASP

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Mol	Chain	Res	Type
1	B	195	LEU
1	B	215	VAL
1	B	222	LEU
1	B	227	ASN
1	B	232	LEU
2	C	5	ARG
2	C	11	GLU
2	C	13	ILE
2	C	15	LEU
2	C	20	GLU
2	C	39	ARG
2	C	69	LEU
2	C	70	GLU
2	C	80	GLN
2	C	81	ASP
2	C	85	GLU
2	C	100	LEU
2	C	103	LYS
2	C	107	LEU
2	C	111	ASP
2	C	140	ILE
2	C	141	HIS
2	C	154	ARG
2	C	179	SER
2	C	194	VAL
2	C	195	LEU
2	C	196	LEU
2	C	198	ARG
2	C	207	LEU
2	C	209	ARG
2	C	217	LEU
2	C	219	GLN
2	C	230	ARG
2	C	242	LEU
2	C	246	ASP
2	C	261	LEU
2	C	274	ARG
2	C	285	LEU
2	C	292	ARG
2	C	297	GLU
2	C	304	LEU
2	C	317	VAL

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Mol	Chain	Res	Type
2	C	322	VAL
2	C	325	ILE
2	C	344	PHE
2	C	361	MET
2	C	367	LEU
2	C	374	ASN
2	C	376	ARG
2	C	393	GLN
2	C	394	PHE
2	C	396	ASP
2	C	410	ILE
2	C	421	GLU
2	C	426	ASP
2	C	428	ARG
2	C	430	VAL
2	C	433	THR
2	C	434	HIS
2	C	438	ILE
2	C	473	ARG
2	C	474	VAL
2	C	495	THR
2	C	543	ASN
2	C	579	VAL
2	C	610	ARG
2	C	620	LEU
2	C	622	GLU
2	C	647	GLN
2	C	680	ASP
2	C	683	ASN
2	C	689	VAL
2	C	690	ILE
2	C	695	LEU
2	C	703	ILE
2	C	713	ARG
2	C	716	LYS
2	C	717	LEU
2	C	729	LEU
2	C	761	PHE
2	C	784	ASP
2	C	788	THR
2	C	790	LEU
2	C	815	LEU

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Mol	Chain	Res	Type
2	C	834	GLN
2	C	848	VAL
2	C	857	ASP
2	C	861	LEU
2	C	863	ASP
2	C	867	VAL
2	C	869	VAL
2	C	871	LEU
2	C	872	ASN
2	C	876	VAL
2	C	887	GLU
2	C	890	LEU
2	C	896	PHE
2	C	900	ARG
2	C	934	PHE
2	C	950	LEU
2	C	953	VAL
2	C	963	LEU
2	C	968	ASP
2	C	972	VAL
2	C	994	ILE
2	C	1000	MET
2	C	1015	LEU
2	C	1026	GLN
2	C	1035	MET
2	C	1053	LEU
2	C	1063	ARG
2	C	1074	GLU
2	C	1088	LEU
2	C	1101	THR
2	C	1104	GLU
2	C	1113	GLU
3	D	16	GLU
3	D	25	GLU
3	D	32	ILE
3	D	47	GLU
3	D	62	LYS
3	D	68	PHE
3	D	69	GLU
3	D	92	HIS
3	D	103	TRP
3	D	104	PHE

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Mol	Chain	Res	Type
3	D	115	LEU
3	D	118	LEU
3	D	124	GLU
3	D	128	TYR
3	D	145	VAL
3	D	154	THR
3	D	155	ASP
3	D	176	ASP
3	D	196	VAL
3	D	216	LEU
3	D	225	ILE
3	D	231	VAL
3	D	233	LYS
3	D	242	LEU
3	D	245	LEU
3	D	246	SER
3	D	251	PHE
3	D	255	GLU
3	D	261	LEU
3	D	266	GLU
3	D	273	ARG
3	D	281	ARG
3	D	289	THR
3	D	292	VAL
3	D	296	GLU
3	D	311	LEU
3	D	313	LEU
3	D	316	HIS
3	D	333	LEU
3	D	335	LEU
3	D	338	GLU
3	D	344	ASP
3	D	350	HIS
3	D	352	ASN
3	D	362	GLN
3	D	374	GLU
3	D	389	GLU
3	D	406	ASP
3	D	421	LEU
3	D	423	ASP
3	D	430	GLU
3	D	439	LEU

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Mol	Chain	Res	Type
3	D	445	ARG
3	D	464	LEU
3	D	497	GLU
3	D	574	LEU
3	D	614	PHE
3	D	619	LEU
3	D	623	VAL
3	D	639	LEU
3	D	640	HIS
3	D	650	LEU
3	D	658	LEU
3	D	660	LYS
3	D	687	VAL
3	D	688	TRP
3	D	694	VAL
3	D	701	LEU
3	D	708	LEU
3	D	717	GLN
3	D	743	ASP
3	D	748	HIS
3	D	754	PHE
3	D	768	ASN
3	D	776	GLU
3	D	780	LYS
3	D	789	LEU
3	D	795	VAL
3	D	817	GLU
3	D	833	GLU
3	D	861	GLN
3	D	863	VAL
3	D	865	THR
3	D	873	LEU
3	D	880	ILE
3	D	897	GLN
3	D	899	LEU
3	D	901	GLN
3	D	903	ASP
3	D	908	LYS
3	D	914	LEU
3	D	958	GLU
3	D	959	GLU
3	D	964	LEU

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Mol	Chain	Res	Type
3	D	965	GLU
3	D	971	LEU
3	D	976	GLN
3	D	1015	TYR
3	D	1025	GLN
3	D	1078	ARG
3	D	1086	LEU
3	D	1094	LEU
3	D	1100	ASP
3	D	1122	LEU
3	D	1130	ARG
3	D	1132	LEU
3	D	1136	LYS
3	D	1137	ARG
3	D	1140	ILE
3	D	1144	LEU
3	D	1158	ARG
3	D	1160	LEU
3	D	1161	GLU
3	D	1184	ARG
3	D	1200	VAL
3	D	1213	ARG
3	D	1267	ARG
3	D	1269	LYS
3	D	1278	ASP
3	D	1285	GLU
3	D	1302	GLU
3	D	1305	LEU
3	D	1308	ASP
3	D	1318	TYR
3	D	1335	LEU
3	D	1342	GLU
3	D	1356	TYR
3	D	1395	LEU
3	D	1421	LEU
3	D	1442	ASN
3	D	1443	THR
3	D	1448	THR
3	D	1462	LEU
3	D	1463	LYS
3	D	1472	ILE
3	D	1497	GLU

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Mol	Chain	Res	Type
3	D	1499	ARG
4	E	37	ASN
4	E	49	ARG
4	E	51	LEU
4	E	56	ASP
4	E	62	THR
4	E	79	LEU
5	F	97	ARG
5	F	108	LEU
5	F	109	LEU
5	F	137	LEU
5	F	153	THR
5	F	175	ASP
5	F	184	GLU
5	F	217	TYR
5	F	225	LEU
5	F	235	LEU
5	F	237	ARG
5	F	244	TYR
5	F	255	THR
5	F	268	ASP
5	F	271	ARG
5	F	279	MET
5	F	282	THR
5	F	291	ARG
5	F	293	LEU
5	F	294	GLN
5	F	319	VAL
5	F	322	THR
5	F	323	LEU
5	F	328	GLU
5	F	336	ILE
5	F	353	LEU
5	F	370	GLU
5	F	409	ARG
5	F	435	ASP
1	G	12	THR
1	G	28	LEU
1	G	32	PHE
1	G	36	LEU
1	G	44	LEU
1	G	51	THR

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Mol	Chain	Res	Type
1	G	54	THR
1	G	61	VAL
1	G	80	LEU
1	G	83	LYS
1	G	85	LEU
1	G	86	VAL
1	G	87	VAL
1	G	113	ASP
1	G	114	PHE
1	G	161	ARG
1	G	186	LEU
1	G	195	LEU
1	G	200	TRP
1	G	206	THR
1	G	209	GLU
1	G	213	GLN
1	G	227	ASN
1	H	19	HIS
1	H	20	TYR
1	H	23	PHE
1	H	30	ARG
1	H	36	LEU
1	H	41	ARG
1	H	51	THR
1	H	54	THR
1	H	58	ILE
1	H	62	LEU
1	H	68	ILE
1	H	74	ASP
1	H	75	VAL
1	H	80	LEU
1	H	100	ILE
1	H	110	ARG
1	H	114	PHE
1	H	162	ILE
1	H	170	ILE
1	H	177	VAL
1	H	186	LEU
1	H	193	ASP
1	H	195	LEU
1	H	215	VAL
1	H	222	LEU

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Mol	Chain	Res	Type
1	H	227	ASN
1	H	232	LEU
2	I	5	ARG
2	I	11	GLU
2	I	13	ILE
2	I	15	LEU
2	I	20	GLU
2	I	39	ARG
2	I	69	LEU
2	I	70	GLU
2	I	80	GLN
2	I	81	ASP
2	I	85	GLU
2	I	100	LEU
2	I	103	LYS
2	I	107	LEU
2	I	111	ASP
2	I	140	ILE
2	I	141	HIS
2	I	154	ARG
2	I	179	SER
2	I	194	VAL
2	I	195	LEU
2	I	196	LEU
2	I	198	ARG
2	I	207	LEU
2	I	209	ARG
2	I	217	LEU
2	I	219	GLN
2	I	230	ARG
2	I	242	LEU
2	I	246	ASP
2	I	261	LEU
2	I	274	ARG
2	I	285	LEU
2	I	292	ARG
2	I	297	GLU
2	I	304	LEU
2	I	317	VAL
2	I	322	VAL
2	I	344	PHE
2	I	361	MET

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Mol	Chain	Res	Type
2	I	367	LEU
2	I	374	ASN
2	I	376	ARG
2	I	393	GLN
2	I	394	PHE
2	I	396	ASP
2	I	410	ILE
2	I	421	GLU
2	I	426	ASP
2	I	428	ARG
2	I	430	VAL
2	I	433	THR
2	I	434	HIS
2	I	438	ILE
2	I	473	ARG
2	I	474	VAL
2	I	495	THR
2	I	516	ARG
2	I	543	ASN
2	I	579	VAL
2	I	610	ARG
2	I	620	LEU
2	I	622	GLU
2	I	647	GLN
2	I	680	ASP
2	I	683	ASN
2	I	689	VAL
2	I	690	ILE
2	I	695	LEU
2	I	703	ILE
2	I	713	ARG
2	I	716	LYS
2	I	717	LEU
2	I	729	LEU
2	I	761	PHE
2	I	784	ASP
2	I	788	THR
2	I	790	LEU
2	I	815	LEU
2	I	834	GLN
2	I	848	VAL
2	I	857	ASP

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Mol	Chain	Res	Type
2	I	861	LEU
2	I	863	ASP
2	I	867	VAL
2	I	869	VAL
2	I	871	LEU
2	I	872	ASN
2	I	876	VAL
2	I	887	GLU
2	I	890	LEU
2	I	896	PHE
2	I	900	ARG
2	I	934	PHE
2	I	950	LEU
2	I	953	VAL
2	I	963	LEU
2	I	968	ASP
2	I	972	VAL
2	I	994	ILE
2	I	1000	MET
2	I	1015	LEU
2	I	1026	GLN
2	I	1035	MET
2	I	1053	LEU
2	I	1063	ARG
2	I	1074	GLU
2	I	1088	LEU
2	I	1101	THR
2	I	1104	GLU
2	I	1113	GLU
3	J	16	GLU
3	J	25	GLU
3	J	32	ILE
3	J	47	GLU
3	J	62	LYS
3	J	68	PHE
3	J	69	GLU
3	J	92	HIS
3	J	103	TRP
3	J	104	PHE
3	J	115	LEU
3	J	118	LEU
3	J	124	GLU

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Mol	Chain	Res	Type
3	J	128	TYR
3	J	145	VAL
3	J	154	THR
3	J	155	ASP
3	J	166	GLN
3	J	180	LYS
3	J	196	VAL
3	J	198	ARG
3	J	204	LEU
3	J	344	ASP
3	J	347	VAL
3	J	355	VAL
3	J	371	ILE
3	J	387	LEU
3	J	393	ILE
3	J	400	VAL
3	J	407	VAL
3	J	410	THR
3	J	421	LEU
3	J	430	GLU
3	J	435	VAL
3	J	464	LEU
3	J	574	LEU
3	J	614	PHE
3	J	619	LEU
3	J	623	VAL
3	J	639	LEU
3	J	640	HIS
3	J	650	LEU
3	J	658	LEU
3	J	660	LYS
3	J	687	VAL
3	J	688	TRP
3	J	694	VAL
3	J	701	LEU
3	J	708	LEU
3	J	717	GLN
3	J	743	ASP
3	J	748	HIS
3	J	754	PHE
3	J	768	ASN
3	J	776	GLU

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Mol	Chain	Res	Type
3	J	780	LYS
3	J	789	LEU
3	J	795	VAL
3	J	817	GLU
3	J	833	GLU
3	J	861	GLN
3	J	863	VAL
3	J	865	THR
3	J	873	LEU
3	J	880	ILE
3	J	897	GLN
3	J	899	LEU
3	J	901	GLN
3	J	903	ASP
3	J	908	LYS
3	J	914	LEU
3	J	958	GLU
3	J	959	GLU
3	J	964	LEU
3	J	965	GLU
3	J	971	LEU
3	J	976	GLN
3	J	1015	TYR
3	J	1025	GLN
3	J	1078	ARG
3	J	1086	LEU
3	J	1094	LEU
3	J	1100	ASP
3	J	1122	LEU
3	J	1130	ARG
3	J	1132	LEU
3	J	1136	LYS
3	J	1137	ARG
3	J	1140	ILE
3	J	1144	LEU
3	J	1158	ARG
3	J	1160	LEU
3	J	1161	GLU
3	J	1184	ARG
3	J	1200	VAL
3	J	1213	ARG
3	J	1267	ARG

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Mol	Chain	Res	Type
3	J	1269	LYS
3	J	1278	ASP
3	J	1285	GLU
3	J	1302	GLU
3	J	1305	LEU
3	J	1308	ASP
3	J	1318	TYR
3	J	1335	LEU
3	J	1342	GLU
3	J	1356	TYR
3	J	1395	LEU
3	J	1421	LEU
3	J	1442	ASN
3	J	1443	THR
3	J	1448	THR
3	J	1462	LEU
3	J	1463	LYS
3	J	1472	ILE
3	J	1497	GLU
3	J	1499	ARG
4	K	37	ASN
4	K	49	ARG
4	K	51	LEU
4	K	56	ASP
4	K	62	THR
4	K	79	LEU
5	L	97	ARG
5	L	108	LEU
5	L	109	LEU
5	L	137	LEU
5	L	153	THR
5	L	175	ASP
5	L	184	GLU
5	L	217	TYR
5	L	225	LEU
5	L	235	LEU
5	L	237	ARG
5	L	244	TYR
5	L	255	THR
5	L	268	ASP
5	L	271	ARG
5	L	279	MET

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Mol	Chain	Res	Type
5	L	282	THR
5	L	291	ARG
5	L	293	LEU
5	L	294	GLN
5	L	319	VAL
5	L	322	THR
5	L	323	LEU
5	L	328	GLU
5	L	336	ILE
5	L	353	LEU
5	L	370	GLU
5	L	409	ARG
5	L	435	ASP
6	M	8	ASP
6	M	52	GLU
6	M	89	ARG
6	M	142	GLN
6	M	157	GLU
6	N	8	ASP
6	N	52	GLU
6	N	80	MET
6	N	142	GLN
6	N	157	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	213	GLN
1	B	63	HIS
1	B	81	ASN
1	B	213	GLN
2	C	80	GLN
2	C	99	GLN
2	C	187	ASN
2	C	374	ASN
2	C	434	HIS
2	C	498	GLN
2	C	538	GLN
2	C	565	GLN
2	C	647	GLN
2	C	683	ASN

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Mol	Chain	Res	Type
2	C	765	GLN
2	C	829	GLN
2	C	899	GLN
2	C	930	GLN
2	C	1026	GLN
2	C	1050	GLN
2	C	1093	GLN
2	C	1107	ASN
3	D	268	HIS
3	D	352	ASN
3	D	640	HIS
3	D	703	ASN
3	D	727	GLN
3	D	756	GLN
3	D	762	GLN
3	D	794	GLN
3	D	855	HIS
3	D	861	GLN
3	D	897	GLN
3	D	917	GLN
3	D	976	GLN
3	D	991	GLN
3	D	1195	GLN
3	D	1353	GLN
3	D	1374	GLN
3	D	1442	ASN
4	E	29	GLN
5	F	98	GLN
5	F	200	GLN
5	F	229	GLN
5	F	233	GLN
5	F	263	ASN
5	F	269	GLN
5	F	284	ASN
5	F	294	GLN
5	F	295	GLN
5	F	417	ASN
1	G	16	GLN
1	G	213	GLN
1	H	63	HIS
1	H	81	ASN
1	H	213	GLN

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Mol	Chain	Res	Type
2	I	80	GLN
2	I	99	GLN
2	I	187	ASN
2	I	374	ASN
2	I	434	HIS
2	I	498	GLN
2	I	565	GLN
2	I	647	GLN
2	I	683	ASN
2	I	765	GLN
2	I	899	GLN
2	I	930	GLN
2	I	999	HIS
2	I	1026	GLN
2	I	1050	GLN
2	I	1093	GLN
2	I	1107	ASN
3	J	166	GLN
3	J	362	GLN
3	J	703	ASN
3	J	727	GLN
3	J	756	GLN
3	J	762	GLN
3	J	794	GLN
3	J	855	HIS
3	J	861	GLN
3	J	897	GLN
3	J	906	GLN
3	J	917	GLN
3	J	976	GLN
3	J	991	GLN
3	J	1103	HIS
3	J	1195	GLN
3	J	1353	GLN
3	J	1374	GLN
3	J	1442	ASN
4	K	28	GLN
4	K	29	GLN
5	L	98	GLN
5	L	200	GLN
5	L	229	GLN
5	L	233	GLN

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Mol	Chain	Res	Type
5	L	263	ASN
5	L	269	GLN
5	L	294	GLN
5	L	295	GLN
5	L	417	ASN
6	M	55	HIS
6	M	101	ASN
6	M	142	GLN
6	N	101	ASN
6	N	142	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	Q	3/4 (75%)	2 (66%)	0
9	T	3/4 (75%)	0	0
All	All	6/8 (75%)	2 (33%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	Q	2	C
9	Q	3	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	227/314 (72%)	-0.23	1 (0%) 92 88	144, 176, 208, 241	0
1	B	227/314 (72%)	-0.41	1 (0%) 92 88	143, 164, 196, 228	0
1	G	227/314 (72%)	-0.03	2 (0%) 84 78	148, 188, 218, 252	0
1	H	227/314 (72%)	-0.34	0 100 100	145, 175, 207, 241	0
2	C	1117/1119 (99%)	-0.19	4 (0%) 92 88	144, 172, 211, 253	0
2	I	1117/1119 (99%)	-0.20	15 (1%) 77 69	144, 182, 221, 270	0
3	D	1490/1524 (97%)	-0.23	3 (0%) 94 93	117, 162, 195, 251	0
3	J	1367/1524 (89%)	-0.20	6 (0%) 92 88	120, 171, 204, 250	0
4	E	93/99 (93%)	-0.23	0 100 100	144, 165, 194, 217	0
4	K	93/99 (93%)	-0.23	0 100 100	144, 179, 206, 228	0
5	F	345/347 (99%)	-0.17	2 (0%) 89 85	144, 179, 222, 245	0
5	L	345/347 (99%)	-0.17	2 (0%) 89 85	145, 187, 225, 258	0
6	M	158/164 (96%)	0.17	5 (3%) 48 39	159, 207, 235, 243	0
6	N	158/164 (96%)	0.42	5 (3%) 48 39	171, 215, 240, 267	0
7	O	48/48 (100%)	0.34	4 (8%) 12 11	157, 217, 256, 270	0
7	R	48/48 (100%)	-0.22	1 (2%) 64 56	163, 207, 251, 276	0
8	P	48/48 (100%)	0.38	4 (8%) 12 11	161, 219, 260, 270	0
8	S	48/48 (100%)	-0.09	1 (2%) 64 56	167, 212, 250, 261	0
9	Q	4/4 (100%)	0.94	1 (25%) 1 2	175, 177, 186, 189	0
9	T	4/4 (100%)	-0.17	0 100 100	165, 183, 184, 196	0
All	All	7391/7962 (92%)	-0.18	57 (0%) 86 80	117, 174, 219, 276	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	187	GLY	4.7
2	I	246	ASP	4.4
3	J	216	LEU	3.4
3	D	1253	THR	3.4
7	O	1	DC	3.4
2	C	58	ASP	3.3
3	J	1253	THR	3.2
5	F	170	THR	3.1
6	M	4	PHE	2.9
8	P	1	DG	2.9
3	J	406	ASP	2.8
7	O	2	DT	2.8
7	O	48	DC	2.7
2	I	649	VAL	2.7
1	G	87	VAL	2.7
7	R	48	DC	2.6
6	N	103	TYR	2.6
6	N	144	LEU	2.6
3	J	64	LYS	2.6
5	L	170	THR	2.5
3	D	446	VAL	2.5
2	C	57	GLY	2.5
8	P	45	DC	2.5
2	I	101	ILE	2.5
8	P	44	DT	2.5
2	I	805	ARG	2.4
2	I	648	ARG	2.4
1	A	187	GLY	2.4
2	I	249	LYS	2.4
2	I	476	ASN	2.4
6	N	59	LEU	2.4
2	C	251	ASP	2.3
2	I	472	ARG	2.3
3	J	407	VAL	2.3
2	I	247	PRO	2.3
8	S	1	DG	2.3
2	I	250	LYS	2.3
5	L	171	VAL	2.2
6	M	49	VAL	2.2
2	I	296	GLY	2.2
3	J	422	ALA	2.2
7	O	3	DT	2.2
2	I	248	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
6	M	59	LEU	2.1
8	P	48	DG	2.1
1	B	137	LYS	2.1
6	M	37	GLN	2.1
3	D	256	SER	2.1
2	I	254	LEU	2.1
6	N	139	GLU	2.1
6	N	4	PHE	2.1
2	I	245	GLY	2.1
2	C	643	VAL	2.0
9	Q	1	U	2.0
6	M	36	TYR	2.0
5	F	171	VAL	2.0
2	I	108	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
11	MG	J	2003	1/1	0.96	0.19	0.07	270,270,270,270	0
10	ZN	J	2001	1/1	0.89	0.14	-0.20	277,277,277,277	0
10	ZN	D	2002	1/1	0.92	0.16	-0.92	237,237,237,237	0
10	ZN	J	2002	1/1	0.95	0.07	-1.14	157,157,157,157	0
10	ZN	D	2001	1/1	0.98	0.10	-1.29	116,116,116,116	0
11	MG	D	2003	1/1	0.97	0.09	-1.89	283,283,283,283	0

6.5 Other polymers [i](#)

There are no such residues in this entry.