



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 05:17 am BST

PDB ID : 1U9I
Title : Crystal Structure of Circadian Clock Protein KaiC with Phosphorylation Sites
Authors : Xu, Y.; Mori, T.; Pattanayek, R.; Pattanayek, S.; Egli, M.; Johnson, C.H.
Deposited on : 2004-08-09
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

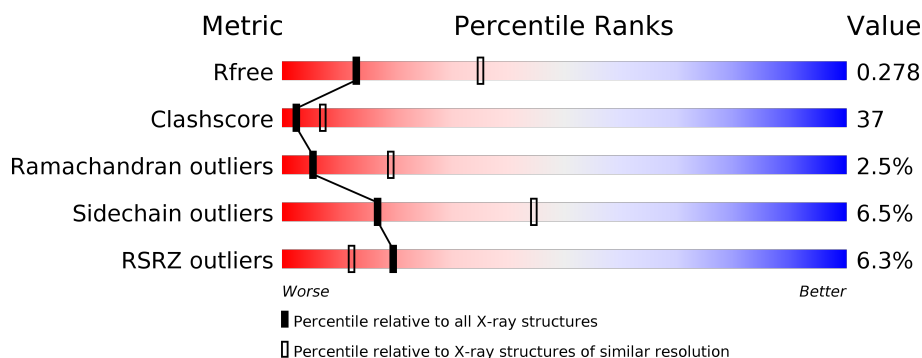
1 Overall quality at a glance

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	519	<div> <div>9%</div> <div> <div>48%</div> <div>40%</div> <div>5%</div> <div>7%</div> </div> </div>
1	B	519	<div> <div>6%</div> <div> <div>47%</div> <div>41%</div> <div>5%</div> <div>7%</div> </div> </div>
1	E	519	<div> <div>6%</div> <div> <div>47%</div> <div>40%</div> <div>6%</div> <div>7%</div> </div> </div>
1	F	519	<div> <div>4%</div> <div> <div>43%</div> <div>43%</div> <div>6%</div> <div>7%</div> </div> </div>
2	C	519	<div> <div>5%</div> <div> <div>42%</div> <div>44%</div> <div>7%</div> <div>7%</div> </div> </div>
2	D	519	<div> <div>4%</div> <div> <div>48%</div> <div>39%</div> <div>5%</div> <div>7%</div> </div> </div>

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	X
1	TPO	B	432	-	-	-	X
1	SEP	E	431	-	-	X	X
1	SEP	F	431	-	-	X	X
1	TPO	F	432	-	-	-	X
2	TPO	C	432	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23375 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 KaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	P	S	0	0	0
			3823	2407	670	729	2	15			
1	B	484	Total	C	N	O	P	S	0	0	0
			3823	2407	670	729	2	15			
1	E	484	Total	C	N	O	P	S	0	0	0
			3823	2407	670	729	2	15			
1	F	484	Total	C	N	O	P	S	0	0	0
			3823	2407	670	729	2	15			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	431	SEP	SER	MODIFIED RESIDUE	UNP Q79PF4
A	432	TPO	THR	MODIFIED RESIDUE	UNP Q79PF4
B	431	SEP	SER	MODIFIED RESIDUE	UNP Q79PF4
B	432	TPO	THR	MODIFIED RESIDUE	UNP Q79PF4
E	431	SEP	SER	MODIFIED RESIDUE	UNP Q79PF4
E	432	TPO	THR	MODIFIED RESIDUE	UNP Q79PF4
F	431	SEP	SER	MODIFIED RESIDUE	UNP Q79PF4
F	432	TPO	THR	MODIFIED RESIDUE	UNP Q79PF4

- Molecule 2 is a protein called KaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	484	Total	C	N	O	P	S	0	0	0
			3819	2407	670	726	1	15			
2	D	484	Total	C	N	O	P	S	0	0	0
			3819	2407	670	726	1	15			

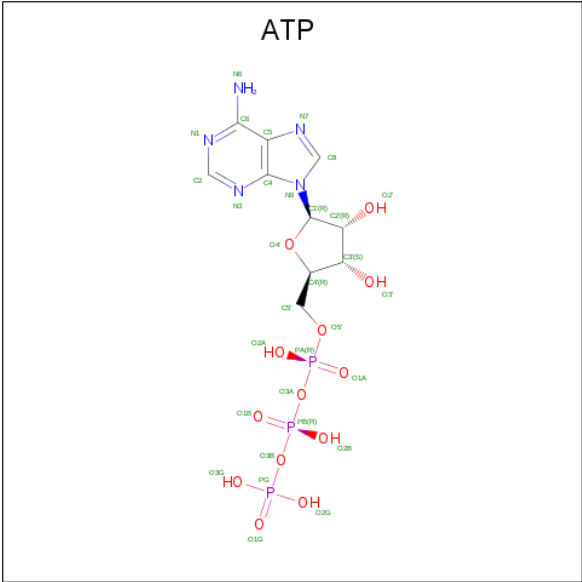
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	432	TPO	THR	MODIFIED RESIDUE	UNP Q79PF4
D	432	TPO	THR	MODIFIED RESIDUE	UNP Q79PF4

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

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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

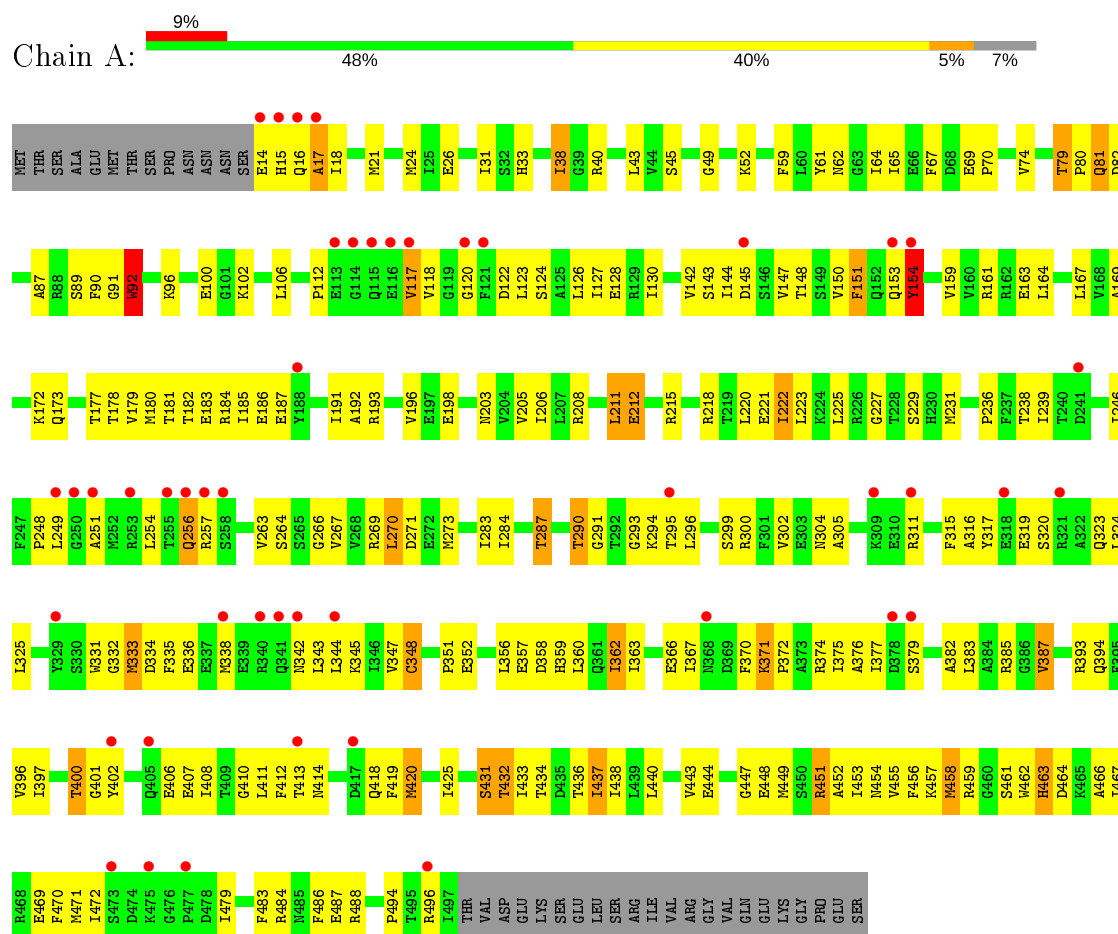
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	8	Total	O	0	0
			8	8		
5	B	5	Total	O	0	0
			5	5		
5	C	7	Total	O	0	0
			7	7		
5	D	13	Total	O	0	0
			13	13		
5	E	10	Total	O	0	0
			10	10		
5	F	24	Total	O	0	0
			24	24		

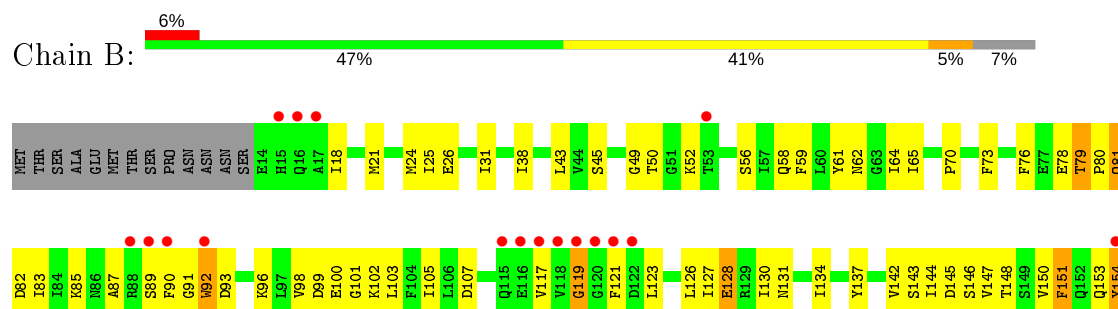
3 Residue-property plots

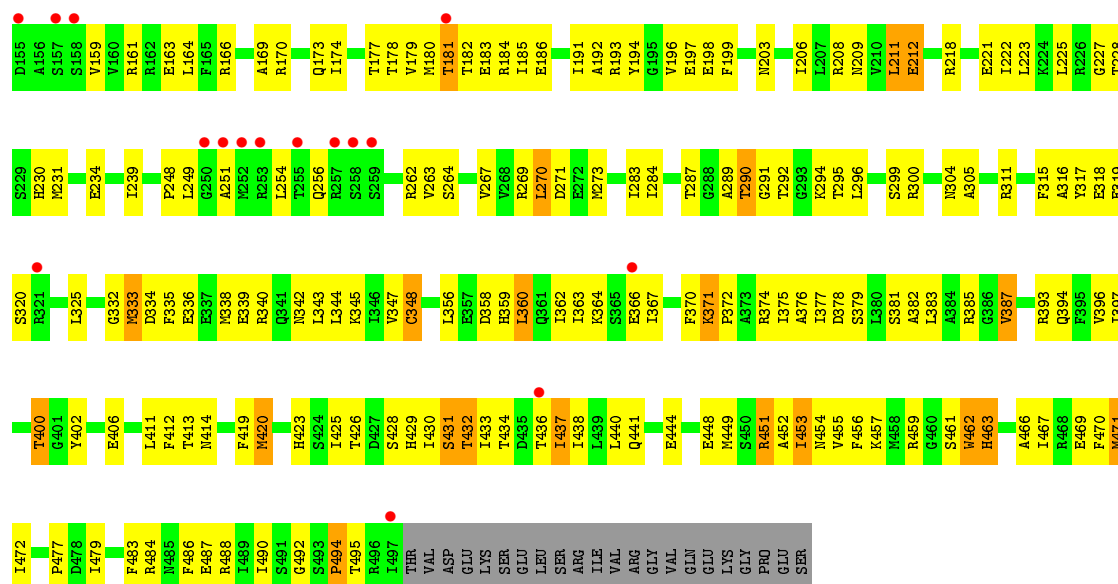
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: KaiC

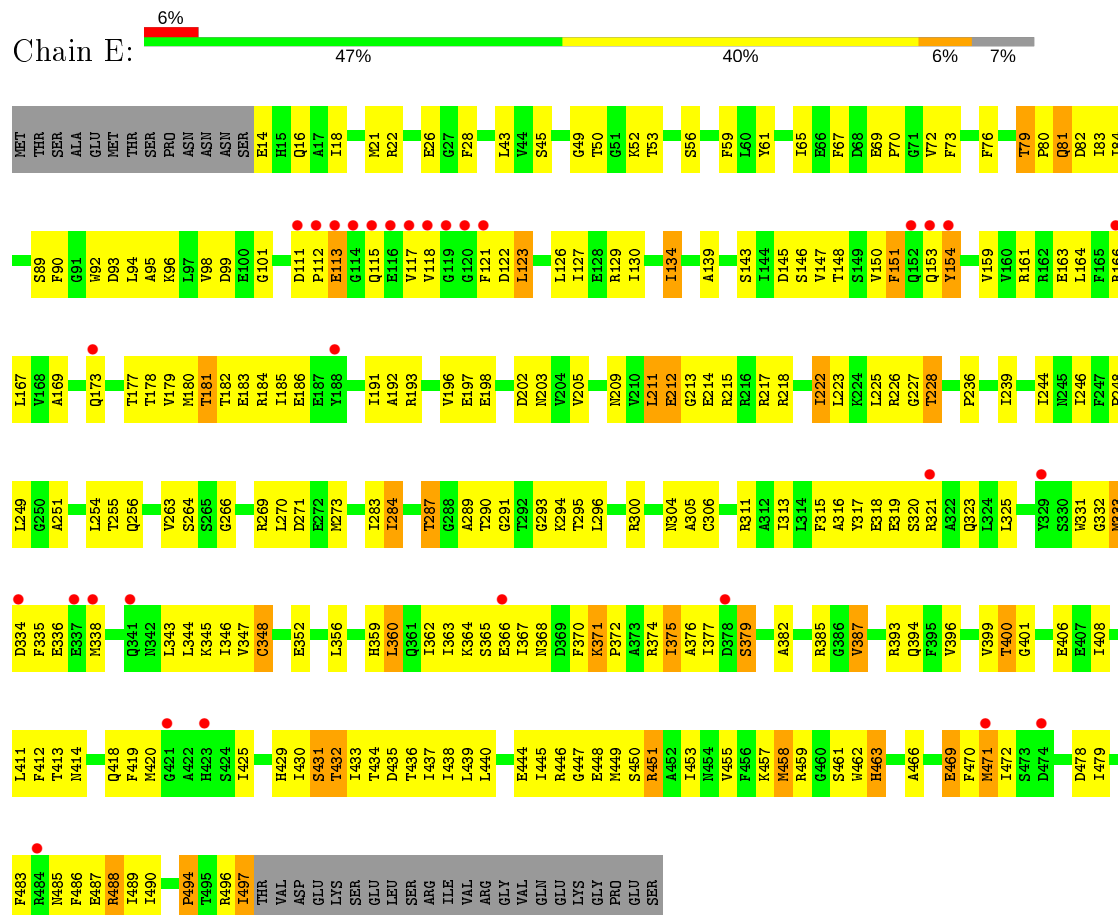


• Molecule 1: KaiC

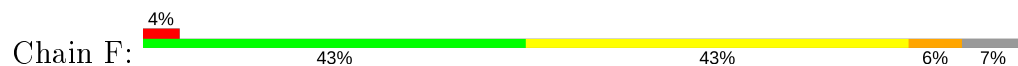


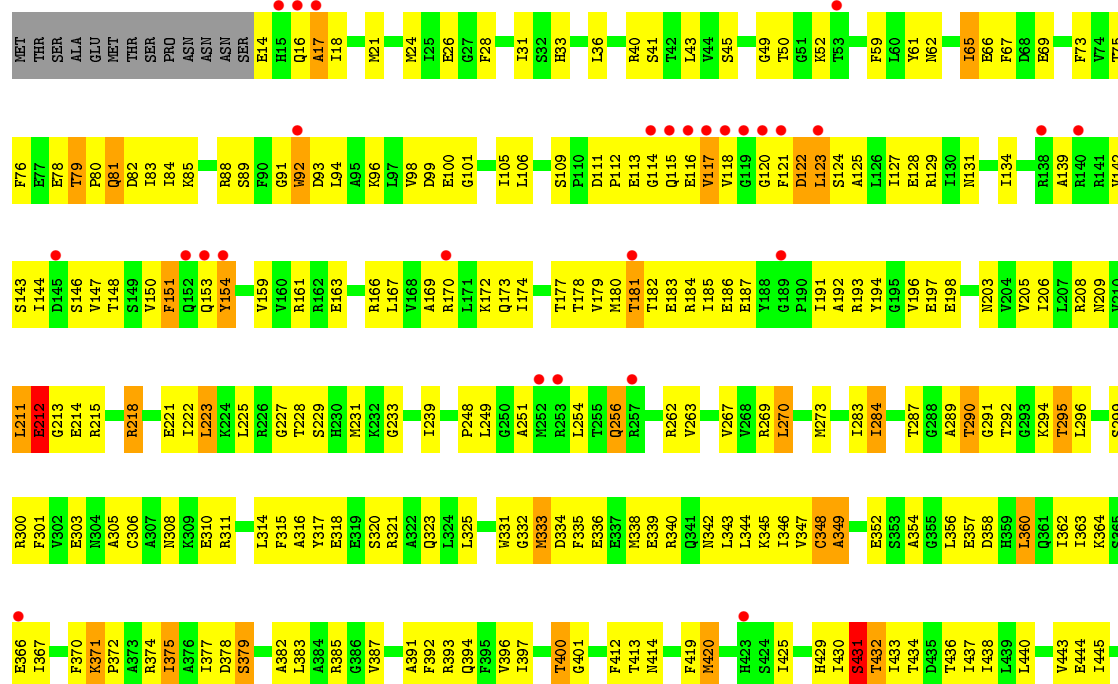


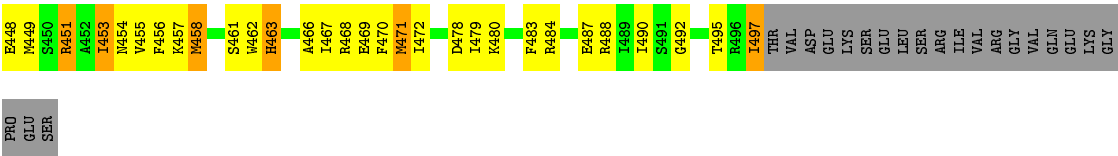
• Molecule 1: KaiC



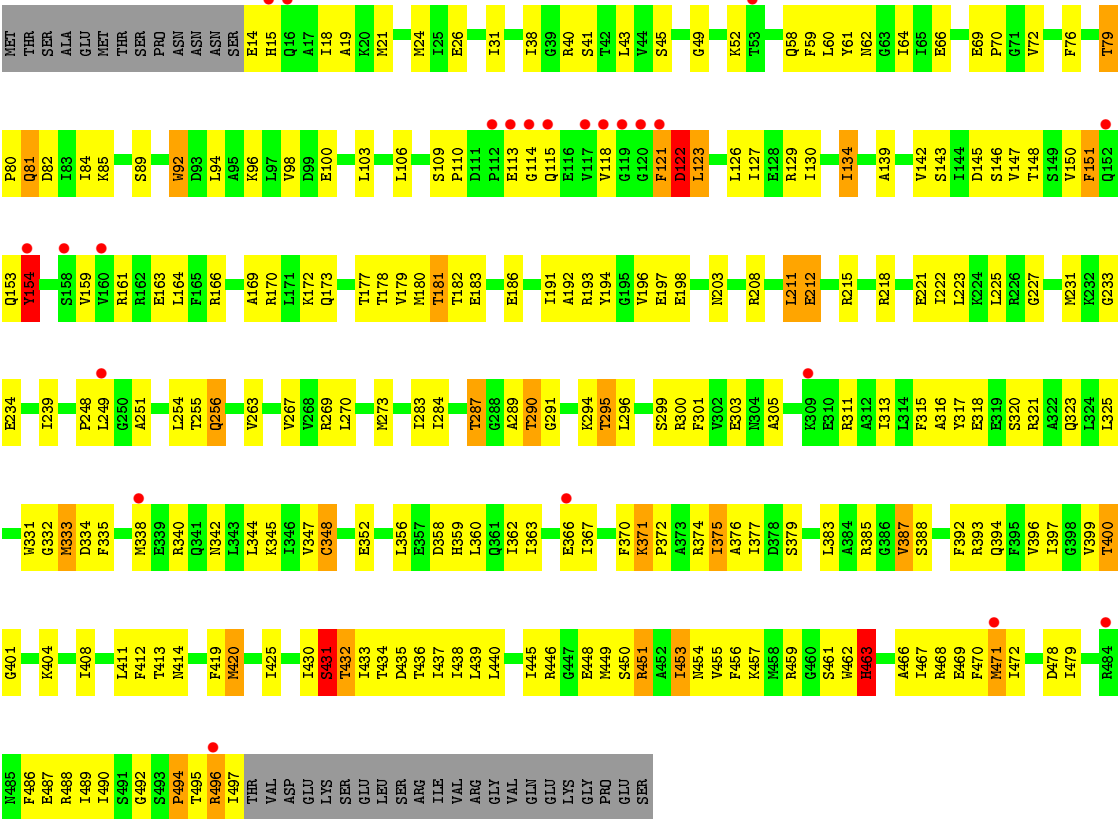
• Molecule 1: KaiC







• Molecule 2: KaiC



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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)	(Not available) (30.00-2.80) 89.7 (29.73-2.83)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.85Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.250 , 0.290 0.245 , 0.278	Depositor DCC
R_{free} test set	4041 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	65.8	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 63.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23375	wwPDB-VP
Average B, all atoms (Å ²)	75.0	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.48	3/3866 (0.1%)	0.65	3/5208 (0.1%)
1	B	0.39	0/3866	0.62	0/5208
1	E	0.42	0/3866	0.65	1/5208 (0.0%)
1	F	0.40	0/3866	0.64	1/5208 (0.0%)
2	C	0.42	2/3872 (0.1%)	0.64	3/5216 (0.1%)
2	D	0.43	1/3872 (0.0%)	0.67	3/5216 (0.1%)
All	All	0.43	6/23208 (0.0%)	0.65	11/31264 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	E	0	2
1	F	0	1
2	C	0	2
2	D	0	2
All	All	0	11

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	92	TRP	CB-CG	12.20	1.72	1.50
1	A	92	TRP	CA-CB	9.80	1.75	1.53
1	A	92	TRP	CG-CD2	-6.71	1.32	1.43
2	C	92	TRP	CG-CD1	-6.26	1.27	1.36
2	C	92	TRP	CA-CB	-5.38	1.42	1.53
2	D	92	TRP	CG-CD2	-5.09	1.34	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	92	TRP	CA-CB-CG	8.38	129.62	113.70
2	C	213	GLY	N-CA-C	-6.51	96.83	113.10
1	A	92	TRP	CB-CG-CD1	6.44	135.38	127.00
1	E	213	GLY	N-CA-C	-6.33	97.27	113.10
2	D	92	TRP	CB-CG-CD1	5.86	134.62	127.00
2	C	92	TRP	CB-CG-CD1	-5.63	119.68	127.00
2	D	92	TRP	CB-CG-CD2	-5.63	119.29	126.60
1	A	92	TRP	CE2-CD2-CG	5.37	111.60	107.30
1	F	114	GLY	N-CA-C	5.36	126.49	113.10
2	C	92	TRP	CB-CG-CD2	5.22	133.39	126.60
1	A	92	TRP	CB-CG-CD2	-5.17	119.87	126.60

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	431	SEP	Mainchain
1	A	432	TPO	Mainchain
1	B	431	SEP	Mainchain
1	B	432	TPO	Mainchain
2	C	431	SER	Mainchain
2	C	432	TPO	Mainchain
2	D	431	SER	Mainchain
2	D	432	TPO	Mainchain
1	E	431	SEP	Mainchain
1	E	432	TPO	Mainchain
1	F	431	SEP	Mainchain

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	3823	0	3811	283	1
1	B	3823	0	3812	296	1
1	E	3823	0	3811	294	0
1	F	3823	0	3810	347	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	3819	0	3813	305	0
2	D	3819	0	3813	320	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	62	0	24	8	0
4	B	62	0	24	8	0
4	C	62	0	24	12	0
4	D	62	0	24	11	0
4	E	62	0	24	8	0
4	F	62	0	24	7	0
5	A	8	0	0	0	0
5	B	5	0	0	0	0
5	C	7	0	0	2	0
5	D	13	0	0	1	0
5	E	10	0	0	2	0
5	F	24	0	0	5	0
All	All	23375	0	23014	1719	1

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 (1719) 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:A:92:TRP:CA	1:A:92:TRP:CB	1.75	1.60
1:E:429:HIS:HA	1:E:431:SEP:O1P	1.46	1.14
1:B:431:SEP:H	1:B:431:SEP:P	1.69	1.14
1:F:313:ILE:HB	1:F:375:ILE:CD1	1.78	1.14
1:B:284:ILE:HD12	1:B:436:THR:HB	1.31	1.13
1:E:290:THR:CG2	1:F:457:LYS:HD3	1.79	1.10
2:D:284:ILE:HD12	2:D:436:THR:HB	1.37	1.07
1:E:263:VAL:HG12	1:E:374:ARG:HH21	1.20	1.07
1:F:305:ALA:HB2	1:F:374:ARG:HD2	1.32	1.06
2:D:486:PHE:CB	2:D:489:ILE:HD11	1.89	1.02
2:C:284:ILE:HD12	2:C:436:THR:HB	1.36	1.02
1:E:284:ILE:HD12	1:E:436:THR:HB	1.41	1.02
1:F:263:VAL:HG12	1:F:374:ARG:HH21	1.19	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:205:VAL:HG22	2:C:222:ILE:HD13	1.39	1.02
1:E:123:LEU:HD13	1:E:166:ARG:HD2	1.41	1.01
2:D:60:LEU:O	2:D:64:ILE:HD13	1.61	1.01
1:A:205:VAL:HG22	1:A:222:ILE:HD12	1.39	1.00
1:E:205:VAL:HG22	1:E:222:ILE:HD12	1.40	1.00
2:D:147:VAL:HG11	2:D:180:MET:HE3	1.41	0.99
1:B:263:VAL:HG12	1:B:374:ARG:HH21	1.27	0.99
1:F:205:VAL:HG22	1:F:222:ILE:HD12	1.44	0.99
2:C:61:TYR:O	2:C:65:ILE:HD13	1.63	0.98
1:A:379:SER:H	1:A:413:THR:HB	1.24	0.97
2:C:287:THR:HG23	2:C:414:ASN:HD22	1.28	0.97
1:E:290:THR:HG22	1:F:457:LYS:HD3	1.46	0.97
2:D:486:PHE:HB3	2:D:489:ILE:HD11	1.46	0.96
2:D:126:LEU:O	2:D:130:ILE:HD13	1.66	0.95
1:A:24:MET:HB2	1:A:62:ASN:HD22	1.32	0.95
1:B:311:ARG:HD2	1:B:371:LYS:HD2	1.45	0.95
1:B:64:ILE:HD12	1:B:102:LYS:HB3	1.49	0.94
1:A:263:VAL:HG12	1:A:374:ARG:HH21	1.29	0.94
1:E:305:ALA:HB2	1:E:374:ARG:HD2	1.50	0.94
2:D:123:LEU:HD12	2:D:166:ARG:HD2	1.50	0.93
1:A:87:ALA:O	1:A:92:TRP:HB2	1.68	0.93
1:A:287:THR:HG23	1:A:414:ASN:HD22	1.31	0.93
2:D:79:THR:HG22	2:D:82:ASP:H	1.32	0.92
1:E:315:PHE:CE2	1:E:366:GLU:OE1	2.21	0.92
1:B:147:VAL:O	1:B:150:VAL:HG12	1.70	0.92
2:D:453:ILE:HG21	2:D:479:ILE:HD12	1.48	0.92
2:C:311:ARG:HD2	2:C:371:LYS:HD2	1.52	0.91
2:C:315:PHE:HE2	2:C:366:GLU:OE1	1.53	0.91
2:D:313:ILE:HD12	2:D:367:ILE:HD13	1.52	0.91
2:D:287:THR:HG23	2:D:414:ASN:HD22	1.36	0.91
1:A:362:ILE:O	1:A:366:GLU:HG3	1.71	0.91
1:F:64:ILE:HD12	1:F:102:LYS:HB3	1.53	0.90
2:C:315:PHE:CE2	2:C:366:GLU:OE1	2.25	0.90
1:F:434:THR:HG23	1:F:437:ILE:HD11	1.53	0.90
1:F:106:LEU:HD11	1:F:129:ARG:CZ	2.02	0.90
1:A:305:ALA:HB2	1:A:374:ARG:HD2	1.54	0.89
1:A:147:VAL:O	1:A:150:VAL:HG12	1.72	0.89
2:D:146:SER:H	2:D:181:THR:HG22	1.37	0.89
1:B:305:ALA:HB2	1:B:374:ARG:HD2	1.53	0.89
1:E:313:ILE:HD12	1:E:367:ILE:HD13	1.53	0.89
1:F:379:SER:H	1:F:413:THR:HB	1.37	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:147:VAL:O	2:C:150:VAL:HG12	1.72	0.88
2:C:495:THR:HA	2:D:487:GLU:OE2	1.73	0.88
1:E:315:PHE:HE2	1:E:366:GLU:OE1	1.56	0.88
1:B:64:ILE:HD11	1:B:70:PRO:HA	1.55	0.88
2:C:14:GLU:HG3	2:C:16:GLN:H	1.39	0.88
1:F:315:PHE:CE2	1:F:366:GLU:OE1	2.26	0.88
1:B:431:SEP:N	1:B:431:SEP:P	2.44	0.88
1:F:313:ILE:HB	1:F:375:ILE:HD11	1.55	0.87
2:D:18:ILE:H	2:D:18:ILE:HD12	1.39	0.86
1:F:123:LEU:HD12	1:F:166:ARG:HD2	1.56	0.86
1:B:31:ILE:HG22	1:B:222:ILE:HD12	1.53	0.86
1:A:147:VAL:HG11	1:A:180:MET:HE3	1.54	0.86
1:E:147:VAL:O	1:E:150:VAL:HG12	1.75	0.86
2:C:147:VAL:HG11	2:C:180:MET:HE3	1.58	0.86
2:C:84:ILE:HD12	2:C:94:LEU:HB2	1.58	0.85
1:E:79:THR:CG2	1:E:81:GLN:HG2	2.06	0.85
2:D:379:SER:H	2:D:413:THR:HB	1.42	0.85
1:E:287:THR:HG23	1:E:414:ASN:HD22	1.42	0.85
1:B:431:SEP:O3P	1:B:431:SEP:N	2.08	0.84
1:E:147:VAL:HG11	1:E:180:MET:HE2	1.59	0.84
1:B:437:ILE:CD1	1:B:457:LYS:HE2	2.07	0.84
2:C:449:MET:CE	2:D:490:ILE:HD11	2.08	0.84
2:D:147:VAL:O	2:D:150:VAL:HG12	1.78	0.84
1:E:263:VAL:HG12	1:E:374:ARG:NH2	1.91	0.84
1:B:263:VAL:HG12	1:B:374:ARG:NH2	1.92	0.83
1:F:263:VAL:HG12	1:F:374:ARG:NH2	1.94	0.83
1:A:311:ARG:HD2	1:A:371:LYS:HD2	1.60	0.83
1:B:434:THR:HG23	1:B:437:ILE:HD11	1.60	0.83
2:D:315:PHE:CE2	2:D:366:GLU:OE1	2.32	0.83
1:A:79:THR:CG2	1:A:81:GLN:HG2	2.09	0.83
2:D:446:ARG:N	2:D:496:ARG:HH12	1.75	0.83
1:E:446:ARG:HE	1:E:496:ARG:NH2	1.77	0.82
1:F:147:VAL:O	1:F:150:VAL:HG12	1.79	0.82
2:D:446:ARG:H	2:D:496:ARG:HH12	1.26	0.82
1:A:434:THR:HG23	1:A:437:ILE:HD11	1.62	0.82
1:B:147:VAL:HG11	1:B:180:MET:HE3	1.62	0.82
2:D:311:ARG:HD2	2:D:371:LYS:HD2	1.61	0.82
1:E:79:THR:HG23	1:E:81:GLN:HG2	1.62	0.82
1:F:347:VAL:HG21	1:F:366:GLU:OE1	1.80	0.82
1:B:191:ILE:HD12	1:B:198:GLU:HG2	1.62	0.82
1:E:449:MET:HG2	1:F:467:ILE:HD11	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:488:ARG:NH2	2:D:488:ARG:HH21	1.78	0.81
1:A:117:VAL:HA	1:A:154:TYR:OH	1.79	0.81
1:B:311:ARG:HD2	1:B:371:LYS:CD	2.10	0.81
1:A:358:ASP:O	1:A:362:ILE:HD13	1.78	0.81
2:D:31:ILE:HG22	2:D:222:ILE:HD12	1.61	0.81
1:A:315:PHE:CE2	1:A:366:GLU:OE1	2.33	0.81
1:A:425:ILE:HB	1:A:431:SEP:O2P	1.80	0.81
2:D:311:ARG:HD2	2:D:371:LYS:CD	2.11	0.81
1:E:311:ARG:HD2	1:E:371:LYS:HD2	1.63	0.81
1:E:379:SER:H	1:E:413:THR:HB	1.43	0.81
1:B:31:ILE:HD13	1:B:231:MET:SD	2.21	0.81
2:C:311:ARG:HD2	2:C:371:LYS:CD	2.10	0.81
1:F:263:VAL:CG1	1:F:374:ARG:HH21	1.92	0.81
1:F:191:ILE:HB	1:F:198:GLU:CG	2.11	0.81
1:A:79:THR:HG22	1:A:82:ASP:H	1.46	0.81
2:D:486:PHE:HB2	2:D:489:ILE:HD11	1.61	0.81
2:C:392:PHE:HE2	2:C:430:ILE:HD11	1.46	0.80
1:B:444:GLU:OE1	2:C:490:ILE:HD12	1.82	0.80
1:F:25:ILE:HD12	1:F:58:GLN:HE21	1.44	0.80
1:B:436:THR:C	1:B:437:ILE:HD12	2.02	0.79
1:E:283:ILE:HD12	1:E:412:PHE:HE1	1.47	0.79
1:F:315:PHE:HE1	1:F:375:ILE:HD12	1.45	0.79
1:F:429:HIS:HA	1:F:431:SEP:O2P	1.82	0.79
1:E:347:VAL:HG21	1:E:366:GLU:OE1	1.83	0.79
2:C:263:VAL:HG12	2:C:374:ARG:HH21	1.48	0.79
2:D:182:THR:HG21	2:D:192:ALA:HB1	1.65	0.79
1:F:287:THR:HG23	1:F:414:ASN:HD22	1.46	0.79
1:B:64:ILE:CD1	1:B:70:PRO:HA	2.13	0.78
1:B:362:ILE:O	1:B:366:GLU:HG3	1.83	0.78
1:B:429:HIS:C	1:B:431:SEP:O1P	2.22	0.78
2:C:347:VAL:HG21	2:C:366:GLU:OE1	1.83	0.78
1:F:79:THR:HG22	1:F:82:ASP:H	1.48	0.78
1:A:263:VAL:HG12	1:A:374:ARG:NH2	1.97	0.78
1:A:311:ARG:HD2	1:A:371:LYS:CD	2.13	0.78
1:B:45:SER:HB3	1:B:182:THR:HB	1.64	0.78
2:D:367:ILE:HD12	2:D:375:ILE:HD11	1.65	0.78
1:A:161:ARG:HB2	1:A:196:VAL:HG11	1.63	0.78
2:D:263:VAL:HG12	2:D:374:ARG:HH21	1.49	0.78
1:F:64:ILE:HD11	1:F:70:PRO:HA	1.66	0.78
1:E:79:THR:HG22	1:E:82:ASP:H	1.48	0.77
1:F:313:ILE:HD12	1:F:367:ILE:HD13	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ARG:HH11	1:A:451:ARG:HG2	1.48	0.77
2:D:425:ILE:HD11	2:D:456:PHE:CE2	2.19	0.77
1:F:161:ARG:HB2	1:F:196:VAL:HG11	1.64	0.77
1:A:436:THR:C	1:A:437:ILE:HD12	2.04	0.77
1:B:24:MET:HB2	1:B:62:ASN:HD22	1.47	0.77
1:F:489:ILE:HA	1:F:494:PRO:HG3	1.65	0.77
1:F:182:THR:HG21	1:F:192:ALA:HB1	1.67	0.77
2:D:287:THR:CG2	2:D:414:ASN:HD22	1.97	0.77
1:B:420:MET:CE	2:C:490:ILE:HD13	2.15	0.77
1:E:290:THR:CG2	1:F:457:LYS:CD	2.61	0.77
2:D:495:THR:HA	1:E:487:GLU:OE2	1.85	0.76
1:E:49:GLY:HA2	4:E:603:ATP:O2B	1.86	0.76
2:C:305:ALA:HB2	2:C:374:ARG:HD2	1.68	0.76
2:D:191:ILE:HB	2:D:198:GLU:CG	2.16	0.76
1:A:347:VAL:HG21	1:A:366:GLU:OE1	1.86	0.76
2:D:489:ILE:HD13	2:D:494:PRO:HB3	1.66	0.76
1:B:263:VAL:CG1	1:B:374:ARG:HH21	1.98	0.76
1:F:436:THR:C	1:F:437:ILE:HD12	2.06	0.76
1:B:191:ILE:HB	1:B:198:GLU:CG	2.16	0.76
2:C:362:ILE:O	2:C:366:GLU:HG3	1.86	0.76
2:C:449:MET:HE3	2:D:490:ILE:HD11	1.66	0.76
1:F:25:ILE:HD12	1:F:58:GLN:NE2	2.00	0.76
1:B:284:ILE:HD12	1:B:436:THR:CB	2.14	0.75
2:D:305:ALA:HB2	2:D:374:ARG:HD2	1.68	0.75
1:E:161:ARG:HB2	1:E:196:VAL:HG11	1.66	0.75
1:A:315:PHE:HE2	1:A:366:GLU:OE1	1.67	0.75
1:B:377:ILE:HD13	1:B:412:PHE:CE2	2.21	0.75
2:C:73:PHE:HB3	2:C:105:ILE:HD13	1.68	0.75
1:A:74:VAL:HB	1:A:144:ILE:HD12	1.68	0.75
1:A:320:SER:HA	1:B:254:LEU:HG	1.67	0.75
1:B:161:ARG:HB2	1:B:196:VAL:HG11	1.68	0.75
2:D:347:VAL:HG21	2:D:366:GLU:OE1	1.87	0.75
2:C:344:LEU:HD22	2:C:345:LYS:N	2.01	0.75
1:A:437:ILE:CD1	1:A:457:LYS:HE2	2.17	0.75
1:E:429:HIS:CA	1:E:431:SEP:O1P	2.32	0.75
1:B:315:PHE:HE2	1:B:366:GLU:OE1	1.69	0.75
1:B:441:GLN:HE22	1:B:490:ILE:HD13	1.51	0.74
2:D:79:THR:CG2	2:D:81:GLN:HG2	2.18	0.74
1:E:363:ILE:O	1:E:367:ILE:HG12	1.87	0.74
1:F:313:ILE:HB	1:F:375:ILE:HD13	1.66	0.74
1:B:43:LEU:HD11	1:B:182:THR:OG1	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:203:ASN:HB3	1:F:225:LEU:HD23	1.68	0.74
1:A:263:VAL:CG1	1:A:374:ARG:HH21	2.01	0.74
1:A:299:SER:HB3	1:A:333:MET:HE1	1.70	0.74
1:B:73:PHE:HB3	1:B:105:ILE:HD13	1.67	0.74
1:B:315:PHE:CE2	1:B:366:GLU:OE1	2.40	0.74
1:A:315:PHE:CD2	1:A:363:ILE:HD12	2.21	0.73
2:C:262:ARG:HH22	2:C:461:SER:HB2	1.52	0.73
1:F:53:THR:HG23	1:F:145:ASP:OD1	1.88	0.73
1:B:347:VAL:HG21	1:B:366:GLU:OE1	1.88	0.73
2:C:367:ILE:HG12	2:C:375:ILE:HD11	1.68	0.73
1:F:362:ILE:O	1:F:366:GLU:HG3	1.89	0.73
1:B:287:THR:HG23	1:B:414:ASN:HD22	1.53	0.73
1:E:123:LEU:HD12	1:E:163:GLU:OE2	1.88	0.73
1:A:457:LYS:HD3	1:F:290:THR:OG1	1.87	0.73
2:D:299:SER:HB3	2:D:333:MET:HE1	1.69	0.73
1:A:64:ILE:HD12	1:A:102:LYS:HB3	1.71	0.73
1:E:269:ARG:HG2	1:E:479:ILE:HB	1.71	0.73
1:F:486:PHE:CB	1:F:489:ILE:HD11	2.19	0.73
2:D:49:GLY:HA2	4:D:522:ATP:O2B	1.88	0.72
1:E:263:VAL:CG1	1:E:374:ARG:HH21	2.00	0.72
2:C:284:ILE:HD11	5:C:529:HOH:O	1.87	0.72
1:E:72:VAL:HG21	1:E:134:ILE:HD12	1.71	0.72
1:F:118:VAL:HG12	1:F:153:GLN:HE22	1.53	0.72
2:D:263:VAL:HG12	2:D:374:ARG:NH2	2.05	0.72
1:A:127:ILE:HD11	1:A:167:LEU:HD12	1.70	0.72
1:E:191:ILE:HD12	1:E:198:GLU:HG2	1.71	0.72
1:E:311:ARG:HD2	1:E:371:LYS:CD	2.20	0.72
1:F:363:ILE:O	1:F:367:ILE:HG12	1.90	0.72
2:D:284:ILE:HD12	2:D:436:THR:CB	2.19	0.72
1:A:287:THR:CG2	1:A:414:ASN:HD22	2.02	0.72
1:E:191:ILE:HB	1:E:198:GLU:CG	2.19	0.72
2:C:269:ARG:HG2	2:C:479:ILE:HB	1.72	0.71
1:B:317:TYR:OH	1:B:363:ILE:HD11	1.90	0.71
1:B:420:MET:HE3	2:C:490:ILE:HD13	1.71	0.71
1:B:49:GLY:HA2	4:B:522:ATP:O2B	1.91	0.71
1:B:127:ILE:HG21	1:B:170:ARG:HG3	1.72	0.71
1:F:315:PHE:HE2	1:F:366:GLU:OE1	1.69	0.71
1:A:254:LEU:HG	1:F:320:SER:HA	1.72	0.71
1:A:377:ILE:HD13	1:A:412:PHE:CE2	2.25	0.71
1:A:437:ILE:HD13	1:A:457:LYS:CG	2.21	0.71
2:C:487:GLU:HG3	2:C:497:ILE:HD11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:392:PHE:HE2	2:D:430:ILE:HD11	1.54	0.71
2:D:284:ILE:CD1	2:D:436:THR:HB	2.18	0.71
1:E:14:GLU:HG3	1:E:16:GLN:H	1.53	0.71
1:F:344:LEU:HD22	1:F:345:LYS:N	2.06	0.71
1:B:426:THR:HB	1:B:431:SEP:O3P	1.91	0.71
2:C:440:LEU:CD2	2:C:453:ILE:HG12	2.20	0.71
2:C:85:LYS:NZ	2:D:14:GLU:HB3	2.05	0.71
1:A:147:VAL:HG11	1:A:180:MET:CE	2.20	0.70
2:D:375:ILE:CD1	2:D:408:ILE:HG21	2.21	0.70
1:F:269:ARG:HG2	1:F:479:ILE:HB	1.72	0.70
1:F:437:ILE:HD13	1:F:457:LYS:CE	2.20	0.70
2:D:315:PHE:HE2	2:D:366:GLU:OE1	1.71	0.70
1:E:446:ARG:HE	1:E:496:ARG:HH22	1.36	0.70
1:E:367:ILE:HD12	1:E:375:ILE:HD11	1.74	0.70
1:E:496:ARG:C	1:E:497:ILE:HD13	2.11	0.70
2:C:392:PHE:CE2	2:C:430:ILE:HD11	2.26	0.70
2:D:161:ARG:HB2	2:D:196:VAL:HG11	1.72	0.70
1:E:325:LEU:HD23	1:E:335:PHE:HB2	1.73	0.70
1:B:123:LEU:HD12	1:B:166:ARG:HD2	1.74	0.70
1:F:299:SER:HB3	1:F:333:MET:HE1	1.74	0.70
1:A:150:VAL:HG13	1:A:151:PHE:N	2.06	0.70
1:F:49:GLY:HA2	4:F:703:ATP:O2B	1.92	0.70
1:F:79:THR:HG23	1:F:81:GLN:HG2	1.74	0.70
1:A:79:THR:HG23	1:A:81:GLN:HG2	1.72	0.69
2:C:123:LEU:HD12	2:C:163:GLU:OE2	1.92	0.69
2:C:299:SER:C	2:C:333:MET:HE1	2.13	0.69
2:C:379:SER:H	2:C:413:THR:HB	1.57	0.69
1:A:211:LEU:O	1:A:212:GLU:HB3	1.92	0.69
1:A:295:THR:HG21	1:A:319:GLU:OE2	1.92	0.69
1:B:182:THR:HG21	1:B:192:ALA:HB1	1.73	0.69
2:C:150:VAL:HG13	2:C:151:PHE:N	2.07	0.69
1:E:284:ILE:HD11	5:E:609:HOH:O	1.93	0.69
1:F:325:LEU:HD23	1:F:335:PHE:HB2	1.74	0.69
1:A:316:ALA:O	1:A:348:CYS:HA	1.92	0.69
1:B:218:ARG:NH1	1:B:239:ILE:HD12	2.08	0.69
1:B:287:THR:HG21	1:B:425:ILE:O	1.92	0.69
2:C:377:ILE:HD12	2:C:412:PHE:CE2	2.28	0.69
2:C:287:THR:HG21	2:C:425:ILE:O	1.92	0.69
1:E:214:GLU:HB3	1:F:234:GLU:HB2	1.73	0.69
1:A:448:GLU:HG2	1:B:466:ALA:HA	1.73	0.69
1:B:437:ILE:HD13	1:B:457:LYS:HE2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:THR:HG23	1:B:81:GLN:HG2	1.75	0.69
1:B:290:THR:OG1	2:C:457:LYS:HD3	1.93	0.69
1:B:448:GLU:HG2	2:C:466:ALA:HA	1.75	0.69
1:F:127:ILE:HD11	1:F:167:LEU:HA	1.75	0.69
1:A:24:MET:CB	1:A:62:ASN:HD22	2.05	0.68
2:D:375:ILE:HD12	2:D:408:ILE:HG21	1.75	0.68
1:F:191:ILE:HG23	1:F:206:ILE:HD11	1.73	0.68
2:C:182:THR:HG21	2:C:192:ALA:HB1	1.75	0.68
1:F:239:ILE:HB	5:F:716:HOH:O	1.94	0.68
1:A:64:ILE:HD11	1:A:70:PRO:HA	1.74	0.68
2:C:191:ILE:HB	2:C:198:GLU:CG	2.23	0.68
1:E:93:ASP:OD2	1:E:96:LYS:HB2	1.93	0.68
1:E:290:THR:HG23	1:F:457:LYS:HD3	1.75	0.68
1:B:437:ILE:HD11	1:B:457:LYS:HE2	1.75	0.68
2:C:325:LEU:HD23	2:C:335:PHE:HB2	1.73	0.68
1:B:299:SER:HB3	1:B:333:MET:HE1	1.76	0.68
1:B:449:MET:CE	2:C:490:ILE:HD11	2.24	0.67
1:E:182:THR:HG21	1:E:192:ALA:HB1	1.75	0.67
1:E:43:LEU:HD11	1:E:182:THR:OG1	1.94	0.67
2:D:377:ILE:HD12	2:D:412:PHE:CE2	2.28	0.67
1:E:61:TYR:CE2	1:E:65:ILE:HG13	2.30	0.67
1:F:16:GLN:HE22	1:F:33:HIS:HB3	1.59	0.67
1:A:437:ILE:N	1:A:437:ILE:HD12	2.08	0.67
2:C:262:ARG:NH2	2:C:461:SER:HB2	2.10	0.67
2:C:344:LEU:HD11	2:C:346:ILE:HD11	1.76	0.67
1:A:182:THR:HG21	1:A:192:ALA:HB1	1.76	0.67
1:A:296:LEU:HD13	1:A:331:TRP:CD2	2.28	0.67
1:B:85:LYS:NZ	2:C:14:GLU:HB3	2.10	0.67
2:D:370:PHE:O	2:D:371:LYS:HD3	1.95	0.67
1:F:437:ILE:CD1	1:F:457:LYS:HE2	2.25	0.67
1:E:123:LEU:O	1:E:127:ILE:HG12	1.94	0.67
1:E:323:GLN:NE2	1:F:459:ARG:HD3	2.10	0.67
1:A:61:TYR:CE2	1:A:65:ILE:HG13	2.30	0.67
1:B:441:GLN:NE2	1:B:490:ILE:HD13	2.10	0.67
2:D:295:THR:HG22	4:D:521:ATP:PA	2.34	0.67
1:F:79:THR:CG2	1:F:81:GLN:HG2	2.25	0.67
1:A:370:PHE:O	1:A:371:LYS:HD3	1.95	0.66
1:B:61:TYR:CE2	1:B:65:ILE:HG13	2.29	0.66
1:F:370:PHE:O	1:F:371:LYS:HG3	1.95	0.66
1:E:447:GLY:O	1:F:467:ILE:HD13	1.95	0.66
1:F:486:PHE:HB2	1:F:489:ILE:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:487:GLU:O	1:E:488:ARG:HB2	1.96	0.66
1:F:144:ILE:CG2	1:F:147:VAL:HG12	2.26	0.66
1:F:52:LYS:HE3	4:F:703:ATP:O1B	1.95	0.66
1:B:24:MET:CB	1:B:62:ASN:HD22	2.08	0.66
2:D:150:VAL:HG13	2:D:151:PHE:N	2.10	0.66
2:C:79:THR:HG23	2:C:81:GLN:HG2	1.76	0.66
1:B:78:GLU:HB2	1:B:83:ILE:HD11	1.78	0.66
1:E:148:THR:OG1	1:E:182:THR:HG23	1.96	0.66
2:D:114:GLY:O	2:D:115:GLN:HG3	1.96	0.66
2:D:43:LEU:HD11	2:D:182:THR:OG1	1.96	0.66
1:A:92:TRP:HE3	1:A:92:TRP:CA	2.09	0.66
1:B:169:ALA:O	1:B:173:GLN:HG3	1.95	0.66
2:D:72:VAL:HG21	2:D:134:ILE:HD12	1.78	0.66
1:E:489:ILE:HA	1:E:494:PRO:HG3	1.76	0.66
2:D:453:ILE:HD13	2:D:454:ASN:N	2.11	0.66
1:F:90:PHE:HB2	1:F:92:TRP:CE2	2.31	0.66
1:B:150:VAL:HG13	1:B:151:PHE:N	2.11	0.65
1:B:283:ILE:HD13	1:B:400:THR:HG23	1.77	0.65
1:B:79:THR:CG2	1:B:81:GLN:HG2	2.25	0.65
2:C:449:MET:HE1	2:D:490:ILE:HD11	1.77	0.65
1:B:425:ILE:HD11	1:B:456:PHE:CE2	2.31	0.65
2:C:321:ARG:HG2	2:C:348:CYS:SG	2.36	0.65
2:D:126:LEU:O	2:D:130:ILE:CD1	2.42	0.65
1:F:147:VAL:HG11	1:F:180:MET:HE2	1.78	0.65
1:B:147:VAL:HG11	1:B:180:MET:CE	2.26	0.65
1:B:483:PHE:HB3	1:B:486:PHE:HD1	1.61	0.65
2:C:31:ILE:HD13	2:C:231:MET:SD	2.37	0.65
2:C:425:ILE:HD11	2:C:456:PHE:CE2	2.30	0.65
1:E:377:ILE:HD12	1:E:412:PHE:CE2	2.30	0.65
1:A:79:THR:HG21	1:A:81:GLN:HG2	1.75	0.65
1:A:96:LYS:O	1:A:100:GLU:HG3	1.96	0.65
1:B:440:LEU:CD2	1:B:453:ILE:HG12	2.26	0.65
2:C:159:VAL:O	2:C:163:GLU:HG2	1.96	0.65
2:D:325:LEU:HD23	2:D:335:PHE:HB2	1.79	0.65
2:D:85:LYS:NZ	1:E:14:GLU:HB3	2.12	0.65
1:A:49:GLY:HA2	4:A:522:ATP:O2B	1.97	0.65
1:F:486:PHE:HE2	1:F:496:ARG:HD2	1.60	0.65
1:B:449:MET:HE3	2:C:490:ILE:HD11	1.77	0.65
2:D:147:VAL:HG11	2:D:180:MET:CE	2.24	0.65
2:D:362:ILE:O	2:D:366:GLU:HG3	1.97	0.65
1:E:150:VAL:HG13	1:E:151:PHE:N	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LYS:N	4:B:522:ATP:O1B	2.24	0.65
2:C:320:SER:HA	2:D:254:LEU:HG	1.79	0.65
1:E:446:ARG:NE	1:E:496:ARG:HH22	1.94	0.65
1:F:283:ILE:HG23	1:F:412:PHE:CE1	2.32	0.65
1:B:18:ILE:HB	1:B:228:THR:HG23	1.79	0.64
1:E:317:TYR:OH	1:E:363:ILE:HD11	1.97	0.64
2:C:263:VAL:HG12	2:C:374:ARG:NH2	2.12	0.64
1:E:344:LEU:HD22	1:E:345:LYS:N	2.12	0.64
1:B:437:ILE:HD13	1:B:457:LYS:CE	2.27	0.64
1:B:453:ILE:HD13	1:B:454:ASN:N	2.12	0.64
1:F:218:ARG:HD2	5:F:706:HOH:O	1.97	0.64
1:F:315:PHE:CE1	1:F:375:ILE:HD12	2.30	0.64
1:F:377:ILE:HD12	1:F:412:PHE:CE2	2.33	0.64
1:B:370:PHE:O	1:B:371:LYS:HD3	1.98	0.64
2:C:295:THR:CG2	4:C:521:ATP:O2A	2.44	0.64
1:E:147:VAL:HG11	1:E:180:MET:CE	2.26	0.64
1:A:45:SER:HB3	1:A:182:THR:HB	1.80	0.64
1:A:218:ARG:CZ	1:A:239:ILE:HD12	2.28	0.64
1:A:317:TYR:OH	1:A:363:ILE:HD11	1.98	0.64
2:D:335:PHE:HA	2:D:338:MET:HG3	1.78	0.64
1:F:117:VAL:HA	1:F:154:TYR:OH	1.98	0.64
2:C:453:ILE:HD13	2:C:454:ASN:N	2.12	0.64
2:D:438:ILE:CD1	2:D:455:VAL:HG22	2.28	0.64
1:E:283:ILE:HD12	1:E:412:PHE:CE1	2.30	0.64
1:F:111:ASP:OD1	1:F:112:PRO:HD2	1.97	0.64
1:F:315:PHE:CE2	1:F:363:ILE:HD12	2.33	0.64
2:C:65:ILE:N	2:C:65:ILE:HD12	2.12	0.64
2:D:146:SER:H	2:D:181:THR:CG2	2.08	0.64
1:A:455:VAL:HG11	1:A:463:HIS:HB2	1.80	0.64
1:B:483:PHE:HB3	1:B:486:PHE:CD1	2.33	0.64
2:C:121:PHE:O	2:C:125:ALA:HB3	1.97	0.64
2:C:21:MET:HE2	2:C:177:THR:HG21	1.79	0.64
2:D:487:GLU:OE1	2:D:497:ILE:HD13	1.98	0.64
1:E:287:THR:CG2	1:E:414:ASN:HD22	2.11	0.64
1:E:269:ARG:HB3	1:E:479:ILE:HD12	1.78	0.64
1:B:344:LEU:HD22	1:B:345:LYS:N	2.13	0.63
2:C:50:THR:HG22	2:C:209:ASN:HB2	1.80	0.63
2:D:295:THR:CG2	4:D:521:ATP:O2A	2.46	0.63
2:D:451:ARG:HH11	2:D:451:ARG:HG2	1.63	0.63
1:E:356:LEU:HD22	1:E:387:VAL:HG11	1.80	0.63
1:E:356:LEU:CD2	1:E:387:VAL:HG11	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:ILE:HD13	1:A:457:LYS:HG2	1.81	0.63
1:A:488:ARG:NE	1:F:488:ARG:HH12	1.96	0.63
1:F:24:MET:HB2	1:F:62:ASN:HD22	1.62	0.63
2:C:469:GLU:HG3	2:C:480:LYS:HE3	1.80	0.63
1:F:315:PHE:CD2	1:F:363:ILE:HD12	2.33	0.63
1:A:257:ARG:NH2	1:A:407:GLU:HG2	2.14	0.63
1:B:437:ILE:HD13	1:B:457:LYS:CG	2.29	0.63
2:C:111:ASP:OD2	2:C:113:GLU:HG2	1.99	0.63
2:C:432:TPO:O1P	2:C:432:TPO:HG21	1.99	0.63
2:C:444:GLU:OE1	2:D:490:ILE:HD12	1.98	0.63
2:C:214:GLU:HB3	2:D:234:GLU:HB2	1.81	0.63
2:C:79:THR:CG2	2:C:81:GLN:HG2	2.29	0.63
2:C:218:ARG:NH1	2:C:239:ILE:HD12	2.14	0.63
2:D:79:THR:HG23	2:D:81:GLN:HG2	1.80	0.63
1:F:440:LEU:CD2	1:F:453:ILE:HG13	2.28	0.63
1:A:437:ILE:HD13	1:A:457:LYS:CE	2.28	0.63
2:D:146:SER:N	2:D:181:THR:HG22	2.10	0.63
2:D:218:ARG:CZ	2:D:239:ILE:HD12	2.29	0.63
1:E:191:ILE:HB	1:E:198:GLU:HG2	1.81	0.63
1:E:382:ALA:O	1:E:385:ARG:HG3	1.98	0.63
1:E:79:THR:HG21	1:E:81:GLN:HG2	1.79	0.63
1:F:437:ILE:HD13	1:F:457:LYS:CG	2.28	0.63
1:E:191:ILE:CD1	1:E:198:GLU:HG2	2.28	0.62
1:E:377:ILE:HD12	1:E:412:PHE:HE2	1.65	0.62
2:D:488:ARG:NH1	1:E:488:ARG:HH21	1.97	0.62
1:A:325:LEU:HD23	1:A:335:PHE:HB2	1.80	0.62
2:C:471:MET:O	2:C:472:ILE:HD13	1.98	0.62
1:E:248:PRO:HB2	1:E:251:ALA:HB3	1.81	0.62
1:A:249:LEU:HD13	1:A:394:GLN:HG2	1.81	0.62
1:B:283:ILE:CD1	1:B:400:THR:HG23	2.29	0.62
2:C:344:LEU:HD22	2:C:345:LYS:H	1.63	0.62
1:F:396:VAL:O	1:F:400:THR:HB	2.00	0.62
1:A:269:ARG:HG2	1:A:479:ILE:HB	1.81	0.62
1:B:437:ILE:HD12	1:B:437:ILE:N	2.14	0.62
2:C:182:THR:HG22	2:C:183:GLU:N	2.14	0.62
2:D:393:ARG:O	2:D:397:ILE:HG12	1.99	0.62
2:C:218:ARG:CZ	2:C:239:ILE:HD12	2.29	0.62
2:C:61:TYR:O	2:C:65:ILE:CD1	2.44	0.62
1:A:437:ILE:HD13	1:A:457:LYS:HE2	1.81	0.62
1:A:64:ILE:CD1	1:A:70:PRO:HA	2.29	0.62
1:B:273:MET:O	1:B:463:HIS:HA	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:PHE:CD2	1:B:363:ILE:HD12	2.34	0.62
2:C:206:ILE:HD11	2:C:223:LEU:HB2	1.81	0.62
2:C:296:LEU:CD2	2:C:472:ILE:HD12	2.29	0.62
2:C:203:ASN:HB3	2:C:225:LEU:HD23	1.81	0.62
2:D:151:PHE:C	2:D:153:GLN:H	2.00	0.62
2:D:182:THR:HG22	2:D:183:GLU:N	2.15	0.62
2:D:295:THR:HG22	4:D:521:ATP:O1A	1.99	0.62
2:D:84:ILE:CD1	2:D:94:LEU:HB2	2.29	0.62
1:F:437:ILE:HD13	1:F:457:LYS:HE2	1.82	0.62
1:A:191:ILE:HB	1:A:198:GLU:CG	2.30	0.62
2:D:290:THR:OG1	1:E:457:LYS:HD3	1.99	0.62
1:B:379:SER:H	1:B:413:THR:HB	1.64	0.62
1:A:49:GLY:CA	4:A:522:ATP:O2B	2.48	0.61
2:D:61:TYR:CE2	2:D:92:TRP:CD1	2.87	0.61
1:F:370:PHE:C	1:F:371:LYS:HG3	2.19	0.61
1:F:451:ARG:HH11	1:F:451:ARG:HG2	1.64	0.61
1:A:451:ARG:NH1	1:A:451:ARG:HG2	2.15	0.61
1:E:115:GLN:OE1	1:E:118:VAL:HG21	2.00	0.61
1:A:184:ARG:O	1:A:185:ILE:HD13	2.00	0.61
1:B:123:LEU:O	1:B:123:LEU:HD13	2.00	0.61
2:C:284:ILE:N	2:C:284:ILE:HD13	2.15	0.61
2:C:431:SER:O	2:C:434:THR:HG22	2.00	0.61
2:D:79:THR:HG21	2:D:81:GLN:HG2	1.82	0.61
1:E:49:GLY:CA	4:E:603:ATP:O2B	2.47	0.61
2:C:148:THR:CG2	2:C:193:ARG:HD2	2.31	0.61
2:C:289:ALA:HB2	2:C:419:PHE:HA	1.80	0.61
2:D:148:THR:CG2	2:D:193:ARG:HD2	2.30	0.61
2:D:72:VAL:HG21	2:D:134:ILE:CD1	2.31	0.61
1:F:134:ILE:HD11	1:F:142:VAL:HG22	1.83	0.61
1:F:64:ILE:CD1	1:F:70:PRO:HA	2.29	0.61
2:C:438:ILE:CD1	2:C:455:VAL:HG22	2.31	0.61
1:E:359:HIS:O	1:E:363:ILE:HG12	2.01	0.61
1:E:284:ILE:HD12	1:E:436:THR:CB	2.24	0.61
1:F:144:ILE:HG22	1:F:147:VAL:HG12	1.83	0.61
1:F:437:ILE:N	1:F:437:ILE:HD12	2.16	0.61
2:C:314:LEU:HB3	2:C:346:ILE:HD13	1.83	0.61
1:A:89:SER:HB2	1:B:227:GLY:O	2.00	0.60
1:B:123:LEU:O	1:B:127:ILE:HG13	2.00	0.60
2:C:191:ILE:HB	2:C:198:GLU:HG2	1.83	0.60
2:C:314:LEU:HD23	2:C:346:ILE:HD12	1.81	0.60
2:D:321:ARG:HG2	2:D:348:CYS:SG	2.41	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:ASP:OD2	1:B:181:THR:HG21	2.00	0.60
1:F:486:PHE:CE2	1:F:496:ARG:HD2	2.36	0.60
1:B:437:ILE:HD13	1:B:457:LYS:HG2	1.82	0.60
2:C:61:TYR:CE2	2:C:65:ILE:HG12	2.35	0.60
2:D:344:LEU:HD22	2:D:345:LYS:N	2.15	0.60
2:D:315:PHE:CZ	2:D:363:ILE:HG23	2.36	0.60
2:D:58:GLN:HG3	2:D:92:TRP:HZ2	1.66	0.60
1:E:79:THR:HG23	1:E:81:GLN:H	1.65	0.60
1:A:382:ALA:O	1:A:385:ARG:HG3	2.02	0.60
1:B:18:ILE:HB	1:B:228:THR:CG2	2.31	0.60
2:D:440:LEU:CD2	2:D:453:ILE:HG12	2.32	0.60
1:B:295:THR:HG21	1:B:319:GLU:OE2	2.01	0.60
1:F:461:SER:OG	1:F:462:TRP:N	2.34	0.60
1:B:438:ILE:HG23	1:B:453:ILE:HD11	1.83	0.60
2:C:287:THR:CG2	2:C:414:ASN:HD22	2.06	0.60
1:F:159:VAL:O	1:F:163:GLU:HG2	2.01	0.60
1:A:344:LEU:HD22	1:A:345:LYS:N	2.17	0.60
1:B:191:ILE:CD1	1:B:198:GLU:HG2	2.31	0.60
2:D:486:PHE:CE2	2:D:496:ARG:HB3	2.37	0.60
1:E:362:ILE:O	1:E:366:GLU:HG3	2.02	0.60
1:F:122:ASP:OD2	1:F:123:LEU:N	2.35	0.60
1:F:127:ILE:HD11	1:F:167:LEU:HD12	1.84	0.60
1:A:14:GLU:HG3	1:A:16:GLN:OE1	2.01	0.60
1:A:52:LYS:HE3	4:A:522:ATP:O1B	2.01	0.60
2:D:79:THR:HG23	2:D:81:GLN:H	1.67	0.60
1:A:79:THR:HG23	1:A:81:GLN:H	1.67	0.60
2:D:194:TYR:O	2:D:196:VAL:HG23	2.01	0.60
2:C:420:MET:CE	2:D:490:ILE:HD13	2.32	0.60
1:F:150:VAL:HG13	1:F:151:PHE:N	2.16	0.60
1:F:377:ILE:HD11	1:F:399:VAL:HG11	1.84	0.60
1:B:218:ARG:CZ	1:B:239:ILE:HD12	2.32	0.59
1:E:461:SER:OG	1:E:462:TRP:N	2.33	0.59
2:D:49:GLY:CA	4:D:522:ATP:O2B	2.49	0.59
1:E:159:VAL:O	1:E:163:GLU:HG2	2.02	0.59
1:E:451:ARG:HH11	1:E:451:ARG:HG2	1.68	0.59
1:F:382:ALA:O	1:F:385:ARG:HG3	2.02	0.59
1:F:467:ILE:N	1:F:467:ILE:HD12	2.17	0.59
1:A:92:TRP:CA	1:A:92:TRP:CE3	2.86	0.59
1:E:432:TPO:HG21	1:E:432:TPO:O1P	2.03	0.59
1:A:21:MET:HB2	1:A:38:ILE:CD1	2.32	0.59
2:D:392:PHE:CE2	2:D:430:ILE:HD11	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:484:ARG:HH11	1:F:484:ARG:HB3	1.68	0.59
1:B:269:ARG:HG2	1:B:479:ILE:HB	1.83	0.59
2:D:385:ARG:NH2	1:E:433:ILE:HD11	2.18	0.59
2:C:290:THR:OG1	2:D:457:LYS:HD3	2.03	0.59
1:A:208:ARG:NH2	1:A:221:GLU:OE2	2.35	0.59
1:A:437:ILE:HD11	1:A:457:LYS:HE2	1.83	0.59
2:C:28:PHE:CZ	2:C:222:ILE:HD11	2.38	0.59
2:D:367:ILE:HG23	2:D:372:PRO:HD2	1.85	0.59
2:D:489:ILE:HD13	2:D:494:PRO:CB	2.33	0.59
1:E:22:ARG:HD3	5:E:612:HOH:O	2.03	0.59
1:E:396:VAL:O	1:E:400:THR:HB	2.03	0.59
1:F:146:SER:H	1:F:181:THR:HG22	1.67	0.59
1:A:290:THR:OG1	1:B:457:LYS:HD3	2.01	0.59
2:D:316:ALA:O	2:D:348:CYS:HA	2.02	0.59
1:E:320:SER:HA	1:F:254:LEU:HG	1.83	0.59
1:B:444:GLU:HB2	2:C:490:ILE:CD1	2.33	0.59
1:E:293:GLY:HA2	4:E:601:ATP:O1A	2.03	0.59
1:F:437:ILE:CD1	1:F:457:LYS:CE	2.81	0.59
2:C:400:THR:HG22	2:C:401:GLY:N	2.18	0.58
2:C:24:MET:HB2	2:C:62:ASN:HD22	1.67	0.58
1:E:273:MET:O	1:E:463:HIS:HA	2.03	0.58
1:E:289:ALA:HB2	1:E:419:PHE:HA	1.84	0.58
1:F:296:LEU:HD13	1:F:331:TRP:CD2	2.37	0.58
1:B:451:ARG:HG2	1:B:451:ARG:HH11	1.68	0.58
2:C:273:MET:O	2:C:463:HIS:HA	2.04	0.58
2:C:52:LYS:HE3	4:C:522:ATP:O1B	2.03	0.58
2:D:400:THR:HG22	2:D:401:GLY:N	2.18	0.58
1:E:148:THR:CG2	1:E:193:ARG:HD2	2.33	0.58
1:F:49:GLY:CA	4:F:703:ATP:O2B	2.51	0.58
1:A:356:LEU:HD13	1:A:387:VAL:HG21	1.85	0.58
1:B:194:TYR:O	1:B:196:VAL:HG23	2.03	0.58
1:B:50:THR:HG22	1:B:209:ASN:HB2	1.85	0.58
2:D:248:PRO:HB2	2:D:251:ALA:HB3	1.86	0.58
1:E:437:ILE:CD1	1:E:457:LYS:HE2	2.33	0.58
1:A:367:ILE:HG12	1:A:375:ILE:HD11	1.84	0.58
1:B:269:ARG:HB3	1:B:479:ILE:HD12	1.84	0.58
2:C:315:PHE:CZ	2:C:363:ILE:HG23	2.38	0.58
2:D:14:GLU:CD	2:D:15:HIS:H	2.07	0.58
1:A:437:ILE:CD1	1:A:457:LYS:CE	2.82	0.58
1:B:78:GLU:CB	1:B:83:ILE:HD11	2.33	0.58
2:C:151:PHE:C	2:C:153:GLN:H	2.05	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:SER:HA	1:A:271:ASP:OD1	2.04	0.58
2:C:79:THR:HG22	2:C:82:ASP:H	1.69	0.58
1:E:470:PHE:CE1	1:E:472:ILE:HD11	2.38	0.58
1:F:293:GLY:HA2	4:F:701:ATP:O1A	2.04	0.58
1:F:79:THR:HG23	1:F:81:GLN:H	1.67	0.58
1:A:126:LEU:HG	1:A:130:ILE:CD1	2.34	0.58
1:A:372:PRO:O	1:A:408:ILE:HD12	2.03	0.58
1:A:396:VAL:O	1:A:400:THR:HB	2.03	0.58
1:A:43:LEU:HD11	1:A:182:THR:OG1	2.04	0.58
1:B:426:THR:HG22	1:B:428:SER:H	1.69	0.58
1:F:316:ALA:O	1:F:348:CYS:HA	2.04	0.58
1:F:311:ARG:HD2	1:F:371:LYS:HE2	1.85	0.58
1:A:379:SER:N	1:A:413:THR:HB	2.06	0.58
2:D:363:ILE:O	2:D:367:ILE:HG12	2.04	0.58
1:F:147:VAL:HG11	1:F:180:MET:CE	2.34	0.58
1:F:194:TYR:O	1:F:196:VAL:HG23	2.04	0.58
1:B:85:LYS:HZ3	2:C:14:GLU:HB3	1.69	0.57
2:D:431:SER:O	2:D:434:THR:HG22	2.03	0.57
1:E:127:ILE:HD11	1:E:167:LEU:HD13	1.84	0.57
1:E:67:PHE:HB2	1:E:69:GLU:HG3	1.86	0.57
1:B:461:SER:OG	1:B:462:TRP:N	2.37	0.57
2:C:142:VAL:O	2:C:178:THR:HA	2.03	0.57
1:F:372:PRO:O	1:F:408:ILE:HD12	2.04	0.57
1:B:432:TPO:HG21	1:B:432:TPO:O1P	2.03	0.57
1:B:49:GLY:CA	4:B:522:ATP:O2B	2.52	0.57
2:D:150:VAL:O	2:D:153:GLN:HG3	2.03	0.57
1:E:169:ALA:O	1:E:173:GLN:HG3	2.03	0.57
1:F:131:ASN:O	1:F:135:GLN:HG3	2.04	0.57
1:F:484:ARG:NH1	1:F:484:ARG:HB3	2.18	0.57
1:B:377:ILE:N	1:B:377:ILE:HD12	2.19	0.57
2:C:88:ARG:NE	2:D:15:HIS:HA	2.18	0.57
2:D:161:ARG:HD2	2:D:196:VAL:HG13	1.86	0.57
1:F:14:GLU:HG2	5:F:723:HOH:O	2.02	0.57
1:F:287:THR:CG2	1:F:414:ASN:HD22	2.17	0.57
2:C:221:GLU:HG3	2:C:233:GLY:O	2.03	0.57
1:F:150:VAL:O	1:F:153:GLN:HG3	2.05	0.57
1:E:315:PHE:CD2	1:E:363:ILE:HD12	2.40	0.57
1:F:191:ILE:HB	1:F:198:GLU:CD	2.24	0.57
1:A:14:GLU:HG3	1:A:15:HIS:H	1.68	0.57
1:A:161:ARG:HD2	1:A:196:VAL:HG13	1.87	0.57
1:A:433:ILE:HD11	1:F:385:ARG:NH2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:486:PHE:HB3	1:F:489:ILE:HD11	1.87	0.57
1:A:273:MET:O	1:A:463:HIS:HA	2.04	0.57
1:A:377:ILE:N	1:A:377:ILE:HD12	2.19	0.57
1:A:432:TPO:O1P	1:A:432:TPO:HG21	2.04	0.57
1:E:372:PRO:HB2	1:E:375:ILE:HD11	1.85	0.57
1:A:315:PHE:CE2	1:A:363:ILE:HD12	2.40	0.57
1:B:87:ALA:O	1:B:92:TRP:HB2	2.05	0.57
2:C:148:THR:HG21	2:C:193:ARG:HD2	1.87	0.57
1:F:169:ALA:O	1:F:173:GLN:HG3	2.05	0.57
1:A:459:ARG:HD3	1:F:323:GLN:NE2	2.20	0.57
2:C:484:ARG:HB3	2:C:484:ARG:NH1	2.19	0.57
2:C:84:ILE:CD1	2:C:94:LEU:HB2	2.31	0.57
1:E:18:ILE:HD11	1:E:227:GLY:C	2.25	0.57
1:E:50:THR:HG22	1:E:209:ASN:HB2	1.86	0.57
1:F:420:MET:HE3	1:F:492:GLY:HA3	1.86	0.57
1:F:429:HIS:CA	1:F:431:SEP:O2P	2.52	0.57
1:B:249:LEU:HD13	1:B:394:GLN:HG2	1.86	0.56
1:B:453:ILE:HD13	1:B:454:ASN:H	1.68	0.56
2:D:283:ILE:CD1	2:D:400:THR:HG23	2.34	0.56
1:E:76:PHE:HZ	1:E:126:LEU:HD21	1.69	0.56
1:E:370:PHE:O	1:E:371:LYS:HD3	2.05	0.56
1:E:453:ILE:HB	1:E:470:PHE:CD2	2.40	0.56
1:F:377:ILE:HD12	1:F:412:PHE:HE2	1.69	0.56
1:A:296:LEU:CD2	1:A:472:ILE:HD12	2.35	0.56
1:B:89:SER:HB2	2:C:227:GLY:O	2.05	0.56
2:C:147:VAL:HG11	2:C:180:MET:CE	2.34	0.56
1:E:28:PHE:HE1	1:E:222:ILE:HD11	1.69	0.56
1:F:134:ILE:HD11	1:F:142:VAL:CG2	2.35	0.56
1:A:124:SER:O	1:A:128:GLU:HG3	2.05	0.56
1:A:74:VAL:CB	1:A:144:ILE:HD12	2.35	0.56
2:C:461:SER:OG	2:C:462:TRP:N	2.36	0.56
1:B:320:SER:HA	2:C:254:LEU:HG	1.87	0.56
2:C:94:LEU:O	2:C:98:VAL:HG23	2.06	0.56
1:A:311:ARG:HA	1:A:343:LEU:O	2.05	0.56
1:A:483:PHE:HB3	1:A:486:PHE:CD1	2.40	0.56
1:B:438:ILE:CD1	1:B:455:VAL:HG22	2.35	0.56
1:F:231:MET:CE	1:F:251:ALA:HB2	2.35	0.56
1:A:287:THR:HG21	1:A:425:ILE:O	2.06	0.56
1:A:436:THR:HG23	1:A:458:MET:HG2	1.88	0.56
2:C:295:THR:HG21	4:C:521:ATP:O2A	2.04	0.56
2:D:24:MET:HG3	2:D:66:GLU:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:203:ASN:HB3	1:E:225:LEU:HD23	1.86	0.56
1:A:92:TRP:HE3	1:A:92:TRP:N	2.03	0.56
2:C:150:VAL:HG13	2:C:151:PHE:H	1.70	0.56
2:C:440:LEU:HD21	2:C:453:ILE:HG12	1.87	0.56
2:D:320:SER:HA	1:E:254:LEU:HG	1.88	0.56
2:D:432:TPO:O1P	2:D:432:TPO:HG21	2.06	0.56
1:F:284:ILE:N	1:F:284:ILE:HD12	2.21	0.56
1:A:127:ILE:HD11	1:A:167:LEU:CD1	2.34	0.56
1:A:151:PHE:C	1:A:153:GLN:H	2.09	0.56
1:B:178:THR:HG22	1:B:179:VAL:N	2.21	0.56
2:D:487:GLU:OE1	2:D:497:ILE:HG21	2.04	0.56
1:F:273:MET:O	1:F:463:HIS:HA	2.06	0.56
1:A:284:ILE:N	1:A:284:ILE:HD12	2.21	0.56
1:A:150:VAL:HG13	1:A:151:PHE:H	1.70	0.56
1:A:74:VAL:CG2	1:A:144:ILE:HD12	2.36	0.56
2:C:218:ARG:HB3	5:C:525:HOH:O	2.05	0.55
2:D:317:TYR:CE2	2:D:383:LEU:HD21	2.41	0.55
2:D:80:PRO:HD2	2:D:81:GLN:NE2	2.21	0.55
1:B:117:VAL:O	1:B:117:VAL:HG12	2.06	0.55
1:B:79:THR:CG2	1:B:82:ASP:H	2.20	0.55
2:D:21:MET:HE1	2:D:177:THR:HB	1.88	0.55
1:F:96:LYS:O	1:F:100:GLU:HG3	2.07	0.55
1:A:466:ALA:HA	1:F:448:GLU:HG2	1.87	0.55
2:C:377:ILE:HD12	2:C:412:PHE:HE2	1.69	0.55
2:D:287:THR:HG21	2:D:425:ILE:O	2.05	0.55
2:D:295:THR:HG21	4:D:521:ATP:O2A	2.05	0.55
1:B:56:SER:HB2	1:B:143:SER:HB3	1.88	0.55
1:B:296:LEU:CD2	1:B:472:ILE:HD12	2.37	0.55
2:C:269:ARG:HB3	2:C:479:ILE:HD13	1.89	0.55
2:C:79:THR:CG2	2:C:82:ASP:H	2.18	0.55
1:F:393:ARG:O	1:F:397:ILE:HG12	2.07	0.55
1:A:363:ILE:O	1:A:367:ILE:HG13	2.05	0.55
2:C:150:VAL:O	2:C:153:GLN:HG3	2.06	0.55
2:D:435:ASP:HA	2:D:459:ARG:HD2	1.87	0.55
1:F:356:LEU:CD2	1:F:387:VAL:HG11	2.36	0.55
1:B:148:THR:CG2	1:B:193:ARG:HD2	2.37	0.55
1:B:367:ILE:HG12	1:B:375:ILE:HD11	1.88	0.55
1:F:248:PRO:HB2	1:F:251:ALA:HB3	1.87	0.55
1:F:338:MET:HB3	1:F:344:LEU:HB3	1.89	0.55
1:A:191:ILE:HG23	1:A:206:ILE:CD1	2.37	0.55
1:B:164:LEU:HD11	1:B:197:GLU:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ALA:O	1:B:348:CYS:HA	2.07	0.55
1:B:85:LYS:HE3	2:C:17:ALA:O	2.07	0.55
1:E:496:ARG:O	1:E:497:ILE:HD13	2.05	0.55
1:F:249:LEU:HD13	1:F:394:GLN:HG2	1.88	0.55
1:A:362:ILE:HG22	1:A:366:GLU:OE2	2.07	0.55
1:B:191:ILE:HB	1:B:198:GLU:CD	2.27	0.55
2:C:185:ILE:HD12	2:C:185:ILE:N	2.21	0.55
2:D:40:ARG:HG2	2:D:172:LYS:HE3	1.88	0.55
1:A:150:VAL:CG1	1:A:151:PHE:N	2.70	0.55
1:B:438:ILE:HD13	1:B:455:VAL:HA	1.89	0.55
2:C:347:VAL:O	2:C:348:CYS:HB2	2.06	0.55
2:D:96:LYS:O	2:D:100:GLU:HG3	2.07	0.55
2:C:80:PRO:O	2:C:84:ILE:HG12	2.07	0.55
2:D:437:ILE:CD1	2:D:457:LYS:HE2	2.37	0.55
1:B:45:SER:CB	1:B:182:THR:HB	2.37	0.54
1:B:283:ILE:C	1:B:284:ILE:HD13	2.27	0.54
1:B:52:LYS:HE3	4:B:522:ATP:O1B	2.07	0.54
1:F:123:LEU:O	1:F:123:LEU:HD13	2.07	0.54
2:C:451:ARG:HH11	2:C:451:ARG:HG2	1.72	0.54
2:D:249:LEU:HD13	2:D:394:GLN:HG2	1.89	0.54
2:D:31:ILE:HD13	2:D:231:MET:SD	2.48	0.54
2:D:80:PRO:O	2:D:84:ILE:HG12	2.07	0.54
1:F:191:ILE:HG23	1:F:206:ILE:CD1	2.37	0.54
1:F:317:TYR:OH	1:F:363:ILE:HD11	2.07	0.54
1:A:294:LYS:N	4:A:521:ATP:O1B	2.41	0.54
1:B:150:VAL:O	1:B:153:GLN:HG3	2.06	0.54
2:C:122:ASP:O	2:C:123:LEU:C	2.45	0.54
2:C:287:THR:HG23	2:C:414:ASN:ND2	2.11	0.54
2:D:356:LEU:HD13	2:D:387:VAL:HG21	1.89	0.54
1:E:290:THR:HG21	1:F:457:LYS:CE	2.36	0.54
1:A:440:LEU:HD23	1:A:453:ILE:HG13	1.89	0.54
1:B:433:ILE:O	1:B:433:ILE:HG22	2.07	0.54
2:C:448:GLU:HG2	2:D:466:ALA:HA	1.89	0.54
2:D:52:LYS:HE3	4:D:522:ATP:O1B	2.08	0.54
1:E:367:ILE:HD12	1:E:375:ILE:CD1	2.38	0.54
1:E:446:ARG:NE	1:E:496:ARG:NH2	2.51	0.54
1:F:121:PHE:O	1:F:125:ALA:N	2.37	0.54
2:C:370:PHE:O	2:C:371:LYS:HD3	2.08	0.54
2:D:311:ARG:HD2	2:D:371:LYS:HD3	1.87	0.54
2:D:470:PHE:CB	2:D:479:ILE:HD13	2.37	0.54
1:F:90:PHE:O	1:F:92:TRP:CD1	2.60	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:THR:HB	4:A:521:ATP:PA	2.48	0.54
1:A:266:GLY:HA3	1:A:300:ARG:O	2.08	0.54
1:A:92:TRP:CB	1:A:92:TRP:N	2.66	0.54
2:D:299:SER:CB	2:D:333:MET:HE1	2.38	0.54
2:D:367:ILE:HD12	2:D:372:PRO:HG2	1.89	0.54
2:D:367:ILE:O	2:D:372:PRO:HD3	2.08	0.54
1:A:203:ASN:HB3	1:A:225:LEU:HD23	1.89	0.54
1:B:363:ILE:O	1:B:367:ILE:HG13	2.08	0.54
2:D:453:ILE:HD13	2:D:454:ASN:H	1.71	0.54
1:E:489:ILE:HD13	1:E:494:PRO:CG	2.37	0.54
1:A:437:ILE:N	1:A:437:ILE:CD1	2.70	0.54
1:E:431:SEP:O	1:E:434:THR:HG22	2.06	0.54
1:E:440:LEU:CD2	1:E:453:ILE:HG13	2.37	0.54
1:F:151:PHE:C	1:F:153:GLN:H	2.11	0.54
1:A:21:MET:HE1	1:A:59:PHE:HZ	1.72	0.54
1:B:437:ILE:CD1	1:B:437:ILE:N	2.69	0.54
2:C:150:VAL:CG1	2:C:151:PHE:N	2.70	0.54
1:E:153:GLN:O	1:F:158:SER:HB2	2.07	0.54
1:E:294:LYS:N	4:E:601:ATP:O1B	2.41	0.54
1:A:248:PRO:HB2	1:A:251:ALA:HB3	1.88	0.54
2:C:111:ASP:C	2:C:113:GLU:H	2.12	0.54
1:E:375:ILE:CD1	1:E:408:ILE:HG21	2.39	0.54
1:F:185:ILE:N	1:F:185:ILE:HD12	2.23	0.54
1:A:400:THR:HG22	1:A:401:GLY:N	2.22	0.53
1:A:438:ILE:CD1	1:A:455:VAL:HG22	2.38	0.53
1:A:290:THR:HG21	1:B:431:SEP:HB3	1.89	0.53
2:C:65:ILE:N	2:C:65:ILE:CD1	2.70	0.53
2:D:148:THR:HG21	2:D:193:ARG:HD2	1.90	0.53
1:A:169:ALA:O	1:A:173:GLN:HG3	2.08	0.53
1:A:440:LEU:CD2	1:A:453:ILE:HG13	2.38	0.53
2:C:89:SER:HB2	2:D:227:GLY:O	2.08	0.53
2:D:377:ILE:HD12	2:D:412:PHE:HE2	1.71	0.53
1:E:356:LEU:HD13	1:E:387:VAL:HG21	1.89	0.53
1:F:93:ASP:OD2	1:F:96:LYS:HB2	2.08	0.53
1:A:461:SER:OG	1:A:462:TRP:N	2.41	0.53
1:B:150:VAL:HG13	1:B:151:PHE:H	1.74	0.53
2:D:332:GLY:O	2:D:333:MET:O	2.26	0.53
2:D:79:THR:CG2	2:D:82:ASP:H	2.15	0.53
1:E:418:GLN:HB2	1:F:423:HIS:O	2.08	0.53
1:F:24:MET:HG3	1:F:66:GLU:HG3	1.89	0.53
1:A:273:MET:O	1:A:464:ASP:N	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:ILE:CD1	1:B:457:LYS:CE	2.84	0.53
2:C:248:PRO:HB2	2:C:251:ALA:HB3	1.89	0.53
1:E:18:ILE:HG13	1:E:228:THR:HG23	1.90	0.53
1:E:295:THR:HG21	1:E:319:GLU:OE2	2.08	0.53
1:F:347:VAL:O	1:F:348:CYS:HB2	2.08	0.53
2:C:169:ALA:O	2:C:173:GLN:HG3	2.08	0.53
2:C:419:PHE:O	2:C:420:MET:HB2	2.09	0.53
1:E:347:VAL:O	1:E:348:CYS:HB2	2.08	0.53
1:F:420:MET:HA	5:F:715:HOH:O	2.07	0.53
1:F:426:THR:OG1	1:F:431:SEP:O1P	2.25	0.53
1:A:21:MET:HE2	1:A:177:THR:HG21	1.90	0.53
1:B:159:VAL:O	1:B:163:GLU:HG2	2.08	0.53
2:D:299:SER:C	2:D:333:MET:HE1	2.29	0.53
1:E:266:GLY:HA2	1:E:304:ASN:HD22	1.73	0.53
1:E:448:GLU:HG2	1:F:466:ALA:HA	1.91	0.53
1:F:182:THR:HG22	1:F:183:GLU:N	2.21	0.53
1:F:208:ARG:NH2	1:F:221:GLU:OE2	2.41	0.53
1:F:317:TYR:CD2	1:F:383:LEU:HD21	2.44	0.53
1:F:149:SER:HA	1:F:152:GLN:HB2	1.90	0.53
1:B:426:THR:CB	1:B:431:SEP:O3P	2.57	0.53
2:C:85:LYS:HZ3	2:D:14:GLU:HB3	1.73	0.53
1:E:76:PHE:CZ	1:E:126:LEU:HD21	2.44	0.53
1:A:74:VAL:HG22	1:A:106:LEU:HD23	1.91	0.53
1:A:91:GLY:C	1:A:92:TRP:HE3	2.12	0.53
2:D:396:VAL:O	2:D:400:THR:HB	2.09	0.53
1:E:244:ILE:HG22	1:E:246:ILE:HD11	1.91	0.53
1:F:122:ASP:HA	1:F:125:ALA:HB3	1.91	0.53
1:F:218:ARG:HB3	5:F:719:HOH:O	2.08	0.53
2:C:206:ILE:N	2:C:206:ILE:HD12	2.24	0.53
2:C:334:ASP:OD1	2:C:336:GLU:HB2	2.09	0.53
2:C:470:PHE:HB2	2:C:478:ASP:O	2.08	0.53
2:D:294:LYS:N	4:D:521:ATP:O1B	2.42	0.53
1:E:146:SER:H	1:E:181:THR:HG22	1.74	0.53
1:B:362:ILE:HG22	1:B:366:GLU:OE2	2.09	0.52
2:D:269:ARG:HG2	2:D:479:ILE:HB	1.89	0.52
1:F:377:ILE:CD1	1:F:399:VAL:HG11	2.38	0.52
1:A:254:LEU:HD23	1:F:348:CYS:HB3	1.91	0.52
2:D:295:THR:HG22	4:D:521:ATP:O2A	2.10	0.52
2:D:453:ILE:CG2	2:D:479:ILE:HD12	2.30	0.52
1:F:406:GLU:HB3	1:F:408:ILE:HG12	1.91	0.52
1:F:431:SEP:HA	1:F:434:THR:HG22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:GLU:CG	1:A:15:HIS:H	2.21	0.52
1:B:429:HIS:HA	1:B:431:SEP:O2P	2.08	0.52
1:E:202:ASP:HA	1:E:226:ARG:HD2	1.90	0.52
1:F:164:LEU:HD11	1:F:197:GLU:HG3	1.90	0.52
1:F:317:TYR:CE2	1:F:383:LEU:HD21	2.43	0.52
1:E:290:THR:CG2	1:F:457:LYS:CE	2.86	0.52
1:A:191:ILE:HG23	1:A:206:ILE:HD11	1.91	0.52
1:B:311:ARG:HA	1:B:343:LEU:O	2.10	0.52
1:A:126:LEU:HG	1:A:130:ILE:HD11	1.91	0.52
1:B:318:GLU:OE2	2:C:432:TPO:O3P	2.27	0.52
2:D:446:ARG:H	2:D:496:ARG:NH1	2.03	0.52
1:A:18:ILE:HD12	1:A:18:ILE:N	2.24	0.52
1:B:64:ILE:HD11	1:B:102:LYS:O	2.09	0.52
2:C:430:ILE:O	2:C:432:TPO:N	2.42	0.52
1:E:372:PRO:HB2	1:E:375:ILE:CD1	2.40	0.52
1:E:80:PRO:HD2	1:E:81:GLN:NE2	2.24	0.52
1:F:440:LEU:HD23	1:F:453:ILE:HG13	1.90	0.52
1:A:438:ILE:HD13	1:A:455:VAL:HA	1.92	0.52
1:B:206:ILE:N	1:B:206:ILE:HD12	2.25	0.52
1:B:356:LEU:HD22	1:B:387:VAL:HG11	1.90	0.52
2:C:311:ARG:HA	2:C:343:LEU:O	2.10	0.52
1:E:70:PRO:HB2	1:E:139:ALA:HA	1.92	0.52
1:F:264:SER:O	1:F:374:ARG:NH2	2.42	0.52
2:C:479:ILE:HD12	2:C:479:ILE:N	2.25	0.52
2:D:347:VAL:O	2:D:348:CYS:HB2	2.10	0.52
2:D:89:SER:HB2	1:E:227:GLY:O	2.09	0.52
1:F:315:PHE:CZ	1:F:363:ILE:HG23	2.44	0.52
1:E:444:GLU:OE1	1:F:490:ILE:HG12	2.09	0.52
1:B:248:PRO:HB2	1:B:251:ALA:HB3	1.92	0.52
2:D:495:THR:O	2:D:497:ILE:HG23	2.10	0.52
1:A:371:LYS:N	1:A:372:PRO:HD3	2.25	0.52
1:B:325:LEU:HD23	1:B:335:PHE:HB2	1.92	0.52
1:B:385:ARG:NE	2:C:432:TPO:O2P	2.42	0.52
2:C:117:VAL:HG12	2:C:117:VAL:O	2.10	0.52
2:D:287:THR:HG23	2:D:414:ASN:ND2	2.17	0.52
2:D:438:ILE:HG23	2:D:453:ILE:HD11	1.91	0.52
2:D:84:ILE:HD12	2:D:94:LEU:HB2	1.90	0.52
1:E:284:ILE:N	1:E:284:ILE:HD13	2.25	0.52
1:F:126:LEU:HG	1:F:130:ILE:HD11	1.92	0.52
1:F:184:ARG:HG2	1:F:191:ILE:O	2.10	0.52
1:A:385:ARG:NE	1:B:432:TPO:O2P	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:472:ILE:HD12	2:D:472:ILE:N	2.24	0.51
2:D:489:ILE:HA	2:D:494:PRO:HG3	1.92	0.51
1:E:348:CYS:HB3	1:F:254:LEU:HD23	1.93	0.51
1:F:115:GLN:HG3	1:F:116:GLU:N	2.25	0.51
2:D:18:ILE:CD1	2:D:18:ILE:H	2.16	0.51
2:D:440:LEU:HD21	2:D:453:ILE:HG12	1.92	0.51
1:E:151:PHE:C	1:E:153:GLN:H	2.14	0.51
1:E:316:ALA:O	1:E:348:CYS:HA	2.10	0.51
1:E:356:LEU:CD1	1:E:387:VAL:HG21	2.40	0.51
1:E:323:GLN:HE21	1:F:459:ARG:HD3	1.74	0.51
1:F:56:SER:HB2	1:F:143:SER:HB2	1.91	0.51
2:C:81:GLN:CD	2:C:81:GLN:H	2.13	0.51
2:C:81:GLN:H	2:C:81:GLN:NE2	2.07	0.51
2:D:267:VAL:CG2	2:D:300:ARG:HG2	2.41	0.51
1:E:123:LEU:C	1:E:127:ILE:HG12	2.31	0.51
1:E:447:GLY:C	1:F:467:ILE:HD13	2.30	0.51
1:F:14:GLU:HG3	1:F:16:GLN:HG3	1.93	0.51
1:F:455:VAL:HG11	1:F:463:HIS:HB2	1.92	0.51
1:A:488:ARG:HE	1:F:488:ARG:HH12	1.56	0.51
2:C:371:LYS:HD3	2:C:371:LYS:O	2.11	0.51
2:C:49:GLY:HA2	4:C:522:ATP:O2B	2.10	0.51
2:D:106:LEU:HD11	2:D:129:ARG:NH2	2.26	0.51
1:E:126:LEU:O	1:E:129:ARG:HB2	2.11	0.51
1:E:496:ARG:HG3	1:E:497:ILE:H	1.75	0.51
1:F:489:ILE:HD13	1:F:494:PRO:CG	2.41	0.51
2:C:111:ASP:O	2:C:113:GLU:N	2.41	0.51
2:D:150:VAL:CG1	2:D:151:PHE:N	2.73	0.51
2:D:170:ARG:HD2	2:D:173:GLN:OE1	2.10	0.51
1:F:291:GLY:N	4:F:701:ATP:O2B	2.44	0.51
1:A:182:THR:HG22	1:A:183:GLU:N	2.26	0.51
2:C:420:MET:HE3	2:D:490:ILE:HD13	1.91	0.51
2:D:21:MET:HE3	2:D:59:PHE:CZ	2.46	0.51
1:E:264:SER:O	1:E:374:ARG:NH2	2.44	0.51
1:F:118:VAL:CG1	1:F:153:GLN:HE22	2.23	0.51
1:F:287:THR:HG21	1:F:425:ILE:O	2.10	0.51
1:A:432:TPO:O2P	1:F:385:ARG:NE	2.44	0.51
1:B:294:LYS:N	4:B:521:ATP:O1B	2.43	0.51
2:C:344:LEU:HD11	2:C:346:ILE:CD1	2.40	0.51
2:D:489:ILE:HD13	2:D:494:PRO:CG	2.41	0.51
1:F:90:PHE:O	1:F:92:TRP:NE1	2.44	0.51
1:B:444:GLU:HB2	2:C:490:ILE:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:362:ILE:HG22	2:D:366:GLU:OE2	2.10	0.51
2:D:84:ILE:HD13	2:D:94:LEU:HB2	1.91	0.51
1:F:148:THR:CG2	1:F:193:ARG:HD2	2.41	0.51
1:F:79:THR:CG2	1:F:82:ASP:H	2.22	0.51
1:A:90:PHE:O	1:A:92:TRP:CE3	2.64	0.51
1:E:300:ARG:HA	1:E:333:MET:HE3	1.93	0.51
1:E:347:VAL:HG12	1:E:348:CYS:N	2.24	0.51
1:E:472:ILE:HD12	1:E:472:ILE:N	2.26	0.51
1:A:266:GLY:HA3	1:A:300:ARG:HG3	1.93	0.50
1:A:484:ARG:HB3	1:A:484:ARG:NH1	2.25	0.50
1:B:150:VAL:CG1	1:B:151:PHE:N	2.73	0.50
2:C:43:LEU:HD11	2:C:182:THR:OG1	2.11	0.50
1:E:130:ILE:O	1:E:134:ILE:HD13	2.10	0.50
1:E:283:ILE:C	1:E:284:ILE:HD13	2.31	0.50
1:B:31:ILE:HA	1:B:231:MET:SD	2.51	0.50
2:C:182:THR:CG2	2:C:183:GLU:N	2.74	0.50
2:D:311:ARG:HD3	2:D:370:PHE:CE1	2.46	0.50
1:F:218:ARG:CZ	1:F:239:ILE:HD12	2.42	0.50
1:A:449:MET:HG2	1:B:467:ILE:HD11	1.93	0.50
1:B:299:SER:C	1:B:333:MET:HE1	2.32	0.50
1:B:264:SER:HB3	1:B:304:ASN:HD21	1.76	0.50
1:B:467:ILE:N	1:B:467:ILE:HD12	2.26	0.50
2:C:114:GLY:O	2:C:115:GLN:HB3	2.11	0.50
2:D:127:ILE:HD13	2:D:170:ARG:HG3	1.93	0.50
1:E:296:LEU:HD13	1:E:331:TRP:CD2	2.47	0.50
1:E:315:PHE:CZ	1:E:363:ILE:HG23	2.46	0.50
1:E:438:ILE:CD1	1:E:455:VAL:HG22	2.42	0.50
1:F:479:ILE:N	1:F:479:ILE:HD12	2.26	0.50
1:A:150:VAL:CG1	1:A:151:PHE:H	2.24	0.50
1:A:21:MET:HE3	1:A:59:PHE:CE1	2.47	0.50
1:B:90:PHE:O	1:B:92:TRP:CZ3	2.64	0.50
2:D:169:ALA:O	2:D:173:GLN:HG3	2.10	0.50
2:D:311:ARG:HD3	2:D:370:PHE:CZ	2.46	0.50
1:B:130:ILE:O	1:B:134:ILE:HG13	2.12	0.50
2:C:191:ILE:H	2:C:191:ILE:HD12	1.75	0.50
1:E:218:ARG:CZ	1:E:239:ILE:HD12	2.42	0.50
1:E:360:LEU:CD2	1:E:364:LYS:HE3	2.42	0.50
1:F:144:ILE:HG21	1:F:147:VAL:HG12	1.94	0.50
1:F:50:THR:HG22	1:F:209:ASN:HB2	1.92	0.50
1:A:67:PHE:HB2	1:A:69:GLU:HG3	1.93	0.50
1:B:123:LEU:HG	1:B:163:GLU:OE2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ARG:HG2	1:B:191:ILE:O	2.11	0.50
1:B:211:LEU:O	1:B:212:GLU:HB3	2.10	0.50
1:B:371:LYS:N	1:B:372:PRO:HD3	2.27	0.50
2:C:332:GLY:O	2:C:333:MET:O	2.30	0.50
2:D:338:MET:HB3	2:D:344:LEU:HB3	1.93	0.50
2:D:375:ILE:HD13	2:D:408:ILE:HG21	1.93	0.50
2:D:433:ILE:HD12	2:D:433:ILE:N	2.27	0.50
1:E:318:GLU:HG2	1:F:432:TPO:O2P	2.12	0.50
1:B:185:ILE:HD11	1:B:193:ARG:NH1	2.26	0.50
1:A:348:CYS:HB3	1:B:254:LEU:HD23	1.93	0.50
1:B:99:ASP:C	1:B:101:GLY:H	2.15	0.50
2:C:396:VAL:O	2:C:400:THR:HB	2.12	0.50
2:C:49:GLY:O	2:C:218:ARG:NH2	2.44	0.50
1:E:332:GLY:O	1:E:333:MET:O	2.30	0.50
1:B:123:LEU:CD1	1:B:166:ARG:HD2	2.40	0.50
1:B:420:MET:SD	2:C:490:ILE:HD13	2.52	0.50
2:C:438:ILE:HD13	2:C:455:VAL:HA	1.94	0.50
2:D:150:VAL:HG13	2:D:151:PHE:H	1.76	0.50
2:D:49:GLY:O	2:D:218:ARG:NH2	2.44	0.50
1:F:218:ARG:NH1	1:F:239:ILE:HD12	2.27	0.50
2:C:348:CYS:O	2:C:349:ALA:HB2	2.12	0.50
2:D:420:MET:HE3	2:D:492:GLY:HA3	1.94	0.50
2:D:439:LEU:HD12	2:D:440:LEU:N	2.27	0.50
2:D:451:ARG:HG2	2:D:451:ARG:NH1	2.25	0.50
2:D:64:ILE:HD12	2:D:64:ILE:N	2.27	0.50
1:E:486:PHE:HB2	1:E:489:ILE:HD11	1.94	0.50
1:E:52:LYS:HE3	4:E:603:ATP:O1B	2.11	0.50
2:D:344:LEU:HD13	2:D:344:LEU:C	2.32	0.49
1:F:432:TPO:HG21	1:F:432:TPO:O3P	2.12	0.49
1:F:439:LEU:HD12	1:F:440:LEU:N	2.27	0.49
1:B:492:GLY:O	1:B:494:PRO:HD3	2.12	0.49
2:D:203:ASN:HB3	2:D:225:LEU:HD23	1.94	0.49
2:C:420:MET:SD	2:D:490:ILE:HD13	2.52	0.49
2:D:85:LYS:HZ3	1:E:14:GLU:HB3	1.75	0.49
1:E:89:SER:HB2	1:F:227:GLY:O	2.12	0.49
1:A:356:LEU:CD1	1:A:387:VAL:HG21	2.41	0.49
1:A:92:TRP:CB	1:A:92:TRP:HA	2.17	0.49
2:C:120:GLY:C	2:C:122:ASP:H	2.16	0.49
2:C:332:GLY:O	2:C:333:MET:C	2.50	0.49
1:E:52:LYS:HD3	1:E:182:THR:O	2.12	0.49
1:E:375:ILE:HD12	1:E:408:ILE:HG21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:25:ILE:HD12	1:F:58:GLN:HG2	1.94	0.49
1:A:451:ARG:HD2	1:A:451:ARG:N	2.27	0.49
1:A:64:ILE:HD11	1:A:102:LYS:O	2.12	0.49
1:A:142:VAL:O	1:A:178:THR:HA	2.13	0.49
1:B:151:PHE:C	1:B:153:GLN:H	2.14	0.49
2:C:150:VAL:CG1	2:C:151:PHE:H	2.24	0.49
2:C:323:GLN:NE2	2:D:459:ARG:HD3	2.27	0.49
1:E:150:VAL:HG13	1:E:151:PHE:H	1.78	0.49
1:F:134:ILE:HD12	1:F:139:ALA:HB3	1.93	0.49
1:F:72:VAL:HG21	1:F:134:ILE:HD13	1.94	0.49
1:F:28:PHE:HE1	1:F:222:ILE:HD11	1.78	0.49
1:F:360:LEU:CD2	1:F:364:LYS:HE3	2.43	0.49
1:F:471:MET:HG3	1:F:478:ASP:HB3	1.94	0.49
1:F:496:ARG:HD3	1:F:496:ARG:N	2.27	0.49
1:A:21:MET:HB2	1:A:38:ILE:HD11	1.95	0.49
1:B:334:ASP:OD1	1:B:336:GLU:HB2	2.12	0.49
1:B:441:GLN:HE22	1:B:490:ILE:HA	1.78	0.49
2:C:106:LEU:HD11	2:C:129:ARG:NH2	2.27	0.49
2:C:134:ILE:HG23	2:C:139:ALA:HB3	1.94	0.49
2:C:352:GLU:OE2	2:C:385:ARG:HD2	2.13	0.49
1:E:496:ARG:HG3	1:E:497:ILE:N	2.28	0.49
1:F:16:GLN:NE2	1:F:33:HIS:HB3	2.27	0.49
1:F:483:PHE:HB3	1:F:486:PHE:CD1	2.47	0.49
1:B:264:SER:HA	1:B:271:ASP:OD1	2.12	0.49
1:B:146:SER:H	1:B:181:THR:CG2	2.26	0.49
1:B:334:ASP:O	1:B:338:MET:HG2	2.13	0.49
2:C:203:ASN:HB3	2:C:225:LEU:CD2	2.43	0.49
2:D:191:ILE:HB	2:D:198:GLU:HG2	1.90	0.49
1:E:28:PHE:CE1	1:E:222:ILE:HD11	2.47	0.49
1:F:23:THR:HB	1:F:25:ILE:HG12	1.94	0.49
1:B:79:THR:HG22	1:B:82:ASP:H	1.77	0.49
1:B:92:TRP:CE3	1:B:92:TRP:CA	2.96	0.49
2:C:28:PHE:CE1	2:C:222:ILE:HD11	2.48	0.49
2:C:440:LEU:HD23	2:C:453:ILE:HG12	1.93	0.49
1:F:283:ILE:HG23	1:F:412:PHE:HE1	1.76	0.49
2:C:356:LEU:HD22	2:C:387:VAL:HG11	1.94	0.49
1:E:255:THR:HG22	1:E:255:THR:O	2.12	0.49
1:E:436:THR:HG23	1:E:458:MET:HG2	1.93	0.49
1:A:144:ILE:N	1:A:144:ILE:HD13	2.28	0.48
1:A:269:ARG:HB3	1:A:479:ILE:HD12	1.94	0.48
1:A:338:MET:HB3	1:A:344:LEU:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:THR:HG22	1:B:183:GLU:N	2.28	0.48
2:C:300:ARG:N	2:C:333:MET:HE1	2.28	0.48
2:D:370:PHE:O	2:D:371:LYS:CD	2.61	0.48
2:D:367:ILE:CD1	2:D:372:PRO:HG2	2.43	0.48
1:E:360:LEU:HD21	1:E:364:LYS:HE3	1.94	0.48
1:F:182:THR:HG21	1:F:192:ALA:CB	2.40	0.48
1:F:211:LEU:O	1:F:212:GLU:HB3	2.12	0.48
1:A:344:LEU:HD22	1:A:345:LYS:H	1.77	0.48
1:B:296:LEU:HD21	1:B:477:PRO:HD3	1.95	0.48
2:D:182:THR:HG21	2:D:192:ALA:CB	2.40	0.48
2:D:94:LEU:O	2:D:98:VAL:HG23	2.12	0.48
1:E:344:LEU:HD22	1:E:345:LYS:H	1.78	0.48
1:F:115:GLN:CG	1:F:116:GLU:H	2.27	0.48
1:A:283:ILE:HD12	1:A:412:PHE:HE1	1.78	0.48
1:B:145:ASP:HA	1:B:181:THR:HB	1.95	0.48
1:B:262:ARG:NH2	1:B:461:SER:HB2	2.28	0.48
2:C:191:ILE:HD12	2:C:191:ILE:N	2.28	0.48
2:C:296:LEU:HD13	2:C:331:TRP:CD2	2.49	0.48
2:D:367:ILE:HD12	2:D:375:ILE:CD1	2.40	0.48
2:D:468:ARG:HH11	2:D:468:ARG:HG2	1.78	0.48
1:E:134:ILE:N	1:E:134:ILE:HD13	2.29	0.48
2:D:151:PHE:C	2:D:153:GLN:N	2.67	0.48
2:D:263:VAL:CG1	2:D:374:ARG:HH21	2.21	0.48
2:D:430:ILE:HA	2:D:433:ILE:HD13	1.96	0.48
1:E:150:VAL:CG1	1:E:151:PHE:N	2.75	0.48
1:E:306:CYS:SG	1:E:344:LEU:HB2	2.53	0.48
1:F:64:ILE:HD11	1:F:102:LYS:O	2.14	0.48
1:F:182:THR:CG2	1:F:183:GLU:N	2.75	0.48
1:F:25:ILE:HD13	1:F:62:ASN:ND2	2.29	0.48
1:A:31:ILE:HD11	1:A:246:ILE:HG21	1.94	0.48
1:B:433:ILE:HD12	1:B:433:ILE:N	2.28	0.48
2:C:31:ILE:HD11	2:C:248:PRO:HB3	1.96	0.48
2:D:445:ILE:HD12	2:D:450:SER:OG	2.13	0.48
1:E:291:GLY:N	4:E:601:ATP:O2B	2.46	0.48
1:A:419:PHE:O	1:A:420:MET:HB2	2.13	0.48
1:B:430:ILE:HA	1:B:433:ILE:HD13	1.95	0.48
1:B:87:ALA:HB1	1:B:92:TRP:HB2	1.95	0.48
1:B:91:GLY:C	1:B:92:TRP:HE3	2.17	0.48
2:C:294:LYS:N	4:C:521:ATP:O1B	2.46	0.48
2:C:49:GLY:CA	4:C:522:ATP:O2B	2.62	0.48
2:D:255:THR:HG22	2:D:255:THR:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:356:LEU:CD2	2:D:387:VAL:HG11	2.44	0.48
2:D:468:ARG:NH1	2:D:468:ARG:HG2	2.29	0.48
1:F:371:LYS:N	1:F:372:PRO:HD3	2.29	0.48
1:F:453:ILE:HB	1:F:470:PHE:CD2	2.49	0.48
1:A:14:GLU:HG3	1:A:15:HIS:N	2.29	0.48
1:A:161:ARG:CB	1:A:196:VAL:HG11	2.39	0.48
1:A:487:GLU:OE1	1:F:495:THR:HA	2.14	0.48
1:A:21:MET:CE	1:A:59:PHE:HZ	2.27	0.48
2:C:283:ILE:C	2:C:284:ILE:HD13	2.33	0.48
2:C:469:GLU:CG	2:C:480:LYS:HE3	2.44	0.48
2:D:130:ILE:N	2:D:130:ILE:HD12	2.29	0.48
2:D:267:VAL:HG22	2:D:300:ARG:HG2	1.96	0.48
2:D:289:ALA:HB2	2:D:419:PHE:HA	1.96	0.48
1:F:274:CYS:HG	1:F:278:PHE:HE2	1.60	0.48
1:F:437:ILE:HD11	1:F:457:LYS:HE2	1.95	0.48
1:A:347:VAL:O	1:A:348:CYS:HB2	2.14	0.48
1:A:434:THR:HG23	1:A:437:ILE:CD1	2.37	0.48
1:B:208:ARG:NH2	1:B:221:GLU:OE2	2.47	0.48
1:B:93:ASP:OD2	1:B:96:LYS:HB2	2.14	0.48
2:C:334:ASP:O	2:C:338:MET:HG2	2.14	0.48
2:C:469:GLU:HB3	2:C:483:PHE:CZ	2.48	0.48
2:D:221:GLU:HG3	2:D:233:GLY:O	2.13	0.48
1:E:72:VAL:HG21	1:E:134:ILE:CD1	2.41	0.48
1:E:182:THR:HG22	1:E:183:GLU:N	2.28	0.48
1:E:99:ASP:C	1:E:101:GLY:H	2.17	0.48
1:F:299:SER:CB	1:F:333:MET:HE1	2.43	0.48
1:A:406:GLU:HB3	1:A:408:ILE:HG12	1.96	0.48
1:A:90:PHE:O	1:A:92:TRP:CZ3	2.66	0.48
1:B:148:THR:HG21	1:B:193:ARG:HD2	1.96	0.48
2:D:332:GLY:O	2:D:333:MET:C	2.51	0.48
2:D:283:ILE:HD13	2:D:400:THR:HG23	1.96	0.48
1:E:123:LEU:HD23	1:E:127:ILE:HD11	1.96	0.48
1:F:291:GLY:HA3	1:F:442:TYR:OH	2.14	0.48
1:A:145:ASP:OD2	1:A:181:THR:HG21	2.14	0.48
2:C:325:LEU:HD23	2:C:335:PHE:CB	2.43	0.48
2:C:290:THR:HG21	2:D:431:SER:HB2	1.95	0.48
1:F:116:GLU:O	1:F:117:VAL:HB	2.14	0.48
1:F:451:ARG:NH1	1:F:472:ILE:HD12	2.28	0.48
1:F:90:PHE:CB	1:F:92:TRP:CE2	2.96	0.48
2:C:205:VAL:CG2	2:C:222:ILE:HD13	2.26	0.47
2:C:371:LYS:N	2:C:372:PRO:HD3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:393:ARG:O	2:C:397:ILE:HG12	2.14	0.47
2:C:295:THR:HG22	4:C:521:ATP:O2A	2.14	0.47
1:E:321:ARG:HG2	1:E:348:CYS:SG	2.54	0.47
1:F:106:LEU:CD1	1:F:129:ARG:CZ	2.85	0.47
1:F:294:LYS:N	4:F:701:ATP:O1B	2.47	0.47
1:A:488:ARG:NH1	1:B:488:ARG:HH21	2.11	0.47
2:C:17:ALA:C	2:C:18:ILE:HD12	2.34	0.47
2:C:471:MET:HG3	2:C:478:ASP:HB3	1.96	0.47
2:D:318:GLU:OE2	1:E:432:TPO:O3P	2.32	0.47
1:B:150:VAL:CG1	1:B:151:PHE:H	2.28	0.47
1:B:197:GLU:CD	1:B:197:GLU:H	2.18	0.47
1:A:89:SER:CB	1:B:227:GLY:O	2.61	0.47
1:B:396:VAL:O	1:B:400:THR:HB	2.14	0.47
2:C:144:ILE:CG2	2:C:147:VAL:HG12	2.44	0.47
2:D:148:THR:OG1	2:D:182:THR:HG23	2.14	0.47
2:D:433:ILE:HG22	2:D:433:ILE:O	2.14	0.47
2:D:451:ARG:NH1	2:D:472:ILE:HD13	2.29	0.47
1:F:21:MET:HE3	1:F:59:PHE:CE1	2.49	0.47
1:F:311:ARG:HA	1:F:343:LEU:O	2.14	0.47
1:F:61:TYR:CE2	1:F:65:ILE:HG13	2.49	0.47
1:B:262:ARG:HH22	1:B:461:SER:HB2	1.79	0.47
2:C:363:ILE:O	2:C:367:ILE:HG13	2.13	0.47
2:C:91:GLY:O	2:C:92:TRP:HE3	1.96	0.47
1:E:148:THR:HG21	1:E:183:GLU:CG	2.45	0.47
1:E:146:SER:H	1:E:181:THR:CG2	2.28	0.47
1:E:311:ARG:HA	1:E:343:LEU:O	2.15	0.47
1:F:178:THR:HG22	1:F:179:VAL:N	2.29	0.47
1:F:191:ILE:HB	1:F:198:GLU:HG3	1.94	0.47
1:A:402:TYR:O	1:A:406:GLU:HB2	2.13	0.47
1:A:459:ARG:HD3	1:F:323:GLN:HE21	1.79	0.47
2:C:185:ILE:HA	5:D:531:HOH:O	2.13	0.47
2:C:357:GLU:HG3	2:C:358:ASP:N	2.29	0.47
1:E:14:GLU:HG3	1:E:16:GLN:N	2.24	0.47
1:E:14:GLU:HG3	1:E:16:GLN:HB2	1.95	0.47
1:F:170:ARG:HD2	1:F:173:GLN:OE1	2.14	0.47
1:F:334:ASP:OD1	1:F:336:GLU:HB2	2.15	0.47
1:F:437:ILE:CD1	1:F:437:ILE:N	2.78	0.47
1:B:344:LEU:HD22	1:B:345:LYS:H	1.79	0.47
2:C:18:ILE:HB	2:C:228:THR:HG23	1.96	0.47
2:C:468:ARG:HG2	2:C:468:ARG:HH11	1.79	0.47
1:E:287:THR:HG21	1:E:425:ILE:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:431:SEP:HA	1:E:434:THR:HG22	1.97	0.47
1:E:448:GLU:HA	1:F:467:ILE:CD1	2.45	0.47
1:E:73:PHE:CE2	1:E:83:ILE:HD13	2.49	0.47
1:F:18:ILE:HG12	1:F:228:THR:HG23	1.95	0.47
1:B:203:ASN:HB3	1:B:225:LEU:HD23	1.97	0.47
1:B:426:THR:HG22	1:B:428:SER:N	2.30	0.47
2:C:295:THR:HG22	4:C:521:ATP:PA	2.55	0.47
1:E:439:LEU:HD12	1:E:440:LEU:N	2.29	0.47
1:E:440:LEU:HD23	1:E:453:ILE:HG13	1.97	0.47
1:F:127:ILE:CD1	1:F:167:LEU:HD12	2.43	0.47
1:F:295:THR:HB	4:F:701:ATP:PA	2.54	0.47
1:F:344:LEU:HD11	1:F:346:ILE:HG13	1.96	0.47
1:F:445:ILE:CD1	1:F:483:PHE:CE2	2.97	0.47
1:A:16:GLN:O	1:A:17:ALA:O	2.32	0.47
1:A:211:LEU:HD12	1:A:215:ARG:O	2.15	0.47
1:A:64:ILE:HD13	1:A:69:GLU:O	2.15	0.47
2:C:122:ASP:O	2:C:124:SER:N	2.47	0.47
2:C:45:SER:CB	2:C:182:THR:HB	2.44	0.47
2:D:142:VAL:O	2:D:178:THR:HA	2.13	0.47
2:D:470:PHE:CE1	2:D:472:ILE:HD11	2.50	0.47
1:F:146:SER:H	1:F:181:THR:CG2	2.27	0.47
1:F:356:LEU:HD21	1:F:387:VAL:HG11	1.97	0.47
1:A:431:SEP:O	1:A:434:THR:HG22	2.15	0.47
1:B:249:LEU:CD1	1:B:394:GLN:HG2	2.44	0.47
2:C:433:ILE:HD12	2:C:433:ILE:N	2.29	0.47
2:D:461:SER:OG	2:D:462:TRP:N	2.47	0.47
2:D:64:ILE:HD12	2:D:69:GLU:O	2.14	0.47
1:F:21:MET:HB2	1:F:38:ILE:HG12	1.97	0.47
1:A:218:ARG:NH1	1:A:239:ILE:HD12	2.29	0.47
1:A:334:ASP:OD1	1:A:336:GLU:HB2	2.14	0.47
1:A:91:GLY:C	1:A:92:TRP:CE3	2.89	0.47
1:B:191:ILE:HB	1:B:198:GLU:HG2	1.96	0.47
1:B:96:LYS:O	1:B:100:GLU:HG3	2.13	0.47
2:C:131:ASN:OD1	2:C:174:ILE:HD12	2.15	0.47
2:C:146:SER:H	2:C:181:THR:HG22	1.79	0.47
2:D:18:ILE:HD13	2:D:227:GLY:O	2.14	0.47
2:D:197:GLU:CD	2:D:197:GLU:H	2.16	0.47
1:F:150:VAL:CG1	1:F:151:PHE:N	2.78	0.47
1:F:45:SER:HB2	1:F:182:THR:HB	1.95	0.47
1:B:451:ARG:HG2	1:B:451:ARG:NH1	2.30	0.47
2:C:267:VAL:HB	2:C:270:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:60:LEU:O	2:D:64:ILE:CD1	2.49	0.47
1:A:484:ARG:HB3	1:A:484:ARG:HH11	1.79	0.46
1:A:92:TRP:HA	1:A:92:TRP:CE3	2.50	0.46
1:B:284:ILE:N	1:B:284:ILE:HD13	2.30	0.46
1:B:377:ILE:HD13	1:B:412:PHE:CD2	2.48	0.46
2:D:191:ILE:HD12	2:D:191:ILE:N	2.31	0.46
2:D:371:LYS:HE2	2:D:371:LYS:O	2.15	0.46
2:D:372:PRO:HB2	2:D:375:ILE:CD1	2.45	0.46
1:E:143:SER:HA	1:E:179:VAL:O	2.16	0.46
1:E:123:LEU:HD21	1:E:167:LEU:HB2	1.96	0.46
2:D:488:ARG:HH12	1:E:488:ARG:HH21	1.61	0.46
1:F:18:ILE:CG1	1:F:228:THR:HG23	2.44	0.46
1:F:76:PHE:HZ	1:F:126:LEU:HD21	1.80	0.46
1:A:249:LEU:CD1	1:A:394:GLN:HG2	2.44	0.46
1:A:92:TRP:HE3	1:A:92:TRP:HA	1.81	0.46
2:C:123:LEU:HD13	2:C:166:ARG:HD2	1.96	0.46
2:C:438:ILE:HG23	2:C:453:ILE:HD11	1.97	0.46
2:D:14:GLU:CG	2:D:15:HIS:H	2.28	0.46
1:E:145:ASP:OD2	1:E:181:THR:HG21	2.15	0.46
2:D:290:THR:HG1	1:E:457:LYS:HD3	1.80	0.46
1:E:435:ASP:HA	1:E:459:ARG:HD2	1.97	0.46
1:E:21:MET:HE3	1:E:59:PHE:CE1	2.51	0.46
2:C:24:MET:CB	2:C:62:ASN:HD22	2.29	0.46
2:C:93:ASP:OD2	2:C:96:LYS:HB2	2.15	0.46
2:D:372:PRO:HB2	2:D:375:ILE:HD11	1.97	0.46
1:E:153:GLN:C	1:F:158:SER:HB2	2.35	0.46
1:F:451:ARG:NH1	1:F:451:ARG:HG2	2.29	0.46
1:A:332:GLY:O	1:A:333:MET:C	2.53	0.46
1:A:376:ALA:HA	1:A:411:LEU:O	2.16	0.46
1:A:21:MET:CE	1:A:59:PHE:CZ	2.97	0.46
1:B:182:THR:HG21	1:B:192:ALA:CB	2.43	0.46
1:B:359:HIS:O	1:B:363:ILE:HG12	2.16	0.46
1:B:393:ARG:O	1:B:397:ILE:HG12	2.15	0.46
2:D:143:SER:HA	2:D:179:VAL:O	2.16	0.46
2:D:178:THR:HG22	2:D:179:VAL:N	2.30	0.46
1:E:127:ILE:CD1	1:E:167:LEU:HD13	2.46	0.46
1:E:161:ARG:CB	1:E:196:VAL:HG11	2.39	0.46
1:A:126:LEU:O	1:A:130:ILE:HG13	2.15	0.46
1:B:142:VAL:O	1:B:178:THR:HA	2.16	0.46
1:B:340:ARG:C	1:B:342:ASN:H	2.18	0.46
1:B:449:MET:CE	2:C:467:ILE:HD11	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:ILE:CD1	1:A:362:ILE:N	2.78	0.46
2:C:393:ARG:HH21	2:C:429:HIS:HB2	1.81	0.46
2:D:203:ASN:HB3	2:D:225:LEU:CD2	2.45	0.46
1:E:451:ARG:NH1	1:E:472:ILE:HD13	2.29	0.46
1:F:106:LEU:CD1	1:F:129:ARG:NH2	2.78	0.46
1:F:356:LEU:HD13	1:F:387:VAL:HG21	1.98	0.46
1:A:231:MET:CE	1:A:251:ALA:HB2	2.46	0.46
1:A:311:ARG:HD2	1:A:371:LYS:HD3	1.96	0.46
1:A:325:LEU:HD23	1:A:335:PHE:CB	2.45	0.46
1:B:130:ILE:HG22	1:B:134:ILE:HD11	1.98	0.46
1:B:332:GLY:O	1:B:333:MET:C	2.54	0.46
2:D:495:THR:HG23	1:E:487:GLU:OE2	2.16	0.46
1:F:127:ILE:HD12	1:F:170:ARG:HB2	1.97	0.46
1:F:321:ARG:HG2	1:F:348:CYS:SG	2.56	0.46
2:C:291:GLY:N	4:C:521:ATP:O2B	2.49	0.46
2:C:335:PHE:O	2:C:339:GLU:HG3	2.15	0.46
1:F:134:ILE:CD1	1:F:139:ALA:HB3	2.45	0.46
1:F:344:LEU:HD22	1:F:345:LYS:H	1.77	0.46
1:B:360:LEU:CD2	1:B:364:LYS:HE3	2.46	0.46
2:C:437:ILE:CD1	2:C:457:LYS:HE2	2.46	0.46
2:C:81:GLN:CD	2:C:81:GLN:N	2.69	0.46
2:D:150:VAL:CG1	2:D:151:PHE:H	2.29	0.46
2:D:182:THR:CG2	2:D:183:GLU:N	2.79	0.46
1:E:72:VAL:CG2	1:E:134:ILE:HD12	2.44	0.46
1:F:115:GLN:HG3	1:F:116:GLU:H	1.81	0.46
1:F:321:ARG:O	1:F:325:LEU:HD12	2.16	0.46
1:A:433:ILE:HD11	1:F:385:ARG:CZ	2.46	0.46
1:B:131:ASN:OD1	1:B:174:ILE:HD12	2.16	0.46
1:B:49:GLY:O	1:B:218:ARG:NH2	2.48	0.46
1:B:264:SER:HB3	1:B:304:ASN:ND2	2.31	0.46
2:C:148:THR:OG1	2:C:182:THR:HG23	2.16	0.46
2:C:36:LEU:HD12	2:C:59:PHE:CE1	2.51	0.46
2:D:273:MET:O	2:D:463:HIS:HA	2.15	0.46
2:D:340:ARG:C	2:D:342:ASN:H	2.19	0.46
2:D:448:GLU:HG2	1:E:466:ALA:HA	1.97	0.46
1:E:344:LEU:C	1:E:344:LEU:HD13	2.36	0.46
1:E:486:PHE:CB	1:E:489:ILE:HD11	2.46	0.46
1:F:289:ALA:HB2	1:F:419:PHE:HA	1.98	0.46
1:A:143:SER:C	1:A:144:ILE:HD13	2.36	0.45
1:A:183:GLU:HB2	1:B:199:PHE:CE1	2.50	0.45
1:A:191:ILE:HB	1:A:198:GLU:HG2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ARG:CB	1:B:196:VAL:HG11	2.42	0.45
1:B:295:THR:HB	4:B:521:ATP:PA	2.56	0.45
2:C:430:ILE:C	2:C:432:TPO:N	2.69	0.45
2:C:88:ARG:HD3	2:D:15:HIS:C	2.37	0.45
2:D:211:LEU:O	2:D:215:ARG:O	2.33	0.45
2:D:301:PHE:CZ	2:D:374:ARG:HD3	2.50	0.45
1:E:325:LEU:HD23	1:E:335:PHE:CB	2.43	0.45
1:F:428:SER:OG	1:F:430:ILE:HG12	2.16	0.45
1:A:150:VAL:O	1:A:153:GLN:HG3	2.16	0.45
1:B:430:ILE:HG22	1:B:430:ILE:O	2.16	0.45
2:D:70:PRO:HB2	2:D:139:ALA:HA	1.97	0.45
1:E:126:LEU:O	1:E:130:ILE:HG13	2.16	0.45
1:E:21:MET:CE	1:E:59:PHE:CZ	2.99	0.45
1:F:145:ASP:OD2	1:F:181:THR:HG21	2.16	0.45
2:C:208:ARG:NH2	2:C:221:GLU:OE2	2.49	0.45
2:D:106:LEU:CD1	2:D:129:ARG:NH2	2.79	0.45
2:D:76:PHE:O	2:D:109:SER:HA	2.16	0.45
2:D:64:ILE:CD1	2:D:64:ILE:N	2.79	0.45
1:F:129:ARG:O	1:F:132:TYR:HB3	2.16	0.45
1:F:24:MET:HB2	1:F:62:ASN:ND2	2.30	0.45
1:F:33:HIS:HD2	1:F:229:SER:OG	1.98	0.45
1:F:356:LEU:HD22	1:F:387:VAL:HG11	1.98	0.45
1:F:371:LYS:HE3	1:F:371:LYS:O	2.16	0.45
1:A:148:THR:CG2	1:A:193:ARG:HD2	2.47	0.45
1:A:454:ASN:CG	1:A:467:ILE:HD13	2.36	0.45
1:B:381:SER:HB3	1:B:414:ASN:OD1	2.16	0.45
1:B:92:TRP:HE3	1:B:92:TRP:CA	2.29	0.45
1:B:429:HIS:CA	1:B:431:SEP:O1P	2.64	0.45
2:C:305:ALA:HB2	2:C:374:ARG:CD	2.43	0.45
2:C:362:ILE:HG22	2:C:366:GLU:OE2	2.16	0.45
2:C:451:ARG:NH1	2:C:451:ARG:HG2	2.31	0.45
2:D:387:VAL:HG12	2:D:388:SER:N	2.31	0.45
1:F:486:PHE:HE2	1:F:496:ARG:CD	2.27	0.45
1:A:323:GLN:NE2	1:B:459:ARG:HD3	2.31	0.45
1:A:315:PHE:CZ	1:A:363:ILE:HG23	2.51	0.45
1:A:375:ILE:O	1:A:410:GLY:HA2	2.16	0.45
1:B:126:LEU:C	1:B:128:GLU:N	2.70	0.45
1:B:317:TYR:CE2	1:B:383:LEU:HD21	2.52	0.45
2:D:164:LEU:HD11	2:D:197:GLU:HG3	1.99	0.45
1:E:211:LEU:O	1:E:212:GLU:HB3	2.15	0.45
1:F:431:SEP:O	1:F:434:THR:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:484:ARG:CB	1:F:484:ARG:NH1	2.79	0.45
1:A:45:SER:CB	1:A:182:THR:HB	2.46	0.45
1:A:418:GLN:HB2	1:B:423:HIS:O	2.17	0.45
1:B:484:ARG:NH1	1:B:484:ARG:HB3	2.32	0.45
1:B:449:MET:HE1	2:C:490:ILE:HD11	1.96	0.45
2:D:492:GLY:O	2:D:494:PRO:HD3	2.17	0.45
1:E:371:LYS:N	1:E:372:PRO:HD3	2.31	0.45
1:E:469:GLU:HB3	1:E:483:PHE:CZ	2.52	0.45
1:F:292:THR:HB	1:F:440:LEU:HB3	1.98	0.45
1:F:443:VAL:HG12	1:F:445:ILE:HG13	1.97	0.45
1:A:80:PRO:HD2	1:A:81:GLN:NE2	2.31	0.45
1:B:431:SEP:N	1:B:431:SEP:O1P	2.50	0.45
1:B:452:ALA:HA	1:B:469:GLU:HA	1.99	0.45
2:C:249:LEU:HD13	2:C:394:GLN:HG2	1.99	0.45
2:C:78:GLU:HB2	2:C:83:ILE:HD11	1.98	0.45
1:A:256:GLN:O	1:F:322:ALA:HB3	2.17	0.45
1:F:357:GLU:HG3	1:F:358:ASP:N	2.32	0.45
1:A:332:GLY:O	1:A:333:MET:O	2.35	0.45
1:A:352:GLU:OE2	1:A:385:ARG:HD2	2.17	0.45
1:B:161:ARG:HD2	1:B:196:VAL:HG13	1.97	0.45
1:B:79:THR:O	1:B:83:ILE:HG12	2.17	0.45
2:C:316:ALA:O	2:C:348:CYS:HA	2.17	0.45
2:C:488:ARG:HH22	2:D:488:ARG:HH21	1.61	0.45
1:E:146:SER:N	1:E:181:THR:HG22	2.32	0.45
1:E:338:MET:HB3	1:E:344:LEU:HB3	1.98	0.45
1:E:90:PHE:HB2	1:E:92:TRP:CE2	2.52	0.45
1:A:118:VAL:HG12	1:A:122:ASP:HB3	1.99	0.45
1:A:433:ILE:HG22	1:A:433:ILE:O	2.17	0.45
1:B:92:TRP:N	1:B:92:TRP:HE3	2.14	0.45
2:C:178:THR:HG22	2:C:179:VAL:N	2.32	0.45
2:C:33:HIS:HD2	2:C:229:SER:OG	2.00	0.45
2:C:24:MET:HG3	2:C:66:GLU:HG3	1.99	0.45
2:D:21:MET:HE3	2:D:59:PHE:CE1	2.52	0.45
2:D:352:GLU:OE2	2:D:385:ARG:HD2	2.17	0.45
2:D:425:ILE:HD11	2:D:456:PHE:CD2	2.52	0.45
2:D:45:SER:HB3	2:D:182:THR:HB	1.98	0.45
1:E:334:ASP:OD1	1:E:336:GLU:HB2	2.16	0.45
1:E:406:GLU:O	1:E:408:ILE:HG13	2.16	0.45
1:E:485:ASN:HD22	1:E:496:ARG:HD3	1.82	0.45
1:E:487:GLU:HB2	1:E:497:ILE:HD11	1.99	0.45
1:A:211:LEU:O	1:A:212:GLU:CB	2.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:VAL:HB	1:A:270:LEU:HB2	1.98	0.44
1:A:356:LEU:HD22	1:A:387:VAL:HG11	1.98	0.44
1:B:317:TYR:CD2	1:B:383:LEU:HD21	2.51	0.44
1:B:402:TYR:O	1:B:406:GLU:HB2	2.17	0.44
1:B:419:PHE:O	1:B:420:MET:HB2	2.17	0.44
2:C:124:SER:O	2:C:128:GLU:HG3	2.17	0.44
2:D:21:MET:CE	2:D:59:PHE:HZ	2.30	0.44
1:E:246:ILE:HD12	1:E:246:ILE:N	2.32	0.44
1:E:332:GLY:O	1:E:333:MET:C	2.55	0.44
1:E:487:GLU:O	1:E:488:ARG:CB	2.64	0.44
1:B:469:GLU:HB3	1:B:483:PHE:CZ	2.52	0.44
2:C:40:ARG:HG2	2:C:172:LYS:HE3	1.99	0.44
2:D:31:ILE:HD11	2:D:248:PRO:HB3	1.99	0.44
2:D:371:LYS:HD3	2:D:371:LYS:O	2.17	0.44
2:D:377:ILE:HD11	2:D:399:VAL:HG11	2.00	0.44
1:E:205:VAL:CG2	1:E:222:ILE:HD12	2.29	0.44
1:F:111:ASP:OD2	1:F:113:GLU:HG3	2.17	0.44
1:E:193:ARG:NH2	1:F:195:GLY:O	2.29	0.44
2:C:187:GLU:O	2:C:208:ARG:HD3	2.18	0.44
1:F:21:MET:CE	1:F:59:PHE:CZ	2.99	0.44
1:F:23:THR:O	1:F:24:MET:HB2	2.18	0.44
1:F:61:TYR:CE1	1:F:92:TRP:HB3	2.52	0.44
1:A:18:ILE:HD13	1:A:227:GLY:O	2.18	0.44
1:A:351:PRO:HB3	1:A:383:LEU:HD23	1.98	0.44
1:B:90:PHE:O	1:B:92:TRP:CE3	2.70	0.44
2:C:443:VAL:HG12	2:C:445:ILE:HG13	1.99	0.44
2:C:73:PHE:HB3	2:C:105:ILE:CD1	2.44	0.44
1:F:43:LEU:HD11	1:F:182:THR:OG1	2.16	0.44
1:A:227:GLY:O	1:F:89:SER:HB2	2.18	0.44
1:B:430:ILE:N	1:B:431:SEP:P	2.90	0.44
2:C:468:ARG:HG2	2:C:468:ARG:NH1	2.32	0.44
2:D:212:GLU:O	2:D:212:GLU:HG2	2.17	0.44
2:D:218:ARG:NH1	2:D:239:ILE:HD12	2.33	0.44
2:D:231:MET:CE	2:D:251:ALA:HB2	2.48	0.44
2:D:440:LEU:HD23	2:D:453:ILE:HG12	1.99	0.44
1:E:290:THR:HG21	1:F:457:LYS:HE2	2.00	0.44
1:E:313:ILE:HD12	1:E:367:ILE:CD1	2.38	0.44
1:F:215:ARG:NE	1:F:215:ARG:HA	2.32	0.44
1:F:363:ILE:N	1:F:363:ILE:HD13	2.32	0.44
1:B:192:ALA:HB3	1:B:197:GLU:OE2	2.18	0.44
1:B:81:GLN:CD	1:B:81:GLN:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:TRP:CE3	1:B:92:TRP:N	2.86	0.44
2:C:146:SER:H	2:C:181:THR:CG2	2.31	0.44
2:C:45:SER:HB3	2:C:182:THR:HB	1.99	0.44
2:C:211:LEU:O	2:C:212:GLU:HB3	2.17	0.44
2:C:335:PHE:HA	2:C:338:MET:HG3	2.00	0.44
2:D:79:THR:HG23	2:D:81:GLN:N	2.31	0.44
1:E:455:VAL:HG11	1:E:463:HIS:HB2	1.99	0.44
1:E:79:THR:CG2	1:E:82:ASP:H	2.26	0.44
1:F:25:ILE:CD1	1:F:58:GLN:HG2	2.48	0.44
1:F:72:VAL:CG2	1:F:134:ILE:HD13	2.48	0.44
1:F:76:PHE:HZ	1:F:126:LEU:CD2	2.30	0.44
1:F:360:LEU:HD21	1:F:364:LYS:HE3	2.00	0.44
1:A:31:ILE:CD1	1:A:246:ILE:HG21	2.48	0.44
1:B:21:MET:HE3	1:B:59:PHE:CE1	2.53	0.44
2:C:151:PHE:C	2:C:153:GLN:N	2.71	0.44
2:C:249:LEU:CD1	2:C:394:GLN:HG2	2.48	0.44
2:D:356:LEU:HD22	2:D:387:VAL:HG11	2.00	0.44
2:D:358:ASP:O	2:D:362:ILE:HG12	2.18	0.44
1:E:148:THR:HG21	1:E:193:ARG:HD2	2.00	0.44
1:F:489:ILE:HD13	1:F:494:PRO:HG2	2.00	0.44
1:A:14:GLU:CG	1:A:15:HIS:N	2.81	0.44
1:B:495:THR:HG23	2:C:487:GLU:OE2	2.18	0.44
2:C:295:THR:HG22	4:C:521:ATP:O1A	2.18	0.44
2:D:122:ASP:HB3	2:D:123:LEU:H	1.43	0.44
2:D:106:LEU:CD1	2:D:129:ARG:HH21	2.31	0.44
2:D:21:MET:HE2	2:D:177:THR:HG21	1.99	0.44
2:D:81:GLN:H	2:D:81:GLN:CD	2.21	0.44
1:E:111:ASP:O	1:E:113:GLU:N	2.51	0.44
1:E:56:SER:HB2	1:E:143:SER:HB2	1.99	0.44
1:E:81:GLN:NE2	1:E:81:GLN:H	2.16	0.44
1:F:467:ILE:N	1:F:467:ILE:CD1	2.81	0.44
1:A:357:GLU:HG3	1:A:358:ASP:N	2.32	0.43
1:A:375:ILE:HD12	1:A:408:ILE:HG21	2.00	0.43
1:A:453:ILE:HB	1:A:470:PHE:CD2	2.52	0.43
1:B:119:GLY:C	1:B:121:PHE:H	2.21	0.43
2:C:88:ARG:HG2	2:C:88:ARG:HH11	1.83	0.43
2:D:211:LEU:HD12	2:D:215:ARG:O	2.18	0.43
2:D:31:ILE:HA	2:D:231:MET:SD	2.58	0.43
1:F:437:ILE:HD13	1:F:457:LYS:HG2	1.99	0.43
1:A:362:ILE:O	1:A:366:GLU:CG	2.54	0.43
1:B:98:VAL:HA	1:B:103:LEU:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:ARG:HH11	1:B:484:ARG:HB3	1.83	0.43
2:C:317:TYR:CE2	2:C:383:LEU:HD21	2.54	0.43
2:C:449:MET:CE	2:D:467:ILE:HD11	2.48	0.43
2:D:291:GLY:N	4:D:521:ATP:O2B	2.50	0.43
2:D:449:MET:HE3	1:E:490:ILE:HD11	2.00	0.43
2:D:98:VAL:HA	2:D:103:LEU:O	2.19	0.43
1:E:376:ALA:HA	1:E:411:LEU:O	2.17	0.43
1:F:340:ARG:C	1:F:342:ASN:H	2.22	0.43
1:B:305:ALA:HB2	1:B:374:ARG:CD	2.38	0.43
1:B:440:LEU:HD21	1:B:453:ILE:HG12	2.00	0.43
1:B:79:THR:HG21	1:B:81:GLN:HG2	2.01	0.43
2:C:338:MET:HB3	2:C:344:LEU:HB3	2.01	0.43
2:D:14:GLU:CG	2:D:15:HIS:N	2.80	0.43
2:C:318:GLU:OE2	2:D:432:TPO:O3P	2.37	0.43
2:D:21:MET:CE	2:D:59:PHE:CZ	3.02	0.43
1:E:451:ARG:HG2	1:E:451:ARG:NH1	2.32	0.43
1:F:332:GLY:O	1:F:333:MET:C	2.56	0.43
1:A:291:GLY:N	4:A:521:ATP:O2B	2.51	0.43
2:C:143:SER:HA	2:C:179:VAL:O	2.18	0.43
1:E:249:LEU:HD13	1:E:394:GLN:HG2	2.01	0.43
1:E:364:LYS:O	1:E:368:ASN:ND2	2.51	0.43
1:E:81:GLN:CD	1:E:81:GLN:H	2.20	0.43
1:F:479:ILE:H	1:F:479:ILE:HD12	1.83	0.43
1:A:178:THR:HG22	1:A:179:VAL:N	2.34	0.43
1:B:81:GLN:H	1:B:81:GLN:NE2	2.16	0.43
2:C:215:ARG:NE	2:C:215:ARG:HA	2.32	0.43
2:C:387:VAL:CG1	2:C:391:ALA:HB3	2.48	0.43
1:E:211:LEU:HD12	1:E:215:ARG:O	2.18	0.43
1:F:381:SER:HB3	1:F:414:ASN:OD1	2.19	0.43
1:A:359:HIS:O	1:A:363:ILE:HG12	2.17	0.43
1:A:87:ALA:HB1	1:A:92:TRP:CB	2.49	0.43
1:B:291:GLY:N	4:B:521:ATP:O2B	2.51	0.43
1:B:80:PRO:HD2	1:B:81:GLN:NE2	2.33	0.43
2:D:437:ILE:HD11	2:D:457:LYS:HE2	1.99	0.43
1:E:45:SER:CB	1:E:182:THR:HB	2.48	0.43
1:E:18:ILE:HD11	1:E:228:THR:N	2.34	0.43
1:E:385:ARG:HA	1:F:393:ARG:HH12	1.83	0.43
1:A:184:ARG:O	1:B:199:PHE:HZ	2.02	0.43
1:A:334:ASP:O	1:A:338:MET:HG2	2.19	0.43
1:A:393:ARG:O	1:A:397:ILE:HG12	2.18	0.43
2:C:118:VAL:O	2:C:118:VAL:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:344:LEU:HD22	2:D:345:LYS:H	1.80	0.43
1:E:150:VAL:CG1	1:E:151:PHE:H	2.32	0.43
1:F:126:LEU:HG	1:F:130:ILE:CD1	2.47	0.43
1:F:191:ILE:CB	1:F:198:GLU:CG	2.90	0.43
1:F:264:SER:HA	1:F:271:ASP:OD1	2.18	0.43
1:F:419:PHE:O	1:F:420:MET:HB2	2.18	0.43
1:A:377:ILE:HD13	1:A:412:PHE:CD2	2.52	0.43
1:A:459:ARG:HH11	1:F:323:GLN:HE22	1.65	0.43
2:C:311:ARG:HD2	2:C:371:LYS:HD3	1.96	0.43
2:C:340:ARG:C	2:C:342:ASN:H	2.22	0.43
1:E:21:MET:HE1	1:E:177:THR:HB	2.01	0.43
1:E:184:ARG:HG2	1:E:191:ILE:O	2.19	0.43
1:F:468:ARG:NH1	1:F:468:ARG:HG2	2.34	0.43
1:F:81:GLN:N	1:F:81:GLN:CD	2.72	0.43
1:B:21:MET:HB2	1:B:38:ILE:HG12	2.01	0.43
2:D:359:HIS:O	2:D:363:ILE:HG13	2.18	0.43
2:D:387:VAL:CG1	2:D:388:SER:N	2.82	0.43
1:E:396:VAL:HG11	1:E:430:ILE:HG21	2.01	0.43
1:A:17:ALA:C	1:A:18:ILE:HD12	2.39	0.43
1:A:299:SER:C	1:A:333:MET:HE1	2.39	0.43
1:A:344:LEU:C	1:A:344:LEU:HD13	2.38	0.43
1:B:56:SER:O	1:B:59:PHE:HB3	2.18	0.43
2:C:360:LEU:CD2	2:C:364:LYS:HE3	2.49	0.43
2:C:67:PHE:HB2	2:C:69:GLU:HG3	1.99	0.43
2:D:317:TYR:CD2	2:D:383:LEU:HD21	2.53	0.43
2:D:430:ILE:O	2:D:432:TPO:N	2.52	0.43
1:F:148:THR:HG21	1:F:183:GLU:HG3	2.01	0.43
1:A:436:THR:CG2	1:A:458:MET:HG2	2.49	0.42
1:B:378:ASP:O	1:B:379:SER:HB3	2.18	0.42
1:B:462:TRP:O	1:B:463:HIS:O	2.35	0.42
2:C:184:ARG:HG2	2:C:191:ILE:O	2.18	0.42
2:C:484:ARG:HH11	2:C:484:ARG:HB3	1.82	0.42
2:D:134:ILE:HD13	2:D:134:ILE:N	2.34	0.42
2:D:256:GLN:HG3	2:D:404:LYS:HD3	2.00	0.42
1:F:191:ILE:HB	1:F:198:GLU:HG2	1.95	0.42
1:F:270:LEU:O	1:F:273:MET:HB2	2.19	0.42
1:A:218:ARG:O	1:A:236:PRO:HA	2.19	0.42
1:A:406:GLU:O	1:A:407:GLU:HB2	2.19	0.42
1:A:65:ILE:O	1:A:65:ILE:HG22	2.18	0.42
1:B:289:ALA:HB2	1:B:419:PHE:HA	2.01	0.42
1:B:470:PHE:HE1	1:B:472:ILE:HD11	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:123:LEU:CD2	2:C:167:LEU:HB2	2.49	0.42
2:C:356:LEU:CD2	2:C:387:VAL:HG11	2.49	0.42
2:C:52:LYS:N	4:C:522:ATP:O1B	2.49	0.42
2:C:65:ILE:H	2:C:65:ILE:CD1	2.32	0.42
2:C:78:GLU:CB	2:C:83:ILE:HD11	2.50	0.42
2:D:486:PHE:HB3	2:D:489:ILE:CD1	2.32	0.42
1:E:400:THR:HG22	1:E:401:GLY:N	2.33	0.42
1:E:446:ARG:HH21	1:E:496:ARG:NH2	2.16	0.42
1:F:106:LEU:HD11	1:F:129:ARG:NH2	2.33	0.42
1:F:142:VAL:O	1:F:178:THR:HA	2.19	0.42
1:F:28:PHE:CE1	1:F:222:ILE:HD11	2.53	0.42
1:F:295:THR:HG21	1:F:319:GLU:OE2	2.19	0.42
1:A:293:GLY:HA2	4:A:521:ATP:O1A	2.19	0.42
1:A:317:TYR:CD2	1:A:383:LEU:HD21	2.54	0.42
1:B:264:SER:O	1:B:374:ARG:NH2	2.51	0.42
1:B:471:MET:O	1:B:472:ILE:HD13	2.19	0.42
1:E:191:ILE:CB	1:E:198:GLU:HG2	2.47	0.42
1:E:437:ILE:HD12	1:E:457:LYS:HE2	1.99	0.42
1:F:111:ASP:OD1	1:F:112:PRO:CD	2.66	0.42
1:F:180:MET:HB3	1:F:180:MET:HE2	1.84	0.42
1:A:33:HIS:HD2	1:A:229:SER:OG	2.02	0.42
2:C:96:LYS:O	2:C:100:GLU:HG3	2.19	0.42
2:C:161:ARG:HB2	2:C:196:VAL:HG11	2.00	0.42
2:C:301:PHE:O	2:C:374:ARG:NH1	2.50	0.42
1:E:53:THR:HG23	1:E:145:ASP:OD1	2.19	0.42
1:E:164:LEU:HD11	1:E:197:GLU:HG3	2.02	0.42
1:E:203:ASN:HB3	1:E:225:LEU:CD2	2.48	0.42
1:F:121:PHE:HD2	1:F:121:PHE:HA	1.74	0.42
1:F:211:LEU:HD12	1:F:215:ARG:O	2.19	0.42
1:F:325:LEU:HD23	1:F:335:PHE:CB	2.45	0.42
1:F:425:ILE:HG22	1:F:426:THR:HG23	2.01	0.42
1:A:425:ILE:HD11	1:A:456:PHE:CE2	2.55	0.42
1:B:146:SER:H	1:B:181:THR:HG22	1.84	0.42
1:A:215:ARG:NH2	1:B:234:GLU:O	2.52	0.42
2:C:123:LEU:O	2:C:124:SER:C	2.58	0.42
2:C:75:THR:HG23	2:C:75:THR:O	2.19	0.42
2:D:296:LEU:HD13	2:D:331:TRP:CD2	2.54	0.42
2:D:334:ASP:O	2:D:338:MET:HG2	2.19	0.42
1:E:148:THR:HG21	1:E:183:GLU:HG3	2.02	0.42
1:E:294:LYS:HB2	4:E:601:ATP:O1B	2.20	0.42
1:F:115:GLN:CG	1:F:116:GLU:N	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:ASP:O	1:F:126:LEU:N	2.33	0.42
1:A:159:VAL:O	1:A:163:GLU:HG2	2.19	0.42
1:A:220:LEU:HD21	1:A:222:ILE:CD1	2.49	0.42
1:A:92:TRP:N	1:A:92:TRP:CE3	2.86	0.42
2:C:308:ASN:O	2:C:310:GLU:HG3	2.20	0.42
2:C:420:MET:HE2	2:C:492:GLY:HA3	2.01	0.42
2:D:123:LEU:HA	2:D:123:LEU:HD22	1.85	0.42
2:D:145:ASP:OD2	2:D:181:THR:HG21	2.20	0.42
2:D:323:GLN:NE2	1:E:459:ARG:HD3	2.34	0.42
2:D:362:ILE:CG2	2:D:366:GLU:OE2	2.67	0.42
2:D:45:SER:CB	2:D:182:THR:HB	2.50	0.42
2:D:64:ILE:CD1	2:D:64:ILE:H	2.33	0.42
1:E:356:LEU:HD21	1:E:387:VAL:HG11	2.00	0.42
1:F:118:VAL:O	1:F:118:VAL:HG22	2.20	0.42
1:F:25:ILE:HD12	1:F:58:GLN:CG	2.50	0.42
1:A:296:LEU:HD23	1:A:472:ILE:HD12	2.01	0.42
1:A:488:ARG:NE	1:F:488:ARG:NH1	2.66	0.42
1:B:21:MET:HE2	1:B:177:THR:HG21	2.02	0.42
2:C:116:GLU:O	2:C:117:VAL:HB	2.19	0.42
2:C:41:SER:HA	2:C:178:THR:O	2.19	0.42
1:E:396:VAL:HG11	1:E:430:ILE:CG2	2.49	0.42
1:A:304:ASN:HB3	1:A:374:ARG:HH12	1.85	0.42
1:A:362:ILE:CG2	1:A:366:GLU:OE2	2.68	0.42
1:B:107:ASP:C	1:B:107:ASP:OD1	2.58	0.42
1:B:336:GLU:OE1	1:B:336:GLU:HA	2.20	0.42
1:B:358:ASP:O	1:B:362:ILE:HG12	2.18	0.42
2:C:292:THR:HB	2:C:440:LEU:HB3	2.02	0.42
2:D:109:SER:HA	2:D:110:PRO:HD3	1.87	0.42
2:D:208:ARG:O	2:D:218:ARG:HA	2.20	0.42
2:D:387:VAL:HG12	2:D:388:SER:O	2.19	0.42
1:E:321:ARG:O	1:E:325:LEU:HD12	2.19	0.42
1:E:81:GLN:CD	1:E:81:GLN:N	2.72	0.42
1:F:119:GLY:HA2	1:F:122:ASP:OD1	2.19	0.42
1:A:52:LYS:HD3	1:A:182:THR:O	2.20	0.42
1:A:443:VAL:CG1	1:A:494:PRO:HG2	2.50	0.42
1:B:292:THR:HB	1:B:440:LEU:HB3	2.02	0.42
1:B:45:SER:HA	1:B:182:THR:O	2.19	0.42
2:D:41:SER:HA	2:D:178:THR:O	2.20	0.42
2:D:412:PHE:CD1	2:D:412:PHE:N	2.88	0.42
1:F:306:CYS:SG	1:F:344:LEU:HB2	2.60	0.42
1:F:356:LEU:CD1	1:F:387:VAL:HG21	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:GLU:O	1:B:494:PRO:HA	2.20	0.42
2:C:214:GLU:C	2:C:215:ARG:HE	2.23	0.42
1:A:291:GLY:O	4:A:521:ATP:H4'	2.20	0.41
2:C:123:LEU:HD11	2:C:163:GLU:O	2.20	0.41
2:D:376:ALA:HA	2:D:411:LEU:O	2.20	0.41
1:E:344:LEU:HD11	1:E:346:ILE:HG13	2.01	0.41
1:A:316:ALA:CB	1:A:324:LEU:HD11	2.50	0.41
1:B:267:VAL:HB	1:B:270:LEU:HB2	2.01	0.41
1:B:360:LEU:HD21	1:B:364:LYS:HE3	2.03	0.41
2:C:123:LEU:HD11	2:C:163:GLU:CA	2.51	0.41
2:D:303:GLU:O	2:D:303:GLU:HG2	2.19	0.41
1:E:84:ILE:HG21	1:E:95:ALA:HB2	2.03	0.41
1:F:269:ARG:HB3	1:F:479:ILE:HD13	2.01	0.41
1:A:447:GLY:C	1:B:467:ILE:HD13	2.41	0.41
1:B:85:LYS:HZ2	2:C:14:GLU:HB3	1.81	0.41
2:C:123:LEU:HD22	2:C:167:LEU:HB2	2.02	0.41
2:C:170:ARG:O	2:C:174:ILE:HG12	2.21	0.41
2:C:52:LYS:HD3	2:C:182:THR:O	2.20	0.41
2:C:197:GLU:OE2	2:C:197:GLU:N	2.36	0.41
2:D:377:ILE:CD1	2:D:399:VAL:HG11	2.51	0.41
1:E:134:ILE:N	1:E:134:ILE:CD1	2.83	0.41
1:E:371:LYS:HD3	1:E:371:LYS:O	2.20	0.41
1:F:113:GLU:O	1:F:114:GLY:O	2.38	0.41
1:F:299:SER:C	1:F:333:MET:HE1	2.41	0.41
1:F:329:TYR:HA	1:F:332:GLY:O	2.20	0.41
1:F:440:LEU:HD21	1:F:453:ILE:HG13	2.02	0.41
1:A:182:THR:CG2	1:A:183:GLU:N	2.84	0.41
1:B:126:LEU:C	1:B:128:GLU:H	2.23	0.41
1:B:178:THR:CG2	1:B:179:VAL:N	2.84	0.41
4:C:521:ATP:C2	2:D:462:TRP:HA	2.56	0.41
1:E:21:MET:CE	1:E:59:PHE:HZ	2.34	0.41
1:F:131:ASN:OD1	1:F:174:ILE:HD12	2.21	0.41
1:F:336:GLU:HB3	1:F:340:ARG:NH2	2.35	0.41
1:B:356:LEU:HD13	1:B:387:VAL:HG21	2.02	0.41
1:B:429:HIS:HA	1:B:431:SEP:O1P	2.19	0.41
2:C:382:ALA:O	2:C:385:ARG:HG3	2.20	0.41
2:C:449:MET:HE3	2:D:467:ILE:HD11	2.03	0.41
2:D:249:LEU:CD1	2:D:394:GLN:HG2	2.51	0.41
1:E:127:ILE:HD13	1:E:127:ILE:N	2.35	0.41
1:E:447:GLY:O	1:F:467:ILE:CD1	2.67	0.41
1:E:469:GLU:CB	1:E:483:PHE:CZ	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:LYS:N	4:E:603:ATP:O1B	2.49	0.41
1:F:161:ARG:CB	1:F:196:VAL:HG11	2.42	0.41
1:A:302:VAL:HG13	1:A:344:LEU:HD23	2.03	0.41
2:C:194:TYR:CD1	2:C:194:TYR:N	2.89	0.41
2:D:24:MET:HB2	2:D:62:ASN:HD22	1.85	0.41
1:E:178:THR:HG22	1:E:179:VAL:N	2.35	0.41
1:E:352:GLU:OE2	1:E:385:ARG:HD2	2.20	0.41
1:F:487:GLU:O	1:F:488:ARG:HB2	2.19	0.41
1:A:40:ARG:HG2	1:A:172:LYS:HE3	2.03	0.41
1:A:183:GLU:OE2	1:B:161:ARG:NH1	2.46	0.41
1:A:451:ARG:CG	1:A:451:ARG:NH1	2.79	0.41
2:C:453:ILE:HD13	2:C:454:ASN:H	1.80	0.41
2:D:159:VAL:O	2:D:163:GLU:HG2	2.21	0.41
1:F:117:VAL:O	1:F:118:VAL:HB	2.21	0.41
1:F:151:PHE:CZ	1:F:160:VAL:HG13	2.55	0.41
1:F:468:ARG:HH11	1:F:468:ARG:HG2	1.85	0.41
1:F:21:MET:HE1	1:F:59:PHE:HZ	1.85	0.41
1:A:299:SER:CB	1:A:333:MET:HE1	2.43	0.41
1:A:311:ARG:HB3	1:A:370:PHE:CE2	2.56	0.41
1:A:483:PHE:HB3	1:A:486:PHE:HD1	1.85	0.41
1:B:300:ARG:HA	1:B:333:MET:HE3	2.03	0.41
2:C:306:CYS:SG	2:C:344:LEU:HB2	2.61	0.41
4:B:521:ATP:H3'	2:C:458:MET:O	2.20	0.41
2:D:488:ARG:HH12	1:E:488:ARG:NH2	2.18	0.41
2:D:489:ILE:CD1	2:D:494:PRO:HB3	2.44	0.41
1:E:249:LEU:CD1	1:E:394:GLN:HG2	2.50	0.41
1:B:126:LEU:HG	1:B:130:ILE:CD1	2.51	0.41
2:C:211:LEU:HD12	2:C:215:ARG:O	2.21	0.41
2:C:21:MET:HE3	2:C:59:PHE:CE1	2.55	0.41
1:E:193:ARG:HH11	1:E:193:ARG:HG2	1.85	0.41
1:A:487:GLU:HG2	1:F:496:ARG:CZ	2.51	0.41
1:A:153:GLN:O	1:A:154:TYR:CB	2.69	0.41
1:B:315:PHE:CD2	1:B:363:ILE:CD1	3.04	0.41
1:B:376:ALA:HA	1:B:411:LEU:O	2.21	0.41
1:B:449:MET:HE3	2:C:467:ILE:HD11	2.02	0.41
2:C:161:ARG:HD2	2:C:196:VAL:HG13	2.03	0.41
1:E:333:MET:HB2	1:E:333:MET:HE2	1.88	0.41
2:D:496:ARG:HG2	1:E:487:GLU:OE1	2.20	0.41
1:F:148:THR:HG21	1:F:183:GLU:CG	2.51	0.41
1:B:127:ILE:HG22	1:B:127:ILE:O	2.20	0.41
1:B:335:PHE:O	1:B:339:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:ALA:O	1:B:385:ARG:HG3	2.21	0.41
2:C:487:GLU:CG	2:C:497:ILE:HD11	2.44	0.41
2:D:130:ILE:O	2:D:134:ILE:HD13	2.21	0.41
2:D:419:PHE:O	2:D:420:MET:HB2	2.21	0.41
4:D:521:ATP:C2	1:E:462:TRP:HA	2.56	0.41
1:E:79:THR:HG23	1:E:81:GLN:CG	2.41	0.41
1:F:220:LEU:C	1:F:220:LEU:HD23	2.41	0.41
1:F:287:THR:HA	1:F:414:ASN:O	2.21	0.41
1:B:25:ILE:HG23	1:B:58:GLN:NE2	2.36	0.40
1:B:91:GLY:C	1:B:92:TRP:CE3	2.95	0.40
2:D:19:ALA:CB	2:D:38:ILE:HD12	2.51	0.40
2:D:471:MET:HG3	2:D:478:ASP:HB3	2.04	0.40
2:D:470:PHE:HB3	2:D:479:ILE:HD13	2.03	0.40
2:D:495:THR:O	2:D:495:THR:HG22	2.21	0.40
2:D:79:THR:HG22	2:D:82:ASP:N	2.16	0.40
1:E:191:ILE:CG2	1:E:198:GLU:HG3	2.51	0.40
1:E:365:SER:HA	1:E:368:ASN:HD22	1.86	0.40
1:E:377:ILE:HD11	1:E:399:VAL:HG11	2.03	0.40
1:E:438:ILE:HD13	1:E:455:VAL:HA	2.04	0.40
1:E:94:LEU:O	1:E:98:VAL:HG23	2.21	0.40
1:F:64:ILE:HD13	1:F:69:GLU:O	2.21	0.40
1:A:164:LEU:HA	1:A:164:LEU:HD23	1.83	0.40
1:A:444:GLU:O	1:A:494:PRO:HD2	2.21	0.40
1:B:225:LEU:HD12	1:B:230:HIS:HB3	2.04	0.40
1:B:429:HIS:HA	1:B:431:SEP:P	2.60	0.40
2:C:123:LEU:HB3	2:C:127:ILE:HD11	2.03	0.40
2:C:144:ILE:HG21	2:C:147:VAL:HG12	2.03	0.40
2:D:191:ILE:HB	2:D:198:GLU:CD	2.40	0.40
2:D:273:MET:CE	2:D:468:ARG:HD2	2.51	0.40
2:D:325:LEU:HD23	2:D:335:PHE:CB	2.48	0.40
1:E:184:ARG:O	1:E:185:ILE:HD13	2.21	0.40
1:E:379:SER:N	1:E:413:THR:HB	2.24	0.40
1:F:357:GLU:HG3	1:F:358:ASP:H	1.87	0.40
1:F:21:MET:CE	1:F:59:PHE:CE1	3.04	0.40
1:A:187:GLU:O	1:A:208:ARG:HD3	2.20	0.40
1:B:148:THR:HA	1:B:151:PHE:CE1	2.57	0.40
1:B:76:PHE:HE1	1:B:144:ILE:CG2	2.33	0.40
2:C:76:PHE:O	2:C:109:SER:HA	2.21	0.40
2:D:121:PHE:N	2:D:121:PHE:CD1	2.89	0.40
2:D:153:GLN:O	2:D:154:TYR:CB	2.69	0.40
1:E:164:LEU:HD23	1:E:164:LEU:HA	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:SER:HA	1:E:181:THR:HG22	2.03	0.40
1:F:123:LEU:HA	1:F:123:LEU:HD22	1.82	0.40
1:F:79:THR:HG21	1:F:81:GLN:HG2	2.01	0.40
1:A:319:GLU:O	1:B:254:LEU:HD21	2.21	0.40
1:B:299:SER:CB	1:B:333:MET:HE1	2.49	0.40
1:B:21:MET:HE3	1:B:59:PHE:CZ	2.56	0.40
2:C:378:ASP:O	2:C:379:SER:HB3	2.22	0.40
2:D:385:ARG:HG2	1:E:393:ARG:NH1	2.37	0.40
1:E:217:ARG:HH21	1:E:236:PRO:HB3	1.86	0.40
1:E:264:SER:HA	1:E:271:ASP:OD1	2.22	0.40
1:E:445:ILE:HD12	1:E:450:SER:OG	2.22	0.40
1:E:471:MET:HG3	1:E:478:ASP:HB3	2.02	0.40
1:F:130:ILE:O	1:F:134:ILE:HG12	2.22	0.40
1:F:249:LEU:CD1	1:F:394:GLN:HG2	2.51	0.40
1:A:283:ILE:HG23	1:A:412:PHE:CE1	2.57	0.40
1:A:452:ALA:HA	1:A:469:GLU:HA	2.04	0.40
2:C:99:ASP:C	2:C:101:GLY:H	2.25	0.40
2:C:256:GLN:H	2:C:256:GLN:HG2	1.70	0.40
2:C:354:ALA:HB1	2:C:358:ASP:HB2	2.04	0.40
2:C:283:ILE:CD1	2:C:400:THR:HG23	2.51	0.40
2:D:123:LEU:HD12	2:D:166:ARG:CD	2.35	0.40
2:D:437:ILE:HD12	2:D:457:LYS:HG2	2.03	0.40
1:F:256:GLN:H	1:F:256:GLN:HG2	1.69	0.40
1:A:16:GLN:O	1:F:88:ARG:HD2	2.21	0.40
1:F:92:TRP:CD1	1:F:92:TRP:N	2.87	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ARG:NH1	1:B:137:TYR:OH[3_755]	2.15	0.05

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	480/519 (92%)	438 (91%)	31 (6%)	11 (2%)	6	21
1	B	480/519 (92%)	430 (90%)	41 (8%)	9 (2%)	8	26
1	E	480/519 (92%)	434 (90%)	31 (6%)	15 (3%)	4	14
1	F	480/519 (92%)	436 (91%)	34 (7%)	10 (2%)	7	23
2	C	481/519 (93%)	431 (90%)	35 (7%)	15 (3%)	4	14
2	D	481/519 (93%)	437 (91%)	32 (7%)	12 (2%)	5	19
All	All	2882/3114 (92%)	2606 (90%)	204 (7%)	72 (2%)	5	19

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ALA
1	A	117	VAL
1	A	154	TYR
1	A	211	LEU
1	A	333	MET
1	A	463	HIS
1	B	154	TYR
1	B	333	MET
1	B	463	HIS
2	C	17	ALA
2	C	117	VAL
2	C	122	ASP
2	C	123	LEU
2	C	154	TYR
2	C	333	MET
2	C	463	HIS
2	D	113	GLU
2	D	122	ASP
2	D	154	TYR
2	D	333	MET
1	E	122	ASP
1	E	154	TYR
1	E	211	LEU
1	E	333	MET
1	E	463	HIS
1	F	114	GLY
1	F	118	VAL

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Mol	Chain	Res	Type
1	F	154	TYR
1	F	333	MET
1	F	463	HIS
1	B	119	GLY
1	B	211	LEU
2	C	431	SER
2	D	431	SER
2	D	463	HIS
1	E	113	GLU
1	E	123	LEU
1	E	387	VAL
1	E	420	MET
1	F	211	LEU
1	A	120	GLY
1	A	387	VAL
1	A	420	MET
1	B	420	MET
2	C	112	PRO
2	C	211	LEU
2	C	349	ALA
2	D	211	LEU
2	D	420	MET
1	E	488	ARG
1	F	117	VAL
1	F	420	MET
2	C	420	MET
2	D	387	VAL
1	E	494	PRO
1	A	348	CYS
1	B	348	CYS
1	B	494	PRO
2	C	348	CYS
2	C	379	SER
2	D	118	VAL
1	E	117	VAL
1	E	348	CYS
1	E	379	SER
2	C	212	GLU
2	D	348	CYS
2	D	494	PRO
1	F	348	CYS
1	A	112	PRO

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Mol	Chain	Res	Type
1	E	112	PRO
1	F	387	VAL
1	B	387	VAL

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	410/442 (93%)	383 (93%)	27 (7%)	16	44
1	B	410/442 (93%)	388 (95%)	22 (5%)	22	53
1	E	410/442 (93%)	384 (94%)	26 (6%)	18	46
1	F	410/442 (93%)	380 (93%)	30 (7%)	14	38
2	C	411/443 (93%)	385 (94%)	26 (6%)	18	46
2	D	411/443 (93%)	382 (93%)	29 (7%)	14	39
All	All	2462/2654 (93%)	2302 (94%)	160 (6%)	17	44

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	38	ILE
1	A	79	THR
1	A	81	GLN
1	A	92	TRP
1	A	123	LEU
1	A	151	PHE
1	A	154	TYR
1	A	186	GLU
1	A	212	GLU
1	A	222	ILE
1	A	223	LEU
1	A	238	THR
1	A	256	GLN
1	A	270	LEU

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Mol	Chain	Res	Type
1	A	287	THR
1	A	290	THR
1	A	342	ASN
1	A	360	LEU
1	A	362	ILE
1	A	371	LYS
1	A	400	THR
1	A	437	ILE
1	A	451	ARG
1	A	458	MET
1	A	471	MET
1	A	496	ARG
1	B	26	GLU
1	B	79	THR
1	B	81	GLN
1	B	92	TRP
1	B	128	GLU
1	B	151	PHE
1	B	154	TYR
1	B	181	THR
1	B	186	GLU
1	B	212	GLU
1	B	223	LEU
1	B	256	GLN
1	B	270	LEU
1	B	290	THR
1	B	360	LEU
1	B	371	LYS
1	B	400	THR
1	B	437	ILE
1	B	451	ARG
1	B	453	ILE
1	B	462	TRP
1	B	471	MET
2	C	26	GLU
2	C	65	ILE
2	C	79	THR
2	C	81	GLN
2	C	151	PHE
2	C	154	TYR
2	C	181	THR
2	C	186	GLU

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Mol	Chain	Res	Type
2	C	212	GLU
2	C	218	ARG
2	C	223	LEU
2	C	256	GLN
2	C	270	LEU
2	C	284	ILE
2	C	290	THR
2	C	295	THR
2	C	303	GLU
2	C	360	LEU
2	C	371	LYS
2	C	375	ILE
2	C	400	THR
2	C	451	ARG
2	C	453	ILE
2	C	458	MET
2	C	471	MET
2	C	497	ILE
2	D	26	GLU
2	D	79	THR
2	D	81	GLN
2	D	121	PHE
2	D	122	ASP
2	D	123	LEU
2	D	134	ILE
2	D	151	PHE
2	D	154	TYR
2	D	181	THR
2	D	186	GLU
2	D	212	GLU
2	D	223	LEU
2	D	256	GLN
2	D	270	LEU
2	D	287	THR
2	D	290	THR
2	D	295	THR
2	D	360	LEU
2	D	371	LYS
2	D	375	ILE
2	D	400	THR
2	D	431	SER
2	D	451	ARG

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Mol	Chain	Res	Type
2	D	453	ILE
2	D	463	HIS
2	D	469	GLU
2	D	471	MET
2	D	496	ARG
1	E	26	GLU
1	E	79	THR
1	E	81	GLN
1	E	121	PHE
1	E	134	ILE
1	E	151	PHE
1	E	154	TYR
1	E	181	THR
1	E	186	GLU
1	E	212	GLU
1	E	222	ILE
1	E	223	LEU
1	E	228	THR
1	E	256	GLN
1	E	270	LEU
1	E	284	ILE
1	E	287	THR
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	469	GLU
1	E	471	MET
1	E	497	ILE
1	F	26	GLU
1	F	45	SER
1	F	53	THR
1	F	79	THR
1	F	81	GLN
1	F	121	PHE
1	F	123	LEU
1	F	151	PHE
1	F	154	TYR
1	F	181	THR
1	F	186	GLU

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Mol	Chain	Res	Type
1	F	212	GLU
1	F	218	ARG
1	F	222	ILE
1	F	223	LEU
1	F	256	GLN
1	F	270	LEU
1	F	290	THR
1	F	342	ASN
1	F	360	LEU
1	F	363	ILE
1	F	371	LYS
1	F	400	THR
1	F	451	ARG
1	F	458	MET
1	F	462	TRP
1	F	471	MET
1	F	487	GLU
1	F	491	SER
1	F	496	ARG

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

Mol	Chain	Res	Type
1	A	33	HIS
1	A	62	ASN
1	A	81	GLN
1	A	209	ASN
1	A	361	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	368	ASN
1	B	414	ASN
1	B	441	GLN
2	C	33	HIS
2	C	62	ASN
2	C	81	GLN
2	C	209	ASN

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Mol	Chain	Res	Type
2	C	368	ASN
2	C	414	ASN
2	D	33	HIS
2	D	81	GLN
2	D	209	ASN
2	D	361	GLN
2	D	368	ASN
2	D	414	ASN
1	E	33	HIS
1	E	81	GLN
1	E	209	ASN
1	E	304	ASN
1	E	361	GLN
1	E	368	ASN
1	E	414	ASN
1	E	441	GLN
1	E	454	ASN
1	F	16	GLN
1	F	33	HIS
1	F	62	ASN
1	F	81	GLN
1	F	135	GLN
1	F	209	ASN
1	F	361	GLN
1	F	368	ASN
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 ⓘ

10 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	TPO	B	432	1	8,10,11	1.12	1 (12%)	10,14,16	1.31	2 (20%)
2	TPO	D	432	2	8,10,11	3.07	2 (25%)	10,14,16	2.07	3 (30%)
1	TPO	F	432	1	8,10,11	3.20	2 (25%)	10,14,16	1.33	1 (10%)
1	TPO	A	432	1	8,10,11	1.01	0	10,14,16	1.57	2 (20%)
2	TPO	C	432	2	8,10,11	3.06	4 (50%)	10,14,16	2.68	3 (30%)
1	TPO	E	432	1	8,10,11	1.34	1 (12%)	10,14,16	2.11	3 (30%)
1	SEP	E	431	1	8,9,10	2.52	3 (37%)	8,12,14	3.39	4 (50%)
1	SEP	F	431	1	8,9,10	1.03	0	8,12,14	3.89	2 (25%)
1	SEP	A	431	1	8,9,10	1.78	2 (25%)	8,12,14	1.44	1 (12%)
1	SEP	B	431	1	8,9,10	1.91	2 (25%)	8,12,14	1.96	3 (37%)

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	TPO	B	432	1	-	1/9/11/13	-
2	TPO	D	432	2	-	1/9/11/13	-
1	TPO	F	432	1	-	7/9/11/13	-
1	TPO	A	432	1	-	1/9/11/13	-
2	TPO	C	432	2	-	2/9/11/13	-
1	TPO	E	432	1	-	1/9/11/13	-
1	SEP	E	431	1	-	4/5/8/10	-
1	SEP	F	431	1	-	4/5/8/10	-
1	SEP	A	431	1	-	3/5/8/10	-
1	SEP	B	431	1	-	4/5/8/10	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	432	TPO	CB-CA	6.99	1.69	1.53
2	C	432	TPO	CB-CA	6.47	1.68	1.53
1	F	432	TPO	CG2-CB	-6.41	1.36	1.51
1	F	432	TPO	CB-CA	-5.81	1.40	1.53
1	E	431	SEP	P-OG	5.34	1.77	1.60
2	C	432	TPO	CA-N	4.16	1.60	1.47
2	D	432	TPO	CA-N	3.77	1.59	1.47
1	A	431	SEP	P-O1P	3.48	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	431	SEP	P-O1P	3.46	1.61	1.50
1	B	431	SEP	P-OG	3.24	1.70	1.60
1	B	431	SEP	P-O1P	3.05	1.60	1.50
1	E	432	TPO	O-C	2.70	1.30	1.19
2	C	432	TPO	CG2-CB	-2.48	1.45	1.51
2	C	432	TPO	O-C	2.38	1.29	1.19
1	E	431	SEP	CB-CA	2.33	1.58	1.52
1	A	431	SEP	P-OG	2.03	1.66	1.60
1	B	432	TPO	O-C	2.02	1.28	1.19

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	431	SEP	P-OG-CB	10.52	147.28	118.30
1	E	431	SEP	P-OG-CB	7.93	140.15	118.30
2	C	432	TPO	O-C-CA	-6.68	107.28	124.78
2	D	432	TPO	O-C-CA	-4.65	112.58	124.78
1	E	432	TPO	O-C-CA	-4.23	113.69	124.78
1	B	431	SEP	O2P-P-OG	4.06	117.53	106.73
1	E	432	TPO	P-OG1-CB	-3.72	111.97	123.21
1	A	432	TPO	P-OG1-CB	-3.66	112.14	123.21
1	E	431	SEP	O3P-P-OG	3.51	116.06	106.73
2	C	432	TPO	CG2-CB-CA	-3.42	106.41	113.16
1	E	432	TPO	CG2-CB-CA	-3.27	106.71	113.16
1	E	431	SEP	OG-P-O1P	3.22	115.52	106.47
2	C	432	TPO	P-OG1-CB	-3.17	113.63	123.21
1	F	432	TPO	P-OG1-CB	-3.14	113.74	123.21
1	A	431	SEP	O2P-P-OG	2.84	114.30	106.73
1	B	432	TPO	O-C-CA	-2.83	117.37	124.78
2	D	432	TPO	P-OG1-CB	-2.80	114.74	123.21
2	D	432	TPO	CG2-CB-CA	-2.80	107.64	113.16
1	B	432	TPO	P-OG1-CB	-2.69	115.09	123.21
1	F	431	SEP	O2P-P-OG	2.53	113.47	106.73
1	B	431	SEP	OG-CB-CA	2.52	110.60	108.14
1	A	432	TPO	O-C-CA	-2.44	118.40	124.78
1	B	431	SEP	P-OG-CB	-2.30	111.97	118.30
1	E	431	SEP	O2P-P-OG	-2.22	100.82	106.73

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	432	TPO	O-C-CA-CB
1	F	432	TPO	N-CA-CB-CG2
1	F	432	TPO	N-CA-CB-OG1
1	F	432	TPO	C-CA-CB-CG2
1	F	432	TPO	O-C-CA-CB
1	F	432	TPO	CG2-CB-OG1-P
1	A	432	TPO	O-C-CA-CB
2	C	432	TPO	O-C-CA-CB
1	E	432	TPO	O-C-CA-CB
1	E	431	SEP	CB-OG-P-O2P
1	F	431	SEP	CA-CB-OG-P
1	F	431	SEP	CB-OG-P-O2P
1	F	431	SEP	CB-OG-P-O3P
1	A	431	SEP	CB-OG-P-O1P
1	A	431	SEP	CB-OG-P-O2P
1	A	431	SEP	CB-OG-P-O3P
1	B	431	SEP	CB-OG-P-O2P
1	B	431	SEP	CB-OG-P-O3P
1	E	431	SEP	CB-OG-P-O1P
1	B	431	SEP	CB-OG-P-O1P
1	E	431	SEP	CA-CB-OG-P
1	B	431	SEP	CA-CB-OG-P
2	C	432	TPO	N-CA-CB-CG2
1	F	432	TPO	CB-OG1-P-O1P
1	E	431	SEP	CB-OG-P-O3P
1	F	431	SEP	CB-OG-P-O1P
1	F	432	TPO	CB-OG1-P-O2P
1	B	432	TPO	O-C-CA-CB

There are no ring outliers.

10 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	432	TPO	2	0
2	D	432	TPO	3	0
1	F	432	TPO	2	0
1	A	432	TPO	2	0
2	C	432	TPO	5	0
1	E	432	TPO	2	0
1	E	431	SEP	4	0
1	F	431	SEP	5	0
1	A	431	SEP	2	0
1	B	431	SEP	13	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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
4	ATP	A	522	-	26,33,33	1.34	3 (11%)	31,52,52	1.83	6 (19%)
4	ATP	C	522	-	26,33,33	1.21	2 (7%)	31,52,52	1.76	4 (12%)
4	ATP	F	701	3	26,33,33	1.43	5 (19%)	31,52,52	1.94	7 (22%)
4	ATP	F	703	-	26,33,33	1.30	2 (7%)	31,52,52	1.79	5 (16%)
4	ATP	D	522	-	26,33,33	1.38	3 (11%)	31,52,52	1.79	5 (16%)
4	ATP	B	522	-	26,33,33	1.35	3 (11%)	31,52,52	1.88	6 (19%)
4	ATP	D	521	3	26,33,33	1.45	5 (19%)	31,52,52	1.93	7 (22%)
4	ATP	B	521	3	26,33,33	1.36	4 (15%)	31,52,52	1.92	6 (19%)
4	ATP	C	521	3	26,33,33	1.45	5 (19%)	31,52,52	1.88	6 (19%)
4	ATP	E	603	-	26,33,33	1.25	2 (7%)	31,52,52	1.81	5 (16%)
4	ATP	A	521	3	26,33,33	1.37	5 (19%)	31,52,52	1.94	7 (22%)
4	ATP	E	601	3	26,33,33	1.45	5 (19%)	31,52,52	1.97	6 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	A	522	-	-	7/18/38/38	0/3/3/3
4	ATP	C	522	-	-	8/18/38/38	0/3/3/3
4	ATP	F	701	3	-	8/18/38/38	0/3/3/3
4	ATP	F	703	-	-	8/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	D	522	-	-	7/18/38/38	0/3/3/3
4	ATP	B	522	-	-	7/18/38/38	0/3/3/3
4	ATP	D	521	3	-	7/18/38/38	0/3/3/3
4	ATP	B	521	3	-	5/18/38/38	0/3/3/3
4	ATP	C	521	3	-	6/18/38/38	0/3/3/3
4	ATP	E	603	-	-	7/18/38/38	0/3/3/3
4	ATP	A	521	3	-	6/18/38/38	0/3/3/3
4	ATP	E	601	3	-	6/18/38/38	0/3/3/3

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	522	ATP	C2-N3	4.36	1.39	1.32
4	F	703	ATP	C2-N3	4.25	1.38	1.32
4	E	601	ATP	C2-N3	4.22	1.38	1.32
4	A	522	ATP	C2-N3	4.07	1.38	1.32
4	C	521	ATP	C2-N3	4.06	1.38	1.32
4	D	522	ATP	C2-N3	4.02	1.38	1.32
4	F	701	ATP	C2-N3	3.97	1.38	1.32
4	D	521	ATP	C2-N3	3.79	1.38	1.32
4	E	603	ATP	C2-N3	3.75	1.38	1.32
4	C	522	ATP	C2-N3	3.74	1.38	1.32
4	A	521	ATP	C2-N3	3.70	1.38	1.32
4	B	521	ATP	C2-N3	3.58	1.37	1.32
4	B	521	ATP	C2-N1	2.89	1.39	1.33
4	F	701	ATP	C2-N1	2.77	1.39	1.33
4	A	522	ATP	C2-N1	2.67	1.38	1.33
4	A	521	ATP	C2-N1	2.66	1.38	1.33
4	E	601	ATP	C2-N1	2.65	1.38	1.33
4	E	601	ATP	C2'-C1'	-2.65	1.49	1.53
4	C	521	ATP	C2'-C1'	-2.63	1.49	1.53
4	A	521	ATP	O4'-C1'	2.63	1.44	1.41
4	D	522	ATP	C2'-C1'	-2.61	1.49	1.53
4	C	521	ATP	C2-N1	2.58	1.38	1.33
4	F	701	ATP	O4'-C1'	2.57	1.44	1.41
4	D	521	ATP	O4'-C1'	2.55	1.44	1.41
4	C	521	ATP	O4'-C1'	2.55	1.44	1.41
4	D	521	ATP	C2-N1	2.48	1.38	1.33
4	D	521	ATP	O2'-C2'	-2.47	1.37	1.43
4	F	701	ATP	C2'-C1'	-2.45	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	521	ATP	C2'-C1'	-2.43	1.50	1.53
4	F	703	ATP	C2-N1	2.36	1.38	1.33
4	B	522	ATP	O4'-C1'	2.34	1.44	1.41
4	B	522	ATP	C2-N1	2.31	1.38	1.33
4	B	521	ATP	O4'-C1'	2.21	1.44	1.41
4	E	601	ATP	O2'-C2'	-2.20	1.37	1.43
4	C	522	ATP	C2'-C1'	-2.19	1.50	1.53
4	D	522	ATP	O4'-C4'	-2.16	1.40	1.45
4	A	521	ATP	C2'-C1'	-2.13	1.50	1.53
4	E	603	ATP	C2'-C1'	-2.08	1.50	1.53
4	E	601	ATP	C4-N3	2.08	1.38	1.35
4	C	521	ATP	O2'-C2'	-2.08	1.38	1.43
4	A	521	ATP	O2'-C2'	-2.04	1.38	1.43
4	B	521	ATP	O2'-C2'	-2.03	1.38	1.43
4	F	701	ATP	C4-N3	2.02	1.38	1.35
4	A	522	ATP	O4'-C1'	2.02	1.43	1.41

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	521	ATP	N3-C2-N1	-5.64	119.86	128.68
4	D	522	ATP	N3-C2-N1	-5.56	119.98	128.68
4	C	522	ATP	N3-C2-N1	-5.54	120.02	128.68
4	E	601	ATP	N3-C2-N1	-5.54	120.02	128.68
4	A	521	ATP	N3-C2-N1	-5.50	120.07	128.68
4	D	521	ATP	N3-C2-N1	-5.50	120.08	128.68
4	E	603	ATP	N3-C2-N1	-5.49	120.09	128.68
4	A	522	ATP	N3-C2-N1	-5.46	120.14	128.68
4	C	521	ATP	N3-C2-N1	-5.44	120.18	128.68
4	F	701	ATP	N3-C2-N1	-5.42	120.21	128.68
4	B	522	ATP	N3-C2-N1	-5.40	120.23	128.68
4	F	703	ATP	N3-C2-N1	-5.30	120.40	128.68
4	F	701	ATP	C4-C5-N7	-4.42	104.80	109.40
4	E	601	ATP	C4-C5-N7	-4.39	104.82	109.40
4	A	521	ATP	C4-C5-N7	-4.31	104.91	109.40
4	F	703	ATP	C4-C5-N7	-4.28	104.94	109.40
4	B	522	ATP	C5-C6-N6	4.27	126.85	120.35
4	C	521	ATP	C4-C5-N7	-4.25	104.97	109.40
4	A	522	ATP	C5-C6-N6	4.20	126.73	120.35
4	B	521	ATP	C4-C5-N7	-4.18	105.04	109.40
4	D	521	ATP	C4-C5-N7	-4.17	105.05	109.40
4	B	522	ATP	C4-C5-N7	-4.17	105.05	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	522	ATP	C4-C5-N7	-4.16	105.06	109.40
4	A	522	ATP	C4-C5-N7	-4.04	105.19	109.40
4	E	603	ATP	C4-C5-N7	-4.02	105.21	109.40
4	F	703	ATP	C5-C6-N6	4.00	126.43	120.35
4	C	522	ATP	C4-C5-N7	-3.90	105.33	109.40
4	F	701	ATP	C5-C6-N6	3.84	126.18	120.35
4	E	603	ATP	C5-C6-N6	3.80	126.13	120.35
4	A	521	ATP	C5-C6-N6	3.77	126.09	120.35
4	D	522	ATP	C5-C6-N6	3.77	126.08	120.35
4	C	522	ATP	C5-C6-N6	3.71	125.99	120.35
4	E	601	ATP	C5-C6-N6	3.67	125.93	120.35
4	E	601	ATP	C3'-C2'-C1'	3.67	106.50	100.98
4	D	521	ATP	C5-C6-N6	3.64	125.88	120.35
4	B	521	ATP	C5-C6-N6	3.60	125.83	120.35
4	D	521	ATP	C3'-C2'-C1'	3.57	106.35	100.98
4	C	521	ATP	C3'-C2'-C1'	3.45	106.17	100.98
4	C	521	ATP	C5-C6-N6	3.39	125.50	120.35
4	A	521	ATP	C3'-C2'-C1'	3.32	105.98	100.98
4	F	701	ATP	C3'-C2'-C1'	3.31	105.96	100.98
4	E	603	ATP	C3'-C2'-C1'	3.17	105.75	100.98
4	B	521	ATP	C3'-C2'-C1'	3.08	105.61	100.98
4	A	522	ATP	C3'-C2'-C1'	2.86	105.29	100.98
4	D	522	ATP	C3'-C2'-C1'	2.82	105.22	100.98
4	B	522	ATP	C3'-C2'-C1'	2.81	105.21	100.98
4	B	521	ATP	PA-O3A-PB	2.70	142.10	132.83
4	D	521	ATP	PA-O3A-PB	2.67	142.00	132.83
4	C	521	ATP	PA-O3A-PB	2.65	141.93	132.83
4	E	601	ATP	PA-O3A-PB	2.62	141.81	132.83
4	A	521	ATP	PA-O3A-PB	2.58	141.67	132.83
4	F	701	ATP	PA-O3A-PB	2.56	141.61	132.83
4	B	522	ATP	N6-C6-N1	-2.49	113.41	118.57
4	B	521	ATP	O5'-PA-O1A	-2.40	99.68	109.07
4	F	703	ATP	C3'-C2'-C1'	2.40	104.59	100.98
4	C	522	ATP	C3'-C2'-C1'	2.31	104.46	100.98
4	E	601	ATP	O5'-PA-O1A	-2.31	100.04	109.07
4	D	521	ATP	O5'-PA-O1A	-2.30	100.10	109.07
4	B	522	ATP	PB-O3B-PG	-2.28	124.99	132.83
4	A	521	ATP	PB-O3B-PG	-2.19	125.31	132.83
4	A	522	ATP	N6-C6-N1	-2.16	114.09	118.57
4	F	701	ATP	PB-O3B-PG	-2.16	125.42	132.83
4	F	703	ATP	N6-C6-N1	-2.15	114.12	118.57
4	E	603	ATP	N6-C6-N1	-2.13	114.15	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	521	ATP	O5'-PA-O1A	-2.13	100.75	109.07
4	F	701	ATP	O5'-PA-O1A	-2.13	100.75	109.07
4	C	521	ATP	O5'-PA-O1A	-2.12	100.80	109.07
4	A	522	ATP	PB-O3B-PG	-2.08	125.68	132.83
4	D	521	ATP	PB-O3B-PG	-2.08	125.70	132.83
4	D	522	ATP	N6-C6-N1	-2.07	114.27	118.57

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	522	ATP	PB-O3B-PG-O3G
4	A	522	ATP	C5'-O5'-PA-O1A
4	A	522	ATP	O4'-C4'-C5'-O5'
4	A	522	ATP	C3'-C4'-C5'-O5'
4	E	601	ATP	PB-O3B-PG-O3G
4	E	601	ATP	PB-O3A-PA-O5'
4	F	701	ATP	PB-O3B-PG-O3G
4	F	701	ATP	PB-O3A-PA-O5'
4	D	522	ATP	PB-O3B-PG-O3G
4	D	522	ATP	C5'-O5'-PA-O1A
4	D	522	ATP	O4'-C4'-C5'-O5'
4	D	522	ATP	C3'-C4'-C5'-O5'
4	C	522	ATP	PB-O3B-PG-O3G
4	C	522	ATP	C5'-O5'-PA-O1A
4	F	703	ATP	PB-O3B-PG-O3G
4	F	703	ATP	C5'-O5'-PA-O1A
4	F	703	ATP	O4'-C4'-C5'-O5'
4	D	521	ATP	PB-O3B-PG-O3G
4	D	521	ATP	PB-O3A-PA-O5'
4	B	521	ATP	PB-O3B-PG-O3G
4	B	521	ATP	PB-O3A-PA-O5'
4	C	521	ATP	PB-O3B-PG-O3G
4	C	521	ATP	PB-O3A-PA-O5'
4	E	603	ATP	PB-O3B-PG-O3G
4	E	603	ATP	C5'-O5'-PA-O1A
4	E	603	ATP	O4'-C4'-C5'-O5'
4	E	603	ATP	C3'-C4'-C5'-O5'
4	A	521	ATP	PB-O3B-PG-O3G
4	A	521	ATP	PB-O3A-PA-O5'
4	B	522	ATP	PB-O3B-PG-O3G
4	C	522	ATP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	C	522	ATP	C3'-C4'-C5'-O5'
4	F	703	ATP	C3'-C4'-C5'-O5'
4	B	522	ATP	O4'-C4'-C5'-O5'
4	B	522	ATP	C3'-C4'-C5'-O5'
4	A	522	ATP	PB-O3A-PA-O1A
4	D	522	ATP	PB-O3A-PA-O5'
4	C	522	ATP	PB-O3A-PA-O5'
4	F	703	ATP	PB-O3A-PA-O5'
4	E	603	ATP	PB-O3A-PA-O5'
4	B	522	ATP	PB-O3A-PA-O5'
4	E	601	ATP	C5'-O5'-PA-O3A
4	F	701	ATP	C5'-O5'-PA-O3A
4	D	521	ATP	C5'-O5'-PA-O3A
4	B	521	ATP	C5'-O5'-PA-O3A
4	C	521	ATP	C5'-O5'-PA-O3A
4	A	521	ATP	C5'-O5'-PA-O3A
4	A	522	ATP	PA-O3A-PB-O2B
4	E	601	ATP	PA-O3A-PB-O2B
4	F	701	ATP	PA-O3A-PB-O2B
4	D	522	ATP	PA-O3A-PB-O2B
4	D	522	ATP	PB-O3A-PA-O1A
4	C	522	ATP	PA-O3A-PB-O2B
4	F	703	ATP	PA-O3A-PB-O2B
4	D	521	ATP	PA-O3A-PB-O2B
4	B	521	ATP	PA-O3A-PB-O2B
4	C	521	ATP	PA-O3A-PB-O2B
4	E	603	ATP	PA-O3A-PB-O2B
4	A	521	ATP	PA-O3A-PB-O2B
4	B	522	ATP	PA-O3A-PB-O2B
4	C	522	ATP	PB-O3A-PA-O1A
4	E	603	ATP	PB-O3A-PA-O1A
4	B	522	ATP	PB-O3A-PA-O1A
4	F	703	ATP	PB-O3A-PA-O1A
4	A	521	ATP	PB-O3A-PA-O2A
4	A	522	ATP	PB-O3A-PA-O5'
4	C	522	ATP	PB-O3B-PG-O1G
4	F	703	ATP	PB-O3B-PG-O1G
4	E	601	ATP	PB-O3B-PG-O2G
4	F	701	ATP	PB-O3B-PG-O2G
4	D	521	ATP	PB-O3B-PG-O2G
4	B	521	ATP	PB-O3B-PG-O2G
4	C	521	ATP	PB-O3B-PG-O2G

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Mol	Chain	Res	Type	Atoms
4	A	521	ATP	PB-O3B-PG-O2G
4	F	701	ATP	PB-O3A-PA-O2A
4	D	521	ATP	PB-O3A-PA-O1A
4	D	521	ATP	PB-O3A-PA-O2A
4	C	521	ATP	PB-O3A-PA-O2A
4	F	701	ATP	C5'-O5'-PA-O1A
4	B	522	ATP	C5'-O5'-PA-O1A
4	E	601	ATP	PB-O3B-PG-O1G
4	F	701	ATP	PB-O3B-PG-O1G

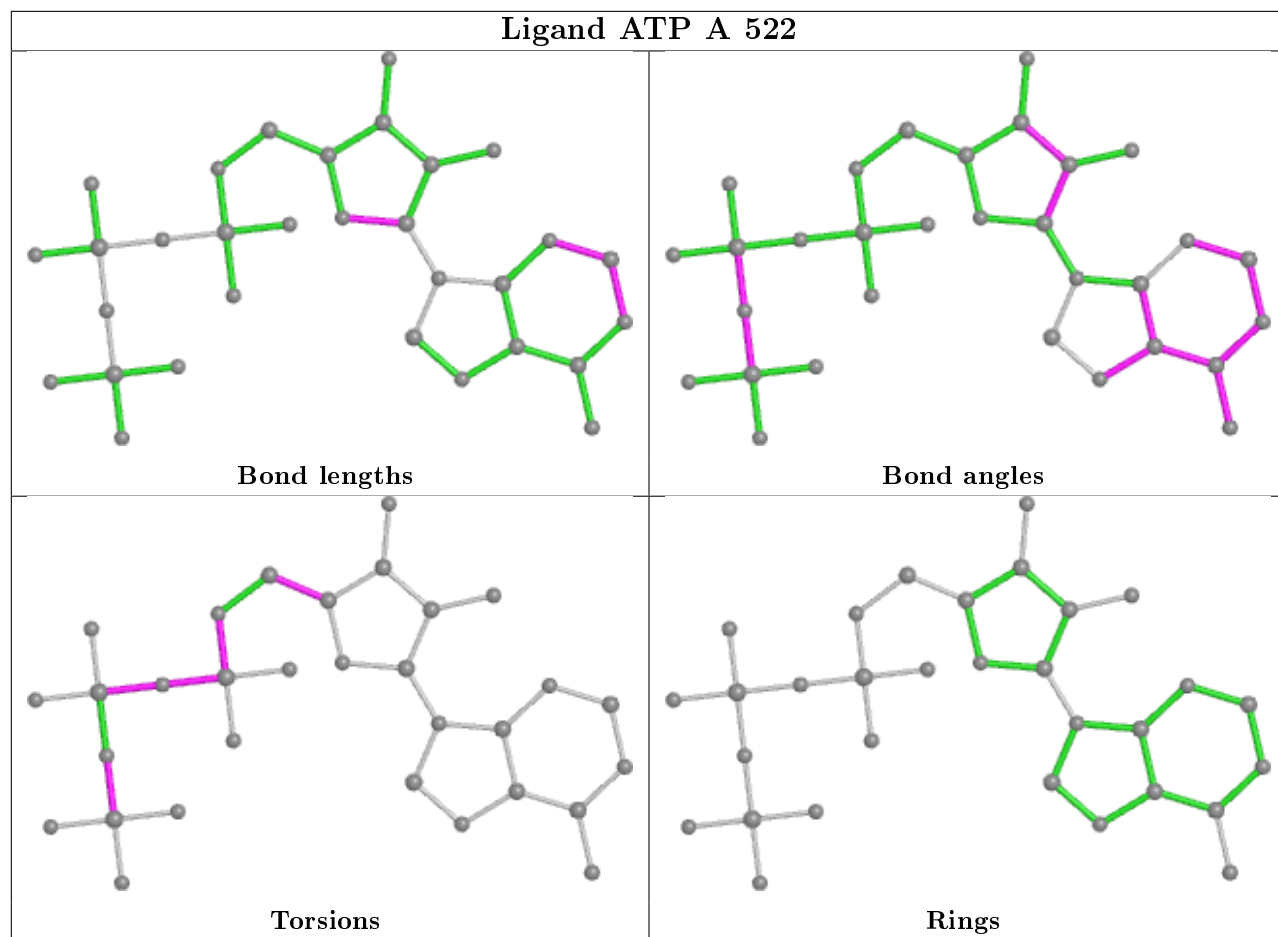
There are no ring outliers.

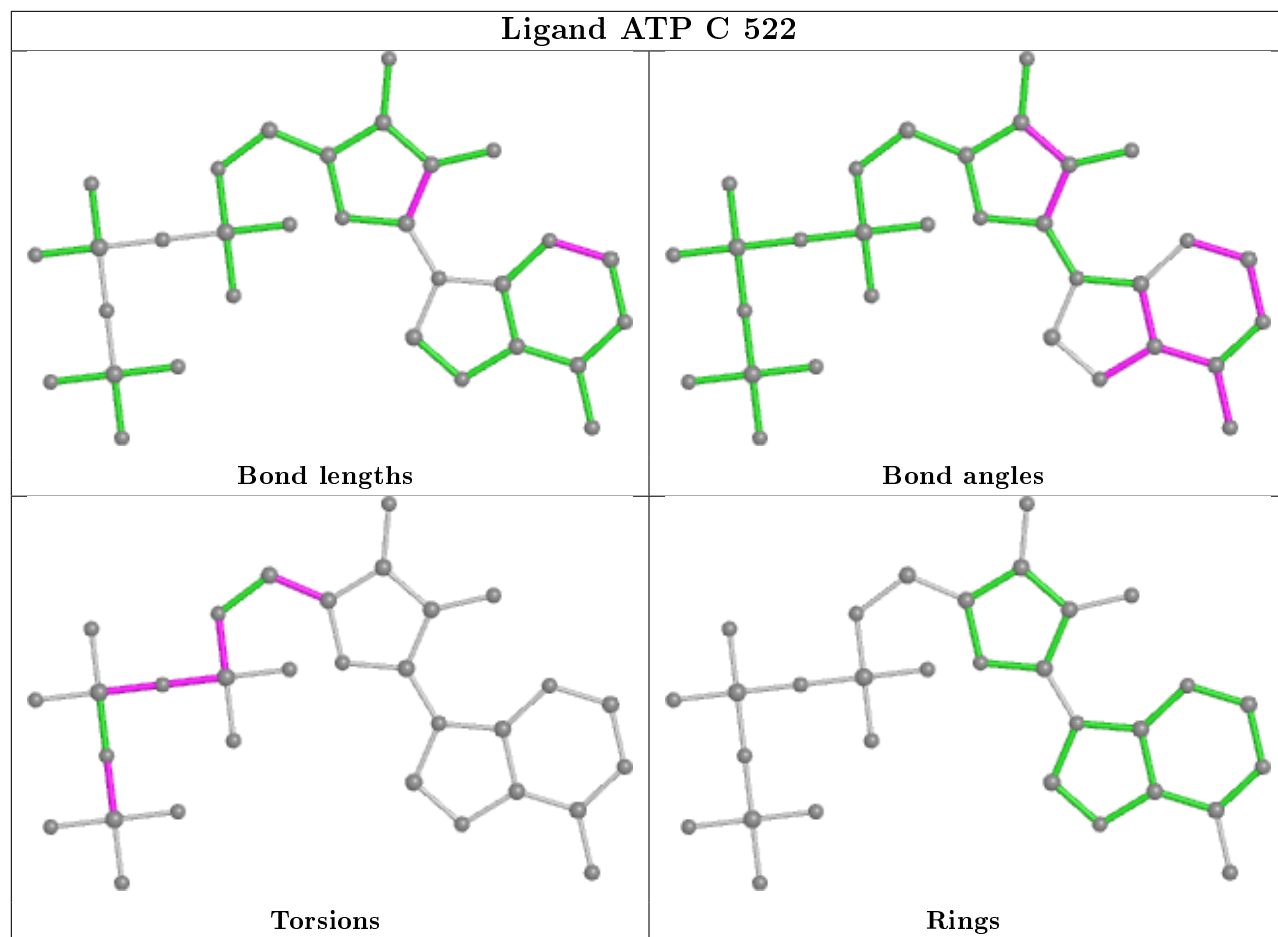
12 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	522	ATP	3	0
4	C	522	ATP	4	0
4	F	701	ATP	4	0
4	F	703	ATP	3	0
4	D	522	ATP	3	0
4	B	522	ATP	4	0
4	D	521	ATP	8	0
4	B	521	ATP	4	0
4	C	521	ATP	8	0
4	E	603	ATP	4	0
4	A	521	ATP	5	0
4	E	601	ATP	4	0

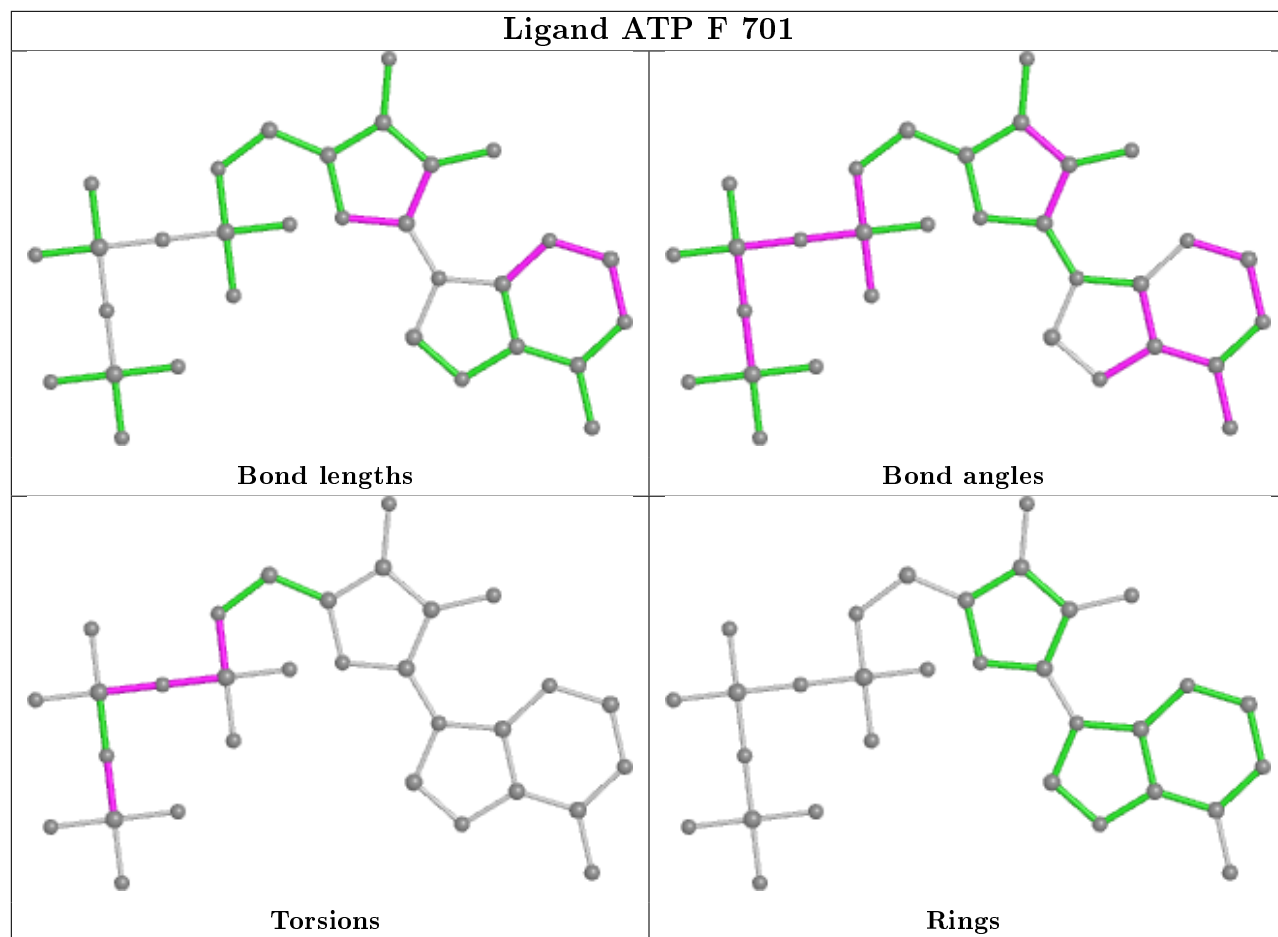
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ATP A 522

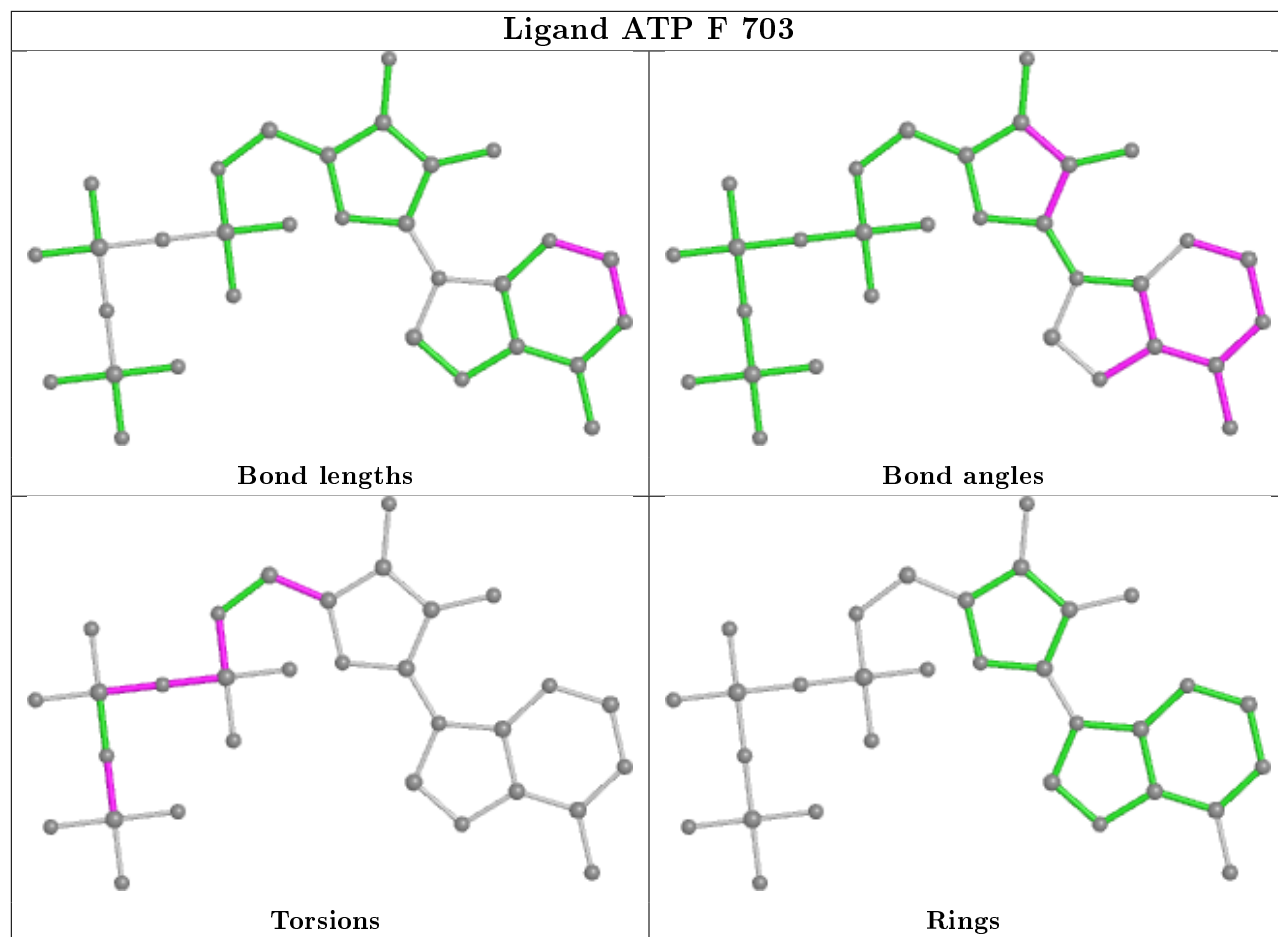


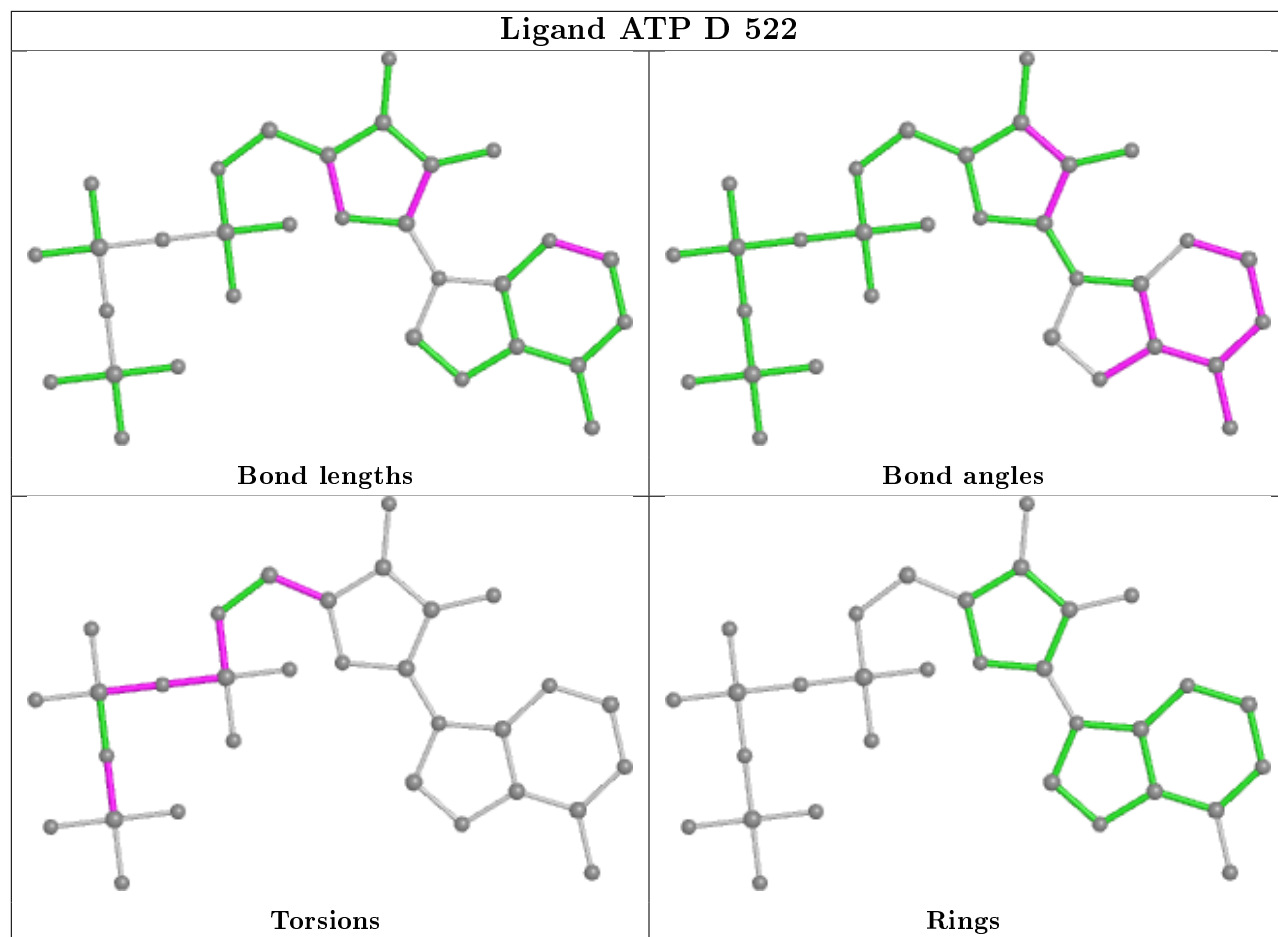


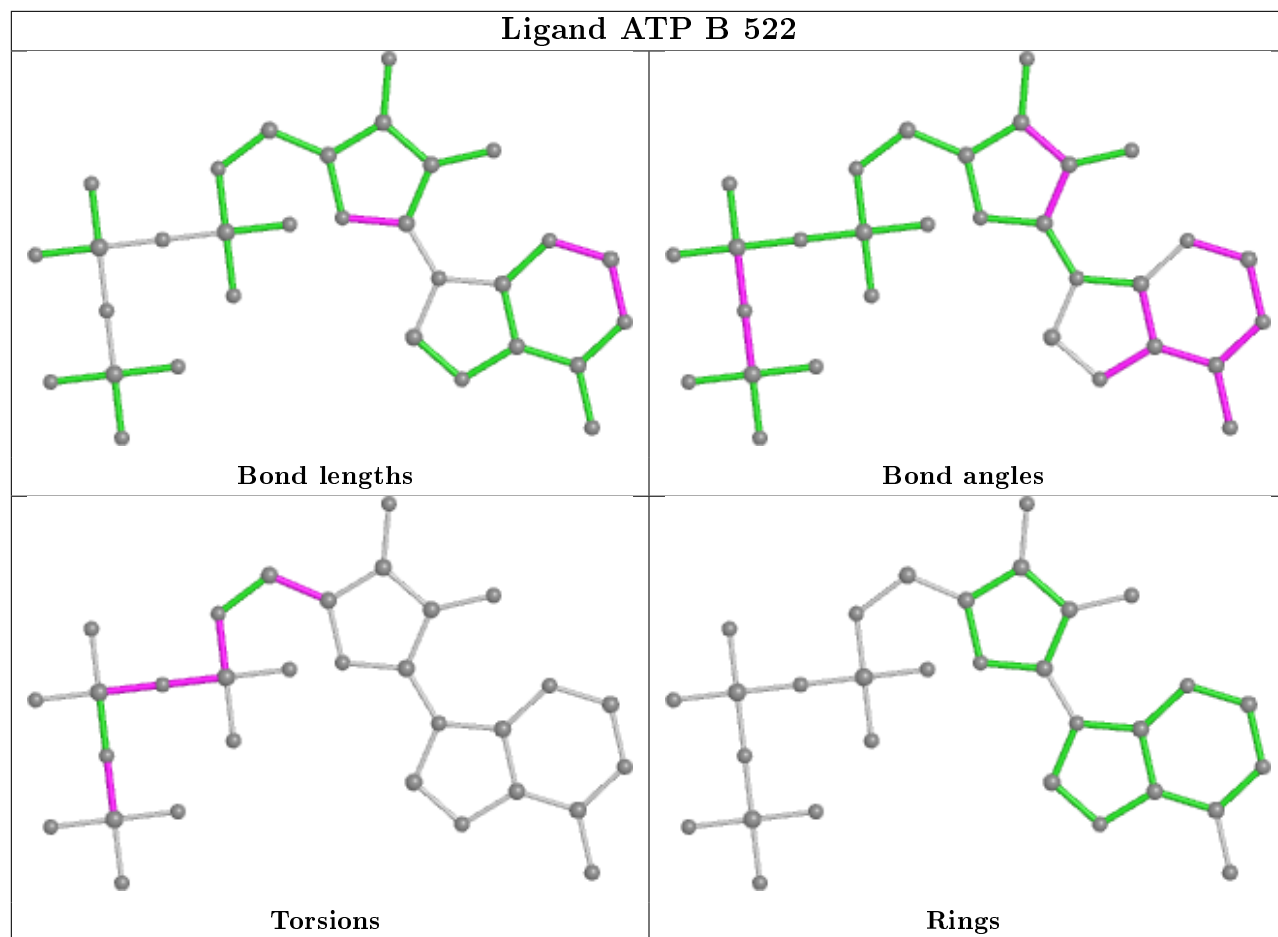
Ligand ATP F 701

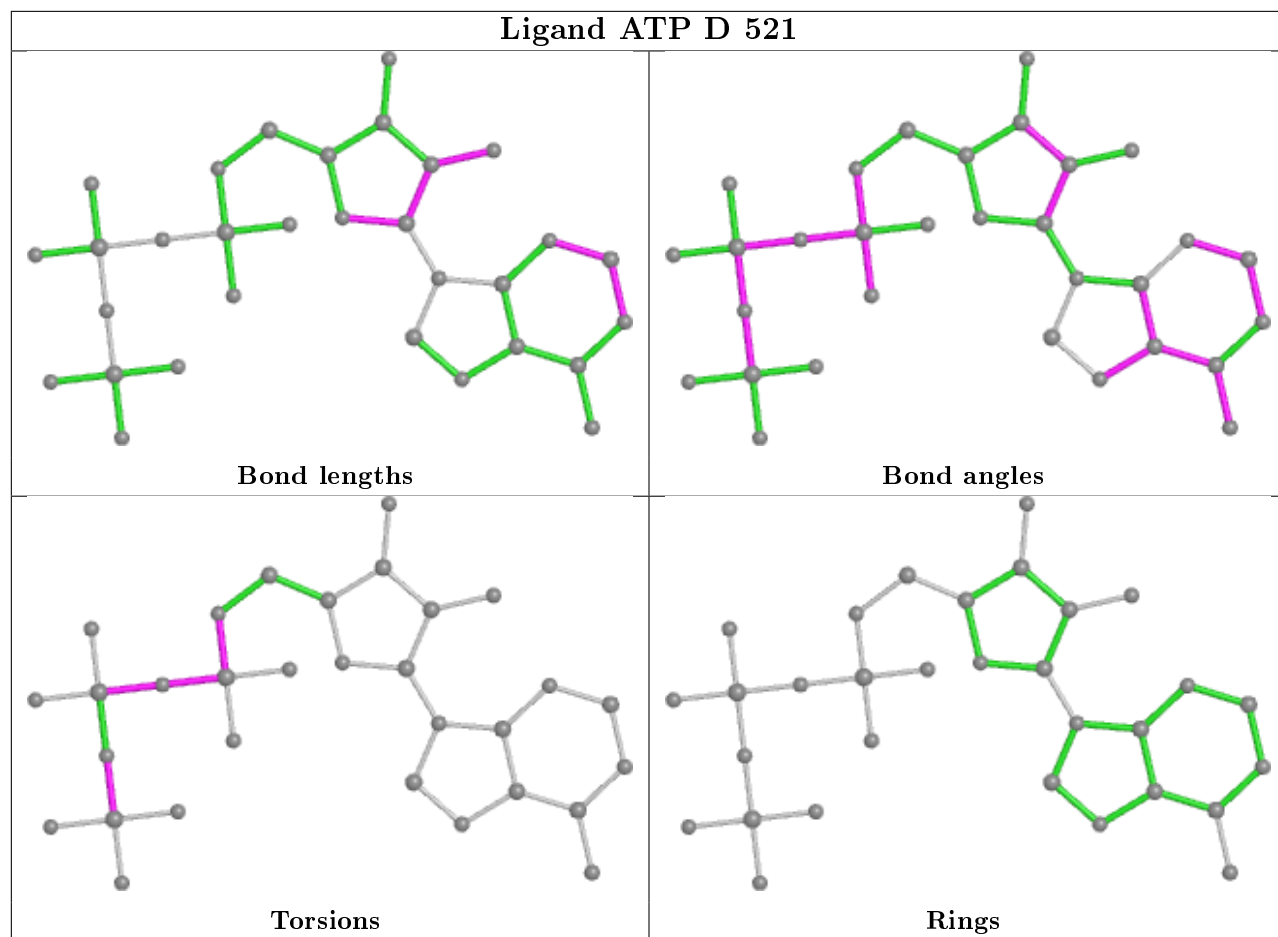


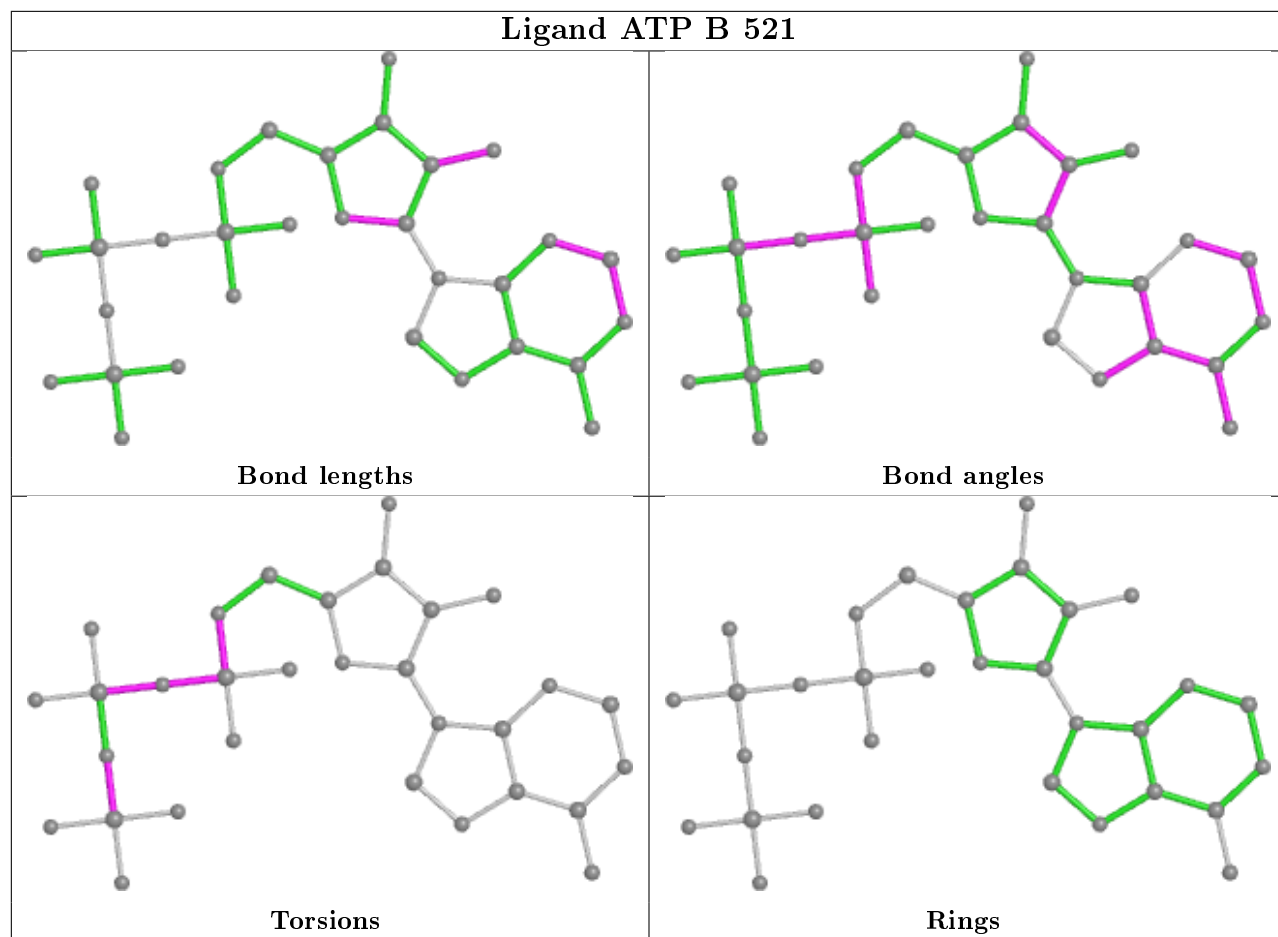
Ligand ATP F 703

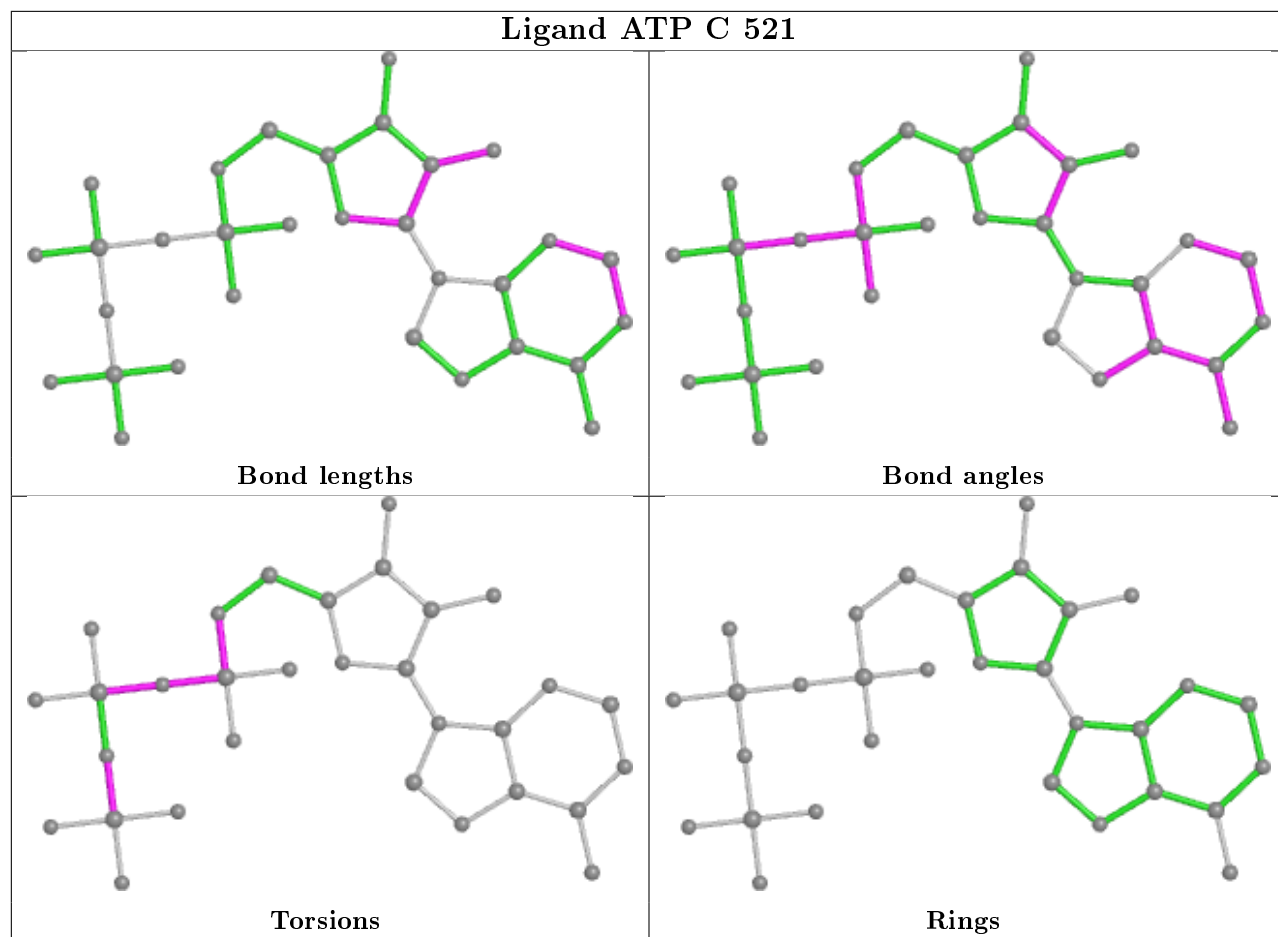




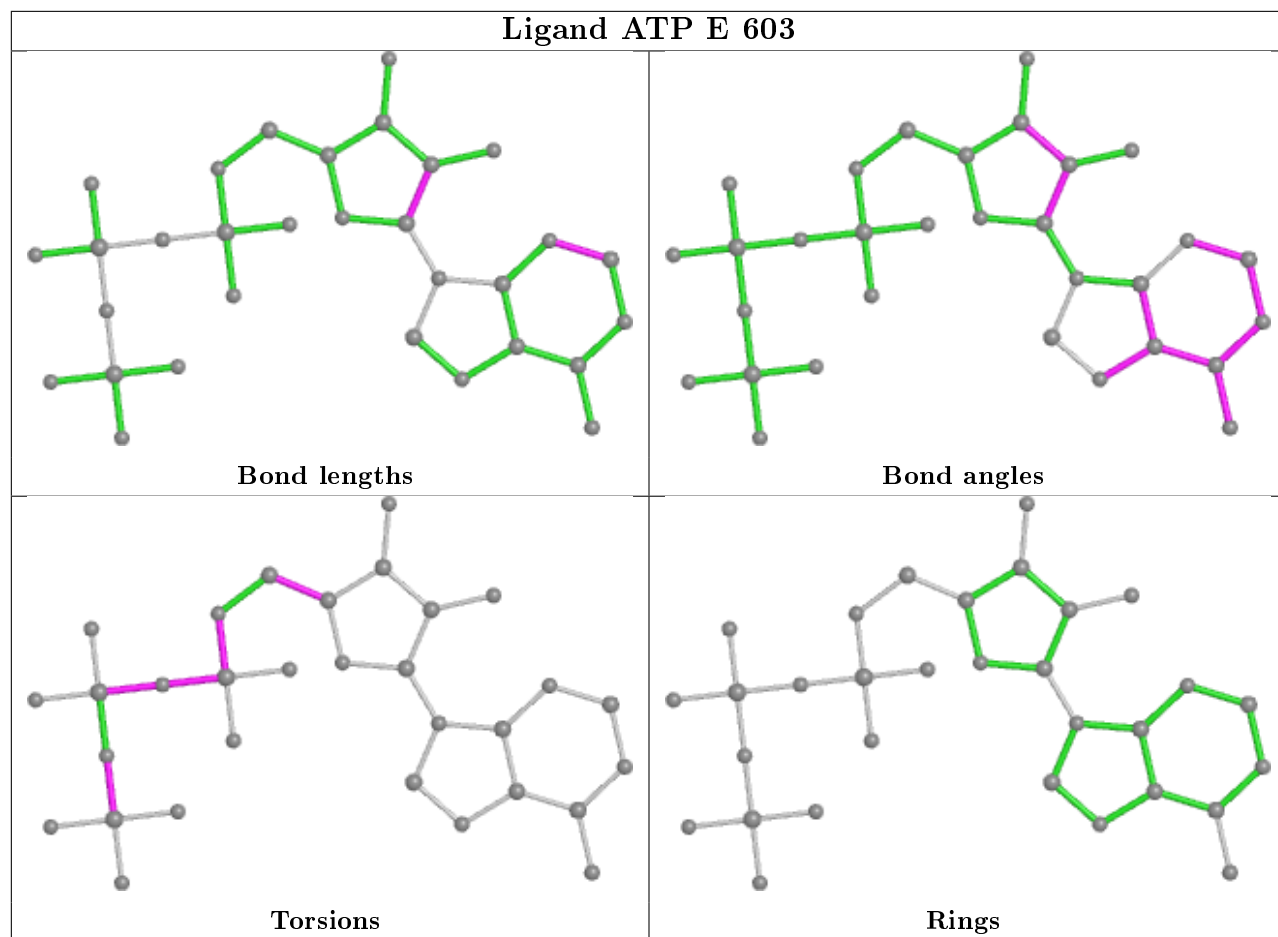




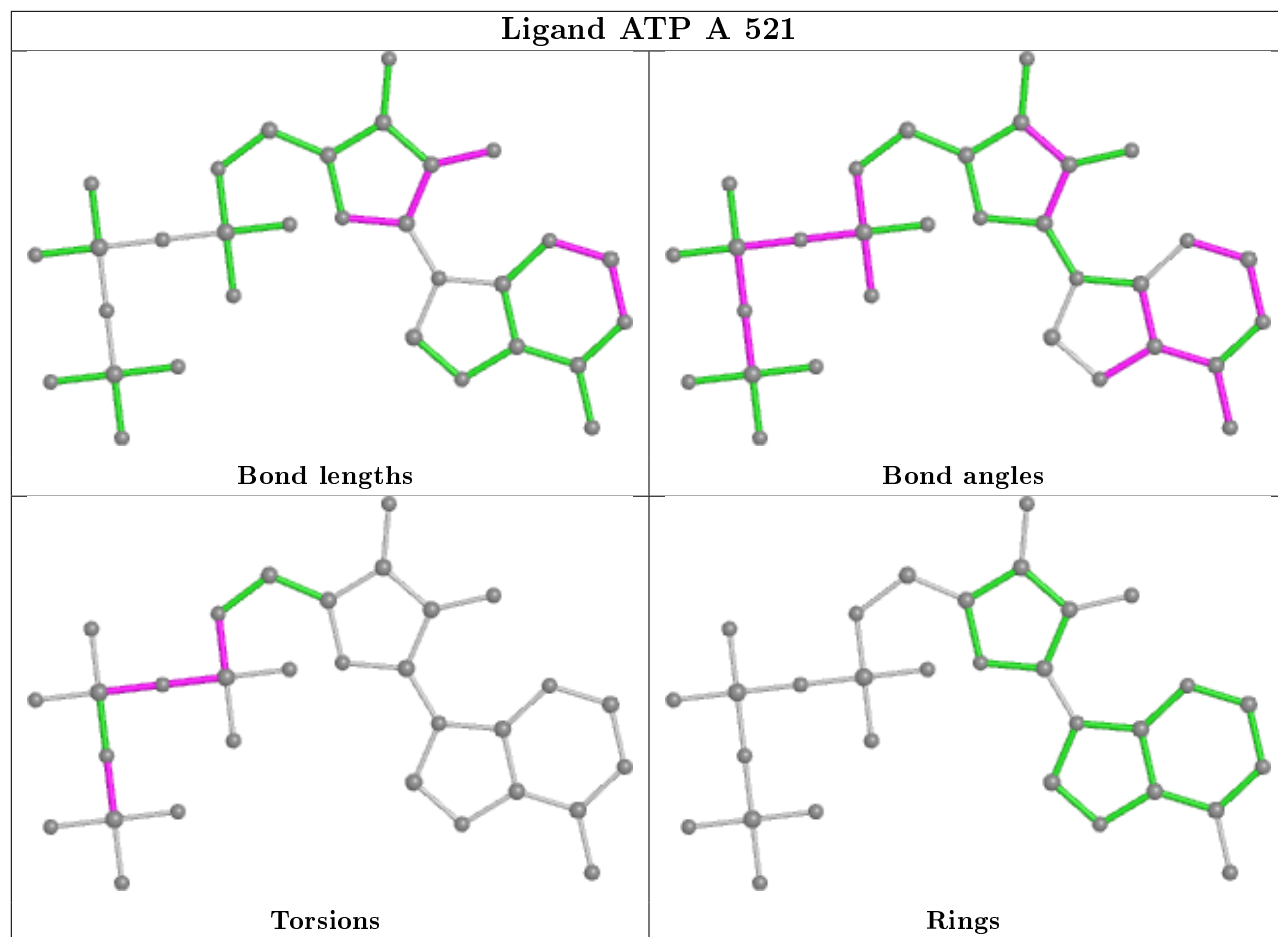


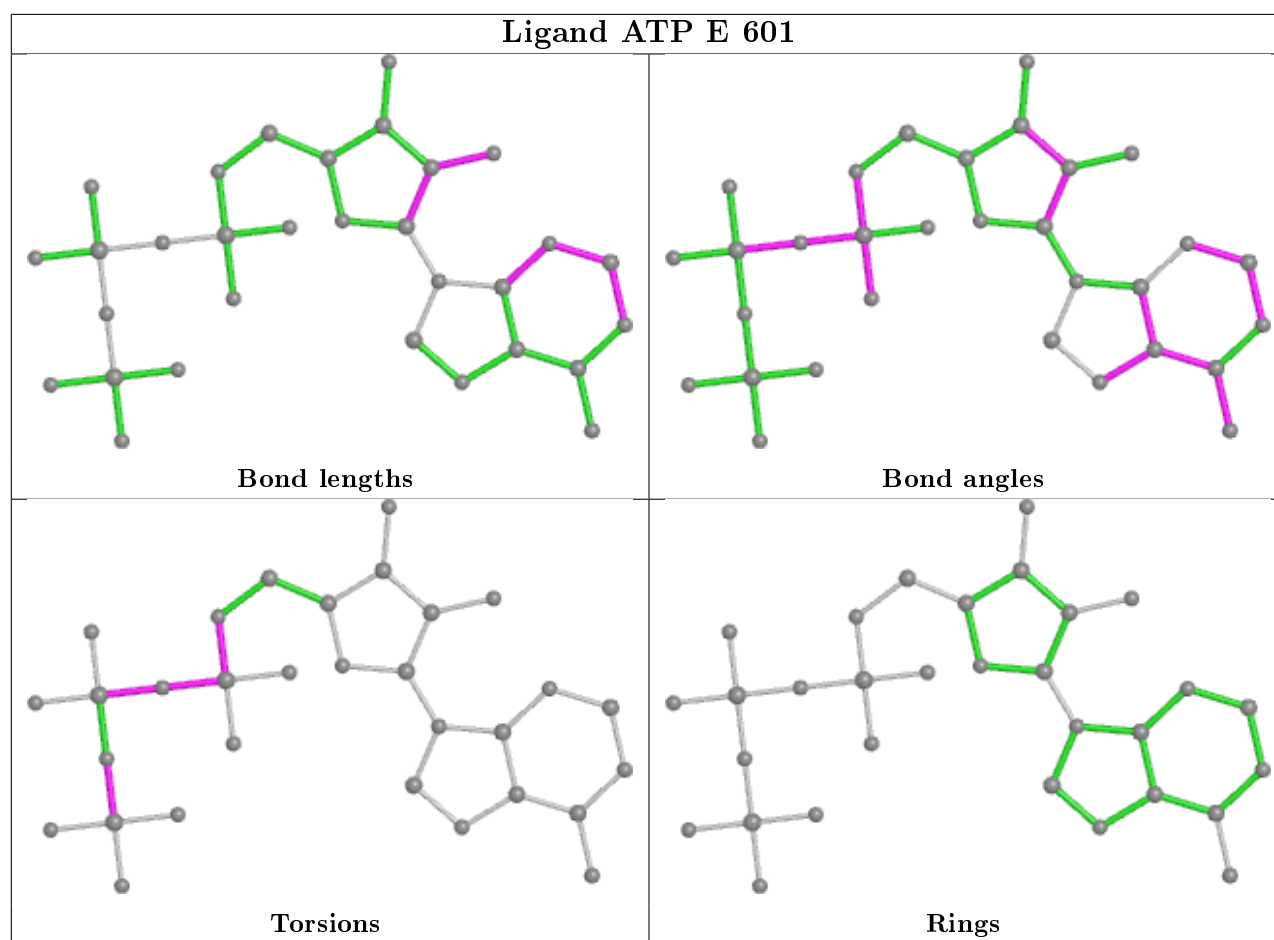


Ligand ATP E 603



Ligand ATP A 521





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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	482/519 (92%)	0.35	46 (9%)	8 4	32, 78, 130, 157	0
1	B	482/519 (92%)	0.43	33 (6%)	17 10	43, 85, 131, 163	0
1	E	482/519 (92%)	0.01	30 (6%)	20 13	23, 62, 109, 158	0
1	F	482/519 (92%)	0.11	22 (4%)	32 22	23, 71, 117, 161	0
2	C	483/519 (93%)	0.21	28 (5%)	23 15	36, 75, 126, 163	0
2	D	483/519 (93%)	0.02	23 (4%)	30 21	29, 60, 112, 163	0
All	All	2894/3114 (92%)	0.19	182 (6%)	20 12	23, 73, 124, 163	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	118	VAL	9.7
1	B	118	VAL	9.1
1	B	116	GLU	8.3
1	B	117	VAL	7.3
2	D	117	VAL	7.2
1	A	121	PHE	7.1
2	D	121	PHE	7.1
2	D	118	VAL	6.9
1	F	154	TYR	6.8
1	F	117	VAL	6.7
2	C	117	VAL	6.5
1	B	121	PHE	6.4
2	C	120	GLY	6.4
2	D	120	GLY	6.3
1	A	257	ARG	6.2
1	A	258	SER	5.3
2	C	119	GLY	5.2
2	D	119	GLY	5.2
1	E	154	TYR	4.9

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Mol	Chain	Res	Type	RSRZ
2	C	17	ALA	4.8
1	B	258	SER	4.7
1	B	154	TYR	4.7
1	E	117	VAL	4.7
1	F	257	ARG	4.6
2	D	113	GLU	4.5
1	B	119	GLY	4.4
1	A	475	LYS	4.3
2	D	154	TYR	4.3
1	B	115	GLN	4.3
1	F	366	GLU	4.3
1	B	15	HIS	4.3
1	B	255	THR	4.1
1	A	251	ALA	4.1
1	B	16	GLN	3.9
2	D	15	HIS	3.8
1	B	366	GLU	3.8
1	F	116	GLU	3.8
1	A	120	GLY	3.8
1	E	366	GLU	3.8
2	C	15	HIS	3.8
2	C	423	HIS	3.8
1	A	154	TYR	3.8
1	E	153	GLN	3.8
2	D	158	SER	3.7
2	C	153	GLN	3.7
1	E	118	VAL	3.7
1	A	253	ARG	3.6
1	F	311	ARG	3.6
1	A	496	ARG	3.5
1	B	321	ARG	3.5
1	A	329	TYR	3.5
1	F	156	ALA	3.4
1	B	257	ARG	3.4
1	F	253	ARG	3.4
1	F	485	ASN	3.4
1	B	157	SER	3.3
1	E	152	GLN	3.3
1	B	155	ASP	3.3
1	F	484	ARG	3.3
1	B	253	ARG	3.2
1	A	311	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	496	ARG	3.2
1	A	295	THR	3.2
1	A	256	GLN	3.2
1	E	474	ASP	3.2
1	A	17	ALA	3.1
1	E	329	TYR	3.1
1	E	120	GLY	3.1
1	F	252	MET	3.1
1	A	114	GLY	3.1
1	F	121	PHE	3.1
2	D	471	MET	3.1
2	C	152	GLN	3.1
2	D	16	GLN	3.1
1	A	341	GLN	3.1
2	C	115	GLN	3.1
1	E	321	ARG	3.1
1	A	16	GLN	3.1
1	A	318	GLU	3.1
1	A	342	ASN	3.0
2	C	154	TYR	3.0
1	B	158	SER	3.0
1	A	241	ASP	3.0
2	D	114	GLY	3.0
1	A	255	THR	2.9
1	A	15	HIS	2.9
1	A	14	GLU	2.9
1	A	116	GLU	2.9
2	C	116	GLU	2.9
1	B	53	THR	2.9
1	F	118	VAL	2.9
1	A	309	LYS	2.8
2	C	366	GLU	2.8
2	D	496	ARG	2.8
1	B	122	ASP	2.8
2	C	138	ARG	2.8
1	E	112	PRO	2.8
1	B	497	ILE	2.8
1	A	115	GLN	2.8
2	C	53	THR	2.7
1	F	340	ARG	2.7
1	B	120	GLY	2.7
1	B	88	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	116	GLU	2.7
1	A	321	ARG	2.7
1	E	119	GLY	2.6
1	A	378	ASP	2.6
1	A	368	ASN	2.6
1	A	113	GLU	2.6
1	B	259	SER	2.6
2	D	249	LEU	2.6
1	A	417	ASP	2.6
1	E	166	ARG	2.6
1	A	153	GLN	2.6
1	E	334	ASP	2.6
2	D	484	ARG	2.6
1	A	249	LEU	2.6
1	E	421	GLY	2.6
2	D	160	VAL	2.6
1	B	250	GLY	2.5
2	C	123	LEU	2.5
2	C	170	ARG	2.5
1	F	321	ARG	2.5
1	E	484	ARG	2.5
1	A	250	GLY	2.5
1	E	121	PHE	2.4
2	C	253	ARG	2.4
2	C	121	PHE	2.4
2	C	140	ARG	2.4
1	E	111	ASP	2.4
1	A	117	VAL	2.4
2	D	366	GLU	2.4
1	E	114	GLY	2.4
2	C	16	GLN	2.3
1	F	255	THR	2.3
1	B	90	PHE	2.3
1	A	338	MET	2.3
1	A	340	ARG	2.3
2	C	92	TRP	2.3
1	B	92	TRP	2.3
1	B	251	ALA	2.3
2	D	338	MET	2.3
1	B	436	THR	2.2
1	E	115	GLN	2.2
2	D	309	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	413	THR	2.2
2	C	189	GLY	2.2
1	F	343	LEU	2.2
1	B	252	MET	2.2
1	E	341	GLN	2.2
1	A	344	LEU	2.2
2	D	112	PRO	2.2
1	A	402	TYR	2.2
1	F	157	SER	2.2
2	C	252	MET	2.2
2	C	145	ASP	2.2
1	A	473	SER	2.2
2	C	181	THR	2.2
1	F	344	LEU	2.1
1	B	17	ALA	2.1
1	E	378	ASP	2.1
2	C	114	GLY	2.1
1	B	181	THR	2.1
1	E	337	GLU	2.1
2	D	115	GLN	2.1
2	D	53	THR	2.1
2	C	257	ARG	2.1
1	B	89	SER	2.1
1	E	113	GLU	2.1
1	E	173	GLN	2.1
1	E	188	TYR	2.1
1	A	188	TYR	2.1
1	A	477	PRO	2.1
1	F	423	HIS	2.0
1	A	145	ASP	2.0
1	A	379	SER	2.0
2	D	152	GLN	2.0
1	F	251	ALA	2.0
1	E	423	HIS	2.0
1	E	338	MET	2.0
1	E	471	MET	2.0
1	A	405	GLN	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. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SEP	E	431	10/11	0.58	0.41	6,59,62,63	0
1	TPO	F	432	11/12	0.59	0.43	5,12,77,78	0
2	TPO	D	432	11/12	0.65	0.39	5,11,63,66	0
1	SEP	F	431	10/11	0.65	0.42	6,82,85,85	0
1	SEP	B	431	10/11	0.65	0.42	6,84,89,90	0
1	TPO	A	432	11/12	0.67	0.43	5,21,84,85	0
1	SEP	A	431	10/11	0.68	0.41	6,81,83,86	0
2	TPO	C	432	11/12	0.68	0.41	5,12,80,81	0
1	TPO	B	432	11/12	0.70	0.40	5,21,85,86	0
1	TPO	E	432	11/12	0.72	0.34	5,12,61,63	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	F	520	1/1	0.53	0.30	21,21,21,21	0
3	MG	B	520	1/1	0.62	0.36	75,75,75,75	0
3	MG	D	520	1/1	0.68	0.24	21,21,21,21	0
3	MG	E	520	1/1	0.77	0.22	21,21,21,21	0
4	ATP	F	701	31/31	0.84	0.28	76,92,116,123	0
4	ATP	A	522	31/31	0.84	0.25	44,56,78,83	0
4	ATP	B	522	31/31	0.84	0.21	45,56,79,83	0
3	MG	A	520	1/1	0.85	0.15	21,21,21,21	0
4	ATP	A	521	31/31	0.86	0.28	77,91,105,114	0
4	ATP	C	522	31/31	0.88	0.24	45,56,79,83	0
4	ATP	D	522	31/31	0.89	0.28	44,56,79,83	0
4	ATP	F	703	31/31	0.90	0.23	44,56,78,82	0
4	ATP	E	601	31/31	0.90	0.23	63,79,103,115	0
4	ATP	B	521	31/31	0.90	0.23	64,75,111,118	0
4	ATP	C	521	31/31	0.92	0.19	50,57,99,112	0
4	ATP	D	521	31/31	0.93	0.24	55,68,91,106	0

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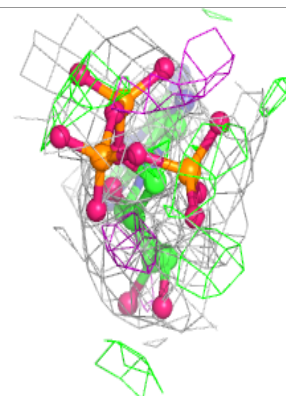
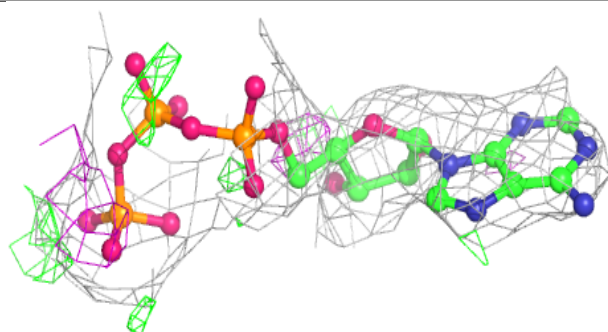
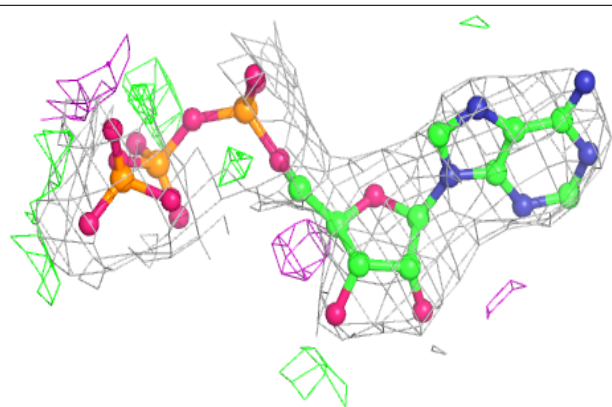
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ATP	E	603	31/31	0.94	0.24	44,56,78,82	0
3	MG	C	520	1/1	0.96	0.10	21,21,21,21	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

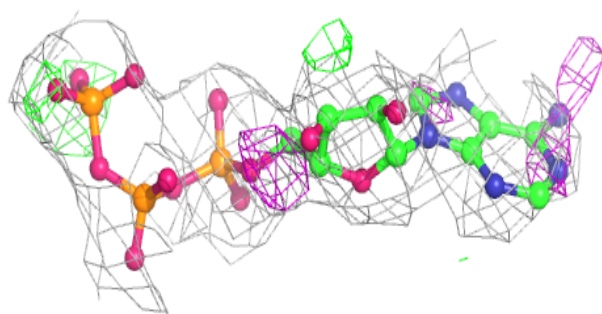
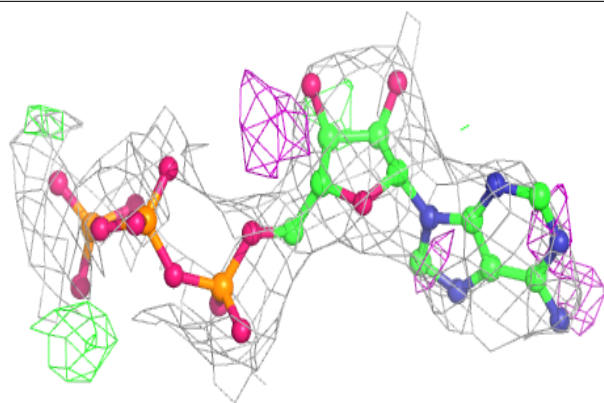
Electron density around ATP F 701:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

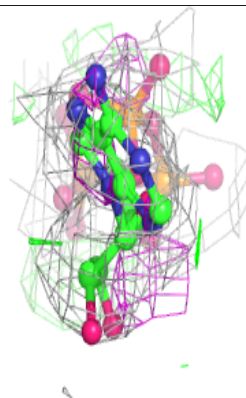
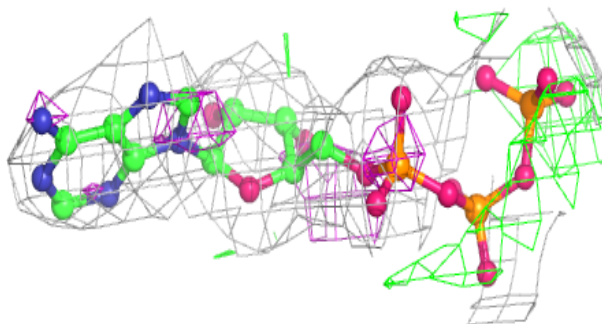
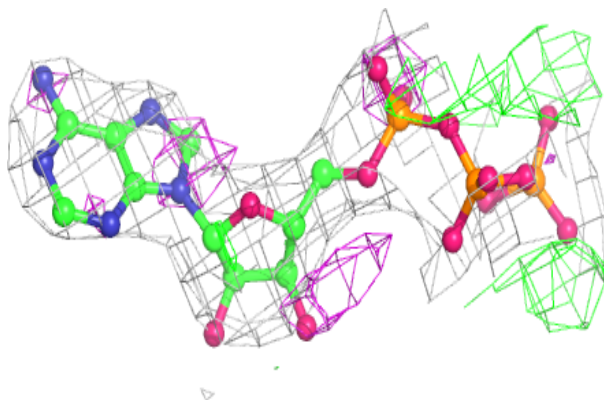


Electron density around ATP A 522:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

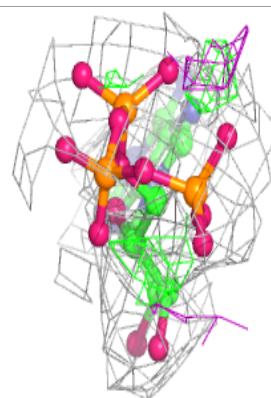
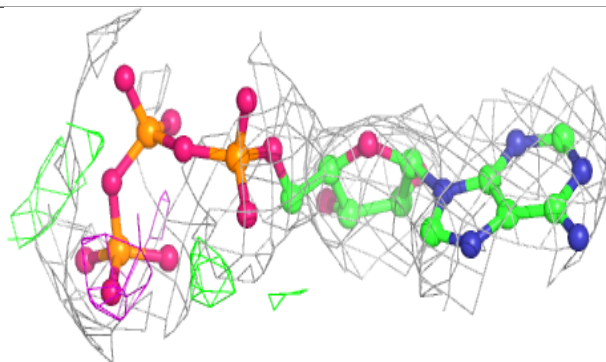
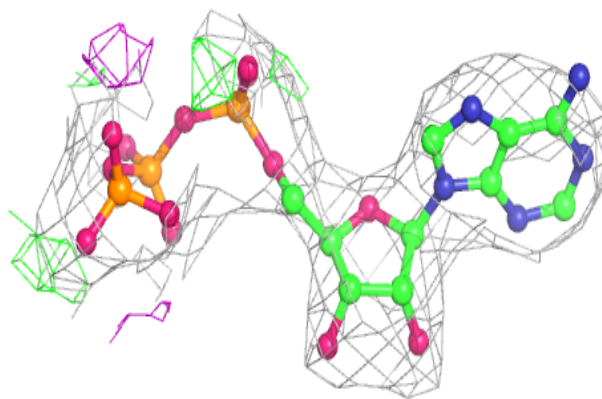
**Electron density around ATP B 522:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

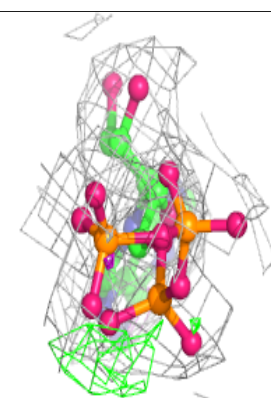
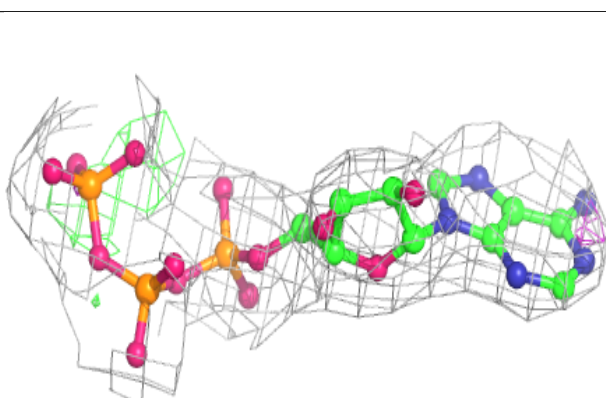
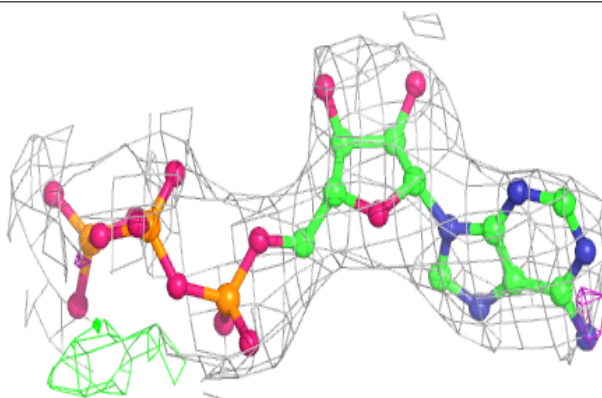


Electron density around ATP A 521:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

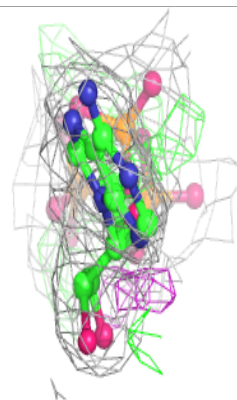
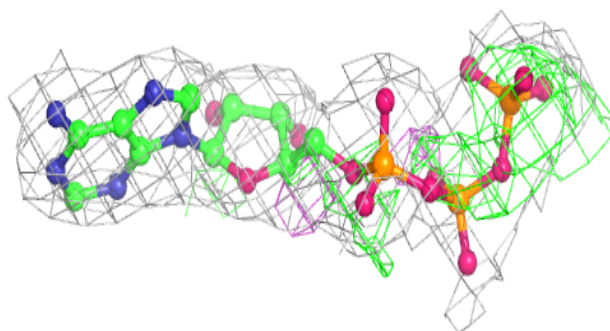
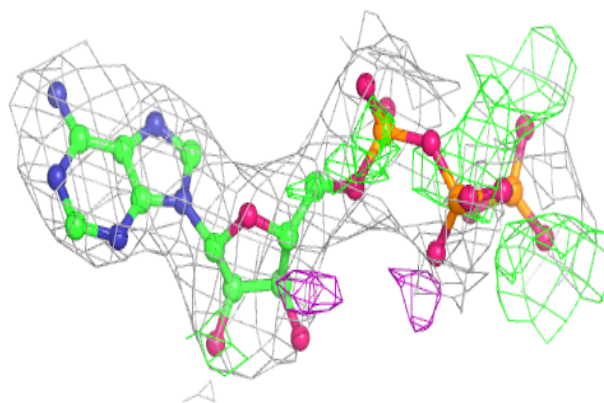
**Electron density around ATP C 522:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

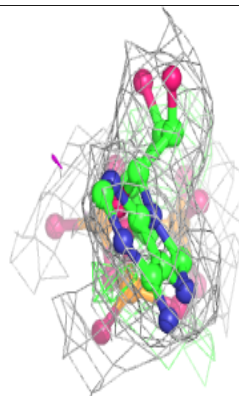
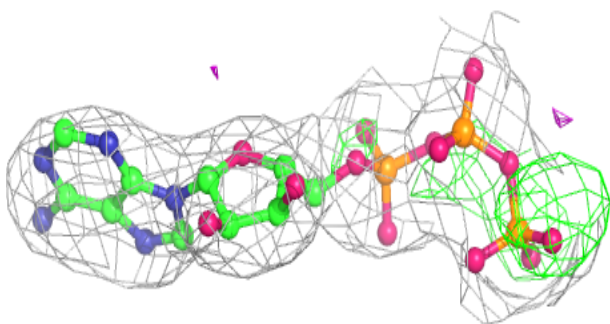
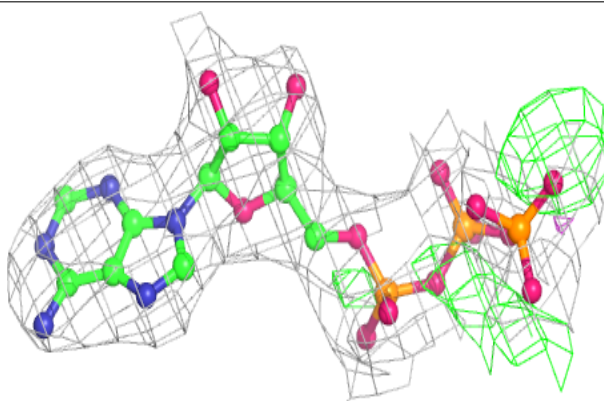


Electron density around ATP D 522:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

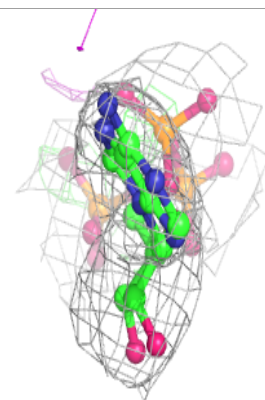
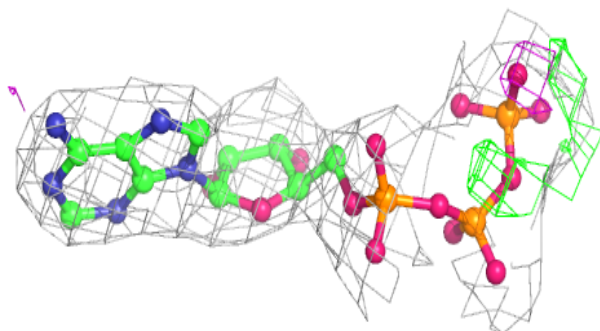
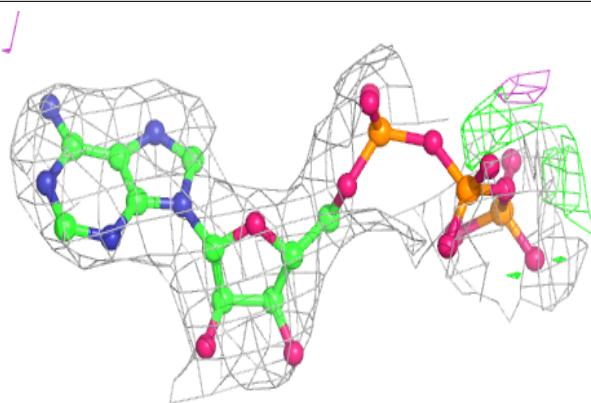
**Electron density around ATP F 703:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

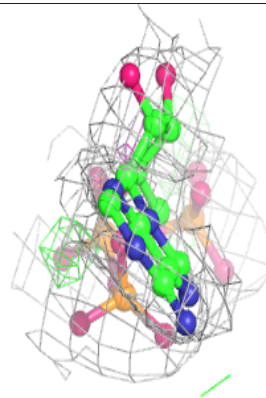
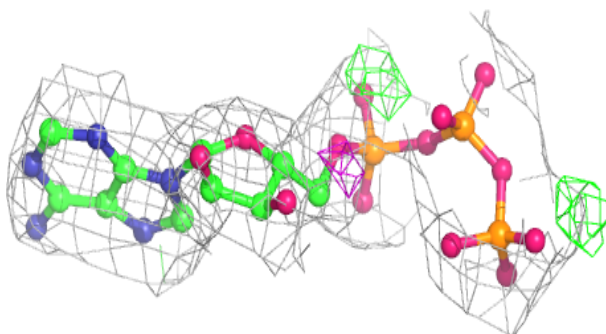
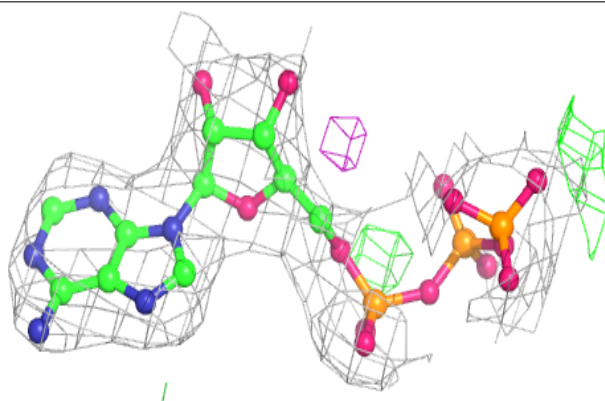


Electron density around ATP E 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

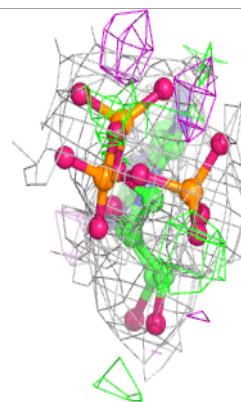
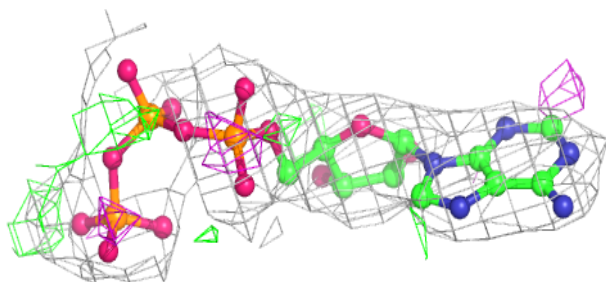
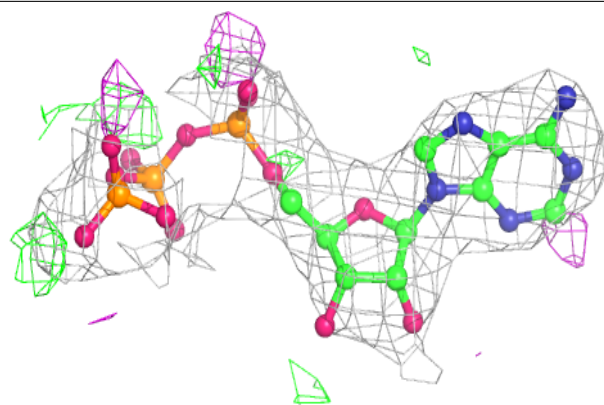
**Electron density around ATP B 521:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

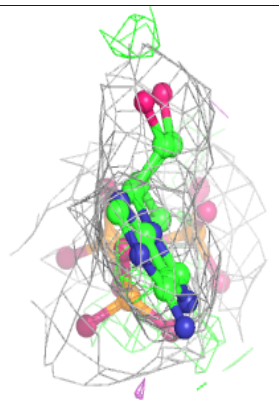
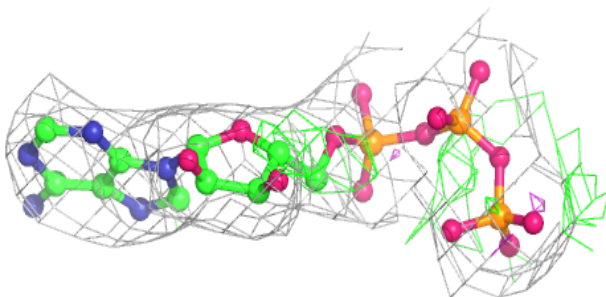
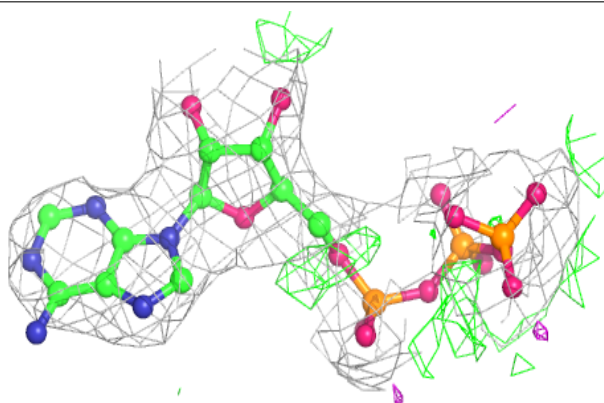


Electron density around ATP C 521:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

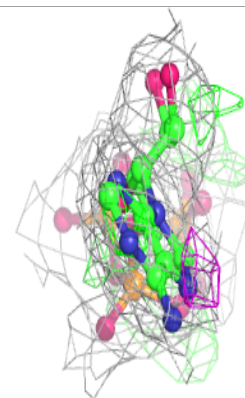
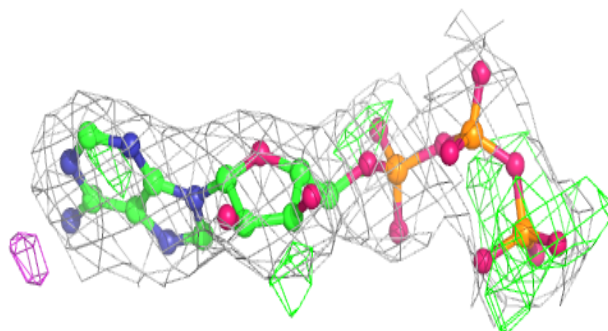
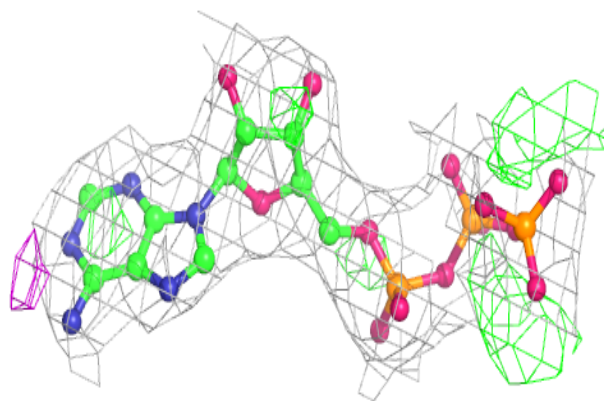
**Electron density around ATP D 521:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ATP E 603:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.