



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:25 PM 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 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/ValidationPDFNotes.html>

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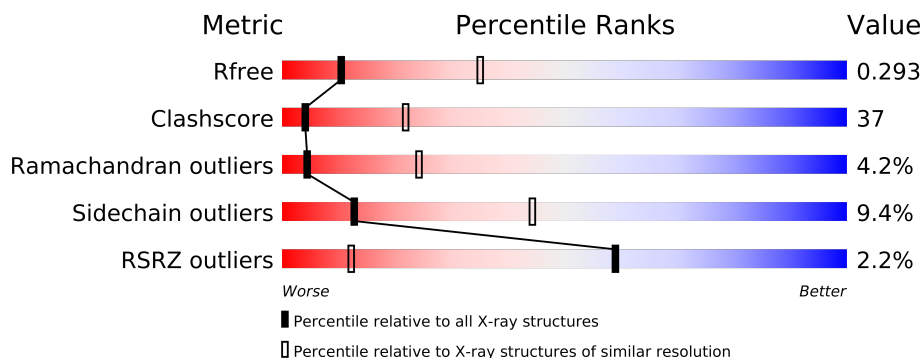
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	519	
2	B	519	
2	C	519	
2	D	519	
2	E	519	
2	F	519	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MG	B	521	-	X
3	MG	B	802	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	MG	C	522	-	X
3	MG	C	803	-	X
3	MG	D	804	-	X
3	MG	F	806	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23930 atoms, of which 0 are hydrogen and 0 are deuterium.

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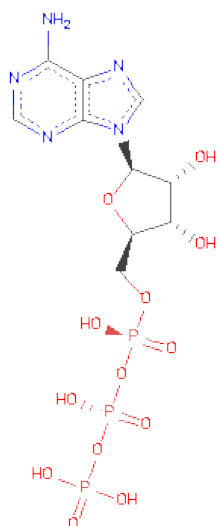
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Chain	Residue	Modelled	Actual	Comment	Reference
E	426	ALA	THR	ENGINEERED	UNP Q79PF4
E	432	ALA	THR	ENGINEERED	UNP Q79PF4
F	426	ALA	THR	ENGINEERED	UNP Q79PF4
F	432	ALA	THR	ENGINEERED	UNP Q79PF4

- 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<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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.

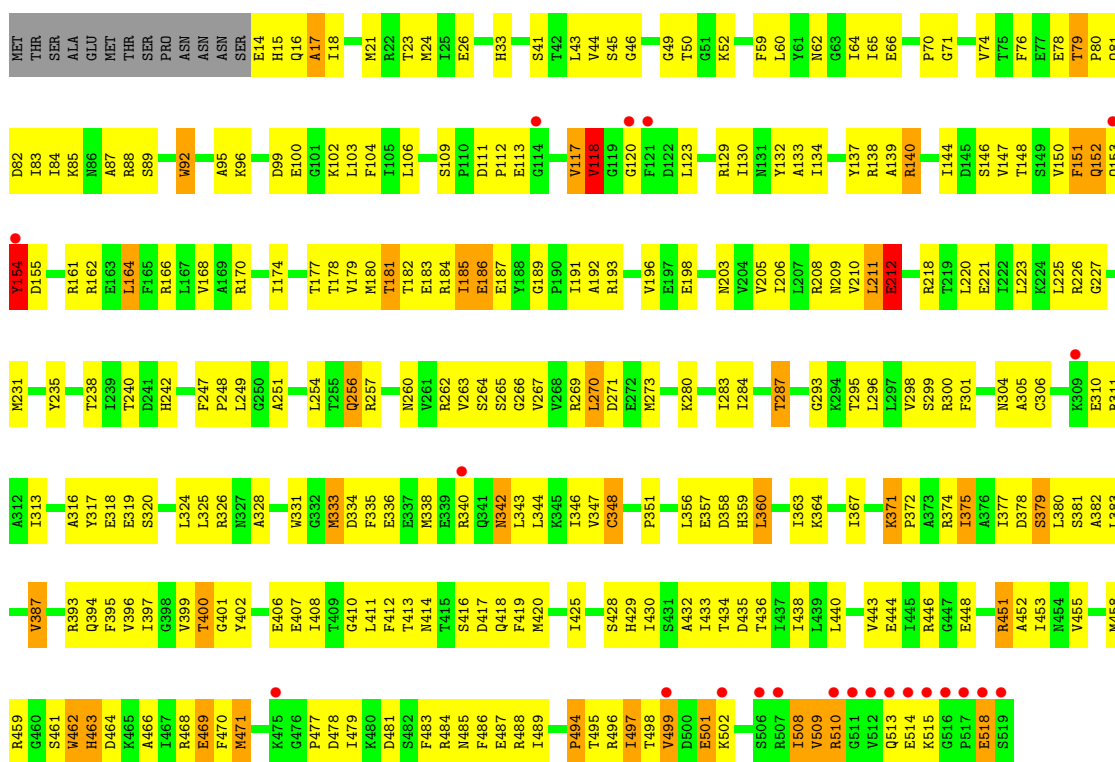
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	21	Total	O	0	0
			21	21		
5	B	12	Total	O	0	0
			12	12		
5	C	23	Total	O	0	0
			23	23		
5	D	37	Total	O	0	0
			37	37		
5	E	34	Total	O	0	0
			34	34		
5	F	40	Total	O	0	0
			40	40		

### 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.

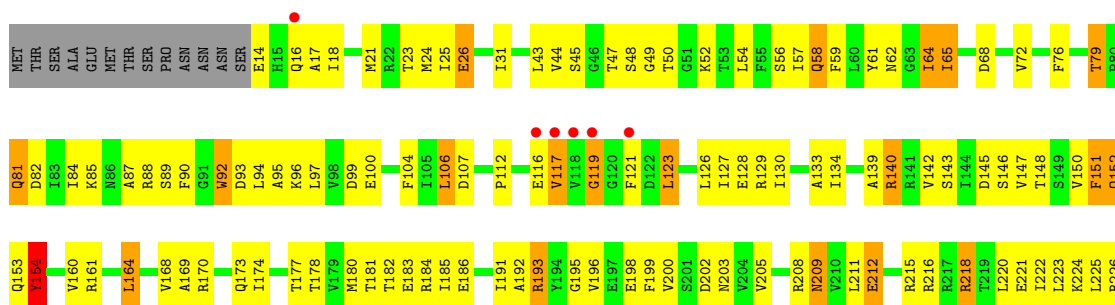
#### • Molecule 1: Circadian clock protein kinase KaiC

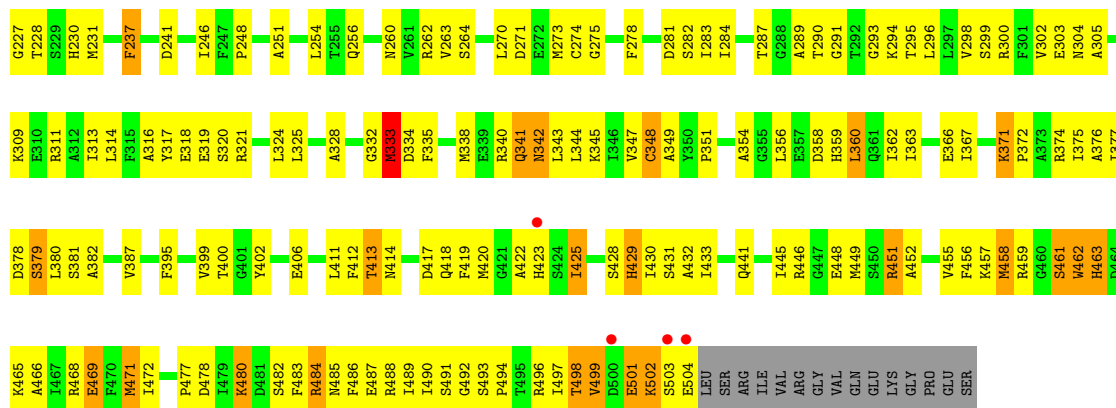
Chain A:



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

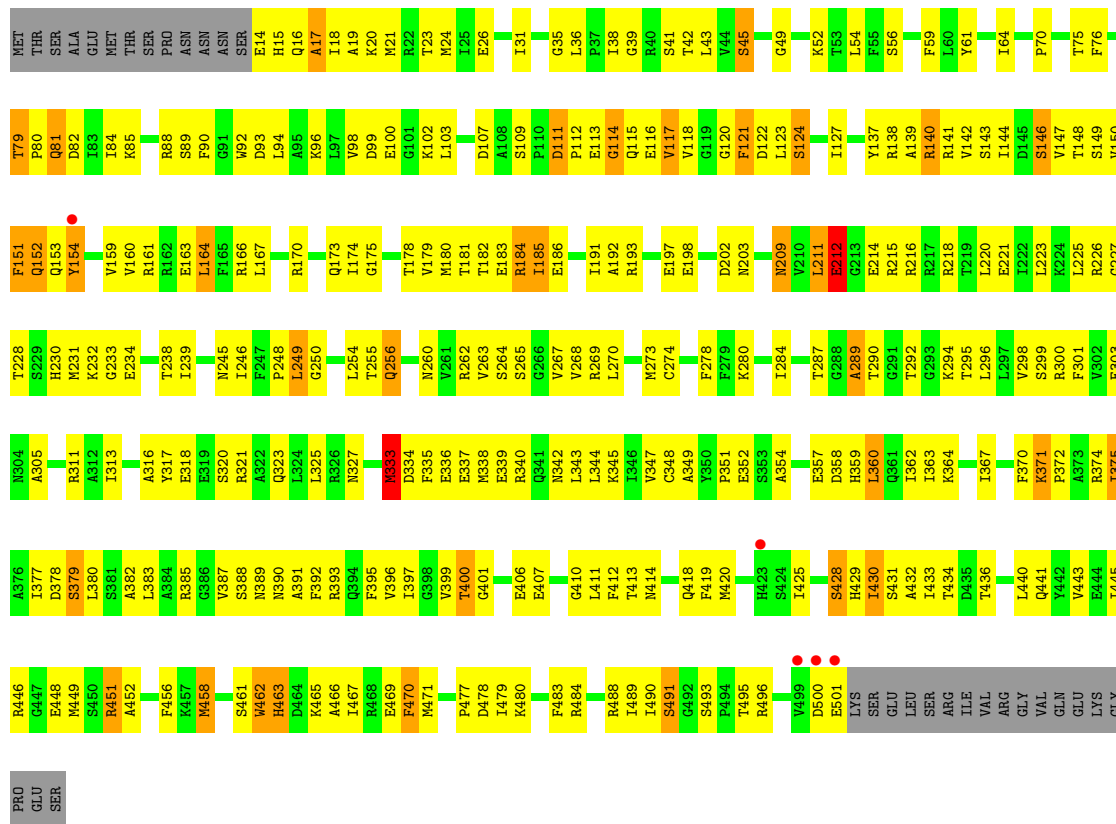
Chain B:





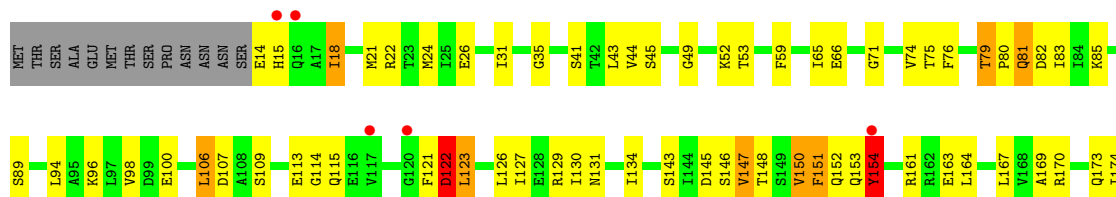
### • Molecule 2: Circadian clock protein kinase KaiC

Chain C:

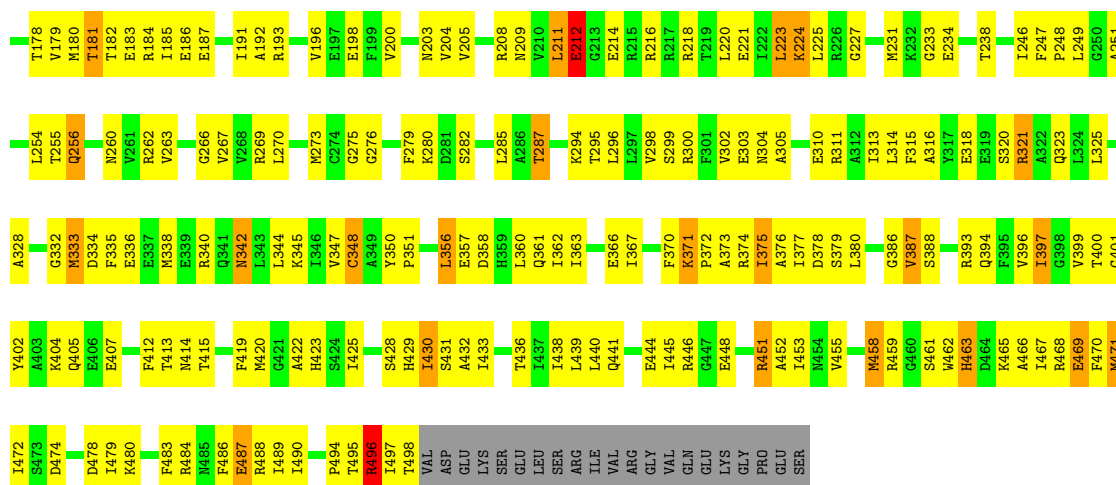


### • Molecule 2: Circadian clock protein kinase KaiC

Chain D:

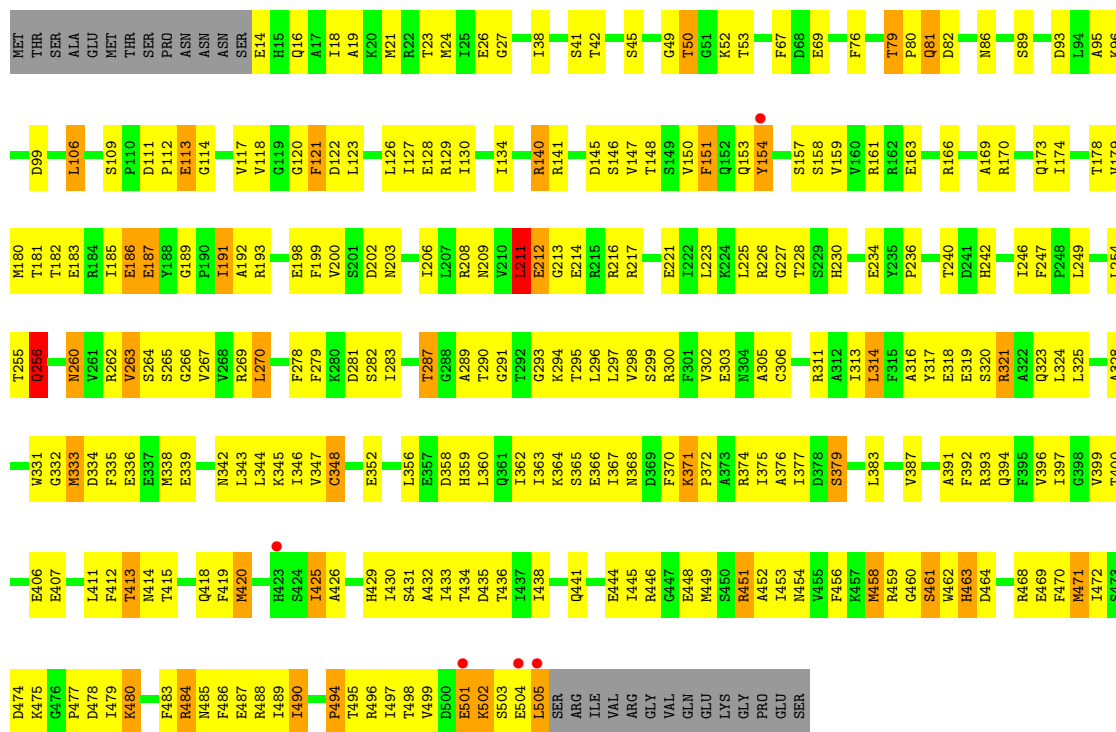






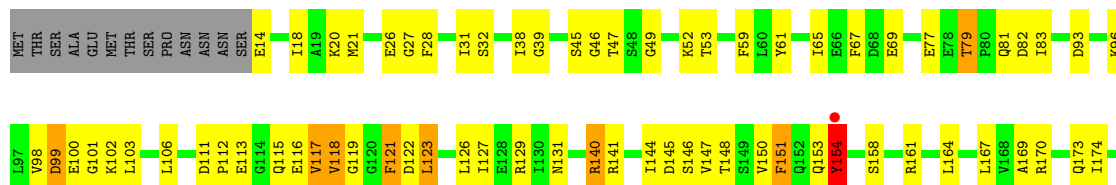
• Molecule 2: Circadian clock protein kinase KaiC

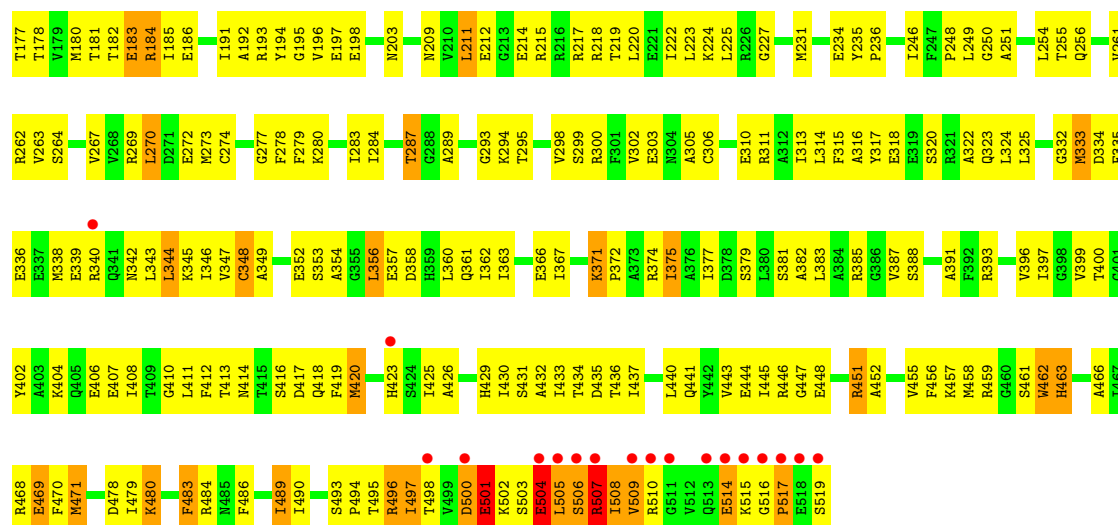
Chain E:



• Molecule 2: Circadian clock protein kinase KaiC

Chain F:





## 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 , 0.293	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 , 26.0	EDS
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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.

## 5 Model quality

### 5.1 Standard geometry

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 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	3846	0	3834	285	0
2	D	3822	0	3815	310	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 37.

All (1736) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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
2:B:263:VAL:CG1	2:B:374:ARG:HH21	1.92	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:352:GLU:H	2:E:352:GLU:CD	2.24	0.40
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	Distance(Å)	Clash(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

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	504/519 (97%)	427 (85%)	54 (11%)	23 (5%)	4	22
2	B	488/519 (94%)	411 (84%)	51 (10%)	26 (5%)	3	18
2	C	485/519 (93%)	420 (87%)	48 (10%)	17 (4%)	6	30
2	D	482/519 (93%)	424 (88%)	44 (9%)	14 (3%)	7	35
2	E	489/519 (94%)	416 (85%)	54 (11%)	19 (4%)	5	26
2	F	503/519 (97%)	422 (84%)	57 (11%)	24 (5%)	4	20
All	All	2951/3114 (95%)	2520 (85%)	308 (10%)	123 (4%)	4	24

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
2	B	484	ARG
2	C	17	ALA
2	C	117	VAL

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Mol	Chain	Res	Type
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
2	E	502	LYS
2	F	212	GLU
2	F	214	GLU

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Mol	Chain	Res	Type
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
2	B	379	SER
2	B	422	ALA
2	B	480	LYS

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Mol	Chain	Res	Type
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%)	14	48
2	B	416/441 (94%)	375 (90%)	41 (10%)	11	40
2	C	413/441 (94%)	373 (90%)	40 (10%)	12	42
2	D	410/441 (93%)	372 (91%)	38 (9%)	13	45
2	E	417/441 (95%)	378 (91%)	39 (9%)	13	44
2	F	429/441 (97%)	389 (91%)	40 (9%)	13	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2515/2647 (95%)	2279 (91%)	236 (9%)	13	44

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
1	A	471	MET
1	A	502	LYS
1	A	508	ILE
1	A	509	VAL

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Mol	Chain	Res	Type
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
2	B	491	SER
2	B	499	VAL
2	B	501	GLU
2	B	502	LYS

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Mol	Chain	Res	Type
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
2	C	500	ASP
2	C	501	GLU
2	D	26	GLU
2	D	79	THR

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Mol	Chain	Res	Type
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
2	E	79	THR
2	E	81	GLN
2	E	99	ASP
2	E	106	LEU

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Mol	Chain	Res	Type
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
2	F	121	PHE
2	F	123	LEU
2	F	140	ARG
2	F	151	PHE

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Mol	Chain	Res	Type
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
1	A	131	ASN
1	A	135	GLN
1	A	152	GLN
1	A	209	ASN

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Mol	Chain	Res	Type
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
2	E	135	GLN
2	E	209	ASN
2	E	256	GLN
2	E	361	GLN

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Mol	Chain	Res	Type
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 chains 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	9,9,10	6.44	3 (33%)	10,12,14	1.20	2 (20%)
2	SEP	C	431	2	9,9,10	5.60	2 (22%)	10,12,14	1.76	3 (30%)
2	SEP	D	431	2	9,9,10	6.86	5 (55%)	10,12,14	3.03	3 (30%)
2	SEP	E	431	2	9,9,10	5.95	4 (44%)	10,12,14	1.18	1 (10%)
2	SEP	F	431	2	9,9,10	5.14	4 (44%)	10,12,14	2.61	2 (20%)

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 (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	431	SEP	O-C	19.96	1.25	1.11
2	B	431	SEP	O-C	18.61	1.24	1.11
2	E	431	SEP	O-C	16.70	1.22	1.11
2	C	431	SEP	O-C	16.17	1.22	1.11
2	F	431	SEP	O-C	14.64	1.21	1.11
2	E	431	SEP	CA-C	4.74	1.57	1.48
2	B	431	SEP	CA-C	3.30	1.54	1.48
2	F	431	SEP	P-O1P	3.23	1.62	1.51
2	D	431	SEP	P-O1P	3.17	1.61	1.51
2	C	431	SEP	P-O1P	3.09	1.61	1.51
2	B	431	SEP	P-O1P	2.95	1.61	1.51
2	E	431	SEP	P-O1P	2.73	1.60	1.51
2	D	431	SEP	CA-C	2.22	1.52	1.48
2	F	431	SEP	CA-C	2.17	1.52	1.48
2	E	431	SEP	P-O3P	2.12	1.62	1.54
2	F	431	SEP	P-O3P	2.05	1.62	1.54
2	D	431	SEP	P-O3P	2.03	1.62	1.54
2	D	431	SEP	P-O2P	2.00	1.62	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	431	SEP	P-OG-CB	-6.94	98.13	118.19
2	D	431	SEP	P-OG-CB	-6.47	99.47	118.19
2	D	431	SEP	OG-CB-CA	6.10	117.33	108.69
2	F	431	SEP	OG-CB-CA	3.98	114.33	108.69
2	C	431	SEP	C-CA-N	3.39	117.21	113.83
2	C	431	SEP	P-OG-CB	-3.04	109.41	118.19
2	E	431	SEP	O3P-P-OG	2.60	113.84	106.65
2	C	431	SEP	OG-CB-CA	2.55	112.30	108.69
2	D	431	SEP	C-CA-N	-2.31	111.52	113.83
2	B	431	SEP	P-OG-CB	-2.20	111.84	118.19
2	B	431	SEP	CB-CA-N	-2.09	101.17	110.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	33,33,33	1.19	2 (6%)	52,52,52	2.07	10 (19%)
4	ATP	A	903	3	33,33,33	1.13	3 (9%)	52,52,52	2.13	10 (19%)
4	ATP	B	901	3	33,33,33	1.12	2 (6%)	52,52,52	2.12	11 (21%)
4	ATP	B	903	3	33,33,33	1.18	3 (9%)	52,52,52	2.19	12 (23%)
4	ATP	C	901	3	33,33,33	1.18	3 (9%)	52,52,52	2.16	12 (23%)
4	ATP	C	903	3	33,33,33	1.05	1 (3%)	52,52,52	2.23	12 (23%)
4	ATP	D	901	3	33,33,33	1.13	3 (9%)	52,52,52	2.17	11 (21%)
4	ATP	D	903	-	33,33,33	1.17	2 (6%)	52,52,52	2.33	14 (26%)
4	ATP	E	901	3	33,33,33	1.15	2 (6%)	52,52,52	2.17	12 (23%)
4	ATP	E	903	-	33,33,33	1.25	3 (9%)	52,52,52	2.10	13 (25%)
4	ATP	F	901	3	33,33,33	1.15	3 (9%)	52,52,52	2.06	11 (21%)
4	ATP	F	903	-	33,33,33	1.08	2 (6%)	52,52,52	2.20	12 (23%)

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	-	0/22/38/38	0/1/3/3
4	ATP	A	903	3	-	0/22/38/38	0/1/3/3
4	ATP	B	901	3	-	0/22/38/38	0/1/3/3
4	ATP	B	903	3	-	0/22/38/38	0/1/3/3
4	ATP	C	901	3	-	0/22/38/38	0/1/3/3
4	ATP	C	903	3	-	0/22/38/38	0/1/3/3
4	ATP	D	901	3	-	0/22/38/38	0/1/3/3
4	ATP	D	903	-	-	0/22/38/38	0/1/3/3
4	ATP	E	901	3	-	0/22/38/38	0/1/3/3
4	ATP	E	903	-	-	0/22/38/38	0/1/3/3
4	ATP	F	901	3	-	0/22/38/38	0/1/3/3
4	ATP	F	903	-	-	0/22/38/38	0/1/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	901	ATP	C2-N3	3.73	1.39	1.32
4	E	903	ATP	C2-N3	3.67	1.39	1.32
4	E	901	ATP	C2-N3	3.63	1.39	1.32
4	B	903	ATP	C2-N3	3.60	1.39	1.32
4	D	901	ATP	C2-N3	3.41	1.38	1.32
4	D	903	ATP	C2-N3	3.40	1.38	1.32
4	C	903	ATP	C2-N3	3.34	1.38	1.32
4	A	901	ATP	C2-N3	3.28	1.38	1.32
4	F	901	ATP	C2-N3	3.23	1.38	1.32
4	A	903	ATP	C2-N3	3.15	1.38	1.32
4	B	901	ATP	C2-N3	3.13	1.38	1.32
4	E	903	ATP	PB-O3B	-3.11	1.54	1.59
4	F	903	ATP	C2-N3	2.85	1.37	1.32
4	D	903	ATP	C4-N3	2.56	1.39	1.35
4	F	901	ATP	O4'-C1'	2.46	1.45	1.41
4	A	901	ATP	O4'-C1'	2.38	1.45	1.41
4	A	903	ATP	O4'-C1'	2.37	1.45	1.41
4	F	903	ATP	C2'-C1'	-2.33	1.50	1.53
4	D	901	ATP	C4-N3	2.30	1.39	1.35
4	B	901	ATP	O4'-C1'	2.27	1.44	1.41
4	C	901	ATP	C2-N1	2.24	1.38	1.33
4	E	901	ATP	C4-N3	2.20	1.39	1.35
4	B	903	ATP	C4-N3	2.17	1.38	1.35
4	F	901	ATP	C2-N1	2.16	1.38	1.33
4	B	903	ATP	C2-N1	2.13	1.38	1.33
4	D	901	ATP	C2-N1	2.13	1.38	1.33
4	A	903	ATP	C2-N1	2.06	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	903	ATP	C2-N1	2.04	1.37	1.33
4	C	901	ATP	O4'-C4'	-2.01	1.40	1.45

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	903	ATP	N3-C2-N1	-11.34	119.23	128.71
4	B	901	ATP	N3-C2-N1	-10.66	119.80	128.71
4	C	903	ATP	N3-C2-N1	-10.56	119.88	128.71
4	A	903	ATP	N3-C2-N1	-10.53	119.90	128.71
4	E	901	ATP	N3-C2-N1	-10.49	119.94	128.71
4	F	903	ATP	N3-C2-N1	-10.45	119.97	128.71
4	B	903	ATP	N3-C2-N1	-10.37	120.04	128.71
4	F	901	ATP	N3-C2-N1	-10.30	120.10	128.71
4	D	901	ATP	N3-C2-N1	-10.21	120.17	128.71
4	A	901	ATP	N3-C2-N1	-10.15	120.22	128.71
4	C	901	ATP	N3-C2-N1	-10.13	120.24	128.71
4	E	903	ATP	N3-C2-N1	-9.69	120.61	128.71
4	E	901	ATP	C4-C5-N7	-5.24	105.04	109.52
4	C	903	ATP	C4-C5-N7	-5.22	105.05	109.52
4	E	903	ATP	C4-C5-N7	-5.19	105.08	109.52
4	B	903	ATP	C4-C5-N7	-5.18	105.09	109.52
4	D	903	ATP	C4-C5-N7	-5.16	105.10	109.52
4	A	903	ATP	C4-C5-N7	-5.12	105.14	109.52
4	D	901	ATP	C4-C5-N7	-5.06	105.19	109.52
4	A	901	ATP	C4-C5-N7	-5.00	105.24	109.52
4	C	901	ATP	C4-C5-N7	-4.98	105.25	109.52
4	F	901	ATP	C4-C5-N7	-4.97	105.27	109.52
4	B	901	ATP	C4-C5-N7	-4.92	105.31	109.52
4	F	903	ATP	C4-C5-N7	-4.90	105.32	109.52
4	F	903	ATP	O3A-PB-O3B	4.89	111.60	101.66
4	D	901	ATP	O3A-PB-O3B	4.64	111.10	101.66
4	D	903	ATP	O3A-PB-O3B	4.50	110.81	101.66
4	C	903	ATP	O3A-PB-O3B	4.22	110.23	101.66
4	B	903	ATP	O3A-PB-O3B	3.80	109.39	101.66
4	C	901	ATP	O3A-PB-O3B	3.59	108.96	101.66
4	C	901	ATP	O4'-C1'-N9	-3.53	105.15	108.44
4	D	901	ATP	O4'-C1'-N9	-3.22	105.45	108.44
4	B	901	ATP	O3A-PB-O3B	3.15	108.08	101.66
4	E	903	ATP	O4'-C1'-N9	-3.14	105.52	108.44
4	E	901	ATP	O4'-C1'-N9	-3.05	105.60	108.44
4	D	903	ATP	C2'-C1'-N9	3.03	121.06	113.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	903	ATP	N6-C6-N1	-2.88	113.72	119.36
4	E	901	ATP	N3-C4-N9	2.83	130.54	125.43
4	D	901	ATP	N3-C4-N9	2.83	130.54	125.43
4	B	903	ATP	O4'-C1'-N9	-2.81	105.83	108.44
4	B	903	ATP	C2'-C1'-N9	2.80	120.45	113.27
4	A	903	ATP	N6-C6-N1	-2.79	113.89	119.36
4	D	903	ATP	N6-C6-N1	-2.78	113.90	119.36
4	C	901	ATP	N3-C4-N9	2.75	130.41	125.43
4	B	903	ATP	N6-C6-N1	-2.70	114.06	119.36
4	B	901	ATP	O2'-C2'-C3'	2.68	120.57	111.83
4	F	903	ATP	N7-C8-N9	-2.67	106.82	114.36
4	E	901	ATP	C8-N7-C5	2.66	111.84	103.58
4	A	901	ATP	N6-C6-N1	-2.65	114.16	119.36
4	E	903	ATP	C8-N7-C5	2.65	111.80	103.58
4	D	901	ATP	C8-N7-C5	2.64	111.76	103.58
4	D	901	ATP	O2B-PB-O3B	2.63	117.63	105.14
4	D	903	ATP	N7-C8-N9	-2.62	106.94	114.36
4	B	903	ATP	C8-N7-C5	2.62	111.71	103.58
4	D	901	ATP	C2'-C1'-N9	2.62	119.99	113.27
4	C	903	ATP	C2'-C1'-N9	2.61	119.97	113.27
4	A	901	ATP	O4'-C1'-N9	-2.61	106.02	108.44
4	C	901	ATP	C8-N7-C5	2.60	111.64	103.58
4	C	903	ATP	C5-C6-N6	2.60	126.60	120.72
4	E	901	ATP	N6-C6-N1	-2.60	114.26	119.36
4	C	903	ATP	N7-C8-N9	-2.60	107.01	114.36
4	C	903	ATP	C8-N7-C5	2.59	111.60	103.58
4	A	901	ATP	C8-N7-C5	2.58	111.59	103.58
4	E	901	ATP	O3A-PB-O3B	2.58	106.90	101.66
4	D	903	ATP	C8-N7-C5	2.57	111.55	103.58
4	E	903	ATP	N3-C4-N9	2.57	130.07	125.43
4	F	903	ATP	N6-C6-N1	-2.57	114.32	119.36
4	B	903	ATP	N3-C4-N9	2.56	130.06	125.43
4	F	901	ATP	N6-C6-N1	-2.56	114.34	119.36
4	B	901	ATP	C8-N7-C5	2.55	111.48	103.58
4	F	901	ATP	C8-N7-C5	2.55	111.48	103.58
4	F	903	ATP	C8-N9-C4	2.54	108.84	106.90
4	A	903	ATP	C5-C6-N6	2.54	126.47	120.72
4	A	903	ATP	C2'-C1'-N9	2.54	119.79	113.27
4	B	901	ATP	N6-C6-N1	-2.54	114.39	119.36
4	A	901	ATP	C2'-C1'-N9	2.53	119.76	113.27
4	A	903	ATP	C8-N7-C5	2.53	111.42	103.58
4	B	901	ATP	N3-C4-N9	2.53	129.99	125.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	ATP	N3-C4-N9	2.52	129.99	125.43
4	D	903	ATP	N3-C4-N9	2.52	129.98	125.43
4	C	901	ATP	O2B-PB-O3B	2.52	117.08	105.14
4	D	903	ATP	O2B-PB-O3B	2.52	117.08	105.14
4	F	901	ATP	N3-C4-N9	2.51	129.97	125.43
4	E	903	ATP	N7-C8-N9	-2.50	107.28	114.36
4	C	901	ATP	C3'-C2'-C1'	2.50	104.82	100.91
4	A	903	ATP	N7-C8-N9	-2.50	107.29	114.36
4	C	903	ATP	O4'-C1'-N9	-2.49	106.12	108.44
4	F	903	ATP	C5-C6-N6	2.48	126.32	120.72
4	D	901	ATP	N6-C6-N1	-2.47	114.51	119.36
4	B	901	ATP	N7-C8-N9	-2.46	107.39	114.36
4	F	903	ATP	C8-N7-C5	2.46	111.22	103.58
4	E	901	ATP	N7-C8-N9	-2.46	107.40	114.36
4	A	901	ATP	C5-C6-N6	2.46	126.28	120.72
4	E	903	ATP	N6-C6-N1	-2.43	114.59	119.36
4	B	903	ATP	N7-C8-N9	-2.43	107.50	114.36
4	D	901	ATP	N7-C8-N9	-2.43	107.50	114.36
4	B	903	ATP	C5-C6-N6	2.42	126.20	120.72
4	A	903	ATP	O3A-PB-O3B	2.42	106.59	101.66
4	C	901	ATP	N7-C8-N9	-2.42	107.52	114.36
4	F	903	ATP	O2B-PB-O3B	2.41	116.56	105.14
4	F	901	ATP	C5-C6-N6	2.40	126.15	120.72
4	A	901	ATP	N7-C8-N9	-2.40	107.58	114.36
4	B	903	ATP	C3'-C2'-C1'	2.38	104.64	100.91
4	F	901	ATP	N7-C8-N9	-2.38	107.62	114.36
4	E	901	ATP	C3'-C2'-C1'	2.38	104.64	100.91
4	F	901	ATP	O4'-C1'-N9	-2.36	106.25	108.44
4	C	901	ATP	N6-C6-N1	-2.35	114.75	119.36
4	F	901	ATP	O3A-PB-O3B	2.34	106.43	101.66
4	F	903	ATP	C2'-C1'-N9	2.33	119.24	113.27
4	D	903	ATP	C5-C6-N6	2.31	125.94	120.72
4	D	903	ATP	C8-N9-C4	2.30	108.65	106.90
4	E	903	ATP	C5-C6-N6	2.29	125.89	120.72
4	E	901	ATP	C5-C6-N6	2.26	125.83	120.72
4	C	903	ATP	O2B-PB-O3B	2.26	115.86	105.14
4	B	901	ATP	O2B-PB-O3B	2.26	115.85	105.14
4	B	901	ATP	C5-C6-N6	2.25	125.81	120.72
4	E	901	ATP	O2B-PB-O3B	2.24	115.78	105.14
4	A	903	ATP	O4'-C1'-N9	-2.24	106.36	108.44
4	C	903	ATP	N3-C4-N9	2.23	129.47	125.43
4	F	903	ATP	C3'-C2'-C1'	2.23	104.40	100.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	901	ATP	O2'-C2'-C3'	2.22	119.05	111.83
4	D	901	ATP	C5-C6-N6	2.22	125.73	120.72
4	E	903	ATP	PB-O3B-PG	-2.21	125.22	131.68
4	A	903	ATP	N3-C4-N9	2.19	129.39	125.43
4	C	903	ATP	C3'-C2'-C1'	2.19	104.33	100.91
4	F	901	ATP	O2'-C2'-C3'	2.16	118.87	111.83
4	C	901	ATP	C5-C6-N6	2.15	125.58	120.72
4	E	903	ATP	C2'-C1'-N9	2.14	118.77	113.27
4	B	901	ATP	C2'-C1'-N9	2.13	118.74	113.27
4	D	903	ATP	O3A-PA-O5'	2.12	112.90	103.41
4	C	901	ATP	O2'-C2'-C3'	2.12	118.74	111.83
4	E	903	ATP	C3'-C2'-C1'	2.08	104.17	100.91
4	D	903	ATP	C2-N3-C4	2.07	119.91	114.01
4	B	903	ATP	O2B-PB-O3B	2.06	114.92	105.14
4	F	901	ATP	C2'-C1'-N9	2.06	118.55	113.27
4	A	901	ATP	O2B-PB-O3B	2.05	114.84	105.14
4	D	903	ATP	O4'-C1'-N9	-2.04	106.55	108.44
4	F	903	ATP	N3-C4-N9	2.04	129.11	125.43
4	E	903	ATP	O2B-PB-O3B	2.03	114.77	105.14
4	E	903	ATP	O3A-PB-O3B	2.00	105.74	101.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.09	22 (4%)	34	7	19, 74, 114, 146	0
2	B	491/519 (94%)	0.03	10 (2%)	62	12	31, 75, 116, 157	0
2	C	488/519 (94%)	-0.10	5 (1%)	79	22	29, 61, 114, 156	0
2	D	485/519 (93%)	-0.18	5 (1%)	79	22	17, 45, 100, 144	0
2	E	492/519 (94%)	-0.08	5 (1%)	79	22	10, 58, 105, 145	0
2	F	506/519 (97%)	0.05	19 (3%)	38	7	14, 73, 116, 135	0
All	All	2968/3114 (95%)	-0.03	66 (2%)	59	12	10, 64, 114, 157	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	517	PRO	5.0
1	A	518	GLU	5.0
1	A	517	PRO	4.8
2	F	518	GLU	4.1
1	A	120	GLY	3.8
2	C	501	GLU	3.6
2	B	119	GLY	3.5
2	F	516	GLY	3.4
2	E	423	HIS	3.3
1	A	515	LYS	3.2
2	C	423	HIS	3.2
2	F	507	ARG	3.1
1	A	516	GLY	3.1
2	F	519	SER	3.0
2	C	500	ASP	3.0
2	E	501	GLU	3.0
2	B	116	GLU	3.0
1	A	507	ARG	2.9
1	A	502	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	F	515	LYS	2.9
1	A	154	TYR	2.8
2	F	506	SER	2.8
2	D	120	GLY	2.8
2	B	121	PHE	2.8
2	B	118	VAL	2.8
1	A	519	SER	2.7
2	F	511	GLY	2.7
1	A	514	GLU	2.7
1	A	511	GLY	2.7
2	D	16	GLN	2.7
2	E	154	TYR	2.6
2	C	499	VAL	2.6
2	F	505	LEU	2.6
2	F	504	GLU	2.6
2	B	16	GLN	2.6
2	F	154	TYR	2.5
2	F	498	THR	2.5
1	A	512	VAL	2.4
1	A	121	PHE	2.4
2	B	117	VAL	2.4
2	F	423	HIS	2.4
1	A	513	GLN	2.4
2	F	514	GLU	2.4
1	A	510	ARG	2.4
1	A	309	LYS	2.4
2	F	513	GLN	2.3
1	A	340	ARG	2.3
1	A	153	GLN	2.2
2	F	500	ASP	2.2
1	A	114	GLY	2.2
2	B	500	ASP	2.2
2	F	510	ARG	2.2
2	F	509	VAL	2.2
2	E	505	LEU	2.2
2	B	503	SER	2.1
2	D	15	HIS	2.1
2	D	117	VAL	2.1
1	A	506	SER	2.1
2	F	340	ARG	2.1
2	E	504	GLU	2.1
2	B	504	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	423	HIS	2.1
2	C	154	TYR	2.1
1	A	499	VAL	2.1
1	A	475	LYS	2.1
2	D	154	TYR	2.0

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

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SEP	D	431	10/11	0.47	2.00	83,89,104,105	0
2	SEP	C	431	10/11	0.40	1.69	77,84,97,97	0
2	SEP	F	431	10/11	0.46	1.60	73,82,88,88	0
2	SEP	E	431	10/11	0.29	0.33	71,78,90,91	0
2	SEP	B	431	10/11	0.29	-0.13	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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	B	802	1/1	0.61	7.92	92,92,92,92	0
3	MG	B	521	1/1	0.42	3.33	33,33,33,33	0
3	MG	F	806	1/1	0.56	3.10	54,54,54,54	0
3	MG	C	803	1/1	0.36	2.48	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	C	522	1/1	0.49	2.17	38,38,38,38	0
3	MG	D	804	1/1	0.44	2.16	17,17,17,17	0
4	ATP	F	903	31/31	0.28	1.55	30,37,41,44	0
3	MG	A	521	1/1	0.28	1.54	23,23,23,23	0
4	ATP	E	903	31/31	0.26	1.35	28,31,46,53	0
4	ATP	C	903	31/31	0.28	1.18	43,48,71,72	0
4	ATP	D	903	31/31	0.23	1.10	24,30,49,50	0
4	ATP	B	901	31/31	0.28	0.82	58,63,74,77	0
4	ATP	A	903	31/31	0.22	0.60	42,49,53,54	0
4	ATP	B	903	31/31	0.24	0.50	57,62,67,70	0
4	ATP	A	901	31/31	0.27	0.17	75,88,90,92	0
4	ATP	F	901	31/31	0.28	0.12	78,89,91,93	0
4	ATP	E	901	31/31	0.29	0.11	60,71,77,78	0
4	ATP	C	901	31/31	0.20	0.10	31,39,42,44	0
4	ATP	D	901	31/31	0.23	0.06	48,52,54,55	0
3	MG	E	805	1/1	0.26	-1.06	25,25,25,25	0
3	MG	A	801	1/1	0.24	-1.71	54,54,54,54	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.