



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:53 AM GMT

PDB ID : 3K0F  
Title : Crystal structure of the phosphorylation-site double mutant T426A/T432A of the KaiC circadian clock protein  
Authors : Pattanayek, R.; Egli, M.; Pattanayek, S.  
Deposited on : 2009-09-24  
Resolution : 3.00 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

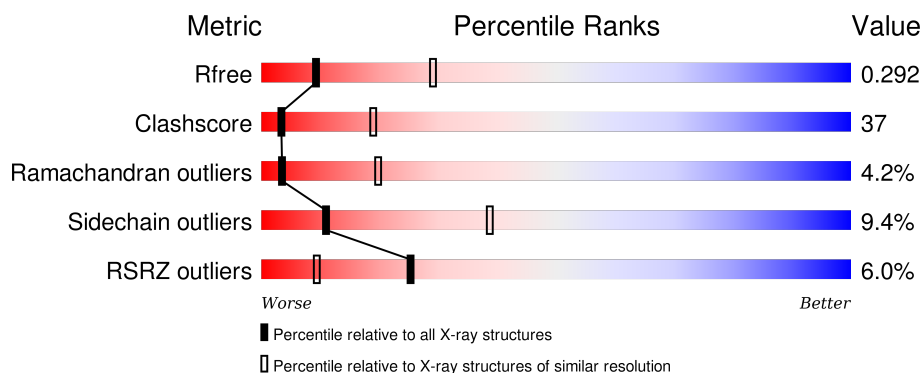
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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. 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	519	<div> <div>9%</div> <div>45%</div> <div>45%</div> <div>7%</div> <div>• •</div> </div>
2	B	519	<div> <div>5%</div> <div>42%</div> <div>44%</div> <div>8%</div> <div>5%</div> </div>
2	C	519	<div> <div>3%</div> <div>40%</div> <div>47%</div> <div>7%</div> <div>6%</div> </div>
2	D	519	<div> <div>4%</div> <div>45%</div> <div>42%</div> <div>6%</div> <div>• 7%</div> </div>
2	E	519	<div> <div>5%</div> <div>43%</div> <div>44%</div> <div>7%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	519	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SEP	B	431	-	-	X	-
2	SEP	D	431	-	-	X	-
3	MG	B	521	-	-	-	X
3	MG	B	802	-	-	-	X
3	MG	C	522	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23930 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 Circadian clock protein kinase KaiC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	S	0	0	0
			3981	2507	701	758	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	426	ALA	THR	ENGINEERED	UNP Q79PF4
A	432	ALA	THR	ENGINEERED	UNP Q79PF4

- Molecule 2 is a protein called Circadian clock protein kinase KaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	491	Total	C	N	O	P	S	0	0	0
			3870	2437	678	739	1	15			
2	C	488	Total	C	N	O	P	S	0	0	0
			3846	2423	674	733	1	15			
2	D	485	Total	C	N	O	P	S	0	0	0
			3822	2409	671	726	1	15			
2	E	492	Total	C	N	O	P	S	0	0	0
			3878	2443	679	740	1	15			
2	F	506	Total	C	N	O	P	S	0	0	0
			3985	2507	701	761	1	15			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	426	ALA	THR	ENGINEERED	UNP Q79PF4
B	432	ALA	THR	ENGINEERED	UNP Q79PF4
C	426	ALA	THR	ENGINEERED	UNP Q79PF4
C	432	ALA	THR	ENGINEERED	UNP Q79PF4
D	426	ALA	THR	ENGINEERED	UNP Q79PF4
D	432	ALA	THR	ENGINEERED	UNP Q79PF4

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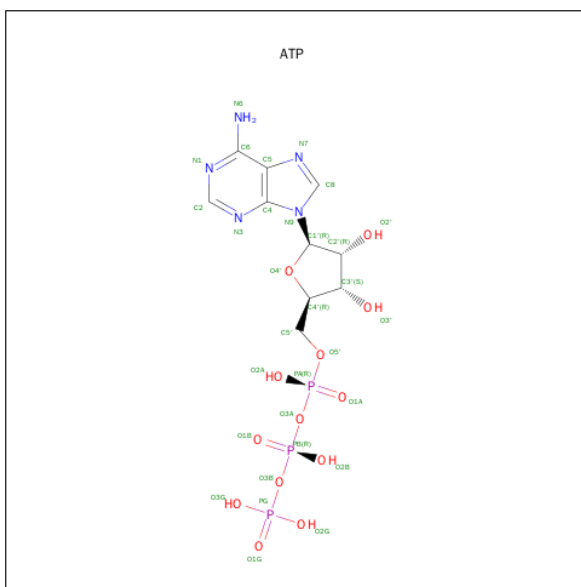
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Chain	Residue	Modelled	Actual	Comment	Reference
E	426	ALA	THR	ENGINEERED	UNP Q79PF4
E	432	ALA	THR	ENGINEERED	UNP Q79PF4
F	426	ALA	THR	ENGINEERED	UNP Q79PF4
F	432	ALA	THR	ENGINEERED	UNP Q79PF4

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	B	2	Total Mg 2 2	0	0
3	C	2	Total Mg 2 2	0	0
3	A	2	Total Mg 2 2	0	0
3	F	1	Total Mg 1 1	0	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

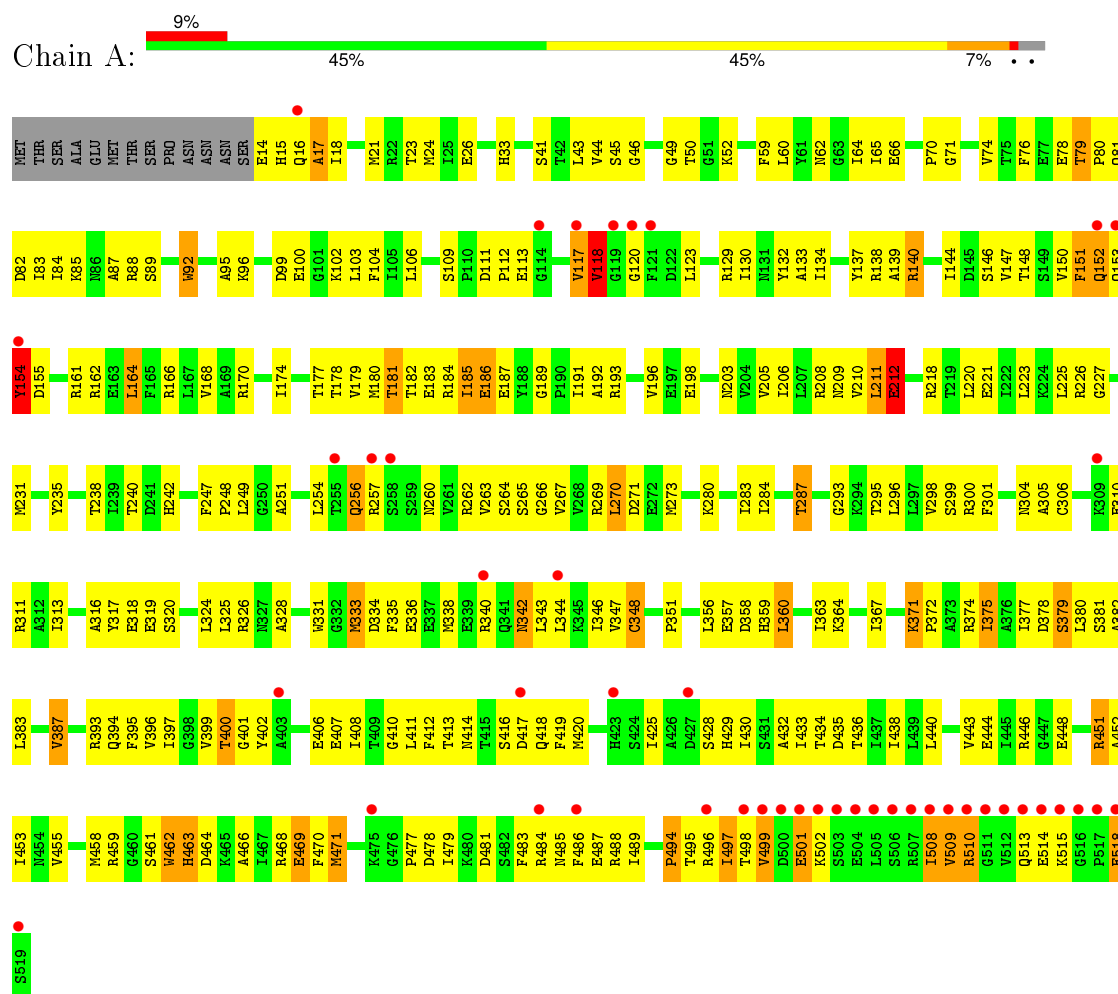
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	21	Total	O	0	0
			21	21		
5	B	12	Total	O	0	0
			12	12		
5	C	23	Total	O	0	0
			23	23		
5	D	37	Total	O	0	0
			37	37		
5	E	34	Total	O	0	0
			34	34		
5	F	40	Total	O	0	0
			40	40		

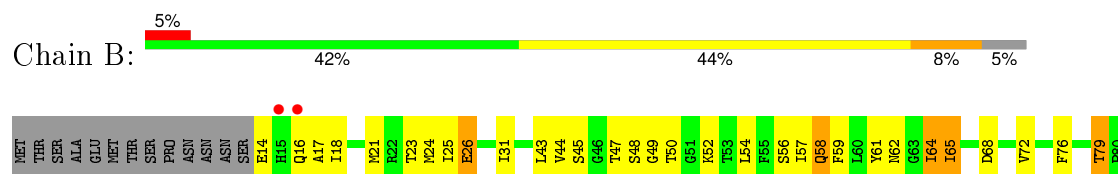
### 3 Residue-property plots

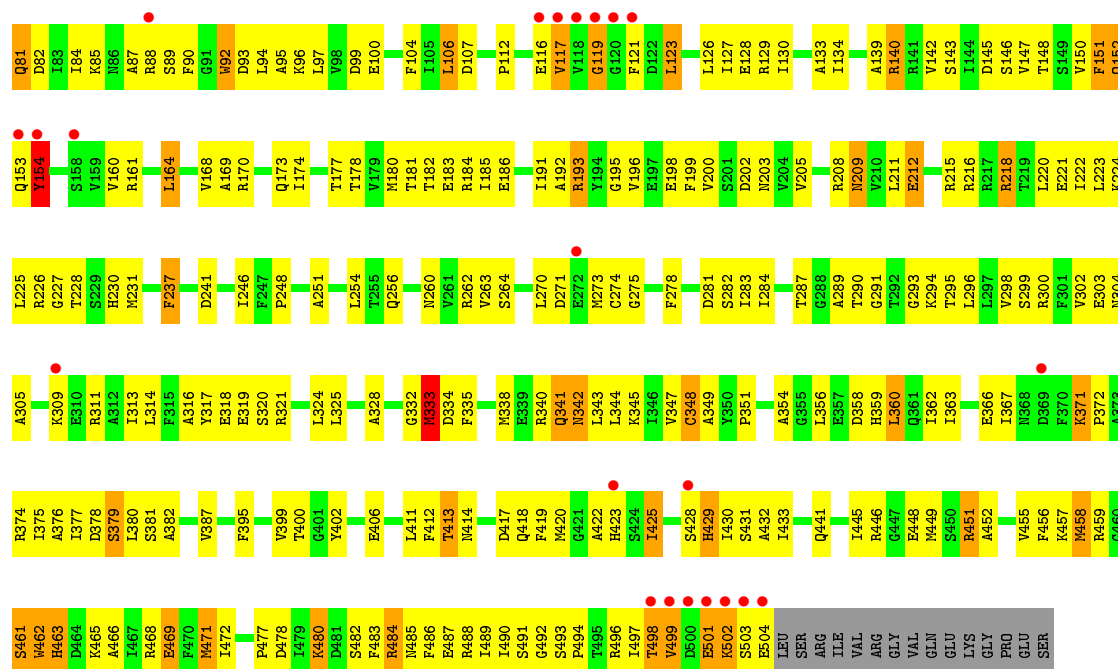
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Circadian clock protein kinase KaiC

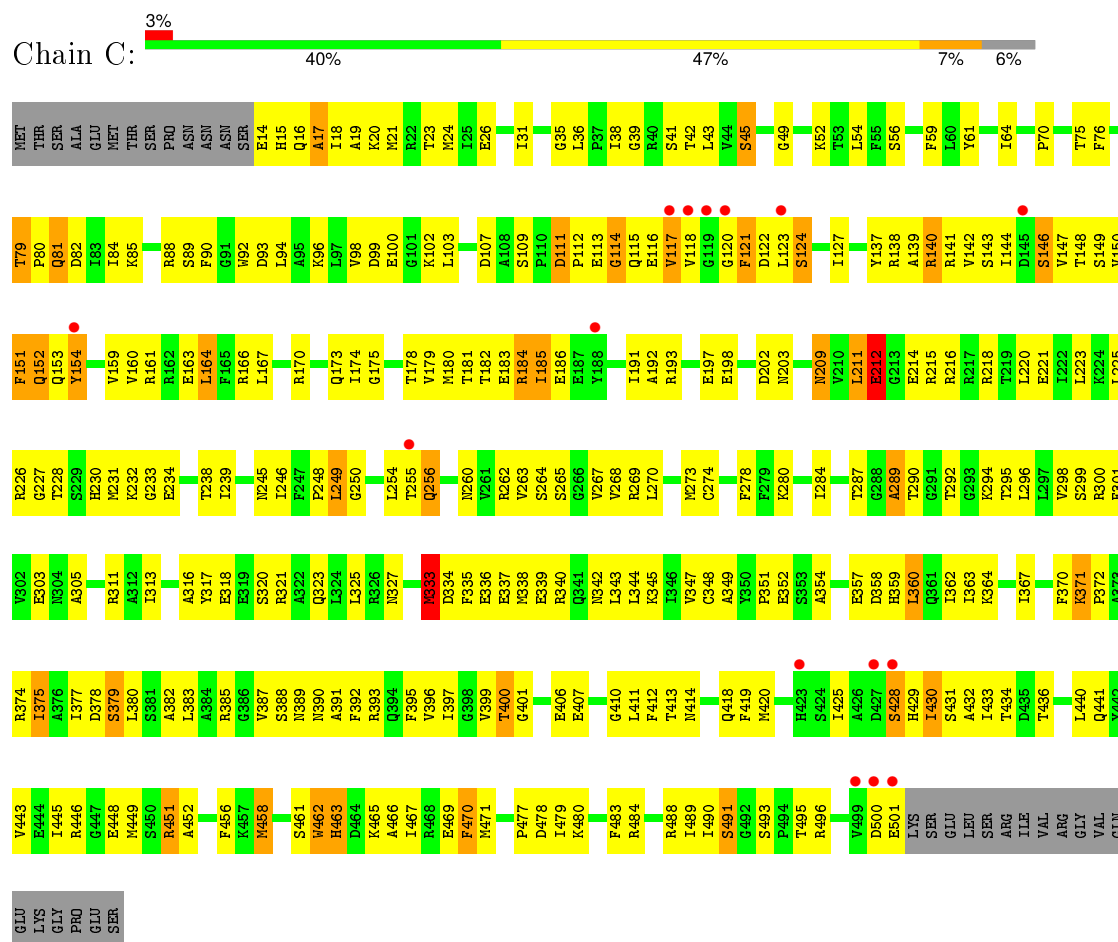


#### • Molecule 2: Circadian clock protein kinase KaiC



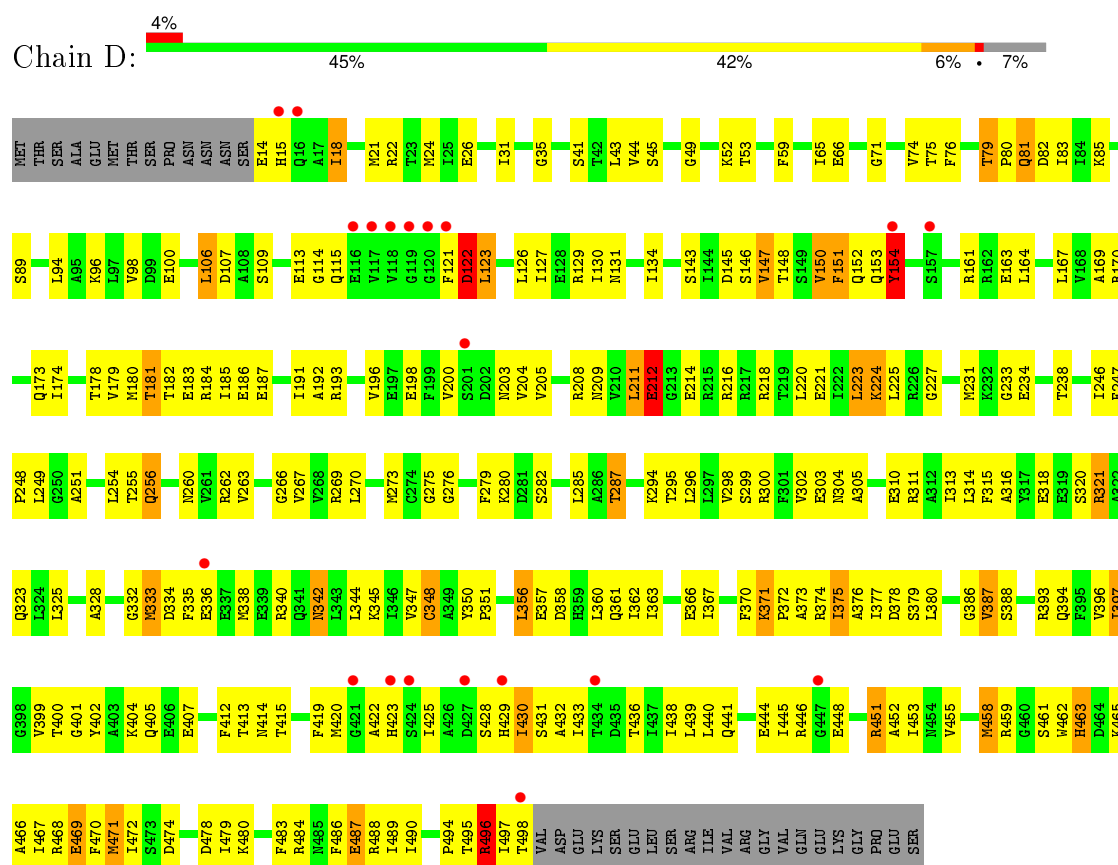


• Molecule 2: Circadian clock protein kinase KaiC

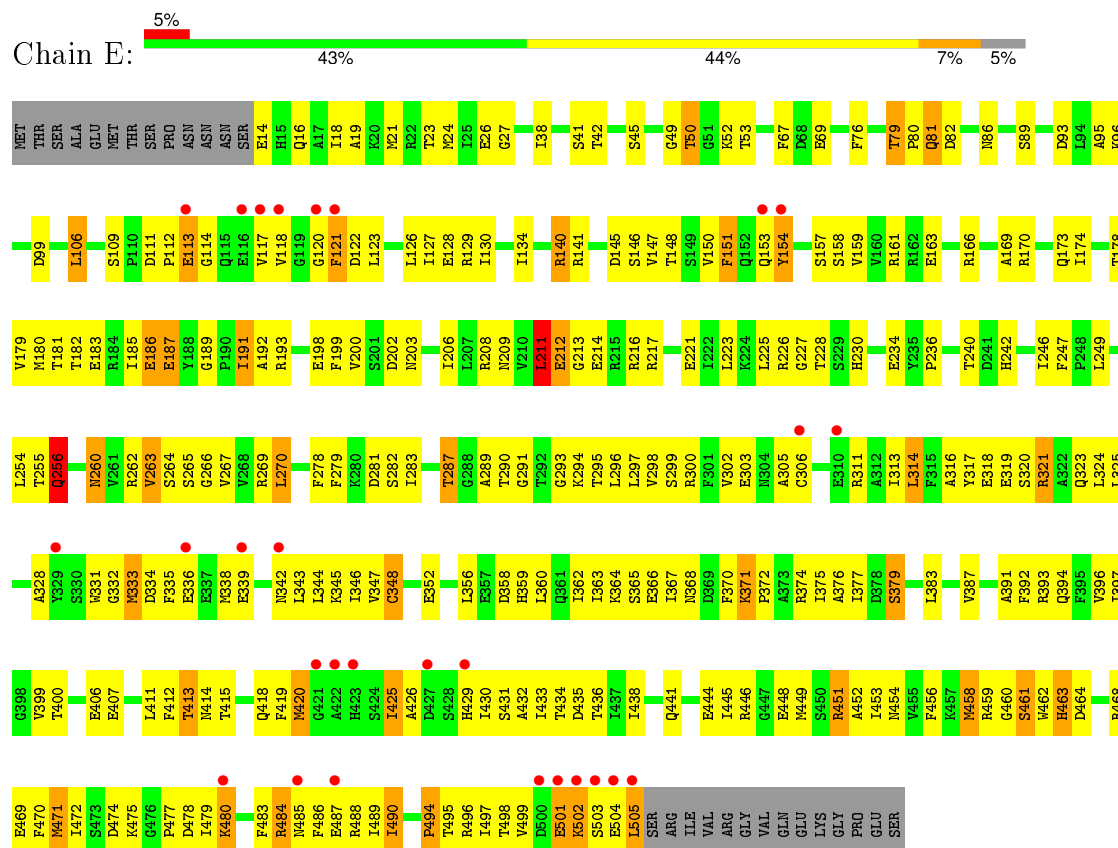


• Molecule 2: Circadian clock protein kinase KaiC

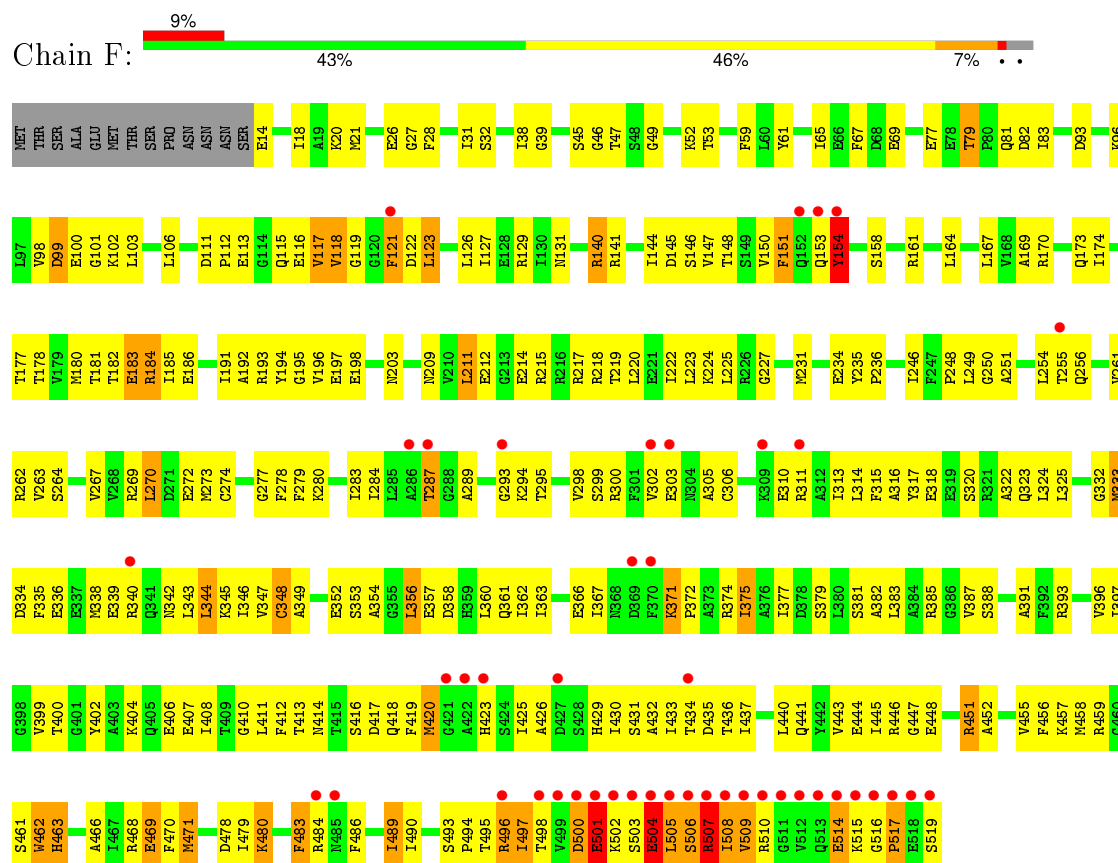




• Molecule 2: Circadian clock protein kinase KaiC



• Molecule 2: Circadian clock protein kinase KaiC



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.93Å 135.41Å 205.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 34.88 – 3.00	Depositor EDS
% Data completeness (in resolution range)	88.5 (30.00-3.00) 95.1 (34.88-3.00)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.39 (at 3.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.229 , 0.288 0.238 , 0.292	Depositor DCC
$R_{free}$ test set	7200 reflections (10.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.3	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 59.5	EDS
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 74993 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	23930	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, ATP, SEP

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	0.38	0/4047	0.65	0/5452
2	B	0.36	0/3924	0.63	0/5286
2	C	0.40	0/3900	0.64	0/5255
2	D	0.43	0/3876	0.68	0/5222
2	E	0.43	0/3932	0.68	1/5297 (0.0%)
2	F	0.41	0/4040	0.70	0/5441
All	All	0.40	0/23719	0.66	1/31953 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	213	GLY	N-CA-C	-5.22	100.04	113.10

There are no chirality outliers.

There are no planarity outliers.

### 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	3981	0	3981	301	0
2	B	3870	0	3858	298	0
2	C	3846	0	3834	285	0
2	D	3822	0	3815	310	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	3878	0	3869	300	0
2	F	3985	0	3980	345	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	62	0	24	7	0
4	B	62	0	24	8	0
4	C	62	0	24	5	0
4	D	62	0	24	3	0
4	E	62	0	24	8	0
4	F	62	0	24	7	0
5	A	21	0	0	7	0
5	B	12	0	0	3	0
5	C	23	0	0	2	0
5	D	37	0	0	6	0
5	E	34	0	0	12	0
5	F	40	0	0	10	0
All	All	23930	0	23481	1736	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 37.

All (1736) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:106:LEU:HD11	2:F:129:ARG:CZ	1.82	1.09
1:A:396:VAL:HG11	1:A:430:ILE:HG21	1.30	1.09
1:A:379:SER:H	1:A:413:THR:HB	1.19	1.03
2:E:356:LEU:HD22	2:E:387:VAL:HG11	1.41	1.02
2:F:305:ALA:HB2	2:F:374:ARG:HD2	1.39	1.00
2:F:420:MET:HA	5:F:520:HOH:O	1.62	0.97
2:C:396:VAL:HG11	2:C:430:ILE:HG21	1.44	0.96
2:B:140:ARG:NH1	2:B:140:ARG:HB3	1.79	0.96
2:B:305:ALA:HB2	2:B:374:ARG:HD2	1.47	0.95
2:B:263:VAL:HG12	2:B:374:ARG:HH21	1.29	0.94
2:B:140:ARG:HH11	2:B:140:ARG:HB3	1.29	0.92
2:B:116:GLU:HG2	2:B:117:VAL:H	1.34	0.92
2:D:305:ALA:HB2	2:D:374:ARG:HD2	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:429:HIS:HA	2:E:431:SEP:O3P	1.68	0.91
1:A:14:GLU:HG3	1:A:15:HIS:H	1.32	0.91
2:C:371:LYS:HD2	2:C:371:LYS:O	1.70	0.91
2:E:14:GLU:HG3	2:E:16:GLN:H	1.35	0.90
2:E:263:VAL:HG12	2:E:374:ARG:HH21	1.35	0.90
2:D:393:ARG:HH21	2:D:429:HIS:HB2	1.38	0.89
2:D:18:ILE:HD12	2:D:18:ILE:H	1.37	0.89
2:E:123:LEU:O	2:E:127:ILE:HG12	1.73	0.89
2:F:393:ARG:O	2:F:397:ILE:HG12	1.74	0.88
2:F:96:LYS:O	2:F:100:GLU:HG3	1.74	0.88
2:F:396:VAL:HG11	2:F:430:ILE:HG23	1.56	0.87
1:A:21:MET:HE2	1:A:177:THR:HG21	1.56	0.87
2:C:290:THR:HG21	2:D:431:SEP:O2P	1.74	0.87
1:A:263:VAL:HG12	1:A:374:ARG:HH21	1.40	0.86
2:B:471:MET:HB3	2:B:480:LYS:NZ	1.89	0.86
2:D:287:THR:HG23	2:D:414:ASN:HD22	1.38	0.86
2:F:283:ILE:HG13	2:F:400:THR:HG23	1.58	0.85
2:D:150:VAL:CG1	2:D:151:PHE:N	2.37	0.85
2:B:79:THR:HG23	2:B:81:GLN:HG2	1.56	0.85
2:F:393:ARG:HH21	2:F:429:HIS:HB2	1.40	0.85
2:E:431:SEP:O	2:E:434:THR:HG22	1.77	0.84
2:F:106:LEU:CD1	2:F:129:ARG:NH2	2.40	0.84
1:A:396:VAL:HG11	1:A:430:ILE:CG2	2.08	0.84
2:D:263:VAL:HG12	2:D:374:ARG:HH21	1.43	0.84
2:C:469:GLU:HG3	2:C:480:LYS:HE3	1.59	0.84
2:B:147:VAL:HG11	2:B:180:MET:HE3	1.60	0.84
2:B:263:VAL:HG12	2:B:374:ARG:NH2	1.92	0.84
2:D:358:ASP:O	2:D:362:ILE:HG12	1.76	0.84
2:D:396:VAL:HG11	2:D:430:ILE:CG2	2.07	0.83
2:B:283:ILE:HG13	2:B:400:THR:HG23	1.59	0.83
2:D:379:SER:H	2:D:413:THR:HB	1.43	0.83
2:E:290:THR:HB	2:F:431:SEP:O1P	1.78	0.83
1:A:211:LEU:O	1:A:212:GLU:HB3	1.79	0.83
2:F:377:ILE:HD11	2:F:399:VAL:HG11	1.61	0.83
2:D:106:LEU:C	2:D:106:LEU:HD12	1.99	0.82
1:A:305:ALA:HB2	1:A:374:ARG:HD2	1.60	0.82
2:E:263:VAL:CG1	2:E:374:ARG:HH21	1.91	0.82
2:E:182:THR:HG21	2:E:192:ALA:HB1	1.62	0.82
1:A:393:ARG:O	1:A:397:ILE:HG12	1.79	0.82
2:C:428:SER:HB2	2:C:430:ILE:HD11	1.62	0.82
2:D:150:VAL:CG1	2:D:151:PHE:H	1.92	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:263:VAL:CG1	2:B:374:ARG:HH21	1.92	0.81
2:D:393:ARG:O	2:D:397:ILE:HG12	1.80	0.81
2:E:53:THR:HG23	2:E:145:ASP:OD1	1.78	0.81
2:C:263:VAL:HG12	2:C:374:ARG:HH21	1.46	0.81
2:E:497:ILE:HG22	2:E:498:THR:H	1.44	0.81
2:D:380:LEU:CD1	2:D:412:PHE:HB3	2.11	0.80
2:D:325:LEU:HD23	2:D:335:PHE:HB2	1.63	0.80
2:F:79:THR:CG2	2:F:81:GLN:HG2	2.11	0.80
1:A:45:SER:HB3	1:A:182:THR:HB	1.61	0.80
2:D:146:SER:H	2:D:181:THR:HG22	1.45	0.80
2:F:486:PHE:CE2	2:F:496:ARG:HD2	2.17	0.80
1:A:320:SER:HA	2:B:254:LEU:HG	1.62	0.80
2:F:500:ASP:O	2:F:501:GLU:HB3	1.81	0.80
1:A:14:GLU:CG	1:A:15:HIS:H	1.95	0.80
2:D:150:VAL:HG13	2:D:151:PHE:N	1.93	0.80
1:A:79:THR:CG2	1:A:81:GLN:HG2	2.11	0.80
2:E:76:PHE:HZ	2:E:126:LEU:HD21	1.47	0.80
2:F:357:GLU:HG3	2:F:358:ASP:H	1.46	0.79
2:B:140:ARG:CB	2:B:140:ARG:HH11	1.94	0.79
2:E:425:ILE:HG22	2:E:426:ALA:N	1.95	0.79
1:A:24:MET:CB	1:A:62:ASN:HD22	1.95	0.79
2:D:299:SER:HB3	2:D:333:MET:HE1	1.63	0.79
2:B:45:SER:HB3	2:B:182:THR:HB	1.64	0.79
2:F:191:ILE:HB	2:F:198:GLU:CG	2.13	0.79
2:F:280:LYS:NZ	2:F:407:GLU:HB3	1.98	0.78
2:F:437:ILE:HD12	2:F:457:LYS:HG2	1.63	0.78
2:E:348:CYS:HB3	2:F:254:LEU:HD23	1.65	0.78
2:B:79:THR:CG2	2:B:81:GLN:HG2	2.12	0.78
2:F:263:VAL:CG1	2:F:374:ARG:HH21	1.97	0.78
2:E:393:ARG:HD2	5:E:524:HOH:O	1.83	0.78
1:A:96:LYS:O	1:A:100:GLU:HG3	1.83	0.78
2:F:379:SER:H	2:F:413:THR:HB	1.48	0.78
1:A:269:ARG:HG2	1:A:479:ILE:HB	1.64	0.78
1:A:508:ILE:H	1:A:508:ILE:HD13	1.49	0.78
1:A:396:VAL:O	1:A:400:THR:HB	1.83	0.78
2:B:43:LEU:HD11	2:B:182:THR:OG1	1.84	0.77
2:E:249:LEU:HD23	5:E:532:HOH:O	1.83	0.77
2:F:106:LEU:CD1	2:F:129:ARG:CZ	2.61	0.77
2:B:419:PHE:CD2	2:C:425:ILE:HD12	2.19	0.77
2:D:269:ARG:HG2	2:D:479:ILE:HB	1.64	0.77
1:A:263:VAL:HG12	1:A:374:ARG:NH2	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:ILE:HB	2:B:198:GLU:CG	2.13	0.77
2:C:449:MET:HE3	2:D:467:ILE:HD11	1.67	0.77
2:D:150:VAL:HG12	2:D:151:PHE:H	1.48	0.77
2:F:161:ARG:HB2	2:F:196:VAL:HG11	1.67	0.77
1:A:360:LEU:HD23	1:A:399:VAL:HG22	1.67	0.77
2:D:152:GLN:O	2:E:158:SER:HB3	1.85	0.77
2:F:263:VAL:HG12	2:F:374:ARG:HH21	1.49	0.76
2:D:431:SEP:C	2:D:433:ILE:H	1.98	0.76
2:C:123:LEU:HD12	2:C:163:GLU:OE2	1.84	0.76
2:D:249:LEU:HB3	5:D:526:HOH:O	1.85	0.76
2:B:24:MET:HB2	2:B:62:ASN:HD22	1.50	0.76
1:A:18:ILE:HD12	1:A:18:ILE:N	2.00	0.76
2:E:293:GLY:HA2	4:E:901:ATP:O1A	1.85	0.76
2:E:396:VAL:HG11	2:E:430:ILE:HG21	1.68	0.76
2:F:515:LYS:HG3	2:F:516:GLY:N	2.01	0.76
2:F:127:ILE:HD11	2:F:167:LEU:HA	1.66	0.76
1:A:466:ALA:HA	2:F:448:GLU:HG2	1.66	0.76
1:A:379:SER:N	1:A:413:THR:HB	2.00	0.75
2:F:486:PHE:HE2	2:F:496:ARG:HD2	1.51	0.75
2:D:191:ILE:HB	2:D:198:GLU:CG	2.15	0.75
2:D:96:LYS:O	2:D:100:GLU:HG3	1.85	0.75
1:A:451:ARG:HH11	1:A:451:ARG:HG2	1.51	0.75
2:C:79:THR:HG23	2:C:81:GLN:HG2	1.66	0.75
2:F:431:SEP:O	2:F:434:THR:HG22	1.87	0.75
2:F:504:GLU:O	2:F:505:LEU:HB2	1.86	0.75
2:C:287:THR:HG21	2:C:425:ILE:O	1.86	0.75
2:D:313:ILE:HG13	2:D:372:PRO:HG3	1.68	0.75
1:A:287:THR:CG2	1:A:414:ASN:HD22	2.00	0.74
2:D:325:LEU:HD22	2:D:336:GLU:HG2	1.69	0.74
2:F:123:LEU:O	2:F:127:ILE:HG12	1.88	0.74
2:E:93:ASP:OD2	2:E:96:LYS:HB2	1.88	0.74
2:C:323:GLN:HE22	2:D:459:ARG:HD3	1.52	0.74
2:C:140:ARG:HB3	2:C:140:ARG:NH1	2.02	0.74
2:C:81:GLN:H	2:C:81:GLN:NE2	1.85	0.74
1:A:24:MET:HB2	1:A:62:ASN:HD22	1.52	0.74
2:F:280:LYS:HZ1	2:F:407:GLU:HB3	1.51	0.74
1:A:147:VAL:HG11	1:A:180:MET:HE3	1.69	0.74
2:F:430:ILE:HG22	2:F:430:ILE:O	1.86	0.74
2:B:191:ILE:HB	2:B:198:GLU:HG3	1.69	0.74
2:D:371:LYS:HD2	2:D:371:LYS:O	1.86	0.74
2:C:305:ALA:HB2	2:C:374:ARG:HD2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:79:THR:CG2	2:D:81:GLN:HG2	2.18	0.73
1:A:78:GLU:HB3	1:A:83:ILE:HD11	1.69	0.73
2:D:393:ARG:NH2	2:D:429:HIS:HB2	2.03	0.73
1:A:140:ARG:HB3	1:A:140:ARG:NH1	2.04	0.73
1:A:287:THR:HG23	1:A:414:ASN:HD22	1.52	0.73
2:C:382:ALA:O	2:C:385:ARG:HG3	1.89	0.73
2:E:387:VAL:HG12	2:E:391:ALA:HB3	1.70	0.73
2:E:269:ARG:HB3	2:E:479:ILE:HD12	1.70	0.73
2:D:486:PHE:HB2	2:D:489:ILE:HD11	1.71	0.72
2:D:147:VAL:HG11	2:D:180:MET:HE3	1.72	0.72
2:E:371:LYS:HD2	2:E:371:LYS:O	1.88	0.72
1:A:191:ILE:HB	1:A:198:GLU:HG2	1.70	0.72
2:E:269:ARG:HG2	2:E:479:ILE:HB	1.71	0.72
2:B:147:VAL:O	2:B:150:VAL:HG12	1.89	0.72
2:B:274:CYS:HG	2:B:278:PHE:HE2	1.35	0.72
2:B:325:LEU:HD23	2:B:335:PHE:HB2	1.70	0.72
2:C:431:SEP:O	2:C:434:THR:HG22	1.90	0.72
2:B:56:SER:HB2	2:B:143:SER:HB3	1.72	0.71
2:B:93:ASP:OD2	2:B:96:LYS:HB2	1.90	0.71
2:F:356:LEU:HD21	2:F:387:VAL:HG11	1.72	0.71
1:A:284:ILE:HB	1:A:411:LEU:HD12	1.70	0.71
2:D:263:VAL:HG12	2:D:374:ARG:NH2	2.03	0.71
1:A:264:SER:HA	1:A:271:ASP:OD1	1.89	0.71
2:E:147:VAL:O	2:E:150:VAL:HG12	1.89	0.71
2:E:485:ASN:HD21	2:E:496:ARG:NH1	1.88	0.71
2:F:203:ASN:HB3	2:F:225:LEU:HD23	1.73	0.71
2:D:287:THR:CG2	2:D:414:ASN:HD22	2.02	0.71
2:C:471:MET:HG3	2:C:478:ASP:HB3	1.71	0.71
1:A:356:LEU:HD13	1:A:387:VAL:HG21	1.71	0.71
2:B:65:ILE:HG22	2:B:65:ILE:O	1.91	0.71
2:D:367:ILE:HG12	2:D:375:ILE:HD11	1.72	0.71
2:C:469:GLU:HB3	2:C:483:PHE:CZ	2.26	0.71
2:B:273:MET:O	2:B:463:HIS:HA	1.90	0.71
2:F:377:ILE:CD1	2:F:399:VAL:HG11	2.20	0.71
2:B:379:SER:HA	2:B:413:THR:HG22	1.73	0.71
1:A:65:ILE:O	1:A:65:ILE:HG22	1.90	0.70
2:F:79:THR:HG22	2:F:82:ASP:H	1.53	0.70
2:D:294:LYS:HZ1	2:D:415:THR:HG23	1.55	0.70
2:B:298:VAL:HG13	2:B:376:ALA:HB1	1.72	0.70
2:D:486:PHE:CB	2:D:489:ILE:HD11	2.21	0.70
2:F:357:GLU:HG3	2:F:358:ASP:N	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:LEU:HG	2:F:320:SER:HA	1.73	0.70
2:F:106:LEU:HD11	2:F:129:ARG:NH2	2.04	0.70
2:D:380:LEU:HD11	2:D:412:PHE:HB3	1.73	0.70
2:C:191:ILE:HB	2:C:198:GLU:CG	2.21	0.70
2:D:422:ALA:HB3	5:D:522:HOH:O	1.92	0.70
2:C:214:GLU:HB3	2:D:234:GLU:HB2	1.73	0.70
2:D:371:LYS:CD	2:D:371:LYS:O	2.39	0.70
2:E:359:HIS:O	2:E:363:ILE:HG13	1.92	0.70
2:C:396:VAL:O	2:C:400:THR:HB	1.92	0.70
2:E:287:THR:HB	5:E:537:HOH:O	1.90	0.70
2:F:49:GLY:HA2	4:F:903:ATP:O2B	1.91	0.70
2:D:294:LYS:NZ	2:D:415:THR:HG23	2.07	0.69
2:F:347:VAL:O	2:F:348:CYS:HB2	1.92	0.69
1:A:247:PHE:HB3	5:A:531:HOH:O	1.91	0.69
2:F:509:VAL:HG12	2:F:510:ARG:H	1.57	0.69
1:A:89:SER:HB2	2:B:227:GLY:O	1.91	0.69
2:B:429:HIS:HB3	2:B:431:SEP:O2P	1.91	0.69
1:A:351:PRO:HB3	1:A:383:LEU:HD23	1.74	0.69
1:A:43:LEU:HD11	1:A:182:THR:OG1	1.93	0.69
2:C:140:ARG:HB3	2:C:140:ARG:HH11	1.57	0.69
2:B:18:ILE:HB	2:B:228:THR:CG2	2.22	0.69
2:C:335:PHE:HA	2:C:338:MET:HG3	1.75	0.69
2:C:344:LEU:HD22	2:C:345:LYS:H	1.57	0.69
2:C:41:SER:HB3	2:C:178:THR:HB	1.75	0.69
2:C:371:LYS:CD	2:C:371:LYS:O	2.40	0.69
2:C:323:GLN:NE2	2:D:459:ARG:HD3	2.08	0.69
2:E:484:ARG:HG2	5:E:525:HOH:O	1.92	0.69
1:A:406:GLU:O	1:A:407:GLU:HB2	1.92	0.69
2:B:363:ILE:O	2:B:367:ILE:HG13	1.91	0.69
2:D:431:SEP:O	2:D:432:ALA:HB3	1.90	0.69
2:D:147:VAL:HG11	2:D:180:MET:CE	2.23	0.69
2:B:351:PRO:HG2	2:B:382:ALA:O	1.92	0.69
2:D:203:ASN:HB3	2:D:225:LEU:HD23	1.74	0.69
1:A:367:ILE:HG12	1:A:375:ILE:HD11	1.74	0.69
2:E:313:ILE:HG13	2:E:372:PRO:HG3	1.74	0.69
1:A:287:THR:HG23	1:A:414:ASN:HB3	1.75	0.69
1:A:257:ARG:NH2	1:A:407:GLU:HG2	2.07	0.68
1:A:446:ARG:HA	1:A:496:ARG:NH2	2.08	0.68
2:D:79:THR:HG23	2:D:81:GLN:HE21	1.57	0.68
2:D:311:ARG:HD2	2:D:371:LYS:CE	2.23	0.68
2:C:273:MET:O	2:C:463:HIS:HA	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:MET:HB3	1:A:235:TYR:OH	1.93	0.68
2:B:81:GLN:H	2:B:81:GLN:NE2	1.92	0.68
2:E:325:LEU:HD23	2:E:335:PHE:HB2	1.75	0.68
2:F:231:MET:HE3	2:F:251:ALA:HB2	1.76	0.68
2:E:444:GLU:OE1	2:F:490:ILE:HG12	1.94	0.68
2:B:299:SER:C	2:B:333:MET:HE1	2.14	0.68
1:A:316:ALA:O	1:A:348:CYS:HA	1.94	0.68
2:B:503:SER:O	2:B:504:GLU:HB2	1.94	0.68
2:D:148:THR:CG2	2:D:193:ARG:HD2	2.24	0.68
2:F:501:GLU:HG3	2:F:502:LYS:N	2.09	0.68
2:D:267:VAL:HG22	2:D:300:ARG:HG2	1.76	0.68
2:C:393:ARG:O	2:C:397:ILE:HG12	1.93	0.68
2:E:287:THR:HG22	2:E:414:ASN:HD22	1.58	0.67
2:C:263:VAL:CG1	2:C:374:ARG:HH21	2.07	0.67
2:E:262:ARG:HH22	2:E:461:SER:HB2	1.60	0.67
1:A:161:ARG:HB2	1:A:196:VAL:HG11	1.75	0.67
2:B:451:ARG:HG2	2:B:451:ARG:HH11	1.59	0.67
1:A:130:ILE:O	1:A:134:ILE:HG13	1.93	0.67
2:C:449:MET:CE	2:D:467:ILE:HD11	2.25	0.67
2:E:263:VAL:HG12	2:E:374:ARG:NH2	2.10	0.67
2:F:387:VAL:HG12	2:F:388:SER:O	1.94	0.67
2:B:18:ILE:HB	2:B:228:THR:HG23	1.75	0.67
1:A:363:ILE:O	1:A:367:ILE:HG13	1.94	0.67
2:E:18:ILE:HG13	2:E:228:THR:HG23	1.76	0.67
1:A:325:LEU:HD23	1:A:335:PHE:HB2	1.77	0.67
2:C:318:GLU:CD	2:D:432:ALA:HB1	2.15	0.67
2:B:493:SER:HB3	2:C:488:ARG:HG2	1.77	0.67
2:D:152:GLN:O	2:E:158:SER:CB	2.43	0.67
2:F:264:SER:O	2:F:374:ARG:NH2	2.26	0.67
2:E:306:CYS:SG	2:E:344:LEU:HB2	2.35	0.67
2:C:85:LYS:NZ	2:D:14:GLU:HB3	2.10	0.67
2:B:367:ILE:HG23	2:B:372:PRO:HD2	1.76	0.66
2:E:42:THR:HA	2:E:203:ASN:HB2	1.75	0.66
2:E:504:GLU:HG2	2:E:505:LEU:H	1.60	0.66
1:A:406:GLU:HB3	1:A:408:ILE:HG13	1.77	0.66
2:E:363:ILE:O	2:E:367:ILE:HG13	1.96	0.66
2:C:269:ARG:HG2	2:C:479:ILE:HB	1.75	0.66
2:C:396:VAL:HG11	2:C:430:ILE:CG2	2.22	0.66
2:E:334:ASP:OD1	2:E:336:GLU:HB2	1.96	0.66
2:D:471:MET:HG3	2:D:478:ASP:HB3	1.76	0.66
2:E:19:ALA:O	2:E:38:ILE:HD12	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:81:GLN:CD	2:C:81:GLN:H	1.97	0.66
1:A:419:PHE:CD2	2:B:425:ILE:HD12	2.30	0.66
2:F:182:THR:HG21	2:F:192:ALA:HB1	1.78	0.66
2:D:318:GLU:OE2	2:E:432:ALA:HB1	1.95	0.66
2:E:461:SER:OG	2:E:462:TRP:N	2.29	0.66
2:C:469:GLU:CG	2:C:480:LYS:HE3	2.25	0.66
2:C:287:THR:HG23	2:C:414:ASN:HD22	1.61	0.66
2:D:79:THR:O	2:D:83:ILE:HD12	1.96	0.66
2:B:123:LEU:O	2:B:127:ILE:HG13	1.95	0.66
2:C:19:ALA:O	2:C:38:ILE:HD12	1.96	0.66
2:E:485:ASN:ND2	2:E:496:ARG:HH11	1.94	0.66
2:C:159:VAL:O	2:C:163:GLU:HG2	1.96	0.65
2:D:14:GLU:CD	2:D:15:HIS:H	1.99	0.65
2:D:212:GLU:HG2	2:D:212:GLU:O	1.95	0.65
2:C:296:LEU:HD21	2:C:477:PRO:HB3	1.77	0.65
2:B:471:MET:HB3	2:B:480:LYS:HZ1	1.60	0.65
2:B:497:ILE:HD12	2:B:499:VAL:HB	1.78	0.65
2:F:287:THR:CG2	2:F:414:ASN:HD22	2.10	0.65
2:E:266:GLY:HA3	2:E:300:ARG:HG3	1.77	0.65
2:F:515:LYS:HG3	2:F:516:GLY:H	1.60	0.65
1:A:356:LEU:CD1	1:A:387:VAL:HG21	2.26	0.65
1:A:299:SER:HB3	1:A:333:MET:HE1	1.77	0.65
2:E:140:ARG:NH1	2:E:140:ARG:HB3	2.12	0.65
2:F:505:LEU:O	2:F:506:SER:HB3	1.96	0.65
2:B:295:THR:HG21	2:B:319:GLU:OE2	1.96	0.65
2:F:197:GLU:N	2:F:197:GLU:OE2	2.22	0.65
2:F:79:THR:HG23	2:F:81:GLN:HG2	1.77	0.65
2:C:363:ILE:O	2:C:367:ILE:HG13	1.97	0.65
2:D:486:PHE:CE2	2:D:496:ARG:HB3	2.31	0.65
2:F:363:ILE:O	2:F:367:ILE:HG13	1.97	0.65
2:C:344:LEU:HD22	2:C:345:LYS:N	2.12	0.65
2:B:211:LEU:HB2	2:B:216:ARG:CZ	2.26	0.65
2:E:191:ILE:HB	2:E:198:GLU:CG	2.27	0.65
2:D:130:ILE:O	2:D:134:ILE:HG13	1.95	0.65
2:E:81:GLN:H	2:E:81:GLN:CD	1.99	0.65
2:B:471:MET:HB3	2:B:480:LYS:HZ3	1.62	0.64
2:F:514:GLU:O	2:F:515:LYS:HB3	1.96	0.64
2:F:53:THR:HG23	2:F:145:ASP:OD1	1.98	0.64
2:E:504:GLU:CG	2:E:505:LEU:H	2.10	0.64
1:A:170:ARG:O	1:A:174:ILE:HG12	1.97	0.64
2:C:148:THR:OG1	2:C:182:THR:HG23	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:ILE:O	2:B:134:ILE:HG13	1.96	0.64
2:E:436:THR:OG1	2:E:458:MET:HG2	1.98	0.64
2:F:269:ARG:HG2	2:F:479:ILE:HB	1.77	0.64
2:D:74:VAL:HG22	2:D:106:LEU:HD23	1.79	0.64
2:C:151:PHE:C	2:C:153:GLN:H	1.98	0.64
2:F:289:ALA:HB2	2:F:419:PHE:HA	1.78	0.64
2:C:396:VAL:CG1	2:C:430:ILE:HG21	2.23	0.64
2:D:446:ARG:HG3	2:D:496:ARG:NH1	2.12	0.64
2:E:485:ASN:ND2	2:E:496:ARG:NH1	2.45	0.64
2:B:79:THR:HG22	2:B:82:ASP:OD2	1.98	0.64
2:F:471:MET:HG3	2:F:478:ASP:HB3	1.78	0.64
2:D:85:LYS:NZ	2:E:14:GLU:HB3	2.12	0.63
2:D:428:SER:HB2	5:D:535:HOH:O	1.96	0.63
2:E:396:VAL:HG11	2:E:430:ILE:CG2	2.28	0.63
2:C:79:THR:CG2	2:C:81:GLN:HG2	2.28	0.63
2:C:31:ILE:HA	2:C:231:MET:SD	2.37	0.63
2:F:79:THR:HB	2:F:82:ASP:OD2	1.98	0.63
2:E:433:ILE:HD12	2:E:433:ILE:N	2.13	0.63
2:C:393:ARG:NH2	2:C:429:HIS:HB2	2.13	0.63
2:F:164:LEU:HD11	2:F:197:GLU:HG3	1.79	0.63
2:B:441:GLN:NE2	2:B:490:ILE:HD13	2.14	0.63
1:A:14:GLU:HG3	1:A:15:HIS:N	2.09	0.63
2:D:446:ARG:N	2:D:496:ARG:HH12	1.95	0.63
1:A:191:ILE:HB	1:A:198:GLU:CG	2.29	0.63
2:C:182:THR:HG21	2:C:192:ALA:HB1	1.79	0.63
2:B:264:SER:HB3	2:B:304:ASN:ND2	2.13	0.63
2:D:178:THR:HG22	2:D:179:VAL:N	2.14	0.63
2:F:344:LEU:HD22	2:F:345:LYS:N	2.14	0.63
2:C:305:ALA:HB2	2:C:374:ARG:CD	2.29	0.63
2:D:335:PHE:HA	2:D:338:MET:HG3	1.79	0.63
2:E:19:ALA:C	2:E:38:ILE:HD12	2.19	0.63
2:F:396:VAL:HG11	2:F:430:ILE:CG2	2.27	0.63
2:E:283:ILE:HG13	2:E:400:THR:HG23	1.80	0.63
1:A:360:LEU:HD23	1:A:399:VAL:CG2	2.28	0.63
2:F:515:LYS:CG	2:F:517:PRO:HD2	2.29	0.63
2:D:316:ALA:O	2:D:348:CYS:HA	1.98	0.63
2:D:114:GLY:O	2:D:115:GLN:HG3	1.99	0.63
2:E:303:GLU:OE2	2:E:333:MET:HB3	1.99	0.63
2:F:515:LYS:HG3	2:F:517:PRO:HD2	1.81	0.62
2:F:20:LYS:C	2:F:38:ILE:HD11	2.19	0.62
2:C:111:ASP:O	2:C:113:GLU:N	2.26	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:GLU:C	1:A:515:LYS:HD2	2.19	0.62
1:A:80:PRO:HD2	1:A:81:GLN:HE21	1.64	0.62
2:E:344:LEU:HD22	2:E:345:LYS:N	2.14	0.62
2:C:191:ILE:HB	2:C:198:GLU:HG2	1.81	0.62
2:B:182:THR:HG21	2:B:192:ALA:HB1	1.81	0.62
2:B:455:VAL:HG11	2:B:463:HIS:HB2	1.80	0.62
2:F:67:PHE:HB2	2:F:69:GLU:HG3	1.80	0.62
2:F:106:LEU:HD11	2:F:129:ARG:NE	2.15	0.62
2:B:320:SER:HA	2:C:254:LEU:HG	1.81	0.62
1:A:140:ARG:HH11	1:A:140:ARG:HA	1.64	0.62
2:F:501:GLU:HG3	2:F:502:LYS:H	1.64	0.62
1:A:381:SER:HB3	1:A:414:ASN:OD1	1.99	0.62
2:C:14:GLU:HG3	2:C:16:GLN:H	1.62	0.62
2:F:106:LEU:HD12	2:F:129:ARG:NH2	2.14	0.62
2:B:47:THR:HG23	5:B:520:HOH:O	1.99	0.62
2:E:379:SER:HA	2:E:413:THR:HG22	1.81	0.62
2:E:471:MET:HG3	2:E:478:ASP:HB3	1.81	0.62
2:D:79:THR:HG23	2:D:81:GLN:HG2	1.81	0.62
2:E:191:ILE:HG13	2:E:206:ILE:HD11	1.81	0.62
2:C:299:SER:C	2:C:333:MET:HE1	2.20	0.62
2:C:225:LEU:HD12	2:C:230:HIS:HB3	1.80	0.61
2:D:255:THR:HG22	2:D:255:THR:O	1.99	0.61
1:A:400:THR:HG21	1:A:433:ILE:CG2	2.29	0.61
2:F:379:SER:HA	2:F:413:THR:HG22	1.81	0.61
2:F:38:ILE:HG22	2:F:39:GLY:N	2.14	0.61
2:F:131:ASN:OD1	2:F:174:ILE:HD12	2.00	0.61
2:C:54:LEU:HD13	2:C:90:PHE:CZ	2.36	0.61
1:A:203:ASN:HB3	1:A:225:LEU:HD23	1.80	0.61
2:F:416:SER:HB3	5:F:557:HOH:O	2.00	0.61
2:E:76:PHE:CZ	2:E:126:LEU:HD21	2.33	0.61
2:E:249:LEU:HD12	2:E:394:GLN:OE1	2.01	0.61
1:A:140:ARG:HH11	1:A:140:ARG:CA	2.13	0.61
2:E:435:ASP:HA	2:E:459:ARG:HD2	1.83	0.61
2:D:148:THR:HG21	2:D:193:ARG:HD2	1.81	0.61
1:A:182:THR:HG21	1:A:192:ALA:HB1	1.83	0.61
1:A:79:THR:HG23	1:A:81:GLN:HG2	1.82	0.61
2:B:293:GLY:O	2:B:296:LEU:HB3	2.00	0.61
2:C:493:SER:HB3	2:D:488:ARG:HG2	1.83	0.61
2:D:273:MET:O	2:D:463:HIS:HA	2.01	0.61
2:D:263:VAL:CG1	2:D:374:ARG:HH21	2.13	0.61
2:D:313:ILE:HD12	2:D:372:PRO:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:LEU:HD22	1:A:387:VAL:HG11	1.83	0.61
2:F:435:ASP:HA	2:F:459:ARG:HD2	1.81	0.61
2:C:311:ARG:HD2	2:C:371:LYS:CE	2.30	0.61
2:D:380:LEU:HD13	2:D:412:PHE:HB3	1.83	0.61
2:C:471:MET:CG	2:C:478:ASP:HB3	2.30	0.61
2:E:45:SER:HB3	2:E:182:THR:HB	1.81	0.60
2:C:79:THR:HG22	2:C:82:ASP:OD2	2.00	0.60
2:C:495:THR:HA	2:D:487:GLU:OE2	2.01	0.60
2:C:461:SER:OG	2:C:462:TRP:N	2.34	0.60
2:E:118:VAL:HG12	2:E:118:VAL:O	2.01	0.60
2:E:305:ALA:HB2	2:E:374:ARG:HD2	1.82	0.60
2:E:377:ILE:HD12	2:E:412:PHE:CE2	2.35	0.60
2:C:147:VAL:HG11	2:C:180:MET:HE2	1.82	0.60
2:F:117:VAL:HA	2:F:154:TYR:OH	2.01	0.60
1:A:78:GLU:HB3	1:A:83:ILE:CD1	2.31	0.60
4:B:901:ATP:H3'	2:C:458:MET:O	2.02	0.60
2:D:247:PHE:CZ	2:D:361:GLN:HB2	2.36	0.60
2:C:36:LEU:HD12	2:C:59:PHE:CE1	2.35	0.60
1:A:433:ILE:HG22	1:A:433:ILE:O	2.00	0.60
2:B:150:VAL:O	2:B:153:GLN:HG3	2.01	0.60
1:A:508:ILE:N	1:A:508:ILE:HD13	2.16	0.60
2:B:184:ARG:C	2:B:185:ILE:HD13	2.21	0.60
2:D:191:ILE:HB	2:D:198:GLU:HG3	1.83	0.60
2:C:317:TYR:HE1	2:C:377:ILE:HG23	1.66	0.60
2:D:303:GLU:OE2	2:D:333:MET:HB3	2.02	0.60
2:E:319:GLU:O	2:F:254:LEU:HD21	2.02	0.60
1:A:360:LEU:O	1:A:360:LEU:HD22	2.01	0.60
2:B:96:LYS:O	2:B:100:GLU:HG3	2.01	0.60
2:E:123:LEU:HD23	2:E:127:ILE:CG1	2.31	0.60
2:D:396:VAL:HG11	2:D:430:ILE:HG23	1.82	0.60
2:D:154:TYR:CD1	2:D:154:TYR:O	2.55	0.60
2:B:430:ILE:O	2:B:431:SEP:C	2.48	0.60
2:E:418:GLN:HB2	2:F:423:HIS:O	2.02	0.60
2:D:295:THR:HG23	2:D:378:ASP:OD2	2.02	0.60
2:F:514:GLU:CB	2:F:519:SER:HB3	2.31	0.60
2:E:140:ARG:CA	2:E:140:ARG:HH11	2.13	0.60
2:E:318:GLU:OE2	2:F:432:ALA:HB1	2.02	0.60
2:F:283:ILE:CG1	2:F:400:THR:HG23	2.29	0.60
2:F:356:LEU:HD11	2:F:387:VAL:HG21	1.82	0.60
2:F:471:MET:SD	2:F:478:ASP:HB3	2.41	0.60
2:C:451:ARG:HH11	2:C:451:ARG:HG2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:374:ARG:HG3	5:E:544:HOH:O	2.02	0.60
2:E:123:LEU:HD13	2:E:166:ARG:HD2	1.83	0.60
2:E:182:THR:HG22	2:E:183:GLU:N	2.17	0.60
2:E:345:LYS:HE2	2:E:366:GLU:OE1	2.02	0.60
1:A:498:THR:HB	1:A:501:GLU:HG3	1.84	0.60
1:A:317:TYR:HE1	1:A:377:ILE:HG23	1.66	0.60
2:E:445:ILE:HG22	2:E:446:ARG:HD2	1.83	0.60
1:A:14:GLU:CG	1:A:15:HIS:N	2.65	0.59
2:D:431:SEP:C	2:D:433:ILE:N	2.61	0.59
2:C:379:SER:H	2:C:413:THR:HB	1.66	0.59
2:C:392:PHE:O	2:C:395:PHE:HB3	2.02	0.59
1:A:212:GLU:O	1:A:212:GLU:HG2	2.02	0.59
2:B:24:MET:CB	2:B:62:ASN:HD22	2.14	0.59
2:E:151:PHE:C	2:E:153:GLN:H	2.05	0.59
2:D:469:GLU:HG2	2:D:480:LYS:HE3	1.84	0.59
1:A:263:VAL:CG1	1:A:374:ARG:HH21	2.12	0.59
2:D:357:GLU:HG3	2:D:358:ASP:N	2.18	0.59
2:D:325:LEU:CD2	2:D:335:PHE:HB2	2.32	0.59
1:A:147:VAL:O	1:A:150:VAL:HG12	2.03	0.59
2:F:20:LYS:NZ	2:F:32:SER:O	2.34	0.59
2:D:45:SER:HB3	2:D:182:THR:HB	1.83	0.59
2:E:296:LEU:HD13	2:E:331:TRP:CD2	2.36	0.59
2:D:31:ILE:HA	2:D:231:MET:SD	2.42	0.59
2:E:400:THR:HG21	2:E:433:ILE:CG2	2.33	0.59
2:B:419:PHE:HD2	2:C:425:ILE:HD12	1.66	0.59
1:A:377:ILE:HD12	1:A:412:PHE:HE2	1.67	0.59
2:D:106:LEU:HD12	2:D:107:ASP:N	2.17	0.59
1:A:79:THR:HG21	1:A:81:GLN:HG2	1.81	0.59
2:C:43:LEU:HD11	2:C:182:THR:OG1	2.03	0.59
2:D:182:THR:HG21	2:D:192:ALA:HB1	1.83	0.59
1:A:438:ILE:CD1	1:A:455:VAL:HG22	2.32	0.59
2:F:404:LYS:HA	5:F:525:HOH:O	2.02	0.59
2:B:151:PHE:C	2:B:153:GLN:H	2.06	0.59
2:C:85:LYS:HZ1	2:D:14:GLU:HB3	1.67	0.59
2:C:182:THR:HG22	2:C:183:GLU:N	2.18	0.59
2:F:471:MET:CG	2:F:478:ASP:HB3	2.32	0.59
2:B:441:GLN:HE22	2:B:490:ILE:HA	1.66	0.59
1:A:448:GLU:HG2	2:B:466:ALA:HA	1.85	0.59
2:E:377:ILE:HD11	2:E:399:VAL:HG11	1.84	0.59
2:E:483:PHE:HB2	2:E:489:ILE:HD11	1.84	0.59
2:E:302:VAL:HG21	2:E:314:LEU:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:425:ILE:HD11	2:F:456:PHE:CE2	2.37	0.59
2:C:123:LEU:HD13	2:C:166:ARG:HD2	1.84	0.59
2:C:140:ARG:CB	2:C:140:ARG:HH11	2.15	0.59
2:F:284:ILE:HB	2:F:411:LEU:HD12	1.85	0.58
2:D:79:THR:HG22	2:D:82:ASP:H	1.68	0.58
2:D:203:ASN:HB3	2:D:225:LEU:CD2	2.33	0.58
2:B:284:ILE:HB	2:B:411:LEU:HD12	1.85	0.58
2:C:94:LEU:O	2:C:98:VAL:HG23	2.03	0.58
2:B:25:ILE:HG23	2:B:58:GLN:NE2	2.18	0.58
2:D:154:TYR:HD1	2:D:154:TYR:O	1.86	0.58
1:A:316:ALA:CB	1:A:324:LEU:HD11	2.33	0.58
2:F:358:ASP:O	2:F:362:ILE:HG12	2.03	0.58
2:D:471:MET:HB3	2:D:480:LYS:NZ	2.18	0.58
2:F:14:GLU:HG2	5:F:533:HOH:O	2.03	0.58
2:F:217:ARG:HH21	2:F:236:PRO:HB3	1.68	0.58
1:A:76:PHE:O	1:A:109:SER:HA	2.03	0.58
1:A:304:ASN:HB3	1:A:374:ARG:HH12	1.68	0.58
1:A:182:THR:HG22	1:A:183:GLU:N	2.18	0.58
2:F:317:TYR:CE2	2:F:383:LEU:HD21	2.37	0.58
2:D:106:LEU:CD1	2:D:129:ARG:NH2	2.66	0.58
1:A:148:THR:HG21	1:A:183:GLU:HG3	1.85	0.58
1:A:79:THR:HG22	1:A:82:ASP:H	1.68	0.58
1:A:140:ARG:HH11	1:A:140:ARG:CB	2.17	0.58
2:B:170:ARG:O	2:B:174:ILE:HG12	2.02	0.58
2:F:317:TYR:CD2	2:F:383:LEU:HD21	2.39	0.58
1:A:418:GLN:HB2	2:B:423:HIS:O	2.04	0.58
2:F:455:VAL:HG11	2:F:463:HIS:HB2	1.85	0.58
2:B:205:VAL:HG22	2:B:222:ILE:HG12	1.85	0.58
2:B:31:ILE:HG22	2:B:222:ILE:HD12	1.84	0.58
2:F:509:VAL:HG12	2:F:510:ARG:N	2.19	0.58
2:C:354:ALA:HB1	2:C:358:ASP:HB2	1.86	0.58
2:C:89:SER:HB2	2:D:227:GLY:O	2.03	0.58
2:E:211:LEU:O	2:E:212:GLU:HB3	2.01	0.58
2:B:45:SER:CB	2:B:182:THR:HB	2.32	0.58
1:A:455:VAL:HG11	1:A:463:HIS:HB2	1.86	0.58
1:A:484:ARG:NH1	1:A:484:ARG:HB3	2.19	0.58
2:F:21:MET:SD	2:F:141:ARG:NE	2.77	0.58
2:D:497:ILE:O	2:D:497:ILE:HD12	2.03	0.58
2:D:262:ARG:HD2	2:D:276:GLY:O	2.03	0.58
2:F:283:ILE:HG23	2:F:412:PHE:CE1	2.37	0.58
2:C:359:HIS:O	2:C:363:ILE:HG13	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:129:ARG:HB3	5:B:525:HOH:O	2.02	0.58
2:E:448:GLU:HG2	2:F:466:ALA:HA	1.84	0.58
1:A:375:ILE:O	1:A:410:GLY:HA2	2.02	0.58
2:D:267:VAL:CG2	2:D:300:ARG:HG2	2.33	0.58
2:B:147:VAL:HG11	2:B:180:MET:CE	2.32	0.58
2:D:496:ARG:HG2	2:E:487:GLU:OE1	2.04	0.58
2:D:451:ARG:NH1	2:D:472:ILE:HD12	2.19	0.58
2:E:377:ILE:CD1	2:E:399:VAL:HG11	2.33	0.57
2:D:184:ARG:HG2	2:D:191:ILE:O	2.03	0.57
2:E:445:ILE:O	2:E:446:ARG:HB2	2.04	0.57
2:E:393:ARG:NH2	5:E:521:HOH:O	2.36	0.57
2:D:431:SEP:O	2:D:432:ALA:CB	2.51	0.57
2:D:106:LEU:HD13	2:D:129:ARG:NH2	2.19	0.57
2:C:263:VAL:HG12	2:C:374:ARG:NH2	2.18	0.57
2:B:284:ILE:HB	2:B:411:LEU:CD1	2.34	0.57
2:E:501:GLU:O	2:E:502:LYS:HG3	2.05	0.57
2:F:508:ILE:HD12	2:F:508:ILE:H	1.70	0.57
2:B:184:ARG:HG2	2:B:191:ILE:O	2.04	0.57
2:F:118:VAL:O	2:F:118:VAL:HG13	2.04	0.57
2:B:358:ASP:O	2:B:362:ILE:HG12	2.03	0.57
2:D:18:ILE:CD1	2:D:18:ILE:H	2.15	0.57
2:E:320:SER:HA	2:F:254:LEU:HG	1.86	0.57
2:C:147:VAL:O	2:C:150:VAL:HG12	2.05	0.57
2:B:31:ILE:HG23	2:B:231:MET:HB2	1.85	0.57
2:F:262:ARG:HA	2:F:278:PHE:O	2.04	0.57
2:D:208:ARG:NH2	2:D:221:GLU:OE2	2.37	0.57
2:C:318:GLU:OE2	2:D:432:ALA:HB1	2.03	0.57
2:D:150:VAL:CG1	2:D:151:PHE:CD2	2.88	0.57
2:E:485:ASN:HD22	2:E:496:ARG:HD3	1.68	0.57
2:C:238:THR:HG22	2:C:239:ILE:H	1.69	0.57
2:C:146:SER:HA	2:C:181:THR:O	2.04	0.57
2:D:148:THR:HA	2:D:151:PHE:CE1	2.40	0.57
2:F:38:ILE:N	2:F:38:ILE:HD12	2.19	0.57
2:D:298:VAL:HG13	2:D:376:ALA:HB1	1.87	0.57
2:F:111:ASP:OD1	2:F:112:PRO:HD2	2.04	0.57
2:F:377:ILE:HD12	2:F:412:PHE:CE2	2.39	0.57
2:D:311:ARG:HD2	2:D:371:LYS:HE3	1.85	0.57
2:B:123:LEU:O	2:B:123:LEU:HD13	2.05	0.57
2:C:225:LEU:HB2	2:C:230:HIS:HD2	1.70	0.57
2:F:440:LEU:HD22	2:F:470:PHE:CE2	2.40	0.57
2:C:347:VAL:O	2:C:348:CYS:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:49:GLY:HA2	4:E:903:ATP:O2B	2.04	0.57
2:F:446:ARG:H	2:F:496:ARG:NH2	2.01	0.57
2:B:23:THR:O	2:B:24:MET:HB2	2.05	0.57
2:C:334:ASP:O	2:C:338:MET:HG2	2.04	0.57
1:A:311:ARG:HD2	1:A:371:LYS:CE	2.35	0.57
2:C:377:ILE:HD11	2:C:399:VAL:HG11	1.85	0.57
2:E:148:THR:HG21	2:E:183:GLU:CG	2.34	0.57
1:A:311:ARG:HA	1:A:343:LEU:O	2.05	0.57
2:F:306:CYS:SG	2:F:344:LEU:HB2	2.45	0.57
1:A:273:MET:O	1:A:463:HIS:HA	2.03	0.57
2:F:215:ARG:NE	2:F:215:ARG:HA	2.19	0.57
1:A:18:ILE:CD1	1:A:18:ILE:N	2.68	0.57
2:D:81:GLN:NE2	2:D:81:GLN:H	2.03	0.57
2:E:504:GLU:HG2	2:E:505:LEU:N	2.19	0.57
2:E:323:GLN:NE2	2:F:459:ARG:HD3	2.20	0.57
2:F:116:GLU:O	2:F:117:VAL:HB	2.05	0.57
2:F:382:ALA:O	2:F:385:ARG:HG3	2.05	0.57
1:A:147:VAL:HG11	1:A:180:MET:CE	2.35	0.56
1:A:469:GLU:HB2	1:A:483:PHE:CZ	2.40	0.56
2:C:323:GLN:HE21	2:C:327:ASN:HD21	1.51	0.56
2:D:22:ARG:NH2	2:D:24:MET:SD	2.78	0.56
2:B:356:LEU:HD22	2:B:387:VAL:HG11	1.87	0.56
1:A:264:SER:HB3	1:A:304:ASN:ND2	2.21	0.56
2:D:185:ILE:HD11	2:D:193:ARG:NH1	2.21	0.56
2:D:377:ILE:CD1	2:D:399:VAL:HG11	2.35	0.56
1:A:24:MET:HB3	1:A:62:ASN:HD22	1.67	0.56
2:B:262:ARG:NH2	2:B:461:SER:HB2	2.20	0.56
1:A:495:THR:HG22	1:A:497:ILE:HG23	1.86	0.56
2:C:148:THR:CG2	2:C:193:ARG:HD2	2.36	0.56
2:C:31:ILE:HG23	2:C:231:MET:HB2	1.88	0.56
2:F:169:ALA:O	2:F:173:GLN:HG3	2.05	0.56
2:F:102:LYS:HE3	5:F:537:HOH:O	2.05	0.56
2:D:169:ALA:O	2:D:173:GLN:HG3	2.05	0.56
1:A:287:THR:HG21	1:A:425:ILE:O	2.05	0.56
2:B:462:TRP:O	2:B:463:HIS:O	2.22	0.56
2:E:289:ALA:HB2	2:E:419:PHE:HA	1.86	0.56
2:B:316:ALA:O	2:B:348:CYS:HA	2.05	0.56
1:A:70:PRO:HA	1:A:102:LYS:O	2.06	0.56
2:F:220:LEU:C	2:F:220:LEU:HD23	2.26	0.56
2:F:303:GLU:OE2	2:F:333:MET:HB3	2.05	0.56
2:E:41:SER:HB2	2:E:178:THR:HB	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:148:THR:HA	2:D:151:PHE:HE1	1.70	0.56
2:B:164:LEU:O	2:B:168:VAL:HG23	2.06	0.56
2:C:433:ILE:HD12	2:C:433:ILE:N	2.21	0.56
2:F:194:TYR:O	2:F:196:VAL:HG23	2.06	0.56
2:B:264:SER:HB3	2:B:304:ASN:HD21	1.70	0.56
1:A:184:ARG:C	1:A:185:ILE:HD13	2.26	0.56
2:E:334:ASP:O	2:E:338:MET:HG2	2.06	0.56
2:B:295:THR:HG23	2:B:378:ASP:OD2	2.06	0.56
2:B:25:ILE:HG23	2:B:58:GLN:HE22	1.69	0.56
2:C:418:GLN:HB2	2:D:423:HIS:O	2.05	0.56
2:E:130:ILE:O	2:E:134:ILE:HG13	2.06	0.56
2:E:264:SER:O	2:E:374:ARG:NH2	2.39	0.56
2:C:419:PHE:CD2	2:D:425:ILE:HD12	2.41	0.56
2:B:150:VAL:HG13	2:B:151:PHE:N	2.20	0.56
2:C:17:ALA:C	2:C:18:ILE:HD12	2.26	0.56
2:F:357:GLU:CG	2:F:358:ASP:H	2.18	0.56
2:E:338:MET:HB3	2:E:344:LEU:HB3	1.88	0.56
2:D:80:PRO:HD2	2:D:81:GLN:NE2	2.21	0.56
1:A:166:ARG:NE	5:A:533:HOH:O	2.38	0.56
2:C:446:ARG:HA	2:C:496:ARG:NH2	2.21	0.56
2:B:52:LYS:N	4:B:903:ATP:O1B	2.36	0.56
2:E:260:ASN:HB2	5:E:546:HOH:O	2.06	0.56
2:E:425:ILE:CG2	2:E:426:ALA:N	2.66	0.55
2:F:191:ILE:CG2	2:F:198:GLU:HG3	2.36	0.55
1:A:306:CYS:SG	1:A:344:LEU:HB2	2.46	0.55
2:D:76:PHE:HZ	2:D:126:LEU:HD21	1.70	0.55
2:D:436:THR:HG23	2:D:458:MET:HG2	1.89	0.55
2:F:393:ARG:NH2	2:F:429:HIS:HB2	2.18	0.55
1:A:21:MET:HE3	1:A:59:PHE:CE1	2.41	0.55
2:B:14:GLU:OE2	2:B:16:GLN:HB2	2.06	0.55
1:A:265:SER:O	1:A:301:PHE:HA	2.06	0.55
1:A:80:PRO:HD2	1:A:81:GLN:NE2	2.22	0.55
2:E:392:PHE:O	2:E:396:VAL:HG23	2.06	0.55
2:E:313:ILE:HG13	2:E:372:PRO:CG	2.37	0.55
2:E:153:GLN:C	2:F:158:SER:HB2	2.26	0.55
2:B:469:GLU:HB2	2:B:483:PHE:CZ	2.41	0.55
2:B:211:LEU:HG	2:B:211:LEU:O	2.05	0.55
2:D:313:ILE:CG1	2:D:372:PRO:HG3	2.36	0.55
2:E:505:LEU:HD12	2:E:505:LEU:O	2.06	0.55
1:A:347:VAL:O	1:A:348:CYS:HB2	2.07	0.55
2:C:123:LEU:HD22	2:C:127:ILE:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:451:ARG:HB3	2:F:470:PHE:CE2	2.40	0.55
2:E:214:GLU:HB3	2:F:234:GLU:HB2	1.88	0.55
2:E:121:PHE:CD1	2:E:121:PHE:N	2.73	0.55
2:B:117:VAL:O	2:B:117:VAL:HG12	2.07	0.55
2:F:161:ARG:CB	2:F:196:VAL:HG11	2.35	0.55
2:C:238:THR:HG22	2:C:239:ILE:N	2.21	0.55
2:C:311:ARG:HD2	2:C:371:LYS:HE3	1.88	0.55
2:F:49:GLY:CA	4:F:903:ATP:O2B	2.54	0.55
2:E:140:ARG:HH11	2:E:140:ARG:CB	2.20	0.55
1:A:351:PRO:HG2	1:A:382:ALA:O	2.07	0.55
1:A:146:SER:HA	1:A:181:THR:O	2.07	0.55
2:D:445:ILE:O	2:D:446:ARG:HB2	2.07	0.55
2:F:299:SER:C	2:F:333:MET:HE1	2.28	0.55
1:A:432:ALA:HB1	2:F:318:GLU:OE2	2.07	0.55
2:C:469:GLU:HB3	2:C:483:PHE:CE1	2.41	0.55
2:F:182:THR:HG21	2:F:192:ALA:CB	2.37	0.55
2:E:441:GLN:HE22	2:E:490:ILE:HA	1.72	0.55
2:E:211:LEU:HD13	2:E:216:ARG:NE	2.22	0.55
2:F:371:LYS:HD2	2:F:371:LYS:O	2.06	0.55
2:E:193:ARG:NH2	2:F:195:GLY:O	2.29	0.54
1:A:298:VAL:HA	1:A:411:LEU:HD23	1.89	0.54
4:A:901:ATP:O3'	2:B:457:LYS:HB2	2.07	0.54
2:C:215:ARG:HA	2:C:215:ARG:NE	2.21	0.54
2:D:342:ASN:HB2	5:D:538:HOH:O	2.06	0.54
2:D:363:ILE:O	2:D:367:ILE:HG13	2.07	0.54
2:B:452:ALA:HA	2:B:468:ARG:O	2.07	0.54
2:F:21:MET:HE1	2:F:59:PHE:HZ	1.72	0.54
2:E:364:LYS:O	2:E:368:ASN:ND2	2.40	0.54
1:A:451:ARG:N	1:A:451:ARG:HD2	2.23	0.54
2:F:287:THR:HG23	2:F:414:ASN:HD22	1.73	0.54
2:C:93:ASP:OD2	2:C:96:LYS:HB2	2.06	0.54
2:D:439:LEU:HD12	2:D:440:LEU:N	2.23	0.54
1:A:191:ILE:HG13	1:A:206:ILE:HD11	1.89	0.54
2:F:316:ALA:O	2:F:348:CYS:HA	2.08	0.54
2:F:144:ILE:HG22	2:F:147:VAL:HG12	1.89	0.54
2:F:287:THR:HG21	2:F:414:ASN:HD22	1.73	0.54
2:F:287:THR:HG23	2:F:414:ASN:HB3	1.89	0.54
2:F:381:SER:HB3	2:F:414:ASN:OD1	2.06	0.54
2:E:191:ILE:CG2	2:E:198:GLU:HG3	2.38	0.54
1:A:273:MET:O	1:A:464:ASP:N	2.34	0.54
2:C:202:ASP:HA	2:C:226:ARG:HD2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:89:SER:HB2	2:E:227:GLY:O	2.07	0.54
1:A:295:THR:HG23	1:A:378:ASP:OD2	2.07	0.54
1:A:356:LEU:HD23	1:A:395:PHE:HB2	1.90	0.54
1:A:65:ILE:O	1:A:65:ILE:CG2	2.56	0.54
2:B:274:CYS:SG	2:B:278:PHE:HE2	2.30	0.54
2:E:14:GLU:HG3	2:E:16:GLN:N	2.15	0.54
2:F:93:ASP:OD2	2:F:96:LYS:HB2	2.08	0.54
2:E:346:ILE:HG22	2:E:348:CYS:SG	2.48	0.54
2:B:340:ARG:C	2:B:342:ASN:H	2.11	0.54
1:A:443:VAL:CG1	1:A:494:PRO:HG2	2.38	0.54
2:E:45:SER:CB	2:E:182:THR:HB	2.37	0.54
2:C:264:SER:O	2:C:374:ARG:NH2	2.39	0.54
1:A:452:ALA:HA	1:A:468:ARG:O	2.08	0.54
2:D:484:ARG:HH11	2:D:484:ARG:HB3	1.73	0.54
2:C:292:THR:HB	2:C:440:LEU:HB3	1.90	0.54
2:B:116:GLU:HG2	2:B:117:VAL:N	2.13	0.53
2:B:296:LEU:HD21	2:B:477:PRO:HD3	1.90	0.53
2:D:469:GLU:HB2	2:D:483:PHE:CZ	2.43	0.53
1:A:461:SER:OG	1:A:462:TRP:N	2.41	0.53
1:A:84:ILE:HG21	1:A:95:ALA:HB2	1.89	0.53
2:B:72:VAL:O	2:B:142:VAL:HG13	2.08	0.53
2:E:499:VAL:HG12	2:E:499:VAL:O	2.08	0.53
2:D:21:MET:O	2:D:35:GLY:HA3	2.07	0.53
2:B:380:LEU:HG	2:B:412:PHE:HB3	1.89	0.53
2:E:183:GLU:OE2	2:F:161:ARG:NH1	2.39	0.53
2:E:371:LYS:CD	2:E:371:LYS:O	2.57	0.53
2:F:509:VAL:CG1	2:F:510:ARG:H	2.17	0.53
2:D:469:GLU:CG	2:D:480:LYS:HE3	2.38	0.53
1:A:184:ARG:O	1:A:185:ILE:HD13	2.09	0.53
2:D:49:GLY:O	2:D:218:ARG:NH2	2.41	0.53
2:E:406:GLU:O	2:E:407:GLU:HB2	2.09	0.53
2:C:419:PHE:O	2:C:420:MET:HB2	2.08	0.53
1:A:399:VAL:HG12	1:A:399:VAL:O	2.09	0.53
2:F:387:VAL:HG13	2:F:391:ALA:HB3	1.90	0.53
2:E:451:ARG:HB2	2:E:470:PHE:O	2.08	0.53
2:B:89:SER:HB2	2:C:227:GLY:O	2.08	0.53
2:C:123:LEU:HD21	2:C:167:LEU:HB2	1.90	0.53
2:D:79:THR:HG21	2:D:81:GLN:HG2	1.90	0.53
1:A:495:THR:HA	2:B:487:GLU:OE2	2.07	0.53
2:E:451:ARG:HG2	2:E:451:ARG:HH11	1.74	0.53
1:A:203:ASN:HB3	1:A:225:LEU:CD2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:ILE:CD1	2:B:97:LEU:HD13	2.38	0.53
2:C:289:ALA:HB2	2:C:419:PHE:HA	1.90	0.53
2:B:182:THR:HG22	2:B:183:GLU:H	1.73	0.53
2:D:377:ILE:HD12	2:D:412:PHE:CE2	2.43	0.53
1:A:52:LYS:HD3	1:A:182:THR:O	2.08	0.53
2:F:489:ILE:HA	2:F:494:PRO:HG3	1.91	0.53
2:F:148:THR:HG21	2:F:193:ARG:HD2	1.89	0.53
2:E:140:ARG:HA	2:E:140:ARG:HH11	1.73	0.53
2:C:148:THR:HG21	2:C:193:ARG:HD2	1.91	0.53
2:F:38:ILE:CG2	2:F:39:GLY:N	2.72	0.53
2:D:75:THR:HG23	2:D:75:THR:O	2.08	0.53
2:B:311:ARG:HD2	2:B:371:LYS:CE	2.38	0.53
2:F:147:VAL:HG11	2:F:180:MET:HE3	1.90	0.53
2:E:453:ILE:HB	2:E:470:PHE:CD2	2.43	0.53
1:A:338:MET:HB3	1:A:344:LEU:HB3	1.90	0.53
1:A:140:ARG:HH11	1:A:140:ARG:HB3	1.74	0.53
2:B:56:SER:O	2:B:59:PHE:HB3	2.09	0.53
2:F:151:PHE:C	2:F:153:GLN:H	2.10	0.53
2:B:441:GLN:HE22	2:B:490:ILE:HD13	1.73	0.53
2:E:303:GLU:HB2	2:E:333:MET:HE1	1.89	0.53
1:A:440:LEU:HD23	1:A:453:ILE:HG13	1.91	0.53
2:B:215:ARG:NH2	2:C:234:GLU:O	2.42	0.53
2:D:214:GLU:HB3	2:E:234:GLU:HB2	1.90	0.53
2:B:300:ARG:N	2:B:333:MET:HE1	2.23	0.53
2:B:483:PHE:O	2:B:485:ASN:N	2.42	0.53
2:C:113:GLU:O	2:C:114:GLY:C	2.47	0.53
1:A:451:ARG:NH1	1:A:451:ARG:HG2	2.20	0.53
2:C:212:GLU:HG2	2:C:212:GLU:O	2.08	0.53
2:D:356:LEU:CD2	2:D:387:VAL:HG11	2.38	0.53
2:D:344:LEU:HD22	2:D:345:LYS:H	1.74	0.53
2:E:316:ALA:O	2:E:348:CYS:HA	2.09	0.53
2:B:93:ASP:OD1	2:B:95:ALA:HB3	2.09	0.53
2:C:211:LEU:HD13	2:C:216:ARG:HD3	1.90	0.53
2:B:371:LYS:O	2:B:371:LYS:CD	2.57	0.53
2:F:117:VAL:O	2:F:118:VAL:HB	2.08	0.53
2:D:170:ARG:O	2:D:174:ILE:HG12	2.09	0.53
2:F:18:ILE:HG13	2:F:227:GLY:HA3	1.91	0.53
1:A:60:LEU:HD22	1:A:71:GLY:HA3	1.92	0.53
1:A:299:SER:C	1:A:333:MET:HE1	2.30	0.52
1:A:469:GLU:HG3	1:A:470:PHE:N	2.24	0.52
2:E:217:ARG:HH21	2:E:236:PRO:HB3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:256:GLN:HG3	2:D:404:LYS:HD3	1.91	0.52
2:B:87:ALA:HB1	2:B:92:TRP:CD1	2.44	0.52
2:D:161:ARG:HB2	2:D:196:VAL:HG11	1.90	0.52
2:D:153:GLN:O	2:D:154:TYR:HB3	2.10	0.52
2:F:79:THR:HG21	2:F:81:GLN:HG2	1.88	0.52
2:D:311:ARG:O	2:D:373:ALA:N	2.34	0.52
2:E:449:MET:HE3	2:F:490:ILE:HD11	1.92	0.52
2:B:483:PHE:HB3	2:B:486:PHE:HD1	1.75	0.52
2:B:496:ARG:HG2	2:B:498:THR:HG23	1.90	0.52
2:F:471:MET:HB3	2:F:480:LYS:NZ	2.24	0.52
2:F:98:VAL:HA	2:F:103:LEU:O	2.08	0.52
2:D:313:ILE:CD1	2:D:372:PRO:CG	2.88	0.52
2:D:471:MET:HE2	2:D:478:ASP:CB	2.39	0.52
2:B:497:ILE:HG13	2:B:498:THR:N	2.24	0.52
2:D:153:GLN:O	2:D:154:TYR:CB	2.56	0.52
1:A:79:THR:O	1:A:83:ILE:HD12	2.10	0.52
2:F:191:ILE:HB	2:F:198:GLU:HG3	1.89	0.52
1:A:269:ARG:HB3	1:A:479:ILE:HD12	1.91	0.52
2:D:313:ILE:CD1	2:D:372:PRO:HG3	2.39	0.52
2:C:284:ILE:HB	2:C:411:LEU:HD12	1.90	0.52
2:B:150:VAL:CG1	2:B:151:PHE:N	2.73	0.52
2:D:191:ILE:CB	2:D:198:GLU:HG3	2.39	0.52
2:B:325:LEU:CD2	2:B:335:PHE:HB2	2.37	0.52
2:F:122:ASP:OD2	2:F:123:LEU:N	2.42	0.52
1:A:359:HIS:O	1:A:363:ILE:HG13	2.09	0.52
2:E:81:GLN:CD	2:E:81:GLN:N	2.62	0.52
2:F:20:LYS:C	2:F:38:ILE:CD1	2.77	0.52
2:B:145:ASP:HA	2:B:181:THR:HB	1.90	0.52
1:A:14:GLU:HG3	1:A:16:GLN:OE1	2.10	0.52
2:E:159:VAL:O	2:E:163:GLU:HG2	2.10	0.52
2:F:501:GLU:CG	2:F:502:LYS:N	2.72	0.52
2:F:119:GLY:HA2	2:F:122:ASP:OD1	2.09	0.52
2:C:114:GLY:O	2:C:115:GLN:HB3	2.08	0.52
1:A:488:ARG:O	1:A:494:PRO:HA	2.09	0.52
2:D:127:ILE:HD11	2:D:167:LEU:HA	1.90	0.52
2:B:202:ASP:HA	2:B:226:ARG:HD2	1.90	0.52
1:A:187:GLU:HG2	1:A:210:VAL:HA	1.91	0.52
2:E:123:LEU:HD23	2:E:127:ILE:HG12	1.91	0.52
1:A:348:CYS:HB3	2:B:254:LEU:HD23	1.91	0.52
2:E:430:ILE:O	2:E:433:ILE:HD13	2.09	0.52
2:D:81:GLN:CD	2:D:81:GLN:H	2.14	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:88:ARG:NE	2:D:15:HIS:HA	2.25	0.52
2:B:483:PHE:HB3	2:B:486:PHE:CD1	2.45	0.52
2:B:216:ARG:NE	2:C:221:GLU:OE1	2.36	0.52
2:B:126:LEU:O	2:B:130:ILE:HG13	2.08	0.52
2:F:32:SER:HB3	2:F:222:ILE:CD1	2.39	0.52
2:F:21:MET:HE3	2:F:59:PHE:CE1	2.43	0.52
2:C:61:TYR:CE1	2:C:92:TRP:HB2	2.45	0.52
2:C:360:LEU:HD22	2:C:364:LYS:HE3	1.92	0.52
1:A:129:ARG:O	1:A:132:TYR:HB3	2.10	0.52
2:E:497:ILE:HG22	2:E:498:THR:N	2.22	0.52
2:E:294:LYS:N	4:E:901:ATP:O1B	2.41	0.52
2:E:191:ILE:HB	2:E:198:GLU:HG3	1.92	0.52
2:C:116:GLU:O	2:C:117:VAL:HB	2.10	0.52
1:A:487:GLU:OE1	2:F:495:THR:HA	2.10	0.52
2:F:263:VAL:HG12	2:F:374:ARG:NH2	2.22	0.51
2:D:151:PHE:C	2:D:153:GLN:H	2.13	0.51
2:D:191:ILE:CG2	2:D:198:GLU:HG3	2.41	0.51
2:D:371:LYS:N	2:D:372:PRO:HD3	2.25	0.51
2:E:150:VAL:HG13	2:E:151:PHE:N	2.25	0.51
1:A:208:ARG:NH2	1:A:221:GLU:OE2	2.43	0.51
1:A:148:THR:HG21	1:A:183:GLU:CG	2.40	0.51
2:B:191:ILE:N	2:B:191:ILE:HD12	2.25	0.51
2:E:486:PHE:HB2	2:E:489:ILE:HD11	1.92	0.51
2:C:298:VAL:O	2:C:301:PHE:HB3	2.10	0.51
2:E:67:PHE:HB2	2:E:69:GLU:HG3	1.92	0.51
2:F:52:LYS:N	4:F:903:ATP:O1B	2.39	0.51
1:A:262:ARG:HH22	1:A:461:SER:HB2	1.74	0.51
1:A:220:LEU:C	1:A:220:LEU:HD23	2.30	0.51
2:D:303:GLU:O	2:D:303:GLU:HG2	2.11	0.51
2:D:486:PHE:HB3	2:D:489:ILE:HD11	1.91	0.51
2:C:462:TRP:O	2:C:463:HIS:O	2.28	0.51
2:B:264:SER:HA	2:B:271:ASP:OD1	2.10	0.51
1:A:111:ASP:C	1:A:113:GLU:H	2.13	0.51
1:A:21:MET:HE3	1:A:59:PHE:HE1	1.75	0.51
2:F:145:ASP:HA	2:F:181:THR:HB	1.93	0.51
2:F:315:PHE:HA	2:F:347:VAL:HB	1.92	0.51
2:E:182:THR:HG21	2:E:192:ALA:CB	2.38	0.51
2:D:332:GLY:O	2:D:333:MET:O	2.29	0.51
2:C:425:ILE:HD11	2:C:456:PHE:CE2	2.46	0.51
2:F:516:GLY:N	2:F:517:PRO:HD2	2.26	0.51
2:D:495:THR:O	2:D:495:THR:HG22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:214:GLU:C	2:C:215:ARG:HE	2.14	0.51
2:F:150:VAL:O	2:F:153:GLN:HG3	2.10	0.51
2:B:25:ILE:HG12	2:B:58:GLN:NE2	2.25	0.51
2:F:311:ARG:HD2	2:F:371:LYS:CE	2.41	0.51
2:B:54:LEU:HD13	2:B:90:PHE:CZ	2.46	0.51
2:E:170:ARG:NH2	5:E:549:HOH:O	2.41	0.51
2:B:195:GLY:HA2	2:B:198:GLU:OE1	2.10	0.51
2:F:344:LEU:HD11	2:F:346:ILE:HG13	1.93	0.51
2:E:186:GLU:HB3	2:E:189:GLY:HA3	1.92	0.51
2:C:443:VAL:HG12	2:C:445:ILE:HG12	1.92	0.51
2:C:452:ALA:HA	2:C:469:GLU:HA	1.92	0.51
2:B:379:SER:OG	2:B:382:ALA:HB2	2.11	0.51
2:B:451:ARG:HG2	2:B:451:ARG:NH1	2.22	0.51
2:E:79:THR:HG23	2:E:81:GLN:HG2	1.92	0.51
2:E:303:GLU:HB2	2:E:333:MET:CE	2.41	0.51
2:C:96:LYS:O	2:C:100:GLU:HG3	2.11	0.51
2:D:320:SER:HA	2:E:254:LEU:HG	1.91	0.51
2:C:290:THR:CG2	2:D:431:SEP:O2P	2.55	0.51
2:B:377:ILE:HD12	2:B:412:PHE:CE2	2.46	0.51
2:D:106:LEU:HD13	2:D:129:ARG:HH21	1.75	0.51
2:F:148:THR:CG2	2:F:193:ARG:HD2	2.41	0.51
2:F:45:SER:HB2	2:F:182:THR:HB	1.93	0.51
2:C:38:ILE:HG22	2:C:39:GLY:N	2.26	0.51
2:E:318:GLU:OE2	2:F:432:ALA:CB	2.59	0.51
2:D:182:THR:HG22	2:D:183:GLU:N	2.25	0.51
2:B:381:SER:HB3	2:B:414:ASN:OD1	2.11	0.51
1:A:293:GLY:HA2	4:A:901:ATP:O1A	2.10	0.51
2:C:178:THR:HG22	2:C:179:VAL:N	2.26	0.51
2:F:293:GLY:HA2	4:F:901:ATP:O1A	2.11	0.51
2:B:104:PHE:HD2	2:B:133:ALA:HB1	1.75	0.51
2:C:123:LEU:O	2:C:124:SER:C	2.49	0.50
2:F:21:MET:HE3	2:F:59:PHE:HE1	1.76	0.50
1:A:186:GLU:HB3	1:A:189:GLY:HA3	1.93	0.50
2:C:42:THR:HA	2:C:203:ASN:HB2	1.93	0.50
2:B:106:LEU:C	2:B:106:LEU:HD12	2.31	0.50
2:C:64:ILE:CD1	2:C:103:LEU:HB2	2.41	0.50
2:C:325:LEU:HD23	2:C:335:PHE:HB2	1.93	0.50
2:E:18:ILE:CG1	2:E:228:THR:HG23	2.41	0.50
2:F:21:MET:HE2	2:F:177:THR:HG21	1.93	0.50
2:B:489:ILE:O	2:B:492:GLY:N	2.44	0.50
2:F:443:VAL:HG12	2:F:445:ILE:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:174:ILE:O	2:F:174:ILE:HG22	2.11	0.50
2:B:281:ASP:O	2:B:282:SER:HB3	2.11	0.50
2:C:184:ARG:C	2:C:185:ILE:HD13	2.32	0.50
2:C:387:VAL:HG12	2:C:388:SER:O	2.12	0.50
2:D:347:VAL:HG12	2:D:348:CYS:N	2.26	0.50
1:A:287:THR:HG23	1:A:414:ASN:ND2	2.25	0.50
1:A:140:ARG:CB	1:A:140:ARG:NH1	2.72	0.50
2:E:504:GLU:OE1	2:E:505:LEU:HD23	2.12	0.50
2:D:461:SER:OG	2:D:462:TRP:N	2.44	0.50
2:F:332:GLY:O	2:F:333:MET:O	2.29	0.50
2:B:248:PRO:HB2	2:B:251:ALA:HB3	1.92	0.50
2:C:170:ARG:O	2:C:174:ILE:HG12	2.11	0.50
1:A:264:SER:HB3	1:A:304:ASN:HD21	1.76	0.50
2:C:469:GLU:CB	2:C:483:PHE:CZ	2.94	0.50
2:F:191:ILE:HG21	2:F:198:GLU:HG3	1.93	0.50
2:E:295:THR:HG21	2:E:319:GLU:OE2	2.11	0.50
2:C:413:THR:CG2	2:C:414:ASN:N	2.74	0.50
1:A:191:ILE:CB	1:A:198:GLU:HG2	2.40	0.50
2:C:262:ARG:NH2	2:C:461:SER:HB2	2.25	0.50
2:C:367:ILE:HG12	2:C:375:ILE:HD11	1.92	0.50
2:D:439:LEU:HD12	2:D:439:LEU:C	2.32	0.50
1:A:266:GLY:HA3	1:A:300:ARG:O	2.12	0.50
2:D:147:VAL:HG23	2:D:151:PHE:CZ	2.46	0.50
2:F:504:GLU:HA	2:F:507:ARG:NE	2.27	0.50
2:E:345:LYS:HB2	2:E:370:PHE:CE2	2.46	0.50
1:A:364:LYS:HG2	1:A:402:TYR:CD2	2.47	0.50
1:A:85:LYS:NZ	2:B:14:GLU:HG3	2.26	0.50
2:F:274:CYS:HG	2:F:278:PHE:HE2	1.60	0.50
1:A:187:GLU:HG3	1:A:208:ARG:HG2	1.92	0.50
2:F:452:ALA:HA	2:F:468:ARG:O	2.12	0.50
2:F:79:THR:HG23	2:F:81:GLN:HE21	1.77	0.50
2:C:160:VAL:O	2:C:164:LEU:HB2	2.12	0.50
2:F:469:GLU:HG2	2:F:480:LYS:HE3	1.92	0.50
2:D:400:THR:HG21	2:D:433:ILE:HG22	1.94	0.50
2:E:332:GLY:O	2:E:333:MET:O	2.30	0.50
2:C:70:PRO:HB2	2:C:139:ALA:HA	1.92	0.50
2:C:137:TYR:O	2:C:138:ARG:HB2	2.11	0.50
2:B:458:MET:HB2	2:B:463:HIS:HD2	1.77	0.50
1:A:371:LYS:N	1:A:372:PRO:HD3	2.27	0.50
2:B:291:GLY:CA	4:B:901:ATP:O2B	2.59	0.50
2:F:371:LYS:HB3	5:F:540:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:VAL:HG22	1:A:300:ARG:HG2	1.93	0.50
2:B:203:ASN:OD1	2:B:225:LEU:HA	2.12	0.50
2:E:123:LEU:CD1	2:E:163:GLU:OE2	2.60	0.49
1:A:364:LYS:HG2	1:A:402:TYR:CE2	2.46	0.49
2:B:273:MET:O	2:B:463:HIS:CA	2.60	0.49
2:B:463:HIS:CE1	2:B:465:LYS:NZ	2.79	0.49
2:E:80:PRO:HD2	2:E:81:GLN:NE2	2.27	0.49
2:C:151:PHE:C	2:C:153:GLN:N	2.66	0.49
2:F:170:ARG:O	2:F:174:ILE:HG12	2.12	0.49
2:E:208:ARG:NH2	2:E:221:GLU:OE2	2.45	0.49
2:C:81:GLN:CD	2:C:81:GLN:N	2.65	0.49
2:C:220:LEU:HD13	2:C:246:ILE:HD11	1.94	0.49
2:D:280:LYS:NZ	2:D:407:GLU:HB3	2.27	0.49
1:A:49:GLY:O	1:A:218:ARG:NH2	2.46	0.49
1:A:316:ALA:HB2	1:A:324:LEU:HD11	1.93	0.49
2:D:269:ARG:HB3	2:D:479:ILE:HD12	1.94	0.49
2:B:371:LYS:O	2:B:371:LYS:HD2	2.12	0.49
2:E:299:SER:HB3	2:E:333:MET:HE2	1.94	0.49
2:F:425:ILE:HG22	2:F:426:ALA:N	2.27	0.49
2:B:360:LEU:HD23	2:B:399:VAL:HG22	1.94	0.49
2:D:65:ILE:HG22	2:D:65:ILE:O	2.13	0.49
1:A:433:ILE:O	1:A:433:ILE:CG2	2.61	0.49
2:F:444:GLU:O	2:F:445:ILE:HD13	2.11	0.49
1:A:295:THR:HG21	1:A:319:GLU:OE2	2.12	0.49
2:D:152:GLN:HG3	2:E:161:ARG:NH1	2.27	0.49
2:E:487:GLU:O	2:E:488:ARG:HB2	2.12	0.49
2:B:294:LYS:N	4:B:901:ATP:O1B	2.46	0.49
2:C:150:VAL:HG13	2:C:151:PHE:N	2.26	0.49
2:F:371:LYS:CD	2:F:371:LYS:O	2.61	0.49
2:B:72:VAL:HG23	2:B:139:ALA:HB2	1.95	0.49
2:F:396:VAL:HG11	2:F:430:ILE:HD12	1.93	0.49
2:E:485:ASN:HD22	2:E:496:ARG:CD	2.26	0.49
2:B:220:LEU:C	2:B:220:LEU:HD23	2.32	0.49
2:B:451:ARG:HD2	2:B:451:ARG:N	2.27	0.49
2:B:486:PHE:CE2	2:B:496:ARG:HB2	2.48	0.49
2:E:140:ARG:HB3	2:E:140:ARG:HH11	1.76	0.49
1:A:225:LEU:O	1:A:226:ARG:C	2.48	0.49
2:B:145:ASP:OD2	2:B:181:THR:HG21	2.12	0.49
2:F:340:ARG:C	2:F:342:ASN:H	2.14	0.49
2:E:311:ARG:HD2	2:E:371:LYS:NZ	2.28	0.49
1:A:161:ARG:HB2	1:A:196:VAL:CG1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:262:ARG:NH1	2:D:275:GLY:O	2.46	0.49
2:F:335:PHE:O	2:F:339:GLU:HG3	2.13	0.49
1:A:351:PRO:CB	1:A:383:LEU:HD23	2.42	0.49
2:F:387:VAL:CG1	2:F:391:ALA:HB3	2.43	0.49
2:F:115:GLN:HG3	2:F:116:GLU:N	2.28	0.49
1:A:46:GLY:HA2	5:A:524:HOH:O	2.11	0.49
2:B:318:GLU:OE2	2:C:432:ALA:HB1	2.12	0.49
2:F:27:GLY:HA3	2:F:246:ILE:HB	1.94	0.49
2:C:389:ASN:HD21	2:C:428:SER:HA	1.78	0.49
2:F:352:GLU:OE2	2:F:385:ARG:HD2	2.12	0.49
2:C:121:PHE:HD1	2:C:121:PHE:H	1.60	0.49
2:B:116:GLU:HG2	2:B:154:TYR:HE2	1.77	0.49
4:A:903:ATP:O3'	2:B:224:LYS:HB2	2.13	0.49
2:B:463:HIS:CE1	2:B:465:LYS:HZ3	2.31	0.49
2:C:215:ARG:HG2	5:C:537:HOH:O	2.13	0.49
2:B:487:GLU:O	2:B:488:ARG:HB2	2.13	0.49
1:A:283:ILE:HG23	1:A:412:PHE:CE1	2.47	0.49
2:E:446:ARG:HD3	5:E:529:HOH:O	2.13	0.49
2:C:18:ILE:HD12	2:C:18:ILE:N	2.28	0.49
2:D:345:LYS:NZ	2:D:366:GLU:OE1	2.42	0.49
1:A:267:VAL:CG2	1:A:300:ARG:HG2	2.42	0.49
2:B:402:TYR:O	2:B:406:GLU:HB2	2.13	0.49
2:D:163:GLU:HA	2:D:163:GLU:OE2	2.13	0.49
2:B:79:THR:HG21	2:B:81:GLN:HG2	1.95	0.48
1:A:79:THR:HG23	1:A:81:GLN:HE21	1.78	0.48
2:D:370:PHE:O	2:D:371:LYS:HG3	2.13	0.48
2:D:471:MET:HB3	2:D:480:LYS:HZ1	1.78	0.48
2:C:150:VAL:CG1	2:C:151:PHE:N	2.75	0.48
1:A:462:TRP:O	1:A:463:HIS:O	2.31	0.48
2:B:31:ILE:HA	2:B:231:MET:HG3	1.94	0.48
2:F:262:ARG:HD2	2:F:277:GLY:O	2.13	0.48
1:A:326:ARG:HG3	2:B:260:ASN:ND2	2.27	0.48
2:F:353:SER:O	2:F:354:ALA:HB2	2.13	0.48
1:A:357:GLU:HG3	1:A:358:ASP:N	2.28	0.48
2:D:145:ASP:OD2	2:D:181:THR:HG21	2.12	0.48
2:B:457:LYS:O	2:B:457:LYS:HG3	2.13	0.48
2:E:191:ILE:HG21	2:E:198:GLU:HG3	1.94	0.48
2:F:269:ARG:O	2:F:272:GLU:HB2	2.12	0.48
2:F:140:ARG:HB3	2:F:140:ARG:HH11	1.78	0.48
2:D:249:LEU:HD13	2:D:394:GLN:HG2	1.95	0.48
2:F:123:LEU:O	2:F:123:LEU:HD13	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:LYS:O	1:A:371:LYS:CD	2.62	0.48
2:D:76:PHE:CZ	2:D:126:LEU:HD21	2.47	0.48
2:F:334:ASP:O	2:F:338:MET:HG2	2.13	0.48
1:A:118:VAL:HG23	1:A:153:GLN:OE1	2.13	0.48
2:E:497:ILE:C	2:E:498:THR:HG23	2.34	0.48
2:F:52:LYS:HD2	2:F:181:THR:HG23	1.96	0.48
2:B:299:SER:C	2:B:333:MET:CE	2.82	0.48
2:F:69:GLU:OE1	2:F:141:ARG:NE	2.45	0.48
2:F:14:GLU:N	5:F:522:HOH:O	2.46	0.48
2:B:448:GLU:HG2	2:C:466:ALA:HA	1.94	0.48
2:B:152:GLN:HG3	2:C:161:ARG:NH1	2.28	0.48
2:D:302:VAL:HG21	2:D:314:LEU:HB2	1.95	0.48
2:B:169:ALA:O	2:B:173:GLN:HG3	2.12	0.48
2:B:161:ARG:HB2	2:B:196:VAL:HG11	1.93	0.48
2:B:471:MET:HG3	2:B:478:ASP:HB3	1.96	0.48
2:F:289:ALA:CB	2:F:419:PHE:HA	2.43	0.48
1:A:117:VAL:HA	1:A:154:TYR:OH	2.13	0.48
2:B:263:VAL:CG1	2:B:374:ARG:NH2	2.65	0.48
2:D:446:ARG:H	2:D:496:ARG:HH12	1.62	0.48
2:B:298:VAL:HG13	2:B:376:ALA:CB	2.41	0.48
2:D:182:THR:CG2	2:D:183:GLU:N	2.75	0.48
1:A:484:ARG:HB3	1:A:484:ARG:HH11	1.78	0.48
1:A:183:GLU:HB2	2:B:199:PHE:CE1	2.48	0.48
2:F:298:VAL:HA	2:F:411:LEU:HD23	1.94	0.48
2:C:449:MET:O	2:D:465:LYS:HB3	2.14	0.48
1:A:436:THR:HG23	1:A:458:MET:HG2	1.96	0.48
2:C:88:ARG:HG2	2:C:88:ARG:HH11	1.79	0.48
2:D:386:GLY:O	2:D:387:VAL:C	2.52	0.48
2:D:344:LEU:HD22	2:D:345:LYS:N	2.29	0.48
2:B:334:ASP:O	2:B:338:MET:HG2	2.14	0.48
2:C:380:LEU:HD21	2:C:412:PHE:HD2	1.79	0.48
2:B:140:ARG:CB	2:B:140:ARG:NH1	2.61	0.48
2:D:357:GLU:HG3	2:D:358:ASP:H	1.78	0.48
2:F:315:PHE:HE1	2:F:375:ILE:HG12	1.79	0.48
2:B:425:ILE:HD11	2:B:456:PHE:CE2	2.49	0.48
1:A:74:VAL:HG22	1:A:106:LEU:HD23	1.96	0.48
2:E:50:THR:HG22	2:E:209:ASN:HB2	1.96	0.48
2:C:441:GLN:HE22	2:C:490:ILE:HD13	1.77	0.48
2:F:402:TYR:O	2:F:406:GLU:HB2	2.13	0.48
2:F:255:THR:O	2:F:255:THR:HG22	2.14	0.48
1:A:137:TYR:O	1:A:138:ARG:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:52:LYS:HD2	2:E:182:THR:O	2.14	0.48
1:A:18:ILE:H	1:A:18:ILE:HD12	1.76	0.48
2:F:461:SER:OG	2:F:462:TRP:N	2.47	0.48
2:F:122:ASP:O	2:F:126:LEU:N	2.43	0.48
2:E:79:THR:CG2	2:E:81:GLN:HG2	2.43	0.48
2:D:76:PHE:O	2:D:109:SER:HA	2.14	0.48
2:D:21:MET:HE3	2:D:59:PHE:CE1	2.48	0.48
2:C:211:LEU:HD12	2:C:215:ARG:O	2.14	0.47
2:B:431:SEP:O	2:B:432:ALA:HB3	2.13	0.47
2:C:488:ARG:HG3	2:C:488:ARG:HH11	1.78	0.47
2:E:451:ARG:NH1	2:E:472:ILE:HD12	2.29	0.47
2:E:178:THR:HG22	2:E:179:VAL:N	2.29	0.47
2:B:445:ILE:O	2:B:446:ARG:HB2	2.13	0.47
1:A:305:ALA:O	1:A:310:GLU:HB2	2.15	0.47
2:C:419:PHE:CG	2:C:419:PHE:O	2.67	0.47
2:B:81:GLN:H	2:B:81:GLN:HE21	1.63	0.47
1:A:81:GLN:CD	1:A:81:GLN:N	2.67	0.47
2:E:321:ARG:O	2:E:325:LEU:HD12	2.14	0.47
2:E:400:THR:HG21	2:E:433:ILE:HG22	1.96	0.47
1:A:462:TRP:HA	4:F:901:ATP:C2	2.49	0.47
2:E:169:ALA:O	2:E:173:GLN:HG3	2.14	0.47
2:E:387:VAL:HG12	2:E:391:ALA:CB	2.41	0.47
2:F:191:ILE:HB	2:F:198:GLU:HG2	1.96	0.47
2:F:437:ILE:HD11	2:F:457:LYS:HE2	1.96	0.47
1:A:284:ILE:HB	1:A:411:LEU:CD1	2.41	0.47
2:B:332:GLY:O	2:B:333:MET:O	2.32	0.47
2:D:31:ILE:HD11	2:D:246:ILE:HG21	1.96	0.47
2:D:220:LEU:HD23	2:D:221:GLU:N	2.28	0.47
2:B:220:LEU:HD13	2:B:246:ILE:CD1	2.44	0.47
2:D:335:PHE:HA	2:D:338:MET:CG	2.44	0.47
2:E:311:ARG:HD2	2:E:371:LYS:CE	2.43	0.47
2:C:463:HIS:O	2:C:465:LYS:HE2	2.14	0.47
2:C:377:ILE:CD1	2:C:399:VAL:HG11	2.44	0.47
2:D:182:THR:HG21	2:D:192:ALA:CB	2.43	0.47
2:D:127:ILE:HG12	2:D:167:LEU:HD12	1.97	0.47
2:D:350:TYR:OH	2:E:256:GLN:NE2	2.47	0.47
1:A:267:VAL:HB	1:A:270:LEU:HB2	1.97	0.47
2:B:317:TYR:HD2	2:B:349:ALA:O	1.97	0.47
2:B:119:GLY:C	2:B:121:PHE:H	2.17	0.47
2:B:148:THR:HG21	2:B:193:ARG:HD2	1.95	0.47
2:F:161:ARG:HB2	2:F:196:VAL:CG1	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:334:ASP:O	2:D:338:MET:HG2	2.14	0.47
2:F:514:GLU:HG2	2:F:519:SER:HB3	1.97	0.47
2:B:273:MET:C	2:B:275:GLY:H	2.18	0.47
2:C:280:LYS:NZ	2:C:407:GLU:HB3	2.29	0.47
1:A:162:ARG:HD2	5:A:529:HOH:O	2.13	0.47
2:E:247:PHE:HB3	5:E:532:HOH:O	2.14	0.47
1:A:287:THR:HA	1:A:414:ASN:O	2.14	0.47
2:B:354:ALA:HB1	2:B:358:ASP:HB2	1.96	0.47
2:D:24:MET:HG3	2:D:66:GLU:HG3	1.97	0.47
2:B:449:MET:CE	2:C:467:ILE:HD11	2.44	0.47
1:A:21:MET:CE	1:A:177:THR:HG21	2.36	0.47
2:D:377:ILE:HD12	2:D:412:PHE:HE2	1.78	0.47
2:F:508:ILE:O	2:F:508:ILE:HG22	2.14	0.47
2:E:462:TRP:O	2:E:463:HIS:CD2	2.67	0.47
2:B:451:ARG:NH2	4:B:901:ATP:O2'	2.48	0.47
2:B:485:ASN:OD1	2:B:485:ASN:N	2.47	0.47
2:E:323:GLN:HE22	2:F:459:ARG:HD3	1.79	0.47
2:F:116:GLU:OE1	2:F:117:VAL:HG23	2.15	0.47
2:D:43:LEU:HD11	2:D:182:THR:OG1	2.14	0.47
2:B:347:VAL:O	2:B:348:CYS:HB2	2.15	0.47
1:A:459:ARG:HD3	2:F:323:GLN:NE2	2.29	0.47
2:D:44:VAL:HA	2:D:205:VAL:O	2.14	0.47
2:E:106:LEU:C	2:E:106:LEU:HD12	2.35	0.47
2:C:400:THR:HG21	2:C:433:ILE:CG2	2.45	0.47
2:C:400:THR:HG22	2:C:401:GLY:N	2.28	0.47
1:A:393:ARG:HH21	1:A:429:HIS:HB2	1.79	0.47
2:F:504:GLU:HB3	2:F:507:ARG:NH2	2.30	0.47
2:B:216:ARG:HB2	2:C:232:LYS:HB3	1.96	0.47
1:A:317:TYR:CE1	1:A:377:ILE:HG23	2.49	0.47
2:B:52:LYS:HE3	4:B:903:ATP:O1B	2.15	0.47
1:A:151:PHE:C	1:A:153:GLN:H	2.18	0.47
2:B:501:GLU:HB2	2:B:502:LYS:H	1.39	0.47
2:C:311:ARG:HA	2:C:343:LEU:O	2.14	0.47
2:B:273:MET:CE	2:B:468:ARG:HD2	2.44	0.47
2:C:211:LEU:O	2:C:212:GLU:HB3	2.14	0.47
2:C:325:LEU:CD2	2:C:335:PHE:HB2	2.45	0.47
2:B:311:ARG:HD2	2:B:371:LYS:HE3	1.97	0.47
1:A:419:PHE:HD2	2:B:425:ILE:HD12	1.78	0.47
2:E:441:GLN:HE22	2:E:490:ILE:HD13	1.80	0.47
4:C:903:ATP:O3'	2:D:224:LYS:HB2	2.15	0.47
2:C:298:VAL:HA	2:C:411:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:ASP:O	2:B:146:SER:OG	2.33	0.47
2:B:220:LEU:HD13	2:B:246:ILE:HD11	1.97	0.47
2:B:218:ARG:HG3	2:B:237:PHE:O	2.15	0.47
1:A:15:HIS:C	1:A:16:GLN:OE1	2.54	0.47
2:E:145:ASP:OD2	2:E:181:THR:HG21	2.15	0.47
2:E:420:MET:CE	2:F:490:ILE:HG13	2.45	0.47
2:B:127:ILE:HG22	2:B:127:ILE:O	2.15	0.47
2:E:191:ILE:CB	2:E:198:GLU:HG3	2.45	0.47
2:C:299:SER:CB	2:C:333:MET:HE1	2.45	0.47
1:A:178:THR:HG22	1:A:179:VAL:N	2.31	0.47
2:B:148:THR:OG1	2:B:182:THR:HG23	2.15	0.46
2:E:146:SER:H	2:E:181:THR:HB	1.79	0.46
2:F:445:ILE:HD12	2:F:486:PHE:CE2	2.50	0.46
2:F:191:ILE:CB	2:F:198:GLU:HG3	2.44	0.46
2:F:388:SER:HA	5:F:542:HOH:O	2.15	0.46
2:F:344:LEU:HD13	2:F:344:LEU:C	2.36	0.46
2:B:64:ILE:HD13	2:B:97:LEU:HD13	1.97	0.46
2:F:334:ASP:OD1	2:F:336:GLU:HB2	2.15	0.46
2:E:281:ASP:O	2:E:282:SER:HB3	2.15	0.46
2:C:484:ARG:HB3	2:C:484:ARG:NH1	2.30	0.46
1:A:191:ILE:HG13	1:A:206:ILE:CD1	2.45	0.46
2:D:323:GLN:HE22	2:E:459:ARG:HD3	1.80	0.46
2:D:223:LEU:O	2:D:224:LYS:HB3	2.15	0.46
2:B:61:TYR:CE1	2:B:92:TRP:HB2	2.50	0.46
2:C:117:VAL:O	2:C:117:VAL:HG12	2.14	0.46
2:C:370:PHE:O	2:C:371:LYS:HG3	2.14	0.46
2:F:433:ILE:HG22	2:F:433:ILE:O	2.15	0.46
1:A:52:LYS:HD2	1:A:181:THR:HG23	1.97	0.46
1:A:248:PRO:HB2	1:A:251:ALA:HB3	1.97	0.46
1:A:393:ARG:NH2	1:A:429:HIS:HB2	2.31	0.46
1:A:49:GLY:CA	4:A:903:ATP:O2B	2.63	0.46
2:C:76:PHE:O	2:C:109:SER:HA	2.15	0.46
2:F:154:TYR:HD1	2:F:154:TYR:O	1.98	0.46
2:C:267:VAL:CG2	2:C:300:ARG:HG2	2.45	0.46
2:C:294:LYS:HB2	4:C:901:ATP:O1B	2.15	0.46
2:D:305:ALA:HB2	2:D:374:ARG:CD	2.33	0.46
2:F:379:SER:H	2:F:413:THR:CB	2.24	0.46
2:C:262:ARG:HH22	2:C:461:SER:HB2	1.81	0.46
2:F:147:VAL:HG23	2:F:148:THR:N	2.30	0.46
2:B:126:LEU:HG	2:B:130:ILE:HD11	1.96	0.46
2:B:49:GLY:HA2	4:B:903:ATP:O2B	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:356:LEU:HD21	2:D:387:VAL:HG11	1.98	0.46
1:A:357:GLU:HG3	1:A:358:ASP:H	1.81	0.46
2:B:208:ARG:O	2:B:218:ARG:HA	2.14	0.46
1:A:471:MET:HG3	1:A:478:ASP:HB3	1.97	0.46
1:A:18:ILE:HD13	1:A:227:GLY:O	2.16	0.46
2:D:191:ILE:HB	2:D:198:GLU:CD	2.35	0.46
2:B:432:ALA:HA	2:B:459:ARG:NH2	2.30	0.46
2:D:452:ALA:HA	2:D:468:ARG:O	2.16	0.46
2:C:370:PHE:C	2:C:371:LYS:HG3	2.36	0.46
2:C:419:PHE:CD1	2:C:419:PHE:O	2.68	0.46
2:B:419:PHE:CD2	2:C:425:ILE:CD1	2.95	0.46
2:D:313:ILE:HG21	2:D:315:PHE:CZ	2.50	0.46
2:B:371:LYS:N	2:B:372:PRO:HD3	2.31	0.46
2:F:144:ILE:CG2	2:F:147:VAL:HG12	2.45	0.46
2:F:147:VAL:CG2	2:F:148:THR:N	2.79	0.46
2:F:294:LYS:N	4:F:901:ATP:O1B	2.45	0.46
1:A:184:ARG:HD3	5:A:524:HOH:O	2.16	0.46
2:D:127:ILE:HG12	2:D:167:LEU:CD1	2.46	0.46
1:A:106:LEU:HD11	1:A:129:ARG:NE	2.30	0.46
2:D:296:LEU:HD12	2:D:296:LEU:O	2.16	0.46
1:A:316:ALA:HB3	1:A:348:CYS:SG	2.56	0.46
2:D:328:ALA:O	2:D:332:GLY:O	2.33	0.46
2:F:316:ALA:HB2	2:F:324:LEU:HD11	1.97	0.46
2:F:311:ARG:HA	2:F:343:LEU:O	2.15	0.46
2:C:360:LEU:CD2	2:C:364:LYS:HE3	2.46	0.46
2:B:225:LEU:HD12	2:B:230:HIS:HB3	1.98	0.46
2:E:148:THR:HG21	2:E:183:GLU:HG3	1.97	0.46
2:F:356:LEU:HD13	2:F:356:LEU:H	1.79	0.46
2:B:425:ILE:H	2:B:425:ILE:HD12	1.81	0.46
2:F:147:VAL:O	2:F:150:VAL:HG12	2.16	0.46
2:C:375:ILE:O	2:C:410:GLY:HA2	2.16	0.46
2:E:441:GLN:NE2	2:E:490:ILE:HD13	2.30	0.46
2:F:451:ARG:HB2	2:F:470:PHE:O	2.15	0.46
2:F:270:LEU:O	2:F:273:MET:N	2.49	0.46
2:B:377:ILE:HD12	2:B:412:PHE:HE2	1.80	0.46
2:E:182:THR:CG2	2:E:183:GLU:N	2.79	0.46
2:F:444:GLU:HB3	2:F:493:SER:HA	1.98	0.46
2:E:76:PHE:O	2:E:109:SER:HA	2.16	0.46
2:D:446:ARG:HG2	5:E:525:HOH:O	2.16	0.46
2:E:267:VAL:HG23	2:E:300:ARG:HG2	1.98	0.46
2:D:247:PHE:HZ	2:D:361:GLN:HB2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:360:LEU:HD23	2:B:399:VAL:CG2	2.46	0.46
2:C:56:SER:HB2	2:C:143:SER:HB3	1.98	0.46
2:F:418:GLN:O	2:F:418:GLN:HG3	2.15	0.46
2:E:200:VAL:O	2:E:200:VAL:HG12	2.15	0.46
2:D:433:ILE:HG22	2:D:433:ILE:O	2.16	0.45
2:B:184:ARG:NH1	5:B:520:HOH:O	2.45	0.45
1:A:360:LEU:HD21	1:A:364:LYS:HE3	1.97	0.45
2:D:249:LEU:CD1	2:D:394:GLN:HG2	2.47	0.45
1:A:425:ILE:HD12	2:F:419:PHE:CD2	2.51	0.45
2:F:145:ASP:OD2	2:F:181:THR:HG21	2.16	0.45
2:F:115:GLN:CG	2:F:116:GLU:H	2.26	0.45
2:D:440:LEU:HD23	2:D:453:ILE:HG13	1.98	0.45
2:F:191:ILE:HB	2:F:198:GLU:CD	2.36	0.45
2:C:470:PHE:HB2	2:C:478:ASP:O	2.15	0.45
2:C:144:ILE:HG21	2:C:147:VAL:HG12	1.98	0.45
2:E:451:ARG:O	2:E:469:GLU:HA	2.16	0.45
2:D:52:LYS:HE3	4:D:903:ATP:O1B	2.16	0.45
2:B:90:PHE:HA	2:B:241:ASP:O	2.15	0.45
2:C:70:PRO:HA	2:C:102:LYS:O	2.16	0.45
2:E:225:LEU:HD12	2:E:230:HIS:HB3	1.98	0.45
1:A:486:PHE:HB2	1:A:489:ILE:HD11	1.98	0.45
2:B:283:ILE:HG23	2:B:412:PHE:CE1	2.50	0.45
2:E:345:LYS:HD2	2:E:370:PHE:CD1	2.51	0.45
2:F:316:ALA:CB	2:F:324:LEU:HD11	2.46	0.45
2:F:164:LEU:CD1	2:F:197:GLU:HG3	2.44	0.45
2:C:164:LEU:HD21	2:C:180:MET:CE	2.46	0.45
1:A:166:ARG:HB2	5:A:533:HOH:O	2.16	0.45
2:F:267:VAL:HG22	2:F:300:ARG:HG2	1.98	0.45
2:D:122:ASP:HB3	2:D:123:LEU:H	1.42	0.45
2:C:21:MET:O	2:C:35:GLY:HA3	2.15	0.45
2:E:358:ASP:O	2:E:362:ILE:HG12	2.16	0.45
2:F:283:ILE:CD1	2:F:400:THR:HG23	2.46	0.45
1:A:319:GLU:O	2:B:254:LEU:HD21	2.15	0.45
2:E:335:PHE:O	2:E:339:GLU:HG3	2.16	0.45
2:E:150:VAL:CG1	2:E:151:PHE:N	2.79	0.45
2:C:52:LYS:HD2	2:C:181:THR:HG23	1.98	0.45
2:C:49:GLY:CA	4:C:903:ATP:O2B	2.64	0.45
2:E:202:ASP:HA	2:E:226:ARG:HD2	1.98	0.45
2:F:121:PHE:HA	2:F:121:PHE:HD2	1.70	0.45
2:E:53:THR:OG1	4:E:903:ATP:O2G	2.35	0.45
1:A:280:LYS:NZ	1:A:407:GLU:HB3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:144:ILE:CG2	2:C:147:VAL:HG12	2.47	0.45
2:E:200:VAL:O	2:E:200:VAL:CG1	2.65	0.45
2:F:219:THR:HA	2:F:235:TYR:O	2.17	0.45
2:D:200:VAL:O	2:D:200:VAL:HG12	2.16	0.45
2:B:451:ARG:HH12	2:B:472:ILE:CD1	2.30	0.45
2:D:320:SER:HB3	2:E:256:GLN:HG2	1.99	0.45
2:F:483:PHE:H	2:F:483:PHE:HD1	1.63	0.45
2:E:23:THR:O	2:E:24:MET:HB2	2.15	0.45
2:D:106:LEU:C	2:D:106:LEU:CD1	2.71	0.45
2:F:500:ASP:O	2:F:501:GLU:CB	2.59	0.45
2:E:425:ILE:HG22	2:E:426:ALA:H	1.77	0.45
2:E:345:LYS:HD2	2:E:370:PHE:CG	2.52	0.45
2:E:344:LEU:HD11	2:E:346:ILE:HG13	1.98	0.45
2:E:18:ILE:HD11	2:E:228:THR:N	2.32	0.45
2:C:354:ALA:HB3	2:C:359:HIS:CE1	2.52	0.45
1:A:377:ILE:HD12	1:A:412:PHE:CE2	2.50	0.45
2:E:446:ARG:HB3	2:F:484:ARG:HG3	1.98	0.45
2:E:265:SER:HB3	2:E:278:PHE:CE1	2.52	0.45
2:B:305:ALA:HB2	2:B:374:ARG:CD	2.30	0.45
2:D:146:SER:H	2:D:181:THR:CG2	2.20	0.45
1:A:24:MET:HB2	1:A:62:ASN:ND2	2.26	0.45
2:D:471:MET:HE2	2:D:478:ASP:HB2	1.98	0.45
2:C:296:LEU:CD2	2:C:477:PRO:HB3	2.44	0.45
2:C:358:ASP:O	2:C:362:ILE:HG12	2.17	0.45
1:A:498:THR:O	1:A:499:VAL:C	2.55	0.45
2:D:484:ARG:HB3	2:D:484:ARG:NH1	2.32	0.45
2:F:441:GLN:HG3	2:F:452:ALA:HB3	1.97	0.45
2:B:203:ASN:HB3	2:B:225:LEU:HD23	1.97	0.45
2:E:113:GLU:HB3	2:E:114:GLY:H	1.62	0.45
2:E:180:MET:HB3	2:E:180:MET:HE2	1.74	0.45
2:C:337:GLU:O	2:C:338:MET:C	2.54	0.45
1:A:311:ARG:HD2	1:A:371:LYS:HE3	1.99	0.45
2:F:182:THR:HG22	2:F:183:GLU:N	2.32	0.45
1:A:416:SER:O	1:A:418:GLN:N	2.50	0.45
2:D:350:TYR:CZ	2:E:254:LEU:HD13	2.52	0.45
2:F:270:LEU:O	2:F:273:MET:HB2	2.17	0.45
2:E:163:GLU:HA	2:E:163:GLU:OE2	2.17	0.45
2:C:111:ASP:OD1	2:C:113:GLU:HG2	2.17	0.45
2:B:215:ARG:NE	2:B:215:ARG:HA	2.32	0.45
2:F:47:THR:HG22	2:F:184:ARG:O	2.17	0.45
2:C:248:PRO:O	2:C:250:GLY:N	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:LEU:HD13	1:A:331:TRP:CD2	2.52	0.45
2:E:344:LEU:HD22	2:E:345:LYS:H	1.79	0.44
2:F:127:ILE:HD13	2:F:167:LEU:HD13	2.00	0.44
2:C:357:GLU:HG3	2:C:358:ASP:N	2.32	0.44
2:F:61:TYR:CZ	2:F:65:ILE:HG13	2.53	0.44
2:E:317:TYR:CE2	2:E:383:LEU:HD21	2.53	0.44
2:C:419:PHE:O	2:C:420:MET:CB	2.65	0.44
2:F:182:THR:CG2	2:F:183:GLU:N	2.81	0.44
2:B:216:ARG:HG2	2:C:233:GLY:HA2	1.98	0.44
2:C:111:ASP:CG	2:C:113:GLU:HG2	2.37	0.44
1:A:458:MET:O	4:F:901:ATP:H3'	2.17	0.44
2:F:483:PHE:N	2:F:483:PHE:CD1	2.85	0.44
2:D:287:THR:HG23	2:D:414:ASN:ND2	2.19	0.44
2:B:148:THR:CG2	2:B:193:ARG:HD2	2.47	0.44
4:E:903:ATP:O1G	2:F:224:LYS:NZ	2.50	0.44
1:A:80:PRO:HB2	1:A:81:GLN:NE2	2.32	0.44
2:F:154:TYR:CD1	2:F:154:TYR:O	2.70	0.44
2:B:356:LEU:HD23	2:B:395:PHE:HB2	1.99	0.44
1:A:111:ASP:O	1:A:113:GLU:N	2.46	0.44
1:A:50:THR:HG22	1:A:209:ASN:HB2	1.99	0.44
1:A:64:ILE:HD11	1:A:103:LEU:HB2	2.00	0.44
2:D:150:VAL:O	2:D:153:GLN:HG3	2.17	0.44
2:F:504:GLU:HB2	2:F:505:LEU:H	1.52	0.44
2:F:504:GLU:HB3	2:F:507:ARG:CZ	2.48	0.44
2:C:79:THR:CG2	2:C:82:ASP:OD2	2.66	0.44
2:C:367:ILE:HG23	2:C:372:PRO:HD2	1.99	0.44
2:D:462:TRP:CE3	2:D:463:HIS:N	2.86	0.44
1:A:87:ALA:O	1:A:92:TRP:CD1	2.71	0.44
2:B:50:THR:HG22	2:B:209:ASN:HB2	1.99	0.44
2:B:147:VAL:CG2	2:B:148:THR:N	2.79	0.44
2:C:38:ILE:CG2	2:C:39:GLY:N	2.80	0.44
1:A:299:SER:CB	1:A:333:MET:HE1	2.46	0.44
2:D:178:THR:CG2	2:D:179:VAL:N	2.77	0.44
2:F:38:ILE:H	2:F:38:ILE:HD12	1.80	0.44
2:E:454:ASN:HD21	2:E:456:PHE:HA	1.82	0.44
2:D:402:TYR:O	2:D:405:GLN:HG2	2.17	0.44
2:E:356:LEU:CD2	2:E:387:VAL:HG11	2.28	0.44
2:E:347:VAL:O	2:E:348:CYS:CB	2.66	0.44
2:E:371:LYS:N	2:E:372:PRO:HD3	2.33	0.44
2:F:145:ASP:O	2:F:146:SER:OG	2.26	0.44
1:A:311:ARG:CZ	1:A:371:LYS:HE3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:144:ILE:HB	2:F:180:MET:HG2	1.99	0.44
2:C:451:ARG:NH1	2:C:451:ARG:HG2	2.31	0.44
2:F:299:SER:O	2:F:333:MET:HE1	2.18	0.44
2:E:186:GLU:OE2	2:E:187:GLU:N	2.51	0.44
2:C:249:LEU:HB3	5:C:521:HOH:O	2.17	0.44
2:E:123:LEU:CD1	2:E:166:ARG:HD2	2.47	0.44
2:D:377:ILE:HD11	2:D:399:VAL:HG11	1.99	0.44
1:A:182:THR:CG2	1:A:183:GLU:N	2.81	0.44
2:F:191:ILE:CB	2:F:198:GLU:CG	2.91	0.44
2:E:294:LYS:O	2:E:298:VAL:HG23	2.18	0.44
2:F:515:LYS:C	2:F:517:PRO:HD2	2.37	0.44
4:A:901:ATP:H3'	2:B:458:MET:O	2.18	0.44
2:F:269:ARG:HG2	2:F:479:ILE:CG2	2.48	0.44
2:F:311:ARG:HD2	2:F:371:LYS:HE3	1.99	0.44
1:A:468:ARG:NH1	1:A:468:ARG:HG2	2.32	0.44
2:C:248:PRO:C	2:C:250:GLY:H	2.21	0.44
2:C:448:GLU:HG2	2:D:466:ALA:HA	1.98	0.44
1:A:400:THR:HG22	1:A:401:GLY:N	2.32	0.44
2:D:147:VAL:HG11	2:D:180:MET:HE2	2.00	0.44
2:B:81:GLN:CD	2:B:81:GLN:H	2.19	0.44
1:A:52:LYS:HE3	4:A:903:ATP:O1B	2.17	0.44
2:D:313:ILE:HG13	2:D:372:PRO:CG	2.41	0.44
2:D:315:PHE:CE2	2:D:347:VAL:HG21	2.53	0.44
1:A:283:ILE:HG23	1:A:412:PHE:CD1	2.53	0.44
1:A:186:GLU:OE2	1:A:187:GLU:N	2.50	0.44
1:A:249:LEU:HD13	1:A:394:GLN:HG2	1.98	0.44
2:B:84:ILE:HG12	2:B:94:LEU:HB2	2.00	0.44
2:D:347:VAL:O	2:D:348:CYS:HB2	2.17	0.44
2:C:352:GLU:OE1	2:C:385:ARG:NH1	2.50	0.44
2:B:428:SER:O	2:B:429:HIS:HB2	2.18	0.44
2:C:142:VAL:O	2:C:178:THR:HA	2.18	0.44
2:D:41:SER:HA	2:D:178:THR:O	2.18	0.44
2:B:21:MET:HE1	2:B:177:THR:HB	1.99	0.44
2:C:23:THR:O	2:C:24:MET:HB2	2.16	0.44
2:C:320:SER:HA	2:D:254:LEU:HG	1.99	0.44
2:E:393:ARG:O	2:E:397:ILE:HG12	2.18	0.43
2:C:215:ARG:NE	2:C:215:ARG:CA	2.81	0.43
2:E:266:GLY:CA	2:E:300:ARG:HG3	2.45	0.43
2:F:21:MET:HE1	2:F:59:PHE:CZ	2.50	0.43
2:C:316:ALA:O	2:C:348:CYS:HA	2.18	0.43
2:D:350:TYR:O	2:D:351:PRO:C	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:482:SER:C	2:B:484:ARG:H	2.21	0.43
2:E:240:THR:C	2:E:242:HIS:H	2.21	0.43
1:A:518:GLU:CD	1:A:518:GLU:H	2.22	0.43
2:F:497:ILE:HD12	2:F:497:ILE:C	2.38	0.43
2:E:431:SEP:HA	2:E:434:THR:HG22	1.99	0.43
2:D:397:ILE:HG12	2:D:397:ILE:H	1.58	0.43
2:D:185:ILE:HD11	2:D:193:ARG:HH12	1.82	0.43
2:B:379:SER:CA	2:B:413:THR:HG22	2.44	0.43
2:E:148:THR:HG21	2:E:183:GLU:HG2	1.99	0.43
1:A:23:THR:O	1:A:24:MET:HB2	2.18	0.43
2:E:486:PHE:CD2	2:E:494:PRO:HB2	2.53	0.43
2:F:356:LEU:CD1	2:F:387:VAL:HG21	2.46	0.43
2:C:164:LEU:HD12	2:C:197:GLU:HG3	2.00	0.43
2:F:269:ARG:HG2	2:F:479:ILE:CB	2.47	0.43
2:B:264:SER:CB	2:B:304:ASN:ND2	2.78	0.43
2:F:115:GLN:CG	2:F:116:GLU:N	2.81	0.43
2:B:49:GLY:CA	4:B:903:ATP:O2B	2.66	0.43
2:D:127:ILE:HD13	2:D:170:ARG:HG3	1.99	0.43
2:C:220:LEU:C	2:C:220:LEU:HD23	2.39	0.43
2:C:340:ARG:C	2:C:342:ASN:H	2.22	0.43
1:A:104:PHE:CD2	1:A:133:ALA:HB1	2.52	0.43
1:A:429:HIS:HB3	5:F:559:HOH:O	2.19	0.43
2:D:285:LEU:HD12	2:D:412:PHE:O	2.18	0.43
2:E:151:PHE:C	2:E:153:GLN:N	2.71	0.43
2:B:461:SER:OG	2:B:462:TRP:N	2.51	0.43
2:C:216:ARG:HG2	2:D:233:GLY:HA2	1.99	0.43
1:A:367:ILE:O	1:A:372:PRO:HD3	2.18	0.43
2:B:127:ILE:HG21	2:B:170:ARG:HG3	2.00	0.43
2:E:140:ARG:NH1	2:E:140:ARG:CB	2.79	0.43
2:E:170:ARG:O	2:E:174:ILE:HG12	2.18	0.43
2:B:471:MET:HE3	2:B:478:ASP:HB3	2.00	0.43
2:D:146:SER:N	2:D:181:THR:HG22	2.24	0.43
2:B:160:VAL:O	2:B:164:LEU:HB2	2.18	0.43
2:F:430:ILE:CG2	2:F:430:ILE:O	2.59	0.43
2:D:396:VAL:HG21	2:D:430:ILE:HG21	1.99	0.43
2:F:194:TYR:O	2:F:195:GLY:C	2.56	0.43
2:F:81:GLN:N	2:F:81:GLN:CD	2.72	0.43
2:E:377:ILE:HD12	2:E:412:PHE:HE2	1.79	0.43
1:A:419:PHE:CD2	2:B:425:ILE:CD1	3.01	0.43
1:A:76:PHE:HE1	1:A:144:ILE:CG2	2.31	0.43
2:D:21:MET:CE	2:D:59:PHE:CZ	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:265:SER:O	2:C:301:PHE:HA	2.19	0.43
2:C:274:CYS:HG	2:C:278:PHE:HE2	1.65	0.43
1:A:513:GLN:O	1:A:513:GLN:HG3	2.17	0.43
1:A:318:GLU:CD	1:A:379:SER:HB2	2.38	0.43
2:D:287:THR:HG21	2:D:425:ILE:O	2.19	0.43
2:D:147:VAL:CG2	2:D:148:THR:N	2.80	0.43
2:D:164:LEU:CD2	2:D:180:MET:HE1	2.48	0.43
2:B:151:PHE:O	2:B:153:GLN:N	2.48	0.43
2:F:507:ARG:O	2:F:508:ILE:C	2.56	0.43
2:F:508:ILE:HD12	2:F:508:ILE:N	2.33	0.43
2:E:79:THR:CG2	2:E:82:ASP:H	2.32	0.43
2:D:183:GLU:HB2	2:E:199:PHE:CE1	2.54	0.43
2:C:284:ILE:HD13	2:C:436:THR:HB	2.00	0.43
2:D:468:ARG:HH11	2:D:468:ARG:HG2	1.82	0.43
2:E:297:LEU:HA	2:E:297:LEU:HD23	1.92	0.43
2:E:52:LYS:HB2	2:E:52:LYS:HE3	1.85	0.43
1:A:62:ASN:O	1:A:66:GLU:HB2	2.18	0.43
2:C:334:ASP:OD1	2:C:336:GLU:HB2	2.19	0.43
2:F:317:TYR:HA	2:F:349:ALA:O	2.18	0.43
2:B:85:LYS:HE3	2:C:17:ALA:O	2.18	0.43
2:D:131:ASN:OD1	2:D:174:ILE:HD12	2.18	0.43
2:C:21:MET:HE3	2:C:141:ARG:NE	2.34	0.43
2:C:120:GLY:O	2:C:122:ASP:N	2.52	0.43
2:D:279:PHE:HB2	2:D:282:SER:HB3	2.00	0.43
1:A:79:THR:HG23	1:A:81:GLN:H	1.83	0.43
2:E:335:PHE:HA	2:E:338:MET:HG3	1.99	0.43
2:E:433:ILE:CD1	2:E:433:ILE:N	2.79	0.43
2:E:93:ASP:OD1	2:E:95:ALA:HB3	2.18	0.43
2:E:311:ARG:HA	2:E:343:LEU:O	2.19	0.43
2:B:287:THR:HG21	2:B:425:ILE:O	2.18	0.43
2:C:182:THR:CG2	2:C:183:GLU:N	2.82	0.43
2:F:32:SER:HB3	2:F:222:ILE:HD11	2.01	0.43
2:B:360:LEU:HD22	2:B:360:LEU:O	2.19	0.43
1:A:249:LEU:CD1	1:A:394:GLN:HG2	2.49	0.43
2:C:351:PRO:HB3	2:C:383:LEU:HA	2.00	0.43
2:B:140:ARG:CA	2:B:140:ARG:HH11	2.30	0.43
2:D:400:THR:HG22	2:D:401:GLY:N	2.33	0.43
2:F:315:PHE:CD2	2:F:347:VAL:HG21	2.54	0.43
2:F:31:ILE:HG23	2:F:231:MET:HB2	2.00	0.43
2:B:497:ILE:HD12	2:B:499:VAL:H	1.84	0.43
2:E:470:PHE:HA	2:E:478:ASP:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:49:GLY:HA2	4:C:903:ATP:O2B	2.18	0.43
2:F:261:VAL:O	2:F:279:PHE:HA	2.19	0.43
2:B:88:ARG:HH11	2:B:88:ARG:HG2	1.84	0.43
2:B:380:LEU:N	2:B:413:THR:O	2.36	0.43
2:F:436:THR:HA	2:F:457:LYS:O	2.19	0.43
2:E:483:PHE:HB2	2:E:489:ILE:CD1	2.47	0.43
2:C:41:SER:HA	2:C:178:THR:O	2.18	0.43
2:B:76:PHE:CZ	2:B:126:LEU:HD21	2.54	0.43
2:E:212:GLU:O	2:E:212:GLU:HG2	2.18	0.43
1:A:468:ARG:HA	1:A:481:ASP:O	2.19	0.43
2:D:387:VAL:HG12	2:D:388:SER:O	2.19	0.43
1:A:104:PHE:HD2	1:A:133:ALA:HB1	1.84	0.43
2:D:266:GLY:HA2	2:D:304:ASN:HD22	1.83	0.43
2:C:428:SER:HB2	2:C:430:ILE:CD1	2.41	0.42
2:E:123:LEU:HD13	2:E:163:GLU:OE2	2.18	0.42
2:F:433:ILE:HD12	2:F:433:ILE:N	2.34	0.42
2:C:489:ILE:C	2:C:491:SER:N	2.70	0.42
2:B:151:PHE:C	2:B:153:GLN:N	2.72	0.42
1:A:49:GLY:HA2	4:A:903:ATP:O2B	2.19	0.42
2:E:347:VAL:HG12	2:E:348:CYS:N	2.34	0.42
2:C:378:ASP:O	2:C:379:SER:CB	2.66	0.42
2:E:376:ALA:HA	2:E:411:LEU:O	2.19	0.42
2:F:356:LEU:CD1	2:F:356:LEU:N	2.82	0.42
2:B:65:ILE:O	2:B:65:ILE:CG2	2.63	0.42
2:E:287:THR:CG2	2:E:414:ASN:HB3	2.49	0.42
2:B:428:SER:O	2:B:429:HIS:CB	2.67	0.42
2:B:367:ILE:CG2	2:B:372:PRO:HD2	2.44	0.42
2:D:471:MET:HE2	2:D:478:ASP:HB3	1.99	0.42
1:A:340:ARG:C	1:A:342:ASN:H	2.21	0.42
1:A:152:GLN:NE2	1:A:193:ARG:HD3	2.34	0.42
2:E:148:THR:OG1	2:E:182:THR:HG23	2.18	0.42
2:E:146:SER:HA	2:E:181:THR:O	2.19	0.42
2:D:332:GLY:C	2:D:333:MET:HG2	2.39	0.42
2:D:184:ARG:HD3	5:D:534:HOH:O	2.19	0.42
1:A:313:ILE:CD1	1:A:372:PRO:HG2	2.49	0.42
2:F:489:ILE:HG22	2:F:490:ILE:N	2.34	0.42
2:F:287:THR:HG23	2:F:414:ASN:ND2	2.34	0.42
2:F:344:LEU:HD13	2:F:344:LEU:O	2.19	0.42
2:B:72:VAL:HG23	2:B:139:ALA:CB	2.49	0.42
2:B:309:LYS:HA	2:B:343:LEU:HD13	2.01	0.42
2:E:324:LEU:O	2:E:328:ALA:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:121:PHE:N	2:D:121:PHE:CD1	2.86	0.42
2:F:295:THR:HG22	2:F:295:THR:O	2.17	0.42
2:E:338:MET:HB3	2:E:344:LEU:CB	2.49	0.42
2:F:514:GLU:HG2	2:F:519:SER:CB	2.49	0.42
2:C:88:ARG:HD3	2:D:15:HIS:O	2.18	0.42
2:D:41:SER:CB	2:D:178:THR:HB	2.48	0.42
2:E:296:LEU:HD21	2:E:477:PRO:HD3	2.00	0.42
2:F:111:ASP:C	2:F:113:GLU:H	2.22	0.42
2:C:209:ASN:HD22	2:C:209:ASN:HA	1.66	0.42
2:C:256:GLN:HG2	2:C:256:GLN:H	1.63	0.42
2:D:419:PHE:CD2	2:E:425:ILE:HD12	2.54	0.42
2:B:25:ILE:HG12	2:B:58:GLN:HE21	1.84	0.42
2:B:44:VAL:HA	2:B:205:VAL:O	2.19	0.42
2:B:354:ALA:HB3	2:B:359:HIS:CE1	2.55	0.42
1:A:151:PHE:O	1:A:153:GLN:N	2.49	0.42
2:D:314:LEU:C	2:D:314:LEU:HD12	2.40	0.42
2:B:344:LEU:HD22	2:B:345:LYS:N	2.35	0.42
1:A:485:ASN:N	1:A:485:ASN:OD1	2.52	0.42
2:F:400:THR:HG21	2:F:433:ILE:HG22	2.01	0.42
1:A:301:PHE:O	1:A:374:ARG:NH1	2.50	0.42
2:F:502:LYS:NZ	2:F:507:ARG:HB3	2.35	0.42
1:A:256:GLN:HG2	2:F:320:SER:HB3	2.00	0.42
2:D:487:GLU:OE1	2:D:497:ILE:HG12	2.18	0.42
2:B:72:VAL:HB	2:B:142:VAL:HG22	2.00	0.42
2:B:54:LEU:HD13	2:B:90:PHE:CE1	2.55	0.42
2:B:302:VAL:HG13	2:B:344:LEU:HD23	2.00	0.42
2:D:248:PRO:HB2	2:D:251:ALA:HB3	2.01	0.42
2:E:415:THR:HG21	2:F:431:SEP:O1P	2.20	0.42
1:A:24:MET:HB2	1:A:62:ASN:HB3	2.01	0.42
1:A:313:ILE:HG13	1:A:372:PRO:CG	2.50	0.42
2:F:287:THR:HA	2:F:414:ASN:O	2.20	0.42
2:C:150:VAL:O	2:C:153:GLN:HG3	2.19	0.42
2:F:269:ARG:HB3	2:F:479:ILE:HD12	2.01	0.42
2:F:274:CYS:HB3	2:F:458:MET:SD	2.59	0.42
1:A:70:PRO:HB2	1:A:139:ALA:HA	2.02	0.42
1:A:306:CYS:HB2	1:A:338:MET:SD	2.59	0.42
2:F:371:LYS:N	2:F:372:PRO:HD3	2.35	0.42
2:D:211:LEU:HD13	2:D:216:ARG:CZ	2.50	0.42
2:E:27:GLY:HA3	2:E:246:ILE:HB	2.02	0.42
2:D:305:ALA:O	2:D:310:GLU:HB2	2.20	0.42
2:B:299:SER:O	2:B:333:MET:CE	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:319:GLU:O	2:C:254:LEU:HD21	2.20	0.42
2:F:406:GLU:C	2:F:408:ILE:H	2.22	0.42
2:F:46:GLY:HA2	2:F:184:ARG:HD2	2.02	0.42
2:B:344:LEU:C	2:B:344:LEU:HD13	2.40	0.42
1:A:334:ASP:OD1	1:A:336:GLU:HB2	2.20	0.42
2:D:438:ILE:HD12	2:D:455:VAL:HG22	2.01	0.42
1:A:16:GLN:O	1:A:17:ALA:O	2.38	0.42
1:A:183:GLU:CB	2:B:199:PHE:CE1	3.03	0.42
2:D:191:ILE:HG21	2:D:198:GLU:HG3	2.01	0.42
2:E:483:PHE:O	2:E:484:ARG:C	2.58	0.42
2:E:311:ARG:HD2	2:E:371:LYS:HE3	2.00	0.42
2:B:296:LEU:O	2:B:299:SER:HB2	2.20	0.42
2:E:452:ALA:HA	2:E:469:GLU:HA	2.01	0.42
2:D:323:GLN:NE2	2:E:459:ARG:HD3	2.35	0.42
1:A:344:LEU:HD11	1:A:346:ILE:HG13	2.02	0.42
2:F:28:PHE:N	2:F:246:ILE:HD12	2.34	0.42
2:B:344:LEU:HD22	2:B:345:LYS:H	1.85	0.42
2:D:444:GLU:HA	2:D:448:GLU:O	2.19	0.42
2:F:313:ILE:HG22	2:F:314:LEU:N	2.34	0.42
2:B:107:ASP:C	2:B:107:ASP:OD1	2.58	0.42
1:A:433:ILE:N	1:A:433:ILE:HD12	2.35	0.42
2:C:430:ILE:O	2:C:433:ILE:HB	2.20	0.42
2:D:53:THR:HG23	2:D:145:ASP:OD1	2.20	0.42
2:E:485:ASN:ND2	2:E:496:ARG:HD3	2.33	0.42
2:D:220:LEU:C	2:D:220:LEU:HD23	2.38	0.42
2:C:406:GLU:O	2:C:407:GLU:HB2	2.20	0.42
2:C:390:ASN:O	2:C:391:ALA:C	2.58	0.42
2:F:397:ILE:HD13	2:F:433:ILE:HG12	2.01	0.42
2:F:498:THR:HB	2:F:500:ASP:O	2.20	0.42
2:F:284:ILE:HD13	2:F:436:THR:HB	2.02	0.42
2:B:290:THR:HB	2:C:431:SEP:O2P	2.20	0.42
4:E:901:ATP:C2	2:F:462:TRP:HA	2.55	0.42
1:A:287:THR:CG2	1:A:414:ASN:ND2	2.77	0.42
2:F:471:MET:HG2	2:F:480:LYS:HE2	2.02	0.42
2:C:317:TYR:HD2	2:C:349:ALA:O	2.03	0.42
1:A:344:LEU:HD13	1:A:344:LEU:C	2.40	0.42
2:F:335:PHE:HA	2:F:338:MET:HG3	2.02	0.42
2:E:464:ASP:OD2	2:E:468:ARG:NH2	2.48	0.42
2:D:94:LEU:O	2:D:98:VAL:HG23	2.20	0.42
2:E:270:LEU:HD21	2:E:438:ILE:HD12	2.02	0.42
2:C:469:GLU:HG3	2:C:480:LYS:CE	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:283:ILE:HG23	2:E:412:PHE:CE1	2.55	0.41
2:F:375:ILE:O	2:F:410:GLY:HA2	2.20	0.41
2:C:335:PHE:O	2:C:339:GLU:HG3	2.20	0.41
2:E:441:GLN:HG3	2:E:452:ALA:HB3	2.02	0.41
2:F:484:ARG:NH1	2:F:484:ARG:HB3	2.34	0.41
2:F:332:GLY:C	2:F:333:MET:HG2	2.40	0.41
2:F:140:ARG:NE	5:F:543:HOH:O	2.52	0.41
2:C:267:VAL:HG23	2:C:300:ARG:HG2	2.00	0.41
2:D:211:LEU:HD13	2:D:216:ARG:NE	2.35	0.41
2:D:287:THR:HG23	2:D:414:ASN:HB3	2.02	0.41
2:F:79:THR:HG23	2:F:81:GLN:H	1.84	0.41
1:A:324:LEU:O	1:A:328:ALA:HB2	2.19	0.41
2:C:80:PRO:HB2	2:C:81:GLN:NE2	2.34	0.41
1:A:425:ILE:HD12	1:A:425:ILE:N	2.35	0.41
2:E:79:THR:HG23	2:E:82:ASP:H	1.85	0.41
2:C:299:SER:HB3	2:C:333:MET:HE1	2.02	0.41
2:B:237:PHE:C	2:B:237:PHE:CD1	2.93	0.41
2:D:441:GLN:HG3	2:D:452:ALA:HB3	2.02	0.41
2:E:240:THR:C	2:E:242:HIS:N	2.72	0.41
2:B:418:GLN:HG3	2:B:418:GLN:O	2.20	0.41
2:D:321:ARG:HG2	2:D:321:ARG:H	1.45	0.41
2:D:495:THR:O	2:D:496:ARG:C	2.56	0.41
1:A:313:ILE:HG13	1:A:372:PRO:HG3	2.01	0.41
2:B:332:GLY:O	2:B:333:MET:C	2.59	0.41
2:F:116:GLU:O	2:F:117:VAL:CB	2.67	0.41
2:D:451:ARG:HB3	2:D:470:PHE:CE2	2.55	0.41
2:D:49:GLY:CA	4:D:903:ATP:O2B	2.69	0.41
2:C:174:ILE:HG22	2:C:174:ILE:O	2.20	0.41
2:D:444:GLU:O	2:D:494:PRO:HD2	2.21	0.41
2:B:324:LEU:O	2:B:328:ALA:HB2	2.20	0.41
2:F:248:PRO:O	2:F:250:GLY:N	2.54	0.41
2:E:393:ARG:HH21	2:E:429:HIS:HB2	1.85	0.41
2:B:182:THR:HG22	2:B:183:GLU:N	2.35	0.41
2:F:505:LEU:O	2:F:506:SER:CB	2.67	0.41
2:C:425:ILE:HB	2:C:431:SEP:O1P	2.21	0.41
2:D:367:ILE:HG12	2:D:375:ILE:CD1	2.46	0.41
2:B:262:ARG:HH22	2:B:461:SER:CB	2.33	0.41
2:F:170:ARG:HH12	2:F:174:ILE:HD11	1.84	0.41
2:C:52:LYS:N	4:C:903:ATP:O1B	2.52	0.41
2:F:140:ARG:HD2	2:F:140:ARG:HA	1.83	0.41
2:B:313:ILE:HG22	2:B:314:LEU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:173:GLN:C	2:C:175:GLY:H	2.23	0.41
2:F:400:THR:HG21	2:F:433:ILE:CG2	2.51	0.41
2:E:49:GLY:CA	4:E:903:ATP:O2B	2.68	0.41
2:C:45:SER:HB2	2:C:182:THR:HB	2.01	0.41
2:F:471:MET:HB3	2:F:480:LYS:HZ1	1.86	0.41
2:E:333:MET:HE3	2:E:333:MET:HB2	1.93	0.41
2:E:314:LEU:C	2:E:314:LEU:HD12	2.41	0.41
2:E:365:SER:HA	2:E:368:ASN:HD22	1.85	0.41
2:E:111:ASP:O	2:E:113:GLU:N	2.53	0.41
1:A:240:THR:C	1:A:242:HIS:H	2.22	0.41
2:E:21:MET:HE1	2:E:141:ARG:HG2	2.01	0.41
2:C:433:ILE:HG22	2:C:433:ILE:O	2.20	0.41
1:A:21:MET:HE1	1:A:59:PHE:HZ	1.85	0.41
1:A:80:PRO:HB2	1:A:81:GLN:HE22	1.86	0.41
2:E:411:LEU:HD12	2:E:412:PHE:N	2.36	0.41
2:F:367:ILE:HG12	2:F:375:ILE:CD1	2.51	0.41
2:B:430:ILE:O	2:B:431:SEP:O	2.38	0.41
1:A:299:SER:C	1:A:333:MET:CE	2.88	0.41
2:C:313:ILE:CD1	2:C:372:PRO:HG3	2.50	0.41
2:B:31:ILE:HA	2:B:231:MET:CG	2.51	0.41
2:C:49:GLY:O	2:C:218:ARG:NH2	2.54	0.41
2:D:298:VAL:HG13	2:D:376:ALA:CB	2.49	0.41
2:B:64:ILE:HD12	2:B:97:LEU:HD13	2.02	0.41
2:C:20:LYS:HB3	2:C:35:GLY:O	2.20	0.41
2:C:75:THR:HG23	2:C:75:THR:O	2.21	0.41
2:F:305:ALA:O	2:F:310:GLU:HB2	2.21	0.41
2:D:396:VAL:O	2:D:400:THR:HB	2.20	0.41
2:D:357:GLU:CG	2:D:358:ASP:N	2.82	0.41
2:D:377:ILE:O	2:D:377:ILE:HG22	2.19	0.41
2:D:496:ARG:NH2	2:E:486:PHE:O	2.54	0.41
1:A:161:ARG:CB	1:A:196:VAL:HG11	2.48	0.41
2:C:76:PHE:HE1	2:C:144:ILE:CG2	2.34	0.41
2:D:151:PHE:C	2:D:153:GLN:N	2.74	0.41
2:F:503:SER:O	2:F:504:GLU:O	2.37	0.41
2:C:80:PRO:HD2	2:C:81:GLN:NE2	2.36	0.41
2:E:483:PHE:O	2:E:485:ASN:N	2.54	0.41
1:A:496:ARG:HG3	2:B:487:GLU:OE1	2.21	0.41
2:F:148:THR:HG21	2:F:183:GLU:HG3	2.03	0.41
2:C:357:GLU:HG3	2:C:358:ASP:H	1.84	0.41
2:B:264:SER:CB	2:B:304:ASN:HD21	2.32	0.41
1:A:380:LEU:HD11	1:A:412:PHE:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:49:GLY:HA2	4:D:903:ATP:O2B	2.21	0.41
2:E:128:GLU:O	2:E:129:ARG:C	2.59	0.41
2:B:212:GLU:HG2	2:B:212:GLU:O	2.16	0.41
1:A:379:SER:OG	1:A:382:ALA:HB2	2.21	0.41
2:B:263:VAL:N	2:B:278:PHE:O	2.53	0.41
2:C:311:ARG:CZ	2:C:371:LYS:HE3	2.51	0.41
2:F:361:GLN:O	2:F:362:ILE:C	2.59	0.41
2:B:191:ILE:N	2:B:191:ILE:CD1	2.84	0.41
2:D:313:ILE:HD12	2:D:372:PRO:CG	2.46	0.41
2:E:486:PHE:HA	2:E:495:THR:O	2.20	0.41
2:E:287:THR:HG23	2:E:414:ASN:HB3	2.02	0.41
2:E:444:GLU:CD	2:F:489:ILE:HB	2.41	0.41
2:E:471:MET:HB3	2:E:480:LYS:HZ1	1.85	0.41
2:E:419:PHE:CD2	2:F:425:ILE:HD12	2.55	0.41
2:D:22:ARG:CZ	2:D:24:MET:SD	3.09	0.41
2:C:446:ARG:HG2	2:C:496:ARG:NH1	2.35	0.41
2:E:265:SER:HB3	2:E:278:PHE:CZ	2.56	0.41
2:F:99:ASP:C	2:F:101:GLY:N	2.74	0.41
2:B:57:ILE:HA	2:B:57:ILE:HD13	1.89	0.41
2:B:283:ILE:HG23	2:B:412:PHE:HE1	1.87	0.41
2:B:380:LEU:HD23	2:B:380:LEU:HA	1.96	0.41
1:A:81:GLN:H	1:A:81:GLN:NE2	2.19	0.41
2:E:291:GLY:N	4:E:901:ATP:O1G	2.53	0.41
2:C:85:LYS:HZ3	2:D:14:GLU:HB3	1.85	0.41
2:F:287:THR:CG2	2:F:414:ASN:ND2	2.82	0.41
2:F:344:LEU:HD11	2:F:346:ILE:CG1	2.51	0.41
2:F:345:LYS:HE2	2:F:366:GLU:OE1	2.21	0.41
2:C:111:ASP:OD2	2:C:113:GLU:HG2	2.21	0.41
2:D:451:ARG:HH11	2:D:451:ARG:HG2	1.85	0.41
2:D:340:ARG:C	2:D:342:ASN:H	2.25	0.41
2:D:484:ARG:CB	2:D:484:ARG:NH1	2.84	0.41
2:B:208:ARG:NH2	2:B:221:GLU:OE2	2.54	0.41
2:C:107:ASP:OD1	2:C:107:ASP:C	2.59	0.41
2:F:507:ARG:HB2	2:F:508:ILE:H	1.72	0.40
2:C:295:THR:HG23	2:C:378:ASP:OD2	2.21	0.40
2:C:88:ARG:HG2	2:C:88:ARG:NH1	2.35	0.40
2:F:294:LYS:HE2	2:F:294:LYS:HB2	1.86	0.40
2:C:152:GLN:HG3	2:D:161:ARG:NH1	2.36	0.40
2:D:200:VAL:O	2:D:200:VAL:CG1	2.68	0.40
2:C:120:GLY:C	2:C:122:ASP:N	2.74	0.40
2:E:352:GLU:H	2:E:352:GLU:CD	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ASN:O	1:A:304:ASN:OD1	2.39	0.40
1:A:96:LYS:HE3	1:A:100:GLU:OE2	2.21	0.40
2:D:315:PHE:CD2	2:D:347:VAL:HG21	2.56	0.40
1:A:256:GLN:O	2:F:322:ALA:HB3	2.21	0.40
2:F:21:MET:CE	2:F:59:PHE:CZ	3.04	0.40
2:E:451:ARG:HG2	2:E:451:ARG:NH1	2.36	0.40
2:F:117:VAL:O	2:F:118:VAL:CB	2.69	0.40
1:A:499:VAL:HG12	1:A:499:VAL:O	2.21	0.40
2:D:204:VAL:HG23	2:D:224:LYS:HE2	2.03	0.40
1:A:444:GLU:O	1:A:494:PRO:HD2	2.21	0.40
2:C:248:PRO:C	2:C:250:GLY:N	2.74	0.40
2:E:279:PHE:CE1	2:E:460:GLY:HA3	2.57	0.40
2:B:68:ASP:OD1	2:B:68:ASP:O	2.40	0.40
2:C:118:VAL:O	2:C:118:VAL:HG12	2.21	0.40
2:D:74:VAL:HG13	2:D:106:LEU:HG	2.02	0.40
2:E:497:ILE:O	2:E:498:THR:HG23	2.21	0.40
2:E:462:TRP:O	2:E:463:HIS:O	2.40	0.40
2:E:79:THR:HG22	2:E:82:ASP:HB2	2.03	0.40
2:B:164:LEU:HB3	2:B:200:VAL:HG11	2.03	0.40
2:B:248:PRO:HB2	2:B:251:ALA:CB	2.50	0.40
1:A:435:ASP:HA	1:A:459:ARG:HD2	2.03	0.40
2:B:341:GLN:O	2:B:343:LEU:HG	2.21	0.40
1:A:164:LEU:HD22	1:A:168:VAL:HG23	2.03	0.40
2:E:86:ASN:O	2:E:89:SER:HB3	2.22	0.40
2:B:184:ARG:CG	2:B:191:ILE:O	2.69	0.40
2:C:80:PRO:O	2:C:84:ILE:HG13	2.20	0.40
1:A:85:LYS:HE3	2:B:18:ILE:HD13	2.04	0.40
1:A:371:LYS:O	1:A:371:LYS:HD2	2.20	0.40
2:E:379:SER:H	2:E:413:THR:CG2	2.35	0.40
2:D:71:GLY:HA3	5:D:532:HOH:O	2.21	0.40
1:A:44:VAL:HG22	1:A:205:VAL:HB	2.02	0.40
1:A:88:ARG:HH11	1:A:88:ARG:HG2	1.87	0.40
1:A:510:ARG:HA	1:A:510:ARG:NE	2.36	0.40
2:C:483:PHE:HB2	2:C:489:ILE:HD13	2.03	0.40
2:B:430:ILE:O	2:B:433:ILE:HB	2.22	0.40
2:C:148:THR:HA	2:C:151:PHE:HE1	1.85	0.40
2:B:76:PHE:CZ	2:B:126:LEU:CD2	3.04	0.40
2:E:471:MET:CE	2:E:478:ASP:HB2	2.51	0.40
1:A:468:ARG:HH11	1:A:468:ARG:HG2	1.86	0.40
2:C:21:MET:SD	2:C:141:ARG:NE	2.94	0.40
1:A:50:THR:HA	5:A:535:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:475:LYS:HB2	5:E:550:HOH:O	2.21	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	504/519 (97%)	427 (85%)	54 (11%)	23 (5%)	3	18
2	B	488/519 (94%)	411 (84%)	51 (10%)	26 (5%)	2	14
2	C	485/519 (93%)	420 (87%)	48 (10%)	17 (4%)	4	24
2	D	482/519 (93%)	424 (88%)	44 (9%)	14 (3%)	6	29
2	E	489/519 (94%)	416 (85%)	54 (11%)	19 (4%)	4	21
2	F	503/519 (97%)	422 (84%)	57 (11%)	24 (5%)	3	17
All	All	2951/3114 (95%)	2520 (85%)	308 (10%)	123 (4%)	3	20

All (123) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ALA
1	A	117	VAL
1	A	154	TYR
1	A	333	MET
1	A	417	ASP
1	A	463	HIS
2	B	65	ILE
2	B	154	TYR
2	B	333	MET
2	B	461	SER
2	B	463	HIS

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Mol	Chain	Res	Type
2	B	484	ARG
2	C	17	ALA
2	C	117	VAL
2	C	154	TYR
2	C	463	HIS
2	D	113	GLU
2	D	122	ASP
2	D	154	TYR
2	D	333	MET
2	D	463	HIS
2	E	154	TYR
2	E	333	MET
2	E	425	ILE
2	E	463	HIS
2	F	118	VAL
2	F	154	TYR
2	F	333	MET
2	F	463	HIS
2	F	504	GLU
2	F	506	SER
2	F	507	ARG
2	F	508	ILE
2	F	509	VAL
1	A	387	VAL
1	A	501	GLU
1	A	510	ARG
2	B	119	GLY
2	B	417	ASP
2	B	420	MET
2	B	429	HIS
2	B	494	PRO
2	C	112	PRO
2	C	333	MET
2	D	387	VAL
2	D	420	MET
2	E	122	ASP
2	E	157	SER
2	E	211	LEU
2	E	256	GLN
2	E	420	MET
2	E	484	ARG
2	E	494	PRO

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Mol	Chain	Res	Type
2	E	502	LYS
2	F	212	GLU
2	F	214	GLU
2	F	249	LEU
2	F	417	ASP
2	F	420	MET
2	F	480	LYS
2	F	489	ILE
2	F	501	GLU
1	A	152	GLN
1	A	211	LEU
1	A	420	MET
1	A	499	VAL
2	B	17	ALA
2	B	289	ALA
2	B	341	GLN
2	C	114	GLY
2	C	124	SER
2	C	289	ALA
2	E	379	SER
2	E	480	LYS
2	F	117	VAL
2	F	517	PRO
1	A	212	GLU
1	A	379	SER
2	B	26	GLU
2	B	348	CYS
2	B	498	THR
2	C	121	PHE
2	C	146	SER
2	C	212	GLU
2	C	249	LEU
2	C	379	SER
2	D	212	GLU
2	E	112	PRO
2	F	211	LEU
2	F	500	ASP
1	A	112	PRO
1	A	118	VAL
1	A	348	CYS
2	B	112	PRO
2	B	152	GLN

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Mol	Chain	Res	Type
2	B	379	SER
2	B	422	ALA
2	B	480	LYS
2	C	149	SER
2	C	152	GLN
2	D	348	CYS
2	D	496	ARG
2	E	348	CYS
2	F	348	CYS
2	F	505	LEU
1	A	477	PRO
1	A	494	PRO
2	B	58	GLN
2	C	268	VAL
2	D	211	LEU
2	D	224	LYS
2	D	430	ILE
2	B	64	ILE
2	E	117	VAL
2	E	120	GLY
1	A	120	GLY
1	A	509	VAL
2	B	425	ILE
2	D	18	ILE
2	E	490	ILE
1	A	497	ILE
2	B	117	VAL
2	F	447	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	430/442 (97%)	392 (91%)	38 (9%)	12	42
2	B	416/441 (94%)	375 (90%)	41 (10%)	10	35
2	C	413/441 (94%)	373 (90%)	40 (10%)	10	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	410/441 (93%)	372 (91%)	38 (9%)	11	39
2	E	417/441 (95%)	378 (91%)	39 (9%)	11	39
2	F	429/441 (97%)	389 (91%)	40 (9%)	11	39
All	All	2515/2647 (95%)	2279 (91%)	236 (9%)	11	39

All (236) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	33	HIS
1	A	41	SER
1	A	79	THR
1	A	92	TRP
1	A	99	ASP
1	A	118	VAL
1	A	123	LEU
1	A	140	ARG
1	A	151	PHE
1	A	154	TYR
1	A	155	ASP
1	A	164	LEU
1	A	181	THR
1	A	185	ILE
1	A	186	GLU
1	A	212	GLU
1	A	223	LEU
1	A	238	THR
1	A	256	GLN
1	A	260	ASN
1	A	270	LEU
1	A	287	THR
1	A	342	ASN
1	A	360	LEU
1	A	371	LYS
1	A	375	ILE
1	A	400	THR
1	A	428	SER
1	A	434	THR
1	A	451	ARG
1	A	462	TRP
1	A	469	GLU

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Mol	Chain	Res	Type
1	A	471	MET
1	A	502	LYS
1	A	508	ILE
1	A	509	VAL
1	A	518	GLU
2	B	26	GLU
2	B	48	SER
2	B	79	THR
2	B	81	GLN
2	B	92	TRP
2	B	99	ASP
2	B	106	LEU
2	B	123	LEU
2	B	128	GLU
2	B	140	ARG
2	B	151	PHE
2	B	154	TYR
2	B	164	LEU
2	B	178	THR
2	B	186	GLU
2	B	193	ARG
2	B	209	ASN
2	B	212	GLU
2	B	218	ARG
2	B	223	LEU
2	B	237	PHE
2	B	256	GLN
2	B	270	LEU
2	B	303	GLU
2	B	321	ARG
2	B	333	MET
2	B	342	ASN
2	B	360	LEU
2	B	366	GLU
2	B	371	LYS
2	B	375	ILE
2	B	413	THR
2	B	451	ARG
2	B	458	MET
2	B	462	TRP
2	B	469	GLU
2	B	471	MET

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Mol	Chain	Res	Type
2	B	491	SER
2	B	499	VAL
2	B	501	GLU
2	B	502	LYS
2	C	15	HIS
2	C	26	GLU
2	C	45	SER
2	C	79	THR
2	C	81	GLN
2	C	99	ASP
2	C	111	ASP
2	C	140	ARG
2	C	151	PHE
2	C	154	TYR
2	C	164	LEU
2	C	184	ARG
2	C	185	ILE
2	C	186	GLU
2	C	209	ASN
2	C	211	LEU
2	C	212	GLU
2	C	223	LEU
2	C	228	THR
2	C	245	ASN
2	C	255	THR
2	C	256	GLN
2	C	260	ASN
2	C	270	LEU
2	C	303	GLU
2	C	321	ARG
2	C	333	MET
2	C	360	LEU
2	C	371	LYS
2	C	375	ILE
2	C	400	THR
2	C	428	SER
2	C	430	ILE
2	C	451	ARG
2	C	458	MET
2	C	462	TRP
2	C	470	PHE
2	C	491	SER

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Mol	Chain	Res	Type
2	C	500	ASP
2	C	501	GLU
2	D	26	GLU
2	D	79	THR
2	D	81	GLN
2	D	106	LEU
2	D	122	ASP
2	D	123	LEU
2	D	143	SER
2	D	147	VAL
2	D	150	VAL
2	D	151	PHE
2	D	154	TYR
2	D	181	THR
2	D	186	GLU
2	D	187	GLU
2	D	209	ASN
2	D	212	GLU
2	D	223	LEU
2	D	238	THR
2	D	256	GLN
2	D	260	ASN
2	D	270	LEU
2	D	287	THR
2	D	321	ARG
2	D	342	ASN
2	D	356	LEU
2	D	360	LEU
2	D	371	LYS
2	D	375	ILE
2	D	397	ILE
2	D	451	ARG
2	D	458	MET
2	D	469	GLU
2	D	471	MET
2	D	474	ASP
2	D	487	GLU
2	D	490	ILE
2	D	496	ARG
2	D	498	THR
2	E	26	GLU
2	E	50	THR

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Mol	Chain	Res	Type
2	E	79	THR
2	E	81	GLN
2	E	99	ASP
2	E	106	LEU
2	E	113	GLU
2	E	121	PHE
2	E	140	ARG
2	E	151	PHE
2	E	154	TYR
2	E	185	ILE
2	E	186	GLU
2	E	187	GLU
2	E	191	ILE
2	E	211	LEU
2	E	212	GLU
2	E	223	LEU
2	E	255	THR
2	E	256	GLN
2	E	260	ASN
2	E	263	VAL
2	E	270	LEU
2	E	287	THR
2	E	314	LEU
2	E	321	ARG
2	E	342	ASN
2	E	360	LEU
2	E	371	LYS
2	E	375	ILE
2	E	413	THR
2	E	451	ARG
2	E	458	MET
2	E	461	SER
2	E	471	MET
2	E	474	ASP
2	E	501	GLU
2	E	503	SER
2	E	505	LEU
2	F	26	GLU
2	F	77	GLU
2	F	79	THR
2	F	83	ILE
2	F	99	ASP

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Mol	Chain	Res	Type
2	F	121	PHE
2	F	123	LEU
2	F	140	ARG
2	F	151	PHE
2	F	154	TYR
2	F	178	THR
2	F	183	GLU
2	F	184	ARG
2	F	185	ILE
2	F	186	GLU
2	F	209	ASN
2	F	211	LEU
2	F	218	ARG
2	F	223	LEU
2	F	256	GLN
2	F	270	LEU
2	F	287	THR
2	F	302	VAL
2	F	325	LEU
2	F	344	LEU
2	F	356	LEU
2	F	360	LEU
2	F	371	LYS
2	F	375	ILE
2	F	451	ARG
2	F	462	TRP
2	F	469	GLU
2	F	471	MET
2	F	483	PHE
2	F	496	ARG
2	F	497	ILE
2	F	501	GLU
2	F	504	GLU
2	F	507	ARG
2	F	514	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	62	ASN
1	A	81	GLN

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Mol	Chain	Res	Type
1	A	131	ASN
1	A	135	GLN
1	A	152	GLN
1	A	209	ASN
1	A	245	ASN
1	A	304	ASN
1	A	323	GLN
1	A	327	ASN
1	A	414	ASN
1	A	441	GLN
2	B	33	HIS
2	B	58	GLN
2	B	62	ASN
2	B	81	GLN
2	B	209	ASN
2	B	260	ASN
2	B	304	ASN
2	B	361	GLN
2	B	368	ASN
2	B	418	GLN
2	B	441	GLN
2	C	33	HIS
2	C	81	GLN
2	C	209	ASN
2	C	245	ASN
2	C	256	GLN
2	C	323	GLN
2	C	361	GLN
2	C	368	ASN
2	C	414	ASN
2	C	441	GLN
2	D	33	HIS
2	D	81	GLN
2	D	209	ASN
2	D	304	ASN
2	D	308	ASN
2	D	323	GLN
2	D	368	ASN
2	D	414	ASN
2	D	441	GLN
2	E	33	HIS
2	E	81	GLN

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Mol	Chain	Res	Type
2	E	135	GLN
2	E	209	ASN
2	E	256	GLN
2	E	361	GLN
2	E	368	ASN
2	E	414	ASN
2	E	441	GLN
2	E	454	ASN
2	E	485	ASN
2	F	16	GLN
2	F	81	GLN
2	F	115	GLN
2	F	135	GLN
2	F	209	ASN
2	F	414	ASN
2	F	454	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SEP	B	431	2	8,9,10	1.50	1 (12%)	8,12,14	1.09	1 (12%)
2	SEP	C	431	2	8,9,10	1.57	1 (12%)	8,12,14	1.91	1 (12%)
2	SEP	D	431	2	8,9,10	1.74	3 (37%)	8,12,14	3.86	1 (12%)
2	SEP	E	431	2	8,9,10	1.51	2 (25%)	8,12,14	1.29	2 (25%)
2	SEP	F	431	2	8,9,10	1.57	2 (25%)	8,12,14	2.70	2 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SEP	B	431	2	-	0/6/8/10	0/0/0/0
2	SEP	C	431	2	-	0/6/8/10	0/0/0/0
2	SEP	D	431	2	-	0/6/8/10	0/0/0/0
2	SEP	E	431	2	-	0/6/8/10	0/0/0/0
2	SEP	F	431	2	-	0/6/8/10	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	431	SEP	P-O2P	2.04	1.62	1.54
2	D	431	SEP	P-O3P	2.07	1.62	1.54
2	F	431	SEP	P-O3P	2.09	1.62	1.54
2	E	431	SEP	P-O3P	2.16	1.62	1.54
2	E	431	SEP	P-O1P	2.79	1.60	1.51
2	B	431	SEP	P-O1P	3.02	1.61	1.51
2	C	431	SEP	P-O1P	3.17	1.61	1.51
2	D	431	SEP	P-O1P	3.25	1.61	1.51
2	F	431	SEP	P-O1P	3.31	1.62	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	431	SEP	O-C-CA	-2.35	119.38	125.49
2	B	431	SEP	O-C-CA	-2.17	119.83	125.49
2	F	431	SEP	O-C-CA	-2.13	119.95	125.49
2	E	431	SEP	O3P-P-OG	2.53	113.84	106.56
2	C	431	SEP	OG-CB-CA	4.72	112.30	108.27
2	F	431	SEP	OG-CB-CA	7.10	114.33	108.27
2	D	431	SEP	OG-CB-CA	10.61	117.33	108.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	431	SEP	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	431	SEP	3	0
2	D	431	SEP	6	0
2	E	431	SEP	3	0
2	F	431	SEP	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 9 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	ATP	A	901	3	24,33,33	1.30	3 (12%)	31,52,52	2.58	6 (19%)
4	ATP	A	903	3	24,33,33	1.27	3 (12%)	31,52,52	2.66	5 (16%)
4	ATP	B	901	3	24,33,33	1.29	3 (12%)	31,52,52	2.61	6 (19%)
4	ATP	B	903	3	24,33,33	1.33	4 (16%)	31,52,52	2.66	6 (19%)
4	ATP	C	901	3	24,33,33	1.37	4 (16%)	31,52,52	2.54	7 (22%)
4	ATP	C	903	3	24,33,33	1.17	1 (4%)	31,52,52	2.69	6 (19%)
4	ATP	D	901	3	24,33,33	1.32	4 (16%)	31,52,52	2.57	6 (19%)
4	ATP	D	903	-	24,33,33	1.31	3 (12%)	31,52,52	2.87	6 (19%)
4	ATP	E	901	3	24,33,33	1.33	4 (16%)	31,52,52	2.61	7 (22%)
4	ATP	E	903	-	24,33,33	1.32	2 (8%)	31,52,52	2.56	7 (22%)
4	ATP	F	901	3	24,33,33	1.33	3 (12%)	31,52,52	2.54	7 (22%)
4	ATP	F	903	-	24,33,33	1.10	2 (8%)	31,52,52	2.62	6 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	A	901	3	-	0/18/38/38	0/3/3/3
4	ATP	A	903	3	-	0/18/38/38	0/3/3/3
4	ATP	B	901	3	-	0/18/38/38	0/3/3/3
4	ATP	B	903	3	-	0/18/38/38	0/3/3/3
4	ATP	C	901	3	-	0/18/38/38	0/3/3/3
4	ATP	C	903	3	-	0/18/38/38	0/3/3/3
4	ATP	D	901	3	-	0/18/38/38	0/3/3/3
4	ATP	D	903	-	-	0/18/38/38	0/3/3/3
4	ATP	E	901	3	-	0/18/38/38	0/3/3/3
4	ATP	E	903	-	-	0/18/38/38	0/3/3/3
4	ATP	F	901	3	-	0/18/38/38	0/3/3/3
4	ATP	F	903	-	-	0/18/38/38	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	901	ATP	O4'-C4'	-2.03	1.40	1.45
4	E	901	ATP	C2-N1	2.00	1.37	1.33
4	B	901	ATP	C4-N3	2.03	1.38	1.35
4	F	903	ATP	C2-N1	2.04	1.37	1.33
4	A	901	ATP	C2-N1	2.06	1.37	1.33
4	D	901	ATP	O4'-C1'	2.11	1.43	1.41
4	E	903	ATP	C2-N1	2.12	1.37	1.33
4	A	903	ATP	C2-N1	2.14	1.38	1.33
4	B	903	ATP	O4'-C1'	2.19	1.44	1.41
4	D	903	ATP	O4'-C1'	2.19	1.44	1.41
4	D	901	ATP	C2-N1	2.21	1.38	1.33
4	B	903	ATP	C2-N1	2.22	1.38	1.33
4	F	901	ATP	C2-N1	2.24	1.38	1.33
4	B	903	ATP	C4-N3	2.25	1.38	1.35
4	E	901	ATP	C4-N3	2.28	1.39	1.35
4	C	901	ATP	C2-N1	2.33	1.38	1.33
4	D	901	ATP	C4-N3	2.39	1.39	1.35
4	C	901	ATP	O4'-C1'	2.42	1.44	1.41
4	E	901	ATP	O4'-C1'	2.44	1.44	1.41
4	D	903	ATP	C4-N3	2.66	1.39	1.35
4	B	901	ATP	O4'-C1'	2.87	1.44	1.41
4	A	903	ATP	O4'-C1'	2.99	1.45	1.41
4	A	901	ATP	O4'-C1'	3.01	1.45	1.41
4	F	901	ATP	O4'-C1'	3.10	1.45	1.41
4	F	903	ATP	C2-N3	3.18	1.37	1.32
4	B	901	ATP	C2-N3	3.49	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	903	ATP	C2-N3	3.51	1.38	1.32
4	F	901	ATP	C2-N3	3.60	1.38	1.32
4	A	901	ATP	C2-N3	3.66	1.38	1.32
4	C	903	ATP	C2-N3	3.72	1.38	1.32
4	D	903	ATP	C2-N3	3.79	1.38	1.32
4	D	901	ATP	C2-N3	3.81	1.38	1.32
4	B	903	ATP	C2-N3	4.01	1.39	1.32
4	E	901	ATP	C2-N3	4.04	1.39	1.32
4	E	903	ATP	C2-N3	4.10	1.39	1.32
4	C	901	ATP	C2-N3	4.16	1.39	1.32

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	903	ATP	N3-C2-N1	-12.62	119.23	128.89
4	B	901	ATP	N3-C2-N1	-11.88	119.80	128.89
4	C	903	ATP	N3-C2-N1	-11.77	119.88	128.89
4	A	903	ATP	N3-C2-N1	-11.74	119.90	128.89
4	E	901	ATP	N3-C2-N1	-11.70	119.94	128.89
4	F	903	ATP	N3-C2-N1	-11.65	119.97	128.89
4	B	903	ATP	N3-C2-N1	-11.57	120.04	128.89
4	F	901	ATP	N3-C2-N1	-11.48	120.10	128.89
4	D	901	ATP	N3-C2-N1	-11.39	120.17	128.89
4	A	901	ATP	N3-C2-N1	-11.32	120.22	128.89
4	C	901	ATP	N3-C2-N1	-11.30	120.24	128.89
4	E	903	ATP	N3-C2-N1	-10.82	120.61	128.89
4	E	901	ATP	C4-C5-N7	-4.83	105.04	109.48
4	C	903	ATP	C4-C5-N7	-4.82	105.05	109.48
4	E	903	ATP	C4-C5-N7	-4.78	105.08	109.48
4	B	903	ATP	C4-C5-N7	-4.77	105.09	109.48
4	D	903	ATP	C4-C5-N7	-4.76	105.10	109.48
4	A	903	ATP	C4-C5-N7	-4.72	105.14	109.48
4	D	901	ATP	C4-C5-N7	-4.66	105.19	109.48
4	A	901	ATP	C4-C5-N7	-4.61	105.24	109.48
4	C	901	ATP	C4-C5-N7	-4.59	105.25	109.48
4	F	901	ATP	C4-C5-N7	-4.58	105.27	109.48
4	B	901	ATP	C4-C5-N7	-4.53	105.31	109.48
4	F	903	ATP	C4-C5-N7	-4.52	105.32	109.48
4	C	903	ATP	N6-C6-N1	-2.56	113.72	119.20
4	A	903	ATP	N6-C6-N1	-2.47	113.89	119.20
4	D	903	ATP	N6-C6-N1	-2.47	113.90	119.20
4	B	903	ATP	N6-C6-N1	-2.39	114.06	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	ATP	N6-C6-N1	-2.35	114.16	119.20
4	E	901	ATP	N6-C6-N1	-2.30	114.26	119.20
4	F	903	ATP	N6-C6-N1	-2.27	114.32	119.20
4	F	901	ATP	N6-C6-N1	-2.27	114.34	119.20
4	B	901	ATP	N6-C6-N1	-2.24	114.39	119.20
4	E	903	ATP	PB-O3B-PG	-2.22	125.22	132.67
4	D	901	ATP	N6-C6-N1	-2.19	114.51	119.20
4	E	903	ATP	N6-C6-N1	-2.15	114.59	119.20
4	C	901	ATP	N6-C6-N1	-2.08	114.75	119.20
4	F	901	ATP	O2B-PB-O3B	2.10	114.62	105.09
4	C	901	ATP	O2'-C2'-C3'	2.12	118.74	111.83
4	E	903	ATP	O2B-PB-O3B	2.13	114.77	105.09
4	A	901	ATP	O2B-PB-O3B	2.15	114.84	105.09
4	F	901	ATP	O2'-C2'-C3'	2.17	118.87	111.83
4	B	903	ATP	O2B-PB-O3B	2.17	114.92	105.09
4	E	901	ATP	O2'-C2'-C3'	2.22	119.05	111.83
4	F	901	ATP	O3A-PA-O5'	2.33	109.13	102.94
4	E	901	ATP	O2B-PB-O3B	2.36	115.78	105.09
4	B	901	ATP	O2B-PB-O3B	2.37	115.85	105.09
4	C	903	ATP	O2B-PB-O3B	2.37	115.86	105.09
4	E	901	ATP	O3A-PA-O5'	2.41	109.34	102.94
4	F	903	ATP	O2B-PB-O3B	2.53	116.56	105.09
4	C	901	ATP	C2'-C1'-N9	2.58	118.23	114.29
4	C	901	ATP	O2B-PB-O3B	2.64	117.08	105.09
4	D	903	ATP	O2B-PB-O3B	2.64	117.08	105.09
4	E	901	ATP	C2'-C1'-N9	2.65	118.34	114.29
4	C	901	ATP	O3A-PA-O5'	2.67	110.02	102.94
4	B	901	ATP	O2'-C2'-C3'	2.69	120.57	111.83
4	D	901	ATP	O2B-PB-O3B	2.76	117.63	105.09
4	D	901	ATP	O3A-PA-O5'	2.77	110.30	102.94
4	F	901	ATP	C2'-C1'-N9	2.78	118.55	114.29
4	A	901	ATP	O3A-PA-O5'	2.79	110.33	102.94
4	B	901	ATP	C2'-C1'-N9	2.91	118.74	114.29
4	E	903	ATP	C2'-C1'-N9	2.93	118.77	114.29
4	A	903	ATP	O3A-PA-O5'	2.99	110.88	102.94
4	F	903	ATP	O3A-PA-O5'	3.13	111.25	102.94
4	B	903	ATP	O3A-PA-O5'	3.19	111.41	102.94
4	F	903	ATP	C2'-C1'-N9	3.24	119.24	114.29
4	E	903	ATP	O3A-PA-O5'	3.32	111.73	102.94
4	C	903	ATP	O3A-PA-O5'	3.33	111.78	102.94
4	A	901	ATP	C2'-C1'-N9	3.58	119.76	114.29
4	A	903	ATP	C2'-C1'-N9	3.60	119.79	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	903	ATP	C2'-C1'-N9	3.72	119.97	114.29
4	D	901	ATP	C2'-C1'-N9	3.73	119.99	114.29
4	D	903	ATP	O3A-PA-O5'	3.76	112.90	102.94
4	B	903	ATP	C2'-C1'-N9	4.03	120.45	114.29
4	D	903	ATP	C2'-C1'-N9	4.43	121.06	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	ATP	3	0
4	A	903	ATP	4	0
4	B	901	ATP	4	0
4	B	903	ATP	4	0
4	C	901	ATP	1	0
4	C	903	ATP	4	0
4	D	903	ATP	3	0
4	E	901	ATP	4	0
4	E	903	ATP	4	0
4	F	901	ATP	4	0
4	F	903	ATP	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	506/519 (97%)	0.34	45 (8%)	12 4	19, 74, 114, 146	0
2	B	490/519 (94%)	0.25	24 (4%)	33 13	31, 75, 116, 157	0
2	C	487/519 (93%)	-0.04	15 (3%)	52 24	29, 61, 114, 156	0
2	D	484/519 (93%)	-0.16	20 (4%)	41 16	17, 45, 100, 144	0
2	E	491/519 (94%)	0.02	28 (5%)	27 10	10, 58, 105, 145	0
2	F	505/519 (97%)	0.27	45 (8%)	12 4	14, 72, 116, 135	0
All	All	2963/3114 (95%)	0.11	177 (5%)	25 9	10, 64, 114, 157	0

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	517	PRO	9.9
2	F	517	PRO	9.9
2	F	519	SER	8.0
1	A	518	GLU	7.8
2	F	506	SER	7.7
1	A	120	GLY	7.7
2	F	518	GLU	6.8
1	A	506	SER	6.6
1	A	519	SER	6.5
2	F	516	GLY	6.5
2	B	116	GLU	6.2
1	A	516	GLY	6.1
1	A	511	GLY	6.1
2	B	503	SER	6.0
2	B	117	VAL	6.0
2	B	119	GLY	6.0
2	C	500	ASP	6.0
2	E	503	SER	5.9
2	D	120	GLY	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	512	VAL	5.8
2	E	423	HIS	5.7
2	C	501	GLU	5.6
1	A	515	LYS	5.6
1	A	513	GLN	5.6
2	C	423	HIS	5.5
1	A	514	GLU	5.4
1	A	154	TYR	5.4
2	D	117	VAL	5.4
2	B	118	VAL	5.3
2	F	507	ARG	5.1
2	E	500	ASP	5.1
2	F	423	HIS	4.9
2	B	121	PHE	4.9
1	A	503	SER	4.9
2	B	500	ASP	4.9
2	F	505	LEU	4.8
2	F	503	SER	4.8
2	E	505	LEU	4.8
2	F	154	TYR	4.8
2	C	499	VAL	4.8
2	F	500	ASP	4.7
1	A	507	ARG	4.7
1	A	153	GLN	4.7
2	E	501	GLU	4.6
2	F	498	THR	4.6
2	F	511	GLY	4.5
1	A	121	PHE	4.5
2	F	514	GLU	4.4
2	F	515	LYS	4.4
2	E	504	GLU	4.3
1	A	119	GLY	4.3
2	D	118	VAL	4.2
1	A	509	VAL	4.1
2	E	153	GLN	4.1
2	F	421	GLY	4.1
2	E	154	TYR	4.0
2	F	504	GLU	4.0
2	B	423	HIS	4.0
2	F	509	VAL	3.9
2	B	16	GLN	3.9
1	A	500	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	152	GLN	3.9
2	F	513	GLN	3.9
2	F	485	ASN	3.9
2	C	427	ASP	3.8
1	A	508	ILE	3.8
2	B	154	TYR	3.8
1	A	502	LYS	3.8
1	A	510	ARG	3.7
2	B	504	GLU	3.7
2	D	121	PHE	3.6
1	A	340	ARG	3.6
2	F	508	ILE	3.6
2	B	501	GLU	3.5
2	C	118	VAL	3.5
2	D	423	HIS	3.5
1	A	427	ASP	3.5
2	D	119	GLY	3.4
2	B	502	LYS	3.4
2	C	154	TYR	3.4
1	A	417	ASP	3.3
2	F	496	ARG	3.3
2	F	501	GLU	3.3
2	F	293	GLY	3.2
2	D	16	GLN	3.2
2	D	336	GLU	3.2
1	A	499	VAL	3.2
2	F	340	ARG	3.1
2	F	512	VAL	3.1
2	C	120	GLY	3.1
2	D	427	ASP	3.1
2	E	421	GLY	3.0
2	B	498	THR	3.0
2	C	188	TYR	3.0
1	A	114	GLY	3.0
2	F	427	ASP	3.0
2	E	118	VAL	2.9
2	E	427	ASP	2.9
2	F	499	VAL	2.9
2	D	154	TYR	2.9
2	E	306	CYS	2.9
2	F	502	LYS	2.9
2	E	502	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	421	GLY	2.8
2	F	255	THR	2.8
1	A	309	LYS	2.8
1	A	504	GLU	2.8
2	F	369	ASP	2.8
1	A	16	GLN	2.7
2	F	311	ARG	2.7
1	A	257	ARG	2.7
1	A	423	HIS	2.6
2	F	510	ARG	2.6
1	A	505	LEU	2.6
1	A	117	VAL	2.6
1	A	501	GLU	2.6
1	A	403	ALA	2.5
2	D	15	HIS	2.5
1	A	258	SER	2.5
2	F	153	GLN	2.5
2	F	434	THR	2.5
2	C	117	VAL	2.5
2	B	88	ARG	2.5
2	E	113	GLU	2.5
2	B	120	GLY	2.5
2	B	369	ASP	2.5
2	D	201	SER	2.5
2	E	116	GLU	2.5
2	B	309	LYS	2.5
2	E	422	ALA	2.4
2	B	428	SER	2.4
2	C	123	LEU	2.4
2	F	370	PHE	2.4
2	E	120	GLY	2.4
2	E	339	GLU	2.4
2	B	153	GLN	2.4
2	D	498	THR	2.4
1	A	496	ARG	2.4
2	D	157	SER	2.3
2	F	484	ARG	2.3
1	A	498	THR	2.3
2	D	434	THR	2.3
2	D	424	SER	2.3
1	A	475	LYS	2.3
2	F	303	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	121	PHE	2.3
2	C	428	SER	2.2
2	E	336	GLU	2.2
1	A	255	THR	2.2
2	C	255	THR	2.2
2	E	310	GLU	2.2
2	D	116	GLU	2.2
2	E	485	ASN	2.2
2	C	119	GLY	2.2
1	A	486	PHE	2.1
2	F	302	VAL	2.1
2	C	145	ASP	2.1
1	A	484	ARG	2.1
2	D	447	GLY	2.1
2	E	329	TYR	2.1
2	D	429	HIS	2.1
2	E	117	VAL	2.1
2	F	152	GLN	2.1
2	E	121	PHE	2.1
2	F	309	LYS	2.1
2	B	158	SER	2.1
2	E	487	GLU	2.1
2	F	422	ALA	2.1
2	B	272	GLU	2.0
2	F	286	ALA	2.0
2	F	287	THR	2.0
2	E	429	HIS	2.0
2	E	480	LYS	2.0
2	B	499	VAL	2.0
1	A	344	LEU	2.0
2	B	15	HIS	2.0
2	E	342	ASN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SEP	C	431	10/11	0.73	0.39	-	77,84,97,97	0
2	SEP	D	431	10/11	0.61	0.47	-	83,89,104,105	0
2	SEP	E	431	10/11	0.83	0.30	-	71,78,90,91	0
2	SEP	F	431	10/11	0.55	0.45	-	73,82,88,88	0
2	SEP	B	431	10/11	0.66	0.30	-	98,101,104,104	0

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	B	802	1/1	0.83	0.58	9.61	92,92,92,92	0
3	MG	B	521	1/1	0.82	0.41	4.36	33,33,33,33	0
3	MG	C	522	1/1	0.91	0.50	2.22	38,38,38,38	0
4	ATP	F	903	31/31	0.90	0.27	1.63	30,37,41,44	0
4	ATP	E	903	31/31	0.92	0.27	1.34	28,31,46,53	0
4	ATP	D	903	31/31	0.93	0.23	1.32	24,30,49,50	0
4	ATP	C	903	31/31	0.90	0.28	1.22	43,48,71,72	0
4	ATP	B	901	31/31	0.90	0.27	0.70	58,63,74,77	0
4	ATP	B	903	31/31	0.89	0.24	0.52	57,62,67,70	0
4	ATP	A	903	31/31	0.94	0.22	0.43	42,49,53,54	0
4	ATP	D	901	31/31	0.92	0.24	0.10	48,52,54,55	0
4	ATP	E	901	31/31	0.90	0.28	0.09	60,71,77,78	0
4	ATP	C	901	31/31	0.94	0.20	0.04	31,39,42,44	0
4	ATP	F	901	31/31	0.90	0.28	-0.04	78,89,91,93	0
4	ATP	A	901	31/31	0.88	0.25	-0.06	75,88,90,92	0
3	MG	A	801	1/1	0.68	0.23	-2.38	54,54,54,54	0
3	MG	A	521	1/1	0.89	0.29	-	23,23,23,23	0
3	MG	D	804	1/1	0.68	0.45	-	17,17,17,17	0
3	MG	C	803	1/1	0.70	0.36	-	16,16,16,16	0
3	MG	E	805	1/1	0.64	0.27	-	25,25,25,25	0
3	MG	F	806	1/1	0.76	0.58	-	54,54,54,54	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.