



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 06:29 am BST

PDB ID : 4XLP  
Title : Crystal structure of T.aquaticus transcription initiation complex containing upstream fork promoter  
Authors : Bae, B.; Darst, S.A.  
Deposited on : 2015-01-13  
Resolution : 4.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

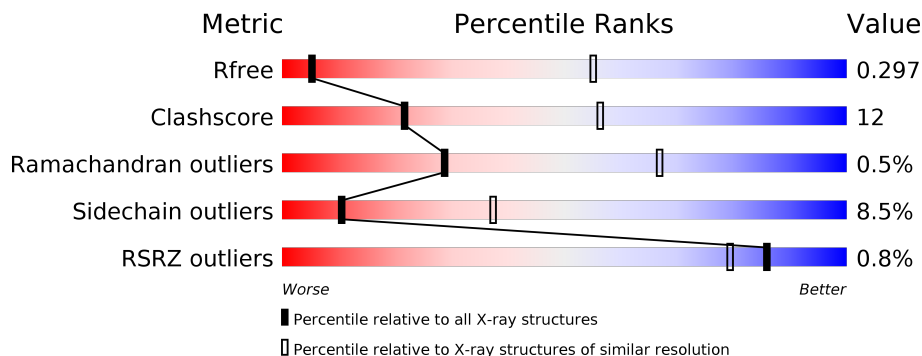
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.













Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	314	
1	B	314	
1	G	314	
1	H	314	
2	C	1119	
2	I	1119	

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Mol	Chain	Length	Quality of chain
3	D	1524	 65% 30% ..
3	J	1524	 60% 27% 10% .
4	E	99	 67% 25% 6% .
4	K	99	 67% 26% 6% .
5	F	347	 65% 32% ..
5	L	347	 63% 33% ..
6	O	30	 70% 30%
6	R	30	 77% 23%
7	P	25	 56% 44%
7	S	25	 52% 48%

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 56454 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
			Total	C	N	O	S			
1	A	227	Total 1770	C 1130	N 303	O 334	S 3	0	0	0
1	B	227	Total 1770	C 1130	N 303	O 334	S 3	0	0	0
1	G	227	Total 1770	C 1130	N 303	O 334	S 3	0	0	0
1	H	227	Total 1770	C 1130	N 303	O 334	S 3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	1112	Total 8739	C 5531	N 1553	O 1632	S 23	0	0	0
2	I	1112	Total 8739	C 5531	N 1553	O 1632	S 23	0	0	0

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

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

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

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

- 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 DNA chain called DNA (30-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	O	30	Total	C	N	O	P	0	0	0
			613	296	109	179	29			
6	R	30	Total	C	N	O	P	0	0	0
			613	296	109	179	29			

- Molecule 7 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	P	25	Total	C	N	O	P	0	0	0
			507	245	91	147	24			
7	S	25	Total	C	N	O	P	0	0	0
			507	245	91	147	24			

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

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

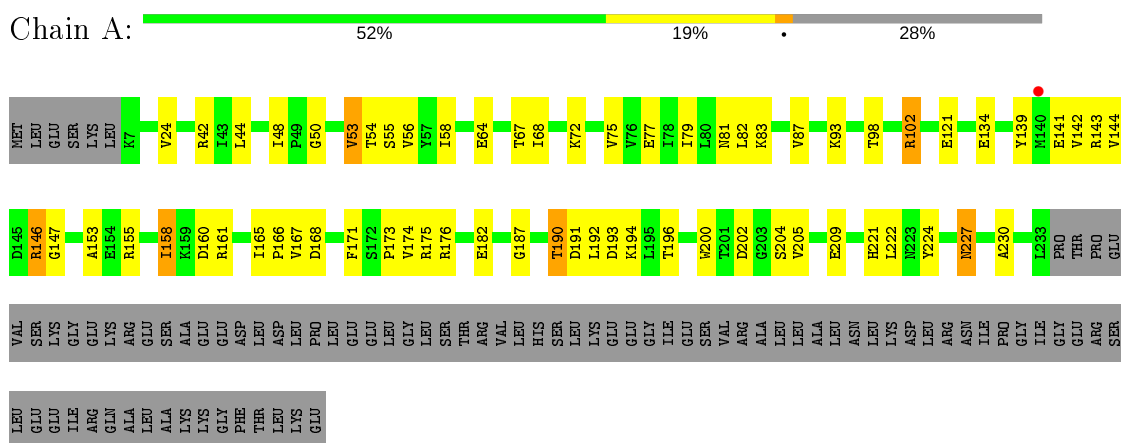
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

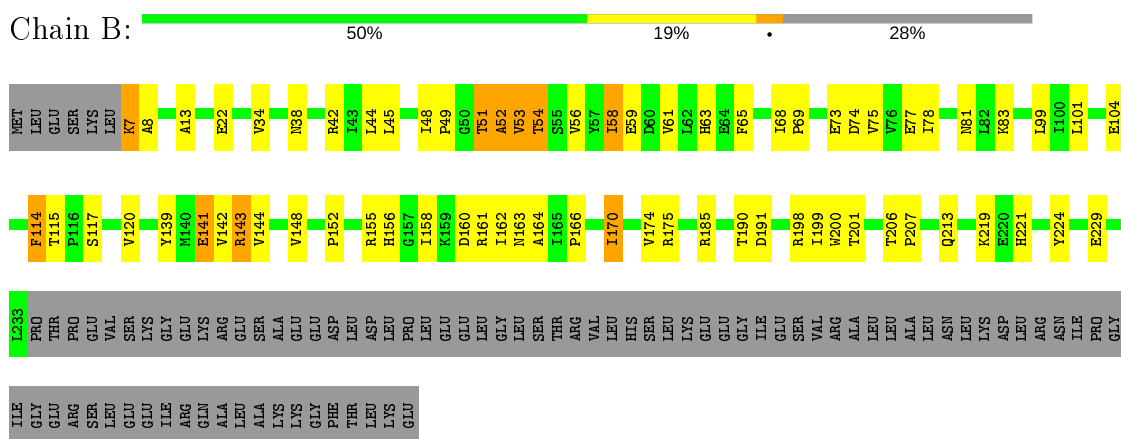
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

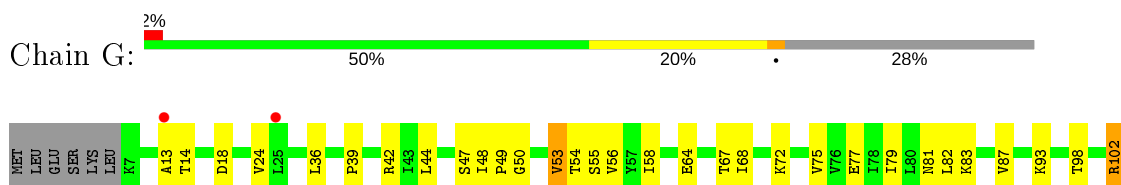
- Molecule 1: DNA-directed RNA polymerase subunit alpha

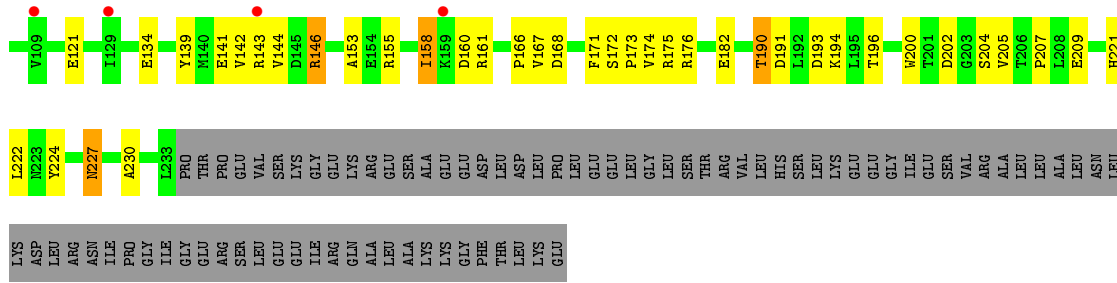


- Molecule 1: DNA-directed RNA polymerase subunit alpha

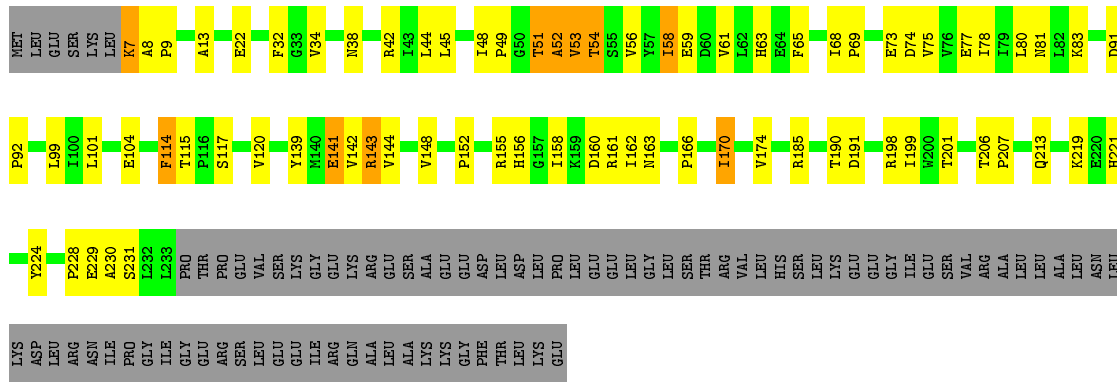


- Molecule 1: DNA-directed RNA polymerase subunit alpha

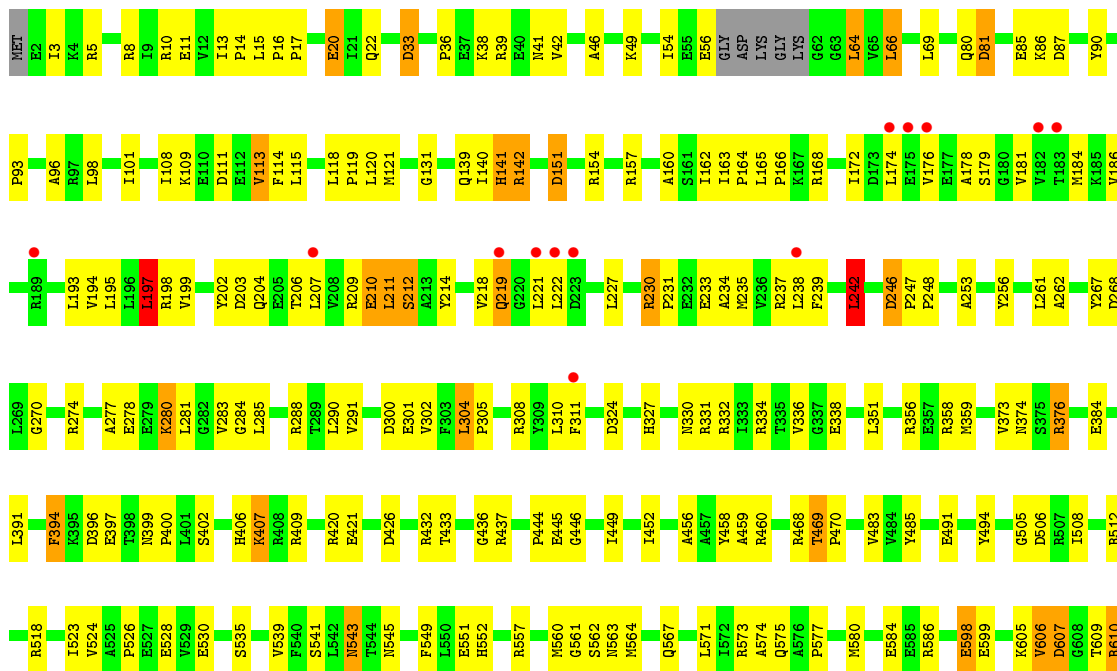


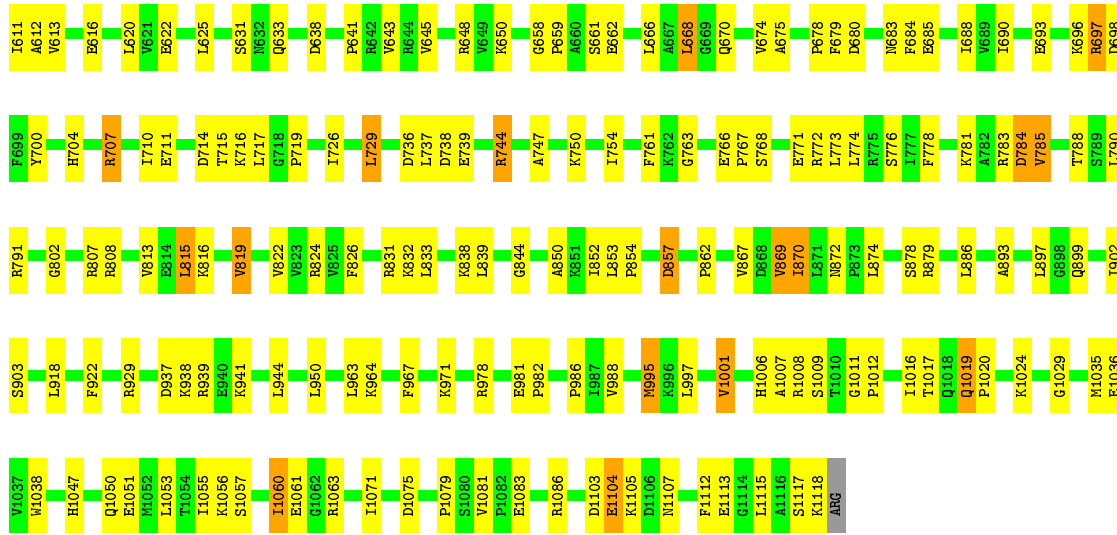


• Molecule 1: DNA-directed RNA polymerase subunit alpha

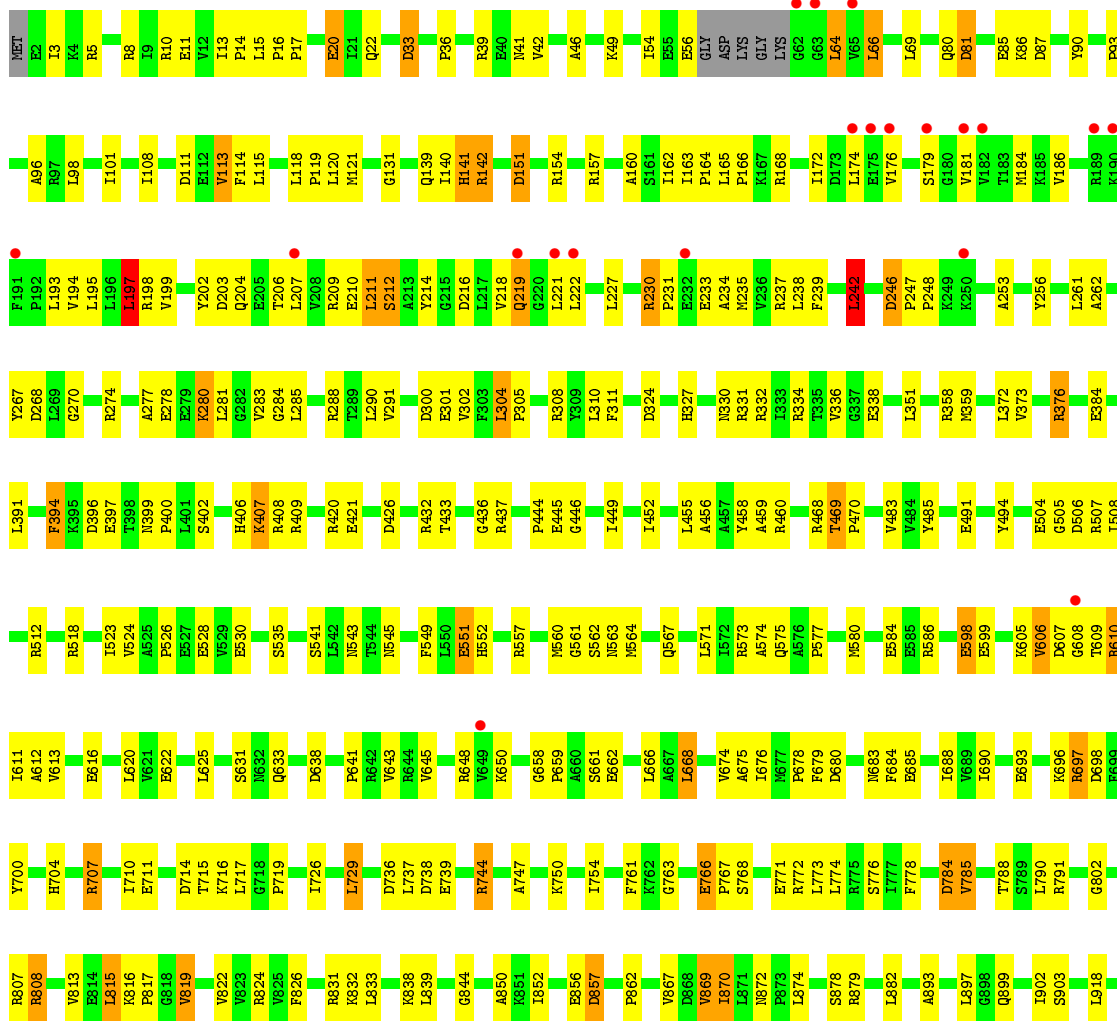


• Molecule 2: DNA-directed RNA polymerase subunit beta

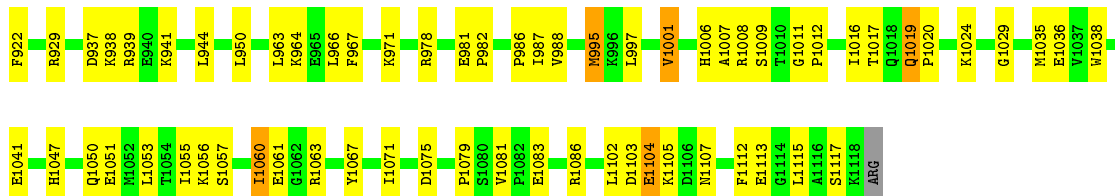




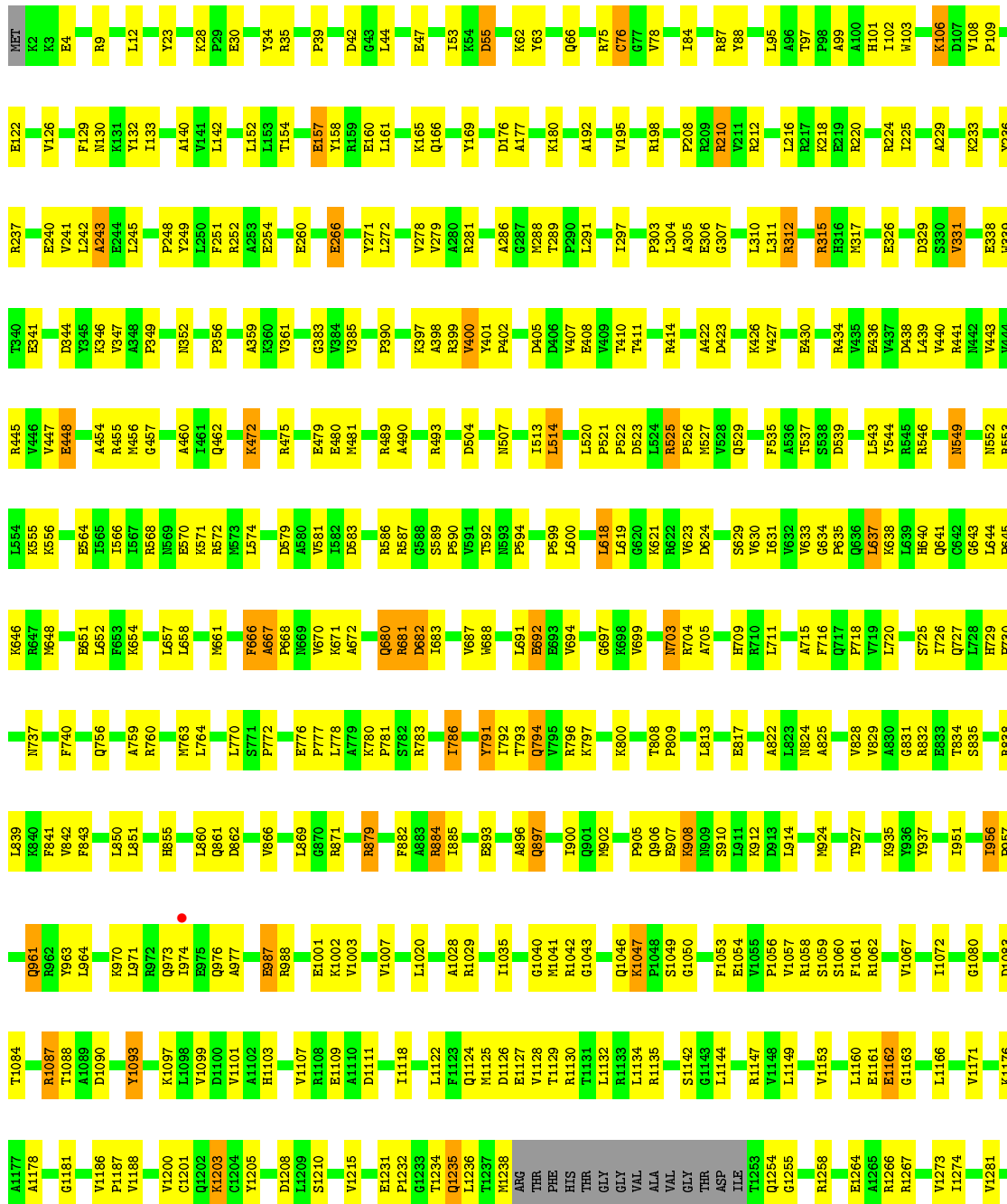
• Molecule 2: DNA-directed RNA polymerase subunit beta

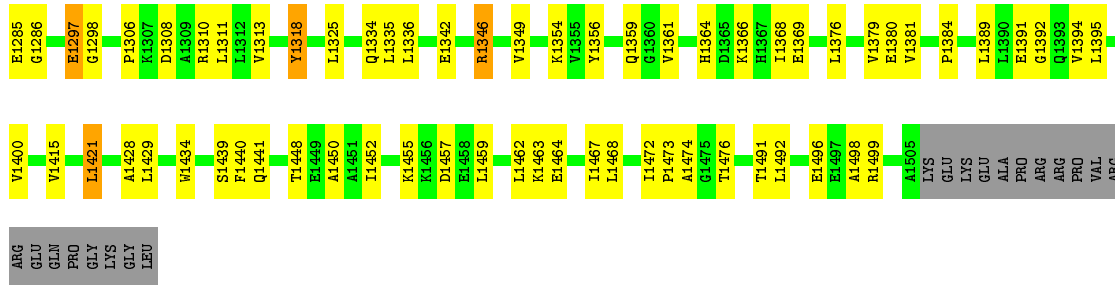




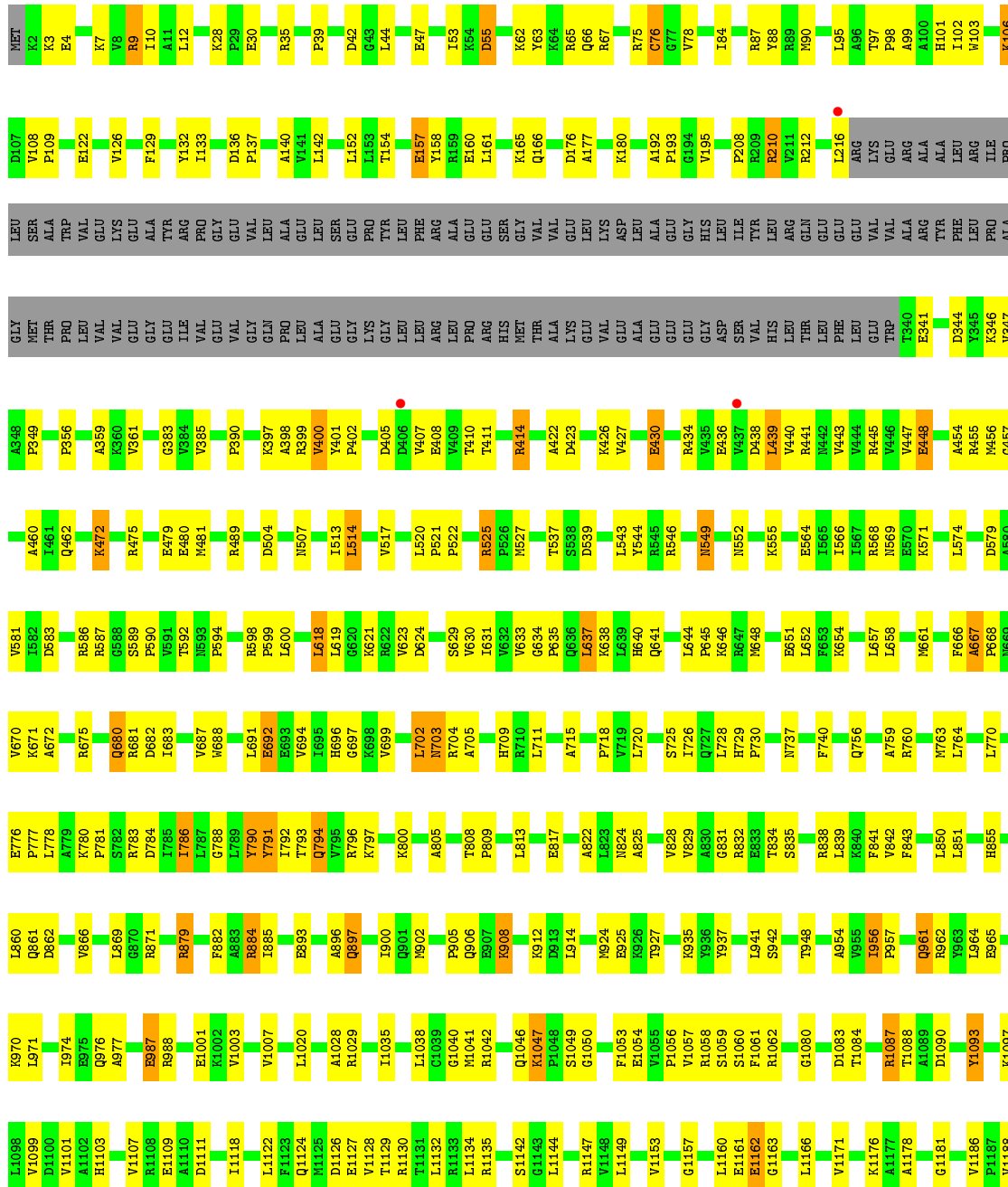


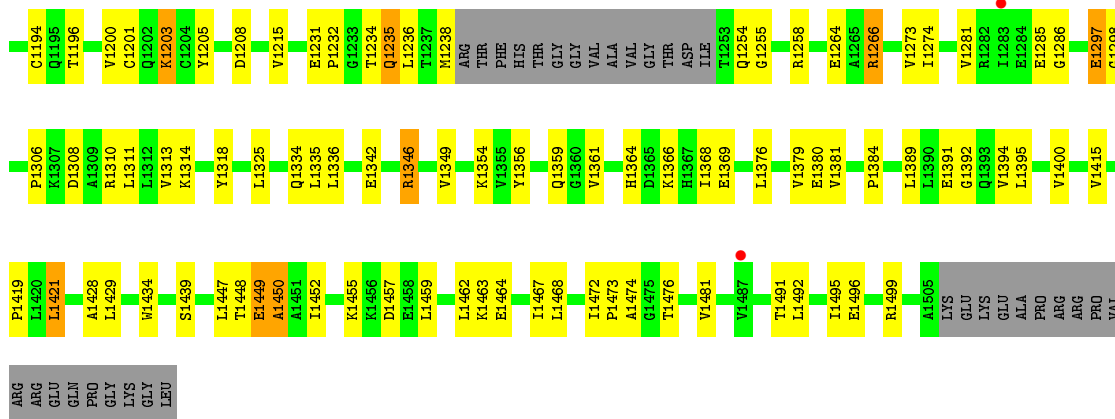
● Molecule 3: DNA-directed RNA polymerase subunit beta'



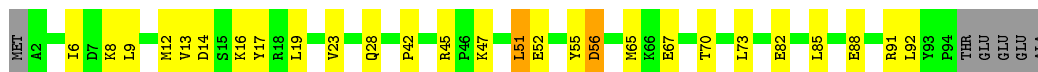


• Molecule 3: DNA-directed RNA polymerase subunit beta'





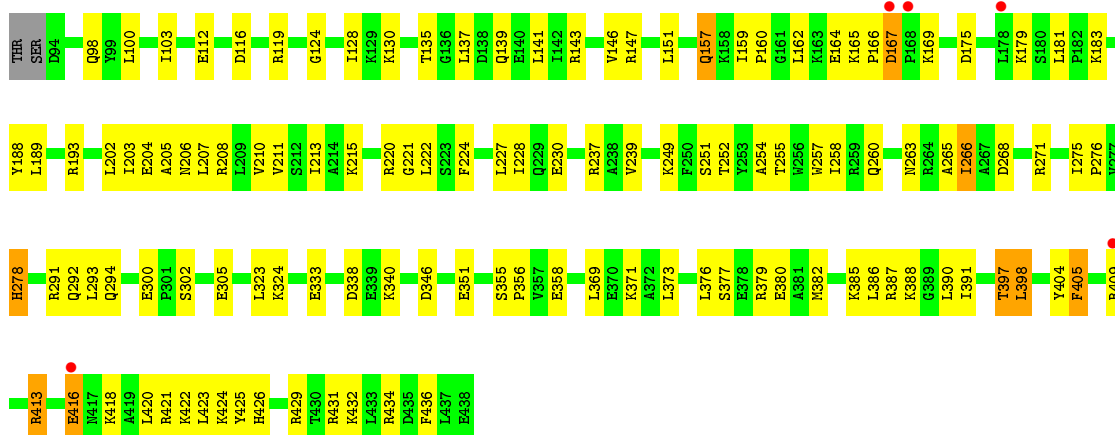
- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 4: DNA-directed RNA polymerase subunit omega

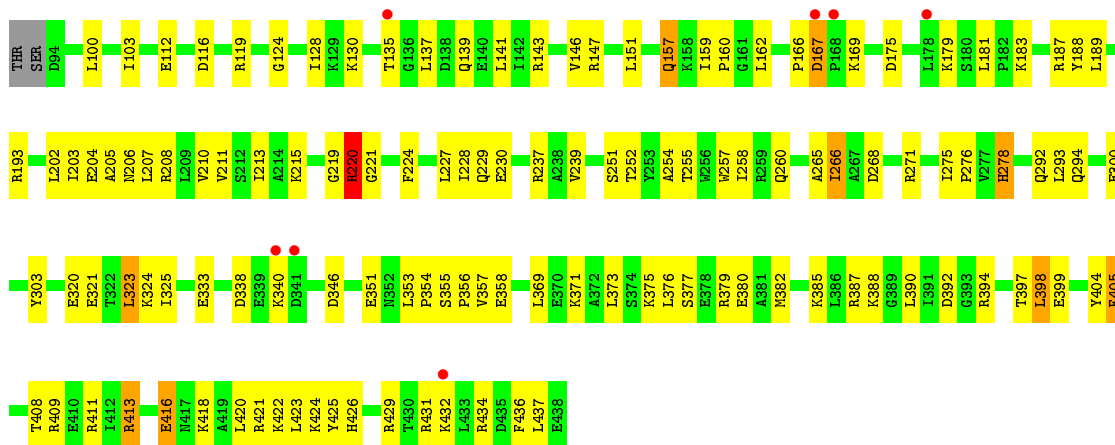


- Molecule 5: RNA polymerase sigma factor SigA

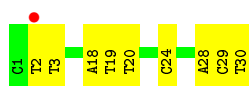


- Molecule 5: RNA polymerase sigma factor SigA

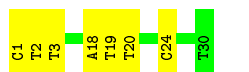




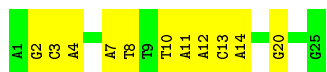
• Molecule 6: DNA (30-MER)



• Molecule 6: DNA (30-MER)



• Molecule 7: DNA (25-MER)



• Molecule 7: DNA (25-MER)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	289.87Å 289.87Å 537.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.03 – 4.00 50.03 – 3.80	Depositor EDS
% Data completeness (in resolution range)	96.3 (50.03-4.00) 85.0 (50.03-3.80)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.92 (at 3.77Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, $R_{free}$	0.257 , 0.297 0.257 , 0.297	Depositor DCC
$R_{free}$ test set	9509 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	135.6	Xtrriage
Anisotropy	0.002	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 107.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.19$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	56454	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	141.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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	0.24	0/1804	0.50	0/2455
1	B	0.24	0/1804	0.50	0/2455
1	G	0.25	0/1804	0.50	0/2455
1	H	0.24	0/1804	0.50	0/2455
2	C	0.24	0/8905	0.49	1/12040 (0.0%)
2	I	0.24	0/8905	0.49	1/12040 (0.0%)
3	D	0.25	0/11963	0.48	1/16165 (0.0%)
3	J	0.25	0/10959	0.48	1/14802 (0.0%)
4	E	0.22	0/783	0.42	0/1054
4	K	0.22	0/783	0.41	0/1054
5	F	0.27	0/2829	0.53	0/3804
5	L	0.28	0/2829	0.54	1/3804 (0.0%)
6	O	0.44	0/687	1.14	0/1059
6	R	0.44	0/687	1.13	0/1059
7	P	0.45	0/568	1.19	0/874
7	S	0.45	0/568	1.19	0/874
All	All	0.26	0/57682	0.54	5/78449 (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	6
2	I	0	5
3	J	0	3
5	F	0	2
5	L	0	3
All	All	0	19

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	J	1286	GLY	N-CA-C	-5.93	98.27	113.10
3	D	1286	GLY	N-CA-C	-5.93	98.28	113.10
5	L	398	LEU	CA-CB-CG	5.44	127.82	115.30
2	C	242	LEU	CA-CB-CG	5.04	126.88	115.30
2	I	242	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	178	ALA	Peptide
2	C	197	LEU	Peptide
2	C	212	SER	Peptide
2	C	230	ARG	Peptide
2	C	737	LEU	Peptide
2	C	850	ALA	Peptide
5	F	159	ILE	Peptide
5	F	397	THR	Peptide
2	I	197	LEU	Peptide
2	I	212	SER	Peptide
2	I	230	ARG	Peptide
2	I	737	LEU	Peptide
2	I	850	ALA	Peptide
3	J	1266	ARG	Peptide
3	J	1449	GLU	Peptide
3	J	790	TYR	Peptide
5	L	159	ILE	Peptide
5	L	219	GLY	Peptide
5	L	220	ARG	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1770	0	1799	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1770	0	1799	43	0
1	G	1770	0	1799	41	0
1	H	1770	0	1799	47	0
2	C	8739	0	8841	242	0
2	I	8739	0	8841	252	0
3	D	11761	0	11976	310	0
3	J	10779	0	10993	292	0
4	E	768	0	784	18	0
4	K	768	0	784	18	0
5	F	2787	0	2866	75	0
5	L	2787	0	2866	80	0
6	O	613	0	343	10	0
6	R	613	0	343	7	0
7	P	507	0	285	7	0
7	S	507	0	285	9	0
8	D	2	0	0	0	0
8	J	2	0	0	0	0
9	D	1	0	0	0	0
9	J	1	0	0	0	0
All	All	56454	0	56403	1341	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 12.

All (1341) 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)
5:L:398:LEU:HG	5:L:409:ARG:HB2	1.45	0.99
5:F:398:LEU:HG	5:F:409:ARG:HB2	1.48	0.91
1:H:53:VAL:HG23	1:H:144:VAL:HG22	1.55	0.88
1:B:53:VAL:HG23	1:B:144:VAL:HG22	1.55	0.86
1:A:42:ARG:HH12	2:C:857:ASP:HB3	1.41	0.86
3:D:977:ALA:HB2	3:J:831:GLY:HA3	1.60	0.83
1:G:42:ARG:HH12	2:I:857:ASP:HB3	1.45	0.80
2:I:64:LEU:HD21	2:I:66:LEU:HD12	1.64	0.79
3:D:770:LEU:HA	3:D:777:PRO:HA	1.65	0.79
2:C:64:LEU:HD21	2:C:66:LEU:HD12	1.65	0.78
3:D:44:LEU:HB3	3:D:525:ARG:HH12	1.50	0.78
3:J:770:LEU:HA	3:J:777:PRO:HA	1.64	0.78
3:J:44:LEU:HB3	3:J:525:ARG:HH12	1.49	0.77
3:J:1111:ASP:OD1	3:J:1203:LYS:NZ	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:408:THR:HG21	6:R:2:DT:H2'	1.65	0.77
3:J:1434:TRP:HB3	3:J:1455:LYS:HD2	1.68	0.76
1:H:53:VAL:HA	1:H:144:VAL:HA	1.68	0.76
3:D:1111:ASP:OD1	3:D:1203:LYS:NZ	2.17	0.75
3:D:160:GLU:HG3	3:D:165:LYS:HD3	1.69	0.75
3:J:160:GLU:HG3	3:J:165:LYS:HD3	1.69	0.74
3:D:1434:TRP:HB3	3:D:1455:LYS:HD2	1.69	0.74
2:I:1063:ARG:HG3	5:L:356:PRO:HG3	1.69	0.74
2:I:432:ARG:HH12	2:I:518:ARG:HH21	1.35	0.74
1:A:53:VAL:HA	1:A:144:VAL:HA	1.69	0.74
3:J:781:PRO:O	3:J:908:LYS:NZ	2.17	0.74
1:B:53:VAL:HA	1:B:144:VAL:HA	1.68	0.73
5:L:213:ILE:HD11	5:L:255:THR:HG22	1.70	0.73
2:C:432:ARG:HH12	2:C:518:ARG:HH21	1.35	0.73
2:I:971:LYS:HB3	2:I:986:PRO:HB2	1.70	0.73
3:D:260:GLU:HB3	3:D:271:TYR:HB2	1.70	0.73
5:F:213:ILE:HD11	5:F:255:THR:HG22	1.69	0.73
2:I:678:PRO:HA	2:I:683:ASN:HD21	1.53	0.73
2:I:1016:ILE:O	3:J:87:ARG:NH2	2.22	0.73
2:C:971:LYS:HB3	2:C:986:PRO:HB2	1.71	0.72
3:D:1254:GLN:HB3	3:D:1258:ARG:HB2	1.70	0.72
3:D:106:LYS:HE2	3:D:587:ARG:HG3	1.70	0.72
1:B:185:ARG:HH12	3:D:692:GLU:HG3	1.52	0.72
2:C:678:PRO:HA	2:C:683:ASN:HD21	1.53	0.72
3:D:781:PRO:O	3:D:908:LYS:NZ	2.17	0.72
1:G:53:VAL:HA	1:G:144:VAL:HA	1.70	0.71
3:J:1254:GLN:HB3	3:J:1258:ARG:HB2	1.70	0.71
2:C:658:GLY:H	2:C:661:SER:HB3	1.55	0.71
3:J:106:LYS:HE2	3:J:587:ARG:HG3	1.71	0.71
3:J:786:ILE:HD12	3:J:1028:ALA:HA	1.72	0.71
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.72	0.71
1:G:102:ARG:HE	1:G:139:TYR:HB2	1.56	0.71
2:I:571:LEU:HB2	2:I:574:ALA:HB2	1.73	0.70
2:C:571:LEU:HB2	2:C:574:ALA:HB2	1.73	0.70
3:J:715:ALA:HB3	3:J:764:LEU:HA	1.73	0.70
2:I:199:VAL:HA	2:I:231:PRO:HB3	1.74	0.70
3:D:786:ILE:HD12	3:D:1028:ALA:HA	1.72	0.70
3:D:668:PRO:HB2	5:F:432:LYS:HG2	1.73	0.70
5:F:413:ARG:HH11	5:F:413:ARG:HG2	1.57	0.70
2:C:22:GLN:HG3	2:C:407:LYS:HG2	1.73	0.69
5:L:413:ARG:HG2	5:L:413:ARG:HH11	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ARG:HE	1:A:139:TYR:HB2	1.56	0.69
2:C:199:VAL:HA	2:C:231:PRO:HB3	1.74	0.69
5:L:220:ARG:HG3	5:L:227:LEU:HD11	1.74	0.69
1:A:190:THR:OG1	1:A:191:ASP:N	2.25	0.69
1:B:59:GLU:HG3	1:B:139:TYR:HB3	1.75	0.68
1:H:59:GLU:HG3	1:H:139:TYR:HB3	1.75	0.68
3:D:1132:LEU:HD12	3:J:1181:GLY:HA3	1.75	0.68
2:I:1075:ASP:OD1	4:K:28:GLN:NE2	2.26	0.68
2:I:142:ARG:HH12	2:I:163:ILE:HG12	1.57	0.68
2:I:698:ASP:OD1	2:I:832:LYS:NZ	2.26	0.68
2:C:142:ARG:HH12	2:C:163:ILE:HG12	1.57	0.68
3:J:1087:ARG:NH2	3:J:1234:THR:O	2.26	0.68
3:D:102:ILE:HD12	3:D:579:ASP:HB3	1.76	0.68
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.75	0.68
1:G:141:GLU:OE2	1:G:161:ARG:NH2	2.26	0.68
2:I:212:SER:HB3	2:I:218:VAL:HG21	1.76	0.68
2:I:437:ARG:NH2	2:I:491:GLU:OE1	2.27	0.68
2:C:437:ARG:NH2	2:C:491:GLU:OE1	2.27	0.68
5:F:220:ARG:HG3	5:F:227:LEU:HD11	1.75	0.68
1:H:185:ARG:HH12	3:J:692:GLU:HG3	1.57	0.68
2:I:15:LEU:O	2:I:586:ARG:NH1	2.27	0.68
2:I:22:GLN:HG3	2:I:407:LYS:HG2	1.74	0.68
2:C:541:SER:O	2:C:545:ASN:ND2	2.25	0.67
2:C:778:PHE:HZ	5:F:434:ARG:HA	1.57	0.67
3:D:1087:ARG:NH2	3:D:1234:THR:O	2.27	0.67
3:D:793:THR:HG21	3:D:906:GLN:HG2	1.76	0.67
2:C:212:SER:HB3	2:C:218:VAL:HG21	1.76	0.67
3:J:102:ILE:HD12	3:J:579:ASP:HB3	1.77	0.67
3:J:793:THR:HG21	3:J:906:GLN:HG2	1.76	0.67
1:A:141:GLU:OE2	1:A:161:ARG:NH2	2.26	0.67
2:I:658:GLY:H	2:I:661:SER:HB3	1.59	0.67
2:I:717:LEU:HD21	2:I:763:GLY:HA2	1.77	0.67
2:C:15:LEU:O	2:C:586:ARG:NH1	2.27	0.67
2:I:87:ASP:OD2	2:I:824:ARG:NH1	2.28	0.67
2:C:168:ARG:HD3	2:C:268:ASP:HB3	1.77	0.67
1:G:190:THR:OG1	1:G:191:ASP:N	2.25	0.67
2:C:773:LEU:HA	5:F:388:LYS:HE3	1.76	0.66
2:C:717:LEU:HD21	2:C:763:GLY:HA2	1.77	0.66
2:I:168:ARG:HD3	2:I:268:ASP:HB3	1.78	0.66
3:J:1042:ARG:HB3	3:J:1057:VAL:HG21	1.77	0.66
3:D:359:ALA:HB3	3:D:385:VAL:HB	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:227:ASN:N	1:G:227:ASN:OD1	2.28	0.66
3:D:1318:TYR:N	3:J:1157:GLY:O	2.19	0.66
3:D:843:PHE:HB2	3:D:866:VAL:HG23	1.78	0.66
2:I:277:ALA:HA	2:I:280:LYS:HG2	1.78	0.65
2:I:680:ASP:OD2	2:I:978:ARG:NH1	2.29	0.65
2:I:750:LYS:HE2	3:J:681:ARG:HD2	1.78	0.65
3:J:843:PHE:HB2	3:J:866:VAL:HG23	1.78	0.65
5:L:382:MET:SD	5:L:385:LYS:NZ	2.66	0.65
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.77	0.65
3:D:1042:ARG:HB3	3:D:1057:VAL:HG21	1.77	0.65
2:I:87:ASP:HA	2:I:131:GLY:HA3	1.77	0.65
2:C:87:ASP:OD2	2:C:824:ARG:NH1	2.30	0.65
2:C:680:ASP:OD2	2:C:978:ARG:NH1	2.28	0.65
2:C:277:ALA:HA	2:C:280:LYS:HG2	1.79	0.65
2:I:86:LYS:HE2	2:I:813:VAL:HG23	1.79	0.65
3:D:800:LYS:HB3	3:D:822:ALA:HB2	1.79	0.65
3:J:359:ALA:HB3	3:J:385:VAL:HB	1.77	0.65
2:I:874:LEU:HD13	3:J:783:ARG:HB3	1.79	0.65
3:D:242:LEU:H	3:D:312:ARG:HA	1.62	0.65
2:C:1083:GLU:OE2	3:D:87:ARG:NH1	2.29	0.65
3:J:882:PHE:HA	3:J:885:ILE:HD12	1.79	0.65
3:D:106:LYS:HG3	3:D:586:ARG:HD3	1.79	0.64
2:C:893:ALA:HB2	2:C:918:LEU:HD22	1.79	0.64
3:D:1472:ILE:HG12	3:D:1474:ALA:H	1.63	0.64
2:C:86:LYS:HE2	2:C:813:VAL:HG23	1.79	0.64
1:B:51:THR:OG1	1:B:52:ALA:N	2.30	0.64
2:I:893:ALA:HB2	2:I:918:LEU:HD22	1.78	0.64
2:C:1060:ILE:HD12	2:C:1061:GLU:H	1.62	0.64
5:F:294:GLN:HE21	5:F:300:GLU:HG2	1.62	0.64
3:J:879:ARG:NE	3:J:902:MET:O	2.26	0.64
5:L:294:GLN:HE21	5:L:300:GLU:HG2	1.62	0.64
3:J:1122:LEU:HD11	3:J:1186:VAL:HG23	1.80	0.64
2:C:698:ASP:OD1	2:C:832:LYS:NZ	2.27	0.63
2:C:598:GLU:HG2	2:C:599:GLU:HG2	1.81	0.63
2:C:1057:SER:HB3	3:D:623:VAL:HG12	1.80	0.63
3:D:882:PHE:HA	3:D:885:ILE:HD12	1.78	0.63
3:J:140:ALA:HB1	3:J:161:LEU:HD23	1.80	0.63
3:J:800:LYS:HB3	3:J:822:ALA:HB2	1.80	0.63
3:J:1472:ILE:HG12	3:J:1474:ALA:H	1.63	0.63
2:I:541:SER:O	2:I:545:ASN:ND2	2.25	0.63
2:I:1060:ILE:HD12	2:I:1061:GLU:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1144:LEU:HD21	3:D:1186:VAL:HG21	1.79	0.63
3:D:140:ALA:HB1	3:D:161:LEU:HD23	1.80	0.63
3:D:407:VAL:HG23	3:D:422:ALA:HB2	1.80	0.63
5:F:377:SER:HB3	5:F:380:GLU:HG2	1.81	0.63
2:I:17:PRO:O	2:I:460:ARG:NH2	2.32	0.63
2:I:598:GLU:HG2	2:I:599:GLU:HG2	1.81	0.63
3:D:233:LYS:HB3	3:D:236:TYR:CZ	2.34	0.62
1:H:141:GLU:OE2	1:H:161:ARG:NH1	2.32	0.62
2:I:160:ALA:HB2	2:I:310:LEU:HD13	1.81	0.62
1:B:141:GLU:OE2	1:B:161:ARG:NH1	2.32	0.62
2:C:17:PRO:O	2:C:460:ARG:NH2	2.33	0.62
5:F:382:MET:SD	5:F:385:LYS:NZ	2.66	0.62
2:C:160:ALA:HB2	2:C:310:LEU:HD13	1.82	0.62
3:J:1144:LEU:HD21	3:J:1186:VAL:HG21	1.81	0.62
3:J:407:VAL:HG23	3:J:422:ALA:HB2	1.80	0.62
2:I:778:PHE:HZ	5:L:434:ARG:HA	1.64	0.62
3:J:568:ARG:HA	3:J:571:LYS:HE2	1.82	0.62
3:J:644:LEU:HB3	3:J:718:PRO:HA	1.82	0.62
3:D:568:ARG:HA	3:D:571:LYS:HE2	1.82	0.62
1:G:77:GLU:O	1:G:81:ASN:ND2	2.33	0.62
2:C:285:LEU:HD11	2:C:301:GLU:HB3	1.82	0.62
5:F:230:GLU:HG3	5:F:265:ALA:HB2	1.82	0.62
1:G:222:LEU:HD23	1:H:219:LYS:HB3	1.82	0.62
1:H:99:LEU:HD11	1:H:120:VAL:HG11	1.81	0.62
2:I:744:ARG:HE	2:I:747:ALA:HB2	1.65	0.62
3:J:397:LYS:NZ	3:J:448:GLU:O	2.32	0.62
2:C:744:ARG:HE	2:C:747:ALA:HB2	1.65	0.61
3:D:97:THR:HG21	3:D:571:LYS:HG3	1.82	0.61
3:D:879:ARG:NE	3:D:902:MET:O	2.26	0.61
3:J:349:PRO:HB3	5:L:112:GLU:HG2	1.80	0.61
1:B:99:LEU:HD11	1:B:120:VAL:HG11	1.81	0.61
2:C:1056:LYS:O	3:D:624:ASP:N	2.25	0.61
2:C:874:LEU:HD13	3:D:783:ARG:HB3	1.82	0.61
5:L:377:SER:HB3	5:L:380:GLU:HG2	1.81	0.61
3:J:106:LYS:HG3	3:J:586:ARG:HD3	1.81	0.61
3:J:439:LEU:HD11	5:L:187:ARG:HB2	1.82	0.61
3:D:1122:LEU:HD11	3:D:1186:VAL:HG23	1.82	0.61
1:A:77:GLU:O	1:A:81:ASN:ND2	2.33	0.61
2:I:710:ILE:HD12	2:I:790:LEU:HB2	1.82	0.61
2:C:710:ILE:HD12	2:C:790:LEU:HB2	1.81	0.61
3:J:667:ALA:HB1	3:J:672:ALA:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1008:ARG:NH2	2:C:1012:PRO:O	2.34	0.60
3:J:592:THR:HG22	3:J:599:PRO:HA	1.83	0.60
5:L:230:GLU:HG3	5:L:265:ALA:HB2	1.83	0.60
2:C:1086:ARG:NH2	3:D:88:TYR:OH	2.32	0.60
2:C:85:GLU:O	2:C:824:ARG:NH2	2.34	0.60
3:D:397:LYS:NZ	3:D:448:GLU:O	2.32	0.60
3:D:644:LEU:HB3	3:D:718:PRO:HA	1.82	0.60
3:D:835:SER:HB3	3:D:838:ARG:HG3	1.83	0.60
2:I:285:LEU:HD11	2:I:301:GLU:HB3	1.82	0.60
3:J:1395:LEU:HD11	3:J:1400:VAL:HB	1.82	0.60
3:J:210:ARG:NH2	3:J:344:ASP:OD2	2.33	0.60
3:J:97:THR:HG21	3:J:571:LYS:HG3	1.82	0.60
3:J:777:PRO:HB2	3:J:912:LYS:HZ1	1.67	0.60
5:F:215:LYS:HA	5:F:224:PHE:HE1	1.67	0.60
3:J:668:PRO:HB2	5:L:432:LYS:HG2	1.82	0.60
3:D:1395:LEU:HD11	3:D:1400:VAL:HB	1.82	0.60
2:I:1008:ARG:NH2	2:I:1012:PRO:O	2.35	0.60
3:D:441:ARG:HH22	3:D:445:ARG:HD3	1.67	0.60
3:D:592:THR:HG22	3:D:599:PRO:HA	1.83	0.60
3:D:780:LYS:HB2	3:D:912:LYS:HZ2	1.66	0.60
1:H:51:THR:OG1	1:H:52:ALA:N	2.30	0.60
3:D:661:MET:HG2	3:D:666:PHE:CZ	2.37	0.60
3:J:28:LYS:HB3	3:J:30:GLU:OE1	2.02	0.59
3:J:835:SER:HB3	3:J:838:ARG:HG3	1.83	0.59
5:L:215:LYS:HA	5:L:224:PHE:HE1	1.67	0.59
3:D:658:LEU:HB3	3:D:670:VAL:HG13	1.84	0.59
2:I:693:GLU:HA	2:I:696:LYS:HG3	1.84	0.59
2:C:693:GLU:HA	2:C:696:LYS:HG3	1.84	0.59
3:D:229:ALA:HB1	3:D:245:LEU:H	1.67	0.59
3:D:436:GLU:OE2	3:D:445:ARG:NH2	2.35	0.59
3:J:436:GLU:OE2	3:J:445:ARG:NH2	2.35	0.59
3:D:680:GLN:HA	3:D:680:GLN:HE21	1.67	0.59
3:D:680:GLN:O	3:D:682:ASP:N	2.30	0.59
3:J:680:GLN:HE21	3:J:680:GLN:HA	1.67	0.59
2:C:711:GLU:HG2	2:C:822:VAL:HG12	1.85	0.59
3:D:210:ARG:NH2	3:D:344:ASP:OD2	2.34	0.59
2:I:397:GLU:HB3	2:I:631:SER:HB2	1.85	0.59
2:I:857:ASP:HB2	2:I:978:ARG:HG2	1.85	0.59
1:G:53:VAL:HG22	1:G:54:THR:H	1.68	0.59
3:J:441:ARG:HH22	3:J:445:ARG:HD3	1.67	0.59
1:B:58:ILE:HD13	1:B:61:VAL:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:697:GLY:O	3:D:760:ARG:NH1	2.35	0.59
3:J:539:ASP:HB3	3:J:600:LEU:HG	1.84	0.59
3:D:1181:GLY:HA3	3:J:1132:LEU:HD12	1.85	0.58
2:I:246:ASP:OD1	2:I:246:ASP:N	2.34	0.58
3:D:566:ILE:HD11	5:F:207:LEU:HD21	1.83	0.58
1:H:58:ILE:HD13	1:H:61:VAL:HB	1.84	0.58
3:J:697:GLY:O	3:J:760:ARG:NH1	2.35	0.58
2:I:711:GLU:HG2	2:I:822:VAL:HG12	1.85	0.58
2:I:1019:GLN:HE22	3:J:621:LYS:HG2	1.69	0.58
2:C:750:LYS:HE2	3:D:681:ARG:HD2	1.85	0.58
2:C:857:ASP:HB2	2:C:978:ARG:HG2	1.85	0.58
2:C:878:SER:HB2	3:D:1029:ARG:HD2	1.84	0.58
2:C:1075:ASP:OD1	4:E:28:GLN:NE2	2.36	0.58
2:C:397:GLU:HB3	2:C:631:SER:HB2	1.85	0.58
2:I:33:ASP:N	2:I:33:ASP:OD1	2.36	0.58
3:D:1274:ILE:HD11	3:D:1334:GLN:HB3	1.84	0.58
3:D:62:LYS:HG3	3:D:63:TYR:N	2.19	0.58
3:J:1274:ILE:HD11	3:J:1334:GLN:HB3	1.84	0.58
5:L:278:HIS:NE2	6:R:20:DT:OP2	2.30	0.58
3:D:539:ASP:HB3	3:D:600:LEU:HG	1.85	0.58
3:J:780:LYS:HB2	3:J:912:LYS:HZ2	1.69	0.58
2:C:198:ARG:HH11	2:C:238:LEU:HD12	1.69	0.57
3:D:1273:VAL:HG23	3:D:1325:LEU:HB2	1.84	0.57
3:D:129:PHE:CE1	3:D:457:GLY:HA3	2.39	0.57
3:D:99:ALA:O	3:D:514:LEU:N	2.37	0.57
1:H:83:LYS:NZ	3:J:842:VAL:O	2.37	0.57
2:I:409:ARG:HD2	2:I:452:ILE:HG22	1.86	0.57
2:I:606:VAL:HG23	2:I:645:VAL:HG22	1.86	0.57
4:K:67:GLU:HB3	4:K:73:LEU:HD11	1.86	0.57
1:A:53:VAL:HG22	1:A:54:THR:H	1.68	0.57
1:A:193:ASP:OD1	2:C:938:LYS:NZ	2.38	0.57
3:D:62:LYS:HG3	3:D:63:TYR:H	1.70	0.57
3:J:1273:VAL:HG23	3:J:1325:LEU:HB2	1.85	0.57
2:I:85:GLU:O	2:I:824:ARG:NH2	2.35	0.57
3:J:711:LEU:HG	3:J:778:LEU:HD23	1.87	0.57
3:D:1491:THR:HG22	4:E:92:LEU:HD12	1.87	0.57
5:F:385:LYS:HB2	5:F:390:LEU:HB2	1.85	0.57
1:H:77:GLU:O	1:H:81:ASN:ND2	2.37	0.57
2:I:494:TYR:HD2	2:I:530:GLU:HG3	1.70	0.57
3:J:489:ARG:NH1	3:J:1391:GLU:OE2	2.37	0.57
3:J:658:LEU:HB3	3:J:670:VAL:HG13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:410:THR:OG1	5:L:193:ARG:NH1	2.38	0.57
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.87	0.57
2:I:198:ARG:HH11	2:I:238:LEU:HD12	1.70	0.57
3:J:99:ALA:O	3:J:514:LEU:N	2.36	0.57
3:D:288:MET:HA	3:D:307:GLY:HA2	1.85	0.57
3:D:241:VAL:HA	3:D:312:ARG:HB3	1.87	0.57
3:D:489:ARG:NH1	3:D:1391:GLU:OE2	2.38	0.57
4:E:67:GLU:HB3	4:E:73:LEU:HD11	1.86	0.57
2:I:470:PRO:HG3	2:I:485:TYR:CZ	2.40	0.57
2:C:606:VAL:HG23	2:C:645:VAL:HG22	1.86	0.57
2:I:64:LEU:HD13	2:I:359:MET:HG2	1.86	0.57
3:J:1376:LEU:HA	3:J:1421:LEU:HA	1.85	0.57
3:D:711:LEU:HG	3:D:778:LEU:HD23	1.87	0.56
2:C:16:PRO:HB2	2:C:460:ARG:HH21	1.70	0.56
2:C:209:ARG:HG3	2:C:210:GLU:H	1.69	0.56
2:C:33:ASP:OD1	2:C:33:ASP:N	2.36	0.56
5:L:385:LYS:HB2	5:L:390:LEU:HB2	1.86	0.56
2:C:470:PRO:HG3	2:C:485:TYR:CZ	2.40	0.56
2:I:468:ARG:HD2	2:I:485:TYR:HB3	1.87	0.56
3:J:472:LYS:HD2	3:J:475:ARG:HH22	1.70	0.56
2:I:141:HIS:NE2	2:I:334:ARG:HD3	2.20	0.56
3:J:208:PRO:HA	3:J:390:PRO:HA	1.87	0.56
2:I:1001:VAL:HG13	3:J:630:VAL:HG12	1.87	0.56
1:B:77:GLU:O	1:B:81:ASN:ND2	2.38	0.56
2:C:278:GLU:HG3	2:C:284:GLY:HA2	1.87	0.56
2:C:409:ARG:HD2	2:C:452:ILE:HG22	1.86	0.56
2:C:13:ILE:HG21	2:C:483:VAL:HG21	1.88	0.56
2:I:1038:TRP:CE2	3:J:1099:VAL:HG11	2.39	0.56
3:D:1376:LEU:HA	3:D:1421:LEU:HA	1.85	0.56
2:C:64:LEU:HD13	2:C:359:MET:HG2	1.87	0.56
2:I:204:GLN:HE22	2:I:222:LEU:HD13	1.70	0.56
2:C:494:TYR:HD2	2:C:530:GLU:HG3	1.70	0.56
3:D:208:PRO:HA	3:D:390:PRO:HA	1.88	0.56
2:I:16:PRO:HB2	2:I:460:ARG:HH21	1.70	0.56
3:J:192:ALA:HB3	3:J:195:VAL:HB	1.87	0.56
2:C:1104:GLU:HG2	2:C:1105:LYS:N	2.21	0.56
2:C:204:GLN:HE22	2:C:222:LEU:HD13	1.70	0.56
3:D:1176:LYS:HD3	3:J:1130:ARG:HH11	1.71	0.56
2:I:1104:GLU:HG2	2:I:1105:LYS:N	2.20	0.56
2:C:246:ASP:N	2:C:246:ASP:OD1	2.34	0.56
2:C:139:GLN:HB2	2:C:391:LEU:HD21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:611:ILE:HD11	2:C:641:PRO:HB3	1.88	0.56
3:D:286:ALA:O	3:D:311:LEU:HA	2.06	0.56
3:J:1194:CYS:SG	3:J:1196:THR:OG1	2.60	0.56
2:C:162:ILE:HB	2:C:172:ILE:HB	1.88	0.56
2:C:468:ARG:HD2	2:C:485:TYR:HB3	1.87	0.56
3:D:1264:GLU:HB3	3:D:1266:ARG:HG3	1.88	0.56
2:I:577:PRO:HG2	2:I:580:MET:HG2	1.87	0.56
2:I:674:VAL:HA	2:I:869:VAL:HG13	1.88	0.56
3:J:661:MET:HG2	3:J:666:PHE:CZ	2.41	0.56
2:C:674:VAL:HA	2:C:869:VAL:HG13	1.87	0.55
2:I:278:GLU:HG3	2:I:284:GLY:HA2	1.87	0.55
2:I:611:ILE:HD11	2:I:641:PRO:HB3	1.88	0.55
3:D:1459:LEU:HD21	3:D:1468:LEU:HG	1.88	0.55
3:D:291:LEU:HB2	3:D:304:LEU:O	2.06	0.55
3:J:546:ARG:HA	3:J:549:ASN:ND2	2.21	0.55
2:C:141:HIS:NE2	2:C:334:ARG:HD3	2.21	0.55
5:F:276:PRO:HB2	5:F:278:HIS:CE1	2.42	0.55
2:I:162:ILE:HB	2:I:172:ILE:HB	1.88	0.55
2:I:209:ARG:HG3	2:I:210:GLU:H	1.69	0.55
2:I:139:GLN:HB2	2:I:391:LEU:HD21	1.88	0.55
2:I:261:LEU:HB3	2:I:291:VAL:HG22	1.89	0.55
5:L:431:ARG:HG3	5:L:434:ARG:HE	1.71	0.55
3:D:988:ARG:NH1	3:D:1054:GLU:OE2	2.35	0.55
2:C:539:VAL:HG21	3:D:1067:VAL:HG11	1.88	0.55
2:C:1071:ILE:HG23	3:D:670:VAL:HG21	1.89	0.55
5:F:431:ARG:HG3	5:F:434:ARG:HE	1.71	0.55
5:L:276:PRO:HB2	5:L:278:HIS:CE1	2.42	0.55
3:J:438:ASP:HB3	3:J:443:VAL:HG12	1.89	0.55
3:J:62:LYS:HG3	3:J:63:TYR:N	2.21	0.55
1:B:101:LEU:HD23	1:B:114:PHE:HA	1.89	0.55
2:C:577:PRO:HG2	2:C:580:MET:HG2	1.87	0.55
2:C:690:ILE:HG13	2:C:852:ILE:HG23	1.89	0.55
3:J:84:ILE:HG23	3:J:88:TYR:HE1	1.72	0.55
3:D:462:GLN:HB2	3:D:513:ILE:HG21	1.89	0.55
3:D:472:LYS:HD2	3:D:475:ARG:HH22	1.71	0.55
1:H:22:GLU:HG2	1:H:198:ARG:HG2	1.88	0.55
4:K:42:PRO:HA	4:K:45:ARG:HG3	1.89	0.55
2:C:1103:ASP:OD1	2:C:1107:ASN:N	2.39	0.55
3:D:84:ILE:HG23	3:D:88:TYR:HE1	1.71	0.55
2:I:179:SER:HB2	2:I:181:VAL:H	1.72	0.55
3:J:1232:PRO:HB2	3:J:1356:TYR:HE2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:GLU:HG2	1:B:198:ARG:HG2	1.88	0.54
3:D:398:ALA:HB2	3:D:447:VAL:HG12	1.89	0.54
3:D:423:ASP:HB2	3:D:426:LYS:HB3	1.90	0.54
3:D:703:ASN:HD22	3:D:704:ARG:N	2.05	0.54
1:G:55:SER:HB2	1:G:158:ILE:HD13	1.89	0.54
2:I:13:ILE:HG21	2:I:483:VAL:HG21	1.89	0.54
2:I:81:ASP:OD1	2:I:81:ASP:N	2.39	0.54
3:J:1364:HIS:CD2	3:J:1366:LYS:HE2	2.43	0.54
3:J:1459:LEU:HD21	3:J:1468:LEU:HG	1.88	0.54
5:L:157:GLN:HG3	5:L:167:ASP:OD1	2.07	0.54
2:I:817:PRO:HG2	5:L:323:LEU:HD22	1.89	0.54
2:C:815:LEU:HD22	2:C:819:VAL:HB	1.89	0.54
1:B:42:ARG:NH1	2:C:981:GLU:OE2	2.40	0.54
1:H:101:LEU:HD23	1:H:114:PHE:HA	1.89	0.54
3:J:988:ARG:NH1	3:J:1054:GLU:OE2	2.35	0.54
3:J:900:ILE:HG12	3:J:914:LEU:HD21	1.89	0.54
3:J:1208:ASP:HB2	3:J:1215:VAL:HA	1.89	0.54
3:D:28:LYS:HB3	3:D:30:GLU:OE1	2.08	0.54
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.90	0.54
2:C:584:GLU:HB3	2:C:666:LEU:H	1.73	0.54
2:I:207:LEU:HD22	2:I:221:LEU:HD21	1.90	0.54
3:J:703:ASN:HD22	3:J:704:ARG:N	2.06	0.54
5:L:220:ARG:H	5:L:220:ARG:HE	1.53	0.54
3:D:1232:PRO:HB2	3:D:1356:TYR:HE2	1.72	0.54
3:D:667:ALA:HB1	3:D:672:ALA:HB3	1.87	0.54
3:D:709:HIS:HB3	3:D:711:LEU:H	1.73	0.54
3:J:133:ILE:HD11	3:J:460:ALA:HB1	1.90	0.54
3:J:1381:VAL:HG21	3:J:1389:LEU:HD23	1.90	0.54
3:D:546:ARG:HA	3:D:549:ASN:ND2	2.22	0.54
3:J:566:ILE:HD11	5:L:207:LEU:HD21	1.89	0.54
2:C:207:LEU:HD22	2:C:221:LEU:HD21	1.90	0.54
2:C:81:ASP:OD1	2:C:81:ASP:N	2.39	0.54
3:D:1364:HIS:CD2	3:D:1366:LYS:HE2	2.43	0.54
4:E:42:PRO:HA	4:E:45:ARG:HG3	1.90	0.54
5:F:387:ARG:NH2	5:F:416:GLU:OE2	2.41	0.54
2:I:815:LEU:HD22	2:I:819:VAL:HB	1.89	0.54
3:J:709:HIS:HB3	3:J:711:LEU:H	1.73	0.54
5:F:252:THR:HG1	6:O:28:DA:H8	1.55	0.54
3:D:133:ILE:HD11	3:D:460:ALA:HB1	1.90	0.54
3:D:900:ILE:HG12	3:D:914:LEU:HD21	1.89	0.54
2:I:1057:SER:HB3	3:J:623:VAL:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1093:TYR:HE1	3:J:1097:LYS:HE3	1.73	0.54
3:J:462:GLN:HB2	3:J:513:ILE:HG21	1.89	0.54
2:I:1083:GLU:OE2	3:J:87:ARG:NH1	2.41	0.54
5:F:254:ALA:O	5:F:258:ILE:HG12	2.08	0.54
2:I:197:LEU:HD22	2:I:207:LEU:HD11	1.89	0.54
5:L:387:ARG:NH2	5:L:416:GLU:OE2	2.41	0.54
2:C:1071:ILE:HG13	3:D:670:VAL:HG11	1.90	0.53
3:D:224:ARG:H	3:D:251:PHE:HE1	1.56	0.53
3:J:704:ARG:NE	3:J:705:ALA:O	2.39	0.53
1:A:55:SER:HB2	1:A:158:ILE:HD13	1.89	0.53
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.89	0.53
2:C:261:LEU:HB3	2:C:291:VAL:HG22	1.89	0.53
2:I:584:GLU:HB3	2:I:666:LEU:H	1.73	0.53
3:J:423:ASP:HB2	3:J:426:LYS:HB3	1.90	0.53
3:J:356:PRO:HB3	3:J:441:ARG:HA	1.89	0.53
4:K:14:ASP:OD1	4:K:14:ASP:N	2.39	0.53
2:C:234:ALA:HA	2:C:237:ARG:HB2	1.91	0.53
3:D:224:ARG:NH2	3:D:254:GLU:OE2	2.41	0.53
3:D:438:ASP:HB3	3:D:443:VAL:HG12	1.89	0.53
3:J:1264:GLU:HB3	3:J:1266:ARG:HG3	1.88	0.53
3:J:1476:THR:HA	4:K:17:TYR:HB3	1.91	0.53
3:J:633:VAL:HG13	3:J:635:PRO:HD3	1.91	0.53
5:L:254:ALA:O	5:L:258:ILE:HG12	2.08	0.53
2:C:675:ALA:HB2	2:C:867:VAL:HG11	1.91	0.53
3:D:1087:ARG:NH1	3:D:1236:LEU:O	2.41	0.53
4:E:6:ILE:HA	4:E:9:LEU:HD12	1.91	0.53
1:H:49:PRO:HA	1:H:148:VAL:HG12	1.90	0.53
2:I:234:ALA:HA	2:I:237:ARG:HB2	1.91	0.53
2:I:987:ILE:HA	3:J:948:THR:HG21	1.90	0.53
1:B:49:PRO:HA	1:B:148:VAL:HG12	1.89	0.53
3:D:1450:ALA:HA	3:D:1455:LYS:HE3	1.91	0.53
3:D:780:LYS:HD3	3:D:912:LYS:HD2	1.91	0.53
5:F:157:GLN:HG3	5:F:167:ASP:OD1	2.08	0.53
5:F:204:GLU:O	5:F:207:LEU:HB2	2.08	0.53
2:I:436:GLY:O	2:I:469:THR:OG1	2.23	0.53
3:J:62:LYS:HG3	3:J:63:TYR:H	1.74	0.53
4:K:6:ILE:HA	4:K:9:LEU:HD12	1.91	0.53
5:L:204:GLU:O	5:L:207:LEU:HB2	2.08	0.53
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.90	0.53
3:D:1208:ASP:HB2	3:D:1215:VAL:HA	1.89	0.53
2:I:833:LEU:HD21	2:I:839:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:400:VAL:HG23	3:J:402:PRO:HD3	1.90	0.53
3:J:398:ALA:HB2	3:J:447:VAL:HG12	1.89	0.53
1:A:222:LEU:HD23	1:B:219:LYS:HB3	1.91	0.53
2:C:197:LEU:HD22	2:C:207:LEU:HD11	1.90	0.53
2:I:773:LEU:HA	5:L:388:LYS:HE3	1.91	0.53
3:D:1381:VAL:HG21	3:D:1389:LEU:HD23	1.90	0.53
2:C:886:LEU:HD21	3:D:951:ILE:HG12	1.90	0.53
2:I:1051:GLU:HB3	2:I:1056:LYS:HG3	1.91	0.53
5:F:278:HIS:NE2	6:O:20:DT:OP2	2.37	0.53
2:C:833:LEU:HD21	2:C:839:LEU:HD11	1.90	0.52
3:D:400:VAL:HG23	3:D:402:PRO:HD3	1.90	0.52
3:J:1118:ILE:HB	3:J:1346:ARG:HH21	1.75	0.52
2:C:16:PRO:HB2	2:C:460:ARG:NH2	2.24	0.52
2:I:160:ALA:HB3	2:I:174:LEU:HB2	1.90	0.52
2:I:324:ASP:HB3	2:I:327:HIS:HB2	1.90	0.52
2:C:172:ILE:HA	2:C:186:VAL:HG22	1.91	0.52
3:D:633:VAL:HG13	3:D:635:PRO:HD3	1.91	0.52
2:I:172:ILE:HA	2:I:186:VAL:HG22	1.91	0.52
3:J:552:ASN:HA	3:J:555:LYS:HE3	1.92	0.52
3:J:780:LYS:HD3	3:J:912:LYS:HD2	1.91	0.52
2:C:773:LEU:HD23	5:F:369:LEU:HD13	1.91	0.52
3:D:1093:TYR:HE1	3:D:1097:LYS:HE3	1.73	0.52
3:D:908:LYS:HE3	3:D:908:LYS:HA	1.90	0.52
2:I:1103:ASP:OD1	2:I:1107:ASN:N	2.41	0.52
2:C:1016:ILE:O	3:D:87:ARG:NH2	2.42	0.52
5:F:202:LEU:HD23	5:F:206:ASN:HD22	1.74	0.52
3:J:122:GLU:O	3:J:126:VAL:HG23	2.10	0.52
2:C:580:MET:O	2:C:903:SER:N	2.35	0.52
1:G:53:VAL:HG23	1:G:144:VAL:HG22	1.92	0.52
3:J:1087:ARG:NH1	3:J:1236:LEU:O	2.42	0.52
5:L:398:LEU:HD21	7:S:21:DT:H72	1.91	0.52
1:A:53:VAL:HG23	1:A:144:VAL:HG22	1.92	0.52
2:C:36:PRO:HA	2:C:39:ARG:HD2	1.92	0.52
2:C:154:ARG:HD2	2:C:157:ARG:HB2	1.92	0.52
2:C:939:ARG:HB3	2:C:982:PRO:HG3	1.92	0.52
3:D:122:GLU:O	3:D:126:VAL:HG23	2.10	0.52
3:D:218:LYS:HD2	3:D:338:GLU:HG2	1.92	0.52
3:D:543:LEU:HB3	3:D:581:VAL:HG22	1.92	0.52
1:A:50:GLY:O	1:A:146:ARG:HB2	2.10	0.52
2:I:707:ARG:HH21	2:I:824:ARG:NE	2.08	0.52
3:J:908:LYS:HA	3:J:908:LYS:HE3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:163:ILE:HD12	2:C:164:PRO:HD2	1.91	0.52
3:D:1118:ILE:HB	3:D:1346:ARG:HH21	1.74	0.52
2:I:163:ILE:HD12	2:I:164:PRO:HD2	1.92	0.52
4:K:88:GLU:HA	4:K:91:ARG:HB2	1.92	0.52
5:L:202:LEU:HD23	5:L:206:ASN:HD22	1.74	0.52
2:C:707:ARG:HH21	2:C:824:ARG:NE	2.07	0.51
4:E:88:GLU:HA	4:E:91:ARG:HB2	1.93	0.51
1:H:42:ARG:NH1	2:I:981:GLU:OE2	2.43	0.51
2:I:239:PHE:HA	2:I:242:LEU:HD12	1.92	0.51
2:I:36:PRO:HA	2:I:39:ARG:HD2	1.92	0.51
2:I:675:ALA:HB2	2:I:867:VAL:HG11	1.91	0.51
2:C:1051:GLU:HB3	2:C:1056:LYS:HG3	1.91	0.51
4:E:14:ASP:N	4:E:14:ASP:OD1	2.37	0.51
2:I:16:PRO:HB2	2:I:460:ARG:NH2	2.24	0.51
3:D:977:ALA:HB2	3:J:831:GLY:CA	2.37	0.51
5:F:271:ARG:HD2	5:F:275:ILE:HD13	1.92	0.51
1:G:13:ALA:HB3	1:H:228:PRO:HB3	1.91	0.51
2:I:351:LEU:HD11	2:I:373:VAL:HG13	1.93	0.51
5:L:411:ARG:HD3	6:R:1:DC:H5'	1.92	0.51
1:B:152:PRO:HD2	1:B:155:ARG:HG3	1.92	0.51
2:C:195:LEU:HG	2:C:238:LEU:HG	1.93	0.51
5:F:166:PRO:HB2	5:F:169:LYS:HB3	1.92	0.51
5:F:252:THR:O	5:F:255:THR:OG1	2.24	0.51
2:I:690:ILE:HG13	2:I:852:ILE:HG23	1.92	0.51
2:C:1047:HIS:HA	2:C:1050:GLN:HB2	1.93	0.51
3:D:1205:TYR:O	3:D:1366:LYS:HD3	2.09	0.51
3:D:1238:MET:O	3:D:1359:GLN:NE2	2.44	0.51
2:C:1115:LEU:HD13	3:D:88:TYR:CE1	2.45	0.51
2:I:612:ALA:HA	2:I:622:GLU:HA	1.92	0.51
3:J:594:PRO:HG2	5:L:221:GLY:HA2	1.92	0.51
2:C:239:PHE:HA	2:C:242:LEU:HD12	1.92	0.51
2:C:1007:ALA:HB2	3:D:648:MET:HG3	1.92	0.51
1:H:34:VAL:HG11	2:I:978:ARG:HB3	1.93	0.51
2:C:351:LEU:HD11	2:C:373:VAL:HG13	1.92	0.51
3:D:266:GLU:HG3	3:D:286:ALA:HB2	1.92	0.51
3:J:680:GLN:O	3:J:682:ASP:N	2.44	0.51
5:L:166:PRO:HB2	5:L:169:LYS:HB3	1.93	0.51
3:D:1142:SER:O	3:D:1364:HIS:ND1	2.44	0.51
3:D:242:LEU:HB3	3:D:311:LEU:O	2.11	0.51
2:I:1071:ILE:HG23	3:J:670:VAL:HG21	1.93	0.51
3:J:1046:GLN:HE21	3:J:1050:GLY:HA2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1384:PRO:HA	3:J:1415:VAL:HG13	1.93	0.51
3:D:129:PHE:HE1	3:D:457:GLY:HA3	1.76	0.51
2:I:154:ARG:HD2	2:I:157:ARG:HB2	1.92	0.51
3:D:552:ASN:HA	3:D:555:LYS:HE3	1.92	0.50
2:I:1016:ILE:HG13	2:I:1017:THR:H	1.76	0.50
2:I:1047:HIS:HA	2:I:1050:GLN:HB2	1.93	0.50
2:I:580:MET:O	2:I:903:SER:N	2.35	0.50
3:J:1205:TYR:O	3:J:1366:LYS:HD3	2.11	0.50
3:J:430:GLU:N	3:J:430:GLU:OE1	2.42	0.50
3:J:543:LEU:HB3	3:J:581:VAL:HG22	1.93	0.50
3:J:629:SER:HB3	3:J:726:ILE:HG13	1.92	0.50
3:D:1384:PRO:HA	3:D:1415:VAL:HG13	1.93	0.50
3:J:1238:MET:O	3:J:1359:GLN:NE2	2.44	0.50
4:K:67:GLU:O	4:K:70:THR:OG1	2.23	0.50
3:J:1491:THR:HG22	4:K:92:LEU:HD12	1.92	0.50
3:D:1476:THR:HA	4:E:17:TYR:HB3	1.93	0.50
2:I:552:HIS:ND1	3:J:1061:PHE:O	2.44	0.50
2:I:939:ARG:HB3	2:I:982:PRO:HG3	1.91	0.50
3:J:675:ARG:HH22	5:L:437:LEU:HG	1.77	0.50
3:J:631:ILE:HG13	3:J:740:PHE:HD2	1.74	0.50
5:L:271:ARG:HD2	5:L:275:ILE:HD13	1.91	0.50
2:C:1016:ILE:HG13	2:C:1017:THR:H	1.76	0.50
2:I:456:ALA:HB3	2:I:459:ALA:HB2	1.93	0.50
4:K:56:ASP:N	4:K:56:ASP:OD1	2.43	0.50
2:C:508:ILE:HD12	2:C:526:PRO:HB3	1.94	0.50
3:D:1046:GLN:HE21	3:D:1050:GLY:HA2	1.75	0.50
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.47	0.50
2:C:778:PHE:CZ	5:F:434:ARG:HA	2.42	0.50
5:F:431:ARG:HG3	5:F:434:ARG:NE	2.27	0.50
3:D:130:ASN:HA	5:F:98:GLN:HE22	1.76	0.50
1:G:83:LYS:HD2	1:G:168:ASP:HB2	1.94	0.50
2:I:202:TYR:HE2	2:I:300:ASP:HB2	1.77	0.50
1:A:83:LYS:HD2	1:A:168:ASP:HB2	1.94	0.50
3:D:237:ARG:HG2	3:D:240:GLU:HB2	1.92	0.50
2:C:436:GLY:O	2:C:469:THR:OG1	2.23	0.50
3:D:252:ARG:HA	3:D:303:PRO:HA	1.92	0.50
4:E:56:ASP:OD1	4:E:56:ASP:N	2.43	0.50
3:J:1281:VAL:HG21	3:J:1313:VAL:HG11	1.93	0.50
3:J:129:PHE:CE1	3:J:457:GLY:HA3	2.46	0.50
5:L:431:ARG:HG3	5:L:434:ARG:NE	2.27	0.50
6:R:2:DT:H2''	6:R:3:DT:H5'	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:346:ASP:N	5:F:346:ASP:OD1	2.44	0.50
3:J:129:PHE:HE1	3:J:457:GLY:HA3	1.77	0.50
3:D:1281:VAL:HG21	3:D:1313:VAL:HG11	1.93	0.50
1:H:152:PRO:HD2	1:H:155:ARG:HG3	1.92	0.50
3:D:777:PRO:HB2	3:D:912:LYS:NZ	2.27	0.49
3:J:76:CYS:HB2	3:J:78:VAL:HG23	1.94	0.49
5:L:421:ARG:O	5:L:424:LYS:HB2	2.12	0.49
2:C:3:ILE:HD11	2:C:902:ILE:HG13	1.94	0.49
3:D:430:GLU:OE1	3:D:430:GLU:N	2.44	0.49
5:F:137:LEU:HB3	5:F:141:LEU:HD23	1.93	0.49
2:I:676:ILE:O	3:J:948:THR:OG1	2.22	0.49
1:G:50:GLY:O	1:G:146:ARG:HB2	2.11	0.49
2:I:1006:HIS:HD2	2:I:1024:LYS:HA	1.77	0.49
2:I:1038:TRP:CE3	3:J:1099:VAL:HG21	2.47	0.49
2:I:1067:TYR:CZ	5:L:357:VAL:HG12	2.47	0.49
1:B:63:HIS:CE1	1:B:65:PHE:HB2	2.48	0.49
2:C:194:VAL:HG12	2:C:207:LEU:HD13	1.94	0.49
2:C:456:ALA:HB3	2:C:459:ALA:HB2	1.93	0.49
3:D:629:SER:HB3	3:D:726:ILE:HG13	1.92	0.49
1:H:143:ARG:NH1	1:H:160:ASP:OD2	2.45	0.49
1:H:162:ILE:HG23	1:H:163:ASN:H	1.78	0.49
2:I:268:ASP:OD1	2:I:288:ARG:HD2	2.13	0.49
3:J:896:ALA:O	3:J:900:ILE:HG13	2.12	0.49
5:L:355:SER:HB3	5:L:358:GLU:HG3	1.94	0.49
2:I:611:ILE:HG13	2:I:625:LEU:HD11	1.94	0.49
3:J:1459:LEU:HA	3:J:1464:GLU:HG3	1.94	0.49
2:C:612:ALA:HA	2:C:622:GLU:HA	1.93	0.49
3:D:1080:GLY:O	3:D:1083:ASP:HB2	2.13	0.49
3:D:1459:LEU:HA	3:D:1464:GLU:HG3	1.94	0.49
5:F:421:ARG:O	5:F:424:LYS:HB2	2.12	0.49
1:H:143:ARG:NH1	1:H:158:ILE:HD11	2.28	0.49
2:I:3:ILE:HD11	2:I:902:ILE:HG13	1.94	0.49
5:L:137:LEU:HB3	5:L:141:LEU:HD23	1.93	0.49
2:I:773:LEU:HD23	5:L:369:LEU:HD13	1.95	0.49
2:C:1008:ARG:HH11	2:C:1029:GLY:N	2.11	0.49
2:C:268:ASP:OD1	2:C:288:ARG:HD2	2.13	0.49
3:D:1126:ASP:HB3	3:D:1129:THR:HB	1.94	0.49
2:I:508:ILE:HD12	2:I:526:PRO:HB3	1.95	0.49
3:J:1495:ILE:HD13	4:K:80:VAL:HB	1.94	0.49
5:L:252:THR:O	5:L:255:THR:OG1	2.22	0.49
1:A:50:GLY:HA3	1:A:171:PHE:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:63:HIS:CE1	1:H:65:PHE:HB2	2.47	0.49
2:I:1008:ARG:HH11	2:I:1029:GLY:N	2.11	0.49
2:C:202:TYR:HE2	2:C:300:ASP:HB2	1.77	0.49
5:F:252:THR:HA	6:O:29:DC:H5	1.76	0.49
3:J:1142:SER:O	3:J:1364:HIS:ND1	2.46	0.49
5:L:116:ASP:OD1	5:L:119:ARG:NH2	2.46	0.49
2:C:611:ILE:HG13	2:C:625:LEU:HD11	1.94	0.49
3:D:704:ARG:NE	3:D:705:ALA:O	2.40	0.49
2:I:1008:ARG:HH21	2:I:1011:GLY:C	2.17	0.49
2:I:195:LEU:HG	2:I:238:LEU:HG	1.94	0.49
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.95	0.48
1:B:143:ARG:NH1	1:B:158:ILE:HD11	2.28	0.48
3:D:834:THR:OG1	3:D:835:SER:N	2.45	0.48
2:I:838:LYS:NZ	2:I:997:LEU:HD12	2.28	0.48
1:B:34:VAL:HG11	2:C:978:ARG:HB3	1.95	0.48
5:F:355:SER:HB3	5:F:358:GLU:HG3	1.94	0.48
2:I:194:VAL:HG12	2:I:207:LEU:HD13	1.94	0.48
3:J:1003:VAL:HG21	3:J:1041:MET:HG2	1.95	0.48
2:C:1006:HIS:HD2	2:C:1024:LYS:HA	1.78	0.48
2:C:768:SER:OG	2:C:771:GLU:HB2	2.13	0.48
3:D:527:MET:HG3	3:D:537:THR:HB	1.94	0.48
1:G:24:VAL:HG22	1:G:196:THR:HG23	1.96	0.48
1:H:45:LEU:HD22	3:J:851:LEU:HD13	1.95	0.48
2:I:56:GLU:HB3	2:I:359:MET:HE1	1.95	0.48
2:I:1007:ALA:HB2	3:J:648:MET:HG3	1.94	0.48
5:L:103:ILE:HD13	5:L:211:VAL:HG21	1.95	0.48
2:C:1060:ILE:H	2:C:1060:ILE:HG13	1.37	0.48
3:D:896:ALA:O	3:D:900:ILE:HG13	2.13	0.48
3:J:1126:ASP:HB3	3:J:1129:THR:HB	1.95	0.48
5:L:146:VAL:HG13	5:L:193:ARG:HG2	1.96	0.48
5:L:379:ARG:HG3	5:L:405:PHE:CE2	2.49	0.48
7:P:7:DA:H1'	7:P:8:DT:H5'	1.96	0.48
2:C:1035:MET:HA	2:C:1038:TRP:CE3	2.49	0.48
2:C:399:ASN:ND2	2:C:402:SER:OG	2.46	0.48
3:D:637:LEU:O	3:D:935:LYS:NZ	2.47	0.48
5:F:103:ILE:HD13	5:F:211:VAL:HG21	1.95	0.48
2:C:638:ASP:H	2:C:659:PRO:HG3	1.79	0.48
2:I:17:PRO:HB2	2:I:20:GLU:HB3	1.95	0.48
2:I:399:ASN:ND2	2:I:402:SER:OG	2.47	0.48
3:J:1080:GLY:O	3:J:1083:ASP:HB2	2.13	0.48
3:J:834:THR:OG1	3:J:835:SER:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1003:VAL:HG21	3:D:1041:MET:HG2	1.96	0.48
3:D:76:CYS:HB2	3:D:78:VAL:HG23	1.95	0.48
2:I:638:ASP:H	2:I:659:PRO:HG3	1.79	0.48
3:J:527:MET:HG3	3:J:537:THR:HB	1.94	0.48
2:C:17:PRO:HB2	2:C:20:GLU:HB3	1.95	0.48
1:G:50:GLY:HA3	1:G:171:PHE:O	2.13	0.48
3:J:1232:PRO:HB3	3:J:1361:VAL:HG11	1.96	0.48
2:C:1019:GLN:HE22	3:D:621:LYS:HG2	1.78	0.48
3:D:777:PRO:HB2	3:D:912:LYS:HZ1	1.78	0.48
2:I:571:LEU:HG	2:I:700:TYR:HA	1.95	0.48
3:J:777:PRO:HB2	3:J:912:LYS:NZ	2.28	0.48
5:L:413:ARG:NH1	5:L:413:ARG:HG2	2.26	0.48
2:C:444:PRO:HA	2:C:563:ASN:HD21	1.79	0.48
2:C:56:GLU:HB3	2:C:359:MET:HE1	1.95	0.48
3:D:618:LEU:HD23	3:D:1467:ILE:HG23	1.96	0.48
2:I:1035:MET:HA	2:I:1038:TRP:CE3	2.48	0.48
2:I:121:MET:HE1	2:I:336:VAL:HG21	1.95	0.48
2:I:262:ALA:HB2	2:I:291:VAL:HG23	1.96	0.48
2:I:683:ASN:HB2	2:I:872:ASN:HB2	1.96	0.48
1:B:45:LEU:HD22	3:D:851:LEU:HD13	1.95	0.47
3:D:594:PRO:HG2	5:F:221:GLY:HA2	1.96	0.47
3:J:618:LEU:HD23	3:J:1467:ILE:HG23	1.96	0.47
2:C:1009:SER:HB3	3:D:651:GLU:O	2.14	0.47
2:C:571:LEU:HG	2:C:700:TYR:HA	1.96	0.47
3:D:272:LEU:O	3:D:279:VAL:N	2.44	0.47
3:D:912:LYS:HE3	3:D:912:LYS:HA	1.95	0.47
5:F:425:TYR:CZ	5:F:429:ARG:HD2	2.49	0.47
2:I:118:LEU:HD12	2:I:119:PRO:HD2	1.96	0.47
2:I:42:VAL:HA	2:I:46:ALA:HB2	1.96	0.47
2:I:768:SER:OG	2:I:771:GLU:HB2	2.13	0.47
3:J:796:ARG:HG3	3:J:861:GLN:HB3	1.97	0.47
1:A:230:ALA:HA	1:B:13:ALA:O	2.14	0.47
2:C:327:HIS:HB3	2:C:330:ASN:HD22	1.80	0.47
3:D:1122:LEU:HD22	3:D:1178:ALA:HB2	1.95	0.47
3:D:1186:VAL:HG12	3:D:1188:VAL:HG23	1.96	0.47
5:F:116:ASP:OD1	5:F:119:ARG:NH2	2.47	0.47
5:F:379:ARG:HG3	5:F:405:PHE:CE2	2.49	0.47
2:I:446:GLY:O	2:I:449:ILE:HG13	2.14	0.47
2:I:878:SER:HB2	3:J:1029:ARG:HD2	1.97	0.47
3:J:637:LEU:O	3:J:935:LYS:NZ	2.47	0.47
3:J:970:LYS:O	3:J:974:ILE:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:224:PHE:CE2	5:L:228:ILE:HD11	2.49	0.47
5:F:224:PHE:CE2	5:F:228:ILE:HD11	2.50	0.47
3:J:1380:GLU:HG3	3:J:1392:GLY:HA2	1.97	0.47
3:J:132:TYR:HA	3:J:456:MET:HB3	1.95	0.47
3:J:809:PRO:HB3	3:J:839:LEU:HD13	1.96	0.47
1:A:64:GLU:O	1:A:75:VAL:HB	2.15	0.47
2:C:683:ASN:HB2	2:C:872:ASN:HB2	1.96	0.47
3:D:1232:PRO:HB3	3:D:1361:VAL:HG11	1.97	0.47
3:D:1349:VAL:HG22	3:D:1368:ILE:HG22	1.97	0.47
1:G:64:GLU:O	1:G:75:VAL:HB	2.14	0.47
2:I:327:HIS:CE1	2:I:433:THR:HG21	2.49	0.47
3:J:1127:GLU:C	3:J:1129:THR:H	2.18	0.47
3:J:1122:LEU:HD22	3:J:1178:ALA:HB2	1.96	0.47
3:J:912:LYS:HE3	3:J:912:LYS:HA	1.96	0.47
1:A:227:ASN:OD1	1:A:227:ASN:N	2.47	0.47
2:C:262:ALA:HB2	2:C:291:VAL:HG23	1.97	0.47
3:D:405:ASP:N	3:D:423:ASP:OD1	2.47	0.47
3:D:850:LEU:HD11	3:D:884:ARG:HH12	1.80	0.47
3:J:1109:GLU:O	3:J:1201:CYS:HB2	2.14	0.47
2:I:1007:ALA:HB1	3:J:652:LEU:HD13	1.95	0.47
3:J:850:LEU:HD11	3:J:884:ARG:HH12	1.79	0.47
6:O:2:DT:H2''	6:O:3:DT:H5'	1.96	0.47
2:C:302:VAL:O	2:C:305:PRO:HD2	2.15	0.47
2:C:446:GLY:O	2:C:449:ILE:HG13	2.14	0.47
2:C:42:VAL:HA	2:C:46:ALA:HB2	1.97	0.47
3:D:1060:SER:OG	3:D:1061:PHE:N	2.48	0.47
3:D:1127:GLU:C	3:D:1129:THR:H	2.18	0.47
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.97	0.47
2:I:971:LYS:HG3	2:I:988:VAL:HG13	1.96	0.47
2:C:1001:VAL:HG13	3:D:630:VAL:HG12	1.95	0.47
2:C:118:LEU:HD12	2:C:119:PRO:HD2	1.96	0.47
2:C:211:LEU:HD22	2:C:218:VAL:HG13	1.97	0.47
2:C:726:ILE:HB	2:C:729:LEU:HB2	1.97	0.47
3:D:1040:GLY:O	3:D:1060:SER:HB2	2.15	0.47
1:H:48:ILE:HG13	1:H:213:GLN:HE21	1.79	0.47
3:J:1040:GLY:O	3:J:1060:SER:HB2	2.15	0.47
7:P:3:DC:H2''	7:P:4:DA:C8	2.50	0.47
3:D:1124:GLN:O	3:D:1132:LEU:HD23	2.15	0.47
3:D:251:PHE:HB3	3:D:305:ALA:H	1.79	0.47
3:D:809:PRO:HB3	3:D:839:LEU:HD13	1.97	0.47
2:I:505:GLY:O	2:I:506:ASP:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1447:LEU:O	3:J:1450:ALA:HB3	2.15	0.47
3:J:666:PHE:CE1	3:J:687:VAL:HG12	2.50	0.47
3:J:860:LEU:H	3:J:860:LEU:HD12	1.80	0.47
2:I:1086:ARG:NH2	3:J:88:TYR:OH	2.46	0.47
5:F:146:VAL:HG13	5:F:193:ARG:HG2	1.96	0.47
2:I:573:ARG:NH1	2:I:697:ARG:HG2	2.29	0.47
3:J:1186:VAL:HG12	3:J:1188:VAL:HG23	1.97	0.47
3:J:1349:VAL:HG22	3:J:1368:ILE:HG22	1.97	0.47
3:J:569:ASN:HD22	5:L:229:GLN:NE2	2.12	0.47
3:J:788:GLY:O	3:J:791:TYR:HB3	2.15	0.47
5:L:425:TYR:CZ	5:L:429:ARG:HD2	2.49	0.47
7:S:7:DA:H1'	7:S:8:DT:H5'	1.96	0.47
1:A:221:HIS:HA	1:A:224:TYR:CD1	2.50	0.47
2:C:971:LYS:HG3	2:C:988:VAL:HG13	1.96	0.47
1:G:205:VAL:HG13	1:G:209:GLU:HB2	1.97	0.47
3:J:657:LEU:HD22	3:J:691:LEU:HD13	1.97	0.47
2:C:151:ASP:OD2	2:C:151:ASP:N	2.48	0.46
2:C:399:ASN:HB2	2:C:400:PRO:HD2	1.97	0.46
2:I:302:VAL:O	2:I:305:PRO:HD2	2.15	0.46
3:J:1124:GLN:O	3:J:1132:LEU:HD23	2.15	0.46
2:C:573:ARG:NH1	2:C:697:ARG:HG2	2.30	0.46
2:I:151:ASP:OD2	2:I:151:ASP:N	2.48	0.46
2:I:304:LEU:HB3	2:I:305:PRO:HD3	1.97	0.46
2:I:575:GLN:HG3	2:I:662:GLU:OE1	2.15	0.46
1:A:187:GLY:HA3	1:A:192:LEU:HD12	1.97	0.46
1:B:48:ILE:HG13	1:B:213:GLN:HE21	1.79	0.46
2:C:142:ARG:HA	2:C:331:ARG:HA	1.97	0.46
2:C:327:HIS:CE1	2:C:433:THR:HG21	2.50	0.46
3:D:1109:GLU:O	3:D:1201:CYS:HB2	2.15	0.46
3:J:405:ASP:N	3:J:423:ASP:OD1	2.48	0.46
3:J:644:LEU:HD12	3:J:645:PRO:HD2	1.97	0.46
5:L:411:ARG:HD3	6:R:1:DC:H6	1.80	0.46
1:A:205:VAL:HG13	1:A:209:GLU:HB2	1.97	0.46
2:C:332:ARG:NH1	2:C:338:GLU:OE2	2.49	0.46
2:C:567:GLN:HB2	2:C:997:LEU:HD13	1.97	0.46
2:C:605:LYS:HG2	2:C:612:ALA:HB3	1.97	0.46
3:D:39:PRO:HG2	3:D:47:GLU:HG3	1.97	0.46
2:I:211:LEU:HD22	2:I:218:VAL:HG13	1.96	0.46
2:I:605:LYS:HG2	2:I:612:ALA:HB3	1.96	0.46
2:I:684:PHE:HE1	3:J:783:ARG:HB2	1.81	0.46
3:J:39:PRO:HG2	3:J:47:GLU:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:575:GLN:HG3	2:C:662:GLU:OE1	2.15	0.46
2:C:971:LYS:HD2	2:C:986:PRO:HG2	1.98	0.46
3:D:132:TYR:HA	3:D:456:MET:HB3	1.96	0.46
3:D:796:ARG:HG3	3:D:861:GLN:HB3	1.97	0.46
2:I:327:HIS:HB3	2:I:330:ASN:HD22	1.80	0.46
2:I:971:LYS:HD2	2:I:986:PRO:HG2	1.98	0.46
3:J:455:ARG:HB2	3:J:460:ALA:HB2	1.96	0.46
7:S:3:DC:H2"	7:S:4:DA:C8	2.50	0.46
3:D:1236:LEU:HD23	3:D:1359:GLN:HG3	1.97	0.46
3:D:455:ARG:HB2	3:D:460:ALA:HB2	1.96	0.46
2:I:396:ASP:HA	2:I:633:GLN:HE22	1.79	0.46
3:J:619:LEU:HD11	3:J:1439:SER:HB2	1.97	0.46
3:J:414:ARG:HA	3:J:414:ARG:HD2	1.61	0.46
2:C:396:ASP:HA	2:C:633:GLN:HE22	1.79	0.46
3:D:317:MET:HG3	3:D:339:TRP:HB3	1.98	0.46
3:D:822:ALA:HB3	3:D:825:ALA:HB2	1.97	0.46
2:I:142:ARG:HA	2:I:331:ARG:HA	1.97	0.46
3:J:1060:SER:OG	3:J:1061:PHE:N	2.48	0.46
1:A:56:VAL:HG22	1:A:142:VAL:HG12	1.98	0.46
2:C:5:ARG:HG2	2:C:10:ARG:HH22	1.81	0.46
2:C:609:THR:OG1	2:C:610:ARG:N	2.49	0.46
3:D:248:PRO:HA	3:D:307:GLY:O	2.15	0.46
3:D:831:GLY:HA3	3:J:977:ALA:HB2	1.98	0.46
3:D:860:LEU:HD12	3:D:860:LEU:H	1.80	0.46
3:J:95:LEU:HD11	3:J:574:LEU:HD11	1.97	0.46
1:B:162:ILE:HG23	1:B:163:ASN:H	1.81	0.46
1:B:174:VAL:HA	1:B:201:THR:HG22	1.98	0.46
5:F:164:GLU:HB3	5:F:165:LYS:H	1.51	0.46
5:F:413:ARG:NH1	5:F:413:ARG:HG2	2.26	0.46
2:I:399:ASN:HB2	2:I:400:PRO:HD2	1.96	0.46
1:A:58:ILE:HG21	1:A:68:ILE:HD13	1.98	0.46
2:C:922:PHE:HB2	2:C:967:PHE:CD2	2.51	0.46
3:D:289:THR:O	3:D:306:GLU:N	2.48	0.46
3:D:644:LEU:HD23	3:D:718:PRO:HB3	1.98	0.46
3:D:869:LEU:HD12	3:D:897:GLN:HG3	1.97	0.46
5:F:130:LYS:HD3	5:F:188:TYR:CE1	2.51	0.46
1:G:221:HIS:HA	1:G:224:TYR:CD1	2.51	0.46
2:I:609:THR:OG1	2:I:610:ARG:N	2.49	0.46
2:I:726:ILE:HB	2:I:729:LEU:HB2	1.97	0.46
7:S:10:DT:H2"	7:S:11:DA:C8	2.51	0.46
2:C:650:LYS:HD2	2:C:650:LYS:HA	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1336:LEU:HD22	3:D:1421:LEU:HB3	1.98	0.45
3:D:657:LEU:HD22	3:D:691:LEU:HD13	1.98	0.45
1:H:174:VAL:HA	1:H:201:THR:HG22	1.99	0.45
1:G:47:SER:HG	1:H:32:PHE:HZ	1.64	0.45
2:I:1036:GLU:OE1	2:I:1036:GLU:N	2.46	0.45
3:J:12:LEU:HG	3:J:507:ASN:HD22	1.81	0.45
3:J:869:LEU:HD12	3:J:897:GLN:HG3	1.97	0.45
5:L:130:LYS:HD3	5:L:188:TYR:CE1	2.51	0.45
2:C:304:LEU:HB3	2:C:305:PRO:HD3	1.97	0.45
1:A:72:LYS:HA	2:C:607:ASP:HA	1.98	0.45
2:C:564:MET:HB3	2:C:997:LEU:HD11	1.97	0.45
1:G:58:ILE:HG21	1:G:68:ILE:HD13	1.98	0.45
2:I:650:LYS:HA	2:I:650:LYS:HD2	1.73	0.45
3:J:108:VAL:HB	3:J:109:PRO:HD3	1.98	0.45
2:C:505:GLY:O	2:C:506:ASP:HB3	2.16	0.45
1:G:56:VAL:HG22	1:G:142:VAL:HG12	1.98	0.45
2:I:808:ARG:NH1	5:L:303:TYR:CE2	2.84	0.45
3:J:1144:LEU:HB3	3:J:1171:VAL:HG22	1.97	0.45
3:D:34:TYR:OH	6:O:20:DT:OP1	2.21	0.45
1:B:143:ARG:NH1	1:B:160:ASP:OD2	2.45	0.45
2:C:121:MET:HE1	2:C:336:VAL:HG21	1.98	0.45
2:C:738:ASP:OD1	2:C:739:GLU:N	2.47	0.45
3:D:704:ARG:NH1	3:D:737:ASN:O	2.49	0.45
3:D:824:ASN:ND2	3:D:862:ASP:OD1	2.46	0.45
5:F:418:LYS:O	5:F:422:LYS:HG3	2.16	0.45
1:G:54:THR:N	1:G:143:ARG:O	2.50	0.45
2:I:90:TYR:CE2	2:I:120:LEU:HB2	2.52	0.45
3:J:1236:LEU:HD23	3:J:1359:GLN:HG3	1.97	0.45
2:C:445:GLU:OE1	2:C:560:MET:HG2	2.17	0.45
2:C:688:ILE:HD12	2:C:839:LEU:HB2	1.99	0.45
5:F:405:PHE:HA	5:F:405:PHE:HD1	1.69	0.45
2:I:14:PRO:HB3	2:I:586:ARG:HH22	1.82	0.45
2:I:332:ARG:NH1	2:I:338:GLU:OE2	2.49	0.45
2:I:922:PHE:HB2	2:I:967:PHE:CD2	2.51	0.45
5:L:418:LYS:O	5:L:422:LYS:HG3	2.17	0.45
2:C:230:ARG:HB2	2:C:231:PRO:CD	2.47	0.45
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.52	0.45
3:D:12:LEU:HG	3:D:507:ASN:HD22	1.82	0.45
3:D:176:ASP:OD1	3:D:177:ALA:N	2.47	0.45
3:D:987:GLU:H	3:D:987:GLU:HG2	1.58	0.45
2:I:247:PRO:HA	2:I:248:PRO:HD3	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:564:MET:HB3	2:I:997:LEU:HD11	1.97	0.45
3:J:67:ARG:HB2	5:L:392:ASP:O	2.16	0.45
3:J:987:GLU:HG2	3:J:987:GLU:H	1.58	0.45
3:D:1231:GLU:OE1	3:D:1235:GLN:NE2	2.50	0.45
3:D:791:TYR:CE2	3:D:792:ILE:HG23	2.52	0.45
5:F:386:LEU:HD23	5:F:386:LEU:HA	1.77	0.45
2:I:235:MET:HG2	2:I:253:ALA:HB1	1.98	0.45
3:J:704:ARG:NH1	3:J:737:ASN:O	2.50	0.45
3:J:791:TYR:CE2	3:J:792:ILE:HG23	2.52	0.45
5:L:346:ASP:OD1	5:L:346:ASP:N	2.44	0.45
7:P:10:DT:H2"	7:P:11:DA:C8	2.51	0.45
1:A:54:THR:N	1:A:143:ARG:O	2.49	0.45
1:B:7:LYS:HB2	1:B:8:ALA:H	1.64	0.45
2:C:761:PHE:HA	2:C:785:VAL:HA	1.98	0.45
2:C:838:LYS:NZ	2:C:997:LEU:HD12	2.31	0.45
3:D:1147:ARG:NH2	3:D:1369:GLU:OE2	2.48	0.45
3:J:644:LEU:HD23	3:J:718:PRO:HB3	1.98	0.45
2:I:1060:ILE:HG21	5:L:353:LEU:HD21	1.99	0.45
1:A:153:ALA:HB2	1:A:167:VAL:C	2.38	0.45
3:D:1448:THR:O	3:D:1452:ILE:HG12	2.17	0.45
2:C:1063:ARG:HG3	5:F:356:PRO:HG3	1.98	0.45
2:I:567:GLN:HB2	2:I:997:LEU:HD13	1.99	0.45
2:I:5:ARG:HG2	2:I:10:ARG:HH22	1.81	0.45
1:A:182:GLU:HB2	1:A:194:LYS:HG3	1.98	0.44
2:C:235:MET:HG2	2:C:253:ALA:HB1	1.98	0.44
2:C:394:PHE:O	2:C:406:HIS:HE1	2.00	0.44
2:C:668:LEU:HB3	2:C:995:MET:SD	2.57	0.44
3:D:55:ASP:N	3:D:55:ASP:OD1	2.50	0.44
2:I:1055:ILE:HD11	2:I:1079:PRO:HD3	1.99	0.44
2:I:394:PHE:O	2:I:406:HIS:HE1	2.00	0.44
2:I:445:GLU:OE1	2:I:560:MET:HG2	2.17	0.44
2:I:1102:LEU:HB2	3:J:7:LYS:HB2	1.99	0.44
3:J:824:ASN:ND2	3:J:862:ASP:OD1	2.47	0.44
5:L:257:TRP:O	5:L:260:GLN:HG3	2.17	0.44
5:L:409:ARG:NH1	7:S:21:DT:O4	2.51	0.44
2:C:90:TYR:CE2	2:C:120:LEU:HB2	2.52	0.44
3:D:543:LEU:HG	3:D:600:LEU:HD23	1.99	0.44
5:F:398:LEU:HB2	7:P:20:DG:OP2	2.16	0.44
2:I:704:HIS:CD2	2:I:831:ARG:HD2	2.52	0.44
1:A:153:ALA:HB1	1:A:166:PRO:HB2	1.98	0.44
2:C:14:PRO:HB3	2:C:586:ARG:HH22	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:108:VAL:HB	3:D:109:PRO:HD3	1.98	0.44
3:D:410:THR:OG1	5:F:193:ARG:NH1	2.50	0.44
5:F:376:LEU:HD21	5:F:423:LEU:HD12	2.00	0.44
2:I:290:LEU:HD23	2:I:302:VAL:HG21	1.99	0.44
3:J:1231:GLU:OE1	3:J:1235:GLN:NE2	2.50	0.44
3:J:788:GLY:HA2	3:J:791:TYR:HB3	1.99	0.44
3:D:1056:PRO:HG2	3:D:1058:ARG:HE	1.83	0.44
3:D:1144:LEU:HB3	3:D:1171:VAL:HG22	1.98	0.44
3:D:619:LEU:HD11	3:D:1439:SER:HB2	1.99	0.44
3:D:961:GLN:O	3:D:964:LEU:HG	2.18	0.44
2:I:11:GLU:HG3	2:I:535:SER:HB2	1.98	0.44
3:J:1153:VAL:HB	3:J:1160:LEU:HB2	1.99	0.44
3:J:62:LYS:HB2	3:J:62:LYS:HE2	1.83	0.44
3:J:829:VAL:HG21	3:J:839:LEU:HD11	2.00	0.44
3:D:101:HIS:ND1	3:D:103:TRP:HB2	2.33	0.44
3:D:759:ALA:HA	3:D:763:MET:HB3	2.00	0.44
4:E:23:VAL:HG21	4:E:65:MET:HE3	1.99	0.44
1:H:8:ALA:HA	1:H:9:PRO:HD3	1.86	0.44
3:J:1336:LEU:HD22	3:J:1421:LEU:HB3	1.98	0.44
3:J:1472:ILE:HA	3:J:1473:PRO:HD3	1.85	0.44
3:J:633:VAL:C	3:J:635:PRO:HD3	2.38	0.44
3:J:634:GLY:O	3:J:637:LEU:HB3	2.18	0.44
6:O:24:DC:H42	7:P:2:DG:H1	1.66	0.44
7:S:11:DA:H4'	7:S:12:DA:OP1	2.18	0.44
3:D:634:GLY:O	3:D:637:LEU:HB3	2.18	0.44
3:D:729:HIS:CG	3:D:730:PRO:HD2	2.53	0.44
3:D:1498:ALA:HB2	4:E:88:GLU:OE2	2.17	0.44
1:G:230:ALA:HA	1:H:13:ALA:O	2.18	0.44
1:H:91:ASP:HA	1:H:92:PRO:HD3	1.87	0.44
2:I:1071:ILE:HG13	3:J:670:VAL:HG11	1.99	0.44
3:J:101:HIS:ND1	3:J:103:TRP:HB2	2.33	0.44
3:J:1147:ARG:NH2	3:J:1369:GLU:OE2	2.48	0.44
3:J:822:ALA:HB3	3:J:825:ALA:HB2	2.00	0.44
1:B:199:ILE:HB	1:B:207:PRO:HB3	2.00	0.44
3:D:154:THR:HG22	3:D:157:GLU:HG2	1.99	0.44
3:D:95:LEU:HD11	3:D:574:LEU:HD11	1.98	0.44
5:F:135:THR:HG23	5:F:181:LEU:HD21	2.00	0.44
3:J:1090:ASP:O	3:J:1093:TYR:HB3	2.18	0.44
3:J:696:HIS:ND1	4:K:57:ASP:OD1	2.50	0.44
1:A:50:GLY:N	1:A:147:GLY:O	2.37	0.44
2:C:767:PRO:HD2	2:C:772:ARG:NH2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:249:LYS:NZ	6:O:29:DC:OP1	2.51	0.44
1:G:153:ALA:HB1	1:G:166:PRO:HB2	1.99	0.44
1:G:182:GLU:HB2	1:G:194:LYS:HG3	1.99	0.44
1:G:56:VAL:HG21	1:G:82:LEU:HD13	1.99	0.44
1:H:161:ARG:HE	1:H:162:ILE:HG22	1.83	0.44
2:I:767:PRO:HD2	2:I:772:ARG:NH2	2.33	0.44
3:J:55:ASP:N	3:J:55:ASP:OD1	2.50	0.44
4:K:8:LYS:O	4:K:12:MET:HG3	2.18	0.44
7:P:11:DA:H4'	7:P:12:DA:OP1	2.18	0.44
3:D:1364:HIS:HD2	3:D:1366:LYS:HB2	1.83	0.44
3:D:224:ARG:N	3:D:251:PHE:HE1	2.16	0.44
3:D:633:VAL:C	3:D:635:PRO:HD3	2.38	0.44
3:D:907:GLU:H	3:D:910:SER:HG	1.65	0.44
5:F:416:GLU:O	5:F:420:LEU:HD23	2.17	0.44
1:H:80:LEU:HD11	3:J:842:VAL:HG12	1.99	0.44
2:I:444:PRO:HA	2:I:563:ASN:HD21	1.82	0.44
2:I:738:ASP:OD1	2:I:739:GLU:N	2.47	0.44
2:I:882:LEU:HD11	3:J:1038:LEU:HD22	1.99	0.44
3:J:12:LEU:HD11	3:J:1452:ILE:HD13	1.99	0.44
3:J:154:THR:HG22	3:J:157:GLU:HG2	1.99	0.44
3:J:654:LYS:O	3:J:658:LEU:HG	2.17	0.44
4:K:23:VAL:HG21	4:K:65:MET:HE3	2.00	0.44
5:L:124:GLY:O	5:L:128:ILE:HG13	2.18	0.44
1:A:175:ARG:HH21	1:A:202:ASP:HB3	1.83	0.43
2:C:165:LEU:HB2	2:C:168:ARG:HG3	1.99	0.43
2:C:204:GLN:HB2	2:C:227:LEU:HD13	2.00	0.43
3:D:30:GLU:OE1	3:D:30:GLU:N	2.51	0.43
1:H:199:ILE:HB	1:H:207:PRO:HB3	2.00	0.43
1:H:73:GLU:HB3	1:H:77:GLU:HB3	1.99	0.43
3:J:759:ALA:HA	3:J:763:MET:HB3	2.00	0.43
1:B:73:GLU:HB3	1:B:77:GLU:HB3	1.99	0.43
2:C:1118:LYS:HB2	3:D:23:TYR:CZ	2.53	0.43
3:D:1090:ASP:O	3:D:1093:TYR:HB3	2.18	0.43
3:D:1147:ARG:HH22	3:D:1369:GLU:CD	2.21	0.43
3:D:520:LEU:O	3:D:525:ARG:NE	2.51	0.43
1:G:175:ARG:HH21	1:G:202:ASP:HB3	1.83	0.43
2:I:1008:ARG:NH1	2:I:1020:PRO:HB3	2.33	0.43
2:I:165:LEU:HB2	2:I:168:ARG:HG3	1.99	0.43
2:I:688:ILE:HD12	2:I:839:LEU:HB2	1.99	0.43
1:B:161:ARG:HE	1:B:162:ILE:HG22	1.82	0.43
2:C:197:LEU:HD22	2:C:207:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:11:GLU:HG3	2:C:535:SER:HB2	2.00	0.43
3:D:1306:PRO:HB2	3:D:1308:ASP:OD1	2.19	0.43
3:D:654:LYS:O	3:D:658:LEU:HG	2.17	0.43
3:D:829:VAL:HG21	3:D:839:LEU:HD11	2.00	0.43
3:D:841:PHE:HB3	3:D:843:PHE:CZ	2.53	0.43
5:F:124:GLY:O	5:F:128:ILE:HG13	2.18	0.43
1:H:158:ILE:H	1:H:166:PRO:HG3	1.83	0.43
1:H:44:LEU:HA	1:H:48:ILE:HD13	2.01	0.43
2:I:675:ALA:O	2:I:870:ILE:HA	2.18	0.43
3:J:521:PRO:HA	3:J:522:PRO:HD3	1.83	0.43
5:L:416:GLU:O	5:L:420:LEU:HD23	2.17	0.43
2:C:1053:LEU:O	3:D:621:LYS:NZ	2.38	0.43
3:D:349:PRO:HB3	5:F:112:GLU:HG2	1.99	0.43
3:J:1147:ARG:HH22	3:J:1369:GLU:CD	2.21	0.43
3:J:1448:THR:O	3:J:1452:ILE:HG12	2.19	0.43
1:A:56:VAL:HG21	1:A:82:LEU:HD13	1.99	0.43
1:B:44:LEU:HA	1:B:48:ILE:HD13	2.01	0.43
2:C:1036:GLU:N	2:C:1036:GLU:OE1	2.47	0.43
2:C:290:LEU:HD23	2:C:302:VAL:HG21	1.98	0.43
3:D:229:ALA:HB1	3:D:243:ALA:HB1	1.99	0.43
3:D:521:PRO:HA	3:D:522:PRO:HD3	1.83	0.43
3:D:666:PHE:CE1	3:D:687:VAL:HG12	2.54	0.43
1:G:153:ALA:HB2	1:G:167:VAL:C	2.38	0.43
2:I:1104:GLU:OE1	3:J:3:LYS:NZ	2.42	0.43
2:I:668:LEU:HB3	2:I:995:MET:SD	2.58	0.43
2:I:704:HIS:HD2	2:I:831:ARG:HD2	1.84	0.43
3:J:1379:VAL:O	3:J:1394:VAL:HA	2.19	0.43
3:J:543:LEU:HG	3:J:600:LEU:HD23	1.99	0.43
2:C:458:TYR:HB3	2:C:470:PRO:HG2	2.01	0.43
2:C:675:ALA:O	2:C:870:ILE:HA	2.18	0.43
3:D:12:LEU:HD11	3:D:1452:ILE:HD13	2.00	0.43
4:E:8:LYS:O	4:E:12:MET:HG3	2.18	0.43
5:F:203:ILE:O	5:F:207:LEU:HG	2.19	0.43
1:G:79:ILE:HA	1:G:82:LEU:HD12	2.01	0.43
2:I:290:LEU:O	2:I:301:GLU:HB2	2.19	0.43
3:J:1056:PRO:HG2	3:J:1058:ARG:HE	1.82	0.43
3:J:841:PHE:HB3	3:J:843:PHE:CZ	2.53	0.43
2:C:242:LEU:HD21	2:C:256:TYR:HE2	1.84	0.43
2:C:736:ASP:HB3	2:C:744:ARG:HG2	2.01	0.43
3:D:1153:VAL:HB	3:D:1160:LEU:HB2	1.99	0.43
3:D:1380:GLU:HG3	3:D:1392:GLY:HA2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:648:MET:O	3:D:652:LEU:HB2	2.18	0.43
3:D:970:LYS:O	3:D:974:ILE:HG13	2.18	0.43
2:I:142:ARG:NH1	2:I:163:ILE:HG12	2.29	0.43
2:I:197:LEU:HD22	2:I:207:LEU:HD21	2.00	0.43
2:I:198:ARG:HH21	2:I:235:MET:HG3	1.83	0.43
2:I:408:ARG:NH1	2:I:455:LEU:O	2.47	0.43
2:I:504:GLU:HG3	2:I:507:ARG:HG3	2.01	0.43
2:I:736:ASP:HB3	2:I:744:ARG:HG2	2.00	0.43
3:J:1364:HIS:HD2	3:J:1366:LYS:HB2	1.83	0.43
6:O:18:DA:H4'	6:O:19:DT:OP1	2.18	0.43
2:C:198:ARG:HH21	2:C:235:MET:HG3	1.83	0.43
2:I:1009:SER:HB3	3:J:651:GLU:O	2.19	0.43
3:J:216:LEU:HD13	3:J:383:GLY:HA2	2.01	0.43
3:J:924:MET:O	3:J:927:THR:OG1	2.30	0.43
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.79	0.43
3:D:1186:VAL:HA	3:D:1187:PRO:HD2	1.94	0.43
3:D:271:TYR:HE2	3:D:281:ARG:HH21	1.67	0.43
3:D:288:MET:HG2	3:D:305:ALA:HB1	2.01	0.43
3:D:62:LYS:HE2	3:D:62:LYS:HB2	1.83	0.43
1:H:48:ILE:HA	1:H:49:PRO:HD2	1.74	0.43
1:H:52:ALA:HB2	1:H:170:ILE:O	2.19	0.43
2:I:219:GLN:H	2:I:219:GLN:HG3	1.41	0.43
5:L:398:LEU:HB3	5:L:399:GLU:H	1.77	0.43
7:S:13:DC:H2''	7:S:14:DA:C8	2.54	0.43
1:A:79:ILE:HA	1:A:82:LEU:HD12	2.01	0.43
1:B:54:THR:OG1	1:B:158:ILE:HG21	2.19	0.43
2:C:853:LEU:HA	2:C:854:PRO:HD3	1.93	0.43
4:E:67:GLU:O	4:E:70:THR:OG1	2.24	0.43
2:I:230:ARG:HB2	2:I:231:PRO:CD	2.49	0.43
2:I:543:ASN:HB2	2:I:562:SER:HB3	2.01	0.43
2:I:561:GLY:HA2	2:I:564:MET:HE2	2.01	0.43
3:J:1255:GLY:O	3:J:1258:ARG:HB3	2.19	0.43
5:L:203:ILE:O	5:L:207:LEU:HG	2.19	0.43
6:R:18:DA:H4'	6:R:19:DT:OP1	2.18	0.43
2:C:1008:ARG:NH1	2:C:1020:PRO:HB3	2.33	0.42
2:C:549:PHE:HB3	2:C:552:HIS:HD2	1.84	0.42
3:D:1379:VAL:O	3:D:1394:VAL:HA	2.19	0.42
3:D:490:ALA:O	3:D:493:ARG:HB3	2.19	0.42
2:I:1019:GLN:HG2	2:I:1019:GLN:H	1.57	0.42
2:I:458:TYR:HB3	2:I:470:PRO:HG2	2.01	0.42
3:J:954:ALA:HB3	3:J:1062:ARG:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:24:DC:H42	7:S:2:DG:H1	1.66	0.42
1:B:117:SER:HB3	1:B:120:VAL:HB	2.01	0.42
2:C:1019:GLN:HG2	2:C:1019:GLN:H	1.57	0.42
3:D:1267:ARG:HG3	3:D:1267:ARG:H	1.53	0.42
3:D:245:LEU:HD11	3:D:249:TYR:HB3	2.01	0.42
3:D:28:LYS:HB2	3:D:42:ASP:HB2	2.01	0.42
1:H:117:SER:HB3	1:H:120:VAL:HB	2.01	0.42
3:J:1107:VAL:HA	3:J:1200:VAL:O	2.18	0.42
3:J:1492:LEU:O	3:J:1496:GLU:HB2	2.19	0.42
3:J:28:LYS:HB2	3:J:42:ASP:HB2	2.01	0.42
3:J:520:LEU:O	3:J:525:ARG:NE	2.51	0.42
3:J:646:LYS:HA	3:J:720:LEU:HD22	2.01	0.42
5:L:376:LEU:HD21	5:L:423:LEU:HD12	2.00	0.42
7:P:13:DC:H2"	7:P:14:DA:C8	2.54	0.42
1:B:158:ILE:H	1:B:166:PRO:HG3	1.84	0.42
3:D:245:LEU:HD12	3:D:307:GLY:HA3	2.00	0.42
2:I:714:ASP:HA	2:I:719:PRO:HA	2.02	0.42
3:J:1314:LYS:HB3	3:J:1314:LYS:HE2	1.87	0.42
1:B:52:ALA:HB2	1:B:170:ILE:O	2.19	0.42
2:C:290:LEU:O	2:C:301:GLU:HB2	2.19	0.42
3:D:1434:TRP:NE1	3:D:1457:ASP:HB2	2.35	0.42
3:D:583:ASP:OD1	3:D:586:ARG:HB2	2.20	0.42
1:G:14:THR:HG23	1:H:231:SER:O	2.19	0.42
1:G:48:ILE:HG22	1:G:173:PRO:HD2	2.01	0.42
1:G:48:ILE:HA	1:G:49:PRO:HD3	1.91	0.42
2:I:376:ARG:HG3	2:I:376:ARG:H	1.57	0.42
2:I:549:PHE:HB3	2:I:552:HIS:HD2	1.85	0.42
2:I:761:PHE:HA	2:I:785:VAL:HA	2.02	0.42
2:I:766:GLU:OE2	3:J:65:ARG:NH2	2.52	0.42
2:C:1055:ILE:HD11	2:C:1079:PRO:HD3	2.00	0.42
2:C:13:ILE:HA	2:C:14:PRO:HD3	1.91	0.42
2:C:168:ARG:O	2:C:267:TYR:HA	2.20	0.42
2:C:242:LEU:HD21	2:C:256:TYR:CE2	2.55	0.42
2:C:561:GLY:HA2	2:C:564:MET:HE2	2.01	0.42
2:C:543:ASN:HB2	2:C:562:SER:HB3	2.01	0.42
2:C:670:GLN:OE1	2:C:700:TYR:N	2.51	0.42
3:D:1255:GLY:O	3:D:1258:ARG:HB3	2.20	0.42
2:I:270:GLY:O	2:I:274:ARG:N	2.43	0.42
3:J:589:SER:HA	3:J:590:PRO:HD3	1.90	0.42
2:I:1019:GLN:NE2	3:J:621:LYS:HG2	2.33	0.42
2:C:1038:TRP:CE3	3:D:1099:VAL:HG21	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1113:GLU:O	2:C:1115:LEU:HG	2.19	0.42
2:C:198:ARG:HB3	2:C:199:VAL:H	1.43	0.42
2:C:704:HIS:HD2	2:C:831:ARG:HD2	1.84	0.42
3:D:1472:ILE:HA	3:D:1473:PRO:HD3	1.85	0.42
3:D:401:TYR:HB3	3:D:427:VAL:HG21	2.02	0.42
5:F:165:LYS:HA	5:F:166:PRO:HD3	1.85	0.42
5:F:385:LYS:HZ3	5:F:391:ILE:HD11	1.85	0.42
2:I:1112:PHE:HB3	2:I:1115:LEU:HB2	2.02	0.42
2:I:184:MET:HB2	2:I:193:LEU:HD23	2.02	0.42
2:I:281:LEU:HB2	2:I:283:VAL:HG22	2.02	0.42
2:I:937:ASP:O	2:I:941:LYS:HG2	2.19	0.42
2:I:1041:GLU:HG2	3:J:1472:ILE:HD12	2.01	0.42
5:L:205:ALA:O	5:L:208:ARG:HB2	2.20	0.42
5:L:224:PHE:O	5:L:228:ILE:HG13	2.19	0.42
2:C:1112:PHE:HB3	2:C:1115:LEU:HB2	2.02	0.42
1:A:42:ARG:NH1	2:C:978:ARG:HA	2.34	0.42
3:D:1162:GLU:OE1	3:D:1163:GLY:N	2.52	0.42
3:J:1162:GLU:OE1	3:J:1163:GLY:N	2.52	0.42
3:J:1434:TRP:NE1	3:J:1457:ASP:HB2	2.35	0.42
3:J:784:ASP:O	3:J:942:SER:OG	2.36	0.42
3:J:961:GLN:O	3:J:964:LEU:HG	2.20	0.42
5:L:210:VAL:HG22	5:L:258:ILE:HD12	2.02	0.42
2:C:184:MET:HB2	2:C:193:LEU:HD23	2.02	0.42
2:C:281:LEU:HB2	2:C:283:VAL:HG22	2.02	0.42
3:D:1101:VAL:HA	3:D:1428:ALA:HB2	2.01	0.42
3:D:1125:MET:HE2	3:D:1132:LEU:HG	2.02	0.42
3:D:671:LYS:HG3	5:F:436:PHE:CZ	2.55	0.42
3:D:683:ILE:HD12	3:D:688:TRP:HZ2	1.84	0.42
3:D:780:LYS:HB2	3:D:912:LYS:NZ	2.35	0.42
2:C:374:ASN:HD21	5:F:291:ARG:NH1	2.18	0.42
1:H:54:THR:OG1	1:H:158:ILE:HG21	2.19	0.42
2:I:874:LEU:O	3:J:1029:ARG:HG2	2.20	0.42
3:J:1297:GLU:HG3	3:J:1298:GLY:N	2.35	0.42
3:J:401:TYR:HB3	3:J:427:VAL:HG21	2.02	0.42
3:J:729:HIS:CG	3:J:730:PRO:HD2	2.54	0.42
1:B:185:ARG:HG3	1:B:190:THR:HA	2.02	0.42
1:B:74:ASP:O	1:B:78:ILE:HG12	2.20	0.42
2:C:198:ARG:NE	2:C:199:VAL:HG23	2.35	0.42
2:C:557:ARG:O	2:C:844:GLY:HA3	2.20	0.42
2:C:944:LEU:HD11	2:C:963:LEU:HG	2.01	0.42
1:G:13:ALA:O	1:H:230:ALA:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:7:LYS:HB2	1:H:8:ALA:H	1.64	0.42
2:I:115:LEU:HD23	2:I:115:LEU:HA	1.76	0.42
2:I:204:GLN:HB2	2:I:227:LEU:HD13	2.00	0.42
2:I:242:LEU:HD21	2:I:256:TYR:CE2	2.55	0.42
2:I:242:LEU:HD21	2:I:256:TYR:HE2	1.84	0.42
3:J:1101:VAL:HA	3:J:1428:ALA:HB2	2.01	0.42
3:J:1306:PRO:HB2	3:J:1308:ASP:OD1	2.19	0.42
3:J:583:ASP:OD1	3:J:586:ARG:HB2	2.19	0.42
5:L:206:ASN:O	5:L:210:VAL:HG23	2.20	0.42
6:O:28:DA:H2''	6:O:29:DC:H5'	2.02	0.42
1:B:48:ILE:HA	1:B:49:PRO:HD2	1.73	0.42
1:B:68:ILE:HD12	1:B:69:PRO:HD2	2.02	0.42
2:C:1008:ARG:HH21	2:C:1011:GLY:C	2.23	0.42
2:C:557:ARG:HG3	2:C:879:ARG:HB3	2.02	0.42
2:C:714:ASP:HA	2:C:719:PRO:HA	2.02	0.42
5:F:206:ASN:O	5:F:210:VAL:HG23	2.20	0.42
1:G:176:ARG:HG3	1:G:200:TRP:CE3	2.55	0.42
3:J:1020:LEU:HG	3:J:1035:ILE:HD12	2.02	0.42
3:J:648:MET:O	3:J:652:LEU:HB2	2.19	0.42
5:L:251:SER:O	5:L:255:THR:HG23	2.20	0.42
5:L:375:LYS:HB3	5:L:375:LYS:HE2	1.82	0.42
2:C:115:LEU:HA	2:C:115:LEU:HD23	1.76	0.41
2:C:198:ARG:HD2	2:C:234:ALA:O	2.20	0.41
2:C:38:LYS:HD2	2:C:38:LYS:HA	1.86	0.41
4:E:51:LEU:HG	4:E:51:LEU:H	1.55	0.41
5:F:205:ALA:O	5:F:208:ARG:HB2	2.20	0.41
5:F:210:VAL:HG22	5:F:258:ILE:HD12	2.02	0.41
5:F:224:PHE:O	5:F:228:ILE:HG13	2.19	0.41
5:F:257:TRP:O	5:F:260:GLN:HG3	2.19	0.41
1:G:172:SER:HA	1:G:173:PRO:HD3	1.77	0.41
2:I:140:ILE:HD11	2:I:331:ARG:HB3	2.02	0.41
2:I:966:LEU:HA	2:I:966:LEU:HD12	1.95	0.41
3:J:956:ILE:HD11	3:J:1062:ARG:HH22	1.85	0.41
3:J:176:ASP:OD1	3:J:177:ALA:N	2.50	0.41
3:J:9:ARG:HG2	3:J:10:ILE:H	1.84	0.41
4:K:16:LYS:HE2	4:K:16:LYS:HB3	1.80	0.41
2:C:179:SER:HB2	2:C:181:VAL:H	1.86	0.41
2:C:937:ASP:O	2:C:941:LYS:HG2	2.20	0.41
3:D:216:LEU:HB3	3:D:218:LYS:HE2	2.02	0.41
3:D:216:LEU:HD13	3:D:383:GLY:HA2	2.01	0.41
3:D:493:ARG:HB2	3:D:493:ARG:HE	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:13:ILE:HA	2:I:14:PRO:HD3	1.87	0.41
3:J:1047:LYS:HG3	3:J:1049:SER:H	1.85	0.41
3:D:1134:LEU:HD13	3:D:1135:ARG:O	2.21	0.41
1:H:68:ILE:HD12	1:H:69:PRO:HD2	2.02	0.41
2:I:1056:LYS:O	3:J:624:ASP:N	2.38	0.41
2:I:166:PRO:C	2:I:168:ARG:H	2.23	0.41
2:I:802:GLY:H	2:I:826:PHE:HB2	1.86	0.41
2:I:862:PRO:HG2	2:I:929:ARG:HH22	1.85	0.41
3:J:1103:HIS:CG	3:J:1463:LYS:HD3	2.55	0.41
3:J:683:ILE:HD12	3:J:688:TRP:HZ2	1.85	0.41
3:J:756:GLN:O	3:J:760:ARG:HG3	2.21	0.41
3:D:973:GLN:HE22	3:J:805:ALA:HB1	1.86	0.41
3:J:957:PRO:HG3	3:J:1007:VAL:HA	2.02	0.41
2:C:356:ARG:HA	2:C:359:MET:SD	2.61	0.41
2:C:754:ILE:HG12	2:C:791:ARG:HG2	2.02	0.41
3:D:266:GLU:CD	3:D:315:ARG:H	2.23	0.41
1:H:185:ARG:HG3	1:H:190:THR:HA	2.02	0.41
3:J:638:LYS:HD3	3:J:640:HIS:CD2	2.56	0.41
5:L:135:THR:HG23	5:L:181:LEU:HD21	2.02	0.41
2:C:93:PRO:HB3	2:C:114:PHE:HE2	1.86	0.41
3:D:957:PRO:HG3	3:D:1007:VAL:HA	2.02	0.41
3:D:1440:PHE:CG	3:D:1441:GLN:HG2	2.56	0.41
3:D:1492:LEU:O	3:D:1496:GLU:HB2	2.19	0.41
3:D:699:VAL:HB	3:D:716:PHE:O	2.21	0.41
4:E:47:LYS:HD2	4:E:47:LYS:HA	1.87	0.41
2:I:168:ARG:O	2:I:267:TYR:HA	2.20	0.41
2:I:198:ARG:HD2	2:I:234:ALA:O	2.20	0.41
2:I:198:ARG:HB3	2:I:199:VAL:H	1.40	0.41
2:I:754:ILE:HG12	2:I:791:ARG:HG2	2.02	0.41
2:I:679:PHE:HB2	2:I:870:ILE:HG21	2.03	0.41
5:L:353:LEU:HA	5:L:354:PRO:HD3	1.95	0.41
2:C:802:GLY:H	2:C:826:PHE:HB2	1.86	0.41
2:C:862:PRO:HG2	2:C:929:ARG:HH22	1.84	0.41
3:D:1107:VAL:HA	3:D:1200:VAL:O	2.20	0.41
3:D:1103:HIS:CG	3:D:1463:LYS:HD3	2.56	0.41
3:D:637:LEU:HD21	3:D:641:GLN:O	2.21	0.41
3:D:646:LYS:HA	3:D:720:LEU:HD22	2.01	0.41
3:D:780:LYS:HD3	3:D:912:LYS:HZ2	1.85	0.41
3:D:924:MET:O	3:D:927:THR:OG1	2.31	0.41
3:D:95:LEU:HG	3:D:574:LEU:HD21	2.03	0.41
2:I:1060:ILE:HG13	2:I:1060:ILE:H	1.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:96:ALA:O	2:I:113:VAL:HG23	2.21	0.41
2:I:944:LEU:HD11	2:I:963:LEU:HG	2.01	0.41
3:J:1149:LEU:HG	3:J:1166:LEU:HD21	2.03	0.41
4:K:13:VAL:HG21	4:K:19:LEU:HB2	2.03	0.41
5:L:202:LEU:HD22	5:L:239:VAL:HG22	2.03	0.41
2:I:817:PRO:HA	5:L:320:GLU:HG3	2.01	0.41
2:C:140:ILE:HD11	2:C:331:ARG:HB3	2.01	0.41
2:C:166:PRO:C	2:C:168:ARG:H	2.23	0.41
2:C:96:ALA:O	2:C:113:VAL:HG23	2.20	0.41
3:D:699:VAL:HG22	3:D:760:ARG:HG2	2.02	0.41
4:E:16:LYS:HE2	4:E:16:LYS:HB3	1.80	0.41
1:H:74:ASP:O	1:H:78:ILE:HG12	2.20	0.41
3:J:1134:LEU:HD13	3:J:1135:ARG:O	2.21	0.41
3:J:1203:LYS:HE3	3:J:1203:LYS:HB2	1.68	0.41
3:J:133:ILE:HG22	3:J:152:LEU:HG	2.03	0.41
3:J:192:ALA:HB1	3:J:193:PRO:HD2	2.02	0.41
3:J:598:ARG:HA	3:J:599:PRO:HD3	1.92	0.41
2:C:164:PRO:HG3	2:C:267:TYR:CE1	2.56	0.41
3:D:1047:LYS:HG3	3:D:1049:SER:H	1.85	0.41
3:D:1043:GLY:O	3:D:1057:VAL:HG22	2.21	0.41
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.56	0.41
3:D:631:ILE:HG13	3:D:740:PHE:HD2	1.85	0.41
1:G:72:LYS:HD2	2:I:606:VAL:HG11	2.01	0.41
3:D:1130:ARG:HH11	3:J:1176:LYS:HD3	1.86	0.41
3:J:95:LEU:HG	3:J:574:LEU:HD21	2.02	0.41
5:L:321:GLU:O	5:L:325:ILE:HG13	2.21	0.41
1:A:165:ILE:HA	1:A:166:PRO:HD3	1.95	0.41
1:B:56:VAL:HG13	1:B:142:VAL:HG12	2.03	0.41
3:D:1072:ILE:HG13	3:D:1072:ILE:H	1.72	0.41
3:D:225:ILE:O	3:D:331:VAL:HG12	2.21	0.41
3:D:956:ILE:HD11	3:D:1062:ARG:HH22	1.85	0.41
5:F:222:LEU:HA	5:F:222:LEU:HD12	1.93	0.41
1:H:56:VAL:HG13	1:H:142:VAL:HG12	2.03	0.41
2:I:93:PRO:HB3	2:I:114:PHE:HE2	1.85	0.41
2:I:198:ARG:NE	2:I:199:VAL:HG23	2.35	0.41
2:I:164:PRO:HG3	2:I:267:TYR:CE1	2.56	0.41
2:I:557:ARG:HG3	2:I:879:ARG:HB3	2.01	0.41
2:I:856:GLU:HG3	2:I:856:GLU:H	1.62	0.41
3:J:133:ILE:HG13	3:J:455:ARG:O	2.21	0.41
3:J:780:LYS:HB2	3:J:912:LYS:NZ	2.35	0.41
3:J:791:TYR:CE2	3:J:941:LEU:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:29:DC:H3'	6:O:30:DT:H71	2.03	0.41
1:A:176:ARG:HG3	1:A:200:TRP:CE3	2.55	0.41
2:C:142:ARG:NH1	2:C:163:ILE:HG12	2.29	0.41
2:C:219:GLN:HG3	2:C:219:GLN:H	1.41	0.41
2:C:679:PHE:HB2	2:C:870:ILE:HG21	2.03	0.41
2:C:781:LYS:NZ	2:C:783:ARG:HA	2.36	0.41
3:D:1232:PRO:HA	3:D:1235:GLN:HE21	1.86	0.41
3:D:1297:GLU:HG3	3:D:1298:GLY:N	2.35	0.41
3:D:638:LYS:HD3	3:D:640:HIS:CD2	2.56	0.41
3:D:794:GLN:HA	3:D:905:PRO:HG3	2.03	0.41
1:G:18:ASP:O	1:G:207:PRO:HD3	2.20	0.41
2:I:214:TYR:CE2	2:I:311:PHE:HB3	2.56	0.41
2:I:922:PHE:CD2	2:I:964:LYS:HG3	2.56	0.41
3:J:925:GLU:OE1	4:K:5:GLY:N	2.52	0.41
1:A:48:ILE:HG22	1:A:173:PRO:HD2	2.01	0.41
1:B:161:ARG:HB3	1:B:164:ALA:HB2	2.03	0.41
2:C:609:THR:OG1	2:C:610:ARG:HD3	2.21	0.41
3:D:783:ARG:NH1	3:D:1029:ARG:HD3	2.36	0.41
3:D:245:LEU:HA	3:D:245:LEU:HD23	1.60	0.41
3:D:523:ASP:O	3:D:526:PRO:HG3	2.21	0.41
3:D:589:SER:HA	3:D:590:PRO:HD3	1.90	0.41
3:D:756:GLN:O	3:D:760:ARG:HG3	2.21	0.41
2:I:1113:GLU:O	2:I:1115:LEU:HG	2.21	0.41
3:J:158:TYR:CE1	3:J:454:ALA:HB3	2.56	0.41
3:J:794:GLN:HA	3:J:905:PRO:HG3	2.02	0.41
3:J:97:THR:HA	3:J:98:PRO:HD3	1.97	0.41
5:L:143:ARG:HE	5:L:147:ARG:NH2	2.19	0.41
3:J:671:LYS:HG3	5:L:436:PHE:CZ	2.56	0.41
2:C:270:GLY:O	2:C:274:ARG:N	2.43	0.40
2:C:280:LYS:HG3	2:C:281:LEU:N	2.36	0.40
3:D:1020:LEU:HG	3:D:1035:ILE:HD12	2.02	0.40
3:D:1231:GLU:HB3	3:D:1232:PRO:HD3	2.03	0.40
3:D:352:ASN:N	3:D:352:ASN:OD1	2.54	0.40
5:F:202:LEU:HD22	5:F:239:VAL:HG22	2.03	0.40
5:F:263:ASN:HA	5:F:266:ILE:HG13	2.03	0.40
2:I:359:MET:HG3	2:I:372:LEU:HD11	2.03	0.40
2:I:557:ARG:O	2:I:844:GLY:HA3	2.20	0.40
3:J:1203:LYS:H	3:J:1203:LYS:HG3	1.62	0.40
3:J:1231:GLU:HB3	3:J:1232:PRO:HD3	2.03	0.40
3:J:1336:LEU:HD11	3:J:1419:PRO:HB2	2.03	0.40
3:J:1462:LEU:HD12	3:J:1463:LYS:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:67:ARG:HD3	5:L:394:ARG:HD3	2.03	0.40
5:L:398:LEU:HB2	7:S:20:DG:OP2	2.20	0.40
2:C:109:LYS:HD2	2:C:109:LYS:HA	1.85	0.40
2:C:922:PHE:CD2	2:C:964:LYS:HG3	2.56	0.40
3:D:133:ILE:HG22	3:D:152:LEU:HG	2.03	0.40
3:D:553:ARG:HD2	3:D:570:GLU:OE1	2.22	0.40
3:D:786:ILE:H	3:D:786:ILE:HG13	1.62	0.40
4:E:13:VAL:HG21	4:E:19:LEU:HB2	2.03	0.40
5:F:143:ARG:HE	5:F:147:ARG:NH2	2.19	0.40
5:F:103:ILE:HD12	5:F:208:ARG:HA	2.04	0.40
5:F:251:SER:O	5:F:255:THR:HG23	2.21	0.40
1:G:193:ASP:OD1	2:I:938:LYS:NZ	2.51	0.40
2:I:280:LYS:HG3	2:I:281:LEU:N	2.36	0.40
3:J:1103:HIS:HB2	3:J:1462:LEU:HD11	2.03	0.40
3:J:136:ASP:HA	3:J:137:PRO:HD2	1.91	0.40
3:J:1481:VAL:HG21	4:K:17:TYR:HB2	2.02	0.40
3:J:956:ILE:HD11	3:J:1062:ARG:NH2	2.36	0.40
3:J:962:ARG:O	3:J:965:GLU:HG2	2.21	0.40
1:B:143:ARG:HH12	1:B:160:ASP:HB2	1.87	0.40
2:C:214:TYR:CE2	2:C:311:PHE:HB3	2.56	0.40
3:D:1103:HIS:HB2	3:D:1462:LEU:HD11	2.03	0.40
3:D:529:GLN:HA	3:D:535:PHE:HA	2.04	0.40
3:D:572:ARG:CZ	5:F:98:GLN:HG2	2.51	0.40
3:D:772:PRO:HG3	3:D:1210:SER:HB3	2.04	0.40
5:F:302:SER:H	5:F:305:GLU:HG2	1.87	0.40
1:G:36:LEU:O	1:G:39:PRO:HD2	2.21	0.40
2:I:1053:LEU:O	3:J:621:LYS:NZ	2.45	0.40
2:I:216:ASP:O	2:I:219:GLN:NE2	2.53	0.40
2:I:683:ASN:OD1	2:I:683:ASN:N	2.53	0.40
3:J:637:LEU:HD21	3:J:641:GLN:O	2.22	0.40
3:J:699:VAL:HG22	3:J:760:ARG:HG2	2.02	0.40
3:J:90:MET:HG2	3:J:521:PRO:HD3	2.04	0.40
3:J:974:ILE:HG22	3:J:988:ARG:HG3	2.02	0.40
5:L:220:ARG:HD3	5:L:266:ILE:HG23	2.04	0.40
1:B:221:HIS:HA	1:B:224:TYR:CD2	2.57	0.40
3:D:1149:LEU:HG	3:D:1166:LEU:HD21	2.03	0.40
3:D:1462:LEU:HD12	3:D:1463:LYS:N	2.36	0.40
2:C:684:PHE:HE1	3:D:783:ARG:HB2	1.86	0.40
3:D:956:ILE:HD11	3:D:1062:ARG:NH2	2.37	0.40
3:D:963:TYR:CE2	3:D:1002:LYS:HD2	2.57	0.40
4:E:82:GLU:O	4:E:85:LEU:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:83:LYS:HE2	1:G:83:LYS:HB3	1.91	0.40
3:J:1232:PRO:HA	3:J:1235:GLN:HE21	1.87	0.40
3:J:514:LEU:HD23	3:J:517:VAL:HG22	2.03	0.40
1:B:175:ARG:HB2	1:B:200:TRP:HB3	2.04	0.40
1:B:83:LYS:NZ	3:D:842:VAL:O	2.54	0.40
2:C:1113:GLU:H	2:C:1113:GLU:HG2	1.65	0.40
2:C:376:ARG:HG3	2:C:376:ARG:H	1.56	0.40
3:D:169:TYR:OH	3:D:198:ARG:N	2.36	0.40
3:D:310:LEU:O	3:D:311:LEU:HG	2.21	0.40
3:D:556:LYS:HA	3:D:556:LYS:HD2	1.86	0.40
1:H:221:HIS:HA	1:H:224:TYR:CD2	2.57	0.40
2:I:551:GLU:H	2:I:551:GLU:HG2	1.62	0.40
2:I:609:THR:OG1	2:I:610:ARG:HD3	2.21	0.40
3:J:1042:ARG:HB3	3:J:1057:VAL:CG2	2.49	0.40
3:J:702:LEU:HD23	3:J:728:LEU:HD13	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	225/314 (72%)	209 (93%)	15 (7%)	1 (0%)	34 71
1	B	225/314 (72%)	208 (92%)	16 (7%)	1 (0%)	34 71
1	G	225/314 (72%)	209 (93%)	15 (7%)	1 (0%)	34 71
1	H	225/314 (72%)	208 (92%)	16 (7%)	1 (0%)	34 71
2	C	1108/1119 (99%)	1045 (94%)	58 (5%)	5 (0%)	29 67
2	I	1108/1119 (99%)	1040 (94%)	62 (6%)	6 (0%)	29 67
3	D	1486/1524 (98%)	1395 (94%)	85 (6%)	6 (0%)	34 71
3	J	1361/1524 (89%)	1281 (94%)	74 (5%)	6 (0%)	34 71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	91/99 (92%)	87 (96%)	4 (4%)	0	100	100
4	K	91/99 (92%)	88 (97%)	3 (3%)	0	100	100
5	F	343/347 (99%)	324 (94%)	17 (5%)	2 (1%)	25	63
5	L	343/347 (99%)	326 (95%)	15 (4%)	2 (1%)	25	63
All	All	6831/7434 (92%)	6420 (94%)	380 (6%)	31 (0%)	29	67

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	VAL
3	D	1128	VAL
1	G	53	VAL
3	J	1128	VAL
2	C	607	ASP
3	D	666	PHE
3	D	681	ARG
3	D	682	ASP
2	I	111	ASP
3	J	791	TYR
3	J	1450	ALA
2	C	111	ASP
2	C	784	ASP
5	F	398	LEU
2	I	606	VAL
5	L	220	ARG
1	B	52	ALA
3	D	243	ALA
1	H	52	ALA
2	I	607	ASP
2	I	608	GLY
2	I	784	ASP
3	J	790	TYR
3	J	1449	GLU
3	D	667	ALA
5	F	160	PRO
5	L	160	PRO
2	C	606	VAL
2	C	870	ILE
2	I	870	ILE
3	J	667	ALA

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/270 (72%)	178 (92%)	16 (8%)	11	38
1	B	194/270 (72%)	177 (91%)	17 (9%)	10	35
1	G	194/270 (72%)	178 (92%)	16 (8%)	11	38
1	H	194/270 (72%)	177 (91%)	17 (9%)	10	35
2	C	931/936 (100%)	847 (91%)	84 (9%)	9	34
2	I	931/936 (100%)	849 (91%)	82 (9%)	10	35
3	D	1252/1281 (98%)	1151 (92%)	101 (8%)	11	39
3	J	1150/1281 (90%)	1057 (92%)	93 (8%)	11	39
4	E	83/88 (94%)	79 (95%)	4 (5%)	25	53
4	K	83/88 (94%)	79 (95%)	4 (5%)	25	53
5	F	296/299 (99%)	266 (90%)	30 (10%)	7	29
5	L	296/299 (99%)	265 (90%)	31 (10%)	7	27
All	All	5798/6288 (92%)	5303 (92%)	495 (8%)	10	37

All (495) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	67	THR
1	A	87	VAL
1	A	93	LYS
1	A	98	THR
1	A	102	ARG
1	A	121	GLU
1	A	134	GLU
1	A	146	ARG
1	A	155	ARG
1	A	158	ILE
1	A	160	ASP
1	A	174	VAL
1	A	190	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	204	SER
1	A	227	ASN
1	B	7	LYS
1	B	38	ASN
1	B	51	THR
1	B	53	VAL
1	B	54	THR
1	B	58	ILE
1	B	75	VAL
1	B	104	GLU
1	B	114	PHE
1	B	115	THR
1	B	141	GLU
1	B	143	ARG
1	B	156	HIS
1	B	170	ILE
1	B	191	ASP
1	B	206	THR
1	B	229	GLU
2	C	8	ARG
2	C	20	GLU
2	C	33	ASP
2	C	41	ASN
2	C	49	LYS
2	C	54	ILE
2	C	64	LEU
2	C	66	LEU
2	C	69	LEU
2	C	80	GLN
2	C	81	ASP
2	C	98	LEU
2	C	101	ILE
2	C	108	ILE
2	C	113	VAL
2	C	141	HIS
2	C	142	ARG
2	C	151	ASP
2	C	176	VAL
2	C	197	LEU
2	C	203	ASP
2	C	206	THR
2	C	210	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	C	211	LEU
2	C	219	GLN
2	C	233	GLU
2	C	242	LEU
2	C	246	ASP
2	C	280	LYS
2	C	304	LEU
2	C	308	ARG
2	C	358	ARG
2	C	376	ARG
2	C	384	GLU
2	C	394	PHE
2	C	407	LYS
2	C	420	ARG
2	C	421	GLU
2	C	426	ASP
2	C	469	THR
2	C	512	ARG
2	C	523	ILE
2	C	524	VAL
2	C	528	GLU
2	C	543	ASN
2	C	551	GLU
2	C	598	GLU
2	C	610	ARG
2	C	613	VAL
2	C	616	GLU
2	C	620	LEU
2	C	643	VAL
2	C	648	ARG
2	C	668	LEU
2	C	685	GLU
2	C	697	ARG
2	C	707	ARG
2	C	715	THR
2	C	716	LYS
2	C	729	LEU
2	C	744	ARG
2	C	766	GLU
2	C	774	LEU
2	C	776	SER
2	C	784	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	C	785	VAL
2	C	788	THR
2	C	807	ARG
2	C	808	ARG
2	C	815	LEU
2	C	816	LYS
2	C	819	VAL
2	C	857	ASP
2	C	869	VAL
2	C	897	LEU
2	C	899	GLN
2	C	950	LEU
2	C	995	MET
2	C	1001	VAL
2	C	1019	GLN
2	C	1060	ILE
2	C	1081	VAL
2	C	1104	GLU
2	C	1117	SER
3	D	4	GLU
3	D	9	ARG
3	D	35	ARG
3	D	53	ILE
3	D	55	ASP
3	D	66	GLN
3	D	75	ARG
3	D	76	CYS
3	D	106	LYS
3	D	142	LEU
3	D	157	GLU
3	D	166	GLN
3	D	180	LYS
3	D	210	ARG
3	D	212	ARG
3	D	220	ARG
3	D	266	GLU
3	D	278	VAL
3	D	297	ILE
3	D	312	ARG
3	D	315	ARG
3	D	326	GLU
3	D	329	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	D	331	VAL
3	D	341	GLU
3	D	346	LYS
3	D	347	VAL
3	D	361	VAL
3	D	399	ARG
3	D	400	VAL
3	D	408	GLU
3	D	411	THR
3	D	414	ARG
3	D	434	ARG
3	D	439	LEU
3	D	440	VAL
3	D	448	GLU
3	D	472	LYS
3	D	479	GLU
3	D	480	GLU
3	D	481	MET
3	D	504	ASP
3	D	514	LEU
3	D	525	ARG
3	D	544	TYR
3	D	549	ASN
3	D	564	GLU
3	D	618	LEU
3	D	637	LEU
3	D	680	GLN
3	D	692	GLU
3	D	694	VAL
3	D	703	ASN
3	D	725	SER
3	D	776	GLU
3	D	786	ILE
3	D	791	TYR
3	D	794	GLN
3	D	797	LYS
3	D	808	THR
3	D	813	LEU
3	D	817	GLU
3	D	828	VAL
3	D	832	ARG
3	D	855	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	D	871	ARG
3	D	879	ARG
3	D	884	ARG
3	D	893	GLU
3	D	897	GLN
3	D	908	LYS
3	D	937	TYR
3	D	956	ILE
3	D	961	GLN
3	D	971	LEU
3	D	976	GLN
3	D	987	GLU
3	D	1001	GLU
3	D	1047	LYS
3	D	1053	PHE
3	D	1059	SER
3	D	1084	THR
3	D	1087	ARG
3	D	1088	THR
3	D	1093	TYR
3	D	1161	GLU
3	D	1162	GLU
3	D	1203	LYS
3	D	1235	GLN
3	D	1285	GLU
3	D	1297	GLU
3	D	1310	ARG
3	D	1311	LEU
3	D	1318	TYR
3	D	1335	LEU
3	D	1342	GLU
3	D	1346	ARG
3	D	1354	LYS
3	D	1421	LEU
3	D	1429	LEU
3	D	1499	ARG
4	E	51	LEU
4	E	52	GLU
4	E	55	TYR
4	E	56	ASP
5	F	100	LEU
5	F	139	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	F	151	LEU
5	F	157	GLN
5	F	162	LEU
5	F	167	ASP
5	F	175	ASP
5	F	179	LYS
5	F	183	LYS
5	F	189	LEU
5	F	237	ARG
5	F	266	ILE
5	F	268	ASP
5	F	278	HIS
5	F	292	GLN
5	F	293	LEU
5	F	323	LEU
5	F	324	LYS
5	F	333	GLU
5	F	338	ASP
5	F	340	LYS
5	F	351	GLU
5	F	371	LYS
5	F	373	LEU
5	F	397	THR
5	F	404	TYR
5	F	405	PHE
5	F	413	ARG
5	F	416	GLU
5	F	426	HIS
1	G	44	LEU
1	G	67	THR
1	G	87	VAL
1	G	93	LYS
1	G	98	THR
1	G	102	ARG
1	G	121	GLU
1	G	134	GLU
1	G	146	ARG
1	G	155	ARG
1	G	158	ILE
1	G	160	ASP
1	G	174	VAL
1	G	190	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	204	SER
1	G	227	ASN
1	H	7	LYS
1	H	38	ASN
1	H	51	THR
1	H	53	VAL
1	H	54	THR
1	H	58	ILE
1	H	75	VAL
1	H	104	GLU
1	H	114	PHE
1	H	115	THR
1	H	141	GLU
1	H	143	ARG
1	H	156	HIS
1	H	170	ILE
1	H	191	ASP
1	H	206	THR
1	H	229	GLU
2	I	8	ARG
2	I	20	GLU
2	I	33	ASP
2	I	41	ASN
2	I	49	LYS
2	I	54	ILE
2	I	64	LEU
2	I	66	LEU
2	I	69	LEU
2	I	80	GLN
2	I	81	ASP
2	I	98	LEU
2	I	101	ILE
2	I	108	ILE
2	I	113	VAL
2	I	141	HIS
2	I	142	ARG
2	I	151	ASP
2	I	176	VAL
2	I	197	LEU
2	I	203	ASP
2	I	206	THR
2	I	211	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	I	219	GLN
2	I	233	GLU
2	I	242	LEU
2	I	246	ASP
2	I	280	LYS
2	I	304	LEU
2	I	308	ARG
2	I	358	ARG
2	I	376	ARG
2	I	384	GLU
2	I	394	PHE
2	I	407	LYS
2	I	420	ARG
2	I	421	GLU
2	I	426	ASP
2	I	469	THR
2	I	512	ARG
2	I	523	ILE
2	I	524	VAL
2	I	528	GLU
2	I	551	GLU
2	I	598	GLU
2	I	610	ARG
2	I	613	VAL
2	I	616	GLU
2	I	620	LEU
2	I	643	VAL
2	I	648	ARG
2	I	668	LEU
2	I	685	GLU
2	I	697	ARG
2	I	707	ARG
2	I	715	THR
2	I	716	LYS
2	I	729	LEU
2	I	744	ARG
2	I	766	GLU
2	I	774	LEU
2	I	776	SER
2	I	784	ASP
2	I	785	VAL
2	I	788	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	I	807	ARG
2	I	808	ARG
2	I	815	LEU
2	I	816	LYS
2	I	819	VAL
2	I	857	ASP
2	I	869	VAL
2	I	897	LEU
2	I	899	GLN
2	I	950	LEU
2	I	995	MET
2	I	1001	VAL
2	I	1019	GLN
2	I	1060	ILE
2	I	1081	VAL
2	I	1104	GLU
2	I	1117	SER
3	J	4	GLU
3	J	9	ARG
3	J	35	ARG
3	J	53	ILE
3	J	55	ASP
3	J	66	GLN
3	J	75	ARG
3	J	76	CYS
3	J	106	LYS
3	J	142	LEU
3	J	157	GLU
3	J	166	GLN
3	J	180	LYS
3	J	210	ARG
3	J	212	ARG
3	J	341	GLU
3	J	346	LYS
3	J	347	VAL
3	J	361	VAL
3	J	399	ARG
3	J	400	VAL
3	J	408	GLU
3	J	411	THR
3	J	414	ARG
3	J	430	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	J	434	ARG
3	J	439	LEU
3	J	440	VAL
3	J	448	GLU
3	J	472	LYS
3	J	479	GLU
3	J	480	GLU
3	J	481	MET
3	J	504	ASP
3	J	514	LEU
3	J	525	ARG
3	J	544	TYR
3	J	549	ASN
3	J	564	GLU
3	J	618	LEU
3	J	637	LEU
3	J	680	GLN
3	J	692	GLU
3	J	694	VAL
3	J	702	LEU
3	J	703	ASN
3	J	725	SER
3	J	776	GLU
3	J	786	ILE
3	J	794	GLN
3	J	797	LYS
3	J	808	THR
3	J	813	LEU
3	J	817	GLU
3	J	828	VAL
3	J	832	ARG
3	J	855	HIS
3	J	871	ARG
3	J	879	ARG
3	J	884	ARG
3	J	893	GLU
3	J	897	GLN
3	J	908	LYS
3	J	937	TYR
3	J	956	ILE
3	J	961	GLN
3	J	971	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	J	976	GLN
3	J	987	GLU
3	J	1001	GLU
3	J	1047	LYS
3	J	1053	PHE
3	J	1059	SER
3	J	1084	THR
3	J	1087	ARG
3	J	1088	THR
3	J	1093	TYR
3	J	1161	GLU
3	J	1162	GLU
3	J	1203	LYS
3	J	1235	GLN
3	J	1285	GLU
3	J	1297	GLU
3	J	1310	ARG
3	J	1311	LEU
3	J	1318	TYR
3	J	1335	LEU
3	J	1342	GLU
3	J	1346	ARG
3	J	1354	LYS
3	J	1421	LEU
3	J	1429	LEU
3	J	1499	ARG
4	K	51	LEU
4	K	52	GLU
4	K	55	TYR
4	K	56	ASP
5	L	100	LEU
5	L	139	GLN
5	L	151	LEU
5	L	157	GLN
5	L	162	LEU
5	L	167	ASP
5	L	175	ASP
5	L	179	LYS
5	L	183	LYS
5	L	189	LEU
5	L	220	ARG
5	L	237	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	L	266	ILE
5	L	268	ASP
5	L	278	HIS
5	L	292	GLN
5	L	293	LEU
5	L	323	LEU
5	L	324	LYS
5	L	333	GLU
5	L	338	ASP
5	L	340	LYS
5	L	351	GLU
5	L	371	LYS
5	L	373	LEU
5	L	397	THR
5	L	404	TYR
5	L	405	PHE
5	L	413	ARG
5	L	416	GLU
5	L	426	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	38	ASN
1	B	63	HIS
1	B	163	ASN
1	B	213	GLN
2	C	41	ASN
2	C	204	GLN
2	C	538	GLN
2	C	563	ASN
2	C	765	GLN
2	C	829	GLN
2	C	843	HIS
2	C	899	GLN
3	D	274	GLN
3	D	483	HIS
3	D	507	ASN
3	D	552	ASN
3	D	569	ASN
3	D	680	GLN
3	D	794	GLN

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Mol	Chain	Res	Type
3	D	973	GLN
3	D	1046	GLN
3	D	1364	HIS
5	F	206	ASN
1	H	38	ASN
1	H	63	HIS
1	H	163	ASN
1	H	213	GLN
2	I	41	ASN
2	I	204	GLN
2	I	538	GLN
2	I	563	ASN
2	I	765	GLN
2	I	829	GLN
2	I	843	HIS
2	I	899	GLN
3	J	483	HIS
3	J	507	ASN
3	J	549	ASN
3	J	552	ASN
3	J	569	ASN
3	J	680	GLN
3	J	1046	GLN
3	J	1364	HIS
5	L	206	ASN
5	L	294	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.



## 5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	227/314 (72%)	-0.17	1 (0%) 92 87	87, 140, 176, 201	0
1	B	227/314 (72%)	-0.29	0 100 100	62, 117, 166, 206	0
1	G	227/314 (72%)	0.16	6 (2%) 56 46	124, 168, 194, 220	0
1	H	227/314 (72%)	-0.11	0 100 100	90, 147, 178, 196	0
2	C	1112/1119 (99%)	-0.14	13 (1%) 79 70	59, 139, 200, 249	0
2	I	1112/1119 (99%)	-0.04	20 (1%) 68 59	80, 159, 207, 252	0
3	D	1490/1524 (97%)	-0.25	1 (0%) 95 94	52, 113, 165, 216	0
3	J	1367/1524 (89%)	-0.18	5 (0%) 92 87	66, 134, 184, 230	0
4	E	93/99 (93%)	-0.21	0 100 100	65, 117, 169, 188	0
4	K	93/99 (93%)	-0.15	0 100 100	92, 145, 192, 221	0
5	F	345/347 (99%)	-0.15	5 (1%) 75 65	76, 146, 205, 235	0
5	L	345/347 (99%)	-0.04	7 (2%) 65 56	100, 161, 214, 248	0
6	O	30/30 (100%)	-0.09	1 (3%) 46 37	107, 178, 224, 227	0
6	R	30/30 (100%)	-0.38	0 100 100	134, 169, 201, 211	0
7	P	25/25 (100%)	-0.07	0 100 100	138, 174, 220, 243	0
7	S	25/25 (100%)	-0.48	0 100 100	141, 177, 196, 203	0
All	All	6975/7544 (92%)	-0.15	59 (0%) 86 79	52, 139, 196, 252	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	207	LEU	4.6
2	I	221	LEU	4.2
2	C	221	LEU	3.7
2	C	222	LEU	3.6
2	C	176	VAL	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	J	216	LEU	3.5
5	L	168	PRO	3.5
2	I	219	GLN	3.5
2	I	222	LEU	3.4
2	I	176	VAL	3.4
5	L	432	LYS	3.2
5	L	167	ASP	3.1
5	L	341	ASP	2.9
2	I	175	GLU	2.9
3	J	406	ASP	2.9
2	I	63	GLY	2.9
1	G	109	VAL	2.7
2	I	182	VAL	2.7
2	C	311	PHE	2.7
2	I	608	GLY	2.7
1	G	13	ALA	2.6
2	I	179	SER	2.6
2	I	181	VAL	2.5
2	I	62	GLY	2.5
2	C	174	LEU	2.5
2	I	174	LEU	2.5
2	I	649	VAL	2.5
3	J	437	VAL	2.5
5	F	168	PRO	2.4
1	G	143	ARG	2.4
2	I	190	LYS	2.4
5	F	416	GLU	2.4
1	A	140	MET	2.4
5	L	178	LEU	2.4
2	C	182	VAL	2.4
5	L	135	THR	2.4
1	G	25	LEU	2.3
2	C	207	LEU	2.3
2	C	175	GLU	2.3
6	O	2	DT	2.3
2	I	191	PHE	2.3
5	F	167	ASP	2.3
1	G	159	LYS	2.3
2	I	232	GLU	2.3
3	J	1487	VAL	2.3
5	F	178	LEU	2.2
5	F	409	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	219	GLN	2.2
3	D	974	ILE	2.2
5	L	340	LYS	2.2
1	G	129	ILE	2.2
2	C	238	LEU	2.1
2	C	183	THR	2.1
2	C	189	ARG	2.1
3	J	1283	ILE	2.1
2	C	223	ASP	2.1
2	I	65	VAL	2.1
2	I	250	LYS	2.1
2	I	189	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
9	MG	D	2003	1/1	0.86	0.15	205,205,205,205	0
8	ZN	J	2002	1/1	0.91	0.09	154,154,154,154	0
9	MG	J	2003	1/1	0.93	0.15	255,255,255,255	0
8	ZN	D	2002	1/1	0.97	0.18	118,118,118,118	0
8	ZN	J	2001	1/1	0.98	0.20	151,151,151,151	0
8	ZN	D	2001	1/1	0.99	0.20	107,107,107,107	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.