



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:15 AM GMT

PDB ID : 3DVL  
Title : Crystal Structure of Full Length Circadian Clock Protein KaiC with Correct Geometry at Phosphorylation Sites  
Authors : Pattanayek, R.; Egli, M.  
Deposited on : 2008-07-18  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

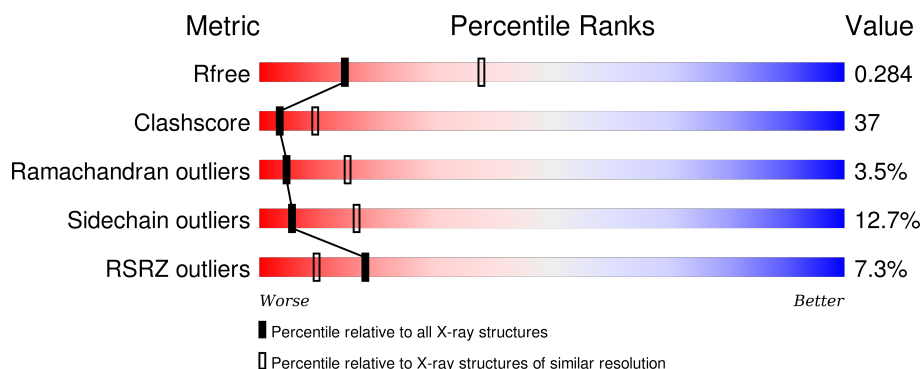
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	519	<div> <div>12%</div> <div>45%</div> <div>42%</div> <div>10%</div> <div>• •</div> </div>
1	B	519	<div> <div>8%</div> <div>43%</div> <div>41%</div> <div>9%</div> <div>• 5%</div> </div>
1	C	519	<div> <div>5%</div> <div>47%</div> <div>36%</div> <div>11%</div> <div>• 6%</div> </div>
1	D	519	<div> <div>4%</div> <div>48%</div> <div>37%</div> <div>7%</div> <div>• 7%</div> </div>
1	E	519	<div> <div>6%</div> <div>46%</div> <div>38%</div> <div>11%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	519	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	SEP	A	431	-	-	X	-
1	TPO	A	432	-	-	X	-
1	SEP	B	431	-	-	X	-
1	TPO	B	432	X	-	X	-
1	SEP	C	431	-	-	X	-
1	TPO	D	432	X	-	-	-
1	TPO	E	432	X	-	-	-
1	TPO	F	432	X	-	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23870 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Circadian clock protein kinase kaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	P	S	0	0	0
			3993	2509	701	766	2	15			
1	B	491	Total	C	N	O	P	S	0	0	0
			3878	2439	678	744	2	15			
1	C	488	Total	C	N	O	P	S	0	0	0
			3850	2425	674	735	1	15			
1	D	485	Total	C	N	O	P	S	0	0	0
			3826	2411	671	728	1	15			
1	E	492	Total	C	N	O	P	S	0	0	0
			3886	2445	679	745	2	15			
1	F	506	Total	C	N	O	P	S	0	0	0
			3993	2509	701	766	2	15			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 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
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

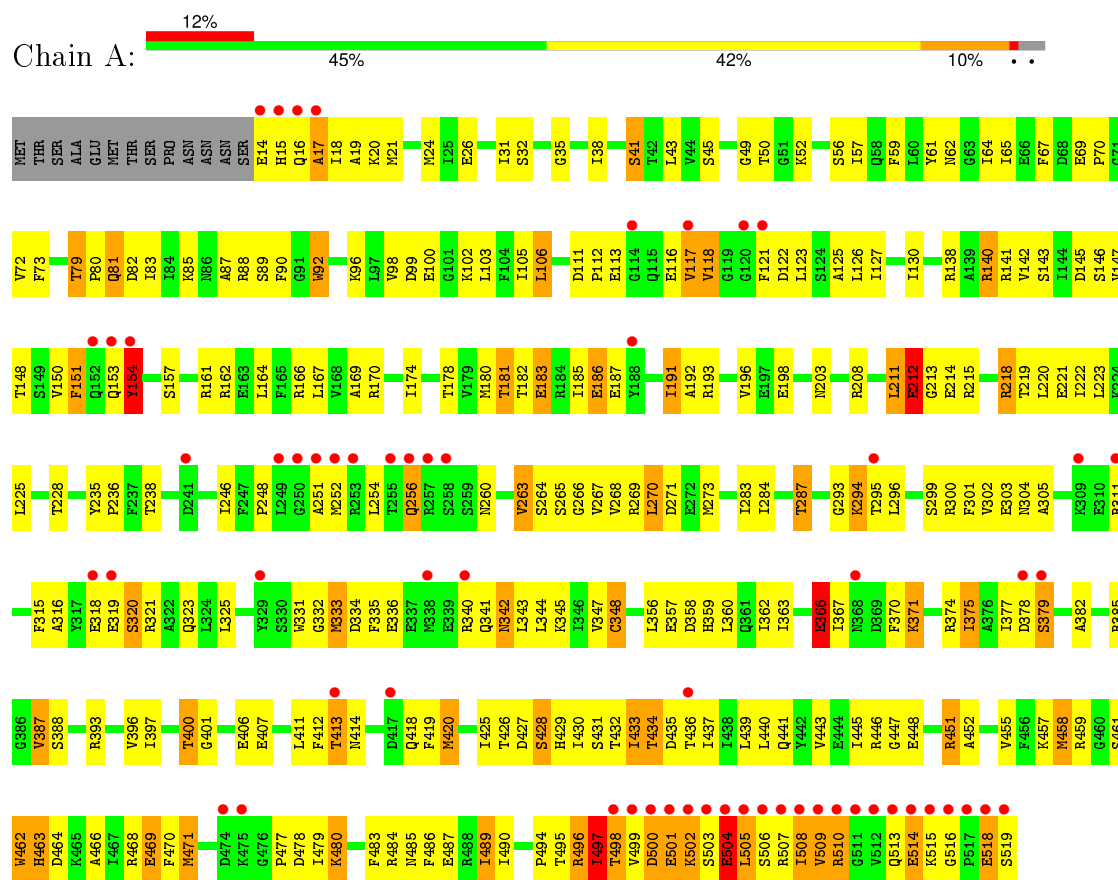
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total 7	O 7	0	0
4	B	5	Total 5	O 5	0	0
4	C	7	Total 7	O 7	0	0
4	D	12	Total 12	O 12	0	0
4	E	10	Total 10	O 10	0	0
4	F	25	Total 25	O 25	0	0

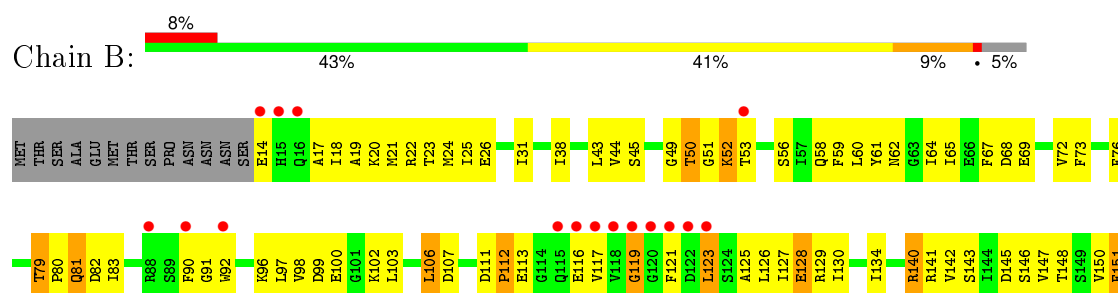
### 3 Residue-property plots

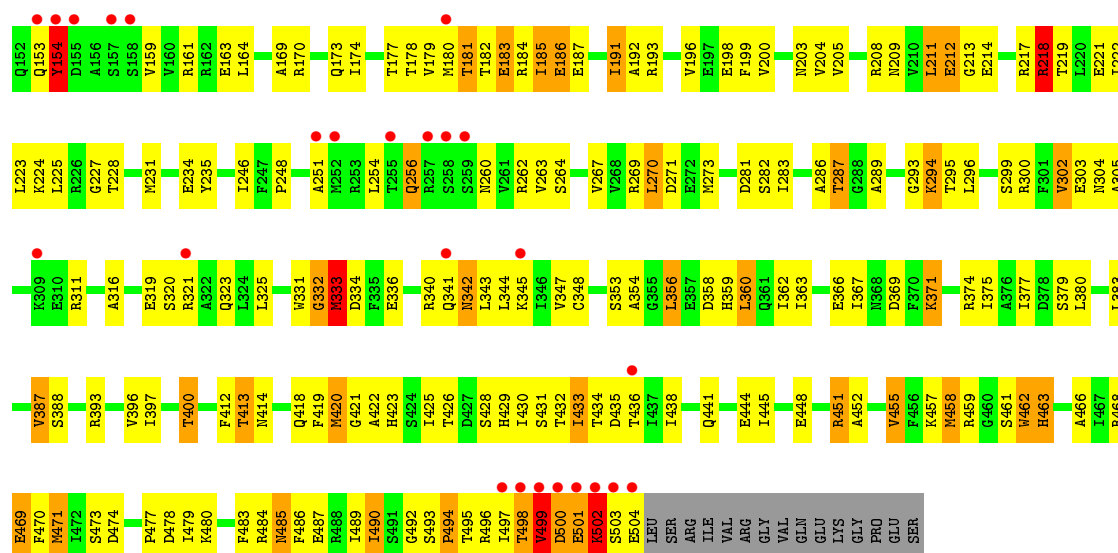
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

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

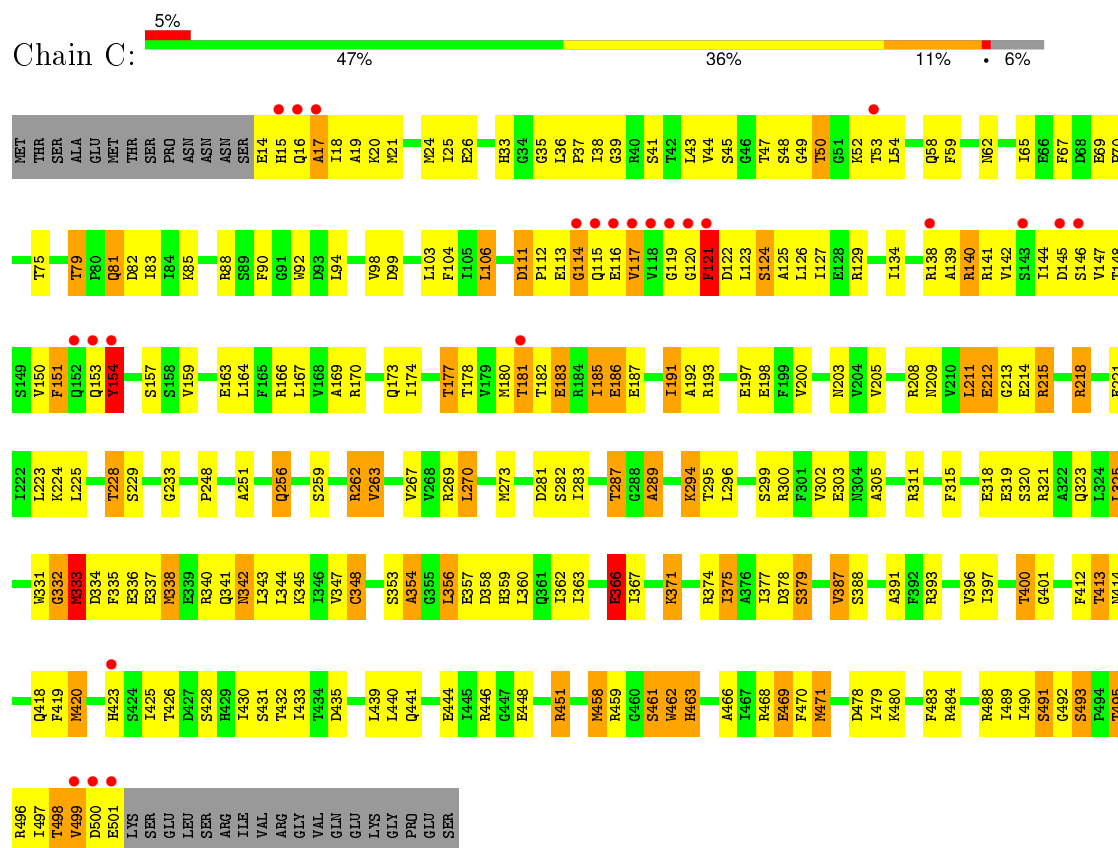


#### • Molecule 1: Circadian clock protein kinase kaiC

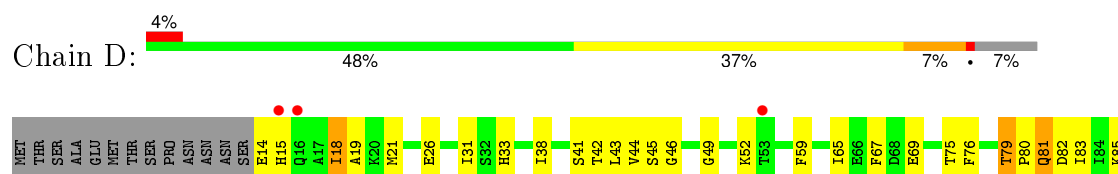




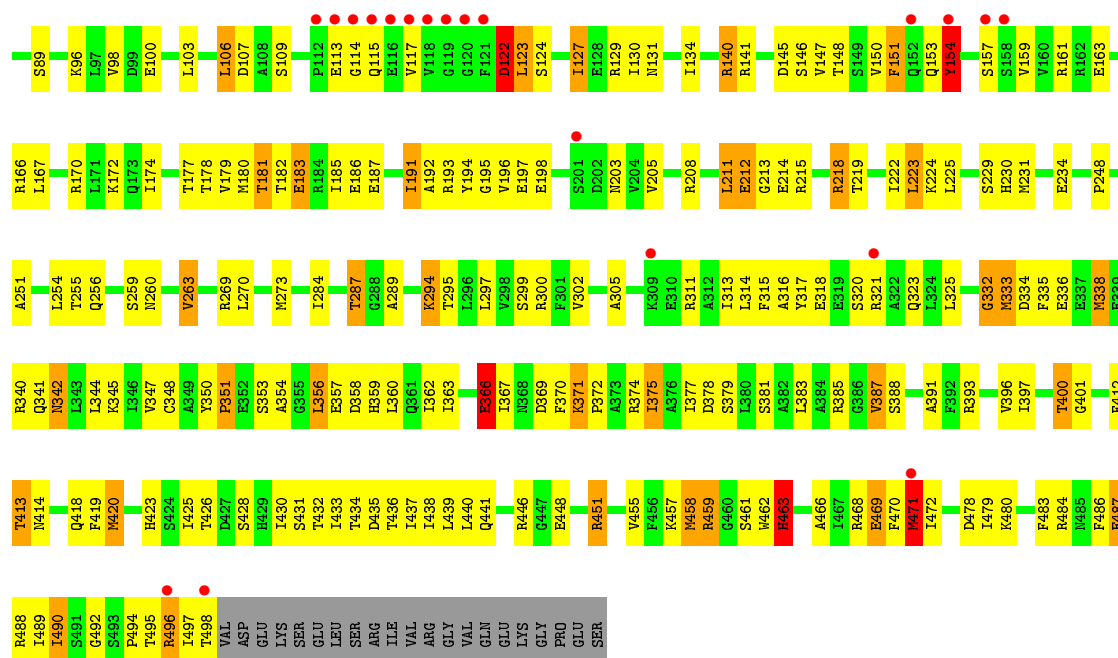
• Molecule 1: Circadian clock protein kinase kaiC



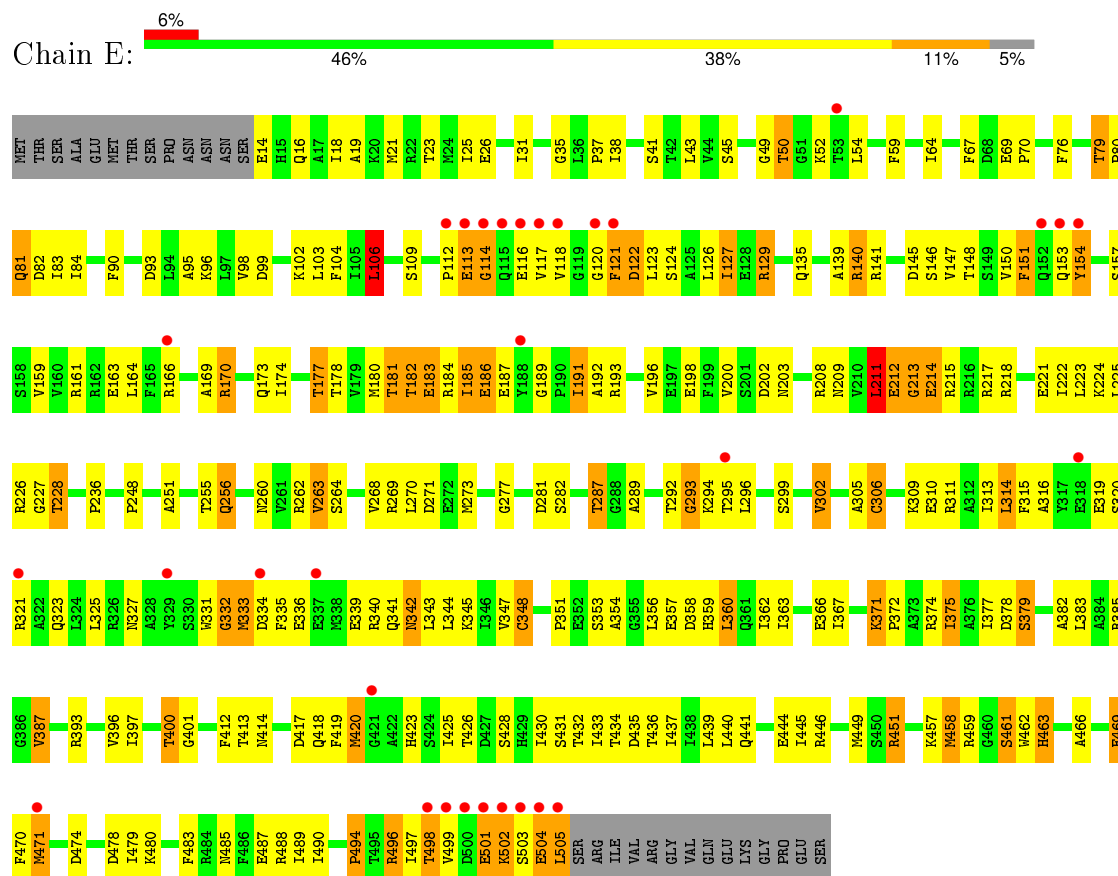
• Molecule 1: Circadian clock protein kinase kaiC







• Molecule 1: Circadian clock protein kinase kaiC



• Molecule 1: Circadian clock protein kinase kaiC



I467	S388	S320	T238	F165	I97	MET
R468		R321	I239	R166	V98	THR
E469	R393	A322		L167	E100	SER
F470		Q323	P248	V168		ALA
M471	V396	L324		A169		GLU
	I397	L325	A251	R170	L103	MET
D478	G398		R252	L171	F104	THR
I479	V399		R253	K172	T105	SER
K480	T400		L254	Q173	L106	PRO
		W331	T255	I174		ASN
F483	E406	Q332	Q256		D111	ASN
R484	E407	M333	R257	T178	P112	SER
M485	I408	D334		V179	E113	SER
F486		F335	N260	M180	G114	E14
	F412	E336		T181	Q115	H15
I489	T413	E337	V263	T182	E116	Q16
I490	M414	M338	S264	E183		
		E339	S265	R184	V117	A19
G491	F419	R340	G266	I185	G119	K20
G492	M420	Q341		E186	G120	M21
S493		M342	R269	E187	F121	R22
P494		L343	L270		D122	T23
T495	H423	L344		I191	L123	M24
R496	S424	K345	M273	A192	S124	I25
I497	I425	I346	C274	R193	A125	E26
T498	I426	V347		V196	L126	
V499	D427	C348	F278	E197	I127	T31
D500	S428	A349		E198	R129	R53
E501	H429	Y350	I283	F199	I130	
K502	I430			V200	M131	I38
S503	S431				Y132	G39
E504	T432	S353	T287	N203		
L505	I433	A354	G288		Y137	T42
S506	T434	G355	A289	R208	R138	L43
R507	D435	L356		N209	A139	V44
I508	T436	E357	T292	V210	R140	S45
Y509	I437	D358	G293	L211	R141	G46
R510	I438	H359	K294	E212		
	L439	L360	T295	G213	I144	G49
G511	L440	Q361	L296	E214	D145	T50
V512		I362			S146	G51
Q513	V443	I363	S299	R217	V147	K52
E514	E444	E366	F301	R218	T148	T53
K515	I445	I367	V302	T219	S149	M62
R446	R446		A305	L220	V150	
G447	G447	R371	C306	E221	F151	I65
E448		P372	I304	I222	Q152	
		R374	A307	L223	Q153	F76
R451	A452	I375	N308	K224	Y154	
A452		A376		L225	D155	
V455	V455	I377	R311		A156	T79
F456	F456	D378	A312	S229	S157	P80
K457	K457	S379	I313	H230	S158	Q81
M458	M458	L380	L314	M231	V159	D82
R459	R459	S381	F315	E234	Y160	I83
G460	G460	L382	A316	T235	R161	
S461	S461	L383	Y317	P236	E162	D83
M462	M462		E318		E163	
H463	H463	V387	E319	F237	L164	K96

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.87Å 135.58Å 204.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 29.73 – 2.83	Depositor EDS
% Data completeness (in resolution range)	89.6 (30.00-2.80) 89.7 (29.73-2.83)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.77 (at 2.85Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.239 , 0.288 0.237 , 0.284	Depositor DCC
$R_{free}$ test set	4041 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.8	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 58.9	EDS
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 87615 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	23870	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, 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	0.96	3/4037 (0.1%)	1.00	3/5437 (0.1%)
1	B	0.83	2/3921 (0.1%)	0.95	5/5282 (0.1%)
1	C	0.87	2/3897 (0.1%)	0.95	2/5251 (0.0%)
1	D	1.00	4/3873 (0.1%)	1.01	2/5218 (0.0%)
1	E	1.01	5/3929 (0.1%)	1.03	5/5293 (0.1%)
1	F	1.00	5/4037 (0.1%)	1.02	4/5437 (0.1%)
All	All	0.95	21/23694 (0.1%)	0.99	21/31918 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	0
1	D	1	0
1	E	1	0
1	F	1	0
All	All	4	0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	366	GLU	CD-OE2	5.99	1.32	1.25
1	B	498	THR	CA-CB	5.92	1.68	1.53
1	F	366	GLU	CD-OE2	5.55	1.31	1.25
1	F	348	CYS	CB-SG	-5.54	1.72	1.81
1	A	366	GLU	CD-OE2	5.54	1.31	1.25
1	D	471	MET	CG-SD	5.52	1.95	1.81
1	C	366	GLU	CD-OE2	5.51	1.31	1.25
1	D	183	GLU	CB-CG	-5.42	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	514	GLU	CG-CD	5.37	1.60	1.51
1	E	306	CYS	CB-SG	5.32	1.91	1.82
1	C	357	GLU	CG-CD	5.31	1.59	1.51
1	D	357	GLU	CG-CD	5.28	1.59	1.51
1	E	357	GLU	CG-CD	5.26	1.59	1.51
1	A	501	GLU	CB-CG	5.25	1.62	1.52
1	E	170	ARG	CG-CD	5.23	1.65	1.51
1	A	504	GLU	CB-CG	5.14	1.61	1.52
1	F	129	ARG	CZ-NH2	5.11	1.39	1.33
1	E	310	GLU	CG-CD	5.10	1.59	1.51
1	B	499	VAL	CA-CB	5.10	1.65	1.54
1	F	76	PHE	CB-CG	-5.06	1.42	1.51
1	E	135	GLN	CG-CD	5.05	1.62	1.51

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	214	GLU	N-CA-C	-6.00	94.81	111.00
1	E	114	GLY	N-CA-C	5.96	128.00	113.10
1	A	516	GLY	N-CA-C	-5.92	98.29	113.10
1	B	218	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	A	116	GLU	N-CA-C	5.84	126.78	111.00
1	E	129	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	E	106	LEU	CA-CB-CG	5.73	128.47	115.30
1	F	193	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	F	332	GLY	N-CA-C	-5.59	99.12	113.10
1	B	332	GLY	N-CA-C	-5.49	99.36	113.10
1	D	332	GLY	N-CA-C	-5.48	99.41	113.10
1	B	502	LYS	N-CA-C	-5.47	96.23	111.00
1	F	141	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	C	332	GLY	N-CA-C	-5.45	99.48	113.10
1	B	455	VAL	N-CA-C	-5.36	96.54	111.00
1	D	459	ARG	C-N-CA	-5.33	111.11	122.30
1	B	217	ARG	NE-CZ-NH1	-5.29	117.65	120.30
1	E	332	GLY	N-CA-C	-5.29	99.87	113.10
1	F	106	LEU	CA-CB-CG	5.07	126.95	115.30
1	A	497	ILE	N-CA-C	5.05	124.64	111.00
1	C	262	ARG	NE-CZ-NH1	-5.00	117.80	120.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	432	TPO	CB
1	D	432	TPO	CB
1	E	432	TPO	CB
1	F	432	TPO	CB

There are no planarity outliers.

## 5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3993	0	3984	320	0
1	B	3878	0	3862	300	0
1	C	3850	0	3836	285	0
1	D	3826	0	3818	283	0
1	E	3886	0	3872	307	0
1	F	3993	0	3982	326	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	62	0	24	11	0
3	B	62	0	24	8	0
3	C	62	0	24	7	0
3	D	62	0	23	6	0
3	E	62	0	24	6	0
3	F	62	0	24	7	0
4	A	7	0	0	0	0
4	B	5	0	0	2	0
4	C	7	0	0	3	0
4	D	12	0	0	2	0
4	E	10	0	0	0	0
4	F	25	0	0	6	0
All	All	23870	0	23497	1727	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 37.

All (1727) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:115:GLN:CG	1:F:116:GLU:H	1.13	1.44
1:B:431:SEP:O	1:B:434:THR:HG22	1.38	1.19
1:D:431:SEP:O	1:D:432:TPO:HB	1.40	1.18
1:F:115:GLN:HG2	1:F:116:GLU:N	1.27	1.14
1:F:486:PHE:HE2	1:F:496:ARG:HD2	1.07	1.13
1:A:14:GLU:HG3	1:A:15:HIS:H	1.08	1.11
1:D:147:VAL:HG11	1:D:180:MET:HE3	1.26	1.09
1:F:305:ALA:HB2	1:F:374:ARG:HD2	1.31	1.09
1:F:115:GLN:HG3	1:F:116:GLU:H	1.08	1.08
1:B:147:VAL:HG11	1:B:180:MET:HE3	1.32	1.08
1:B:140:ARG:HH11	1:B:140:ARG:HB3	1.16	1.08
1:F:431:SEP:O	1:F:434:THR:HG22	1.54	1.07
1:F:115:GLN:CG	1:F:116:GLU:N	1.87	1.06
1:B:21:MET:HE1	1:B:141:ARG:HG2	1.38	1.04
1:D:146:SER:H	1:D:181:THR:HG22	1.21	1.04
1:C:21:MET:HE3	1:C:141:ARG:HG2	1.36	1.04
1:E:146:SER:H	1:E:181:THR:HG22	1.22	1.04
1:A:79:THR:CG2	1:A:81:GLN:HG2	1.87	1.03
1:F:486:PHE:CE2	1:F:496:ARG:HD2	1.93	1.01
1:E:214:GLU:HB3	1:F:234:GLU:HB2	1.42	1.01
1:C:123:LEU:HD12	1:C:163:GLU:OE2	1.61	0.99
1:F:140:ARG:HB3	1:F:140:ARG:HH11	1.29	0.98
1:E:505:LEU:O	1:E:505:LEU:HG	1.60	0.98
1:E:305:ALA:HB2	1:E:374:ARG:HD2	1.46	0.98
1:F:146:SER:H	1:F:181:THR:HG22	1.25	0.97
1:D:446:ARG:N	1:D:496:ARG:HH12	1.60	0.97
1:B:79:THR:HG22	1:B:82:ASP:H	1.29	0.97
1:D:79:THR:HG22	1:D:82:ASP:H	1.25	0.97
1:C:262:ARG:HH22	1:C:461:SER:HB2	1.32	0.95
1:A:305:ALA:HB2	1:A:374:ARG:HD2	1.46	0.95
1:E:501:GLU:O	1:E:502:LYS:HG3	1.67	0.95
1:F:79:THR:HG22	1:F:82:ASP:H	1.31	0.95
1:A:451:ARG:HH11	1:A:451:ARG:HG2	1.29	0.95
1:B:441:GLN:HE22	1:B:490:ILE:HD13	1.32	0.94
1:E:431:SEP:O	1:E:434:THR:HG22	1.69	0.93
1:B:305:ALA:HB2	1:B:374:ARG:HD2	1.49	0.93
1:D:371:LYS:HD3	1:D:371:LYS:O	1.69	0.93
1:E:263:VAL:HG12	1:E:374:ARG:HH21	1.34	0.92
1:E:79:THR:CG2	1:E:81:GLN:HG2	2.00	0.91
1:C:147:VAL:HG11	1:C:180:MET:HE2	1.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:ASP:OD2	1:B:181:THR:HG21	1.71	0.90
1:B:379:SER:HA	1:B:413:THR:HG22	1.53	0.90
1:E:123:LEU:HD22	1:E:166:ARG:HD2	1.54	0.89
1:C:140:ARG:HB3	1:C:140:ARG:HH11	1.36	0.89
1:A:79:THR:HG23	1:A:81:GLN:HG2	1.53	0.88
1:A:147:VAL:HG11	1:A:180:MET:HE2	1.54	0.88
1:B:140:ARG:NH1	1:B:140:ARG:HB3	1.88	0.87
1:C:123:LEU:HD13	1:C:166:ARG:HD2	1.55	0.87
1:F:287:THR:CG2	1:F:414:ASN:HD22	1.85	0.87
1:C:287:THR:CG2	1:C:414:ASN:HD22	1.87	0.87
1:B:263:VAL:HG12	1:B:374:ARG:HH21	1.40	0.87
1:A:14:GLU:CG	1:A:15:HIS:H	1.84	0.86
1:F:287:THR:HG23	1:F:414:ASN:HB3	1.54	0.86
1:F:203:ASN:HB3	1:F:225:LEU:HD23	1.56	0.86
1:F:45:SER:HB2	1:F:182:THR:HB	1.58	0.86
1:D:123:LEU:HD12	1:D:166:ARG:HD2	1.57	0.86
1:C:146:SER:H	1:C:181:THR:HG22	1.41	0.86
1:A:318:GLU:OE2	1:B:432:TPO:HG21	1.76	0.85
1:F:426:THR:HG22	1:F:428:SER:H	1.38	0.85
1:A:24:MET:HB2	1:A:62:ASN:HD22	1.41	0.85
1:F:191:ILE:HB	1:F:198:GLU:CG	2.07	0.85
1:A:140:ARG:HH11	1:A:140:ARG:HB3	1.40	0.85
1:D:305:ALA:HB2	1:D:374:ARG:HD2	1.58	0.85
1:D:182:THR:HG21	1:D:192:ALA:HB1	1.59	0.85
1:B:147:VAL:O	1:B:150:VAL:HG12	1.76	0.85
1:B:140:ARG:CB	1:B:140:ARG:HH11	1.89	0.85
1:D:191:ILE:HB	1:D:198:GLU:CG	2.07	0.85
1:C:305:ALA:HB2	1:C:374:ARG:HD2	1.59	0.84
1:A:287:THR:CG2	1:A:414:ASN:HD22	1.89	0.84
1:E:79:THR:HG23	1:E:81:GLN:HG2	1.57	0.84
1:B:79:THR:CG2	1:B:81:GLN:HG2	2.07	0.84
1:D:287:THR:CG2	1:D:414:ASN:HD22	1.89	0.84
1:F:509:VAL:O	1:F:512:VAL:HG23	1.76	0.84
1:C:52:LYS:HE3	3:C:903:ATP:O1B	1.78	0.84
1:C:347:VAL:O	1:C:348:CYS:HB2	1.77	0.84
1:A:433:ILE:HG22	1:A:433:ILE:O	1.77	0.83
1:F:145:ASP:OD2	1:F:181:THR:HG21	1.78	0.83
1:C:182:THR:HG21	1:C:192:ALA:HB1	1.61	0.83
1:E:146:SER:N	1:E:181:THR:HG22	1.92	0.83
1:E:432:TPO:OG1	1:E:433:ILE:HD12	1.78	0.83
1:A:14:GLU:HG3	1:A:15:HIS:N	1.91	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:505:LEU:O	1:E:505:LEU:CG	2.27	0.83
1:A:498:THR:HB	1:A:501:GLU:HG3	1.59	0.83
1:F:504:GLU:HB3	1:F:507:ARG:NH2	1.92	0.83
1:D:446:ARG:H	1:D:496:ARG:HH12	1.20	0.82
1:E:287:THR:CG2	1:E:414:ASN:HD22	1.92	0.82
1:C:147:VAL:O	1:C:150:VAL:HG12	1.79	0.82
1:A:147:VAL:O	1:A:150:VAL:HG12	1.80	0.82
1:A:379:SER:HA	1:A:413:THR:HG22	1.60	0.82
1:D:146:SER:N	1:D:181:THR:HG22	1.95	0.81
1:B:191:ILE:HB	1:B:198:GLU:CG	2.10	0.81
1:F:515:LYS:HG3	1:F:516:GLY:N	1.95	0.81
1:A:79:THR:HG22	1:A:82:ASP:H	1.44	0.81
1:D:147:VAL:HG11	1:D:180:MET:CE	2.07	0.81
1:C:262:ARG:NH2	1:C:461:SER:HB2	1.94	0.81
1:E:433:ILE:HG22	1:E:433:ILE:O	1.80	0.80
1:F:263:VAL:HG12	1:F:374:ARG:HH21	1.45	0.80
1:A:211:LEU:O	1:A:212:GLU:HB3	1.81	0.80
1:A:79:THR:HG21	1:A:81:GLN:HG2	1.62	0.80
1:C:67:PHE:HB2	1:C:69:GLU:HG3	1.60	0.80
1:D:106:LEU:C	1:D:106:LEU:HD12	2.01	0.80
1:D:79:THR:O	1:D:83:ILE:HD12	1.82	0.80
1:C:287:THR:HG23	1:C:414:ASN:HD22	1.47	0.80
1:F:148:THR:HG21	1:F:183:GLU:HG3	1.64	0.80
1:B:377:ILE:HD12	1:B:412:PHE:CE2	2.17	0.80
1:C:495:THR:HA	1:D:487:GLU:OE2	1.81	0.80
1:E:79:THR:HG22	1:E:82:ASP:H	1.47	0.79
1:D:315:PHE:CZ	1:D:363:ILE:HG23	2.16	0.79
1:F:263:VAL:CG1	1:F:374:ARG:HH21	1.95	0.79
1:E:426:THR:HG22	1:E:428:SER:H	1.47	0.79
1:A:419:PHE:CD2	1:B:425:ILE:HD12	2.17	0.79
1:D:299:SER:C	1:D:333:MET:HE1	2.01	0.79
1:A:87:ALA:O	1:A:92:TRP:CD1	2.36	0.79
1:D:446:ARG:H	1:D:496:ARG:NH1	1.80	0.79
1:B:287:THR:HG23	1:B:414:ASN:HD22	1.47	0.79
1:E:147:VAL:O	1:E:150:VAL:HG12	1.82	0.79
1:F:293:GLY:HA2	3:F:901:ATP:O1A	1.81	0.79
1:F:502:LYS:NZ	1:F:507:ARG:HB3	1.98	0.79
1:D:311:ARG:HD2	1:D:371:LYS:HD2	1.63	0.78
1:B:471:MET:HB3	1:B:480:LYS:NZ	1.98	0.78
1:E:461:SER:OG	1:E:462:TRP:N	2.16	0.78
1:E:67:PHE:HB2	1:E:69:GLU:HG3	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:GLN:NE2	1:B:490:ILE:HD13	1.98	0.78
1:B:191:ILE:HB	1:B:198:GLU:CD	2.04	0.78
1:E:485:ASN:ND2	1:E:496:ARG:HH11	1.82	0.78
1:C:79:THR:HG22	1:C:82:ASP:H	1.49	0.78
1:A:455:VAL:HG11	1:A:463:HIS:HB2	1.63	0.78
1:E:371:LYS:HD2	1:E:371:LYS:O	1.84	0.78
1:F:486:PHE:HE2	1:F:496:ARG:CD	1.95	0.78
1:D:344:LEU:HD13	1:D:344:LEU:C	2.04	0.78
1:E:191:ILE:HB	1:E:198:GLU:CG	2.14	0.77
1:F:218:ARG:HD2	4:F:522:HOH:O	1.85	0.77
1:A:41:SER:HB3	1:A:178:THR:HB	1.67	0.77
1:F:509:VAL:O	1:F:512:VAL:CG2	2.32	0.77
1:F:147:VAL:HG11	1:F:180:MET:HE2	1.67	0.77
1:A:299:SER:C	1:A:333:MET:HE1	2.05	0.77
1:A:263:VAL:HG12	1:A:374:ARG:HH21	1.49	0.77
1:B:43:LEU:HD11	1:B:182:THR:OG1	1.85	0.77
1:E:504:GLU:OE1	1:E:505:LEU:HD23	1.84	0.76
1:B:79:THR:HG23	1:B:81:GLN:HG2	1.66	0.76
3:B:901:ATP:H3'	1:C:458:MET:O	1.85	0.76
1:F:420:MET:HA	4:F:532:HOH:O	1.83	0.76
1:B:127:ILE:HG21	1:B:170:ARG:HG3	1.67	0.76
1:F:146:SER:N	1:F:181:THR:HG22	2.01	0.76
1:A:426:THR:HG22	1:A:428:SER:H	1.51	0.76
1:F:515:LYS:HG3	1:F:516:GLY:H	1.50	0.76
1:E:14:GLU:HG3	1:E:16:GLN:H	1.50	0.76
1:B:429:HIS:HA	1:B:431:SEP:O1P	1.85	0.76
1:F:191:ILE:HB	1:F:198:GLU:CD	2.06	0.76
1:F:439:LEU:HD12	1:F:440:LEU:N	2.01	0.76
1:B:419:PHE:CD2	1:C:425:ILE:HD12	2.21	0.76
1:A:371:LYS:O	1:A:371:LYS:HD3	1.86	0.76
1:E:334:ASP:OD1	1:E:336:GLU:HB2	1.86	0.75
1:C:151:PHE:C	1:C:153:GLN:H	1.90	0.75
1:A:117:VAL:HA	1:A:154:TYR:OH	1.86	0.75
1:F:185:ILE:HD11	1:F:193:ARG:NH1	2.01	0.75
1:E:146:SER:H	1:E:181:THR:CG2	2.00	0.75
1:E:371:LYS:CD	1:E:371:LYS:O	2.35	0.75
1:D:140:ARG:HH11	1:D:140:ARG:HB3	1.50	0.75
1:B:263:VAL:CG1	1:B:374:ARG:HH21	2.00	0.75
1:E:140:ARG:HB3	1:E:140:ARG:HH11	1.51	0.75
1:B:146:SER:H	1:B:181:THR:HG22	1.52	0.75
1:D:431:SEP:O	1:D:432:TPO:CB	2.27	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:437:ILE:HD12	1:F:457:LYS:HG2	1.68	0.74
1:D:419:PHE:CD2	1:E:425:ILE:HD12	2.23	0.74
1:F:53:THR:HG23	1:F:145:ASP:OD1	1.85	0.74
1:B:377:ILE:HD12	1:B:412:PHE:HE2	1.52	0.74
1:A:316:ALA:O	1:A:348:CYS:HA	1.88	0.74
1:E:289:ALA:HB2	1:E:419:PHE:HA	1.68	0.74
1:B:147:VAL:HG11	1:B:180:MET:CE	2.14	0.74
1:D:446:ARG:N	1:D:496:ARG:NH1	2.35	0.74
1:D:379:SER:HA	1:D:413:THR:HG22	1.67	0.74
1:E:145:ASP:OD2	1:E:181:THR:HG21	1.87	0.74
1:B:24:MET:HB2	1:B:62:ASN:HD22	1.52	0.74
1:E:356:LEU:HD22	1:E:387:VAL:HG11	1.69	0.74
1:C:81:GLN:H	1:C:81:GLN:NE2	1.85	0.74
1:E:419:PHE:CD2	1:F:425:ILE:HD12	2.23	0.74
1:D:203:ASN:HB3	1:D:225:LEU:HD23	1.70	0.73
1:B:363:ILE:O	1:B:367:ILE:HG13	1.88	0.73
1:B:182:THR:HG21	1:B:192:ALA:HB1	1.68	0.73
1:D:146:SER:H	1:D:181:THR:CG2	1.99	0.73
1:A:377:ILE:HD12	1:A:412:PHE:CE2	2.22	0.73
1:E:294:LYS:HB2	3:E:901:ATP:O1B	1.88	0.73
1:D:147:VAL:O	1:D:150:VAL:HG12	1.88	0.73
1:A:127:ILE:HD11	1:A:167:LEU:HD12	1.69	0.73
1:E:148:THR:HG21	1:E:183:GLU:HG3	1.68	0.73
1:F:461:SER:OG	1:F:462:TRP:N	2.20	0.73
1:B:296:LEU:HD21	1:B:477:PRO:HD3	1.70	0.73
1:C:121:PHE:H	1:C:121:PHE:HD1	1.35	0.73
1:E:287:THR:HG23	1:E:414:ASN:HD22	1.54	0.73
1:F:140:ARG:NH1	1:F:140:ARG:HB3	2.04	0.73
1:D:191:ILE:HB	1:D:198:GLU:HG3	1.68	0.73
1:D:287:THR:HG23	1:D:414:ASN:HB3	1.68	0.73
1:E:191:ILE:CG2	1:E:198:GLU:HG3	2.19	0.73
1:F:140:ARG:CB	1:F:140:ARG:HH11	2.02	0.73
1:D:106:LEU:HD12	1:D:107:ASP:N	2.04	0.73
1:B:299:SER:C	1:B:333:MET:HE1	2.10	0.73
1:D:148:THR:OG1	1:D:182:THR:HG23	1.89	0.72
1:C:123:LEU:HD22	1:C:127:ILE:HD11	1.69	0.72
1:C:79:THR:CG2	1:C:81:GLN:HG2	2.18	0.72
1:C:451:ARG:HH11	1:C:451:ARG:HG2	1.52	0.72
1:A:426:THR:HB	1:A:431:SEP:O2P	1.89	0.72
1:C:79:THR:O	1:C:83:ILE:HD12	1.89	0.72
1:A:140:ARG:HB3	1:A:140:ARG:NH1	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:LEU:HD13	1:A:331:TRP:CD2	2.24	0.72
1:E:323:GLN:HE22	1:F:459:ARG:HD3	1.53	0.72
1:A:145:ASP:OD2	1:A:181:THR:HG21	1.89	0.72
1:F:191:ILE:HB	1:F:198:GLU:HG3	1.71	0.72
1:E:212:GLU:O	1:E:213:GLY:C	2.28	0.72
1:A:431:SEP:O	1:A:434:THR:HG22	1.89	0.72
1:D:203:ASN:HB3	1:D:225:LEU:CD2	2.19	0.72
1:D:106:LEU:HD11	1:D:129:ARG:NH2	2.04	0.72
1:E:263:VAL:CG1	1:E:374:ARG:HH21	2.03	0.72
1:B:52:LYS:HB2	3:B:903:ATP:O1B	1.90	0.72
1:A:65:ILE:O	1:A:65:ILE:HG22	1.88	0.72
1:E:19:ALA:O	1:E:38:ILE:HD12	1.89	0.72
1:C:218:ARG:HB3	4:C:522:HOH:O	1.88	0.72
1:D:486:PHE:HB2	1:D:489:ILE:HD11	1.72	0.72
1:C:140:ARG:HB3	1:C:140:ARG:NH1	2.05	0.72
1:F:182:THR:HG22	1:F:183:GLU:N	2.05	0.72
1:E:497:ILE:O	1:E:498:THR:OG1	2.06	0.72
1:E:426:THR:HG22	1:E:428:SER:N	2.04	0.71
1:D:426:THR:HG22	1:D:428:SER:H	1.53	0.71
1:D:263:VAL:HG12	1:D:374:ARG:HH21	1.55	0.71
1:E:191:ILE:HG21	1:E:198:GLU:HG3	1.70	0.71
1:C:191:ILE:HB	1:C:198:GLU:CG	2.19	0.71
1:E:418:GLN:HB2	1:F:423:HIS:O	1.89	0.71
1:D:497:ILE:O	1:D:497:ILE:HD12	1.90	0.71
1:C:123:LEU:HD21	1:C:167:LEU:HB2	1.72	0.71
1:E:396:VAL:O	1:E:400:THR:HB	1.89	0.71
1:B:462:TRP:O	1:B:463:HIS:O	2.08	0.71
1:D:79:THR:CG2	1:D:81:GLN:HG2	2.19	0.71
1:C:45:SER:HB2	1:C:182:THR:HB	1.72	0.71
1:C:315:PHE:CZ	1:C:363:ILE:HG23	2.26	0.71
1:A:446:ARG:HA	1:A:496:ARG:NH2	2.05	0.71
1:E:499:VAL:HG12	1:E:499:VAL:O	1.89	0.71
1:B:497:ILE:HG13	1:B:498:THR:N	2.04	0.71
1:C:140:ARG:HH11	1:C:140:ARG:CB	2.04	0.71
1:F:21:MET:HE1	1:F:141:ARG:HG2	1.72	0.71
1:D:295:THR:HG23	1:D:378:ASP:OD2	1.90	0.71
1:F:299:SER:C	1:F:333:MET:HE1	2.09	0.71
1:E:432:TPO:HG21	1:E:432:TPO:O1P	1.88	0.70
1:C:79:THR:HG23	1:C:81:GLN:HG2	1.71	0.70
1:D:387:VAL:HG12	1:D:388:SER:N	2.05	0.70
1:D:439:LEU:HD12	1:D:440:LEU:N	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:VAL:HG12	1:B:374:ARG:NH2	2.06	0.70
1:A:287:THR:HG23	1:A:414:ASN:HD22	1.56	0.70
1:F:379:SER:HA	1:F:413:THR:HG22	1.74	0.70
1:B:397:ILE:HD13	1:B:433:ILE:HG21	1.72	0.70
1:A:425:ILE:HB	1:A:431:SEP:O1P	1.91	0.70
1:F:161:ARG:HB2	1:F:196:VAL:HG11	1.73	0.70
1:A:266:GLY:HA3	1:A:300:ARG:O	1.91	0.70
1:A:451:ARG:NH1	1:A:451:ARG:HG2	1.99	0.70
1:A:147:VAL:HG11	1:A:180:MET:CE	2.21	0.70
1:F:239:ILE:HB	4:F:533:HOH:O	1.90	0.70
1:F:182:THR:HG21	1:F:192:ALA:HB1	1.74	0.70
1:A:499:VAL:HG12	1:A:499:VAL:O	1.92	0.70
1:B:65:ILE:HG22	1:B:65:ILE:O	1.90	0.70
1:D:79:THR:HG23	1:D:81:GLN:H	1.57	0.70
1:E:123:LEU:CD2	1:E:127:ILE:HD11	2.21	0.70
1:B:273:MET:O	1:B:463:HIS:HA	1.91	0.70
1:F:378:ASP:OD1	1:F:413:THR:HG21	1.91	0.70
1:B:287:THR:CG2	1:B:414:ASN:HD22	2.05	0.69
1:D:451:ARG:HH11	1:D:451:ARG:HG2	1.57	0.69
1:C:379:SER:HA	1:C:413:THR:HG22	1.73	0.69
1:E:273:MET:O	1:E:463:HIS:HA	1.92	0.69
1:B:18:ILE:HB	1:B:228:THR:HG23	1.73	0.69
1:D:496:ARG:HG2	1:E:487:GLU:OE1	1.92	0.69
1:A:311:ARG:HD2	1:A:371:LYS:CE	2.22	0.69
1:B:169:ALA:O	1:B:173:GLN:HG3	1.92	0.69
1:C:14:GLU:HG3	1:C:16:GLN:H	1.58	0.69
1:A:318:GLU:HG2	1:B:432:TPO:O3P	1.92	0.69
1:D:151:PHE:C	1:D:153:GLN:H	1.95	0.69
1:C:203:ASN:HB3	1:C:225:LEU:HD23	1.74	0.69
1:A:49:GLY:HA2	3:A:903:ATP:O2B	1.93	0.69
1:F:115:GLN:HG2	1:F:116:GLU:CA	2.21	0.69
1:D:345:LYS:NZ	1:D:366:GLU:CG	2.55	0.69
1:B:451:ARG:HG2	1:B:451:ARG:HH11	1.56	0.69
1:A:89:SER:HB2	1:B:227:GLY:O	1.93	0.69
1:F:502:LYS:HZ1	1:F:507:ARG:HB3	1.55	0.69
1:C:289:ALA:HB2	1:C:419:PHE:HA	1.73	0.69
1:D:145:ASP:OD2	1:D:181:THR:HG21	1.93	0.69
1:F:191:ILE:CB	1:F:198:GLU:HG3	2.23	0.69
1:A:377:ILE:HD12	1:A:412:PHE:HE2	1.58	0.69
1:A:64:ILE:HG22	1:A:65:ILE:HD13	1.75	0.69
1:B:498:THR:OG1	1:C:499:VAL:HG21	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:ARG:O	1:C:397:ILE:HG12	1.91	0.69
1:B:334:ASP:OD1	1:B:336:GLU:HB2	1.93	0.69
1:F:334:ASP:OD1	1:F:336:GLU:HB2	1.93	0.69
1:C:371:LYS:HD3	1:C:371:LYS:O	1.92	0.69
1:F:430:ILE:O	1:F:431:SEP:C	2.40	0.69
1:A:287:THR:HG23	1:A:414:ASN:HB3	1.75	0.69
1:C:461:SER:OG	1:C:462:TRP:N	2.25	0.68
1:A:118:VAL:HG12	1:A:122:ASP:HB3	1.75	0.68
1:C:126:LEU:O	1:C:129:ARG:HB2	1.91	0.68
1:C:146:SER:N	1:C:181:THR:HG22	2.08	0.68
1:E:356:LEU:CD2	1:E:387:VAL:HG11	2.23	0.68
1:F:347:VAL:O	1:F:348:CYS:HB2	1.93	0.68
1:C:287:THR:HG23	1:C:414:ASN:HB3	1.74	0.68
1:F:81:GLN:H	1:F:81:GLN:NE2	1.91	0.68
1:F:147:VAL:O	1:F:150:VAL:HG12	1.93	0.68
1:F:287:THR:HG23	1:F:414:ASN:HD22	1.58	0.68
1:F:14:GLU:HG2	4:F:540:HOH:O	1.93	0.68
1:A:459:ARG:HD3	1:F:323:GLN:NE2	2.09	0.68
1:A:505:LEU:HD12	1:A:505:LEU:O	1.94	0.68
1:A:18:ILE:HD12	1:A:18:ILE:N	2.08	0.68
1:D:106:LEU:CD1	1:D:129:ARG:NH2	2.57	0.68
1:B:497:ILE:HD12	1:B:499:VAL:H	1.59	0.68
1:B:295:THR:HG21	1:B:319:GLU:OE2	1.93	0.67
1:A:495:THR:HG22	1:A:497:ILE:HG23	1.76	0.67
1:D:31:ILE:HG22	1:D:222:ILE:HD12	1.75	0.67
1:A:363:ILE:O	1:A:367:ILE:HG13	1.94	0.67
1:A:248:PRO:HB2	1:A:251:ALA:HB3	1.76	0.67
1:F:273:MET:O	1:F:463:HIS:HA	1.94	0.67
1:A:140:ARG:HH11	1:A:140:ARG:CB	2.08	0.67
1:D:367:ILE:HG12	1:D:375:ILE:HD11	1.75	0.67
1:A:263:VAL:CG1	1:A:374:ARG:HH21	2.07	0.67
1:F:504:GLU:HA	1:F:507:ARG:NE	2.09	0.67
1:A:90:PHE:HB2	1:A:92:TRP:CE2	2.30	0.67
1:A:293:GLY:HA2	3:A:901:ATP:O1A	1.95	0.67
1:A:92:TRP:HD1	1:A:92:TRP:O	1.78	0.67
1:C:106:LEU:HD13	1:C:129:ARG:NH2	2.10	0.67
1:A:273:MET:O	1:A:463:HIS:HA	1.95	0.67
1:D:21:MET:HE1	1:D:141:ARG:HG2	1.75	0.67
1:E:123:LEU:HD22	1:E:166:ARG:CD	2.24	0.67
1:F:504:GLU:HB3	1:F:507:ARG:CZ	2.24	0.67
1:B:81:GLN:H	1:B:81:GLN:NE2	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:THR:HG22	1:C:183:GLU:H	1.59	0.66
1:F:471:MET:HB3	1:F:480:LYS:NZ	2.10	0.66
1:E:344:LEU:C	1:E:344:LEU:HD13	2.15	0.66
1:F:371:LYS:CD	1:F:371:LYS:O	2.43	0.66
1:F:289:ALA:HB2	1:F:419:PHE:HA	1.78	0.66
1:D:334:ASP:OD1	1:D:336:GLU:HB2	1.95	0.66
1:D:316:ALA:O	1:D:348:CYS:HA	1.96	0.66
1:B:305:ALA:HB2	1:B:374:ARG:CD	2.24	0.66
1:D:370:PHE:O	1:D:371:LYS:HD2	1.95	0.66
1:B:461:SER:OG	1:B:462:TRP:N	2.27	0.66
1:C:273:MET:O	1:C:463:HIS:HA	1.96	0.66
1:A:295:THR:HG21	1:A:319:GLU:OE2	1.95	0.66
1:B:426:THR:HG22	1:B:428:SER:H	1.60	0.66
1:E:323:GLN:NE2	1:F:459:ARG:HD3	2.09	0.66
1:B:497:ILE:HD12	1:B:499:VAL:HB	1.76	0.66
1:F:363:ILE:O	1:F:367:ILE:HG13	1.96	0.66
1:B:119:GLY:C	1:B:121:PHE:H	1.99	0.66
1:D:441:GLN:HE22	1:D:490:ILE:HD12	1.61	0.66
1:A:80:PRO:HB3	1:A:105:ILE:HG21	1.77	0.66
1:D:371:LYS:CD	1:D:371:LYS:O	2.42	0.66
1:D:182:THR:HG22	1:D:183:GLU:N	2.10	0.66
1:F:14:GLU:HG3	1:F:16:GLN:HG3	1.77	0.66
1:C:334:ASP:OD1	1:C:336:GLU:HB2	1.96	0.66
1:C:263:VAL:HG12	1:C:374:ARG:HH21	1.61	0.65
1:D:345:LYS:HZ2	1:D:366:GLU:HG2	1.59	0.65
1:E:439:LEU:HD12	1:E:440:LEU:N	2.11	0.65
1:D:191:ILE:CB	1:D:198:GLU:HG3	2.27	0.65
1:A:49:GLY:CA	3:A:903:ATP:O2B	2.43	0.65
1:E:435:ASP:HA	1:E:459:ARG:HD2	1.76	0.65
1:B:106:LEU:C	1:B:106:LEU:HD12	2.17	0.65
1:B:293:GLY:HA2	3:B:901:ATP:O1A	1.96	0.65
1:D:344:LEU:HD13	1:D:345:LYS:N	2.12	0.65
1:C:371:LYS:CD	1:C:371:LYS:O	2.43	0.65
1:A:311:ARG:HD2	1:A:371:LYS:HD2	1.78	0.65
1:D:435:ASP:HA	1:D:459:ARG:HD2	1.78	0.65
1:D:345:LYS:NZ	1:D:366:GLU:HG2	2.12	0.65
1:C:106:LEU:C	1:C:106:LEU:HD12	2.17	0.65
1:B:79:THR:HG21	1:B:81:GLN:HG2	1.77	0.65
1:A:151:PHE:C	1:A:153:GLN:H	2.00	0.65
1:E:148:THR:OG1	1:E:182:THR:HG23	1.96	0.65
1:E:263:VAL:HG12	1:E:374:ARG:NH2	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:SER:HB3	1:B:182:THR:HB	1.78	0.65
1:C:470:PHE:HB2	1:C:478:ASP:O	1.97	0.65
1:E:359:HIS:O	1:E:363:ILE:HG13	1.97	0.65
1:D:486:PHE:CB	1:D:489:ILE:HD11	2.27	0.65
1:E:79:THR:HG23	1:E:81:GLN:HE21	1.60	0.65
1:E:269:ARG:HG2	1:E:479:ILE:HB	1.79	0.65
1:A:146:SER:H	1:A:181:THR:HG22	1.61	0.65
1:A:459:ARG:HD3	1:F:323:GLN:HE22	1.62	0.65
1:D:385:ARG:NH2	1:E:432:TPO:O3P	2.27	0.65
1:C:419:PHE:O	1:C:420:MET:HB2	1.96	0.65
1:B:311:ARG:HD2	1:B:371:LYS:CE	2.27	0.64
1:B:371:LYS:HD3	1:B:371:LYS:O	1.97	0.64
1:F:79:THR:CG2	1:F:81:GLN:HG2	2.27	0.64
1:C:182:THR:HG22	1:C:183:GLU:N	2.12	0.64
1:D:469:GLU:HG3	1:D:470:PHE:N	2.12	0.64
1:E:497:ILE:HG22	1:E:498:THR:H	1.63	0.64
1:B:148:THR:HG21	1:B:183:GLU:HG3	1.78	0.64
1:E:93:ASP:OD2	1:E:96:LYS:HB2	1.97	0.64
1:C:41:SER:HB3	1:C:178:THR:HB	1.78	0.64
1:E:377:ILE:HD12	1:E:412:PHE:CE2	2.31	0.64
1:F:311:ARG:HD2	1:F:371:LYS:CE	2.27	0.64
1:A:79:THR:O	1:A:83:ILE:HD12	1.97	0.64
1:F:146:SER:H	1:F:181:THR:CG2	2.03	0.64
1:D:311:ARG:HD2	1:D:371:LYS:CD	2.28	0.64
1:F:151:PHE:C	1:F:153:GLN:H	2.01	0.64
1:A:334:ASP:OD1	1:A:336:GLU:HB2	1.97	0.64
1:A:96:LYS:O	1:A:100:GLU:HG3	1.98	0.64
1:E:151:PHE:C	1:E:153:GLN:H	2.01	0.64
1:B:24:MET:CB	1:B:62:ASN:HD22	2.09	0.64
1:A:396:VAL:O	1:A:400:THR:HB	1.97	0.64
1:E:43:LEU:HD11	1:E:182:THR:OG1	1.97	0.64
1:B:471:MET:HB3	1:B:480:LYS:HZ1	1.62	0.64
1:F:344:LEU:HD22	1:F:345:LYS:N	2.12	0.64
1:D:345:LYS:HZ3	1:D:366:GLU:CG	2.11	0.64
1:F:471:MET:HG2	1:F:480:LYS:HE2	1.79	0.64
1:A:419:PHE:CD2	1:B:425:ILE:CD1	2.81	0.64
1:E:462:TRP:O	1:E:463:HIS:O	2.16	0.64
1:F:455:VAL:HG11	1:F:463:HIS:HB2	1.79	0.64
1:C:311:ARG:HD2	1:C:371:LYS:HD2	1.80	0.64
1:D:313:ILE:CD1	1:D:372:PRO:HG3	2.28	0.64
1:F:296:LEU:HD13	1:F:331:TRP:CD2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:LYS:HE3	3:D:903:ATP:O1B	1.98	0.64
1:A:371:LYS:O	1:A:371:LYS:CD	2.45	0.64
1:A:315:PHE:CZ	1:A:363:ILE:HG23	2.33	0.64
1:C:18:ILE:HD12	1:C:18:ILE:N	2.12	0.64
1:D:223:LEU:O	1:D:223:LEU:HD22	1.98	0.64
1:C:159:VAL:O	1:C:163:GLU:HG2	1.97	0.63
1:D:311:ARG:HD2	1:D:371:LYS:CE	2.28	0.63
1:F:122:ASP:O	1:F:126:LEU:N	2.30	0.63
1:A:420:MET:CE	1:B:490:ILE:HG21	2.29	0.63
1:D:393:ARG:O	1:D:397:ILE:HG12	1.98	0.63
1:D:345:LYS:HZ3	1:D:366:GLU:CD	2.02	0.63
1:B:371:LYS:O	1:B:371:LYS:CD	2.47	0.63
1:C:305:ALA:HB2	1:C:374:ARG:CD	2.29	0.63
1:F:147:VAL:HG11	1:F:180:MET:CE	2.28	0.63
1:D:400:THR:HG22	1:D:401:GLY:N	2.13	0.63
1:F:120:GLY:HA2	1:F:123:LEU:HB2	1.80	0.63
1:E:496:ARG:O	1:E:497:ILE:HD13	1.99	0.63
1:B:496:ARG:HG2	1:B:498:THR:HG23	1.81	0.63
1:E:186:GLU:OE2	1:E:187:GLU:N	2.31	0.63
1:F:377:ILE:HD12	1:F:412:PHE:CE2	2.34	0.63
1:D:340:ARG:O	1:D:342:ASN:N	2.31	0.63
1:D:79:THR:HG23	1:D:81:GLN:HE21	1.64	0.62
1:A:503:SER:C	1:A:504:GLU:HG3	2.20	0.62
1:C:451:ARG:NH1	1:C:451:ARG:HG2	2.14	0.62
1:C:170:ARG:O	1:C:174:ILE:HG12	1.99	0.62
1:A:24:MET:CB	1:A:62:ASN:HD22	2.11	0.62
1:E:446:ARG:NH2	1:E:496:ARG:NH2	2.47	0.62
1:B:170:ARG:O	1:B:174:ILE:HG12	1.99	0.62
1:A:21:MET:HE1	1:A:141:ARG:HG2	1.81	0.62
1:D:14:GLU:CD	1:D:15:HIS:H	2.03	0.62
1:F:31:ILE:HG22	1:F:222:ILE:HD12	1.80	0.62
1:C:269:ARG:HG2	1:C:479:ILE:HB	1.80	0.62
1:D:182:THR:HG22	1:D:183:GLU:H	1.62	0.62
1:B:146:SER:H	1:B:181:THR:CG2	2.13	0.62
1:B:19:ALA:O	1:B:38:ILE:HD12	1.99	0.62
1:C:419:PHE:CD1	1:C:420:MET:HG3	2.34	0.62
1:A:323:GLN:HE22	1:B:459:ARG:HD3	1.64	0.62
1:B:444:GLU:OE2	1:C:489:ILE:HG13	1.99	0.62
1:E:123:LEU:HD23	1:E:127:ILE:HD11	1.80	0.62
1:C:145:ASP:OD2	1:C:181:THR:HG21	1.98	0.62
1:F:119:GLY:C	1:F:122:ASP:OD2	2.38	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:PHE:C	1:B:153:GLN:H	2.03	0.62
1:E:159:VAL:O	1:E:163:GLU:HG2	2.00	0.62
1:E:148:THR:OG1	1:E:182:THR:CG2	2.47	0.62
1:C:203:ASN:HB3	1:C:225:LEU:CD2	2.29	0.62
1:C:17:ALA:C	1:C:18:ILE:HD12	2.19	0.62
1:C:19:ALA:O	1:C:38:ILE:HD12	1.99	0.62
1:A:14:GLU:HG3	1:A:16:GLN:OE1	1.99	0.62
1:A:263:VAL:HG12	1:A:374:ARG:NH2	2.14	0.62
1:C:52:LYS:HD3	1:C:182:THR:O	2.00	0.62
1:B:311:ARG:HD2	1:B:371:LYS:HD2	1.81	0.62
1:E:161:ARG:HB2	1:E:196:VAL:HG11	1.80	0.62
1:D:486:PHE:CE2	1:D:496:ARG:HB3	2.34	0.62
1:D:14:GLU:OE1	1:D:14:GLU:HA	1.99	0.62
1:D:377:ILE:HD12	1:D:412:PHE:CE2	2.35	0.62
1:B:146:SER:N	1:B:181:THR:HG22	2.14	0.62
1:F:231:MET:CE	1:F:251:ALA:HB2	2.29	0.62
1:F:263:VAL:HG12	1:F:374:ARG:NH2	2.15	0.62
1:E:148:THR:HG21	1:E:183:GLU:CG	2.30	0.62
1:B:418:GLN:HG3	1:B:418:GLN:O	1.99	0.61
1:A:441:GLN:O	1:A:441:GLN:HG3	2.00	0.61
1:A:432:TPO:O1P	1:A:432:TPO:HG21	2.00	0.61
1:F:508:ILE:O	1:F:508:ILE:HG22	2.00	0.61
1:F:248:PRO:HB2	1:F:251:ALA:HB3	1.81	0.61
1:D:418:GLN:HB2	1:E:423:HIS:O	1.99	0.61
1:E:170:ARG:O	1:E:174:ILE:HG12	2.00	0.61
1:A:323:GLN:NE2	1:B:459:ARG:HD3	2.15	0.61
1:F:79:THR:HG23	1:F:81:GLN:HG2	1.82	0.61
1:F:356:LEU:CD2	1:F:387:VAL:HG11	2.30	0.61
1:F:24:MET:HB2	1:F:62:ASN:HD22	1.64	0.61
1:D:231:MET:CE	1:D:251:ALA:HB2	2.31	0.61
1:E:299:SER:C	1:E:333:MET:HE1	2.21	0.61
1:A:85:LYS:NZ	1:B:14:GLU:HG3	2.15	0.61
1:D:49:GLY:O	1:D:218:ARG:NH2	2.34	0.61
1:D:81:GLN:NE2	1:D:81:GLN:H	1.99	0.61
1:E:140:ARG:NH1	1:E:140:ARG:HB3	2.15	0.61
1:B:379:SER:CA	1:B:413:THR:HG22	2.29	0.61
1:B:191:ILE:HB	1:B:198:GLU:HG3	1.82	0.61
1:D:140:ARG:HB3	1:D:140:ARG:NH1	2.15	0.61
1:D:41:SER:HB3	1:D:178:THR:HB	1.83	0.61
1:A:320:SER:HA	1:B:254:LEU:HG	1.81	0.61
1:F:305:ALA:HB2	1:F:374:ARG:CD	2.20	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:VAL:O	1:C:153:GLN:HG3	2.01	0.61
1:A:486:PHE:HB2	1:A:489:ILE:HD11	1.82	0.61
1:A:435:ASP:HA	1:A:459:ARG:HD2	1.81	0.61
1:C:296:LEU:HD13	1:C:331:TRP:CD2	2.36	0.61
1:B:283:ILE:HD12	1:B:412:PHE:HE1	1.65	0.61
1:E:14:GLU:HG3	1:E:16:GLN:N	2.15	0.61
1:F:19:ALA:O	1:F:38:ILE:HD12	2.01	0.61
1:B:117:VAL:O	1:B:117:VAL:HG12	2.01	0.61
1:D:446:ARG:H	1:D:496:ARG:HH22	1.48	0.60
1:F:371:LYS:HD3	1:F:371:LYS:O	2.00	0.60
1:F:340:ARG:O	1:F:342:ASN:N	2.33	0.60
1:C:340:ARG:O	1:C:342:ASN:N	2.33	0.60
1:E:79:THR:HG21	1:E:81:GLN:HG2	1.79	0.60
1:C:347:VAL:O	1:C:348:CYS:CB	2.45	0.60
1:A:273:MET:O	1:A:464:ASP:N	2.31	0.60
1:E:347:VAL:HG12	1:E:348:CYS:N	2.15	0.60
1:A:16:GLN:O	1:A:17:ALA:O	2.20	0.60
1:B:287:THR:HG21	1:B:425:ILE:O	2.01	0.60
1:A:347:VAL:O	1:A:348:CYS:HB2	2.01	0.60
1:F:420:MET:HE3	1:F:492:GLY:HA3	1.83	0.60
1:D:471:MET:HG3	1:D:478:ASP:HB3	1.82	0.60
1:B:91:GLY:O	1:B:92:TRP:HD1	1.84	0.60
1:C:400:THR:HG22	1:C:401:GLY:N	2.16	0.60
1:A:67:PHE:HB2	1:A:69:GLU:HG3	1.83	0.60
1:A:504:GLU:C	1:A:506:SER:H	2.05	0.60
1:D:347:VAL:O	1:D:348:CYS:HB2	2.01	0.60
1:E:436:THR:HG23	1:E:458:MET:HG3	1.82	0.60
1:C:148:THR:OG1	1:C:182:THR:HG23	2.02	0.60
1:A:52:LYS:HE3	3:A:903:ATP:O1B	2.02	0.60
1:F:123:LEU:HD12	1:F:166:ARG:HD2	1.83	0.60
1:A:318:GLU:OE2	1:B:432:TPO:CG2	2.48	0.60
1:E:433:ILE:CG2	1:E:433:ILE:O	2.47	0.60
1:F:504:GLU:O	1:F:505:LEU:HB2	1.99	0.60
1:B:493:SER:HB3	1:C:488:ARG:HG2	1.82	0.60
1:D:19:ALA:C	1:D:38:ILE:HD12	2.21	0.60
1:A:126:LEU:HG	1:A:130:ILE:CD1	2.32	0.60
1:C:363:ILE:O	1:C:367:ILE:HG13	2.02	0.60
1:B:469:GLU:HB2	1:B:483:PHE:CZ	2.36	0.60
1:A:420:MET:HE1	1:B:490:ILE:HG21	1.84	0.60
1:D:79:THR:HG22	1:D:82:ASP:N	2.07	0.60
1:C:396:VAL:HG11	1:C:430:ILE:HG23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:ILE:HB	1:D:198:GLU:CD	2.21	0.59
1:D:396:VAL:O	1:D:400:THR:HB	2.02	0.59
1:F:316:ALA:O	1:F:348:CYS:HA	2.02	0.59
1:B:426:THR:HB	1:B:431:SEP:O3P	2.02	0.59
1:D:446:ARG:H	1:D:496:ARG:NH2	2.00	0.59
1:E:315:PHE:CZ	1:E:363:ILE:HG23	2.36	0.59
1:E:382:ALA:O	1:E:385:ARG:HG3	2.01	0.59
1:F:159:VAL:O	1:F:163:GLU:HG2	2.01	0.59
1:F:218:ARG:HB3	4:F:536:HOH:O	2.02	0.59
1:E:268:VAL:O	1:E:271:ASP:HB2	2.03	0.59
1:F:123:LEU:O	1:F:127:ILE:HG12	2.01	0.59
1:D:79:THR:HG21	1:D:81:GLN:HG2	1.82	0.59
1:D:287:THR:HG23	1:D:414:ASN:HD22	1.64	0.59
1:D:130:ILE:O	1:D:134:ILE:HG13	2.02	0.59
1:C:462:TRP:O	1:C:463:HIS:O	2.20	0.59
1:C:419:PHE:CD2	1:D:425:ILE:HD12	2.37	0.59
1:C:431:SEP:C	1:C:432:TPO:HG22	2.33	0.59
1:F:106:LEU:C	1:F:106:LEU:HD12	2.23	0.59
1:E:248:PRO:HB2	1:E:251:ALA:HB3	1.85	0.59
1:D:131:ASN:OD1	1:D:174:ILE:HD12	2.02	0.59
1:D:79:THR:HG23	1:D:81:GLN:HG2	1.84	0.59
1:F:451:ARG:HH11	1:F:451:ARG:HG2	1.67	0.59
1:E:316:ALA:O	1:E:348:CYS:HA	2.03	0.59
1:A:418:GLN:HB2	1:B:423:HIS:O	2.02	0.59
1:C:497:ILE:C	1:C:498:THR:HG22	2.23	0.59
1:F:191:ILE:CG2	1:F:198:GLU:HG3	2.33	0.59
1:A:379:SER:H	1:A:413:THR:HB	1.67	0.59
1:F:377:ILE:HD12	1:F:412:PHE:HE2	1.66	0.58
1:E:140:ARG:HH11	1:E:140:ARG:CB	2.16	0.58
1:F:269:ARG:HG2	1:F:479:ILE:HB	1.85	0.58
1:A:269:ARG:HG2	1:A:479:ILE:HB	1.85	0.58
1:F:471:MET:HG3	1:F:478:ASP:HB3	1.86	0.58
1:B:98:VAL:HA	1:B:103:LEU:O	2.02	0.58
1:E:296:LEU:HD13	1:E:331:TRP:CD2	2.38	0.58
1:D:446:ARG:HG3	1:D:496:ARG:NH1	2.18	0.58
1:D:263:VAL:HG12	1:D:374:ARG:NH2	2.19	0.58
1:A:432:TPO:OG1	1:A:433:ILE:HD12	2.03	0.58
1:F:503:SER:O	1:F:504:GLU:O	2.21	0.58
3:A:901:ATP:H3'	1:B:458:MET:O	2.03	0.58
1:D:248:PRO:HB2	1:D:251:ALA:HB3	1.86	0.58
1:A:106:LEU:HD12	1:A:106:LEU:C	2.24	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:393:ARG:O	1:F:397:ILE:HG12	2.03	0.58
1:A:166:ARG:HG3	1:F:112:PRO:O	2.02	0.58
1:C:294:LYS:HB2	3:C:901:ATP:O1B	2.04	0.58
1:A:513:GLN:O	1:A:513:GLN:HG3	2.04	0.58
1:E:400:THR:HG22	1:E:401:GLY:N	2.19	0.58
1:A:461:SER:OG	1:A:462:TRP:N	2.36	0.58
1:F:378:ASP:HB3	4:F:520:HOH:O	2.04	0.58
1:B:65:ILE:O	1:B:65:ILE:CG2	2.52	0.58
1:A:191:ILE:HB	1:A:198:GLU:CG	2.33	0.58
1:A:208:ARG:NH2	1:A:221:GLU:OE2	2.37	0.58
1:B:471:MET:HB3	1:B:480:LYS:HZ3	1.69	0.58
1:E:485:ASN:HD21	1:E:496:ARG:NH1	2.02	0.58
1:C:471:MET:HG3	1:C:478:ASP:HB3	1.85	0.58
1:C:147:VAL:HG11	1:C:180:MET:CE	2.31	0.58
1:E:377:ILE:HD12	1:E:412:PHE:HE2	1.68	0.58
1:A:400:THR:HG22	1:A:401:GLY:N	2.18	0.58
1:E:295:THR:HG23	1:E:378:ASP:OD2	2.04	0.58
1:C:344:LEU:HD22	1:C:345:LYS:N	2.19	0.58
1:F:50:THR:HG22	1:F:209:ASN:HB2	1.86	0.58
1:A:344:LEU:HD13	1:A:344:LEU:C	2.24	0.58
1:C:151:PHE:C	1:C:153:GLN:N	2.55	0.58
1:A:496:ARG:HG3	1:B:487:GLU:OE1	2.03	0.58
1:A:52:LYS:N	3:A:903:ATP:O1B	2.28	0.58
1:A:21:MET:CE	1:A:59:PHE:CZ	2.87	0.58
1:E:281:ASP:O	1:E:282:SER:HB3	2.04	0.58
1:B:356:LEU:HD22	1:B:387:VAL:HG11	1.86	0.58
1:D:79:THR:CG2	1:D:82:ASP:H	2.10	0.58
1:C:79:THR:CG2	1:C:82:ASP:H	2.16	0.58
1:E:203:ASN:HB3	1:E:225:LEU:HD23	1.86	0.58
1:F:305:ALA:CB	1:F:374:ARG:HD2	2.20	0.57
1:C:444:GLU:OE2	1:D:489:ILE:HG12	2.03	0.57
1:C:33:HIS:HD2	1:C:229:SER:OG	1.87	0.57
1:F:182:THR:HG22	1:F:183:GLU:H	1.69	0.57
1:A:462:TRP:O	1:A:463:HIS:O	2.21	0.57
1:C:88:ARG:HD3	1:D:15:HIS:O	2.04	0.57
1:C:426:THR:HG22	1:C:428:SER:H	1.69	0.57
1:E:358:ASP:O	1:E:362:ILE:HG12	2.03	0.57
1:D:495:THR:HA	1:E:487:GLU:OE2	2.04	0.57
1:B:45:SER:CB	1:B:182:THR:HB	2.34	0.57
1:A:252:MET:HE3	1:F:350:TYR:CE1	2.39	0.57
1:B:264:SER:HB3	1:B:304:ASN:HD21	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:79:THR:HG23	1:F:81:GLN:H	1.70	0.57
1:E:81:GLN:H	1:E:81:GLN:NE2	2.02	0.57
1:A:448:GLU:HG2	1:B:466:ALA:HA	1.87	0.57
1:B:435:ASP:HA	1:B:459:ARG:HD2	1.86	0.57
1:C:248:PRO:HB2	1:C:251:ALA:HB3	1.86	0.57
1:E:41:SER:HB3	1:E:178:THR:HB	1.84	0.57
1:E:123:LEU:CD2	1:E:166:ARG:HD2	2.30	0.57
1:A:430:ILE:O	1:A:431:SEP:C	2.53	0.57
1:C:431:SEP:C	1:C:432:TPO:CG2	2.82	0.57
1:E:469:GLU:HB2	1:E:483:PHE:CZ	2.40	0.57
1:F:123:LEU:O	1:F:123:LEU:HD13	2.04	0.57
1:C:146:SER:H	1:C:181:THR:CG2	2.16	0.57
1:E:19:ALA:C	1:E:38:ILE:HD12	2.25	0.57
1:F:295:THR:HG23	1:F:378:ASP:OD2	2.04	0.57
1:C:419:PHE:O	1:C:420:MET:CB	2.51	0.57
1:A:182:THR:HG21	1:A:192:ALA:HB1	1.86	0.57
1:C:21:MET:HE3	1:C:141:ARG:CG	2.25	0.57
1:A:61:TYR:CE1	1:A:92:TRP:HB2	2.39	0.57
1:D:471:MET:HB3	1:D:480:LYS:NZ	2.20	0.57
1:B:264:SER:HB3	1:B:304:ASN:ND2	2.19	0.57
1:E:76:PHE:CZ	1:E:126:LEU:HD21	2.40	0.57
1:F:484:ARG:NH1	1:F:484:ARG:HB3	2.19	0.57
1:D:45:SER:HB2	1:D:182:THR:HB	1.87	0.56
1:D:419:PHE:CD2	1:E:425:ILE:CD1	2.86	0.56
1:F:118:VAL:O	1:F:118:VAL:HG13	2.05	0.56
1:E:123:LEU:CD1	1:E:163:GLU:OE2	2.53	0.56
1:F:122:ASP:HA	1:F:125:ALA:HB3	1.87	0.56
1:E:426:THR:HG21	1:E:430:ILE:HG12	1.87	0.56
1:C:45:SER:CB	1:C:182:THR:HB	2.35	0.56
1:E:287:THR:HG23	1:E:414:ASN:HB3	1.88	0.56
1:C:81:GLN:H	1:C:81:GLN:CD	2.06	0.56
1:B:161:ARG:HB2	1:B:196:VAL:HG11	1.85	0.56
1:A:345:LYS:HZ3	1:A:366:GLU:HG2	1.70	0.56
1:B:248:PRO:HB2	1:B:251:ALA:HB3	1.86	0.56
1:D:446:ARG:H	1:D:496:ARG:CZ	2.16	0.56
1:A:211:LEU:HD12	1:A:215:ARG:O	2.06	0.56
1:B:497:ILE:HG13	1:B:498:THR:H	1.69	0.56
1:B:448:GLU:HG2	1:C:466:ALA:HA	1.88	0.56
1:D:96:LYS:O	1:D:100:GLU:HG3	2.05	0.56
1:D:151:PHE:C	1:D:153:GLN:N	2.58	0.56
1:F:436:THR:OG1	1:F:458:MET:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:901:ATP:O3'	1:B:457:LYS:HB2	2.05	0.56
1:B:130:ILE:O	1:B:134:ILE:HG13	2.06	0.56
1:B:430:ILE:O	1:B:431:SEP:C	2.53	0.56
1:B:150:VAL:O	1:B:153:GLN:HG3	2.06	0.56
1:B:451:ARG:HG2	1:B:451:ARG:NH1	2.20	0.56
1:E:76:PHE:HZ	1:E:126:LEU:HD21	1.69	0.56
1:F:294:LYS:N	3:F:901:ATP:O1B	2.39	0.56
1:D:387:VAL:CG1	1:D:388:SER:N	2.69	0.56
1:B:52:LYS:N	3:B:903:ATP:O1B	2.38	0.56
1:A:311:ARG:HD2	1:A:371:LYS:CD	2.35	0.56
1:F:111:ASP:C	1:F:113:GLU:H	2.07	0.56
1:F:117:VAL:O	1:F:118:VAL:HB	2.06	0.56
1:B:79:THR:CG2	1:B:82:ASP:H	2.12	0.56
1:C:49:GLY:O	1:C:218:ARG:NH2	2.39	0.56
1:E:485:ASN:HD21	1:E:496:ARG:HH11	1.50	0.56
1:F:150:VAL:O	1:F:153:GLN:HG3	2.06	0.56
1:F:118:VAL:HG22	1:F:122:ASP:HB3	1.88	0.55
1:C:104:PHE:CE2	1:C:106:LEU:HB2	2.41	0.55
1:C:43:LEU:HD11	1:C:182:THR:OG1	2.05	0.55
1:A:495:THR:HG22	1:A:497:ILE:CG2	2.36	0.55
1:D:178:THR:HG22	1:D:179:VAL:N	2.21	0.55
1:F:96:LYS:O	1:F:100:GLU:HG3	2.06	0.55
1:F:396:VAL:HG11	1:F:430:ILE:CG2	2.36	0.55
1:A:501:GLU:O	1:A:503:SER:N	2.39	0.55
1:E:147:VAL:HG11	1:E:180:MET:HE2	1.89	0.55
1:E:345:LYS:HZ3	1:E:366:GLU:CD	2.09	0.55
1:D:469:GLU:HB2	1:D:483:PHE:CZ	2.42	0.55
1:E:49:GLY:CA	3:E:903:ATP:O2B	2.54	0.55
1:C:356:LEU:HD22	1:C:387:VAL:HG11	1.87	0.55
1:D:140:ARG:HH11	1:D:140:ARG:CB	2.19	0.55
1:B:159:VAL:O	1:B:163:GLU:HG2	2.07	0.55
1:E:501:GLU:O	1:E:502:LYS:CG	2.49	0.55
1:B:191:ILE:CB	1:B:198:GLU:HG3	2.36	0.55
1:F:435:ASP:HA	1:F:459:ARG:HD2	1.87	0.55
1:B:294:LYS:HB2	3:B:901:ATP:O1B	2.07	0.55
1:D:439:LEU:HD12	1:D:439:LEU:C	2.27	0.55
1:D:67:PHE:HB2	1:D:69:GLU:HG3	1.89	0.55
1:B:213:GLY:O	1:B:214:GLU:HB2	2.06	0.55
1:D:148:THR:CG2	1:D:193:ARG:HD2	2.37	0.55
1:A:433:ILE:CG2	1:A:433:ILE:O	2.50	0.55
1:E:496:ARG:HG3	1:E:497:ILE:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:ILE:HD12	1:D:412:PHE:HE2	1.72	0.55
1:A:393:ARG:O	1:A:397:ILE:HG12	2.06	0.55
1:B:485:ASN:N	1:B:485:ASN:OD1	2.33	0.55
1:E:123:LEU:HD21	1:E:127:ILE:HD11	1.87	0.55
1:C:53:THR:HG23	1:C:145:ASP:OD1	2.05	0.55
1:A:211:LEU:O	1:A:212:GLU:CB	2.52	0.55
1:F:49:GLY:HA2	3:F:903:ATP:O2B	2.06	0.55
1:B:340:ARG:C	1:B:342:ASN:H	2.11	0.55
1:A:57:ILE:HD13	1:A:73:PHE:CE1	2.42	0.55
1:B:184:ARG:HG2	1:B:191:ILE:O	2.06	0.55
1:F:315:PHE:CZ	1:F:363:ILE:HG23	2.41	0.55
1:C:493:SER:HB3	1:D:488:ARG:HG2	1.89	0.55
1:A:439:LEU:HD12	1:A:440:LEU:N	2.21	0.55
1:C:377:ILE:HD12	1:C:412:PHE:CE2	2.42	0.55
1:C:20:LYS:HE3	1:C:228:THR:HG21	1.89	0.55
1:B:148:THR:OG1	1:B:182:THR:HG23	2.07	0.54
1:A:65:ILE:O	1:A:65:ILE:CG2	2.54	0.54
1:C:18:ILE:HG21	1:C:37:PRO:HB3	1.89	0.54
1:F:340:ARG:C	1:F:342:ASN:H	2.10	0.54
1:C:435:ASP:HA	1:C:459:ARG:HD2	1.89	0.54
1:E:121:PHE:CD1	1:E:121:PHE:N	2.74	0.54
1:B:503:SER:O	1:B:504:GLU:HB2	2.05	0.54
1:D:127:ILE:HD11	1:D:167:LEU:HA	1.87	0.54
1:A:484:ARG:HB3	1:A:484:ARG:NH1	2.21	0.54
1:C:148:THR:HG21	1:C:183:GLU:HG3	1.89	0.54
1:D:340:ARG:C	1:D:342:ASN:H	2.11	0.54
1:C:113:GLU:O	1:C:114:GLY:C	2.45	0.54
1:B:316:ALA:O	1:B:348:CYS:HA	2.07	0.54
1:A:203:ASN:HB3	1:A:225:LEU:HD23	1.89	0.54
1:B:426:THR:HG22	1:B:428:SER:N	2.23	0.54
1:D:191:ILE:CG2	1:D:198:GLU:HG3	2.37	0.54
1:D:354:ALA:HB3	1:D:359:HIS:NE2	2.23	0.54
1:E:437:ILE:CD1	1:E:457:LYS:HE2	2.37	0.54
1:E:31:ILE:HG22	1:E:222:ILE:HD12	1.89	0.54
1:E:449:MET:HE3	1:F:490:ILE:HD11	1.88	0.54
1:C:169:ALA:O	1:C:173:GLN:HG3	2.08	0.54
1:A:451:ARG:N	1:A:451:ARG:HD2	2.23	0.54
1:A:283:ILE:HD12	1:A:412:PHE:HE1	1.73	0.54
1:A:148:THR:HG21	1:A:183:GLU:HG3	1.88	0.54
1:A:148:THR:OG1	1:A:182:THR:HG23	2.08	0.54
1:C:117:VAL:O	1:C:117:VAL:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:ARG:NH2	1:C:221:GLU:OE2	2.40	0.54
1:A:161:ARG:HB2	1:A:196:VAL:HG11	1.89	0.54
1:F:119:GLY:HA2	1:F:122:ASP:OD1	2.08	0.54
1:E:211:LEU:O	1:E:212:GLU:HB3	2.07	0.54
1:C:367:ILE:HG12	1:C:375:ILE:HD11	1.89	0.54
1:C:441:GLN:HE22	1:C:490:ILE:HD13	1.72	0.54
1:A:79:THR:HG23	1:A:81:GLN:H	1.73	0.54
1:F:148:THR:HG21	1:F:183:GLU:CG	2.37	0.54
1:C:148:THR:CG2	1:C:193:ARG:HD2	2.38	0.54
1:E:485:ASN:ND2	1:E:496:ARG:NH1	2.52	0.54
1:B:360:LEU:HD22	1:B:360:LEU:O	2.08	0.54
1:D:489:ILE:HA	1:D:494:PRO:HG3	1.89	0.54
1:D:451:ARG:HG2	1:D:451:ARG:NH1	2.22	0.54
1:B:311:ARG:HD2	1:B:371:LYS:CD	2.38	0.54
1:C:356:LEU:CD2	1:C:387:VAL:HG11	2.38	0.54
1:B:213:GLY:O	1:B:214:GLU:CB	2.56	0.54
1:C:150:VAL:HG13	1:C:151:PHE:N	2.22	0.54
1:E:306:CYS:SG	1:E:344:LEU:HB2	2.48	0.54
1:E:471:MET:HB3	1:E:480:LYS:NZ	2.23	0.54
1:B:358:ASP:O	1:B:362:ILE:HG12	2.08	0.54
1:B:31:ILE:HG22	1:B:222:ILE:HD12	1.89	0.54
1:F:504:GLU:HA	1:F:507:ARG:HE	1.73	0.54
1:A:311:ARG:HA	1:A:343:LEU:O	2.07	0.54
1:C:359:HIS:O	1:C:363:ILE:HG13	2.07	0.54
1:B:483:PHE:HB3	1:B:486:PHE:CD1	2.43	0.54
1:B:116:GLU:HG2	1:B:117:VAL:H	1.73	0.54
1:E:18:ILE:HG13	1:E:228:THR:HG23	1.89	0.54
1:D:161:ARG:HB2	1:D:196:VAL:HG11	1.89	0.54
1:D:150:VAL:O	1:D:153:GLN:HG3	2.07	0.53
1:B:340:ARG:O	1:B:342:ASN:N	2.41	0.53
1:A:79:THR:HG23	1:A:81:GLN:CG	2.34	0.53
1:E:320:SER:HA	1:F:254:LEU:HG	1.89	0.53
1:A:19:ALA:C	1:A:38:ILE:HD12	2.29	0.53
1:A:510:ARG:HA	1:A:510:ARG:NE	2.23	0.53
1:E:123:LEU:O	1:E:127:ILE:CG1	2.56	0.53
1:B:38:ILE:HA	1:B:177:THR:CG2	2.37	0.53
1:E:471:MET:HG2	1:E:480:LYS:HE2	1.90	0.53
1:A:264:SER:HA	1:A:271:ASP:OD1	2.08	0.53
1:E:118:VAL:HG12	1:E:118:VAL:O	2.09	0.53
1:C:300:ARG:N	1:C:333:MET:HE1	2.23	0.53
1:A:503:SER:O	1:A:504:GLU:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:LEU:C	1:D:106:LEU:CD1	2.75	0.53
1:A:126:LEU:HG	1:A:130:ILE:HD12	1.90	0.53
1:C:164:LEU:HB3	1:C:200:VAL:HG11	1.89	0.53
1:F:489:ILE:HA	1:F:494:PRO:HG3	1.91	0.53
1:B:79:THR:O	1:B:83:ILE:HD12	2.08	0.53
1:E:356:LEU:HD13	1:E:387:VAL:HG21	1.91	0.53
1:E:489:ILE:HA	1:E:494:PRO:HG3	1.90	0.53
1:B:67:PHE:HB2	1:B:69:GLU:HG3	1.89	0.53
1:D:43:LEU:HD11	1:D:182:THR:OG1	2.08	0.53
1:A:419:PHE:O	1:A:420:MET:HB2	2.08	0.53
1:A:150:VAL:HG13	1:A:151:PHE:N	2.23	0.53
1:F:498:THR:HB	1:F:500:ASP:O	2.08	0.53
1:D:318:GLU:OE2	1:D:379:SER:CB	2.56	0.53
1:C:488:ARG:HH11	1:C:488:ARG:HG3	1.72	0.53
1:F:49:GLY:CA	3:F:903:ATP:O2B	2.56	0.53
1:C:221:GLU:HG3	1:C:233:GLY:O	2.08	0.53
1:F:505:LEU:O	1:F:506:SER:HB3	2.09	0.53
1:A:457:LYS:HB2	3:F:901:ATP:O3'	2.08	0.53
1:B:262:ARG:NH2	1:B:461:SER:HB2	2.23	0.53
1:C:323:GLN:HE22	1:D:459:ARG:HD3	1.74	0.53
1:C:431:SEP:O	1:C:432:TPO:HG23	2.09	0.53
1:D:212:GLU:HG2	1:D:212:GLU:O	2.08	0.53
1:B:305:ALA:CB	1:B:374:ARG:HD2	2.32	0.53
1:A:426:THR:HG22	1:A:428:SER:N	2.21	0.53
1:D:300:ARG:N	1:D:333:MET:HE1	2.23	0.53
1:A:92:TRP:CD1	1:A:92:TRP:O	2.59	0.53
1:A:458:MET:O	3:F:901:ATP:H3'	2.09	0.53
1:F:311:ARG:HG3	1:F:371:LYS:NZ	2.24	0.53
1:B:353:SER:O	1:B:354:ALA:HB2	2.08	0.53
1:D:294:LYS:HB2	3:D:901:ATP:O1B	2.08	0.53
1:E:325:LEU:CD2	1:E:335:PHE:HB2	2.38	0.53
1:F:122:ASP:OD2	1:F:123:LEU:N	2.42	0.53
1:E:123:LEU:HD23	1:E:127:ILE:CD1	2.38	0.53
1:C:287:THR:HG21	1:C:425:ILE:O	2.08	0.53
1:F:148:THR:CG2	1:F:193:ARG:HD2	2.39	0.53
1:C:52:LYS:HB2	3:C:903:ATP:O1B	2.09	0.53
1:E:191:ILE:CB	1:E:198:GLU:CG	2.87	0.53
1:C:311:ARG:HD2	1:C:371:LYS:CE	2.38	0.53
1:C:430:ILE:O	1:C:432:TPO:N	2.42	0.53
1:E:437:ILE:HD12	1:E:457:LYS:HE2	1.90	0.53
1:D:359:HIS:O	1:D:363:ILE:HG13	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:GLY:O	1:A:333:MET:O	2.27	0.52
1:A:146:SER:N	1:A:181:THR:HG22	2.24	0.52
1:F:379:SER:H	1:F:413:THR:HB	1.74	0.52
1:A:43:LEU:HD11	1:A:182:THR:OG1	2.08	0.52
1:F:208:ARG:NH2	1:F:221:GLU:OE2	2.42	0.52
1:E:255:THR:O	1:E:255:THR:HG22	2.08	0.52
1:C:119:GLY:HA2	1:C:122:ASP:OD1	2.09	0.52
1:A:419:PHE:CE2	1:B:425:ILE:HD12	2.44	0.52
1:F:500:ASP:O	1:F:501:GLU:HB3	2.09	0.52
1:E:451:ARG:HH11	1:E:451:ARG:HG2	1.74	0.52
1:A:367:ILE:HG12	1:A:375:ILE:HD11	1.90	0.52
1:C:426:THR:HG21	1:C:430:ILE:HG12	1.90	0.52
1:A:451:ARG:CG	1:A:451:ARG:NH1	2.65	0.52
1:D:42:THR:HG23	1:D:203:ASN:HB2	1.90	0.52
1:C:123:LEU:O	1:C:126:LEU:N	2.42	0.52
1:F:79:THR:HG23	1:F:81:GLN:HE21	1.74	0.52
1:F:191:ILE:HG21	1:F:198:GLU:HG3	1.92	0.52
1:F:501:GLU:HG3	1:F:502:LYS:N	2.25	0.52
1:A:267:VAL:HB	1:A:270:LEU:HB2	1.91	0.52
1:D:255:THR:HG22	1:D:255:THR:O	2.09	0.52
1:F:396:VAL:O	1:F:400:THR:HB	2.10	0.52
1:B:79:THR:HG23	1:B:81:GLN:HE21	1.74	0.52
1:F:191:ILE:CB	1:F:198:GLU:CG	2.80	0.52
1:D:353:SER:O	1:D:354:ALA:HB2	2.10	0.52
1:F:52:LYS:HE3	3:F:903:ATP:O1B	2.09	0.52
1:E:50:THR:HG22	1:E:209:ASN:HB2	1.90	0.52
1:A:15:HIS:C	1:A:16:GLN:OE1	2.47	0.52
1:F:161:ARG:HB2	1:F:196:VAL:CG1	2.39	0.52
1:E:469:GLU:HG3	1:E:470:PHE:N	2.24	0.52
1:D:211:LEU:HD12	1:D:215:ARG:O	2.10	0.52
1:A:213:GLY:O	1:A:214:GLU:HB2	2.09	0.52
1:D:65:ILE:HG22	1:D:65:ILE:O	2.08	0.52
1:E:441:GLN:HE22	1:E:490:ILE:HD13	1.74	0.52
1:C:111:ASP:O	1:C:113:GLU:N	2.39	0.52
1:D:80:PRO:HD2	1:D:81:GLN:NE2	2.25	0.52
1:E:191:ILE:HB	1:E:198:GLU:CD	2.30	0.52
1:B:96:LYS:O	1:B:100:GLU:HG3	2.09	0.52
1:F:509:VAL:HG12	1:F:510:ARG:H	1.75	0.52
1:B:436:THR:HG23	1:B:458:MET:HG3	1.92	0.52
1:B:91:GLY:O	1:B:92:TRP:CD1	2.63	0.52
1:C:186:GLU:OE2	1:C:187:GLU:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:THR:HG22	1:B:179:VAL:N	2.25	0.52
1:A:471:MET:HB3	1:A:480:LYS:NZ	2.24	0.52
1:F:148:THR:OG1	1:F:182:THR:HG23	2.10	0.52
1:C:79:THR:C	1:C:83:ILE:HD12	2.29	0.52
1:A:294:LYS:N	3:A:901:ATP:O1B	2.43	0.52
1:F:104:PHE:CE2	1:F:106:LEU:HB2	2.44	0.52
1:F:353:SER:O	1:F:354:ALA:HB2	2.10	0.52
1:A:151:PHE:C	1:A:153:GLN:N	2.64	0.51
1:D:419:PHE:CE2	1:E:425:ILE:HD12	2.44	0.51
1:C:336:GLU:OE1	1:C:336:GLU:HA	2.10	0.51
1:E:433:ILE:HD12	1:E:433:ILE:N	2.25	0.51
1:A:300:ARG:N	1:A:333:MET:HE1	2.25	0.51
1:A:370:PHE:O	1:A:371:LYS:HD2	2.09	0.51
1:F:502:LYS:HZ2	1:F:507:ARG:HB3	1.74	0.51
1:B:52:LYS:HD3	1:B:182:THR:O	2.10	0.51
1:A:89:SER:CB	1:B:227:GLY:O	2.59	0.51
1:E:123:LEU:O	1:E:127:ILE:HG13	2.10	0.51
1:E:262:ARG:NH2	1:E:461:SER:HB2	2.26	0.51
1:C:191:ILE:HB	1:C:198:GLU:HG3	1.91	0.51
1:A:294:LYS:HB2	3:A:901:ATP:O1B	2.10	0.51
1:D:81:GLN:CD	1:D:81:GLN:H	2.14	0.51
1:B:38:ILE:HA	1:B:177:THR:HG23	1.92	0.51
1:A:359:HIS:O	1:A:363:ILE:HG13	2.10	0.51
1:A:340:ARG:O	1:A:342:ASN:N	2.44	0.51
1:B:286:ALA:HA	1:B:438:ILE:O	2.11	0.51
1:F:497:ILE:HD12	1:F:497:ILE:C	2.30	0.51
1:D:432:TPO:H2	1:D:434:THR:HG22	1.74	0.51
1:D:45:SER:CB	1:D:182:THR:HB	2.41	0.51
1:B:191:ILE:CG2	1:B:198:GLU:HG3	2.40	0.51
1:F:515:LYS:CG	1:F:517:PRO:HD2	2.41	0.51
1:E:379:SER:H	1:E:413:THR:HB	1.76	0.51
1:E:471:MET:HG3	1:E:478:ASP:HB3	1.92	0.51
1:A:213:GLY:O	1:A:214:GLU:CB	2.59	0.51
1:A:325:LEU:HD23	1:A:335:PHE:HB2	1.92	0.51
1:D:332:GLY:O	1:D:333:MET:O	2.28	0.51
1:E:191:ILE:HB	1:E:198:GLU:HG3	1.91	0.51
1:F:270:LEU:O	1:F:273:MET:HB2	2.11	0.51
1:B:486:PHE:CE2	1:B:496:ARG:HB2	2.46	0.51
1:B:64:ILE:HG22	1:B:65:ILE:HD13	1.93	0.51
1:B:161:ARG:HB2	1:B:196:VAL:CG1	2.40	0.51
1:E:49:GLY:HA2	3:E:903:ATP:O2B	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:THR:HG23	1:A:81:GLN:HE21	1.76	0.51
1:C:340:ARG:C	1:C:342:ASN:H	2.14	0.51
1:B:246:ILE:O	1:B:248:PRO:HD3	2.10	0.51
1:A:56:SER:HB2	1:A:143:SER:HB3	1.92	0.51
1:C:134:ILE:HG23	1:C:139:ALA:HB3	1.91	0.51
1:A:425:ILE:HD12	1:F:419:PHE:CE2	2.46	0.51
1:D:385:ARG:HG2	1:E:393:ARG:NH1	2.26	0.51
1:C:79:THR:HG21	1:C:81:GLN:HG2	1.91	0.51
1:D:335:PHE:HA	1:D:338:MET:HG3	1.93	0.51
1:D:19:ALA:O	1:D:38:ILE:HD12	2.11	0.51
1:C:295:THR:HG21	1:C:319:GLU:OE2	2.11	0.51
1:A:220:LEU:C	1:A:220:LEU:HD23	2.31	0.51
1:D:484:ARG:NH1	1:D:484:ARG:HB3	2.25	0.51
1:C:123:LEU:HD11	1:C:163:GLU:O	2.10	0.51
1:B:79:THR:HG23	1:B:81:GLN:H	1.75	0.51
1:F:81:GLN:N	1:F:81:GLN:NE2	2.59	0.51
1:B:289:ALA:HB2	1:B:419:PHE:HA	1.92	0.51
1:E:191:ILE:CB	1:E:198:GLU:HG3	2.41	0.51
1:F:439:LEU:C	1:F:439:LEU:HD12	2.30	0.51
1:B:119:GLY:C	1:B:121:PHE:N	2.62	0.51
1:F:170:ARG:O	1:F:174:ILE:HG12	2.11	0.51
1:C:120:GLY:O	1:C:122:ASP:N	2.44	0.50
1:D:496:ARG:CG	1:E:487:GLU:OE1	2.59	0.50
1:B:49:GLY:O	1:B:218:ARG:NH2	2.44	0.50
1:B:148:THR:CG2	1:B:193:ARG:HD2	2.42	0.50
1:B:336:GLU:OE1	1:B:336:GLU:HA	2.11	0.50
1:F:344:LEU:HD22	1:F:345:LYS:H	1.76	0.50
1:F:231:MET:HE1	1:F:251:ALA:HB2	1.93	0.50
1:C:299:SER:C	1:C:333:MET:HE1	2.31	0.50
1:C:24:MET:HB2	1:C:62:ASN:HD22	1.76	0.50
1:F:151:PHE:C	1:F:153:GLN:N	2.64	0.50
1:F:462:TRP:O	1:F:463:HIS:O	2.28	0.50
1:F:106:LEU:HD13	1:F:129:ARG:CZ	2.41	0.50
1:C:344:LEU:HD22	1:C:345:LYS:H	1.75	0.50
1:E:84:ILE:HG21	1:E:95:ALA:HB2	1.94	0.50
1:A:18:ILE:CD1	1:A:18:ILE:N	2.74	0.50
1:A:436:THR:HG23	1:A:458:MET:HG3	1.93	0.50
1:E:347:VAL:O	1:E:348:CYS:HB2	2.11	0.50
1:F:120:GLY:O	1:F:123:LEU:HB3	2.11	0.50
1:E:169:ALA:O	1:E:173:GLN:HG3	2.11	0.50
1:D:191:ILE:CB	1:D:198:GLU:CG	2.86	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:262:ARG:HH22	1:E:461:SER:HB2	1.76	0.50
1:F:437:ILE:CD1	1:F:457:LYS:HE2	2.41	0.50
1:C:420:MET:CE	1:D:490:ILE:HG21	2.41	0.50
1:C:431:SEP:O	1:C:432:TPO:CG2	2.59	0.50
1:D:273:MET:CE	1:D:468:ARG:HD2	2.41	0.50
1:A:318:GLU:CD	1:B:432:TPO:CG2	2.80	0.50
1:D:313:ILE:HD11	1:D:372:PRO:HG3	1.94	0.50
1:C:38:ILE:HA	1:C:177:THR:HG23	1.94	0.50
1:B:418:GLN:HB2	1:C:423:HIS:O	2.11	0.50
1:E:146:SER:CA	1:E:181:THR:HG22	2.41	0.50
1:B:287:THR:HG23	1:B:414:ASN:HB3	1.94	0.50
1:E:363:ILE:O	1:E:367:ILE:HG13	2.12	0.50
1:D:159:VAL:O	1:D:163:GLU:HG2	2.12	0.50
1:D:79:THR:HG23	1:D:81:GLN:N	2.26	0.50
1:F:509:VAL:HG12	1:F:510:ARG:N	2.27	0.50
1:A:295:THR:HG23	1:A:378:ASP:OD2	2.11	0.50
1:B:483:PHE:HB3	1:B:486:PHE:HD1	1.76	0.50
1:D:451:ARG:HB3	1:D:470:PHE:CE2	2.47	0.50
1:F:471:MET:CG	1:F:478:ASP:HB3	2.42	0.50
1:C:323:GLN:NE2	1:D:459:ARG:HD3	2.27	0.50
1:E:441:GLN:HE22	1:E:490:ILE:HA	1.77	0.50
1:A:266:GLY:HA3	1:A:300:ARG:HG3	1.93	0.50
1:C:419:PHE:HD1	1:C:420:MET:HG3	1.75	0.50
1:F:19:ALA:C	1:F:38:ILE:HD12	2.32	0.50
1:A:254:LEU:HG	1:F:320:SER:HA	1.94	0.50
1:B:269:ARG:HG2	1:B:479:ILE:HB	1.94	0.50
1:D:433:ILE:HG22	1:D:433:ILE:O	2.10	0.50
1:F:396:VAL:HG11	1:F:430:ILE:HG21	1.92	0.49
1:A:425:ILE:HD12	1:F:419:PHE:CD2	2.46	0.49
1:C:495:THR:HG22	1:D:487:GLU:OE2	2.11	0.49
1:C:38:ILE:HA	1:C:177:THR:CG2	2.42	0.49
1:B:50:THR:HG22	1:B:209:ASN:HB2	1.94	0.49
1:C:36:LEU:HD12	1:C:59:PHE:CE1	2.46	0.49
1:C:287:THR:HG23	1:C:414:ASN:ND2	2.22	0.49
1:B:377:ILE:HD12	1:B:412:PHE:CD2	2.46	0.49
1:D:396:VAL:HG11	1:D:430:ILE:HG23	1.93	0.49
1:F:20:LYS:C	1:F:38:ILE:HD11	2.31	0.49
1:B:31:ILE:HA	1:B:231:MET:SD	2.52	0.49
1:A:340:ARG:C	1:A:342:ASN:H	2.15	0.49
1:D:468:ARG:NH1	1:D:468:ARG:HG2	2.27	0.49
1:C:54:LEU:HD13	1:C:90:PHE:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ILE:HG21	1:B:198:GLU:HG3	1.94	0.49
1:B:81:GLN:CD	1:B:81:GLN:H	2.15	0.49
1:C:52:LYS:N	3:C:903:ATP:O1B	2.42	0.49
1:E:151:PHE:C	1:E:153:GLN:N	2.64	0.49
1:A:191:ILE:HB	1:A:198:GLU:CD	2.32	0.49
1:C:111:ASP:OD1	1:C:113:GLU:HG2	2.12	0.49
1:F:131:ASN:OD1	1:F:174:ILE:HD12	2.13	0.49
1:B:126:LEU:HD12	1:B:129:ARG:HD3	1.93	0.49
1:F:79:THR:CG2	1:F:82:ASP:H	2.13	0.49
1:A:218:ARG:O	1:A:236:PRO:HA	2.13	0.49
1:C:311:ARG:HD2	1:C:371:LYS:CD	2.42	0.49
1:F:471:MET:HB3	1:F:480:LYS:HZ3	1.77	0.49
1:F:406:GLU:HB3	1:F:408:ILE:HG13	1.94	0.49
1:F:121:PHE:O	1:F:125:ALA:N	2.41	0.49
1:F:356:LEU:HD21	1:F:387:VAL:HG11	1.94	0.49
1:E:430:ILE:O	1:E:431:SEP:C	2.60	0.49
1:D:263:VAL:CG1	1:D:374:ARG:HH21	2.21	0.49
1:C:54:LEU:HD13	1:C:90:PHE:CZ	2.48	0.49
1:C:469:GLU:HB2	1:C:483:PHE:CZ	2.47	0.49
1:F:356:LEU:HD22	1:F:387:VAL:HG11	1.95	0.49
1:A:267:VAL:O	1:A:271:ASP:OD2	2.31	0.49
1:C:70:PRO:HG2	1:C:138:ARG:O	2.12	0.49
1:E:21:MET:CE	1:E:59:PHE:CZ	2.96	0.49
1:A:17:ALA:C	1:A:18:ILE:HD12	2.33	0.49
1:D:148:THR:OG1	1:D:182:THR:CG2	2.60	0.49
1:B:455:VAL:HG11	1:B:463:HIS:HB2	1.93	0.49
1:A:356:LEU:HD22	1:A:387:VAL:HG11	1.93	0.49
1:E:79:THR:HG23	1:E:81:GLN:H	1.76	0.49
1:B:419:PHE:CD2	1:C:425:ILE:CD1	2.93	0.49
1:F:182:THR:CG2	1:F:183:GLU:N	2.75	0.49
1:C:67:PHE:CB	1:C:69:GLU:HG3	2.40	0.49
3:B:903:ATP:O3'	1:C:224:LYS:HB2	2.13	0.49
1:B:20:LYS:HE3	1:B:228:THR:HG21	1.95	0.49
1:F:471:MET:HB3	1:F:480:LYS:HZ1	1.77	0.49
1:A:471:MET:HG2	1:A:480:LYS:HE2	1.94	0.49
1:D:151:PHE:O	1:D:153:GLN:N	2.42	0.48
1:F:501:GLU:HG3	1:F:502:LYS:H	1.78	0.48
1:D:299:SER:HB3	1:D:333:MET:CE	2.42	0.48
1:E:211:LEU:O	1:E:212:GLU:CB	2.61	0.48
1:D:347:VAL:O	1:D:348:CYS:CB	2.60	0.48
1:C:332:GLY:O	1:C:333:MET:O	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:461:SER:OG	1:D:462:TRP:N	2.45	0.48
1:F:169:ALA:O	1:F:173:GLN:HG3	2.12	0.48
1:B:203:ASN:HB3	1:B:225:LEU:HD23	1.95	0.48
1:C:325:LEU:CD2	1:C:335:PHE:HB2	2.43	0.48
1:E:417:ASP:O	1:F:424:SER:HB3	2.13	0.48
1:B:431:SEP:O	1:B:434:THR:CG2	2.33	0.48
1:A:81:GLN:H	1:A:81:GLN:CD	2.16	0.48
1:A:419:PHE:HD1	1:A:420:MET:HG3	1.77	0.48
1:A:127:ILE:HD11	1:A:167:LEU:CD1	2.41	0.48
1:C:471:MET:HB3	1:C:480:LYS:NZ	2.27	0.48
1:E:186:GLU:HB3	1:E:189:GLY:HA3	1.95	0.48
1:F:340:ARG:C	1:F:342:ASN:N	2.66	0.48
1:B:323:GLN:NE2	1:C:459:ARG:HD3	2.28	0.48
1:A:19:ALA:O	1:A:38:ILE:HD12	2.13	0.48
1:B:25:ILE:HG12	1:B:58:GLN:NE2	2.29	0.48
1:B:396:VAL:O	1:B:400:THR:HB	2.13	0.48
1:F:426:THR:CG2	1:F:428:SER:OG	2.60	0.48
1:C:263:VAL:CG1	1:C:374:ARG:HH21	2.27	0.48
1:A:483:PHE:HB3	1:A:486:PHE:CD1	2.47	0.48
1:E:104:PHE:CE2	1:E:106:LEU:HB2	2.48	0.48
3:D:903:ATP:O3'	1:E:224:LYS:HB2	2.14	0.48
1:D:363:ILE:O	1:D:367:ILE:HG13	2.13	0.48
1:F:311:ARG:HD2	1:F:371:LYS:HD2	1.95	0.48
1:F:311:ARG:HG3	1:F:371:LYS:HZ1	1.78	0.48
1:E:348:CYS:HB3	1:F:254:LEU:HD23	1.95	0.48
1:F:484:ARG:HH11	1:F:484:ARG:HB3	1.78	0.48
1:F:65:ILE:HG22	1:F:65:ILE:O	2.12	0.48
1:C:58:GLN:HG3	1:C:92:TRP:CH2	2.48	0.48
1:E:487:GLU:O	1:E:488:ARG:HB2	2.13	0.48
1:A:433:ILE:N	1:A:433:ILE:HD12	2.29	0.48
1:A:49:GLY:O	1:A:218:ARG:NH2	2.47	0.48
1:C:41:SER:HA	1:C:178:THR:O	2.13	0.48
1:E:18:ILE:HD11	1:E:227:GLY:C	2.34	0.48
1:B:281:ASP:O	1:B:282:SER:HB3	2.13	0.48
1:F:325:LEU:CD2	1:F:335:PHE:HB2	2.44	0.48
1:E:311:ARG:HD2	1:E:371:LYS:CE	2.44	0.48
1:C:44:VAL:HA	1:C:205:VAL:O	2.14	0.48
1:A:81:GLN:H	1:A:81:GLN:NE2	2.11	0.48
1:E:123:LEU:HD23	1:E:127:ILE:CG1	2.43	0.48
1:D:323:GLN:NE2	1:E:459:ARG:HD3	2.28	0.48
1:C:396:VAL:O	1:C:400:THR:HB	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:ILE:HG22	1:D:174:ILE:O	2.13	0.48
1:A:387:VAL:HG12	1:A:388:SER:N	2.28	0.48
1:F:514:GLU:HB3	1:F:519:SER:HB3	1.96	0.48
1:F:79:THR:O	1:F:83:ILE:HD12	2.14	0.48
1:C:49:GLY:CA	3:C:903:ATP:O2B	2.62	0.48
1:B:387:VAL:HG12	1:B:388:SER:N	2.29	0.48
1:E:185:ILE:HD11	1:E:193:ARG:NH1	2.29	0.48
1:E:52:LYS:HD3	1:E:182:THR:O	2.13	0.48
1:C:81:GLN:N	1:C:81:GLN:CD	2.66	0.48
1:E:336:GLU:HA	1:E:336:GLU:OE1	2.14	0.48
1:B:311:ARG:HA	1:B:343:LEU:O	2.13	0.48
1:A:121:PHE:O	1:A:125:ALA:HB2	2.14	0.48
1:A:70:PRO:HA	1:A:102:LYS:O	2.14	0.48
1:E:79:THR:O	1:E:83:ILE:HD12	2.14	0.47
1:C:305:ALA:CB	1:C:374:ARG:HD2	2.39	0.47
1:D:21:MET:CE	1:D:59:PHE:CZ	2.98	0.47
1:B:347:VAL:O	1:B:348:CYS:HB2	2.13	0.47
1:C:98:VAL:HA	1:C:103:LEU:O	2.14	0.47
1:B:396:VAL:HG11	1:B:430:ILE:CG2	2.45	0.47
1:A:153:GLN:O	1:A:154:TYR:CB	2.62	0.47
1:F:426:THR:HG22	1:F:428:SER:N	2.18	0.47
1:D:388:SER:OG	1:D:391:ALA:CB	2.62	0.47
1:E:444:GLU:OE1	1:F:490:ILE:HG12	2.13	0.47
1:B:208:ARG:NH2	1:B:221:GLU:OE2	2.47	0.47
1:F:420:MET:HE3	1:F:420:MET:HB3	1.79	0.47
1:E:497:ILE:O	1:E:498:THR:CB	2.62	0.47
1:C:367:ILE:HG12	1:C:375:ILE:CD1	2.44	0.47
1:B:61:TYR:CE1	1:B:92:TRP:HB3	2.49	0.47
1:A:514:GLU:HA	1:A:514:GLU:OE1	2.11	0.47
1:D:98:VAL:HA	1:D:103:LEU:O	2.15	0.47
1:A:98:VAL:HA	1:A:103:LEU:O	2.13	0.47
1:C:354:ALA:HB1	1:C:358:ASP:HB2	1.95	0.47
1:A:502:LYS:O	1:A:502:LYS:HG3	2.14	0.47
1:D:52:LYS:HD3	1:D:182:THR:O	2.14	0.47
1:B:419:PHE:HD1	1:B:420:MET:HG3	1.79	0.47
1:A:469:GLU:HB2	1:A:483:PHE:CZ	2.49	0.47
1:D:356:LEU:HD21	1:D:387:VAL:HG11	1.96	0.47
1:C:311:ARG:HA	1:C:343:LEU:O	2.14	0.47
1:F:283:ILE:HG23	1:F:412:PHE:CE1	2.49	0.47
1:E:332:GLY:O	1:E:333:MET:O	2.32	0.47
1:E:271:ASP:OD1	1:E:277:GLY:HA2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ARG:NE	1:B:432:TPO:O2P	2.47	0.47
1:D:150:VAL:HG13	1:D:151:PHE:N	2.28	0.47
1:B:123:LEU:HD13	1:B:127:ILE:HD11	1.97	0.47
1:D:356:LEU:CD2	1:D:387:VAL:HG11	2.43	0.47
1:E:344:LEU:HD22	1:E:345:LYS:N	2.29	0.47
1:D:269:ARG:HB3	1:D:479:ILE:HD12	1.97	0.47
1:B:60:LEU:HD12	1:B:73:PHE:HB2	1.96	0.47
1:B:111:ASP:O	1:B:113:GLU:N	2.47	0.47
1:B:431:SEP:C	1:B:434:THR:HG22	2.32	0.47
3:B:901:ATP:C5	1:C:461:SER:O	2.68	0.47
1:D:289:ALA:HB2	1:D:419:PHE:HA	1.94	0.47
1:A:170:ARG:O	1:A:174:ILE:HG12	2.15	0.47
1:C:320:SER:HA	1:D:254:LEU:HG	1.95	0.47
1:B:150:VAL:HG13	1:B:151:PHE:N	2.29	0.47
1:D:81:GLN:CD	1:D:81:GLN:N	2.68	0.47
1:B:294:LYS:N	3:B:901:ATP:O1B	2.48	0.47
1:F:184:ARG:HG2	1:F:191:ILE:O	2.15	0.47
1:D:305:ALA:HB2	1:D:374:ARG:CD	2.37	0.47
1:E:311:ARG:HA	1:E:343:LEU:O	2.15	0.47
1:C:451:ARG:NH1	1:C:451:ARG:CG	2.77	0.47
1:A:486:PHE:CD2	1:A:496:ARG:HA	2.50	0.47
1:F:311:ARG:HD2	1:F:371:LYS:NZ	2.29	0.47
1:F:104:PHE:HE2	1:F:106:LEU:HB2	1.80	0.47
1:B:264:SER:HA	1:B:271:ASP:OD1	2.14	0.47
1:A:45:SER:CB	1:A:182:THR:HB	2.43	0.47
1:E:76:PHE:HZ	1:E:126:LEU:CD2	2.28	0.47
1:E:471:MET:HB3	1:E:480:LYS:HZ1	1.78	0.47
1:E:18:ILE:HD13	1:E:227:GLY:HA3	1.94	0.47
1:A:32:SER:HB3	1:A:222:ILE:HD11	1.97	0.47
1:B:212:GLU:HG2	1:B:212:GLU:O	2.15	0.47
1:A:87:ALA:HB1	1:A:92:TRP:CD1	2.50	0.47
1:D:412:PHE:N	1:D:412:PHE:CD1	2.83	0.47
1:F:451:ARG:NH1	1:F:451:ARG:HG2	2.30	0.47
1:E:18:ILE:CG1	1:E:228:THR:HG23	2.44	0.47
1:E:345:LYS:NZ	1:E:366:GLU:CG	2.78	0.47
1:A:268:VAL:O	1:A:271:ASP:HB2	2.15	0.47
1:D:468:ARG:HH11	1:D:468:ARG:HG2	1.78	0.47
1:B:211:LEU:O	1:B:212:GLU:HB3	2.13	0.47
1:C:448:GLU:HG2	1:D:466:ALA:HA	1.97	0.47
1:B:21:MET:HE3	1:B:141:ARG:NE	2.30	0.47
1:A:80:PRO:HD2	1:A:81:GLN:HE21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:SER:H	1:A:181:THR:CG2	2.27	0.47
1:D:323:GLN:HE22	1:E:459:ARG:HD3	1.79	0.47
1:A:182:THR:HG22	1:A:183:GLU:N	2.30	0.47
1:A:356:LEU:CD2	1:A:387:VAL:HG11	2.44	0.47
1:F:65:ILE:O	1:F:65:ILE:CG2	2.61	0.47
1:D:213:GLY:O	1:D:214:GLU:HB2	2.15	0.47
1:E:313:ILE:HD11	1:E:372:PRO:HG3	1.97	0.47
1:A:487:GLU:OE1	1:F:496:ARG:HD3	2.16	0.46
1:B:80:PRO:HD2	1:B:81:GLN:NE2	2.30	0.46
1:F:81:GLN:N	1:F:81:GLN:CD	2.69	0.46
1:B:51:GLY:O	1:B:52:LYS:C	2.54	0.46
1:B:18:ILE:HB	1:B:228:THR:CG2	2.44	0.46
1:F:197:GLU:H	1:F:197:GLU:CD	2.18	0.46
1:A:420:MET:HB3	1:A:420:MET:HE3	1.84	0.46
1:A:150:VAL:CG1	1:A:151:PHE:N	2.78	0.46
1:E:147:VAL:HG11	1:E:180:MET:CE	2.45	0.46
1:B:182:THR:HG22	1:B:183:GLU:N	2.30	0.46
1:E:344:LEU:HD22	1:E:345:LYS:H	1.81	0.46
1:B:323:GLN:HE22	1:C:459:ARG:HD3	1.79	0.46
1:B:125:ALA:O	1:B:128:GLU:HB2	2.15	0.46
1:C:353:SER:O	1:C:354:ALA:HB2	2.14	0.46
1:E:313:ILE:HG13	1:E:372:PRO:HG3	1.97	0.46
1:B:219:THR:HA	1:B:235:TYR:O	2.14	0.46
1:D:350:TYR:O	1:D:351:PRO:C	2.51	0.46
1:F:117:VAL:HG13	1:F:154:TYR:OH	2.16	0.46
1:E:79:THR:HG23	1:E:81:GLN:NE2	2.30	0.46
1:B:356:LEU:CD2	1:B:387:VAL:HG11	2.44	0.46
1:E:49:GLY:O	1:E:218:ARG:NH2	2.49	0.46
1:F:514:GLU:CB	1:F:519:SER:HB3	2.46	0.46
1:A:186:GLU:OE2	1:A:187:GLU:N	2.49	0.46
1:F:360:LEU:O	1:F:360:LEU:HD22	2.15	0.46
1:A:164:LEU:HA	1:A:164:LEU:HD23	1.69	0.46
1:B:419:PHE:CE2	1:C:425:ILE:HD12	2.49	0.46
1:B:90:PHE:O	1:B:92:TRP:NE1	2.48	0.46
1:C:377:ILE:HD12	1:C:412:PHE:HE2	1.79	0.46
1:A:356:LEU:HD13	1:A:387:VAL:HG21	1.97	0.46
1:C:468:ARG:HG2	1:C:468:ARG:HH11	1.80	0.46
1:F:486:PHE:CE2	1:F:496:ARG:CD	2.81	0.46
1:E:166:ARG:O	1:E:169:ALA:HB3	2.15	0.46
1:D:345:LYS:HZ2	1:D:366:GLU:CG	2.23	0.46
1:D:340:ARG:C	1:D:342:ASN:N	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:387:VAL:HG12	1:C:388:SER:N	2.31	0.46
1:E:340:ARG:O	1:E:342:ASN:N	2.49	0.46
1:A:490:ILE:HD13	1:A:490:ILE:HA	1.84	0.46
1:F:115:GLN:HG3	1:F:116:GLU:N	1.94	0.46
3:E:901:ATP:H3'	1:F:458:MET:O	2.16	0.46
1:B:300:ARG:N	1:B:333:MET:HE1	2.30	0.46
1:A:447:GLY:HA2	1:B:489:ILE:HD12	1.96	0.46
1:F:336:GLU:OE1	1:F:336:GLU:HA	2.16	0.46
1:E:483:PHE:HB2	1:E:489:ILE:HD11	1.97	0.46
1:B:125:ALA:O	1:B:129:ARG:HG3	2.16	0.46
1:A:518:GLU:HB2	1:A:519:SER:H	1.55	0.46
1:B:56:SER:HB2	1:B:143:SER:HB3	1.98	0.46
1:C:446:ARG:HA	1:C:496:ARG:NH2	2.30	0.46
1:B:441:GLN:HE22	1:B:490:ILE:HA	1.80	0.46
1:F:287:THR:HG23	1:F:414:ASN:ND2	2.29	0.46
1:E:148:THR:HG1	1:E:182:THR:HG23	1.79	0.46
1:E:140:ARG:HA	1:E:140:ARG:HD2	1.60	0.46
1:B:23:THR:O	1:B:24:MET:HB2	2.15	0.46
1:A:497:ILE:O	1:A:497:ILE:CD1	2.64	0.46
1:A:191:ILE:HG21	1:A:198:GLU:HG3	1.97	0.46
1:B:164:LEU:HA	1:B:164:LEU:HD23	1.66	0.46
1:A:287:THR:HG21	1:A:425:ILE:O	2.16	0.46
1:A:429:HIS:O	1:A:432:TPO:O2P	2.33	0.46
1:F:504:GLU:HB3	1:F:507:ARG:HH21	1.77	0.46
1:C:191:ILE:HB	1:C:198:GLU:CD	2.35	0.46
1:C:430:ILE:O	1:C:433:ILE:HG12	2.16	0.46
1:D:170:ARG:O	1:D:174:ILE:HG12	2.16	0.46
1:F:317:TYR:CD2	1:F:383:LEU:HD21	2.51	0.46
1:B:432:TPO:C	1:B:434:THR:H	2.29	0.46
1:F:446:ARG:H	1:F:496:ARG:NH2	2.14	0.46
1:F:264:SER:O	1:F:374:ARG:NH2	2.47	0.46
1:E:499:VAL:CG1	1:E:499:VAL:O	2.61	0.46
1:B:397:ILE:HD11	1:B:433:ILE:CD1	2.46	0.46
1:E:313:ILE:CD1	1:E:372:PRO:HG3	2.46	0.46
1:E:202:ASP:HA	1:E:226:ARG:HD2	1.97	0.46
1:B:379:SER:H	1:B:413:THR:CG2	2.29	0.46
1:A:504:GLU:C	1:A:506:SER:N	2.68	0.46
1:E:305:ALA:HB2	1:E:374:ARG:CD	2.32	0.45
1:C:150:VAL:CG1	1:C:151:PHE:N	2.80	0.45
1:B:492:GLY:O	1:B:494:PRO:HD3	2.17	0.45
1:C:19:ALA:C	1:C:38:ILE:HD12	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:SER:HB3	1:A:182:THR:HB	1.97	0.45
1:A:161:ARG:HB2	1:A:196:VAL:CG1	2.47	0.45
1:C:50:THR:HG22	1:C:209:ASN:HB2	1.98	0.45
1:C:185:ILE:HA	4:D:527:HOH:O	2.15	0.45
1:A:487:GLU:OE1	1:F:495:THR:HA	2.16	0.45
1:B:151:PHE:C	1:B:153:GLN:N	2.69	0.45
1:E:81:GLN:H	1:E:81:GLN:CD	2.19	0.45
1:E:45:SER:HB2	1:E:182:THR:HB	1.97	0.45
1:D:338:MET:H	1:D:338:MET:HG2	1.58	0.45
1:F:256:GLN:H	1:F:256:GLN:HG2	1.46	0.45
1:A:485:ASN:N	1:A:485:ASN:OD1	2.39	0.45
1:F:433:ILE:HG22	1:F:433:ILE:O	2.15	0.45
1:D:79:THR:HG23	1:D:81:GLN:NE2	2.31	0.45
1:D:106:LEU:HD11	1:D:129:ARG:CZ	2.45	0.45
1:A:455:VAL:HG11	1:A:463:HIS:CB	2.39	0.45
1:B:483:PHE:HB2	1:B:489:ILE:HD11	1.99	0.45
1:B:64:ILE:HG21	1:B:97:LEU:HD13	1.98	0.45
1:C:471:MET:CG	1:C:478:ASP:HB3	2.47	0.45
1:F:38:ILE:HG22	1:F:39:GLY:N	2.31	0.45
1:B:91:GLY:C	1:B:92:TRP:CD1	2.90	0.45
1:E:441:GLN:NE2	1:E:490:ILE:HD13	2.31	0.45
1:C:187:GLU:O	1:C:208:ARG:HD3	2.17	0.45
1:D:455:VAL:HG11	1:D:463:HIS:HB2	1.97	0.45
1:C:325:LEU:HD23	1:C:335:PHE:HB2	1.98	0.45
1:C:211:LEU:O	1:C:212:GLU:HB3	2.16	0.45
1:E:353:SER:O	1:E:354:ALA:HB2	2.16	0.45
1:A:432:TPO:O1P	1:A:432:TPO:CG2	2.65	0.45
1:A:436:THR:OG1	1:A:458:MET:HG2	2.17	0.45
1:F:344:LEU:HD11	1:F:346:ILE:HG13	1.97	0.45
1:C:430:ILE:HG23	1:C:433:ILE:HD11	1.98	0.45
1:D:448:GLU:HG2	1:E:466:ALA:HA	1.98	0.45
1:C:439:LEU:HD12	1:C:440:LEU:N	2.31	0.45
1:D:436:THR:HG23	1:D:458:MET:HG3	1.98	0.45
1:C:144:ILE:HG21	1:C:147:VAL:HG12	1.99	0.45
1:D:122:ASP:HB3	1:D:123:LEU:H	1.44	0.45
1:E:345:LYS:HZ3	1:E:366:GLU:CG	2.30	0.45
1:C:164:LEU:HD23	1:C:164:LEU:HA	1.69	0.45
1:D:44:VAL:HG22	1:D:205:VAL:HB	1.98	0.45
1:D:146:SER:CA	1:D:181:THR:HG22	2.45	0.45
1:C:123:LEU:O	1:C:124:SER:C	2.54	0.45
1:F:79:THR:HG21	1:F:81:GLN:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:393:ARG:O	1:E:397:ILE:HG12	2.17	0.45
1:A:455:VAL:CG1	1:A:463:HIS:HB2	2.39	0.45
1:A:311:ARG:HD2	1:A:371:LYS:HE3	1.97	0.45
1:D:426:THR:HG21	1:D:430:ILE:HG12	1.98	0.45
1:B:469:GLU:HG3	1:B:470:PHE:N	2.30	0.45
1:C:14:GLU:CG	1:C:16:GLN:HB2	2.46	0.45
1:F:469:GLU:HG3	1:F:470:PHE:N	2.32	0.45
1:E:116:GLU:O	1:E:118:VAL:HG23	2.16	0.45
1:F:217:ARG:HH21	1:F:236:PRO:HB3	1.81	0.45
1:B:21:MET:HE1	1:B:141:ARG:CG	2.29	0.45
1:E:497:ILE:C	1:E:498:THR:HG23	2.37	0.45
1:D:379:SER:H	1:D:413:THR:HB	1.82	0.45
1:B:296:LEU:HD13	1:B:331:TRP:CD2	2.52	0.45
1:A:21:MET:CE	1:A:59:PHE:HZ	2.28	0.45
1:A:85:LYS:O	1:A:88:ARG:HB2	2.17	0.45
1:A:57:ILE:CD1	1:A:73:PHE:CE1	3.00	0.45
1:E:325:LEU:HD23	1:E:335:PHE:HB2	1.98	0.45
1:D:147:VAL:CG2	1:D:148:THR:N	2.79	0.45
1:E:146:SER:HA	1:E:181:THR:O	2.17	0.45
1:D:344:LEU:C	1:D:344:LEU:CD1	2.78	0.45
1:A:496:ARG:O	1:A:497:ILE:HG23	2.16	0.45
1:C:85:LYS:NZ	1:D:14:GLU:HB3	2.32	0.45
1:C:488:ARG:NH1	1:C:488:ARG:HG3	2.31	0.45
1:A:471:MET:HG3	1:A:478:ASP:HB3	1.97	0.45
1:B:126:LEU:C	1:B:128:GLU:N	2.68	0.45
1:E:313:ILE:CD1	1:E:372:PRO:CG	2.95	0.45
1:B:141:ARG:HB2	4:B:521:HOH:O	2.17	0.45
1:A:153:GLN:O	1:A:154:TYR:CG	2.70	0.45
1:A:266:GLY:O	1:A:300:ARG:CG	2.65	0.45
1:F:266:GLY:O	1:F:300:ARG:CG	2.65	0.45
1:F:137:TYR:O	1:F:138:ARG:HB2	2.17	0.45
1:A:504:GLU:O	1:A:506:SER:N	2.49	0.45
1:B:191:ILE:CB	1:B:198:GLU:CG	2.87	0.45
1:B:499:VAL:C	1:B:501:GLU:H	2.21	0.45
1:A:183:GLU:OE2	1:B:161:ARG:NH1	2.47	0.45
1:F:186:GLU:OE2	1:F:187:GLU:N	2.50	0.45
1:B:302:VAL:HG13	1:B:344:LEU:HD23	1.99	0.45
1:B:21:MET:CE	1:B:59:PHE:CZ	3.00	0.44
1:E:496:ARG:C	1:E:497:ILE:HD13	2.37	0.44
1:A:273:MET:O	1:A:463:HIS:CA	2.63	0.44
1:F:371:LYS:HD2	1:F:371:LYS:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:ASP:O	1:C:362:ILE:HG12	2.17	0.44
1:A:219:THR:HA	1:A:235:TYR:O	2.17	0.44
1:B:267:VAL:HB	1:B:270:LEU:HB2	1.98	0.44
1:B:186:GLU:OE2	1:B:187:GLU:N	2.50	0.44
1:D:52:LYS:N	3:D:903:ATP:O1B	2.50	0.44
1:C:144:ILE:CG2	1:C:147:VAL:HG12	2.46	0.44
1:D:338:MET:HB2	1:D:344:LEU:HB3	1.99	0.44
1:A:146:SER:HA	1:A:181:THR:O	2.17	0.44
1:E:211:LEU:HD12	1:E:215:ARG:O	2.16	0.44
1:A:469:GLU:HG3	1:A:470:PHE:N	2.31	0.44
1:F:451:ARG:HB3	1:F:470:PHE:CE2	2.53	0.44
1:C:215:ARG:HB3	4:C:521:HOH:O	2.17	0.44
1:A:318:GLU:CD	1:B:432:TPO:HG23	2.37	0.44
1:B:487:GLU:O	1:B:494:PRO:HA	2.17	0.44
1:C:318:GLU:CD	1:C:379:SER:HB2	2.38	0.44
1:A:203:ASN:HB3	1:A:225:LEU:CD2	2.47	0.44
1:C:75:THR:HG23	1:C:75:THR:O	2.17	0.44
1:D:31:ILE:HA	1:D:231:MET:SD	2.58	0.44
1:C:426:THR:HG22	1:C:428:SER:N	2.33	0.44
1:A:191:ILE:CG2	1:A:198:GLU:HG3	2.47	0.44
1:C:116:GLU:O	1:C:117:VAL:HB	2.16	0.44
1:D:269:ARG:HG2	1:D:479:ILE:HB	1.99	0.44
1:E:164:LEU:HD23	1:E:164:LEU:HA	1.65	0.44
1:B:107:ASP:C	1:B:107:ASP:OD1	2.56	0.44
1:D:197:GLU:CD	1:D:197:GLU:H	2.19	0.44
1:B:21:MET:HE3	1:B:141:ARG:CZ	2.48	0.44
1:D:381:SER:HB3	1:D:414:ASN:OD1	2.18	0.44
1:E:485:ASN:OD1	1:E:485:ASN:N	2.42	0.44
1:A:273:MET:SD	1:A:468:ARG:HD2	2.57	0.44
1:F:20:LYS:O	1:F:38:ILE:HD11	2.17	0.44
1:E:18:ILE:CD1	1:E:227:GLY:HA3	2.48	0.44
1:F:33:HIS:HD2	1:F:229:SER:OG	1.98	0.44
1:C:21:MET:HE1	1:C:59:PHE:CZ	2.52	0.44
1:B:146:SER:HA	1:B:181:THR:HG22	2.00	0.44
1:F:43:LEU:HD11	1:F:182:THR:OG1	2.17	0.44
1:E:432:TPO:OG1	1:E:433:ILE:CD1	2.56	0.44
1:D:344:LEU:HD22	1:D:345:LYS:H	1.82	0.44
1:B:262:ARG:HH22	1:B:461:SER:HB2	1.82	0.44
1:C:419:PHE:CD2	1:D:425:ILE:CD1	3.00	0.44
1:C:18:ILE:CD1	1:C:18:ILE:N	2.81	0.44
1:F:220:LEU:C	1:F:220:LEU:HD23	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:GLU:CG	1:A:15:HIS:N	2.57	0.44
1:B:146:SER:CA	1:B:181:THR:HG22	2.47	0.44
1:F:504:GLU:CA	1:F:507:ARG:HE	2.31	0.44
1:E:147:VAL:CG2	1:E:148:THR:N	2.80	0.44
1:C:315:PHE:CE1	1:C:363:ILE:HG23	2.52	0.44
1:F:311:ARG:HD2	1:F:371:LYS:CD	2.48	0.44
1:F:127:ILE:HD11	1:F:167:LEU:HD12	2.00	0.44
1:A:81:GLN:N	1:A:81:GLN:CD	2.71	0.44
1:A:452:ALA:HA	1:A:468:ARG:O	2.17	0.44
1:E:292:THR:OG1	1:E:294:LYS:HD3	2.18	0.44
1:D:89:SER:HB2	1:E:227:GLY:O	2.17	0.44
1:C:120:GLY:C	1:C:122:ASP:N	2.71	0.44
1:F:180:MET:HB3	1:F:180:MET:HE2	1.75	0.44
1:C:419:PHE:CE2	1:D:425:ILE:HD12	2.53	0.44
1:E:347:VAL:O	1:E:348:CYS:CB	2.64	0.44
1:D:65:ILE:O	1:D:65:ILE:CG2	2.66	0.44
1:B:344:LEU:C	1:B:344:LEU:HD13	2.38	0.44
1:A:466:ALA:HA	1:F:448:GLU:HG2	1.99	0.44
1:F:313:ILE:HG13	1:F:372:PRO:HG3	2.00	0.44
1:C:418:GLN:HB2	1:D:423:HIS:O	2.18	0.44
1:D:311:ARG:HG3	1:D:371:LYS:NZ	2.32	0.43
1:A:378:ASP:OD1	1:A:413:THR:HG21	2.18	0.43
1:B:184:ARG:C	1:B:185:ILE:HD13	2.38	0.43
1:E:212:GLU:CG	1:E:213:GLY:N	2.79	0.43
3:A:901:ATP:C5	1:B:461:SER:O	2.71	0.43
1:A:496:ARG:O	1:A:497:ILE:CG2	2.66	0.43
1:F:295:THR:HG21	1:F:319:GLU:OE2	2.17	0.43
1:C:294:LYS:N	3:C:901:ATP:O1B	2.51	0.43
1:E:313:ILE:HG13	1:E:372:PRO:CG	2.48	0.43
1:D:33:HIS:HD2	1:D:229:SER:OG	2.01	0.43
1:C:123:LEU:O	1:C:125:ALA:N	2.51	0.43
1:E:396:VAL:HG11	1:E:430:ILE:CG2	2.48	0.43
1:E:293:GLY:HA2	3:E:901:ATP:O1A	2.18	0.43
1:C:433:ILE:HG21	1:C:433:ILE:HD13	1.74	0.43
1:F:156:ALA:O	1:F:159:VAL:HG23	2.18	0.43
1:B:340:ARG:C	1:B:342:ASN:N	2.71	0.43
1:F:452:ALA:HB1	1:F:467:ILE:HG22	1.99	0.43
1:B:490:ILE:HD13	1:B:490:ILE:HA	1.75	0.43
1:E:123:LEU:HD23	1:E:127:ILE:HG13	1.99	0.43
1:E:497:ILE:O	1:E:498:THR:HG23	2.18	0.43
1:D:318:GLU:OE2	1:D:379:SER:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:332:GLY:O	1:F:333:MET:O	2.36	0.43
1:A:499:VAL:CG1	1:A:499:VAL:O	2.64	0.43
1:F:344:LEU:HD13	1:F:344:LEU:C	2.39	0.43
1:B:126:LEU:C	1:B:128:GLU:H	2.21	0.43
1:A:357:GLU:HG3	1:A:358:ASP:N	2.33	0.43
1:F:430:ILE:HG22	1:F:433:ILE:HB	2.01	0.43
1:C:121:PHE:HB3	1:C:125:ALA:HB3	2.01	0.43
1:E:445:ILE:O	1:E:446:ARG:HB2	2.18	0.43
1:F:31:ILE:HG22	1:F:222:ILE:CD1	2.47	0.43
1:B:418:GLN:CG	1:B:418:GLN:O	2.66	0.43
1:C:340:ARG:C	1:C:342:ASN:N	2.71	0.43
1:E:295:THR:HG21	1:E:319:GLU:OE2	2.18	0.43
1:B:76:PHE:CZ	1:B:126:LEU:HD21	2.53	0.43
1:C:94:LEU:O	1:C:98:VAL:HG23	2.18	0.43
1:D:46:GLY:HA2	4:D:520:HOH:O	2.17	0.43
1:C:121:PHE:N	1:C:121:PHE:CD1	2.77	0.43
1:F:81:GLN:H	1:F:81:GLN:CD	2.19	0.43
1:F:203:ASN:HB3	1:F:225:LEU:CD2	2.38	0.43
1:D:426:THR:HG22	1:D:428:SER:N	2.28	0.43
1:F:299:SER:HB3	1:F:333:MET:HE1	2.00	0.43
1:C:497:ILE:O	1:C:498:THR:HG22	2.19	0.43
1:B:164:LEU:HB3	1:B:200:VAL:HG11	2.00	0.43
1:A:507:ARG:HG3	1:A:508:ILE:N	2.33	0.43
1:A:305:ALA:HB2	1:A:374:ARG:CD	2.33	0.43
1:B:359:HIS:O	1:B:363:ILE:HG13	2.19	0.43
1:E:38:ILE:HA	1:E:177:THR:HG23	2.00	0.43
1:B:204:VAL:HG23	1:B:224:LYS:HG2	2.01	0.43
1:B:500:ASP:O	1:B:503:SER:HB2	2.18	0.43
1:F:178:THR:HG22	1:F:179:VAL:N	2.34	0.43
1:E:64:ILE:HD13	1:E:102:LYS:HB3	2.00	0.43
1:E:54:LEU:HD13	1:E:90:PHE:CE1	2.54	0.43
1:F:486:PHE:CB	1:F:489:ILE:HD11	2.48	0.43
1:E:273:MET:O	1:E:463:HIS:CA	2.62	0.43
1:A:169:ALA:HB3	1:F:112:PRO:HB3	2.00	0.43
1:A:325:LEU:CD2	1:A:335:PHE:HB2	2.49	0.43
1:F:358:ASP:O	1:F:362:ILE:HG12	2.19	0.43
1:A:265:SER:O	1:A:301:PHE:HA	2.18	0.43
1:B:345:LYS:HZ2	1:B:366:GLU:HG2	1.84	0.43
1:E:70:PRO:HB2	1:E:139:ALA:HA	2.01	0.43
1:C:484:ARG:HB3	1:C:484:ARG:NH1	2.34	0.43
1:F:255:THR:O	1:F:255:THR:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:PHE:O	1:C:153:GLN:N	2.43	0.43
1:A:429:HIS:HA	1:A:431:SEP:O2P	2.18	0.43
3:C:903:ATP:PG	1:D:224:LYS:HZ2	2.41	0.43
1:A:87:ALA:O	1:A:92:TRP:NE1	2.51	0.43
1:E:356:LEU:CD1	1:E:387:VAL:HG21	2.49	0.43
1:E:292:THR:O	1:E:451:ARG:NH1	2.52	0.43
1:E:383:LEU:HD23	1:E:383:LEU:HA	1.83	0.43
1:A:162:ARG:CZ	1:F:116:GLU:HG2	2.49	0.43
1:A:487:GLU:HG2	1:F:496:ARG:CZ	2.48	0.43
1:D:148:THR:HG21	1:D:193:ARG:HD2	2.01	0.43
1:D:496:ARG:HE	1:E:487:GLU:HG2	1.83	0.43
1:E:79:THR:HG23	1:E:81:GLN:CG	2.36	0.43
1:E:180:MET:HB3	1:E:180:MET:HE2	1.79	0.43
1:E:344:LEU:C	1:E:344:LEU:CD1	2.86	0.43
1:F:367:ILE:HG12	1:F:375:ILE:HD11	2.01	0.43
1:C:142:VAL:O	1:C:178:THR:HA	2.18	0.43
1:C:47:THR:O	1:C:48:SER:C	2.55	0.43
1:B:53:THR:HG23	1:B:145:ASP:OD1	2.19	0.43
1:A:425:ILE:CD1	1:F:419:PHE:CD2	3.01	0.43
1:C:193:ARG:NH2	1:D:195:GLY:O	2.28	0.43
1:F:507:ARG:O	1:F:508:ILE:C	2.57	0.43
1:B:299:SER:HB3	1:B:333:MET:HE1	2.01	0.43
1:C:191:ILE:CG2	1:C:198:GLU:HG3	2.49	0.43
1:A:445:ILE:HD12	1:A:486:PHE:CZ	2.54	0.43
1:F:38:ILE:CG2	1:F:39:GLY:N	2.82	0.43
1:C:396:VAL:HG11	1:C:430:ILE:CG2	2.48	0.43
1:F:484:ARG:CB	1:F:484:ARG:NH1	2.81	0.43
3:E:903:ATP:O3G	1:F:224:LYS:NZ	2.51	0.43
1:D:317:TYR:CE2	1:D:383:LEU:HD21	2.53	0.43
1:F:468:ARG:NH1	1:F:468:ARG:HG2	2.34	0.43
1:F:123:LEU:HA	1:F:123:LEU:HD22	1.90	0.42
1:D:153:GLN:O	1:D:154:TYR:CB	2.66	0.42
1:B:471:MET:HE3	1:B:473:SER:OG	2.19	0.42
1:E:311:ARG:HD2	1:E:371:LYS:HE3	2.01	0.42
1:E:419:PHE:O	1:E:420:MET:O	2.36	0.42
1:E:106:LEU:HD13	1:E:129:ARG:CZ	2.49	0.42
1:C:468:ARG:HG2	1:C:468:ARG:NH1	2.33	0.42
1:E:23:THR:C	1:E:25:ILE:H	2.22	0.42
1:F:46:GLY:HA2	1:F:184:ARG:HD2	2.00	0.42
1:D:85:LYS:NZ	1:E:14:GLU:HB3	2.34	0.42
1:F:161:ARG:CB	1:F:196:VAL:HG11	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:GLU:OE1	1:C:340:ARG:NH1	2.52	0.42
1:A:484:ARG:HB3	1:A:484:ARG:HH11	1.84	0.42
1:E:217:ARG:HH21	1:E:236:PRO:HB3	1.84	0.42
1:D:18:ILE:H	1:D:18:ILE:HD12	1.83	0.42
1:F:223:LEU:HD23	1:F:223:LEU:HA	1.81	0.42
1:E:123:LEU:HD13	1:E:163:GLU:OE2	2.18	0.42
1:A:332:GLY:O	1:A:333:MET:C	2.58	0.42
1:B:311:ARG:HD2	1:B:371:LYS:HE3	2.01	0.42
1:F:387:VAL:HG12	1:F:388:SER:N	2.35	0.42
1:F:469:GLU:HB2	1:F:483:PHE:CZ	2.54	0.42
1:A:72:VAL:O	1:A:142:VAL:HA	2.19	0.42
1:D:420:MET:HE3	1:D:492:GLY:HA3	1.99	0.42
1:F:200:VAL:O	1:F:200:VAL:HG12	2.18	0.42
1:B:44:VAL:HG22	1:B:205:VAL:HB	2.01	0.42
1:B:21:MET:CE	1:B:141:ARG:HG2	2.27	0.42
1:D:191:ILE:HG21	1:D:198:GLU:HG3	2.00	0.42
1:C:311:ARG:HD2	1:C:371:LYS:NZ	2.34	0.42
1:E:302:VAL:HG13	1:E:344:LEU:HD23	2.01	0.42
1:E:489:ILE:O	1:E:490:ILE:C	2.57	0.42
1:A:31:ILE:HD11	1:A:246:ILE:HG21	2.01	0.42
1:E:208:ARG:NH2	1:E:221:GLU:OE2	2.51	0.42
1:F:302:VAL:HG12	1:F:303:GLU:N	2.35	0.42
1:F:127:ILE:CD1	1:F:167:LEU:HD12	2.49	0.42
1:A:82:ASP:O	1:A:83:ILE:C	2.57	0.42
1:E:264:SER:O	1:E:374:ARG:NH2	2.51	0.42
1:E:79:THR:O	1:E:80:PRO:C	2.57	0.42
1:F:42:THR:HG23	1:F:203:ASN:HB2	2.02	0.42
1:D:287:THR:HA	1:D:414:ASN:O	2.20	0.42
1:A:498:THR:HB	1:A:501:GLU:CG	2.41	0.42
1:E:43:LEU:HD12	1:E:43:LEU:HA	1.82	0.42
1:A:311:ARG:HB3	1:A:370:PHE:CE2	2.55	0.42
1:F:437:ILE:HD11	1:F:457:LYS:HE2	2.02	0.42
1:E:451:ARG:HG2	1:E:451:ARG:NH1	2.33	0.42
1:C:419:PHE:CG	1:C:419:PHE:O	2.72	0.42
1:C:88:ARG:HD3	1:D:15:HIS:C	2.40	0.42
1:A:169:ALA:CB	1:F:112:PRO:HB3	2.50	0.42
1:E:379:SER:HA	1:E:413:THR:HG22	2.00	0.42
1:E:203:ASN:HB3	1:E:225:LEU:CD2	2.48	0.42
1:A:514:GLU:HB3	1:A:515:LYS:HD2	2.02	0.42
1:C:211:LEU:HD12	1:C:215:ARG:O	2.19	0.42
1:A:508:ILE:H	1:A:508:ILE:HD13	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:VAL:O	1:B:142:VAL:HA	2.20	0.42
1:F:338:MET:H	1:F:338:MET:HG2	1.68	0.42
1:B:383:LEU:HD23	1:B:383:LEU:HA	1.81	0.42
1:B:420:MET:HE3	1:B:420:MET:HB3	1.73	0.42
1:F:191:ILE:HG12	1:F:198:GLU:HG2	2.01	0.42
1:C:263:VAL:HG12	1:C:374:ARG:NH2	2.33	0.42
1:A:503:SER:C	1:A:504:GLU:CG	2.88	0.42
1:B:22:ARG:NH2	1:B:24:MET:SD	2.92	0.42
1:D:490:ILE:HA	1:D:490:ILE:HD12	1.91	0.42
1:D:437:ILE:HD12	1:D:457:LYS:HG2	2.00	0.42
1:D:187:GLU:O	1:D:208:ARG:HD3	2.20	0.42
1:B:21:MET:HE2	1:B:59:PHE:CZ	2.54	0.42
1:C:123:LEU:HA	1:C:123:LEU:HD23	1.79	0.42
1:F:509:VAL:HG23	1:F:509:VAL:H	1.46	0.42
1:D:388:SER:OG	1:D:391:ALA:HB2	2.18	0.42
1:C:489:ILE:O	1:C:490:ILE:C	2.56	0.42
1:F:24:MET:HB2	1:F:62:ASN:ND2	2.33	0.42
1:A:443:VAL:CG1	1:A:494:PRO:HG2	2.50	0.42
1:E:256:GLN:HG2	1:E:256:GLN:H	1.51	0.42
1:F:485:ASN:N	1:F:485:ASN:OD1	2.47	0.42
1:D:153:GLN:O	1:D:154:TYR:CG	2.72	0.42
1:C:21:MET:O	1:C:35:GLY:HA3	2.20	0.42
1:F:287:THR:HG23	1:F:414:ASN:CB	2.37	0.42
1:C:148:THR:HG1	1:C:182:THR:HG23	1.85	0.42
1:B:471:MET:HG3	1:B:478:ASP:HB3	2.02	0.42
1:E:419:PHE:CD2	1:F:425:ILE:CD1	3.00	0.42
1:F:238:THR:HG22	1:F:239:ILE:N	2.34	0.42
1:D:451:ARG:NH1	1:D:472:ILE:HD12	2.34	0.42
1:F:367:ILE:HG12	1:F:375:ILE:CD1	2.49	0.42
1:C:38:ILE:HG22	1:C:39:GLY:N	2.34	0.42
1:E:378:ASP:OD1	1:E:413:THR:HG21	2.19	0.42
1:C:345:LYS:NZ	1:C:366:GLU:CG	2.82	0.42
1:A:70:PRO:HG2	1:A:138:ARG:O	2.19	0.42
1:B:421:GLY:O	1:B:422:ALA:C	2.56	0.42
1:B:452:ALA:HA	1:B:468:ARG:O	2.19	0.42
1:E:360:LEU:HD22	1:E:360:LEU:O	2.20	0.42
1:A:406:GLU:O	1:A:407:GLU:HB2	2.19	0.42
1:C:121:PHE:O	1:C:122:ASP:C	2.58	0.42
1:D:140:ARG:HD2	1:D:140:ARG:HA	1.82	0.42
1:E:323:GLN:HE21	1:E:327:ASN:HD21	1.68	0.42
1:B:492:GLY:C	1:B:494:PRO:HD3	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:315:PHE:HE1	1:E:375:ILE:CD1	2.33	0.42
1:D:194:TYR:O	1:D:196:VAL:HG23	2.19	0.42
1:E:164:LEU:HB3	1:E:200:VAL:HG11	2.02	0.42
1:D:33:HIS:CD2	1:D:230:HIS:HA	2.55	0.42
1:B:484:ARG:NH1	1:B:484:ARG:HB3	2.34	0.42
1:B:256:GLN:H	1:B:256:GLN:HG2	1.55	0.42
1:D:208:ARG:O	1:D:218:ARG:HA	2.20	0.42
1:E:345:LYS:NZ	1:E:366:GLU:HG2	2.35	0.42
1:B:119:GLY:O	1:B:121:PHE:N	2.53	0.42
1:C:283:ILE:HD12	1:C:412:PHE:HE1	1.85	0.42
1:D:114:GLY:O	1:D:115:GLN:HG3	2.20	0.42
1:B:68:ASP:OD2	1:B:102:LYS:HE3	2.19	0.42
1:D:52:LYS:HB2	3:D:903:ATP:O1B	2.20	0.41
1:A:426:THR:HG22	1:A:427:ASP:N	2.35	0.41
1:A:311:ARG:HD2	1:A:371:LYS:NZ	2.35	0.41
1:C:344:LEU:HD13	1:C:344:LEU:C	2.41	0.41
1:E:106:LEU:HD13	1:E:129:ARG:NH2	2.35	0.41
1:A:514:GLU:C	1:A:515:LYS:HD2	2.40	0.41
1:F:443:VAL:HG12	1:F:445:ILE:HG12	2.02	0.41
1:E:150:VAL:HG13	1:E:151:PHE:N	2.35	0.41
1:F:144:ILE:CG2	1:F:147:VAL:HG12	2.50	0.41
1:B:332:GLY:O	1:B:333:MET:O	2.38	0.41
1:A:486:PHE:CE2	1:A:496:ARG:HA	2.55	0.41
1:B:445:ILE:HD12	1:B:486:PHE:CZ	2.55	0.41
1:E:161:ARG:CB	1:E:196:VAL:HG11	2.48	0.41
1:E:76:PHE:O	1:E:109:SER:HA	2.19	0.41
1:A:256:GLN:HG2	1:A:256:GLN:H	1.52	0.41
1:E:314:LEU:C	1:E:314:LEU:HD12	2.41	0.41
1:B:153:GLN:O	1:B:154:TYR:CB	2.68	0.41
1:F:140:ARG:HD2	1:F:140:ARG:HA	1.95	0.41
1:E:505:LEU:O	1:E:505:LEU:CD1	2.69	0.41
1:D:370:PHE:O	1:D:371:LYS:CD	2.67	0.41
1:F:185:ILE:CD1	1:F:193:ARG:NH1	2.79	0.41
1:A:430:ILE:O	1:A:432:TPO:N	2.53	0.41
1:E:182:THR:HG21	1:E:192:ALA:HB1	2.01	0.41
1:E:336:GLU:O	1:E:339:GLU:HB2	2.21	0.41
1:B:451:ARG:HB3	1:B:470:PHE:CE2	2.55	0.41
1:C:378:ASP:OD1	1:C:413:THR:HG21	2.20	0.41
1:C:489:ILE:O	1:C:492:GLY:N	2.47	0.41
1:C:489:ILE:C	1:C:491:SER:N	2.71	0.41
1:A:183:GLU:HB2	1:B:199:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:GLY:O	1:C:115:GLN:HB3	2.20	0.41
1:A:510:ARG:HD2	1:A:510:ARG:N	2.35	0.41
1:E:21:MET:HE1	1:E:141:ARG:HG2	2.01	0.41
1:F:164:LEU:HD11	1:F:197:GLU:HG3	2.01	0.41
1:D:297:LEU:HD23	1:D:297:LEU:HA	1.82	0.41
1:E:122:ASP:HB3	1:E:123:LEU:H	1.70	0.41
1:F:419:PHE:O	1:F:420:MET:HB2	2.19	0.41
1:D:224:LYS:O	1:D:225:LEU:HD23	2.20	0.41
1:F:504:GLU:CA	1:F:507:ARG:NE	2.81	0.41
1:F:292:THR:HB	1:F:440:LEU:HB3	2.02	0.41
1:E:412:PHE:N	1:E:412:PHE:CD1	2.88	0.41
1:E:76:PHE:CZ	1:E:126:LEU:CD2	3.02	0.41
1:E:21:MET:O	1:E:35:GLY:HA3	2.20	0.41
1:A:20:LYS:HD3	1:A:35:GLY:O	2.19	0.41
1:F:213:GLY:O	1:F:214:GLU:HB2	2.20	0.41
1:C:256:GLN:HG2	1:C:256:GLN:H	1.47	0.41
1:B:81:GLN:CD	1:B:81:GLN:N	2.73	0.41
1:C:153:GLN:O	1:C:154:TYR:CG	2.74	0.41
1:E:289:ALA:CB	1:E:419:PHE:HA	2.45	0.41
1:D:21:MET:CE	1:D:59:PHE:HZ	2.33	0.41
1:E:344:LEU:HD13	1:E:345:LYS:N	2.34	0.41
1:D:471:MET:HB3	1:D:480:LYS:HZ3	1.84	0.41
1:F:484:ARG:CB	1:F:484:ARG:CZ	2.98	0.41
1:C:387:VAL:CG1	1:C:391:ALA:HB3	2.50	0.41
1:D:438:ILE:CD1	1:D:455:VAL:HG22	2.51	0.41
1:F:516:GLY:N	1:F:517:PRO:HD2	2.36	0.41
1:E:147:VAL:HG23	1:E:148:THR:N	2.35	0.41
1:E:446:ARG:CZ	1:E:496:ARG:NH2	2.84	0.41
1:A:296:LEU:HD21	1:A:477:PRO:HD3	2.02	0.41
1:B:273:MET:O	1:B:463:HIS:CA	2.63	0.41
1:B:501:GLU:HB2	1:B:502:LYS:H	1.39	0.41
1:C:14:GLU:HG3	1:C:16:GLN:HB2	2.01	0.41
1:F:23:THR:O	1:F:24:MET:HB2	2.20	0.41
1:A:345:LYS:NZ	1:A:366:GLU:HG2	2.35	0.41
1:C:332:GLY:O	1:C:333:MET:C	2.58	0.41
1:D:273:MET:SD	1:D:468:ARG:HD2	2.61	0.41
1:C:281:ASP:O	1:C:282:SER:HB3	2.21	0.41
1:C:267:VAL:HB	1:C:270:LEU:HB2	2.03	0.41
1:C:65:ILE:HG22	1:C:65:ILE:O	2.20	0.41
1:D:314:LEU:C	1:D:314:LEU:HD12	2.40	0.41
1:F:116:GLU:C	1:F:117:VAL:HG23	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:165:PHE:O	1:F:166:ARG:C	2.58	0.41
1:B:141:ARG:HD2	4:B:521:HOH:O	2.19	0.41
1:A:430:ILE:O	1:A:433:ILE:N	2.54	0.41
1:E:432:TPO:O2P	1:E:433:ILE:HD11	2.20	0.41
1:E:345:LYS:HZ2	1:E:366:GLU:HG2	1.85	0.41
1:F:93:ASP:OD2	1:F:96:LYS:HB2	2.21	0.41
1:D:75:THR:HG23	1:D:75:THR:O	2.19	0.41
1:A:382:ALA:HB2	1:B:432:TPO:O3P	2.21	0.41
1:F:379:SER:CA	1:F:413:THR:HG22	2.47	0.41
1:C:338:MET:HB2	1:C:344:LEU:HB3	2.03	0.41
1:E:483:PHE:CB	1:E:489:ILE:HD11	2.51	0.41
1:A:471:MET:HE2	1:A:478:ASP:CB	2.50	0.41
1:D:273:MET:O	1:D:463:HIS:HA	2.20	0.41
1:D:150:VAL:CG1	1:D:151:PHE:N	2.84	0.41
1:A:432:TPO:P	1:A:433:ILE:CD1	3.09	0.41
1:D:315:PHE:CE2	1:D:363:ILE:HG23	2.54	0.41
1:A:436:THR:HG23	1:A:458:MET:CG	2.51	0.41
1:C:81:GLN:N	1:C:81:GLN:NE2	2.63	0.41
1:B:20:LYS:C	1:B:38:ILE:HD11	2.41	0.41
1:B:19:ALA:C	1:B:38:ILE:HD12	2.41	0.41
1:C:420:MET:HE3	1:C:420:MET:HB3	1.69	0.41
1:D:21:MET:CE	1:D:141:ARG:HG2	2.46	0.41
1:B:106:LEU:CD1	1:B:106:LEU:C	2.89	0.41
1:C:471:MET:HB3	1:C:480:LYS:HZ3	1.85	0.41
1:A:400:THR:CG2	1:A:401:GLY:N	2.83	0.41
1:F:377:ILE:HD11	1:F:399:VAL:HG11	2.02	0.41
1:A:21:MET:CE	1:A:59:PHE:CE1	3.04	0.41
1:F:357:GLU:HG3	1:F:358:ASP:N	2.36	0.41
1:E:113:GLU:HB3	1:E:114:GLY:H	1.75	0.41
1:F:306:CYS:C	1:F:308:ASN:N	2.72	0.41
1:C:197:GLU:CD	1:C:197:GLU:H	2.14	0.41
1:D:358:ASP:O	1:D:362:ILE:HG12	2.20	0.41
1:E:148:THR:CG2	1:E:193:ARG:HD2	2.51	0.41
1:E:148:THR:OG1	1:E:182:THR:HG22	2.21	0.41
1:C:79:THR:HG23	1:C:81:GLN:H	1.86	0.41
1:A:505:LEU:CD1	1:A:505:LEU:O	2.65	0.41
1:E:306:CYS:O	1:E:309:LYS:N	2.41	0.41
1:A:484:ARG:CZ	1:A:484:ARG:CB	2.99	0.41
1:A:340:ARG:C	1:A:342:ASN:N	2.74	0.41
1:F:274:CYS:HG	1:F:278:PHE:HE2	1.69	0.41
1:D:182:THR:CG2	1:D:183:GLU:N	2.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:GLY:C	1:C:122:ASP:H	2.24	0.40
1:B:79:THR:C	1:B:83:ILE:HD12	2.41	0.40
1:B:79:THR:HG23	1:B:81:GLN:CG	2.42	0.40
1:C:79:THR:HG23	1:C:81:GLN:HE21	1.87	0.40
3:A:903:ATP:O3'	1:B:224:LYS:HB2	2.21	0.40
1:C:269:ARG:NE	4:C:525:HOH:O	2.33	0.40
1:D:41:SER:HA	1:D:178:THR:O	2.21	0.40
1:A:148:THR:HG1	1:A:182:THR:HG23	1.84	0.40
1:B:76:PHE:HZ	1:B:126:LEU:HD21	1.84	0.40
1:B:219:THR:HB	1:B:234:GLU:HB3	2.03	0.40
1:A:284:ILE:HB	1:A:411:LEU:HD12	2.02	0.40
1:D:76:PHE:O	1:D:109:SER:HA	2.21	0.40
1:A:362:ILE:HG22	1:A:362:ILE:O	2.21	0.40
1:F:127:ILE:HD11	1:F:167:LEU:CD1	2.51	0.40
1:D:49:GLY:HA2	3:D:903:ATP:O2B	2.21	0.40
1:D:495:THR:HG23	1:E:487:GLU:OE2	2.21	0.40
1:F:203:ASN:CB	1:F:225:LEU:HD23	2.39	0.40
1:E:345:LYS:NZ	1:E:366:GLU:OE1	2.55	0.40
1:D:471:MET:CG	1:D:478:ASP:HB3	2.51	0.40
1:C:44:VAL:HG22	1:C:205:VAL:HB	2.03	0.40
1:D:383:LEU:HD23	1:D:383:LEU:HA	1.81	0.40
1:F:98:VAL:HA	1:F:103:LEU:O	2.21	0.40
1:A:111:ASP:C	1:A:113:GLU:H	2.24	0.40
1:D:371:LYS:C	1:D:371:LYS:CD	2.89	0.40
1:D:315:PHE:CE1	1:D:363:ILE:HG23	2.56	0.40
1:E:184:ARG:HG2	1:E:191:ILE:O	2.22	0.40
1:D:396:VAL:HG11	1:D:430:ILE:CG2	2.50	0.40
1:C:18:ILE:CG2	1:C:37:PRO:HB3	2.51	0.40
1:A:264:SER:HB3	1:A:304:ASN:HD21	1.86	0.40
1:D:462:TRP:O	1:D:463:HIS:O	2.39	0.40
1:B:60:LEU:CD1	1:B:73:PHE:HB2	2.50	0.40
1:E:356:LEU:HD21	1:E:387:VAL:HG11	2.02	0.40
1:D:497:ILE:HG13	1:D:497:ILE:H	1.78	0.40
1:B:393:ARG:O	1:B:397:ILE:HG12	2.21	0.40
1:F:129:ARG:O	1:F:132:TYR:HB3	2.21	0.40
1:C:25:ILE:HG23	1:C:58:GLN:NE2	2.36	0.40
1:B:441:GLN:HG3	1:B:441:GLN:O	2.21	0.40
1:A:140:ARG:HD2	1:A:140:ARG:HA	1.84	0.40
1:C:148:THR:HG21	1:C:193:ARG:HD2	2.02	0.40
1:E:193:ARG:HH11	1:E:193:ARG:HG2	1.86	0.40
1:A:437:ILE:CD1	1:A:457:LYS:HE2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:371:LYS:HD3	1:E:371:LYS:O	2.19	0.40
1:D:344:LEU:HD22	1:D:345:LYS:N	2.37	0.40
1:E:449:MET:HE3	1:F:467:ILE:HD11	2.02	0.40
1:D:219:THR:HB	1:D:234:GLU:HB3	2.03	0.40
1:E:98:VAL:HA	1:E:103:LEU:O	2.22	0.40
1:B:380:LEU:HD23	1:B:380:LEU:HA	1.98	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	502/519 (97%)	445 (89%)	35 (7%)	22 (4%)	3	10
1	B	487/519 (94%)	430 (88%)	45 (9%)	12 (2%)	7	24
1	C	484/519 (93%)	433 (90%)	32 (7%)	19 (4%)	4	12
1	D	481/519 (93%)	433 (90%)	37 (8%)	11 (2%)	8	26
1	E	488/519 (94%)	416 (85%)	53 (11%)	19 (4%)	4	12
1	F	502/519 (97%)	442 (88%)	39 (8%)	21 (4%)	3	11
All	All	2944/3114 (94%)	2599 (88%)	241 (8%)	104 (4%)	4	15

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ALA
1	A	154	TYR
1	A	211	LEU
1	A	333	MET
1	A	387	VAL
1	A	463	HIS

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Mol	Chain	Res	Type
1	A	502	LYS
1	A	509	VAL
1	B	154	TYR
1	B	333	MET
1	B	341	GLN
1	B	387	VAL
1	B	463	HIS
1	C	17	ALA
1	C	112	PRO
1	C	117	VAL
1	C	124	SER
1	C	154	TYR
1	C	333	MET
1	C	341	GLN
1	C	463	HIS
1	D	122	ASP
1	D	154	TYR
1	D	333	MET
1	D	387	VAL
1	D	463	HIS
1	E	122	ASP
1	E	154	TYR
1	E	211	LEU
1	E	333	MET
1	E	420	MET
1	E	463	HIS
1	F	118	VAL
1	F	154	TYR
1	F	333	MET
1	F	463	HIS
1	F	501	GLU
1	F	504	GLU
1	F	506	SER
1	F	507	ARG
1	F	508	ILE
1	F	509	VAL
1	F	510	ARG
1	A	117	VAL
1	A	157	SER
1	A	341	GLN
1	A	500	ASP
1	A	505	LEU

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Mol	Chain	Res	Type
1	B	17	ALA
1	B	119	GLY
1	B	211	LEU
1	B	420	MET
1	C	121	PHE
1	C	379	SER
1	C	387	VAL
1	D	18	ILE
1	D	113	GLU
1	D	341	GLN
1	D	420	MET
1	E	117	VAL
1	E	120	GLY
1	E	213	GLY
1	E	341	GLN
1	E	387	VAL
1	E	502	LYS
1	F	117	VAL
1	F	157	SER
1	F	211	LEU
1	F	341	GLN
1	A	379	SER
1	A	420	MET
1	B	112	PRO
1	C	114	GLY
1	C	211	LEU
1	C	499	VAL
1	E	157	SER
1	E	498	THR
1	F	420	MET
1	A	480	LYS
1	A	504	GLU
1	B	52	LYS
1	C	289	ALA
1	C	354	ALA
1	D	211	LEU
1	E	293	GLY
1	A	433	ILE
1	B	494	PRO
1	C	157	SER
1	E	348	CYS
1	E	379	SER

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Mol	Chain	Res	Type
1	F	354	ALA
1	F	500	ASP
1	F	517	PRO
1	A	212	GLU
1	A	348	CYS
1	C	213	GLY
1	C	348	CYS
1	D	157	SER
1	E	494	PRO
1	F	112	PRO
1	A	112	PRO
1	A	497	ILE
1	F	387	VAL
1	E	112	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	430/442 (97%)	372 (86%)	58 (14%)	5	14
1	B	417/442 (94%)	364 (87%)	53 (13%)	5	16
1	C	414/442 (94%)	357 (86%)	57 (14%)	4	13
1	D	411/442 (93%)	358 (87%)	53 (13%)	5	16
1	E	418/442 (95%)	368 (88%)	50 (12%)	6	19
1	F	430/442 (97%)	380 (88%)	50 (12%)	7	20
All	All	2520/2652 (95%)	2199 (87%)	321 (13%)	5	16

All (321) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	41	SER
1	A	50	THR
1	A	79	THR

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Mol	Chain	Res	Type
1	A	81	GLN
1	A	92	TRP
1	A	99	ASP
1	A	106	LEU
1	A	118	VAL
1	A	123	LEU
1	A	140	ARG
1	A	151	PHE
1	A	154	TYR
1	A	181	THR
1	A	183	GLU
1	A	185	ILE
1	A	186	GLU
1	A	191	ILE
1	A	193	ARG
1	A	212	GLU
1	A	218	ARG
1	A	223	LEU
1	A	228	THR
1	A	238	THR
1	A	256	GLN
1	A	260	ASN
1	A	263	VAL
1	A	270	LEU
1	A	287	THR
1	A	294	LYS
1	A	302	VAL
1	A	303	GLU
1	A	320	SER
1	A	321	ARG
1	A	342	ASN
1	A	360	LEU
1	A	366	GLU
1	A	371	LYS
1	A	375	ILE
1	A	400	THR
1	A	413	THR
1	A	428	SER
1	A	434	THR
1	A	451	ARG
1	A	458	MET
1	A	462	TRP

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Mol	Chain	Res	Type
1	A	469	GLU
1	A	471	MET
1	A	489	ILE
1	A	496	ARG
1	A	498	THR
1	A	500	ASP
1	A	504	GLU
1	A	508	ILE
1	A	509	VAL
1	A	510	ARG
1	A	514	GLU
1	A	518	GLU
1	B	26	GLU
1	B	50	THR
1	B	79	THR
1	B	81	GLN
1	B	99	ASP
1	B	106	LEU
1	B	112	PRO
1	B	123	LEU
1	B	128	GLU
1	B	140	ARG
1	B	151	PHE
1	B	154	TYR
1	B	181	THR
1	B	183	GLU
1	B	185	ILE
1	B	186	GLU
1	B	191	ILE
1	B	212	GLU
1	B	218	ARG
1	B	223	LEU
1	B	256	GLN
1	B	260	ASN
1	B	270	LEU
1	B	287	THR
1	B	294	LYS
1	B	302	VAL
1	B	303	GLU
1	B	320	SER
1	B	321	ARG
1	B	325	LEU

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Mol	Chain	Res	Type
1	B	333	MET
1	B	342	ASN
1	B	356	LEU
1	B	360	LEU
1	B	369	ASP
1	B	371	LYS
1	B	375	ILE
1	B	400	THR
1	B	413	THR
1	B	433	ILE
1	B	451	ARG
1	B	458	MET
1	B	462	TRP
1	B	469	GLU
1	B	471	MET
1	B	474	ASP
1	B	485	ASN
1	B	490	ILE
1	B	495	THR
1	B	499	VAL
1	B	500	ASP
1	B	501	GLU
1	B	502	LYS
1	C	15	HIS
1	C	26	GLU
1	C	50	THR
1	C	79	THR
1	C	81	GLN
1	C	99	ASP
1	C	106	LEU
1	C	111	ASP
1	C	121	PHE
1	C	140	ARG
1	C	151	PHE
1	C	154	TYR
1	C	177	THR
1	C	181	THR
1	C	183	GLU
1	C	185	ILE
1	C	186	GLU
1	C	191	ILE
1	C	212	GLU

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Mol	Chain	Res	Type
1	C	214	GLU
1	C	215	ARG
1	C	218	ARG
1	C	223	LEU
1	C	228	THR
1	C	256	GLN
1	C	259	SER
1	C	263	VAL
1	C	270	LEU
1	C	287	THR
1	C	294	LYS
1	C	302	VAL
1	C	303	GLU
1	C	321	ARG
1	C	325	LEU
1	C	333	MET
1	C	338	MET
1	C	342	ASN
1	C	356	LEU
1	C	360	LEU
1	C	366	GLU
1	C	371	LYS
1	C	375	ILE
1	C	400	THR
1	C	413	THR
1	C	420	MET
1	C	451	ARG
1	C	458	MET
1	C	461	SER
1	C	462	TRP
1	C	469	GLU
1	C	471	MET
1	C	491	SER
1	C	493	SER
1	C	495	THR
1	C	498	THR
1	C	500	ASP
1	C	501	GLU
1	D	26	GLU
1	D	79	THR
1	D	81	GLN
1	D	106	LEU

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Mol	Chain	Res	Type
1	D	117	VAL
1	D	122	ASP
1	D	123	LEU
1	D	124	SER
1	D	127	ILE
1	D	140	ARG
1	D	151	PHE
1	D	154	TYR
1	D	172	LYS
1	D	177	THR
1	D	181	THR
1	D	185	ILE
1	D	186	GLU
1	D	191	ILE
1	D	212	GLU
1	D	218	ARG
1	D	223	LEU
1	D	256	GLN
1	D	259	SER
1	D	260	ASN
1	D	263	VAL
1	D	270	LEU
1	D	284	ILE
1	D	287	THR
1	D	294	LYS
1	D	302	VAL
1	D	320	SER
1	D	321	ARG
1	D	325	LEU
1	D	338	MET
1	D	342	ASN
1	D	351	PRO
1	D	356	LEU
1	D	360	LEU
1	D	366	GLU
1	D	369	ASP
1	D	371	LYS
1	D	375	ILE
1	D	400	THR
1	D	413	THR
1	D	451	ARG
1	D	458	MET

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Mol	Chain	Res	Type
1	D	463	HIS
1	D	469	GLU
1	D	471	MET
1	D	487	GLU
1	D	490	ILE
1	D	496	ARG
1	D	498	THR
1	E	26	GLU
1	E	37	PRO
1	E	50	THR
1	E	79	THR
1	E	81	GLN
1	E	99	ASP
1	E	106	LEU
1	E	113	GLU
1	E	121	PHE
1	E	124	SER
1	E	127	ILE
1	E	140	ARG
1	E	151	PHE
1	E	154	TYR
1	E	177	THR
1	E	181	THR
1	E	182	THR
1	E	183	GLU
1	E	185	ILE
1	E	186	GLU
1	E	191	ILE
1	E	211	LEU
1	E	212	GLU
1	E	223	LEU
1	E	228	THR
1	E	256	GLN
1	E	260	ASN
1	E	263	VAL
1	E	270	LEU
1	E	287	THR
1	E	302	VAL
1	E	314	LEU
1	E	321	ARG
1	E	342	ASN
1	E	351	PRO

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Mol	Chain	Res	Type
1	E	360	LEU
1	E	371	LYS
1	E	375	ILE
1	E	400	THR
1	E	451	ARG
1	E	458	MET
1	E	461	SER
1	E	469	GLU
1	E	471	MET
1	E	474	ASP
1	E	496	ARG
1	E	501	GLU
1	E	503	SER
1	E	504	GLU
1	E	505	LEU
1	F	26	GLU
1	F	45	SER
1	F	79	THR
1	F	81	GLN
1	F	99	ASP
1	F	106	LEU
1	F	115	GLN
1	F	121	PHE
1	F	123	LEU
1	F	140	ARG
1	F	151	PHE
1	F	154	TYR
1	F	172	LYS
1	F	181	THR
1	F	183	GLU
1	F	185	ILE
1	F	186	GLU
1	F	191	ILE
1	F	212	GLU
1	F	218	ARG
1	F	223	LEU
1	F	256	GLN
1	F	260	ASN
1	F	263	VAL
1	F	270	LEU
1	F	287	THR
1	F	321	ARG

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Mol	Chain	Res	Type
1	F	325	LEU
1	F	342	ASN
1	F	356	LEU
1	F	360	LEU
1	F	366	GLU
1	F	371	LYS
1	F	375	ILE
1	F	381	SER
1	F	400	THR
1	F	413	THR
1	F	451	ARG
1	F	458	MET
1	F	462	TRP
1	F	469	GLU
1	F	471	MET
1	F	496	ARG
1	F	497	ILE
1	F	499	VAL
1	F	501	GLU
1	F	504	GLU
1	F	505	LEU
1	F	507	ARG
1	F	514	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	33	HIS
1	A	62	ASN
1	A	81	GLN
1	A	209	ASN
1	A	245	ASN
1	A	323	GLN
1	A	368	ASN
1	A	414	ASN
1	A	441	GLN
1	B	16	GLN
1	B	62	ASN
1	B	81	GLN
1	B	209	ASN
1	B	260	ASN

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Mol	Chain	Res	Type
1	B	304	ASN
1	B	361	GLN
1	B	368	ASN
1	B	414	ASN
1	B	441	GLN
1	C	33	HIS
1	C	62	ASN
1	C	81	GLN
1	C	209	ASN
1	C	256	GLN
1	C	323	GLN
1	C	368	ASN
1	C	389	ASN
1	C	414	ASN
1	C	441	GLN
1	D	33	HIS
1	D	81	GLN
1	D	209	ASN
1	D	256	GLN
1	D	304	ASN
1	D	368	ASN
1	D	389	ASN
1	D	414	ASN
1	D	441	GLN
1	E	33	HIS
1	E	81	GLN
1	E	209	ASN
1	E	256	GLN
1	E	304	ASN
1	E	323	GLN
1	E	361	GLN
1	E	368	ASN
1	E	414	ASN
1	E	441	GLN
1	E	454	ASN
1	F	33	HIS
1	F	62	ASN
1	F	81	GLN
1	F	115	GLN
1	F	209	ASN
1	F	256	GLN
1	F	368	ASN

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Mol	Chain	Res	Type
1	F	414	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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
1	SEP	A	431	1	8,9,10	2.03	3 (37%)	8,12,14	3.65	2 (25%)
1	TPO	A	432	1	8,10,11	0.58	0	7,14,16	1.37	1 (14%)
1	SEP	B	431	1	8,9,10	1.92	1 (12%)	8,12,14	2.57	1 (12%)
1	TPO	B	432	1	8,10,11	0.48	0	7,14,16	1.42	1 (14%)
1	SEP	C	431	1	4,5,10	0.76	0	2,5,14	1.80	1 (50%)
1	TPO	C	432	1	8,10,11	1.29	1 (12%)	7,14,16	1.49	1 (14%)
1	SEP	D	431	1	4,5,10	1.52	1 (25%)	2,5,14	0.89	0
1	TPO	D	432	1	8,10,11	1.33	1 (12%)	7,14,16	1.96	3 (42%)
1	SEP	E	431	1	8,9,10	2.38	3 (37%)	8,12,14	2.78	3 (37%)
1	TPO	E	432	1	8,10,11	1.06	0	7,14,16	1.41	2 (28%)
1	SEP	F	431	1	8,9,10	1.92	3 (37%)	8,12,14	1.11	0
1	TPO	F	432	1	8,10,11	3.36	7 (87%)	7,14,16	5.63	4 (57%)

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
1	SEP	A	431	1	-	0/6/8/10	0/0/0/0
1	TPO	A	432	1	-	0/8/11/13	0/0/0/0
1	SEP	B	431	1	-	0/6/8/10	0/0/0/0
1	TPO	B	432	1	1/1/3/4	0/8/11/13	0/0/0/0
1	SEP	C	431	1	-	0/2/4/10	0/0/0/0
1	TPO	C	432	1	-	0/8/11/13	0/0/0/0
1	SEP	D	431	1	-	0/2/4/10	0/0/0/0
1	TPO	D	432	1	1/1/3/4	0/8/11/13	0/0/0/0
1	SEP	E	431	1	-	0/6/8/10	0/0/0/0
1	TPO	E	432	1	1/1/3/4	0/8/11/13	0/0/0/0
1	SEP	F	431	1	-	0/6/8/10	0/0/0/0
1	TPO	F	432	1	1/1/3/4	1/8/11/13	0/0/0/0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	432	TPO	P-O2P	-6.02	1.33	1.54
1	F	432	TPO	CG2-CB	-3.64	1.42	1.51
1	F	432	TPO	P-O1P	-3.64	1.39	1.51
1	F	432	TPO	P-OG1	-2.81	1.51	1.60
1	F	432	TPO	CB-CA	-2.58	1.49	1.54
1	F	432	TPO	O-C	-2.44	1.08	1.19
1	F	432	TPO	P-O3P	-2.33	1.46	1.54
1	E	431	SEP	CB-CA	2.03	1.58	1.52
1	F	431	SEP	P-O2P	2.07	1.62	1.54
1	F	431	SEP	P-O3P	2.37	1.63	1.54
1	D	432	TPO	CG2-CB	2.44	1.57	1.51
1	C	432	TPO	P-O1P	2.67	1.60	1.51
1	A	431	SEP	CB-CA	2.82	1.60	1.52
1	A	431	SEP	P-O3P	2.83	1.64	1.54
1	D	431	SEP	O-C	2.89	1.33	1.19
1	E	431	SEP	P-O2P	3.50	1.67	1.54
1	A	431	SEP	P-O2P	3.85	1.68	1.54
1	F	431	SEP	P-O1P	4.16	1.64	1.51
1	B	431	SEP	P-O1P	4.78	1.66	1.51
1	E	431	SEP	P-O1P	5.16	1.68	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	432	TPO	CG2-CB-CA	-9.27	94.31	113.17
1	A	431	SEP	OG-CB-CA	-7.86	101.57	108.27
1	E	431	SEP	OG-CB-CA	-5.58	103.52	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	432	TPO	OG1-P-O1P	-2.68	100.42	107.11
1	D	432	TPO	CG2-CB-CA	-2.67	107.73	113.17
1	C	431	SEP	O-C-CA	-2.46	119.09	125.49
1	E	431	SEP	O2P-P-O1P	-2.36	102.99	110.58
1	E	432	TPO	O-C-CA	-2.27	119.44	125.44
1	B	432	TPO	O-C-CA	-2.20	119.63	125.44
1	D	432	TPO	O-C-CA	-2.07	119.96	125.44
1	A	432	TPO	O-C-CA	-2.05	120.03	125.44
1	E	432	TPO	O2P-P-O1P	2.02	117.08	110.58
1	C	432	TPO	O3P-P-O2P	2.60	117.28	107.38
1	D	432	TPO	O3P-P-O2P	2.84	118.19	107.38
1	E	431	SEP	O3P-P-OG	4.20	118.66	106.56
1	F	432	TPO	O3P-P-O1P	4.46	124.93	110.58
1	A	431	SEP	OG-P-O1P	5.80	121.90	107.14
1	B	431	SEP	OG-CB-CA	6.35	113.69	108.27
1	F	432	TPO	C-CA-N	10.29	131.32	109.83

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	E	432	TPO	CB
1	D	432	TPO	CB
1	B	432	TPO	CB
1	F	432	TPO	CB

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	F	432	TPO	OG1-CB-CA-N

There are no ring outliers.

11 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	431	SEP	5	0
1	A	432	TPO	6	0
1	B	431	SEP	6	0
1	B	432	TPO	8	0
1	C	431	SEP	4	0
1	C	432	TPO	5	0
1	D	431	SEP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	432	TPO	3	0
1	E	431	SEP	2	0
1	E	432	TPO	5	0
1	F	431	SEP	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 6 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$
3	ATP	A	901	-	24,33,33	1.49	4 (16%)	31,52,52	2.61	7 (22%)
3	ATP	A	903	-	24,33,33	1.58	5 (20%)	31,52,52	2.62	8 (25%)
3	ATP	B	901	-	24,33,33	1.57	4 (16%)	31,52,52	2.69	7 (22%)
3	ATP	B	903	-	24,33,33	1.77	3 (12%)	31,52,52	2.98	11 (35%)
3	ATP	C	901	-	24,33,33	1.50	4 (16%)	31,52,52	2.46	6 (19%)
3	ATP	C	903	-	24,33,33	1.31	2 (8%)	31,52,52	2.96	8 (25%)
3	ATP	D	901	-	24,33,33	1.54	4 (16%)	31,52,52	2.71	6 (19%)
3	ATP	D	903	-	24,33,33	1.72	4 (16%)	31,52,52	3.06	9 (29%)
3	ATP	E	901	-	24,33,33	1.56	3 (12%)	31,52,52	2.65	7 (22%)
3	ATP	E	903	-	24,33,33	1.73	8 (33%)	31,52,52	2.69	11 (35%)
3	ATP	F	901	-	24,33,33	1.66	5 (20%)	31,52,52	2.67	9 (29%)
3	ATP	F	903	-	24,33,33	1.52	4 (16%)	31,52,52	2.73	7 (22%)

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
3	ATP	A	901	-	-	0/18/38/38	0/3/3/3
3	ATP	A	903	-	-	0/18/38/38	0/3/3/3
3	ATP	B	901	-	-	0/18/38/38	0/3/3/3
3	ATP	B	903	-	-	0/18/38/38	0/3/3/3
3	ATP	C	901	-	-	0/18/38/38	0/3/3/3
3	ATP	C	903	-	-	0/18/38/38	0/3/3/3
3	ATP	D	901	-	-	0/18/38/38	0/3/3/3
3	ATP	D	903	-	-	0/18/38/38	0/3/3/3
3	ATP	E	901	-	-	0/18/38/38	0/3/3/3
3	ATP	E	903	-	-	0/18/38/38	0/3/3/3
3	ATP	F	901	-	-	0/18/38/38	0/3/3/3
3	ATP	F	903	-	-	0/18/38/38	0/3/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	903	ATP	O4'-C4'	-3.80	1.36	1.45
3	C	903	ATP	O4'-C4'	-3.36	1.37	1.45
3	C	901	ATP	PB-O1B	-3.16	1.39	1.51
3	D	903	ATP	PB-O1B	-3.07	1.39	1.51
3	D	903	ATP	PB-O2B	-3.05	1.41	1.54
3	E	903	ATP	PB-O1B	-2.93	1.40	1.51
3	B	901	ATP	PB-O1B	-2.62	1.41	1.51
3	F	903	ATP	PB-O1B	-2.61	1.41	1.51
3	D	901	ATP	O2'-C2'	-2.56	1.36	1.43
3	E	901	ATP	PB-O1B	-2.53	1.41	1.51
3	E	903	ATP	C6-N6	-2.50	1.27	1.34
3	F	903	ATP	C6-N6	-2.47	1.27	1.34
3	E	903	ATP	PA-O1A	-2.46	1.42	1.51
3	E	903	ATP	O4'-C4'	-2.38	1.39	1.45
3	A	901	ATP	PB-O1B	-2.32	1.42	1.51
3	E	903	ATP	PB-O2B	-2.28	1.45	1.54
3	E	903	ATP	C2'-C3'	-2.26	1.47	1.53
3	E	903	ATP	C8-N7	-2.20	1.30	1.34
3	A	903	ATP	PB-O2B	-2.15	1.45	1.54
3	C	901	ATP	O4'-C4'	-2.14	1.40	1.45
3	A	903	ATP	PB-O1B	-2.12	1.43	1.51
3	C	901	ATP	PB-O2B	-2.07	1.46	1.54
3	F	901	ATP	PB-O1B	-2.02	1.43	1.51
3	A	901	ATP	C2-N1	2.13	1.38	1.33
3	E	903	ATP	C2-N3	2.41	1.36	1.32
3	D	901	ATP	C3'-C4'	2.42	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	901	ATP	C2-N1	2.55	1.38	1.33
3	F	903	ATP	C2-N1	2.67	1.39	1.33
3	D	901	ATP	C2-N3	2.71	1.37	1.32
3	F	901	ATP	O4'-C1'	2.75	1.44	1.41
3	C	903	ATP	C2-N3	2.76	1.37	1.32
3	B	901	ATP	C2-N3	2.77	1.37	1.32
3	A	903	ATP	O4'-C1'	2.97	1.45	1.41
3	D	901	ATP	O4'-C1'	2.98	1.45	1.41
3	E	901	ATP	C4-N3	3.03	1.40	1.35
3	B	901	ATP	C2-N1	3.11	1.39	1.33
3	A	903	ATP	C2-N3	3.18	1.37	1.32
3	A	903	ATP	C2-N1	3.30	1.40	1.33
3	A	901	ATP	O4'-C1'	3.34	1.45	1.41
3	A	901	ATP	C2-N3	3.51	1.38	1.32
3	D	903	ATP	C2-N3	3.56	1.38	1.32
3	B	901	ATP	C4-N3	3.61	1.40	1.35
3	F	901	ATP	C4-N3	3.68	1.41	1.35
3	B	903	ATP	O4'-C1'	3.77	1.46	1.41
3	F	903	ATP	C2-N3	3.90	1.39	1.32
3	F	901	ATP	C2-N3	3.94	1.39	1.32
3	C	901	ATP	C2-N3	4.11	1.39	1.32
3	B	903	ATP	C4-N3	4.20	1.41	1.35
3	E	901	ATP	C2-N3	4.22	1.39	1.32
3	B	903	ATP	C2-N3	4.66	1.40	1.32

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	903	ATP	N3-C2-N1	-12.58	119.26	128.89
3	D	901	ATP	N3-C2-N1	-12.34	119.44	128.89
3	B	901	ATP	N3-C2-N1	-12.34	119.45	128.89
3	B	903	ATP	N3-C2-N1	-12.32	119.46	128.89
3	D	903	ATP	N3-C2-N1	-12.21	119.55	128.89
3	E	901	ATP	N3-C2-N1	-11.87	119.81	128.89
3	A	901	ATP	N3-C2-N1	-11.39	120.17	128.89
3	F	901	ATP	N3-C2-N1	-11.35	120.20	128.89
3	E	903	ATP	N3-C2-N1	-10.87	120.57	128.89
3	F	903	ATP	N3-C2-N1	-10.61	120.77	128.89
3	A	903	ATP	N3-C2-N1	-10.60	120.78	128.89
3	C	901	ATP	N3-C2-N1	-10.10	121.16	128.89
3	D	903	ATP	C4-C5-N7	-5.57	104.35	109.48
3	F	903	ATP	C4-C5-N7	-5.17	104.72	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	903	ATP	C4-C5-N7	-4.74	105.12	109.48
3	C	901	ATP	C4-C5-N7	-4.73	105.13	109.48
3	A	901	ATP	C4-C5-N7	-4.54	105.31	109.48
3	F	901	ATP	C4-C5-N7	-4.48	105.36	109.48
3	E	901	ATP	C4-C5-N7	-4.18	105.63	109.48
3	C	903	ATP	C4-C5-N7	-4.16	105.65	109.48
3	E	903	ATP	C4-C5-N7	-4.03	105.77	109.48
3	B	903	ATP	C4-C5-N7	-3.96	105.84	109.48
3	B	901	ATP	C4-C5-N7	-3.39	106.36	109.48
3	B	903	ATP	C1'-N9-C4	-3.32	121.93	126.94
3	D	901	ATP	C4-C5-N7	-3.25	106.49	109.48
3	A	903	ATP	C1'-N9-C4	-3.20	122.11	126.94
3	A	903	ATP	N6-C6-N1	-2.78	113.23	119.20
3	E	901	ATP	N6-C6-N1	-2.76	113.29	119.20
3	F	903	ATP	N6-C6-N1	-2.71	113.39	119.20
3	C	903	ATP	C1'-N9-C4	-2.65	122.95	126.94
3	B	903	ATP	N6-C6-N1	-2.61	113.61	119.20
3	F	901	ATP	N6-C6-N1	-2.45	113.94	119.20
3	C	903	ATP	O5'-PA-O1A	-2.44	100.13	109.62
3	E	903	ATP	O3G-PG-O1G	-2.26	103.31	110.58
3	D	903	ATP	C1'-N9-C4	-2.22	123.60	126.94
3	D	903	ATP	N6-C6-N1	-2.21	114.46	119.20
3	E	903	ATP	C1'-N9-C4	-2.18	123.65	126.94
3	F	901	ATP	C1'-N9-C4	-2.15	123.69	126.94
3	A	901	ATP	N6-C6-N1	-2.12	114.66	119.20
3	B	903	ATP	PB-O3B-PG	-2.01	125.93	132.67
3	E	903	ATP	C4'-O4'-C1'	2.01	111.93	109.72
3	C	903	ATP	O2G-PG-O1G	2.01	117.06	110.58
3	E	901	ATP	O2B-PB-O3B	2.03	114.29	105.09
3	E	903	ATP	O2B-PB-O3A	2.05	114.37	105.09
3	A	903	ATP	O2B-PB-O3B	2.06	114.42	105.09
3	F	901	ATP	O2B-PB-O3A	2.06	114.46	105.09
3	B	901	ATP	C4'-O4'-C1'	2.08	112.00	109.72
3	B	903	ATP	O2B-PB-O3A	2.08	114.53	105.09
3	E	901	ATP	O2'-C2'-C3'	2.14	118.80	111.83
3	B	903	ATP	O2G-PG-O1G	2.15	117.50	110.58
3	A	901	ATP	O2'-C2'-C3'	2.16	118.86	111.83
3	A	903	ATP	PA-O3A-PB	2.17	138.81	132.73
3	B	901	ATP	O2'-C2'-C3'	2.20	118.97	111.83
3	D	903	ATP	O2G-PG-O1G	2.23	117.77	110.58
3	B	901	ATP	O2B-PB-O3A	2.26	115.37	105.09
3	E	903	ATP	O2B-PB-O3B	2.35	115.77	105.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	901	ATP	O2B-PB-O3A	2.39	115.94	105.09
3	F	903	ATP	O2B-PB-O3B	2.39	115.95	105.09
3	F	903	ATP	O2G-PG-O1G	2.42	118.37	110.58
3	E	903	ATP	C2'-C1'-N9	2.45	118.04	114.29
3	C	901	ATP	O2'-C2'-C3'	2.49	119.91	111.83
3	A	901	ATP	O2B-PB-O3B	2.52	116.53	105.09
3	C	901	ATP	O2B-PB-O3A	2.56	116.69	105.09
3	E	903	ATP	O2G-PG-O1G	2.60	118.96	110.58
3	D	903	ATP	O2B-PB-O3B	2.61	116.95	105.09
3	C	903	ATP	O2B-PB-O3B	2.61	116.95	105.09
3	D	903	ATP	PA-O3A-PB	2.62	140.08	132.73
3	F	901	ATP	O2B-PB-O3B	2.72	117.45	105.09
3	E	903	ATP	PA-O3A-PB	2.77	140.50	132.73
3	D	901	ATP	C2'-C1'-N9	2.78	118.54	114.29
3	B	903	ATP	O2'-C2'-C3'	2.84	121.07	111.83
3	F	901	ATP	O2'-C2'-C3'	2.87	121.15	111.83
3	B	903	ATP	O4'-C1'-N9	2.88	114.12	108.10
3	B	903	ATP	O2B-PB-O3B	2.92	118.34	105.09
3	A	903	ATP	C2'-C1'-N9	2.95	118.79	114.29
3	E	901	ATP	C2'-C1'-N9	3.05	118.95	114.29
3	B	901	ATP	O2B-PB-O3B	3.09	119.09	105.09
3	A	901	ATP	C2'-C1'-N9	3.12	119.06	114.29
3	C	901	ATP	O2B-PB-O3B	3.28	119.97	105.09
3	A	901	ATP	O3A-PA-O5'	3.32	111.74	102.94
3	E	901	ATP	O3A-PA-O5'	3.38	111.90	102.94
3	D	901	ATP	O2B-PB-O3B	3.46	120.78	105.09
3	B	901	ATP	O3A-PA-O5'	3.62	112.54	102.94
3	F	901	ATP	O3A-PA-O5'	3.71	112.78	102.94
3	C	903	ATP	C2'-C1'-N9	3.79	120.09	114.29
3	F	901	ATP	C2'-C1'-N9	3.82	120.13	114.29
3	D	901	ATP	O3A-PA-O5'	3.89	113.25	102.94
3	C	901	ATP	O3A-PA-O5'	3.98	113.50	102.94
3	A	903	ATP	O3A-PA-O5'	4.10	113.80	102.94
3	F	903	ATP	C2'-C1'-N9	4.42	121.05	114.29
3	D	903	ATP	C2'-C1'-N9	5.27	122.34	114.29
3	B	903	ATP	O3A-PA-O5'	5.42	117.31	102.94
3	E	903	ATP	O3A-PA-O5'	5.42	117.32	102.94
3	F	903	ATP	O3A-PA-O5'	5.56	117.68	102.94
3	D	903	ATP	O3A-PA-O5'	5.79	118.29	102.94
3	C	903	ATP	O3A-PA-O5'	6.15	119.25	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	ATP	6	0
3	A	903	ATP	5	0
3	B	901	ATP	5	0
3	B	903	ATP	3	0
3	C	901	ATP	2	0
3	C	903	ATP	5	0
3	D	901	ATP	1	0
3	D	903	ATP	5	0
3	E	901	ATP	3	0
3	E	903	ATP	3	0
3	F	901	ATP	4	0
3	F	903	ATP	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	504/519 (97%)	0.46	60 (11%) 6 3	29, 76, 127, 154	0
1	B	489/519 (94%)	0.36	41 (8%) 14 6	24, 82, 128, 160	0
1	C	486/519 (93%)	0.11	24 (4%) 33 22	33, 73, 124, 160	0
1	D	483/519 (93%)	-0.09	23 (4%) 34 23	27, 58, 109, 160	0
1	E	490/519 (94%)	-0.01	31 (6%) 23 14	20, 60, 107, 155	0
1	F	504/519 (97%)	0.17	38 (7%) 17 9	20, 69, 114, 158	0
All	All	2956/3114 (94%)	0.17	217 (7%) 18 10	20, 71, 121, 160	0

All (217) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	117	VAL	8.6
1	E	505	LEU	8.3
1	D	121	PHE	8.1
1	F	516	GLY	7.9
1	B	117	VAL	7.8
1	A	517	PRO	7.6
1	E	503	SER	7.6
1	F	517	PRO	7.5
1	A	518	GLU	7.3
1	A	519	SER	7.3
1	D	118	VAL	7.2
1	D	120	GLY	7.2
1	C	118	VAL	7.2
1	D	119	GLY	7.1
1	A	506	SER	7.1
1	D	117	VAL	7.0
1	F	519	SER	6.8
1	B	500	ASP	6.8
1	A	503	SER	6.7

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Mol	Chain	Res	Type	RSRZ
1	B	498	THR	6.3
1	B	121	PHE	6.3
1	B	118	VAL	6.2
1	E	499	VAL	6.1
1	A	257	ARG	6.0
1	A	120	GLY	5.9
1	A	511	GLY	5.9
1	A	508	ILE	5.9
1	F	506	SER	5.8
1	A	515	LYS	5.7
1	A	507	ARG	5.7
1	F	515	LYS	5.7
1	E	154	TYR	5.6
1	A	513	GLN	5.6
1	C	499	VAL	5.6
1	C	501	GLU	5.6
1	B	116	GLU	5.6
1	A	516	GLY	5.5
1	F	154	TYR	5.4
1	A	152	GLN	5.3
1	F	518	GLU	5.2
1	B	258	SER	5.2
1	F	509	VAL	5.1
1	A	514	GLU	5.1
1	C	117	VAL	5.1
1	B	119	GLY	5.0
1	A	258	SER	4.9
1	A	509	VAL	4.9
1	B	503	SER	4.9
1	E	500	ASP	4.8
1	A	251	ALA	4.8
1	C	120	GLY	4.7
1	B	158	SER	4.7
1	B	154	TYR	4.7
1	F	513	GLN	4.7
1	B	255	THR	4.6
1	A	500	ASP	4.6
1	F	514	GLU	4.5
1	A	510	ARG	4.5
1	A	498	THR	4.4
1	A	121	PHE	4.4
1	F	512	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	F	505	LEU	4.4
1	C	423	HIS	4.3
1	E	117	VAL	4.2
1	B	15	HIS	4.2
1	E	501	GLU	4.2
1	F	507	ARG	4.2
1	A	252	MET	4.1
1	F	508	ILE	4.1
1	B	499	VAL	4.1
1	F	311	ARG	4.0
1	D	498	THR	4.0
1	C	500	ASP	3.9
1	A	368	ASN	3.9
1	E	504	GLU	3.9
1	C	154	TYR	3.9
1	A	504	GLU	3.8
1	F	500	ASP	3.8
1	E	153	GLN	3.8
1	A	295	THR	3.8
1	A	502	LYS	3.8
1	A	512	VAL	3.8
1	E	121	PHE	3.7
1	F	503	SER	3.7
1	A	117	VAL	3.7
1	B	504	GLU	3.7
1	B	321	ARG	3.7
1	D	113	GLU	3.7
1	A	505	LEU	3.7
1	F	511	GLY	3.6
1	B	16	GLN	3.6
1	B	502	LYS	3.6
1	A	249	LEU	3.6
1	B	115	GLN	3.6
1	C	53	THR	3.6
1	A	114	GLY	3.6
1	E	321	ARG	3.5
1	D	154	TYR	3.5
1	C	15	HIS	3.5
1	B	259	SER	3.5
1	F	510	ARG	3.5
1	B	501	GLU	3.4
1	C	115	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	115	GLN	3.4
1	B	157	SER	3.4
1	C	119	GLY	3.4
1	D	158	SER	3.3
1	C	17	ALA	3.3
1	D	53	THR	3.3
1	B	257	ARG	3.3
1	F	321	ARG	3.3
1	E	116	GLU	3.3
1	F	504	GLU	3.2
1	A	338	MET	3.2
1	A	311	ARG	3.2
1	A	17	ALA	3.2
1	A	14	GLU	3.2
1	D	16	GLN	3.2
1	E	112	PRO	3.2
1	C	152	GLN	3.1
1	F	253	ARG	3.1
1	D	112	PRO	3.1
1	A	499	VAL	3.0
1	A	475	LYS	3.0
1	E	118	VAL	3.0
1	B	53	THR	3.0
1	B	120	GLY	3.0
1	A	255	THR	3.0
1	F	255	THR	3.0
1	F	501	GLU	3.0
1	E	152	GLN	3.0
1	A	154	TYR	3.0
1	A	318	GLU	2.9
1	C	145	ASP	2.9
1	D	15	HIS	2.9
1	E	329	TYR	2.8
1	D	471	MET	2.8
1	A	309	LYS	2.8
1	B	252	MET	2.8
1	A	15	HIS	2.8
1	C	121	PHE	2.8
1	D	114	GLY	2.8
1	F	485	ASN	2.7
1	A	329	TYR	2.7
1	F	502	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	502	LYS	2.7
1	B	88	ARG	2.7
1	E	113	GLU	2.6
1	A	474	ASP	2.6
1	F	498	THR	2.6
1	F	121	PHE	2.6
1	A	253	ARG	2.6
1	A	501	GLU	2.6
1	F	157	SER	2.6
1	A	153	GLN	2.6
1	A	188	TYR	2.6
1	B	92	TRP	2.6
1	A	378	ASP	2.5
1	E	498	THR	2.5
1	A	250	GLY	2.5
1	C	153	GLN	2.5
1	C	146	SER	2.5
1	B	155	ASP	2.5
1	E	120	GLY	2.5
1	C	138	ARG	2.4
1	A	16	GLN	2.4
1	A	241	ASP	2.4
1	B	123	LEU	2.4
1	A	413	THR	2.4
1	B	497	ILE	2.4
1	B	180	MET	2.4
1	C	16	GLN	2.4
1	C	143	SER	2.4
1	B	122	ASP	2.4
1	D	496	ARG	2.4
1	E	114	GLY	2.4
1	B	14	GLU	2.4
1	E	166	ARG	2.4
1	F	340	ARG	2.3
1	B	345	LYS	2.3
1	E	188	TYR	2.3
1	A	340	ARG	2.3
1	D	321	ARG	2.3
1	D	201	SER	2.3
1	F	329	TYR	2.3
1	F	118	VAL	2.3
1	B	153	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	421	GLY	2.3
1	A	319	GLU	2.3
1	E	471	MET	2.3
1	B	309	LYS	2.2
1	B	436	THR	2.2
1	E	295	THR	2.2
1	D	157	SER	2.2
1	D	116	GLU	2.2
1	C	181	THR	2.2
1	F	257	ARG	2.2
1	C	116	GLU	2.2
1	D	115	GLN	2.2
1	E	318	GLU	2.1
1	C	114	GLY	2.1
1	D	152	GLN	2.1
1	E	53	THR	2.1
1	B	90	PHE	2.1
1	A	417	ASP	2.1
1	A	379	SER	2.1
1	B	341	GLN	2.1
1	B	251	ALA	2.1
1	E	334	ASP	2.1
1	E	337	GLU	2.1
1	F	496	ARG	2.1
1	A	436	THR	2.0
1	F	252	MET	2.0
1	F	337	GLU	2.0
1	D	309	LYS	2.0
1	A	256	GLN	2.0
1	F	484	ARG	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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	TPO	C	432	11/12	0.65	0.35	-	10,19,77,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	TPO	A	432	11/12	0.73	0.33	-	19,19,19,19	0
1	TPO	E	432	11/12	0.75	0.27	-	17,18,22,23	0
1	TPO	D	432	11/12	0.80	0.27	-	19,19,19,19	0
1	SEP	E	431	10/11	0.57	0.37	-	13,56,60,60	0
1	SEP	D	431	6/11	0.79	0.25	-	57,63,68,70	0
1	SEP	C	431	6/11	0.80	0.34	-	75,79,81,84	0
1	SEP	B	431	10/11	0.78	0.29	-	29,81,86,88	0
1	SEP	A	431	10/11	0.78	0.33	-	17,78,80,83	0
1	SEP	F	431	10/11	0.68	0.36	-	13,79,83,83	0
1	TPO	B	432	11/12	0.76	0.31	-	29,29,29,29	0
1	TPO	F	432	11/12	0.79	0.30	-	16,20,74,75	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	B	802	1/1	0.79	0.32	1.47	73,73,73,73	0
3	ATP	D	903	31/31	0.94	0.25	1.29	42,53,76,80	0
3	ATP	F	903	31/31	0.94	0.22	1.22	42,53,76,79	0
3	ATP	E	903	31/31	0.96	0.23	1.18	42,53,76,80	0
3	ATP	D	901	31/31	0.95	0.23	0.93	53,65,88,104	0
3	ATP	F	901	31/31	0.88	0.25	0.55	74,89,113,120	0
3	ATP	C	901	31/31	0.95	0.19	0.50	47,55,96,109	0
3	ATP	A	901	31/31	0.84	0.32	0.49	75,88,102,112	0
3	ATP	B	901	31/31	0.92	0.21	0.46	61,73,109,115	0
3	ATP	C	903	31/31	0.91	0.22	0.37	42,54,76,80	0
3	ATP	E	901	31/31	0.89	0.25	0.25	61,76,100,113	0
3	ATP	A	903	31/31	0.88	0.21	0.12	42,54,76,80	0
3	ATP	B	903	31/31	0.87	0.18	-0.61	43,54,76,80	0
2	MG	F	806	1/1	0.97	0.14	-	18,18,18,18	0
2	MG	C	803	1/1	0.90	0.12	-	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	D	804	1/1	0.93	0.17	-	18,18,18,18	0
2	MG	E	805	1/1	0.86	0.11	-	18,18,18,18	0
2	MG	A	801	1/1	0.97	0.12	-	18,18,18,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.