



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2021 – 04:32 PM EDT

PDB ID : 3K0E
Title : Crystal structure of the phosphorylation-site mutant T426N of the KaiC circadian clock protein
Authors : Pattanayek, R.; Egli, M.; Pattanayek, S.
Deposited on : 2009-09-24
Resolution : 3.20 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 : 2.23.2
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) : 2.23.2

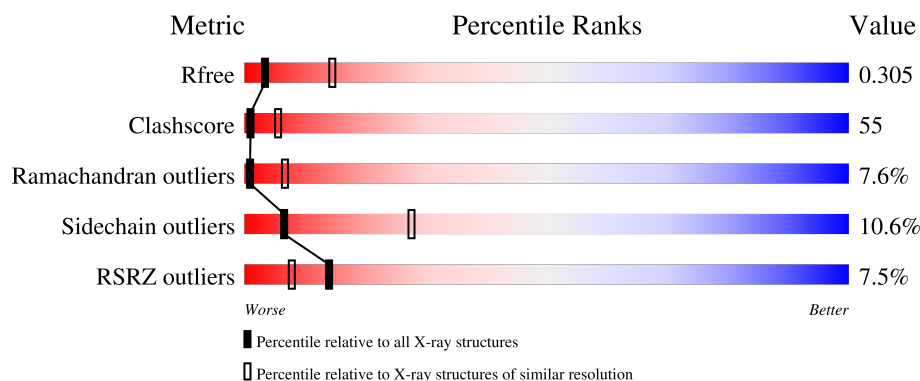
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 of 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>12%</div> <div>29%</div> <div>57%</div> <div>11%</div> <div>• •</div> </div>
1	B	519	<div> <div>7%</div> <div>27%</div> <div>54%</div> <div>13%</div> <div>• 5%</div> </div>
1	C	519	<div> <div>5%</div> <div>29%</div> <div>53%</div> <div>12%</div> <div>• 6%</div> </div>
1	D	519	<div> <div>4%</div> <div>30%</div> <div>52%</div> <div>11%</div> <div>• 7%</div> </div>
1	E	519	<div> <div>6%</div> <div>31%</div> <div>55%</div> <div>9%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	519	

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

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

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 23897 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	P	S	0	0	0
			3994	2509	702	766	2	15			
1	B	491	Total	C	N	O	P	S	0	0	0
			3879	2439	679	744	2	15			
1	C	488	Total	C	N	O	P	S	0	0	0
			3855	2425	675	738	2	15			
1	D	485	Total	C	N	O	P	S	0	0	0
			3831	2411	672	731	2	15			
1	E	492	Total	C	N	O	P	S	0	0	0
			3887	2445	680	745	2	15			
1	F	506	Total	C	N	O	P	S	0	0	0
			3994	2509	702	766	2	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	426	ASN	THR	engineered mutation	UNP Q79PF4
B	426	ASN	THR	engineered mutation	UNP Q79PF4
C	426	ASN	THR	engineered mutation	UNP Q79PF4
D	426	ASN	THR	engineered mutation	UNP Q79PF4
E	426	ASN	THR	engineered mutation	UNP Q79PF4
F	426	ASN	THR	engineered mutation	UNP Q79PF4

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

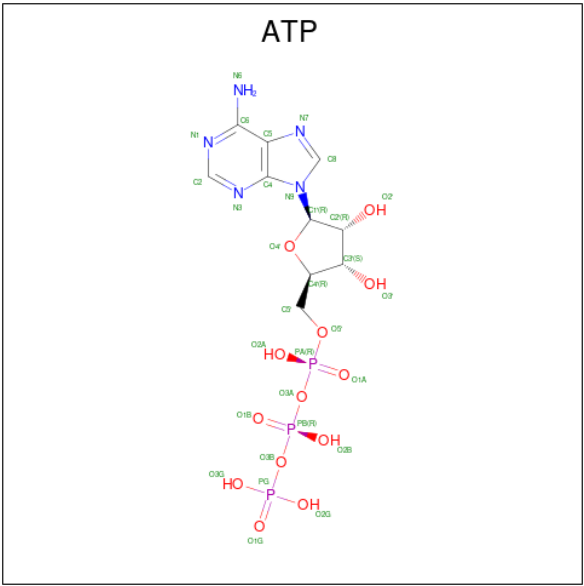
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Mg	0	0
			4	4		
2	B	4	Total	Mg	0	0
			4	4		
2	C	4	Total	Mg	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	3	Total	Mg	0	0
			3	3		
2	E	2	Total	Mg	0	0
			2	2		
2	F	3	Total	Mg	0	0
			3	3		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

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

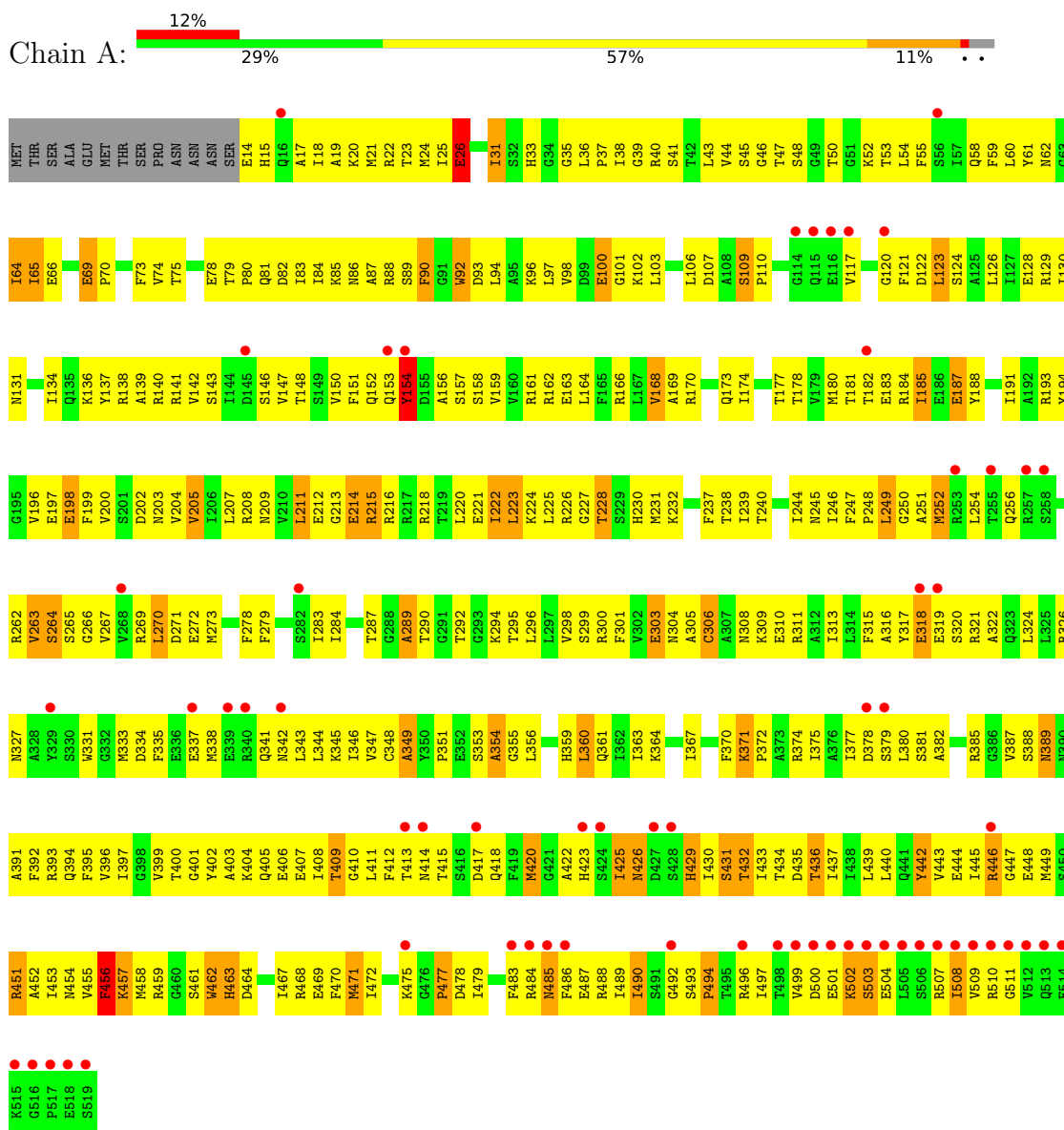
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O	0	0
			8	8		
4	B	4	Total	O	0	0
			4	4		
4	C	6	Total	O	0	0
			6	6		
4	D	19	Total	O	0	0
			19	19		
4	E	11	Total	O	0	0
			11	11		
4	F	17	Total	O	0	0
			17	17		

3 Residue-property plots

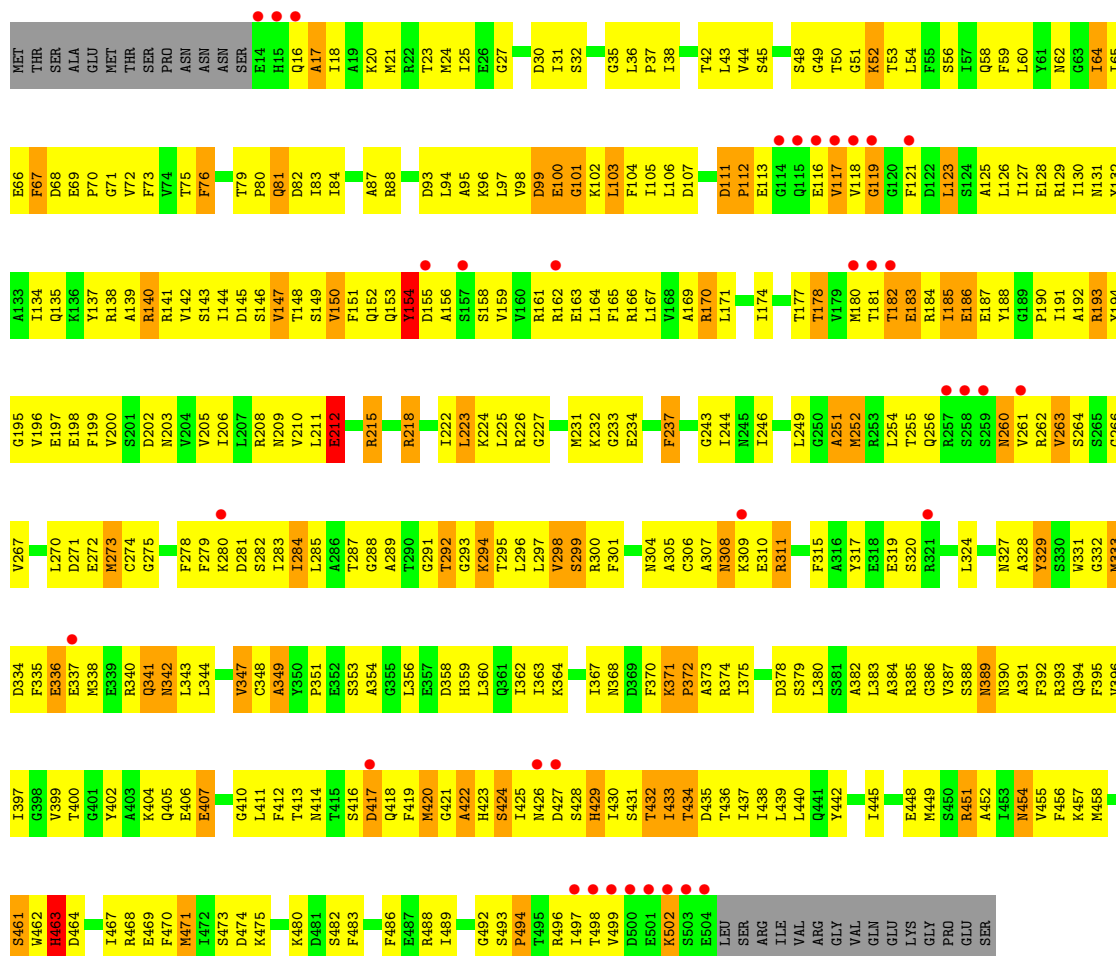
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

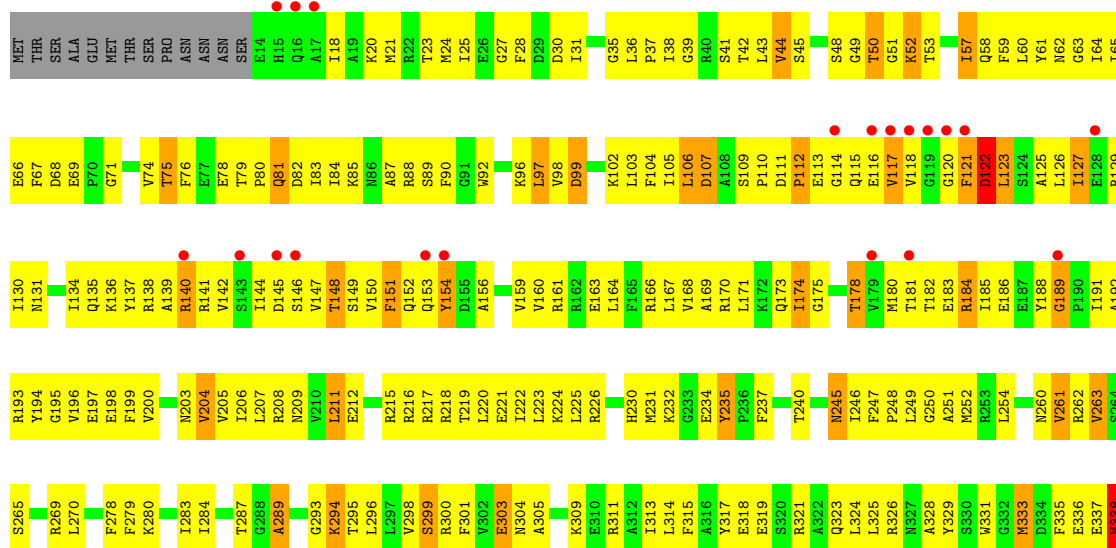


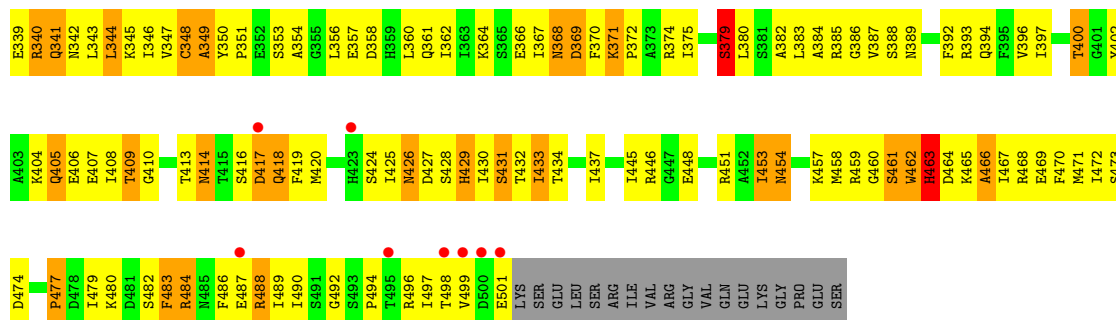
• Molecule 1: Circadian clock protein kinase KaiC



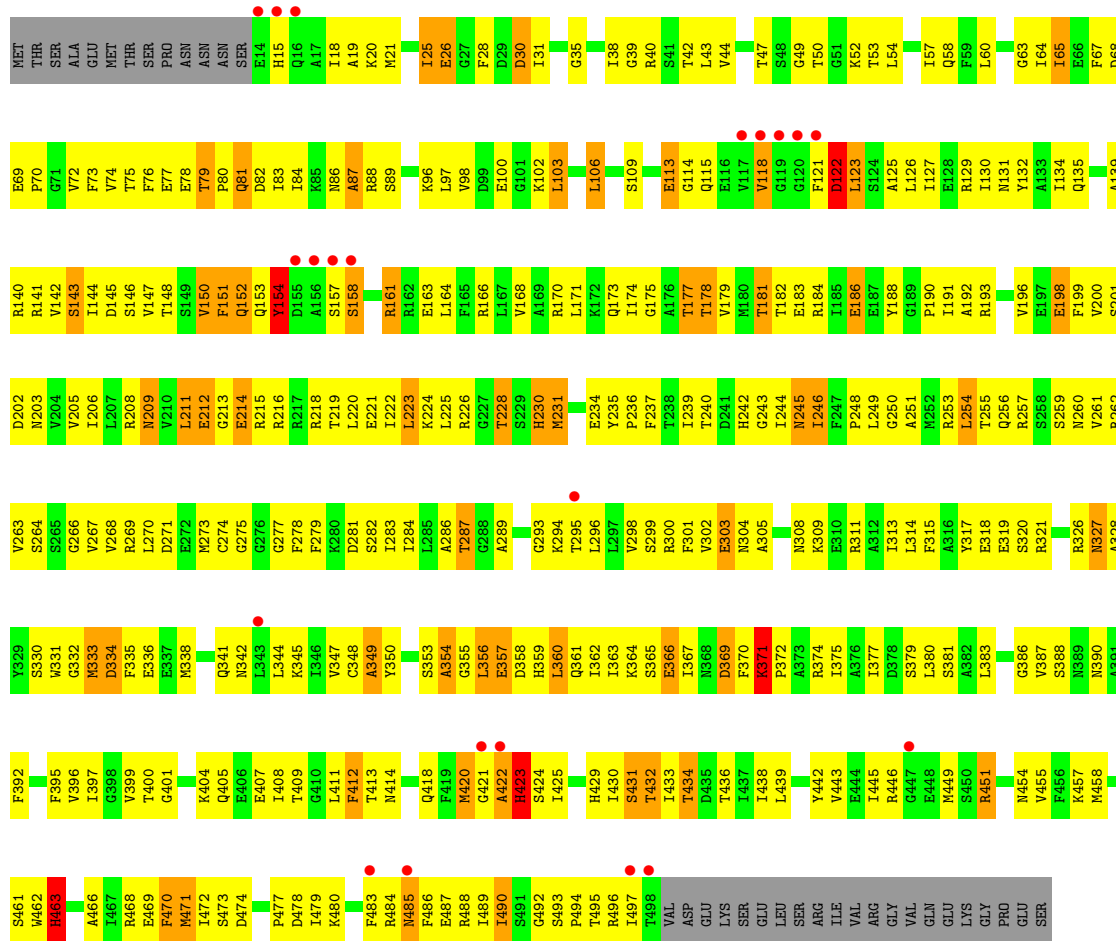


• Molecule 1: Circadian clock protein kinase KaiC

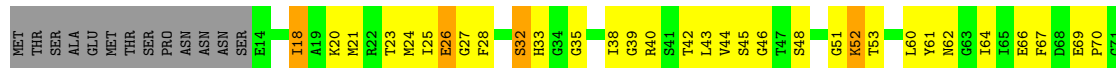


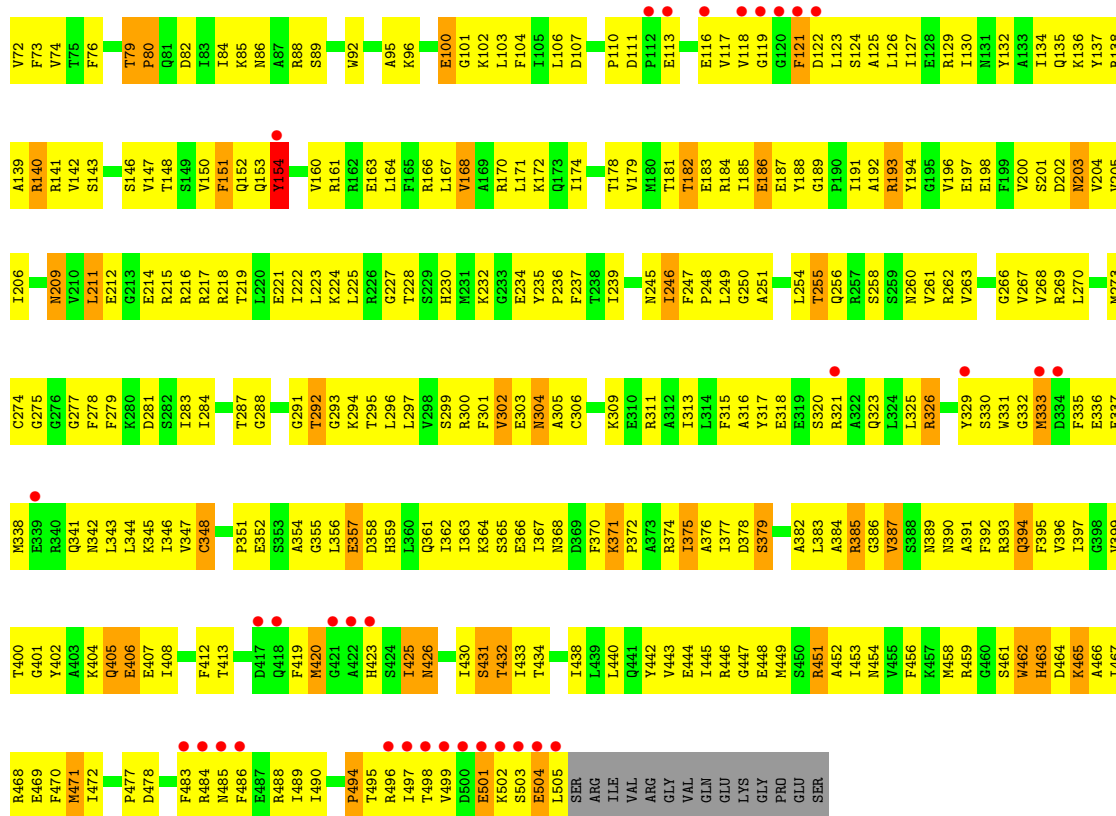


● Molecule 1: Circadian clock protein kinase KaiC

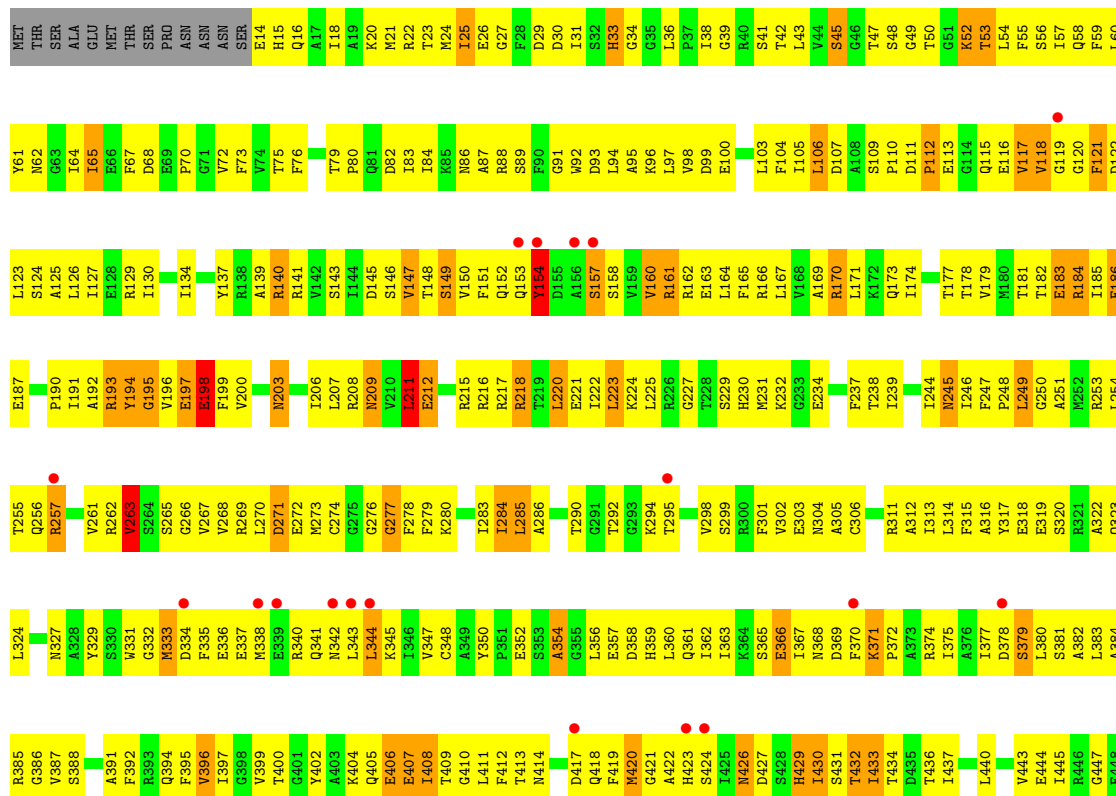


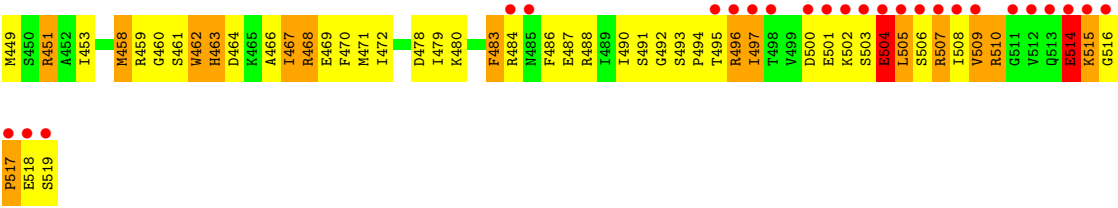
● Molecule 1: Circadian clock protein kinase KaiC





● Molecule 1: Circadian clock protein kinase KaiC





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.50Å 135.83Å 204.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 29.89 – 3.17	Depositor EDS
% Data completeness (in resolution range)	85.3 (30.00-3.20) 91.4 (29.89-3.17)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 3.18Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.250 , 0.320 0.233 , 0.305	Depositor DCC
R_{free} test set	5782 reflections (9.50%)	wwPDB-VP
Wilson B-factor (Å ²)	85.9	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 63.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.036 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23897	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, SEP, ATP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	0/4038	0.67	0/5438
1	B	0.39	0/3922	0.64	0/5283
1	C	0.43	0/3898	0.69	0/5252
1	D	0.50	0/3874	0.73	0/5219
1	E	0.48	0/3930	0.72	0/5294
1	F	0.46	0/4038	0.71	1/5438 (0.0%)
All	All	0.45	0/23700	0.70	1/31924 (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	C	0	1
1	D	0	1
1	E	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	25	ILE	N-CA-C	-5.53	96.06	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	235	TYR	Sidechain
1	D	132	TYR	Sidechain
1	E	188	TYR	Sidechain

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	3994	0	3982	450	0
1	B	3879	0	3859	442	0
1	C	3855	0	3836	442	0
1	D	3831	0	3816	453	0
1	E	3887	0	3870	428	0
1	F	3994	0	3982	550	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	3	0	0	0	0
2	E	2	0	0	0	0
2	F	3	0	0	0	0
3	A	62	0	24	2	0
3	B	62	0	24	7	0
3	C	62	0	24	5	0
3	D	62	0	24	8	0
3	E	62	0	24	9	0
3	F	62	0	24	4	0
4	A	8	0	0	2	0
4	B	4	0	0	2	0
4	C	6	0	0	2	0
4	D	19	0	0	17	0
4	E	11	0	0	3	0
4	F	17	0	0	9	0
All	All	23897	0	23489	2615	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 55.

All (2615) 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:24:MET:HB2	1:A:62:ASN:HD22	1.14	1.13
1:B:147:VAL:HG11	1:B:180:MET:HE2	1.29	1.13
1:D:211:LEU:HB2	1:D:216:ARG:HD3	1.18	1.11
1:F:191:ILE:CB	1:F:198:GLU:HG3	1.82	1.09
1:B:379:SER:H	1:B:413:THR:HB	1.14	1.08
1:F:191:ILE:HB	1:F:198:GLU:CG	1.84	1.08
1:A:215:ARG:HH12	1:B:233:GLY:HA3	1.18	1.06
1:E:140:ARG:HB3	1:E:140:ARG:HH11	1.13	1.06
1:A:379:SER:H	1:A:413:THR:HB	1.21	1.06
1:F:305:ALA:HB2	1:F:374:ARG:HD2	1.38	1.05
1:C:379:SER:H	1:C:413:THR:HB	1.18	1.05
1:C:191:ILE:HG23	1:C:206:ILE:HD11	1.34	1.04
1:F:161:ARG:HB2	1:F:196:VAL:HG11	1.39	1.04
1:F:514:GLU:HG2	1:F:519:SER:HB3	1.38	1.04
1:B:305:ALA:HB2	1:B:374:ARG:HD2	1.35	1.03
1:B:140:ARG:HB3	1:B:140:ARG:HH11	1.23	1.03
1:F:115:GLN:HG2	1:F:116:GLU:H	1.20	1.03
1:C:42:THR:HA	1:C:203:ASN:HB2	1.37	1.02
1:A:437:ILE:HD13	1:A:457:LYS:HE3	1.37	1.02
1:A:299:SER:HB3	1:A:333:MET:HE1	1.42	1.02
1:D:371:LYS:HD2	1:D:371:LYS:O	1.58	1.02
1:F:315:PHE:HE1	1:F:375:ILE:HD11	1.26	1.01
1:A:146:SER:H	1:A:181:THR:HB	1.24	1.00
1:E:451:ARG:H	1:E:451:ARG:HD2	1.26	1.00
1:E:164:LEU:HD11	1:E:197:GLU:HG3	1.37	1.00
1:F:432:TPO:O	1:F:433:ILE:HG12	1.61	0.98
1:D:311:ARG:HD2	1:D:371:LYS:HE3	1.45	0.98
1:A:488:ARG:HE	1:F:488:ARG:HH12	1.08	0.98
1:F:79:THR:HG23	1:F:82:ASP:H	1.29	0.98
1:B:170:ARG:HB3	1:B:170:ARG:HH11	1.27	0.97
1:D:263:VAL:HG12	1:D:374:ARG:HH21	1.29	0.97
1:C:31:ILE:HA	1:C:231:MET:HG3	1.47	0.96
1:F:280:LYS:HE2	1:F:407:GLU:HB3	1.49	0.94
1:A:287:THR:HG22	1:A:414:ASN:HB3	1.50	0.94
1:C:134:ILE:HG23	1:C:139:ALA:HB3	1.49	0.94
1:F:191:ILE:HB	1:F:198:GLU:HG3	0.96	0.94
1:F:371:LYS:O	1:F:371:LYS:HD2	1.65	0.94
1:A:130:ILE:O	1:A:134:ILE:HG13	1.68	0.94
1:D:486:PHE:HB3	1:D:489:ILE:HD11	1.50	0.94
1:A:263:VAL:HG12	1:A:374:ARG:HH21	1.31	0.93
1:D:211:LEU:HD22	1:D:216:ARG:NH1	1.84	0.93
1:E:305:ALA:HB2	1:E:374:ARG:HD2	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:145:ASP:HA	1:F:181:THR:HG22	1.48	0.93
1:F:269:ARG:HA	1:F:272:GLU:OE2	1.68	0.92
1:A:161:ARG:HB2	1:A:196:VAL:HG11	1.50	0.92
1:F:115:GLN:HG2	1:F:116:GLU:N	1.86	0.91
1:E:497:ILE:HG22	1:E:498:THR:H	1.35	0.91
1:C:182:THR:HG22	1:C:183:GLU:H	1.34	0.91
1:B:25:ILE:HG12	1:B:58:GLN:HE21	1.35	0.91
1:B:358:ASP:O	1:B:362:ILE:HG12	1.70	0.91
1:F:25:ILE:HD12	1:F:58:GLN:HG2	1.52	0.90
1:A:426:ASN:OD1	1:A:429:HIS:HA	1.69	0.90
1:A:375:ILE:O	1:A:410:GLY:HA2	1.72	0.90
1:C:413:THR:HG22	1:C:414:ASN:H	1.32	0.90
1:F:207:LEU:HD21	1:F:220:LEU:HD12	1.54	0.90
1:F:194:TYR:O	1:F:196:VAL:HG23	1.72	0.90
1:D:269:ARG:HG2	1:D:479:ILE:HB	1.51	0.90
1:F:269:ARG:HG2	1:F:479:ILE:HB	1.50	0.90
1:D:31:ILE:HA	1:D:231:MET:HG3	1.52	0.89
1:F:72:VAL:HG21	1:F:134:ILE:HD13	1.53	0.89
1:A:488:ARG:HH12	1:B:488:ARG:NH2	1.71	0.89
1:A:263:VAL:CG1	1:A:374:ARG:HH21	1.85	0.89
1:B:116:GLU:HG2	1:B:117:VAL:H	1.38	0.88
1:B:263:VAL:HG12	1:B:374:ARG:HH21	1.39	0.88
1:C:425:ILE:HD12	1:C:425:ILE:H	1.37	0.88
1:D:317:TYR:CE2	1:D:383:LEU:HD21	2.09	0.88
1:E:148:THR:HG21	1:E:183:GLU:HG2	1.56	0.88
1:B:88:ARG:HH22	1:B:95:ALA:HB2	1.38	0.88
1:B:334:ASP:OD1	1:B:336:GLU:HB2	1.74	0.88
1:C:305:ALA:HB2	1:C:374:ARG:HD2	1.56	0.87
1:F:117:VAL:HA	1:F:154:TYR:OH	1.74	0.87
1:D:296:LEU:HD13	4:D:536:HOH:O	1.74	0.87
1:B:194:TYR:O	1:B:196:VAL:HG23	1.75	0.87
1:B:294:LYS:HB3	1:B:413:THR:HG23	1.56	0.87
1:E:359:HIS:O	1:E:363:ILE:HG12	1.75	0.87
1:A:70:PRO:HB2	1:A:139:ALA:HA	1.57	0.87
1:C:262:ARG:HH22	1:C:461:SER:HB2	1.36	0.87
1:D:296:LEU:HD11	1:D:477:PRO:HD3	1.55	0.87
1:E:18:ILE:HG13	1:E:228:THR:HG23	1.55	0.86
1:A:170:ARG:HG2	1:F:112:PRO:HB2	1.56	0.86
1:F:285:LEU:HD12	1:F:286:ALA:N	1.89	0.86
1:D:211:LEU:HB2	1:D:216:ARG:CD	2.03	0.86
1:D:492:GLY:O	1:D:494:PRO:HD3	1.76	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:LEU:HD21	1:A:360:LEU:HD11	1.56	0.86
1:A:320:SER:HA	1:B:254:LEU:HG	1.58	0.86
1:A:359:HIS:O	1:A:363:ILE:HD13	1.76	0.86
1:C:296:LEU:HD21	1:C:477:PRO:HB3	1.55	0.85
1:A:213:GLY:O	1:A:214:GLU:HB2	1.75	0.85
1:B:396:VAL:HG21	1:B:430:ILE:HD12	1.57	0.85
1:E:147:VAL:O	1:E:150:VAL:HG12	1.76	0.85
1:D:21:MET:HE2	1:D:177:THR:HG21	1.59	0.85
1:D:25:ILE:HG12	1:D:58:GLN:HE21	1.40	0.85
1:E:140:ARG:HB3	1:E:140:ARG:NH1	1.92	0.85
1:A:263:VAL:HG23	1:A:278:PHE:O	1.77	0.84
1:B:187:GLU:HG2	1:B:210:VAL:HG22	1.57	0.84
1:A:488:ARG:NE	1:F:488:ARG:HH12	1.74	0.84
1:A:264:SER:HB3	1:A:304:ASN:HD21	1.41	0.84
1:B:97:LEU:HB2	1:B:103:LEU:HD23	1.57	0.84
1:E:266:GLY:HA2	1:E:304:ASN:HD22	1.43	0.84
1:A:311:ARG:NH1	1:A:371:LYS:HE3	1.92	0.84
1:B:185:ILE:HD13	1:B:185:ILE:H	1.41	0.84
1:C:309:LYS:HA	1:C:343:LEU:HD13	1.59	0.84
1:C:79:THR:O	1:C:83:ILE:HG13	1.78	0.84
1:F:379:SER:H	1:F:413:THR:HB	1.43	0.84
1:B:493:SER:HB3	1:C:488:ARG:HG2	1.59	0.84
1:C:393:ARG:NH2	1:C:429:HIS:HB2	1.93	0.84
1:A:120:GLY:HA2	1:A:166:ARG:HH12	1.42	0.83
1:A:488:ARG:HH12	1:B:488:ARG:HH21	1.20	0.83
1:F:148:THR:HG21	1:F:183:GLU:HG3	1.59	0.83
1:B:88:ARG:NH1	1:B:93:ASP:HA	1.92	0.83
1:A:147:VAL:HG11	1:A:180:MET:HE2	1.60	0.83
1:D:79:THR:HG22	1:D:82:ASP:H	1.43	0.83
1:B:64:ILE:HG22	1:B:65:ILE:HD13	1.59	0.83
1:F:426:ASN:OD1	1:F:430:ILE:HG13	1.77	0.83
1:A:215:ARG:NH1	1:B:233:GLY:HA3	1.93	0.83
1:F:262:ARG:O	1:F:263:VAL:HG13	1.79	0.83
1:F:284:ILE:HG23	1:F:436:THR:HB	1.60	0.82
1:F:115:GLN:CG	1:F:116:GLU:H	1.86	0.82
1:C:294:LYS:HB2	3:C:901:ATP:O1B	1.79	0.82
1:D:263:VAL:CG1	1:D:374:ARG:HH21	1.91	0.82
1:A:348:CYS:HB3	1:B:254:LEU:HD23	1.62	0.82
1:C:486:PHE:HD2	1:C:494:PRO:HB2	1.42	0.82
1:F:284:ILE:HB	1:F:411:LEU:HD12	1.61	0.82
1:F:299:SER:HB3	1:F:333:MET:HE1	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:VAL:HG12	1:C:262:ARG:H	1.43	0.82
1:B:341:GLN:O	1:B:343:LEU:HG	1.78	0.82
1:F:266:GLY:HA2	1:F:304:ASN:HD22	1.45	0.82
1:A:31:ILE:HG22	1:A:231:MET:HB2	1.61	0.82
1:D:191:ILE:HB	1:D:198:GLU:CD	2.00	0.82
1:E:325:LEU:HD23	1:E:335:PHE:HB2	1.60	0.82
1:A:446:ARG:HA	1:A:496:ARG:NH2	1.94	0.82
1:D:354:ALA:HB3	1:D:359:HIS:NE2	1.94	0.82
1:C:413:THR:HG22	1:C:414:ASN:N	1.93	0.82
1:C:156:ALA:HB3	1:C:159:VAL:HG23	1.61	0.81
1:E:485:ASN:HD22	1:E:496:ARG:HD3	1.43	0.81
1:F:140:ARG:HB3	1:F:140:ARG:HH11	1.43	0.81
1:B:306:CYS:SG	1:B:344:LEU:HB2	2.19	0.81
1:B:497:ILE:HD12	1:B:499:VAL:H	1.42	0.81
1:B:161:ARG:NH2	1:B:199:PHE:HB2	1.95	0.81
1:E:153:GLN:O	1:F:158:SER:HB2	1.79	0.81
1:B:285:LEU:CD2	1:B:426:ASN:HD21	1.93	0.81
1:B:425:ILE:H	1:B:425:ILE:HD12	1.44	0.80
1:F:23:THR:OG1	1:F:25:ILE:HG12	1.81	0.80
1:A:14:GLU:HG3	1:A:15:HIS:H	1.46	0.80
1:A:469:GLU:HG2	1:A:470:PHE:N	1.97	0.80
1:E:140:ARG:HH11	1:E:140:ARG:CB	1.93	0.80
1:D:379:SER:H	1:D:413:THR:HB	1.47	0.80
1:A:311:ARG:HA	1:A:343:LEU:O	1.81	0.80
1:B:308:ASN:O	1:B:310:GLU:HG3	1.82	0.80
1:D:42:THR:HG23	1:D:203:ASN:HB2	1.64	0.80
1:D:486:PHE:CB	1:D:489:ILE:HD11	2.12	0.80
1:F:515:LYS:HG3	1:F:516:GLY:H	1.45	0.80
1:D:25:ILE:HG12	1:D:58:GLN:NE2	1.95	0.80
1:D:311:ARG:HD2	1:D:371:LYS:CE	2.11	0.80
1:E:150:VAL:HG13	1:E:151:PHE:H	1.46	0.80
1:F:79:THR:HG22	1:F:82:ASP:OD2	1.82	0.80
1:A:84:ILE:HG23	1:A:94:LEU:HB2	1.64	0.79
1:F:60:LEU:HA	4:F:526:HOH:O	1.81	0.79
1:A:266:GLY:HA3	1:A:300:ARG:HG3	1.65	0.79
1:C:262:ARG:HH22	1:C:461:SER:CB	1.95	0.79
1:C:25:ILE:HG23	1:C:58:GLN:HE22	1.47	0.79
1:D:321:ARG:HG3	1:E:255:THR:HG22	1.63	0.79
1:E:150:VAL:HG13	1:E:151:PHE:N	1.98	0.79
1:D:171:LEU:HD12	1:D:178:THR:HG21	1.64	0.79
1:B:191:ILE:HB	1:B:198:GLU:CD	2.02	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:363:ILE:O	1:F:367:ILE:HG12	1.82	0.79
1:C:384:ALA:HB2	1:C:392:PHE:CE1	2.17	0.79
1:E:446:ARG:NH2	1:E:496:ARG:HH22	1.81	0.79
1:E:278:PHE:CZ	1:E:438:ILE:HD11	2.18	0.78
1:A:469:GLU:HG2	1:A:470:PHE:H	1.48	0.78
1:F:315:PHE:CE1	1:F:375:ILE:HD11	2.15	0.78
1:A:215:ARG:HA	1:A:215:ARG:CZ	2.13	0.78
1:D:396:VAL:HG11	1:D:430:ILE:HG23	1.66	0.78
1:F:406:GLU:HB3	1:F:408:ILE:HG13	1.65	0.78
1:A:211:LEU:HD13	1:A:216:ARG:HE	1.48	0.78
1:A:14:GLU:CG	1:A:15:HIS:H	1.97	0.78
1:A:488:ARG:NH1	1:B:488:ARG:HH21	1.82	0.78
1:A:264:SER:HB3	1:A:304:ASN:ND2	1.99	0.78
1:B:294:LYS:HB2	3:B:901:ATP:O1B	1.84	0.78
1:C:469:GLU:HG3	1:C:480:LYS:HB2	1.66	0.78
1:D:211:LEU:HD22	1:D:216:ARG:HH12	1.46	0.78
1:E:311:ARG:HD2	1:E:371:LYS:HE3	1.65	0.78
1:F:161:ARG:HB2	1:F:196:VAL:CG1	2.13	0.78
1:B:354:ALA:HB1	1:B:358:ASP:HB2	1.67	0.77
1:C:469:GLU:HG3	1:C:480:LYS:HE3	1.65	0.77
1:D:130:ILE:O	1:D:134:ILE:HG12	1.84	0.77
1:E:45:SER:HB2	1:E:182:THR:HG22	1.66	0.77
1:A:21:MET:HE3	1:A:141:ARG:CZ	2.13	0.77
1:E:163:GLU:HA	1:E:163:GLU:OE2	1.82	0.77
1:D:219:THR:HG22	1:D:236:PRO:HA	1.65	0.77
1:E:452:ALA:HA	1:E:469:GLU:HA	1.66	0.77
1:F:336:GLU:O	1:F:340:ARG:HG3	1.82	0.77
1:D:161:ARG:HB2	1:D:196:VAL:HG11	1.66	0.77
1:E:358:ASP:O	1:E:362:ILE:HG13	1.85	0.77
1:A:380:LEU:HD21	1:A:412:PHE:HD2	1.49	0.77
1:E:273:MET:O	1:E:463:HIS:HA	1.84	0.77
1:A:47:THR:O	1:A:50:THR:HG23	1.84	0.77
1:B:311:ARG:HG2	1:B:343:LEU:HA	1.64	0.77
1:B:311:ARG:HB3	1:B:370:PHE:CE2	2.20	0.77
1:A:147:VAL:HG11	1:A:180:MET:CE	2.15	0.77
1:E:218:ARG:HB3	1:E:237:PHE:CE2	2.20	0.77
1:D:147:VAL:O	1:D:150:VAL:HG12	1.85	0.76
1:F:469:GLU:HB2	1:F:483:PHE:HE1	1.50	0.76
1:A:269:ARG:HB3	1:A:479:ILE:HD13	1.68	0.76
1:B:215:ARG:NH1	1:B:215:ARG:HA	2.01	0.76
1:F:504:GLU:O	1:F:505:LEU:HB2	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:PHE:O	1:C:125:ALA:HB3	1.85	0.76
1:D:215:ARG:HA	1:D:215:ARG:HE	1.50	0.76
1:B:496:ARG:HG2	1:B:498:THR:HG23	1.66	0.76
1:D:146:SER:H	1:D:181:THR:HG22	1.50	0.76
1:C:433:ILE:HG13	1:C:433:ILE:O	1.86	0.76
1:B:80:PRO:HG2	1:B:107:ASP:HB2	1.68	0.75
1:E:400:THR:HG21	1:E:433:ILE:HG22	1.68	0.75
1:A:24:MET:CB	1:A:62:ASN:HD22	1.97	0.75
1:C:148:THR:HA	1:C:151:PHE:HE1	1.50	0.75
1:A:52:LYS:HB3	1:A:181:THR:HG23	1.67	0.75
1:F:195:GLY:HA2	1:F:198:GLU:OE2	1.86	0.75
1:D:263:VAL:HG12	1:D:374:ARG:NH2	2.02	0.75
1:A:317:TYR:HE1	1:A:377:ILE:HG23	1.50	0.75
1:F:426:ASN:H	1:F:426:ASN:HD22	1.32	0.75
1:D:218:ARG:HH12	1:E:232:LYS:HE2	1.52	0.75
1:A:93:ASP:OD2	1:A:96:LYS:HB2	1.87	0.74
1:A:209:ASN:OD1	1:A:216:ARG:HD2	1.87	0.74
1:E:469:GLU:HB3	1:E:483:PHE:CE1	2.22	0.74
1:B:43:LEU:HD11	1:B:182:THR:OG1	1.86	0.74
1:B:185:ILE:HD13	1:B:185:ILE:N	2.01	0.74
1:C:80:PRO:O	1:C:84:ILE:HG12	1.86	0.74
1:C:488:ARG:HH21	1:D:488:ARG:NH2	1.84	0.74
1:A:24:MET:HB2	1:A:62:ASN:ND2	1.98	0.74
1:A:202:ASP:HA	1:A:226:ARG:HD2	1.70	0.74
1:A:267:VAL:HG23	1:A:300:ARG:HG2	1.68	0.74
1:D:431:SEP:HA	1:D:434:THR:CG2	2.16	0.74
1:F:305:ALA:CB	1:F:374:ARG:HD2	2.17	0.74
1:A:227:GLY:O	1:A:228:THR:HG23	1.87	0.74
1:B:206:ILE:N	1:B:206:ILE:HD12	2.03	0.74
1:D:211:LEU:CB	1:D:216:ARG:HD3	2.09	0.74
1:B:130:ILE:O	1:B:134:ILE:HG12	1.87	0.74
1:D:266:GLY:HA2	1:D:304:ASN:HD22	1.52	0.74
1:E:299:SER:C	1:E:333:MET:HE1	2.08	0.74
1:A:79:THR:CG2	1:A:81:GLN:HG2	2.18	0.74
1:A:425:ILE:HB	1:A:426:ASN:ND2	2.02	0.74
1:B:140:ARG:HB3	1:B:140:ARG:NH1	2.01	0.74
1:D:20:LYS:HE3	1:D:228:THR:HG21	1.69	0.74
1:F:443:VAL:HG12	1:F:445:ILE:HD11	1.70	0.74
1:B:283:ILE:HG12	1:B:400:THR:HG23	1.69	0.74
1:C:413:THR:CG2	1:C:414:ASN:H	2.01	0.74
1:B:287:THR:HG21	1:B:425:ILE:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:359:HIS:O	1:F:363:ILE:HD13	1.88	0.73
1:A:46:GLY:HA2	1:A:184:ARG:HD3	1.70	0.73
1:A:445:ILE:HD11	1:A:483:PHE:HE2	1.52	0.73
1:E:203:ASN:HB3	1:E:225:LEU:HD23	1.69	0.73
1:E:445:ILE:CG2	1:E:446:ARG:HD2	2.18	0.73
1:D:305:ALA:HB2	1:D:374:ARG:HD2	1.71	0.73
1:A:487:GLU:OE1	1:F:495:THR:HA	1.89	0.73
1:B:64:ILE:HG21	1:B:97:LEU:HD13	1.69	0.73
1:B:294:LYS:HB3	1:B:413:THR:CG2	2.19	0.73
1:C:340:ARG:C	1:C:342:ASN:H	1.90	0.73
1:E:261:VAL:HG12	1:E:262:ARG:N	2.03	0.73
1:E:287:THR:HG22	1:E:288:GLY:N	2.02	0.73
1:D:321:ARG:HG2	1:D:348:CYS:SG	2.28	0.73
1:B:147:VAL:HG23	1:B:151:PHE:HE1	1.54	0.72
1:D:38:ILE:HA	1:D:177:THR:HG23	1.71	0.72
1:D:344:LEU:HD22	1:D:345:LYS:H	1.53	0.72
1:D:367:ILE:CD1	1:D:375:ILE:HD11	2.19	0.72
1:D:367:ILE:HD12	1:D:375:ILE:HD11	1.71	0.72
1:D:287:THR:HG22	1:D:414:ASN:HD22	1.53	0.72
1:E:338:MET:HB3	1:E:344:LEU:HB2	1.71	0.72
1:F:336:GLU:HB3	1:F:340:ARG:NH2	2.03	0.72
1:A:164:LEU:HD23	1:A:168:VAL:HG22	1.70	0.72
1:A:191:ILE:HD12	1:A:198:GLU:HG2	1.72	0.72
1:E:191:ILE:HB	1:E:198:GLU:HG3	1.70	0.72
1:A:215:ARG:NH1	1:A:215:ARG:HA	2.04	0.72
1:C:471:MET:HB3	1:C:480:LYS:HE2	1.70	0.72
1:D:347:VAL:HG12	1:D:348:CYS:N	2.04	0.72
1:E:123:LEU:HD21	1:E:166:ARG:HD2	1.70	0.72
1:E:148:THR:HG21	1:E:183:GLU:CG	2.20	0.72
1:F:26:GLU:HB3	1:F:245:ASN:ND2	2.04	0.72
1:C:36:LEU:HD12	1:C:59:PHE:CE1	2.25	0.72
1:C:263:VAL:CG1	1:C:374:ARG:HH21	2.02	0.72
1:D:142:VAL:HB	1:D:178:THR:HG23	1.72	0.72
1:F:497:ILE:H	1:F:497:ILE:HD13	1.55	0.72
1:A:232:LYS:H	1:A:232:LYS:HD2	1.53	0.72
1:D:262:ARG:NH2	1:D:461:SER:HB2	2.04	0.72
1:D:296:LEU:HD12	1:D:296:LEU:O	1.90	0.72
1:D:53:THR:HG23	1:D:57:ILE:CD1	2.18	0.72
1:F:26:GLU:HB3	1:F:245:ASN:HD21	1.55	0.72
1:A:363:ILE:O	1:A:367:ILE:HG13	1.89	0.71
1:C:461:SER:OG	1:C:462:TRP:N	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:73:PHE:HE2	1:F:75:THR:HB	1.55	0.71
1:B:195:GLY:HA2	1:B:198:GLU:OE2	1.90	0.71
1:C:263:VAL:HG12	1:C:374:ARG:HH21	1.55	0.71
1:A:440:LEU:HD23	1:A:453:ILE:HG13	1.72	0.71
1:E:245:ASN:HD22	1:E:247:PHE:HE2	1.38	0.71
1:F:313:ILE:HD12	1:F:345:LYS:HB3	1.72	0.71
1:C:171:LEU:HD13	1:C:178:THR:HG21	1.72	0.71
1:E:313:ILE:HD12	1:E:367:ILE:HD13	1.72	0.71
1:F:161:ARG:CB	1:F:196:VAL:HG11	2.18	0.71
1:B:170:ARG:HB3	1:B:170:ARG:NH1	2.04	0.71
1:C:387:VAL:HG12	1:C:388:SER:N	2.05	0.71
1:F:382:ALA:O	1:F:385:ARG:HG3	1.91	0.71
1:B:292:THR:HB	1:B:440:LEU:HB2	1.73	0.71
1:C:269:ARG:HG2	1:C:479:ILE:HB	1.73	0.71
1:C:484:ARG:HB3	1:C:484:ARG:NH1	2.06	0.71
1:D:304:ASN:HB3	1:D:374:ARG:HH12	1.56	0.71
1:F:486:PHE:CE2	1:F:496:ARG:HB3	2.25	0.71
1:A:437:ILE:CD1	1:A:457:LYS:HE3	2.17	0.70
1:C:74:VAL:HG22	1:C:106:LEU:HD23	1.73	0.70
1:F:169:ALA:O	1:F:173:GLN:HG3	1.90	0.70
1:B:146:SER:H	1:B:181:THR:HB	1.54	0.70
1:B:205:VAL:HG22	1:B:222:ILE:HG12	1.74	0.70
1:C:45:SER:CB	1:C:182:THR:HB	2.21	0.70
1:D:79:THR:HG22	1:D:82:ASP:N	2.06	0.70
1:F:443:VAL:CG1	1:F:445:ILE:HD11	2.22	0.70
1:B:18:ILE:H	1:B:18:ILE:HD12	1.55	0.70
1:D:220:LEU:HD13	1:D:246:ILE:CD1	2.22	0.70
1:D:425:ILE:H	1:D:425:ILE:HD12	1.56	0.70
1:E:356:LEU:HD11	1:E:387:VAL:HG21	1.71	0.70
1:F:515:LYS:HG3	1:F:516:GLY:N	2.07	0.70
1:E:387:VAL:HG12	1:E:391:ALA:HB3	1.71	0.70
1:E:451:ARG:HG2	1:E:451:ARG:HH11	1.56	0.70
1:E:26:GLU:O	1:E:246:ILE:HG12	1.91	0.70
1:E:371:LYS:HD2	1:E:371:LYS:O	1.92	0.70
1:B:106:LEU:HD23	1:B:130:ILE:HD13	1.73	0.69
1:F:396:VAL:HG11	1:F:430:ILE:CG2	2.22	0.69
1:B:18:ILE:HD12	1:B:18:ILE:N	2.07	0.69
1:D:203:ASN:HB3	1:D:225:LEU:HD23	1.73	0.69
1:F:64:ILE:HG21	1:F:97:LEU:HD13	1.73	0.69
1:C:247:PHE:HZ	1:C:361:GLN:HG3	1.55	0.69
1:D:81:GLN:HA	1:D:84:ILE:HD12	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:283:ILE:HG23	1:E:412:PHE:HE1	1.56	0.69
1:E:469:GLU:HB3	1:E:483:PHE:HE1	1.55	0.69
1:B:328:ALA:HA	1:B:331:TRP:CE3	2.26	0.69
1:F:315:PHE:CD2	1:F:347:VAL:HG21	2.27	0.69
1:B:492:GLY:O	1:B:494:PRO:HD3	1.93	0.69
1:D:366:GLU:HA	1:D:366:GLU:OE2	1.92	0.69
1:D:431:SEP:C	1:D:433:ILE:H	2.05	0.69
1:E:74:VAL:HG22	1:E:106:LEU:HD23	1.74	0.69
1:C:44:VAL:HG22	1:C:205:VAL:HB	1.74	0.69
1:D:212:GLU:HG2	1:D:212:GLU:O	1.91	0.69
1:F:345:LYS:HD2	1:F:370:PHE:CD1	2.27	0.69
1:A:426:ASN:HD21	1:A:431:SEP:HB2	1.58	0.69
1:B:351:PRO:HG2	1:B:382:ALA:O	1.92	0.69
1:C:185:ILE:HG21	1:D:190:PRO:HB3	1.75	0.69
1:E:363:ILE:O	1:E:367:ILE:HG12	1.93	0.69
1:D:451:ARG:HG2	1:D:451:ARG:HH11	1.56	0.69
1:E:323:GLN:NE2	1:F:459:ARG:HD3	2.07	0.69
1:A:70:PRO:HA	1:A:102:LYS:O	1.93	0.69
1:B:430:ILE:O	1:B:433:ILE:HG12	1.92	0.69
1:C:280:LYS:O	1:C:409:THR:HG23	1.91	0.69
1:E:278:PHE:HZ	1:E:438:ILE:HD11	1.56	0.69
1:E:375:ILE:HD13	1:E:376:ALA:N	2.08	0.69
1:A:21:MET:HE2	1:A:59:PHE:CZ	2.28	0.68
1:A:316:ALA:HB3	1:A:348:CYS:SG	2.33	0.68
1:B:264:SER:HB3	1:B:304:ASN:HD21	1.58	0.68
1:B:25:ILE:HG23	1:B:58:GLN:HE22	1.58	0.68
1:D:182:THR:HG21	1:D:192:ALA:HB1	1.76	0.68
1:E:24:MET:CB	1:E:62:ASN:HD22	2.07	0.68
1:F:211:LEU:O	1:F:212:GLU:HB3	1.93	0.68
1:F:294:LYS:HB3	1:F:413:THR:HG23	1.75	0.68
1:A:40:ARG:HH22	1:F:86:ASN:ND2	1.91	0.68
1:F:25:ILE:CD1	1:F:58:GLN:HG2	2.22	0.68
1:F:405:GLN:HG3	1:F:406:GLU:OE1	1.92	0.68
1:A:485:ASN:O	1:A:497:ILE:HG13	1.92	0.68
1:C:25:ILE:HG12	1:C:58:GLN:HE21	1.58	0.68
1:D:374:ARG:HG2	1:D:409:THR:HB	1.75	0.68
1:F:94:LEU:O	1:F:98:VAL:HG23	1.92	0.68
1:A:164:LEU:HD22	1:A:200:VAL:CG1	2.24	0.68
1:E:269:ARG:HH22	1:E:468:ARG:NH2	1.91	0.68
1:E:337:GLU:OE2	1:E:341:GLN:HG3	1.94	0.68
1:F:317:TYR:OH	1:F:363:ILE:HD11	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LEU:HD22	1:A:200:VAL:HG11	1.76	0.68
1:B:186:GLU:HB3	1:B:190:PRO:HD2	1.75	0.68
1:C:147:VAL:O	1:C:150:VAL:HG12	1.93	0.68
1:D:328:ALA:HB1	4:D:540:HOH:O	1.93	0.68
1:E:171:LEU:HA	1:E:174:ILE:HD12	1.75	0.68
1:F:445:ILE:HA	1:F:496:ARG:NH1	2.09	0.68
1:A:264:SER:CB	1:A:304:ASN:HD21	2.06	0.68
1:D:348:CYS:O	1:D:349:ALA:HB2	1.94	0.68
1:A:283:ILE:HD12	1:A:412:PHE:HE1	1.59	0.68
1:F:345:LYS:HB2	1:F:370:PHE:CE1	2.29	0.68
1:B:56:SER:HB2	1:B:143:SER:HB3	1.76	0.67
1:C:31:ILE:CA	1:C:231:MET:HG3	2.24	0.67
1:A:439:LEU:HD12	1:A:440:LEU:H	1.59	0.67
1:A:443:VAL:HG13	1:A:494:PRO:HG2	1.76	0.67
1:C:82:ASP:HA	1:C:85:LYS:HB3	1.76	0.67
1:C:358:ASP:O	1:C:362:ILE:HG12	1.93	0.67
1:D:211:LEU:HD13	1:D:216:ARG:HH11	1.58	0.67
1:D:333:MET:HG2	4:D:538:HOH:O	1.95	0.67
1:D:363:ILE:O	1:D:367:ILE:HG12	1.94	0.67
1:F:47:THR:O	1:F:50:THR:HG23	1.95	0.67
1:C:173:GLN:C	1:C:175:GLY:H	1.98	0.67
1:F:170:ARG:HH12	1:F:174:ILE:HG13	1.59	0.67
1:F:311:ARG:HD2	1:F:371:LYS:HE3	1.77	0.67
1:F:151:PHE:CE1	1:F:160:VAL:HG13	2.29	0.67
1:B:379:SER:OG	1:B:382:ALA:HB2	1.95	0.67
1:B:425:ILE:HG21	1:B:437:ILE:HG23	1.75	0.67
1:C:25:ILE:HG23	1:C:58:GLN:NE2	2.08	0.67
1:C:106:LEU:HD21	1:C:130:ILE:HA	1.77	0.67
1:C:185:ILE:HD12	1:C:185:ILE:N	2.09	0.67
1:C:451:ARG:HG2	1:C:451:ARG:HH11	1.60	0.67
1:E:27:GLY:N	4:E:526:HOH:O	2.26	0.67
1:F:42:THR:HG23	1:F:203:ASN:HB2	1.77	0.67
1:B:285:LEU:HD12	1:B:412:PHE:O	1.95	0.67
1:C:170:ARG:O	1:C:174:ILE:HG12	1.95	0.67
1:E:283:ILE:HG23	1:E:412:PHE:CE1	2.30	0.67
1:F:187:GLU:HG3	1:F:208:ARG:HG2	1.75	0.67
1:A:41:SER:HA	1:A:178:THR:O	1.94	0.67
1:A:370:PHE:HD2	1:A:372:PRO:HG3	1.59	0.67
1:A:374:ARG:O	1:A:375:ILE:HD12	1.95	0.67
1:A:393:ARG:O	1:A:397:ILE:HG12	1.94	0.67
1:C:43:LEU:HD23	1:C:204:VAL:HG13	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:SER:O	1:D:333:MET:HE1	1.95	0.67
1:F:406:GLU:O	1:F:408:ILE:HG13	1.94	0.67
1:E:335:PHE:HA	1:E:338:MET:HG3	1.75	0.67
1:A:21:MET:CE	1:A:59:PHE:CZ	2.78	0.67
1:A:445:ILE:HD11	1:A:483:PHE:CE2	2.29	0.67
1:B:56:SER:O	1:B:59:PHE:HB3	1.95	0.67
1:B:88:ARG:NH2	1:B:95:ALA:HB2	2.10	0.67
1:C:379:SER:N	1:C:413:THR:HB	2.02	0.67
1:F:170:ARG:HH12	1:F:174:ILE:CG1	2.07	0.67
1:A:170:ARG:HD2	1:A:173:GLN:OE1	1.95	0.66
1:F:497:ILE:O	1:F:497:ILE:HG12	1.95	0.66
1:D:257:ARG:NH1	1:D:407:GLU:HG3	2.10	0.66
1:C:64:ILE:HG13	1:C:69:GLU:O	1.95	0.66
1:C:194:TYR:O	1:C:196:VAL:HG23	1.95	0.66
1:D:79:THR:CG2	1:D:81:GLN:HG2	2.24	0.66
1:E:300:ARG:N	1:E:333:MET:HE1	2.09	0.66
1:F:484:ARG:HB3	1:F:484:ARG:NH1	2.10	0.66
1:A:256:GLN:O	1:F:322:ALA:HB3	1.96	0.66
1:D:248:PRO:O	1:D:250:GLY:N	2.26	0.66
1:E:356:LEU:HD22	1:E:387:VAL:HG11	1.76	0.66
1:E:448:GLU:HG2	1:F:466:ALA:HA	1.78	0.66
1:A:449:MET:HG2	1:B:467:ILE:HD11	1.76	0.66
1:B:32:SER:OG	1:B:35:GLY:HA2	1.95	0.66
1:D:347:VAL:O	1:D:348:CYS:HB2	1.94	0.66
1:A:469:GLU:HB2	1:A:483:PHE:CZ	2.30	0.66
1:B:327:ASN:ND2	1:C:459:ARG:HB3	2.11	0.66
1:C:146:SER:H	1:C:181:THR:HB	1.60	0.66
1:D:248:PRO:C	1:D:250:GLY:H	1.98	0.66
1:E:315:PHE:CE2	1:E:347:VAL:HG21	2.30	0.66
1:E:426:ASN:H	1:E:426:ASN:ND2	1.93	0.66
1:F:57:ILE:HD11	1:F:83:ILE:HG23	1.77	0.66
1:A:471:MET:HG3	1:A:478:ASP:HB3	1.77	0.66
1:B:171:LEU:HD13	1:B:178:THR:HG21	1.78	0.66
1:F:316:ALA:CB	1:F:324:LEU:HD11	2.25	0.66
1:F:375:ILE:O	1:F:410:GLY:HA2	1.95	0.66
1:A:159:VAL:O	1:A:163:GLU:HG2	1.96	0.66
1:A:193:ARG:NH2	1:B:195:GLY:O	2.28	0.66
1:B:24:MET:HB2	1:B:62:ASN:HD22	1.60	0.66
1:B:94:LEU:O	1:B:98:VAL:HG23	1.96	0.66
1:B:203:ASN:HB3	1:B:225:LEU:HD23	1.77	0.66
1:D:220:LEU:HD23	1:D:221:GLU:N	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:LEU:CD1	1:E:197:GLU:HG3	2.18	0.66
1:E:203:ASN:HB3	1:E:225:LEU:CD2	2.26	0.66
1:E:401:GLY:O	1:E:405:GLN:HG2	1.96	0.66
1:F:381:SER:HB3	1:F:414:ASN:OD1	1.95	0.66
1:F:426:ASN:HD22	1:F:426:ASN:N	1.90	0.66
1:A:21:MET:HE1	1:A:141:ARG:HG2	1.76	0.66
1:A:79:THR:HG23	1:A:80:PRO:HD2	1.77	0.66
1:C:296:LEU:CD2	1:C:477:PRO:HB3	2.26	0.66
1:E:266:GLY:HA2	1:E:304:ASN:ND2	2.11	0.66
1:F:208:ARG:O	1:F:218:ARG:HA	1.96	0.66
1:C:52:LYS:H	1:C:207:LEU:HD12	1.61	0.66
1:C:218:ARG:HB3	4:C:521:HOH:O	1.96	0.66
1:D:79:THR:CG2	1:D:82:ASP:H	2.08	0.66
1:F:285:LEU:HB3	1:F:437:ILE:HD13	1.77	0.66
1:F:294:LYS:HG3	1:F:440:LEU:HD12	1.77	0.66
1:A:21:MET:HE2	1:A:59:PHE:HZ	1.59	0.65
3:C:903:ATP:O2'	1:D:230:HIS:NE2	2.29	0.65
1:E:451:ARG:H	1:E:451:ARG:CD	2.06	0.65
1:B:106:LEU:CD2	1:B:130:ILE:HD13	2.26	0.65
1:D:123:LEU:HD11	1:D:163:GLU:HB3	1.79	0.65
1:D:274:CYS:SG	1:D:455:VAL:HG21	2.37	0.65
1:D:287:THR:CG2	1:D:414:ASN:HD22	2.08	0.65
1:A:356:LEU:HD22	1:A:387:VAL:HG11	1.78	0.65
1:E:311:ARG:HD2	1:E:371:LYS:CE	2.27	0.65
1:F:47:THR:HG23	4:F:522:HOH:O	1.96	0.65
1:A:54:LEU:CD2	1:A:244:ILE:HG13	2.27	0.65
1:A:73:PHE:CE2	1:A:83:ILE:HD13	2.32	0.65
1:C:65:ILE:HG22	1:C:65:ILE:O	1.97	0.65
1:E:18:ILE:HD11	1:E:227:GLY:HA3	1.79	0.65
1:F:262:ARG:HH22	1:F:461:SER:HB2	1.62	0.65
1:C:185:ILE:CG2	1:D:190:PRO:HB3	2.27	0.65
1:C:451:ARG:HB2	1:C:470:PHE:O	1.96	0.65
1:D:18:ILE:HD12	1:D:40:ARG:HH12	1.62	0.65
1:A:74:VAL:HG22	1:A:106:LEU:HD23	1.78	0.65
1:A:237:PHE:HB3	1:A:246:ILE:HG12	1.78	0.65
1:A:490:ILE:O	1:A:490:ILE:HG22	1.97	0.65
1:E:150:VAL:CG1	1:E:151:PHE:H	2.10	0.65
1:F:247:PHE:HB3	1:F:249:LEU:HD21	1.78	0.65
1:A:388:SER:HB3	1:A:391:ALA:CB	2.27	0.65
1:A:479:ILE:H	1:A:479:ILE:HD12	1.61	0.65
1:A:507:ARG:HD2	1:A:507:ARG:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:PHE:HD1	1:C:121:PHE:H	1.42	0.65
1:D:65:ILE:CD1	1:D:97:LEU:HD11	2.27	0.65
1:B:335:PHE:O	1:B:338:MET:HB2	1.97	0.64
1:D:80:PRO:O	1:D:84:ILE:HG13	1.97	0.64
1:E:218:ARG:HB2	4:E:528:HOH:O	1.97	0.64
1:E:451:ARG:HD2	1:E:451:ARG:N	2.07	0.64
1:B:170:ARG:O	1:B:174:ILE:HG12	1.97	0.64
1:C:317:TYR:CE1	1:C:383:LEU:HD21	2.32	0.64
1:D:240:THR:O	1:D:243:GLY:N	2.26	0.64
1:E:152:GLN:HG3	1:F:161:ARG:NH1	2.13	0.64
1:E:287:THR:HG22	1:E:288:GLY:H	1.59	0.64
1:F:274:CYS:HG	1:F:278:PHE:HE2	1.43	0.64
1:C:425:ILE:H	1:C:425:ILE:CD1	2.10	0.64
1:D:461:SER:OG	1:D:462:TRP:N	2.30	0.64
1:E:186:GLU:OE2	1:E:187:GLU:N	2.30	0.64
1:F:317:TYR:CE2	1:F:383:LEU:HD21	2.32	0.64
1:F:514:GLU:O	1:F:515:LYS:HB3	1.96	0.64
1:A:40:ARG:HH22	1:F:86:ASN:HD21	1.43	0.64
1:C:279:PHE:CE1	1:C:460:GLY:HA3	2.31	0.64
1:F:335:PHE:HA	1:F:338:MET:CG	2.28	0.64
1:A:96:LYS:HG2	1:A:100:GLU:OE1	1.97	0.64
1:C:45:SER:HB2	1:C:182:THR:HB	1.78	0.64
1:E:248:PRO:HB2	1:E:251:ALA:HB3	1.78	0.64
1:F:392:PHE:O	1:F:396:VAL:HG23	1.98	0.64
1:A:296:LEU:HD22	1:A:472:ILE:HD12	1.79	0.64
1:B:88:ARG:HG2	1:B:88:ARG:HH11	1.61	0.64
1:C:413:THR:O	1:C:414:ASN:HB2	1.98	0.64
1:E:486:PHE:HA	1:E:495:THR:O	1.98	0.64
1:F:197:GLU:N	1:F:197:GLU:OE2	2.30	0.64
1:F:280:LYS:CE	1:F:407:GLU:HB3	2.25	0.64
1:D:65:ILE:HD11	1:D:97:LEU:HD11	1.79	0.64
1:B:161:ARG:HB2	1:B:196:VAL:CG1	2.28	0.64
1:E:67:PHE:HB2	1:E:69:GLU:HG3	1.79	0.64
1:A:140:ARG:HA	1:A:140:ARG:HH11	1.61	0.64
1:D:53:THR:HG23	1:D:57:ILE:HD11	1.78	0.64
1:D:171:LEU:CD1	1:D:178:THR:HG21	2.28	0.64
1:E:345:LYS:HB2	1:E:370:PHE:CE2	2.33	0.64
1:A:90:PHE:HB2	1:A:92:TRP:CE2	2.33	0.64
1:A:426:ASN:ND2	1:A:426:ASN:N	2.46	0.64
1:B:417:ASP:O	1:C:424:SER:HB2	1.98	0.64
1:E:301:PHE:O	1:E:374:ARG:NH1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:182:THR:HG22	1:F:183:GLU:O	1.97	0.64
1:F:470:PHE:HB3	1:F:479:ILE:HD13	1.79	0.64
1:D:148:THR:CG2	1:D:193:ARG:HD2	2.27	0.63
1:D:257:ARG:CZ	1:D:407:GLU:HG3	2.28	0.63
1:E:126:LEU:CD1	1:E:130:ILE:HD11	2.28	0.63
1:A:432:TPO:HB	1:F:318:GLU:OE2	1.97	0.63
1:E:164:LEU:O	1:E:168:VAL:HG23	1.98	0.63
1:A:41:SER:OG	1:A:178:THR:HB	1.99	0.63
1:A:371:LYS:N	1:A:372:PRO:HD3	2.13	0.63
1:C:150:VAL:HG13	1:C:151:PHE:N	2.13	0.63
1:E:445:ILE:HG23	1:E:446:ARG:HD2	1.79	0.63
1:F:96:LYS:O	1:F:100:GLU:HG3	1.98	0.63
1:F:184:ARG:NH1	1:F:186:GLU:O	2.31	0.63
1:F:502:LYS:NZ	1:F:507:ARG:HG2	2.14	0.63
1:A:14:GLU:HG3	1:A:15:HIS:N	2.12	0.63
1:A:379:SER:N	1:A:413:THR:HB	2.04	0.63
1:A:388:SER:HB3	1:A:391:ALA:HB2	1.80	0.63
1:B:88:ARG:HH11	1:B:93:ASP:HA	1.62	0.63
1:B:126:LEU:O	1:B:130:ILE:HG12	1.98	0.63
1:B:449:MET:HG2	1:C:467:ILE:HD11	1.81	0.63
1:C:211:LEU:HA	1:C:216:ARG:HD3	1.80	0.63
1:D:283:ILE:HG12	1:D:400:THR:HG23	1.80	0.63
1:D:431:SEP:C	1:D:432:TPO:HG22	2.29	0.63
1:F:316:ALA:HB2	1:F:324:LEU:HD11	1.79	0.63
1:D:25:ILE:HD11	1:D:58:GLN:HB3	1.81	0.63
1:E:249:LEU:HD12	1:E:394:GLN:OE1	1.98	0.63
1:F:263:VAL:O	1:F:277:GLY:HA3	1.98	0.63
1:F:269:ARG:HH12	1:F:468:ARG:CD	2.12	0.63
1:A:408:ILE:HG22	1:A:409:THR:N	2.14	0.63
1:B:162:ARG:NH1	1:B:162:ARG:HB2	2.14	0.63
1:C:220:LEU:HD23	1:C:221:GLU:N	2.14	0.63
1:D:182:THR:HG22	1:D:183:GLU:N	2.12	0.63
1:D:208:ARG:HG2	1:D:208:ARG:HH11	1.62	0.63
1:E:80:PRO:HG2	1:E:107:ASP:HB2	1.81	0.63
1:E:321:ARG:HD2	1:F:255:THR:HG23	1.80	0.63
1:B:52:LYS:N	3:B:903:ATP:O1B	2.31	0.63
1:B:309:LYS:HA	1:B:343:LEU:HD13	1.80	0.63
1:C:331:TRP:HH2	3:C:901:ATP:O2A	1.82	0.63
1:C:426:ASN:ND2	1:C:431:SEP:HB3	2.13	0.63
1:C:465:LYS:HE2	1:C:465:LYS:N	2.12	0.63
1:D:150:VAL:CG1	1:D:151:PHE:N	2.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:418:GLN:NE2	1:F:422:ALA:HA	2.14	0.63
1:D:38:ILE:HA	1:D:177:THR:CG2	2.28	0.63
1:D:150:VAL:HG13	1:D:151:PHE:N	2.12	0.63
1:B:44:VAL:HG22	1:B:205:VAL:HB	1.81	0.63
1:B:497:ILE:HB	1:B:499:VAL:HG23	1.80	0.63
1:D:235:TYR:CD2	1:D:248:PRO:HA	2.34	0.63
1:D:235:TYR:HD2	1:D:248:PRO:HA	1.63	0.63
1:D:283:ILE:HD13	1:D:404:LYS:HE3	1.80	0.63
1:A:183:GLU:HB2	1:B:199:PHE:CZ	2.34	0.62
1:A:490:ILE:HG21	1:F:419:PHE:HE1	1.64	0.62
1:B:141:ARG:HD2	4:B:520:HOH:O	1.98	0.62
1:C:23:THR:O	1:C:24:MET:HB2	1.98	0.62
1:C:473:SER:OG	1:C:474:ASP:N	2.30	0.62
1:D:211:LEU:CB	1:D:216:ARG:HH11	2.12	0.62
1:E:395:PHE:O	1:E:399:VAL:HG23	1.99	0.62
1:F:27:GLY:HA3	1:F:246:ILE:HB	1.81	0.62
1:F:432:TPO:HG21	1:F:432:TPO:O1P	1.98	0.62
1:A:211:LEU:HD13	1:A:216:ARG:NE	2.12	0.62
1:B:437:ILE:HG12	1:B:457:LYS:HG2	1.80	0.62
1:E:123:LEU:CD2	1:E:166:ARG:HD2	2.29	0.62
1:F:146:SER:H	1:F:181:THR:HG22	1.64	0.62
1:A:364:LYS:HG2	1:A:402:TYR:CD2	2.34	0.62
1:A:377:ILE:HD13	1:A:412:PHE:CE2	2.34	0.62
1:D:151:PHE:O	1:D:153:GLN:N	2.32	0.62
1:F:47:THR:N	1:F:50:THR:HG21	2.14	0.62
1:F:397:ILE:HD11	1:F:433:ILE:HG21	1.81	0.62
1:C:21:MET:O	1:C:35:GLY:HA3	1.99	0.62
1:A:218:ARG:HH12	1:B:232:LYS:HE2	1.64	0.62
1:A:477:PRO:O	1:A:479:ILE:HD12	2.00	0.62
1:C:279:PHE:HE1	1:C:460:GLY:HA3	1.65	0.62
1:D:79:THR:HG23	1:D:81:GLN:HG2	1.81	0.62
1:E:313:ILE:HG13	1:E:372:PRO:HG3	1.82	0.62
1:A:405:GLN:C	1:A:407:GLU:H	2.01	0.62
1:C:64:ILE:CG2	1:C:102:LYS:HB3	2.30	0.62
1:C:81:GLN:NE2	1:C:81:GLN:H	1.98	0.62
1:C:261:VAL:HG12	1:C:262:ARG:N	2.11	0.62
1:D:379:SER:HA	1:D:413:THR:HG22	1.80	0.62
1:D:400:THR:HG21	1:D:433:ILE:HG22	1.82	0.62
1:E:446:ARG:HH21	1:E:496:ARG:HH22	1.44	0.62
1:B:161:ARG:HH22	1:B:199:PHE:HB2	1.64	0.62
1:D:208:ARG:HD2	1:D:234:GLU:OE1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:ASN:HA	4:D:535:HOH:O	2.00	0.62
1:E:123:LEU:HD23	1:E:124:SER:N	2.14	0.62
1:F:248:PRO:O	1:F:250:GLY:N	2.32	0.62
1:A:54:LEU:HD21	1:A:244:ILE:HG13	1.80	0.62
1:A:199:PHE:CE1	1:F:183:GLU:HB3	2.35	0.62
1:B:449:MET:HE3	1:C:490:ILE:HD11	1.82	0.62
1:C:140:ARG:NH1	1:C:140:ARG:HB3	2.14	0.62
1:C:483:PHE:HB2	1:C:489:ILE:HD13	1.81	0.62
1:E:32:SER:OG	1:E:35:GLY:N	2.32	0.62
1:F:203:ASN:HB3	1:F:225:LEU:CD2	2.29	0.62
1:A:334:ASP:O	1:A:338:MET:HG2	1.99	0.62
1:B:385:ARG:NH1	1:C:397:ILE:HD11	2.15	0.62
1:C:65:ILE:HD11	1:C:97:LEU:HD21	1.81	0.62
1:A:65:ILE:O	1:A:65:ILE:HG22	1.99	0.62
1:A:131:ASN:HA	1:A:134:ILE:HD12	1.81	0.62
1:A:294:LYS:NZ	1:A:415:THR:HA	2.15	0.62
1:C:64:ILE:H	1:C:64:ILE:HD12	1.65	0.62
1:C:64:ILE:HG22	1:C:64:ILE:O	2.00	0.62
1:C:247:PHE:HE2	1:C:364:LYS:HD2	1.65	0.62
1:F:21:MET:HE1	1:F:141:ARG:HG2	1.81	0.62
1:F:270:LEU:HA	1:F:273:MET:SD	2.40	0.62
1:F:396:VAL:HG11	1:F:430:ILE:HG23	1.82	0.62
1:B:148:THR:HG21	1:B:193:ARG:HD2	1.81	0.61
1:D:259:SER:HB3	1:D:281:ASP:OD2	2.00	0.61
1:A:497:ILE:HD12	1:A:497:ILE:O	1.99	0.61
1:B:25:ILE:HG23	1:B:58:GLN:NE2	2.15	0.61
1:B:145:ASP:OD2	1:B:181:THR:HG21	1.99	0.61
1:B:363:ILE:O	1:B:367:ILE:HG13	2.00	0.61
1:B:418:GLN:O	1:B:422:ALA:HB2	2.00	0.61
1:B:430:ILE:HA	1:B:433:ILE:HD11	1.80	0.61
1:C:43:LEU:HD12	1:C:180:MET:O	2.00	0.61
1:C:75:THR:HG23	1:C:107:ASP:HA	1.82	0.61
1:C:471:MET:HB3	1:C:480:LYS:CE	2.30	0.61
1:A:364:LYS:HG2	1:A:402:TYR:CE2	2.35	0.61
1:E:142:VAL:HB	1:E:178:THR:OG1	2.00	0.61
1:F:458:MET:SD	1:F:461:SER:HB3	2.40	0.61
1:B:445:ILE:HG13	1:B:483:PHE:HE2	1.66	0.61
1:C:80:PRO:CG	1:C:107:ASP:HB2	2.29	0.61
1:D:287:THR:HG23	1:D:414:ASN:HB3	1.81	0.61
1:F:182:THR:HG21	1:F:192:ALA:HB1	1.81	0.61
1:B:131:ASN:O	1:B:135:GLN:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:379:SER:HA	1:D:413:THR:O	2.00	0.61
1:C:76:PHE:O	1:C:109:SER:HA	2.01	0.61
1:D:211:LEU:HB2	1:D:216:ARG:HH11	1.65	0.61
1:D:215:ARG:HA	1:D:215:ARG:NE	2.16	0.61
1:E:89:SER:HB2	1:F:227:GLY:O	2.00	0.61
1:E:123:LEU:HD13	1:E:163:GLU:OE2	1.99	0.61
1:E:261:VAL:HG12	1:E:262:ARG:H	1.64	0.61
1:F:335:PHE:HA	1:F:338:MET:HG2	1.83	0.61
1:F:406:GLU:C	1:F:408:ILE:H	2.04	0.61
1:A:405:GLN:HG3	1:A:406:GLU:N	2.15	0.61
1:B:31:ILE:HG23	1:B:231:MET:HB2	1.82	0.61
1:C:212:GLU:O	1:C:212:GLU:HG2	2.00	0.61
1:F:269:ARG:HG2	1:F:479:ILE:CB	2.29	0.61
1:B:360:LEU:HD11	1:B:364:LYS:HE3	1.83	0.61
1:C:116:GLU:O	1:C:117:VAL:HB	2.00	0.61
1:C:335:PHE:HA	1:C:338:MET:HG3	1.82	0.61
1:F:280:LYS:NZ	1:F:280:LYS:HB3	2.16	0.61
1:F:387:VAL:HG12	1:F:391:ALA:HB3	1.83	0.61
1:A:25:ILE:HD12	1:A:58:GLN:NE2	2.15	0.61
1:A:227:GLY:HA3	1:F:86:ASN:OD1	2.01	0.61
1:C:393:ARG:O	1:C:397:ILE:HG12	2.01	0.61
1:C:148:THR:HA	1:C:151:PHE:CE1	2.35	0.61
1:D:245:ASN:CG	1:D:361:GLN:HE22	2.04	0.61
1:F:444:GLU:O	1:F:494:PRO:HD2	2.01	0.61
1:B:129:ARG:O	1:B:132:TYR:HB3	2.01	0.60
1:C:31:ILE:HA	1:C:231:MET:CG	2.27	0.60
1:C:48:SER:HB2	1:D:199:PHE:CE1	2.36	0.60
1:C:53:THR:HG23	1:C:145:ASP:OD1	2.01	0.60
1:C:64:ILE:HG12	1:C:102:LYS:O	2.01	0.60
1:C:384:ALA:HB2	1:C:392:PHE:CD1	2.35	0.60
1:B:202:ASP:HA	1:B:226:ARG:HD2	1.82	0.60
1:D:53:THR:CG2	1:D:57:ILE:HD13	2.31	0.60
1:D:115:GLN:OE1	1:D:118:VAL:HG21	2.01	0.60
1:E:365:SER:HA	1:E:368:ASN:ND2	2.16	0.60
1:F:218:ARG:HB3	4:F:532:HOH:O	2.01	0.60
1:B:38:ILE:HA	1:B:177:THR:HG23	1.83	0.60
1:B:117:VAL:O	1:B:117:VAL:HG12	2.02	0.60
1:B:149:SER:HB3	1:C:161:ARG:NH2	2.17	0.60
1:C:396:VAL:HG21	1:C:430:ILE:HD12	1.82	0.60
1:C:396:VAL:HG11	1:C:430:ILE:HG23	1.82	0.60
1:E:485:ASN:ND2	1:E:496:ARG:HD3	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:LEU:HD11	1:A:182:THR:OG1	2.01	0.60
1:E:150:VAL:CG1	1:E:151:PHE:N	2.65	0.60
1:E:431:SEP:O	1:E:434:THR:HG22	2.02	0.60
1:F:26:GLU:OE1	1:F:245:ASN:ND2	2.34	0.60
1:F:49:GLY:HA2	3:F:903:ATP:O2B	2.01	0.60
1:A:23:THR:HB	1:A:25:ILE:HG12	1.84	0.60
1:A:25:ILE:HD12	1:A:58:GLN:HE21	1.66	0.60
1:B:58:GLN:HG2	1:B:58:GLN:O	2.02	0.60
1:C:106:LEU:CD2	1:C:130:ILE:HA	2.32	0.60
1:C:118:VAL:HA	1:C:121:PHE:CD1	2.37	0.60
1:D:123:LEU:HD12	1:D:163:GLU:OE2	2.01	0.60
1:E:24:MET:HB3	1:E:62:ASN:HD22	1.65	0.60
1:A:490:ILE:N	1:A:490:ILE:HD12	2.16	0.60
1:E:103:LEU:HD12	1:E:104:PHE:H	1.67	0.60
1:F:315:PHE:CE2	1:F:347:VAL:HG21	2.36	0.60
1:A:265:SER:O	1:A:301:PHE:HA	2.00	0.60
1:A:439:LEU:HD12	1:A:440:LEU:N	2.16	0.60
1:B:385:ARG:HH12	1:C:397:ILE:CD1	2.15	0.60
1:C:387:VAL:HG12	1:C:388:SER:H	1.65	0.60
1:D:462:TRP:O	1:D:463:HIS:O	2.20	0.60
1:E:404:LYS:C	1:E:406:GLU:H	2.05	0.60
1:F:263:VAL:HB	1:F:374:ARG:HH21	1.65	0.60
1:B:103:LEU:HD11	1:B:105:ILE:HG13	1.83	0.60
1:B:147:VAL:O	1:B:150:VAL:HG12	2.00	0.60
1:E:214:GLU:HB3	1:F:234:GLU:HB2	1.81	0.60
1:E:392:PHE:O	1:E:395:PHE:HB3	2.02	0.60
1:F:209:ASN:ND2	1:F:216:ARG:HD2	2.17	0.60
1:B:304:ASN:HB3	1:B:374:ARG:HH12	1.67	0.60
1:C:137:TYR:O	1:C:138:ARG:HB2	2.01	0.60
1:E:153:GLN:C	1:F:158:SER:HB2	2.21	0.60
1:E:305:ALA:CB	1:E:374:ARG:HD2	2.28	0.60
1:E:454:ASN:CG	1:E:467:ILE:HD13	2.22	0.60
1:A:295:THR:HG23	1:A:378:ASP:OD2	2.02	0.60
1:B:96:LYS:HG2	1:B:100:GLU:OE1	2.02	0.60
1:B:264:SER:HB3	1:B:304:ASN:ND2	2.17	0.60
1:D:270:LEU:O	1:D:270:LEU:HD13	2.02	0.60
1:B:356:LEU:HD23	1:B:395:PHE:HB2	1.83	0.59
1:C:76:PHE:O	1:C:110:PRO:HD3	2.02	0.59
1:C:98:VAL:HG22	1:C:103:LEU:HG	1.82	0.59
1:C:247:PHE:HD2	1:C:364:LYS:HZ2	1.50	0.59
1:B:144:ILE:HD12	1:B:144:ILE:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:ARG:NH2	1:D:190:PRO:O	2.35	0.59
1:E:266:GLY:HA3	1:E:300:ARG:CG	2.32	0.59
1:E:317:TYR:CE2	1:E:383:LEU:HD21	2.36	0.59
1:F:265:SER:HA	1:F:301:PHE:HD1	1.67	0.59
1:A:44:VAL:HG13	1:A:205:VAL:HG12	1.84	0.59
1:A:266:GLY:CA	1:A:300:ARG:HG3	2.32	0.59
1:A:446:ARG:HA	1:A:496:ARG:HH22	1.65	0.59
1:B:191:ILE:HB	1:B:198:GLU:OE2	2.02	0.59
1:B:205:VAL:C	1:B:206:ILE:HD12	2.23	0.59
1:C:382:ALA:O	1:C:385:ARG:HG2	2.01	0.59
1:D:311:ARG:HD3	1:D:370:PHE:CE1	2.37	0.59
1:E:396:VAL:HG21	1:E:430:ILE:CD1	2.32	0.59
1:D:206:ILE:HD12	1:D:206:ILE:N	2.17	0.59
1:E:146:SER:HA	1:E:181:THR:O	2.02	0.59
1:E:379:SER:HA	1:E:413:THR:O	2.02	0.59
1:C:406:GLU:O	1:C:408:ILE:HG13	2.02	0.59
1:D:31:ILE:HA	1:D:231:MET:CG	2.29	0.59
1:E:168:VAL:O	1:E:171:LEU:HB2	2.02	0.59
1:F:141:ARG:HD2	4:F:526:HOH:O	2.01	0.59
1:A:185:ILE:HD12	1:A:185:ILE:N	2.18	0.59
1:A:256:GLN:HG2	1:F:320:SER:HB3	1.85	0.59
1:A:436:THR:OG1	1:A:458:MET:HG2	2.02	0.59
1:B:44:VAL:HA	1:B:205:VAL:O	2.02	0.59
1:C:467:ILE:N	1:C:467:ILE:HD12	2.18	0.59
1:F:248:PRO:C	1:F:250:GLY:H	2.06	0.59
1:F:471:MET:CG	1:F:478:ASP:HB3	2.32	0.59
1:A:420:MET:N	4:A:521:HOH:O	2.32	0.59
1:B:36:LEU:HD12	1:B:59:PHE:CE1	2.37	0.59
1:F:269:ARG:CG	1:F:479:ILE:HB	2.28	0.59
1:A:380:LEU:HD21	1:A:412:PHE:CD2	2.35	0.59
1:A:434:THR:HG23	1:A:437:ILE:HD11	1.85	0.59
1:B:64:ILE:HG22	1:B:65:ILE:N	2.18	0.59
1:B:264:SER:HA	1:B:271:ASP:OD1	2.03	0.59
1:B:315:PHE:CE2	1:B:347:VAL:HG21	2.38	0.59
1:B:341:GLN:O	1:B:343:LEU:N	2.36	0.59
1:C:197:GLU:OE2	1:C:197:GLU:N	2.33	0.59
1:D:370:PHE:O	1:D:371:LYS:HG3	2.02	0.59
1:A:379:SER:HB3	1:A:382:ALA:HB2	1.84	0.59
1:B:266:GLY:HA3	1:B:300:ARG:O	2.03	0.59
1:B:402:TYR:O	1:B:406:GLU:HB2	2.03	0.59
1:B:436:THR:HA	1:B:457:LYS:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:VAL:O	1:C:262:ARG:HG2	2.03	0.59
1:D:371:LYS:O	1:D:371:LYS:CD	2.44	0.59
1:F:80:PRO:HG2	1:F:107:ASP:HB2	1.84	0.59
1:E:356:LEU:CD1	1:E:387:VAL:HG21	2.32	0.59
1:A:263:VAL:HG12	1:A:374:ARG:NH2	2.10	0.58
1:E:152:GLN:HG3	1:F:161:ARG:HH11	1.67	0.58
1:F:22:ARG:HA	1:F:29:ASP:OD1	2.02	0.58
1:A:142:VAL:HG12	1:A:143:SER:N	2.18	0.58
1:A:147:VAL:O	1:A:150:VAL:HG12	2.03	0.58
1:B:273:MET:CE	1:B:468:ARG:HD2	2.34	0.58
1:D:154:TYR:O	1:D:154:TYR:HD1	1.86	0.58
1:D:436:THR:OG1	1:D:458:MET:HG2	2.03	0.58
1:E:302:VAL:O	1:E:305:ALA:HB3	2.02	0.58
1:A:389:ASN:C	1:A:389:ASN:HD22	2.06	0.58
1:C:468:ARG:HG2	1:C:482:SER:HB3	1.85	0.58
1:D:431:SEP:HA	1:D:434:THR:HG22	1.85	0.58
1:A:313:ILE:HG21	1:A:315:PHE:CZ	2.38	0.58
1:A:479:ILE:HD12	1:A:479:ILE:N	2.18	0.58
1:C:419:PHE:O	1:C:420:MET:HB2	2.04	0.58
1:E:164:LEU:CB	1:E:200:VAL:HG11	2.33	0.58
1:F:203:ASN:HB3	1:F:225:LEU:HD23	1.84	0.58
1:F:453:ILE:HG21	1:F:479:ILE:CD1	2.34	0.58
1:D:44:VAL:HG22	1:D:205:VAL:HB	1.84	0.58
1:D:211:LEU:CG	1:D:216:ARG:HH11	2.16	0.58
1:D:220:LEU:HD13	1:D:246:ILE:HD12	1.83	0.58
1:F:104:PHE:HB2	1:F:137:TYR:CE2	2.39	0.58
1:E:451:ARG:HG2	1:E:451:ARG:NH1	2.18	0.58
1:F:285:LEU:HD12	1:F:286:ALA:H	1.67	0.58
1:F:384:ALA:HB2	1:F:392:PHE:CE1	2.39	0.58
1:A:508:ILE:HD13	1:A:508:ILE:N	2.17	0.58
1:B:293:GLY:O	1:B:296:LEU:N	2.36	0.58
1:B:493:SER:HB3	1:C:488:ARG:CG	2.31	0.58
1:C:309:LYS:HA	1:C:343:LEU:CD1	2.33	0.58
1:D:57:ILE:HD12	1:D:57:ILE:N	2.19	0.58
1:D:163:GLU:OE2	1:D:163:GLU:HA	2.04	0.58
1:F:70:PRO:HB2	1:F:139:ALA:HA	1.85	0.58
1:F:94:LEU:HB3	1:F:103:LEU:HD23	1.86	0.58
1:F:207:LEU:CD2	1:F:220:LEU:HD12	2.30	0.58
1:F:263:VAL:HB	1:F:374:ARG:NH2	2.17	0.58
1:C:486:PHE:CD2	1:C:494:PRO:HB2	2.33	0.58
1:E:170:ARG:O	1:E:174:ILE:HG13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:ASP:HA	1:B:181:THR:HB	1.85	0.58
1:B:436:THR:HG23	1:B:458:MET:HG2	1.85	0.58
1:C:385:ARG:NH1	1:D:397:ILE:HD11	2.19	0.58
1:D:264:SER:HB3	1:D:304:ASN:ND2	2.19	0.58
1:E:21:MET:HE1	1:E:141:ARG:HG2	1.84	0.58
1:E:245:ASN:ND2	1:E:247:PHE:HE2	2.01	0.58
1:B:70:PRO:HA	1:B:102:LYS:O	2.03	0.58
1:B:186:GLU:OE2	1:B:187:GLU:N	2.37	0.58
1:E:464:ASP:OD2	1:E:466:ALA:HB3	2.04	0.58
1:F:266:GLY:HA2	1:F:304:ASN:ND2	2.15	0.58
1:F:518:GLU:HG2	1:F:519:SER:H	1.69	0.58
1:A:437:ILE:HD13	1:A:457:LYS:CE	2.25	0.57
1:D:224:LYS:HA	1:D:230:HIS:HE1	1.68	0.57
1:D:262:ARG:HH22	1:D:461:SER:HB2	1.66	0.57
1:D:431:SEP:O	1:D:433:ILE:N	2.36	0.57
1:E:217:ARG:HH21	1:E:236:PRO:HB3	1.68	0.57
1:F:41:SER:HA	1:F:178:THR:O	2.04	0.57
1:F:197:GLU:H	1:F:197:GLU:CD	2.05	0.57
1:D:425:ILE:HD12	1:D:425:ILE:N	2.19	0.57
1:E:315:PHE:CD2	1:E:347:VAL:HG21	2.39	0.57
1:A:218:ARG:NH1	1:B:232:LYS:HE2	2.19	0.57
1:A:320:SER:CA	1:B:254:LEU:HG	2.31	0.57
1:B:49:GLY:HA2	3:B:903:ATP:O2B	2.05	0.57
1:C:23:THR:HG21	1:C:28:PHE:CD2	2.38	0.57
1:D:211:LEU:CD2	1:D:216:ARG:NH1	2.65	0.57
1:D:356:LEU:H	1:D:356:LEU:HD12	1.69	0.57
1:E:72:VAL:HG21	1:E:134:ILE:HD13	1.86	0.57
1:E:430:ILE:O	1:E:431:SEP:C	2.53	0.57
1:E:446:ARG:HH21	1:E:496:ARG:NH2	2.01	0.57
1:E:461:SER:OG	1:E:462:TRP:N	2.36	0.57
1:A:509:VAL:O	1:A:509:VAL:HG12	2.04	0.57
1:B:425:ILE:HG21	1:B:437:ILE:CG2	2.34	0.57
1:B:438:ILE:HD12	1:B:455:VAL:HG22	1.85	0.57
1:C:31:ILE:HG23	1:C:231:MET:HB2	1.86	0.57
1:C:64:ILE:HG23	1:C:102:LYS:HB3	1.85	0.57
1:C:217:ARG:HA	1:C:357:GLU:OE1	2.05	0.57
1:F:170:ARG:HB3	1:F:170:ARG:NH1	2.20	0.57
1:F:270:LEU:O	1:F:273:MET:N	2.37	0.57
1:B:416:SER:O	1:B:418:GLN:N	2.38	0.57
1:C:262:ARG:NH2	1:C:461:SER:HB2	2.14	0.57
1:D:284:ILE:HG13	1:D:436:THR:HB	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:311:ARG:HG2	1:E:343:LEU:HA	1.86	0.57
1:D:28:PHE:CE1	1:D:222:ILE:HD11	2.39	0.57
1:D:341:GLN:O	1:D:342:ASN:HB2	2.05	0.57
1:A:94:LEU:O	1:A:97:LEU:HB2	2.04	0.57
1:A:289:ALA:O	1:A:292:THR:HG23	2.05	0.57
1:B:329:TYR:HD2	1:B:329:TYR:O	1.86	0.57
1:C:371:LYS:N	1:C:372:PRO:HD3	2.20	0.57
1:C:453:ILE:HG23	1:C:454:ASN:N	2.18	0.57
1:D:331:TRP:CD2	4:D:536:HOH:O	2.57	0.57
1:F:429:HIS:ND1	1:F:429:HIS:O	2.37	0.57
1:B:282:SER:HB2	1:B:435:ASP:HB2	1.87	0.57
1:F:111:ASP:OD1	1:F:112:PRO:HD2	2.05	0.57
1:C:41:SER:OG	1:C:168:VAL:HG13	2.05	0.57
1:C:354:ALA:HB1	1:C:358:ASP:HB2	1.87	0.57
1:B:371:LYS:HD2	1:B:371:LYS:O	2.05	0.57
1:D:294:LYS:N	3:D:901:ATP:O1B	2.38	0.57
1:E:287:THR:CG2	1:E:288:GLY:H	2.18	0.57
1:F:72:VAL:CG2	1:F:134:ILE:HD13	2.31	0.57
1:F:360:LEU:HG	1:F:395:PHE:CD1	2.40	0.57
1:C:50:THR:HG21	1:C:207:LEU:C	2.25	0.56
1:C:156:ALA:O	1:C:160:VAL:HG23	2.05	0.56
1:C:300:ARG:HA	1:C:333:MET:CE	2.34	0.56
1:D:330:SER:CB	4:D:535:HOH:O	2.53	0.56
1:F:515:LYS:CG	1:F:516:GLY:H	2.15	0.56
1:A:508:ILE:HD13	1:A:508:ILE:H	1.70	0.56
1:B:237:PHE:HB3	1:B:246:ILE:HG13	1.86	0.56
1:B:383:LEU:HD13	1:B:395:PHE:CE2	2.40	0.56
1:E:406:GLU:O	1:E:407:GLU:HB2	2.05	0.56
1:F:317:TYR:CD2	1:F:383:LEU:HD21	2.40	0.56
1:F:418:GLN:HG3	1:F:422:ALA:HA	1.86	0.56
1:B:18:ILE:H	1:B:18:ILE:CD1	2.19	0.56
1:B:21:MET:HB2	1:B:38:ILE:CG1	2.35	0.56
1:B:469:GLU:HB3	1:B:483:PHE:CE1	2.40	0.56
1:C:45:SER:HB3	1:C:182:THR:HB	1.87	0.56
1:C:69:GLU:HB3	1:C:140:ARG:HB2	1.87	0.56
1:C:80:PRO:HG2	1:C:107:ASP:HB2	1.86	0.56
1:C:159:VAL:O	1:C:163:GLU:HG2	2.05	0.56
1:D:311:ARG:CD	1:D:371:LYS:HE3	2.26	0.56
1:E:52:LYS:HB3	1:E:181:THR:HG23	1.86	0.56
1:E:266:GLY:HA3	1:E:300:ARG:HG3	1.86	0.56
1:E:315:PHE:HB3	1:E:317:TYR:HE1	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:400:THR:O	1:F:404:LYS:HG3	2.05	0.56
1:F:470:PHE:HA	1:F:478:ASP:O	2.05	0.56
1:F:487:GLU:HG3	1:F:497:ILE:HD11	1.88	0.56
1:A:21:MET:CE	1:A:59:PHE:HZ	2.18	0.56
1:B:38:ILE:HA	1:B:177:THR:CG2	2.35	0.56
1:C:170:ARG:HD2	1:C:173:GLN:OE1	2.05	0.56
1:C:313:ILE:HG12	1:C:345:LYS:HB3	1.86	0.56
1:E:392:PHE:O	1:E:395:PHE:N	2.39	0.56
1:F:111:ASP:C	1:F:113:GLU:H	2.08	0.56
1:A:249:LEU:HD13	1:A:394:GLN:HG2	1.87	0.56
1:D:161:ARG:HD2	1:D:196:VAL:CG1	2.35	0.56
1:D:296:LEU:HD22	4:D:536:HOH:O	2.06	0.56
1:E:72:VAL:HG12	1:E:73:PHE:N	2.20	0.56
1:F:471:MET:HG3	1:F:478:ASP:HB3	1.88	0.56
1:A:267:VAL:CG2	1:A:300:ARG:HG2	2.36	0.56
1:A:375:ILE:HD13	1:A:408:ILE:HG21	1.87	0.56
1:A:468:ARG:NH1	1:A:468:ARG:HG2	2.19	0.56
1:B:191:ILE:HB	1:B:198:GLU:CG	2.35	0.56
1:B:418:GLN:O	1:B:418:GLN:HG3	2.06	0.56
1:D:215:ARG:HE	1:D:215:ARG:CA	2.16	0.56
1:D:349:ALA:H	1:E:254:LEU:HD23	1.70	0.56
1:E:287:THR:CG2	1:E:288:GLY:N	2.68	0.56
1:F:191:ILE:CG1	1:F:198:GLU:HG3	2.35	0.56
1:A:256:GLN:HG3	1:A:404:LYS:HD3	1.87	0.56
1:B:315:PHE:HB3	1:B:317:TYR:CE1	2.41	0.56
1:B:473:SER:C	1:B:475:LYS:H	2.09	0.56
1:C:49:GLY:O	1:C:218:ARG:NH2	2.39	0.56
1:C:340:ARG:C	1:C:342:ASN:N	2.59	0.56
1:D:47:THR:O	1:D:50:THR:HG23	2.06	0.56
1:D:98:VAL:HG23	1:D:103:LEU:HD23	1.86	0.56
1:D:114:GLY:O	1:D:115:GLN:HG3	2.06	0.56
1:D:161:ARG:HD2	1:D:196:VAL:HG13	1.86	0.56
1:E:485:ASN:ND2	1:E:496:ARG:HH11	2.04	0.56
1:F:432:TPO:C	1:F:434:THR:H	2.19	0.56
1:B:183:GLU:OE2	1:C:161:ARG:NH1	2.36	0.56
1:B:451:ARG:H	1:B:451:ARG:HD2	1.69	0.56
1:D:76:PHE:O	1:D:109:SER:HA	2.06	0.56
1:D:145:ASP:OD2	1:D:181:THR:HG21	2.05	0.56
1:F:430:ILE:O	1:F:432:TPO:O	2.23	0.56
1:A:248:PRO:O	1:A:250:GLY:N	2.39	0.56
1:A:267:VAL:HG11	1:A:479:ILE:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:ILE:N	1:C:144:ILE:HD12	2.21	0.56
1:D:486:PHE:HE2	1:D:496:ARG:HH11	1.54	0.56
1:F:313:ILE:HD11	1:F:372:PRO:HG3	1.88	0.56
1:B:356:LEU:HD11	1:B:387:VAL:HG21	1.88	0.56
1:D:202:ASP:HA	1:D:226:ARG:HD2	1.88	0.56
1:D:257:ARG:CZ	1:D:407:GLU:CG	2.83	0.56
1:D:451:ARG:HB3	1:D:470:PHE:CE2	2.41	0.56
1:D:471:MET:HG2	1:D:480:LYS:HE2	1.88	0.56
1:E:80:PRO:O	1:E:84:ILE:HG13	2.06	0.56
1:F:365:SER:HA	1:F:368:ASN:ND2	2.20	0.56
1:F:509:VAL:HG12	1:F:510:ARG:H	1.70	0.56
1:A:61:TYR:O	1:A:65:ILE:HG12	2.06	0.55
1:C:340:ARG:O	1:C:342:ASN:N	2.39	0.55
1:D:293:GLY:HA2	3:D:901:ATP:O1A	2.06	0.55
1:E:40:ARG:HG3	1:E:172:LYS:NZ	2.21	0.55
1:E:74:VAL:HG11	1:E:76:PHE:HE1	1.71	0.55
1:F:256:GLN:HE21	1:F:404:LYS:HB2	1.69	0.55
1:F:418:GLN:O	1:F:422:ALA:HB2	2.06	0.55
1:A:161:ARG:NH2	1:F:149:SER:HB3	2.22	0.55
1:B:51:GLY:O	1:B:54:LEU:HB3	2.07	0.55
1:B:327:ASN:HD21	1:C:459:ARG:HB3	1.70	0.55
3:B:901:ATP:C2	1:C:462:TRP:HA	2.41	0.55
1:C:25:ILE:HG12	1:C:58:GLN:NE2	2.21	0.55
1:E:377:ILE:HD12	1:E:412:PHE:CE2	2.41	0.55
1:A:46:GLY:HA2	1:A:184:ARG:CD	2.35	0.55
1:C:338:MET:HB2	1:C:344:LEU:HD12	1.89	0.55
1:F:302:VAL:CG1	1:F:344:LEU:HG	2.35	0.55
1:A:21:MET:HE3	1:A:141:ARG:NE	2.21	0.55
1:B:147:VAL:HG11	1:B:180:MET:CE	2.20	0.55
1:C:269:ARG:NE	4:C:524:HOH:O	2.32	0.55
1:C:425:ILE:HD12	1:C:425:ILE:N	2.13	0.55
1:D:72:VAL:HG21	1:D:134:ILE:HD13	1.89	0.55
1:D:259:SER:OG	1:D:261:VAL:HG23	2.06	0.55
1:E:119:GLY:HA2	1:E:122:ASP:HB3	1.88	0.55
1:E:211:LEU:O	1:E:212:GLU:HB3	2.05	0.55
1:F:115:GLN:CG	1:F:116:GLU:N	2.57	0.55
1:F:486:PHE:HE2	1:F:496:ARG:HD2	1.70	0.55
1:B:311:ARG:HD2	1:B:371:LYS:CE	2.36	0.55
1:E:28:PHE:O	1:E:32:SER:HB3	2.06	0.55
1:F:186:GLU:CD	1:F:187:GLU:H	2.10	0.55
1:A:298:VAL:HG22	1:A:411:LEU:CD2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:PHE:CD2	1:C:347:VAL:HG21	2.41	0.55
1:C:360:LEU:HD21	1:C:364:LYS:HE3	1.89	0.55
1:D:214:GLU:HG2	1:E:234:GLU:CB	2.37	0.55
1:E:18:ILE:CD1	1:E:227:GLY:HA3	2.36	0.55
1:E:291:GLY:HA3	1:E:442:TYR:OH	2.06	0.55
1:E:326:ARG:O	1:E:329:TYR:N	2.39	0.55
1:A:223:LEU:HD21	1:F:216:ARG:HH21	1.70	0.55
1:A:269:ARG:O	1:A:272:GLU:HB2	2.06	0.55
1:A:294:LYS:HG3	1:A:440:LEU:HD12	1.88	0.55
1:B:438:ILE:CD1	1:B:455:VAL:HG22	2.37	0.55
1:C:52:LYS:H	1:C:207:LEU:CD1	2.20	0.55
1:C:347:VAL:O	1:C:348:CYS:HB2	2.07	0.55
1:D:200:VAL:O	1:D:200:VAL:HG12	2.06	0.55
1:D:449:MET:HE2	1:D:449:MET:HA	1.89	0.55
1:E:344:LEU:HD13	1:E:345:LYS:N	2.21	0.55
1:A:341:GLN:HB3	1:A:343:LEU:HG	1.88	0.55
1:B:191:ILE:HD12	1:B:198:GLU:HG2	1.89	0.55
1:C:305:ALA:HB2	1:C:374:ARG:CD	2.34	0.55
1:D:39:GLY:N	1:D:177:THR:HG23	2.22	0.55
1:F:148:THR:CG2	1:F:193:ARG:HD2	2.37	0.55
1:A:61:TYR:CZ	1:A:65:ILE:HG13	2.41	0.55
1:B:24:MET:CB	1:B:62:ASN:HD22	2.19	0.55
1:C:360:LEU:CD2	1:C:364:LYS:HE3	2.36	0.55
1:E:18:ILE:CG1	1:E:228:THR:HG23	2.33	0.55
1:E:426:ASN:HD22	1:E:426:ASN:N	2.05	0.55
1:F:191:ILE:HG23	1:F:206:ILE:HD11	1.89	0.55
1:F:298:VAL:O	1:F:301:PHE:HB3	2.06	0.55
1:A:163:GLU:HA	1:A:163:GLU:OE2	2.07	0.55
1:C:280:LYS:C	1:C:409:THR:HG23	2.27	0.55
1:D:65:ILE:O	1:D:65:ILE:HG22	2.07	0.55
1:D:152:GLN:OE1	1:E:161:ARG:HD2	2.07	0.55
1:E:426:ASN:ND2	1:E:426:ASN:N	2.54	0.55
1:A:283:ILE:HG13	1:A:400:THR:HG23	1.88	0.54
1:A:444:GLU:HB3	1:A:493:SER:HA	1.90	0.54
1:B:263:VAL:CG1	1:B:374:ARG:HH21	2.14	0.54
1:B:347:VAL:O	1:B:348:CYS:HB2	2.05	0.54
1:C:126:LEU:O	1:C:129:ARG:N	2.39	0.54
1:C:317:TYR:CD1	1:C:383:LEU:HD21	2.42	0.54
1:D:451:ARG:NH1	1:D:472:ILE:HD13	2.22	0.54
1:E:116:GLU:O	1:E:118:VAL:HG23	2.07	0.54
1:E:445:ILE:HG22	1:E:446:ARG:HD2	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:292:THR:HB	1:F:440:LEU:HB3	1.89	0.54
1:A:215:ARG:HH22	1:B:234:GLU:N	2.04	0.54
1:A:468:ARG:HG2	1:A:468:ARG:HH11	1.71	0.54
1:D:287:THR:CG2	1:D:414:ASN:HB3	2.36	0.54
1:D:331:TRP:CE2	4:D:536:HOH:O	2.53	0.54
1:B:73:PHE:CE2	1:B:83:ILE:HD13	2.42	0.54
1:C:64:ILE:HD12	1:C:64:ILE:N	2.23	0.54
1:D:211:LEU:CD1	1:D:216:ARG:HH11	2.19	0.54
1:D:298:VAL:O	1:D:302:VAL:HG23	2.07	0.54
1:D:451:ARG:HH11	1:D:472:ILE:HD13	1.72	0.54
1:F:451:ARG:HG2	1:F:451:ARG:HH11	1.73	0.54
1:B:203:ASN:HB3	1:B:225:LEU:CD2	2.37	0.54
1:C:328:ALA:O	1:C:331:TRP:N	2.39	0.54
1:C:341:GLN:O	1:C:343:LEU:HG	2.07	0.54
1:E:302:VAL:HG13	1:E:344:LEU:CD2	2.38	0.54
1:E:485:ASN:HD21	1:E:496:ARG:NH1	2.05	0.54
1:F:170:ARG:O	1:F:174:ILE:HG13	2.07	0.54
1:F:313:ILE:HB	1:F:375:ILE:CD1	2.38	0.54
1:A:327:ASN:HB3	1:A:331:TRP:CZ3	2.42	0.54
1:A:455:VAL:HG11	1:A:463:HIS:HB2	1.90	0.54
1:C:184:ARG:C	1:C:185:ILE:HD12	2.27	0.54
1:C:417:ASP:HB3	1:D:429:HIS:CE1	2.42	0.54
1:C:469:GLU:CG	1:C:480:LYS:HB2	2.35	0.54
1:C:471:MET:O	1:C:471:MET:HG3	2.08	0.54
1:E:267:VAL:HG22	1:E:477:PRO:CG	2.38	0.54
1:F:215:ARG:HA	1:F:215:ARG:NE	2.22	0.54
1:B:161:ARG:HB2	1:B:196:VAL:HG11	1.89	0.54
1:B:203:ASN:OD1	1:B:225:LEU:HA	2.08	0.54
1:B:434:THR:HG21	1:B:437:ILE:HD11	1.89	0.54
1:D:264:SER:HA	1:D:271:ASP:OD1	2.08	0.54
1:E:263:VAL:CG1	1:E:374:ARG:HH21	2.20	0.54
1:E:338:MET:HB3	1:E:344:LEU:CB	2.37	0.54
1:F:122:ASP:OD2	1:F:123:LEU:N	2.41	0.54
1:F:124:SER:OG	1:F:166:ARG:NH1	2.41	0.54
1:F:146:SER:H	1:F:181:THR:CG2	2.20	0.54
1:F:331:TRP:HE1	1:F:472:ILE:CG2	2.21	0.54
1:F:406:GLU:O	1:F:408:ILE:N	2.41	0.54
1:A:52:LYS:CB	1:A:181:THR:HG23	2.36	0.54
1:A:298:VAL:HG22	1:A:411:LEU:HD23	1.90	0.54
1:A:311:ARG:HH11	1:A:371:LYS:HE3	1.73	0.54
1:A:353:SER:O	1:A:354:ALA:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:THR:O	1:A:404:LYS:HB2	2.07	0.54
1:D:191:ILE:HB	1:D:198:GLU:OE2	2.08	0.54
1:E:76:PHE:CE2	1:E:150:VAL:HB	2.43	0.54
1:F:80:PRO:CG	1:F:107:ASP:HB2	2.38	0.54
1:F:262:ARG:HH22	1:F:461:SER:CB	2.20	0.54
1:B:458:MET:HB2	1:B:463:HIS:HD2	1.73	0.54
1:C:114:GLY:O	1:C:115:GLN:HB3	2.08	0.54
1:E:130:ILE:N	1:E:130:ILE:HD12	2.23	0.54
1:F:140:ARG:HB3	1:F:140:ARG:NH1	2.18	0.54
1:A:377:ILE:HD12	1:A:377:ILE:N	2.23	0.54
1:B:73:PHE:HE2	1:B:83:ILE:HD13	1.72	0.54
1:C:18:ILE:HD12	1:C:18:ILE:N	2.23	0.54
1:D:182:THR:CG2	1:D:183:GLU:N	2.71	0.54
1:D:299:SER:C	1:D:333:MET:HE1	2.28	0.54
1:F:302:VAL:HG21	1:F:314:LEU:HD13	1.90	0.54
1:F:509:VAL:HG12	1:F:510:ARG:N	2.22	0.54
1:A:134:ILE:CD1	1:A:174:ILE:HG21	2.38	0.54
1:B:52:LYS:HB2	3:B:903:ATP:O1B	2.07	0.54
1:D:421:GLY:O	1:D:423:HIS:N	2.41	0.54
1:E:341:GLN:O	1:E:342:ASN:HB2	2.07	0.54
1:B:152:GLN:HG3	1:C:161:ARG:NH1	2.23	0.53
1:B:193:ARG:NH2	1:C:195:GLY:O	2.40	0.53
1:B:249:LEU:HD12	1:B:394:GLN:HG2	1.90	0.53
1:B:356:LEU:HD12	1:B:356:LEU:N	2.21	0.53
1:B:445:ILE:CD1	1:B:494:PRO:HG2	2.38	0.53
1:D:53:THR:CG2	1:D:57:ILE:CD1	2.86	0.53
1:C:52:LYS:HB3	1:C:181:THR:HG23	1.90	0.53
1:C:301:PHE:CE2	1:C:374:ARG:HD3	2.43	0.53
1:C:426:ASN:ND2	1:C:426:ASN:N	2.56	0.53
1:A:254:LEU:HD13	1:F:350:TYR:CZ	2.43	0.53
1:C:191:ILE:HB	1:C:198:GLU:CG	2.38	0.53
1:D:471:MET:HE2	1:D:478:ASP:HB3	1.90	0.53
1:E:32:SER:OG	1:E:32:SER:O	2.26	0.53
1:E:364:LYS:HG3	1:E:402:TYR:CE2	2.42	0.53
1:F:16:GLN:HE22	1:F:33:HIS:HB3	1.73	0.53
1:F:73:PHE:C	1:F:73:PHE:CD2	2.81	0.53
1:F:118:VAL:O	1:F:118:VAL:HG13	2.08	0.53
1:F:184:ARG:HD2	4:F:522:HOH:O	2.07	0.53
1:F:469:GLU:CG	1:F:470:PHE:N	2.70	0.53
1:A:136:LYS:HD3	1:A:137:TYR:CE1	2.43	0.53
1:B:62:ASN:O	1:B:66:GLU:HB2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:454:ASN:OD1	1:C:467:ILE:HG13	2.08	0.53
1:D:28:PHE:HE1	1:D:222:ILE:HD11	1.71	0.53
1:D:63:GLY:HA2	1:D:141:ARG:CZ	2.38	0.53
1:D:157:SER:O	1:D:196:VAL:HG21	2.09	0.53
3:E:901:ATP:H2'	1:F:458:MET:O	2.09	0.53
1:F:217:ARG:HH22	1:F:394:GLN:HE22	1.56	0.53
1:F:273:MET:O	1:F:464:ASP:N	2.38	0.53
1:F:313:ILE:HG23	1:F:345:LYS:O	2.07	0.53
1:A:14:GLU:CG	1:A:15:HIS:N	2.64	0.53
1:B:390:ASN:O	1:B:392:PHE:N	2.42	0.53
1:C:211:LEU:HD22	1:C:216:ARG:NE	2.22	0.53
1:E:383:LEU:C	1:E:385:ARG:H	2.12	0.53
1:F:14:GLU:HG3	1:F:15:HIS:N	2.24	0.53
1:B:432:TPO:C	1:B:433:ILE:HD13	2.39	0.53
1:C:173:GLN:O	1:C:175:GLY:N	2.42	0.53
1:D:30:ASP:OD2	1:D:30:ASP:N	2.42	0.53
1:D:344:LEU:HD13	1:D:345:LYS:N	2.23	0.53
1:E:24:MET:HG3	1:E:66:GLU:HG3	1.90	0.53
1:E:320:SER:HA	1:F:254:LEU:HG	1.90	0.53
1:F:311:ARG:CD	1:F:371:LYS:HE3	2.38	0.53
1:A:396:VAL:HG11	1:A:430:ILE:HD12	1.91	0.53
1:D:218:ARG:NH1	1:E:232:LYS:HE2	2.21	0.53
1:E:497:ILE:HG22	1:E:498:THR:N	2.14	0.53
1:A:82:ASP:O	1:A:85:LYS:HB3	2.09	0.53
1:A:264:SER:HA	1:A:271:ASP:OD1	2.08	0.53
1:B:191:ILE:HD12	1:B:198:GLU:CG	2.38	0.53
1:E:85:LYS:O	1:E:88:ARG:HB2	2.08	0.53
1:E:444:GLU:OE1	1:F:490:ILE:HG12	2.09	0.53
1:F:18:ILE:HG13	1:F:227:GLY:HA3	1.89	0.53
1:F:61:TYR:O	1:F:64:ILE:HB	2.08	0.53
1:F:194:TYR:CD1	1:F:194:TYR:N	2.76	0.53
1:F:518:GLU:HG2	1:F:519:SER:N	2.23	0.53
1:A:45:SER:CB	1:A:182:THR:HB	2.38	0.53
1:B:434:THR:CG2	1:B:437:ILE:HD11	2.38	0.53
1:D:21:MET:O	1:D:35:GLY:HA3	2.08	0.53
1:D:301:PHE:HZ	1:D:409:THR:HG22	1.74	0.53
1:D:356:LEU:O	1:D:359:HIS:N	2.42	0.53
1:E:18:ILE:HD11	1:E:228:THR:N	2.24	0.53
1:E:347:VAL:HG12	1:E:348:CYS:N	2.23	0.53
1:F:148:THR:HG21	1:F:193:ARG:HD2	1.90	0.53
1:F:470:PHE:CB	1:F:479:ILE:HD13	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:MET:HA	1:A:449:MET:CE	2.39	0.53
1:B:206:ILE:N	1:B:206:ILE:CD1	2.71	0.53
1:B:379:SER:N	1:B:413:THR:HB	2.00	0.53
1:B:380:LEU:N	1:B:413:THR:O	2.42	0.53
1:C:63:GLY:HA3	1:C:141:ARG:CZ	2.39	0.53
1:C:118:VAL:O	1:C:118:VAL:HG12	2.08	0.53
1:C:468:ARG:HA	1:C:482:SER:HA	1.90	0.53
1:D:19:ALA:HB1	1:D:38:ILE:HD12	1.91	0.53
1:D:193:ARG:HG2	1:D:193:ARG:HH11	1.73	0.53
1:E:164:LEU:HB2	1:E:200:VAL:HG11	1.91	0.53
1:A:207:LEU:HD21	1:A:220:LEU:HD12	1.91	0.52
1:A:467:ILE:HG12	1:F:447:GLY:O	2.09	0.52
1:B:433:ILE:HD13	1:B:433:ILE:N	2.24	0.52
1:C:182:THR:HG22	1:C:183:GLU:N	2.14	0.52
1:D:367:ILE:HD11	1:D:375:ILE:CD1	2.39	0.52
1:D:431:SEP:C	1:D:433:ILE:N	2.67	0.52
1:E:40:ARG:HG3	1:E:172:LYS:HZ1	1.74	0.52
1:F:145:ASP:HA	1:F:181:THR:CG2	2.29	0.52
1:A:435:ASP:OD1	1:A:459:ARG:NH1	2.42	0.52
1:B:185:ILE:N	1:B:185:ILE:CD1	2.71	0.52
1:B:392:PHE:O	1:B:395:PHE:N	2.39	0.52
1:C:71:GLY:O	1:C:103:LEU:HA	2.09	0.52
1:C:211:LEU:HD22	1:C:216:ARG:CZ	2.38	0.52
1:C:487:GLU:O	1:C:488:ARG:HB2	2.08	0.52
1:D:401:GLY:O	1:D:405:GLN:HG2	2.09	0.52
1:D:451:ARG:HG2	1:D:451:ARG:NH1	2.23	0.52
1:E:84:ILE:HG21	1:E:95:ALA:HB2	1.90	0.52
1:E:193:ARG:NH2	1:F:195:GLY:O	2.41	0.52
1:F:106:LEU:C	1:F:106:LEU:HD12	2.30	0.52
1:F:516:GLY:N	1:F:517:PRO:HD2	2.24	0.52
1:A:161:ARG:HB2	1:A:196:VAL:CG1	2.33	0.52
1:B:38:ILE:HG23	1:B:177:THR:OG1	2.09	0.52
1:D:211:LEU:CB	1:D:216:ARG:NH1	2.72	0.52
1:D:355:GLY:O	1:D:356:LEU:C	2.48	0.52
1:F:185:ILE:HD11	1:F:193:ARG:NH1	2.24	0.52
1:F:283:ILE:HG23	1:F:412:PHE:CE1	2.43	0.52
1:F:379:SER:N	1:F:413:THR:HB	2.18	0.52
1:F:486:PHE:CZ	1:F:496:ARG:HB3	2.44	0.52
1:A:317:TYR:HB3	1:A:351:PRO:HG3	1.91	0.52
1:A:453:ILE:HB	1:A:470:PHE:CE2	2.44	0.52
1:E:451:ARG:HH12	1:E:472:ILE:CD1	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:274:CYS:SG	1:F:278:PHE:HE2	2.33	0.52
1:A:150:VAL:HG13	1:A:151:PHE:CD2	2.44	0.52
1:C:486:PHE:CE2	1:C:496:ARG:HG2	2.45	0.52
1:D:330:SER:HB2	4:D:537:HOH:O	2.09	0.52
1:E:211:LEU:HD13	1:E:216:ARG:NH1	2.24	0.52
1:F:344:LEU:HD22	1:F:345:LYS:N	2.24	0.52
1:F:368:ASN:C	1:F:370:PHE:H	2.12	0.52
1:F:432:TPO:O	1:F:433:ILE:CG1	2.47	0.52
1:A:52:LYS:HD2	1:A:181:THR:HG23	1.91	0.52
1:A:215:ARG:NH1	1:B:232:LYS:O	2.43	0.52
1:A:405:GLN:C	1:A:407:GLU:N	2.63	0.52
1:A:484:ARG:HB3	1:A:484:ARG:NH1	2.24	0.52
1:B:192:ALA:HB3	1:B:197:GLU:OE2	2.10	0.52
1:B:348:CYS:O	1:B:349:ALA:HB2	2.10	0.52
1:B:497:ILE:HD13	1:B:499:VAL:HG23	1.91	0.52
1:C:96:LYS:O	1:C:99:ASP:N	2.43	0.52
1:D:121:PHE:O	1:D:122:ASP:O	2.27	0.52
1:D:214:GLU:HG2	1:E:234:GLU:HB2	1.92	0.52
1:E:24:MET:HB2	1:E:62:ASN:HD22	1.74	0.52
1:B:332:GLY:C	1:B:333:MET:HG2	2.29	0.52
1:C:21:MET:HB2	1:C:38:ILE:HG12	1.91	0.52
1:C:27:GLY:HA2	1:C:30:ASP:OD2	2.08	0.52
1:C:488:ARG:NH2	1:D:488:ARG:HH22	2.08	0.52
1:D:79:THR:HG22	1:D:82:ASP:CB	2.40	0.52
1:D:219:THR:HG22	1:D:236:PRO:CA	2.35	0.52
1:D:330:SER:HB2	4:D:535:HOH:O	2.09	0.52
1:F:117:VAL:HG22	1:F:154:TYR:HE2	1.75	0.52
1:B:71:GLY:O	1:B:103:LEU:HA	2.09	0.52
1:B:273:MET:O	1:B:464:ASP:N	2.37	0.52
1:C:20:LYS:HD3	1:C:35:GLY:O	2.09	0.52
1:E:311:ARG:HD2	1:E:371:LYS:NZ	2.25	0.52
1:E:386:GLY:O	1:E:387:VAL:O	2.28	0.52
1:E:396:VAL:HG21	1:E:430:ILE:HD12	1.91	0.52
1:A:161:ARG:CB	1:A:196:VAL:HG11	2.33	0.52
1:B:21:MET:HB2	1:B:38:ILE:HD11	1.92	0.52
1:B:99:ASP:C	1:B:101:GLY:H	2.13	0.52
1:B:264:SER:OG	1:B:271:ASP:OD2	2.26	0.52
1:C:79:THR:CG2	1:C:82:ASP:OD2	2.58	0.52
1:C:314:LEU:HD23	1:C:346:ILE:HG23	1.90	0.52
1:C:488:ARG:HH21	1:D:488:ARG:HH22	1.57	0.52
1:C:488:ARG:NH2	1:D:488:ARG:NH2	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:LEU:O	1:E:129:ARG:N	2.43	0.52
1:E:375:ILE:HG22	1:E:408:ILE:HG22	1.91	0.52
1:A:279:PHE:HD1	1:A:279:PHE:H	1.58	0.52
1:C:396:VAL:HG12	1:C:433:ILE:HD11	1.91	0.52
1:D:75:THR:HG23	1:D:75:THR:O	2.10	0.52
1:D:438:ILE:HG22	1:D:439:LEU:N	2.24	0.52
1:F:178:THR:HG22	1:F:179:VAL:N	2.23	0.52
1:F:406:GLU:HB3	1:F:408:ILE:CG1	2.37	0.52
1:F:443:VAL:HG12	1:F:445:ILE:CD1	2.39	0.52
1:B:162:ARG:CB	1:B:162:ARG:HH11	2.23	0.51
1:B:299:SER:HG	1:B:335:PHE:HZ	1.57	0.51
1:C:298:VAL:O	1:C:301:PHE:HB3	2.09	0.51
1:E:48:SER:HB2	1:F:199:PHE:CE1	2.45	0.51
1:E:293:GLY:HA2	3:E:901:ATP:PA	2.50	0.51
1:E:318:GLU:HG2	1:F:432:TPO:HG21	1.92	0.51
1:E:425:ILE:HG22	1:E:426:ASN:N	2.25	0.51
1:F:73:PHE:CE2	1:F:83:ILE:HD13	2.44	0.51
1:F:311:ARG:CD	1:F:370:PHE:O	2.58	0.51
1:A:45:SER:HB3	1:A:182:THR:HB	1.92	0.51
1:A:248:PRO:C	1:A:250:GLY:H	2.13	0.51
1:A:487:GLU:HG3	1:F:496:ARG:CZ	2.41	0.51
1:A:503:SER:O	1:A:504:GLU:HB2	2.11	0.51
1:F:279:PHE:HE1	1:F:460:GLY:HA3	1.75	0.51
1:A:158:SER:HB3	1:F:153:GLN:C	2.30	0.51
1:A:224:LYS:HB3	1:F:49:GLY:HA3	1.91	0.51
1:A:426:ASN:ND2	1:A:431:SEP:HB2	2.25	0.51
1:C:74:VAL:HB	1:C:144:ILE:HA	1.92	0.51
1:C:79:THR:HG22	1:C:82:ASP:OD2	2.10	0.51
1:C:150:VAL:CG1	1:C:151:PHE:N	2.73	0.51
1:C:313:ILE:HB	1:C:375:ILE:HD12	1.92	0.51
1:D:493:SER:HB3	1:E:488:ARG:HG2	1.92	0.51
1:E:137:TYR:O	1:E:138:ARG:HB2	2.11	0.51
1:E:302:VAL:HG13	1:E:344:LEU:HD21	1.91	0.51
1:F:84:ILE:HA	1:F:94:LEU:HD12	1.91	0.51
1:F:117:VAL:O	1:F:118:VAL:HB	2.09	0.51
1:F:285:LEU:HD21	1:F:430:ILE:HD12	1.93	0.51
1:A:89:SER:HB2	1:B:227:GLY:O	2.10	0.51
1:A:488:ARG:HA	1:F:493:SER:CB	2.41	0.51
1:B:116:GLU:CG	1:B:154:TYR:HE2	2.23	0.51
1:C:116:GLU:O	1:C:117:VAL:CB	2.58	0.51
1:E:100:GLU:O	1:E:102:LYS:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:292:THR:HB	1:E:440:LEU:HB3	1.91	0.51
1:E:321:ARG:HG2	1:E:348:CYS:SG	2.50	0.51
1:A:311:ARG:HB3	1:A:370:PHE:CE2	2.45	0.51
1:A:426:ASN:N	1:A:426:ASN:HD22	2.09	0.51
1:B:210:VAL:HG12	1:B:211:LEU:O	2.10	0.51
1:C:404:LYS:O	1:C:407:GLU:N	2.42	0.51
1:D:211:LEU:HB2	1:D:216:ARG:NH1	2.24	0.51
1:D:314:LEU:O	1:D:314:LEU:HG	2.09	0.51
1:E:283:ILE:HG13	1:E:400:THR:HG23	1.91	0.51
1:E:292:THR:HG21	1:E:440:LEU:O	2.11	0.51
1:E:375:ILE:HD13	1:E:375:ILE:C	2.31	0.51
1:F:354:ALA:HB3	1:F:359:HIS:CE1	2.46	0.51
1:A:443:VAL:HG13	1:A:494:PRO:CG	2.41	0.51
1:B:251:ALA:O	1:B:252:MET:C	2.48	0.51
1:C:301:PHE:CE2	1:C:374:ARG:HB3	2.45	0.51
1:D:31:ILE:CA	1:D:231:MET:HG3	2.33	0.51
1:D:60:LEU:CD1	1:D:73:PHE:HB2	2.40	0.51
1:F:47:THR:C	1:F:50:THR:HG23	2.30	0.51
1:F:54:LEU:O	1:F:55:PHE:C	2.49	0.51
1:B:20:LYS:HA	1:B:37:PRO:HA	1.93	0.51
1:B:311:ARG:HD2	1:B:371:LYS:HE3	1.92	0.51
1:C:161:ARG:HD2	1:C:196:VAL:HG13	1.91	0.51
1:C:164:LEU:HD11	1:C:197:GLU:HG3	1.93	0.51
1:D:443:VAL:HG12	1:D:445:ILE:HG12	1.92	0.51
1:E:302:VAL:CG1	1:E:344:LEU:HD21	2.41	0.51
1:F:192:ALA:HB3	1:F:197:GLU:OE2	2.10	0.51
1:F:332:GLY:O	1:F:333:MET:O	2.27	0.51
1:A:488:ARG:NH1	1:B:488:ARG:NH2	2.47	0.51
1:B:84:ILE:HG12	1:B:94:LEU:HB2	1.93	0.51
1:B:164:LEU:O	1:B:167:LEU:N	2.44	0.51
1:B:197:GLU:OE2	1:B:197:GLU:N	2.41	0.51
1:B:451:ARG:HB3	1:B:470:PHE:CE2	2.46	0.51
1:B:497:ILE:HD12	1:B:498:THR:N	2.26	0.51
1:B:498:THR:HG21	1:C:499:VAL:HG21	1.93	0.51
1:C:43:LEU:N	1:C:203:ASN:O	2.42	0.51
1:C:173:GLN:C	1:C:175:GLY:N	2.63	0.51
1:D:74:VAL:HB	1:D:144:ILE:HG23	1.91	0.51
1:E:191:ILE:CB	1:E:198:GLU:HG3	2.40	0.51
1:E:296:LEU:HD13	1:E:331:TRP:CD2	2.46	0.51
1:E:449:MET:HG2	1:F:467:ILE:HD11	1.93	0.51
1:E:483:PHE:O	1:E:486:PHE:HD1	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:126:LEU:O	1:F:129:ARG:N	2.44	0.51
1:B:140:ARG:HH11	1:B:140:ARG:CB	2.09	0.51
1:B:237:PHE:CB	1:B:246:ILE:HG13	2.40	0.51
1:B:256:GLN:NE2	1:B:404:LYS:HB3	2.25	0.51
1:C:321:ARG:O	1:C:325:LEU:HG	2.11	0.51
1:C:356:LEU:CD1	1:C:387:VAL:HG21	2.41	0.51
1:D:146:SER:N	1:D:181:THR:HG22	2.22	0.51
1:D:163:GLU:O	1:D:166:ARG:HB3	2.10	0.51
1:F:294:LYS:N	3:F:901:ATP:O1B	2.44	0.51
1:F:329:TYR:O	1:F:332:GLY:N	2.44	0.51
1:B:297:LEU:O	1:B:298:VAL:C	2.49	0.51
1:C:296:LEU:HD23	1:C:472:ILE:HD12	1.92	0.51
1:E:344:LEU:HD13	1:E:344:LEU:C	2.31	0.51
1:F:52:LYS:HB2	3:F:903:ATP:O1B	2.11	0.51
1:F:147:VAL:O	1:F:150:VAL:HG12	2.11	0.51
1:F:200:VAL:O	1:F:200:VAL:HG12	2.11	0.51
1:A:313:ILE:HG13	1:A:372:PRO:HG2	1.93	0.50
1:B:150:VAL:HG12	1:B:151:PHE:CD1	2.46	0.50
1:D:344:LEU:HD22	1:D:345:LYS:N	2.24	0.50
1:E:505:LEU:HD12	1:E:505:LEU:C	2.31	0.50
1:A:84:ILE:O	1:A:87:ALA:HB3	2.11	0.50
1:A:305:ALA:HB2	1:A:374:ARG:HD2	1.93	0.50
1:E:126:LEU:O	1:E:130:ILE:HD13	2.10	0.50
1:E:329:TYR:HA	1:E:332:GLY:O	2.11	0.50
1:E:400:THR:HG21	1:E:433:ILE:CG2	2.40	0.50
1:F:42:THR:OG1	1:F:203:ASN:ND2	2.42	0.50
1:F:418:GLN:HE21	1:F:422:ALA:HA	1.77	0.50
1:F:500:ASP:O	1:F:501:GLU:HB3	2.11	0.50
1:A:248:PRO:HB2	1:A:251:ALA:HB3	1.92	0.50
1:A:262:ARG:HH12	1:A:461:SER:HB2	1.75	0.50
1:B:64:ILE:HG21	1:B:97:LEU:CD1	2.38	0.50
1:D:146:SER:H	1:D:181:THR:CG2	2.21	0.50
1:D:471:MET:HE2	1:D:478:ASP:CB	2.42	0.50
1:E:76:PHE:CD2	1:E:150:VAL:HB	2.47	0.50
1:E:123:LEU:O	1:E:126:LEU:HB3	2.12	0.50
1:E:361:GLN:O	1:E:365:SER:N	2.44	0.50
1:F:217:ARG:HH22	1:F:394:GLN:NE2	2.09	0.50
1:A:296:LEU:HD13	1:A:331:TRP:CE2	2.46	0.50
1:A:315:PHE:HD1	1:A:377:ILE:HG13	1.76	0.50
1:A:451:ARG:HD2	1:A:451:ARG:N	2.27	0.50
1:B:64:ILE:HG12	1:B:97:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ASP:OD1	1:B:159:VAL:HG11	2.10	0.50
1:B:454:ASN:C	1:B:454:ASN:OD1	2.50	0.50
1:C:426:ASN:H	1:C:426:ASN:HD22	1.59	0.50
1:D:123:LEU:O	1:D:127:ILE:HG12	2.12	0.50
1:F:284:ILE:HD13	1:F:411:LEU:HD13	1.94	0.50
1:F:298:VAL:O	1:F:302:VAL:HG23	2.10	0.50
1:B:80:PRO:HB3	1:B:105:ILE:CG2	2.41	0.50
1:B:156:ALA:O	1:B:159:VAL:HB	2.12	0.50
1:B:311:ARG:HD2	1:B:371:LYS:NZ	2.26	0.50
1:C:66:GLU:C	1:C:67:PHE:CD1	2.84	0.50
1:C:111:ASP:OD2	1:C:113:GLU:HG2	2.11	0.50
1:D:148:THR:HG21	1:D:183:GLU:CG	2.42	0.50
1:D:279:PHE:HB2	1:D:282:SER:OG	2.11	0.50
1:E:52:LYS:O	1:E:53:THR:C	2.49	0.50
1:E:130:ILE:O	1:E:134:ILE:HG12	2.11	0.50
1:E:499:VAL:O	1:E:499:VAL:HG12	2.11	0.50
1:F:313:ILE:HB	1:F:375:ILE:HD12	1.93	0.50
1:F:497:ILE:HD13	1:F:497:ILE:N	2.24	0.50
1:A:249:LEU:CD1	1:A:394:GLN:HG2	2.42	0.50
1:A:484:ARG:HB3	1:A:484:ARG:HH11	1.76	0.50
1:C:152:GLN:NE2	1:C:194:TYR:OH	2.45	0.50
1:D:154:TYR:O	1:D:154:TYR:CD1	2.64	0.50
1:D:387:VAL:HG12	1:D:388:SER:N	2.26	0.50
1:E:193:ARG:HB3	1:E:194:TYR:CD1	2.46	0.50
1:F:336:GLU:HB3	1:F:340:ARG:HH21	1.75	0.50
1:F:496:ARG:H	1:F:496:ARG:HD3	1.77	0.50
1:B:123:LEU:O	1:B:127:ILE:HG13	2.12	0.50
1:B:367:ILE:HG23	1:B:372:PRO:HD2	1.94	0.50
1:C:393:ARG:NH2	1:C:429:HIS:CB	2.72	0.50
1:D:150:VAL:CG1	1:D:151:PHE:H	2.25	0.50
1:D:443:VAL:HG11	1:D:483:PHE:CE2	2.46	0.50
1:E:237:PHE:HB3	1:E:246:ILE:HG23	1.93	0.50
1:E:356:LEU:HD12	1:E:356:LEU:N	2.26	0.50
1:E:485:ASN:HD21	1:E:496:ARG:HH11	1.56	0.50
1:F:21:MET:HE3	1:F:141:ARG:NE	2.27	0.50
1:C:215:ARG:HA	1:C:215:ARG:NE	2.26	0.50
1:C:225:LEU:HB2	1:C:230:HIS:HD2	1.76	0.50
1:D:253:ARG:O	1:D:255:THR:N	2.36	0.50
1:D:259:SER:OG	1:D:260:ASN:N	2.43	0.50
1:D:299:SER:HB3	1:D:335:PHE:CZ	2.46	0.50
1:D:313:ILE:HD12	1:D:372:PRO:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:LEU:HD23	1:E:270:LEU:C	2.32	0.50
1:E:311:ARG:HD3	1:E:370:PHE:CE1	2.46	0.50
1:F:76:PHE:HZ	1:F:126:LEU:HD22	1.77	0.50
1:F:294:LYS:HD3	1:F:294:LYS:H	1.77	0.50
1:A:40:ARG:NH2	1:F:86:ASN:HD21	2.08	0.50
1:A:425:ILE:HG12	1:F:419:PHE:CD2	2.46	0.50
1:C:131:ASN:O	1:C:135:GLN:HG3	2.12	0.50
1:C:245:ASN:C	1:C:245:ASN:HD22	2.13	0.50
1:C:349:ALA:H	1:D:254:LEU:HD22	1.76	0.50
1:C:453:ILE:HD13	1:C:454:ASN:H	1.77	0.50
1:D:356:LEU:H	1:D:356:LEU:CD1	2.25	0.50
1:D:446:ARG:H	1:D:496:ARG:NH2	2.09	0.50
1:E:260:ASN:HA	1:E:279:PHE:HE2	1.77	0.50
1:A:162:ARG:HE	1:F:153:GLN:HG2	1.77	0.49
1:D:18:ILE:CG1	1:D:228:THR:HG23	2.42	0.49
1:D:38:ILE:CG2	1:D:39:GLY:N	2.75	0.49
1:D:43:LEU:HD11	1:D:182:THR:OG1	2.12	0.49
1:D:317:TYR:CD2	1:D:383:LEU:HD21	2.47	0.49
1:E:126:LEU:HD12	1:E:130:ILE:HD11	1.93	0.49
1:E:371:LYS:N	1:E:372:PRO:HD3	2.26	0.49
1:F:262:ARG:HD2	1:F:276:GLY:O	2.12	0.49
1:F:265:SER:HB3	1:F:278:PHE:CE1	2.47	0.49
1:A:247:PHE:HZ	1:A:361:GLN:HB2	1.76	0.49
1:E:44:VAL:HG22	1:E:205:VAL:HB	1.94	0.49
1:E:453:ILE:HG12	1:E:454:ASN:N	2.27	0.49
1:F:29:ASP:O	1:F:34:GLY:N	2.45	0.49
1:F:123:LEU:O	1:F:127:ILE:HG13	2.12	0.49
1:F:445:ILE:HD11	1:F:483:PHE:HE2	1.76	0.49
1:A:194:TYR:O	1:A:196:VAL:HG23	2.13	0.49
1:A:445:ILE:CD1	1:A:483:PHE:HE2	2.23	0.49
1:B:389:ASN:O	1:B:392:PHE:HB3	2.12	0.49
1:C:50:THR:CG2	1:C:207:LEU:HB3	2.41	0.49
1:D:143:SER:OG	1:D:179:VAL:HB	2.13	0.49
1:D:412:PHE:N	1:D:412:PHE:CD1	2.79	0.49
1:E:193:ARG:HG2	1:E:193:ARG:HH11	1.76	0.49
1:E:218:ARG:NH2	1:E:239:ILE:HD12	2.28	0.49
1:E:262:ARG:NH1	1:E:275:GLY:O	2.45	0.49
1:E:383:LEU:C	1:E:385:ARG:N	2.66	0.49
1:F:222:ILE:N	4:F:527:HOH:O	2.42	0.49
1:F:335:PHE:HA	1:F:338:MET:HG3	1.94	0.49
1:A:254:LEU:HD13	1:F:350:TYR:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ILE:HG22	1:A:430:ILE:O	2.11	0.49
1:A:437:ILE:HG22	1:A:456:PHE:HB2	1.92	0.49
1:B:103:LEU:HD12	1:B:104:PHE:N	2.27	0.49
1:C:404:LYS:O	1:C:406:GLU:N	2.46	0.49
1:D:449:MET:HB2	1:E:465:LYS:HB3	1.94	0.49
1:E:281:ASP:OD1	1:E:407:GLU:OE1	2.30	0.49
3:E:901:ATP:C2	1:F:462:TRP:HA	2.46	0.49
1:F:116:GLU:O	1:F:117:VAL:HB	2.12	0.49
1:F:270:LEU:C	1:F:270:LEU:HD23	2.33	0.49
1:F:440:LEU:HD23	1:F:453:ILE:HG13	1.93	0.49
1:F:514:GLU:CG	1:F:519:SER:HB3	2.27	0.49
1:A:86:ASN:O	1:A:89:SER:HB3	2.12	0.49
1:A:191:ILE:CD1	1:A:198:GLU:HG2	2.41	0.49
1:B:285:LEU:HD22	1:B:426:ASN:HD21	1.76	0.49
1:C:80:PRO:HB3	1:C:105:ILE:HG21	1.95	0.49
1:D:392:PHE:HE2	1:D:430:ILE:HD11	1.77	0.49
1:A:37:PRO:HG2	1:A:203:ASN:HD21	1.78	0.49
1:A:39:GLY:O	1:A:40:ARG:HG3	2.13	0.49
1:A:69:GLU:HG2	1:A:140:ARG:HB2	1.94	0.49
1:A:403:ALA:HB1	1:A:408:ILE:HB	1.95	0.49
1:A:490:ILE:HD12	1:A:490:ILE:H	1.77	0.49
1:B:299:SER:HB3	1:B:333:MET:CE	2.43	0.49
1:D:231:MET:SD	1:D:251:ALA:HB2	2.53	0.49
1:D:332:GLY:O	1:D:333:MET:C	2.51	0.49
1:E:345:LYS:HD2	1:E:370:PHE:CG	2.48	0.49
1:F:38:ILE:HA	1:F:177:THR:CG2	2.43	0.49
1:F:47:THR:H	1:F:50:THR:HG21	1.76	0.49
1:A:18:ILE:HG21	1:A:37:PRO:HB3	1.94	0.49
1:A:93:ASP:OD2	1:A:96:LYS:CB	2.58	0.49
1:A:381:SER:HB3	1:A:414:ASN:OD1	2.13	0.49
1:A:447:GLY:O	1:A:448:GLU:HG2	2.13	0.49
1:B:187:GLU:OE2	1:B:208:ARG:HG2	2.12	0.49
1:C:211:LEU:O	1:C:215:ARG:O	2.31	0.49
1:D:65:ILE:O	1:D:65:ILE:CG2	2.61	0.49
1:E:121:PHE:O	1:E:125:ALA:HB3	2.12	0.49
1:E:218:ARG:N	4:E:528:HOH:O	2.44	0.49
1:F:273:MET:O	1:F:463:HIS:HA	2.13	0.49
1:F:303:GLU:OE2	1:F:333:MET:HB3	2.13	0.49
1:A:146:SER:N	1:A:181:THR:HB	2.08	0.49
1:A:298:VAL:HA	1:A:411:LEU:CD2	2.42	0.49
1:A:316:ALA:O	1:A:348:CYS:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:140:ARG:HH11	1:F:140:ARG:CB	2.20	0.49
1:F:185:ILE:HD11	1:F:193:ARG:HH12	1.78	0.49
1:F:345:LYS:HB2	1:F:370:PHE:CZ	2.48	0.49
1:F:432:TPO:HG23	1:F:433:ILE:N	2.27	0.49
1:A:191:ILE:HB	1:A:198:GLU:CG	2.43	0.49
1:B:237:PHE:C	1:B:237:PHE:CD1	2.86	0.49
1:B:462:TRP:O	1:B:463:HIS:CG	2.65	0.49
1:C:88:ARG:CZ	1:D:15:HIS:HA	2.43	0.49
1:C:318:GLU:C	1:C:319:GLU:HG3	2.32	0.49
1:D:53:THR:HG22	1:D:57:ILE:HD13	1.95	0.49
1:D:86:ASN:O	1:D:88:ARG:N	2.45	0.49
1:D:301:PHE:CE2	1:D:411:LEU:HB3	2.48	0.49
1:D:358:ASP:O	1:D:361:GLN:N	2.46	0.49
1:E:247:PHE:HE1	1:E:357:GLU:O	1.96	0.49
1:F:106:LEU:HD11	1:F:129:ARG:CZ	2.42	0.49
1:F:184:ARG:HH21	1:F:191:ILE:HA	1.77	0.49
1:F:380:LEU:HD12	1:F:430:ILE:HD13	1.95	0.49
1:F:406:GLU:C	1:F:408:ILE:N	2.65	0.49
1:C:451:ARG:HG2	1:C:451:ARG:NH1	2.28	0.49
1:D:333:MET:HE3	4:D:540:HOH:O	2.12	0.49
1:D:338:MET:HB3	1:D:344:LEU:HB3	1.95	0.49
1:D:345:LYS:NZ	1:D:366:GLU:OE1	2.43	0.49
1:D:367:ILE:HD11	1:D:375:ILE:HD11	1.94	0.49
1:D:371:LYS:N	1:D:372:PRO:HD3	2.28	0.49
1:D:420:MET:HG3	1:D:442:TYR:HB2	1.95	0.49
3:E:903:ATP:O1G	1:F:224:LYS:NZ	2.41	0.49
1:A:356:LEU:CD2	1:A:387:VAL:HG11	2.41	0.48
1:B:23:THR:HG22	1:B:59:PHE:CD1	2.48	0.48
1:B:359:HIS:O	1:B:360:LEU:C	2.51	0.48
1:D:347:VAL:CG1	1:D:348:CYS:N	2.76	0.48
1:E:258:SER:HA	1:E:281:ASP:CG	2.33	0.48
1:E:309:LYS:HA	1:E:343:LEU:CD1	2.43	0.48
1:E:451:ARG:HH12	1:E:472:ILE:HD12	1.78	0.48
1:F:61:TYR:CE2	1:F:65:ILE:HG13	2.48	0.48
1:F:347:VAL:HG12	1:F:348:CYS:N	2.28	0.48
1:F:445:ILE:N	1:F:445:ILE:HD12	2.28	0.48
1:A:207:LEU:CD2	1:A:220:LEU:HD12	2.43	0.48
1:A:344:LEU:HD22	1:A:345:LYS:N	2.27	0.48
1:A:452:ALA:C	1:A:470:PHE:HE2	2.17	0.48
1:C:120:GLY:C	1:C:122:ASP:N	2.66	0.48
1:C:151:PHE:CE2	1:C:160:VAL:HG13	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:LYS:N	3:D:903:ATP:O1B	2.46	0.48
1:D:294:LYS:HB2	3:D:901:ATP:O1B	2.13	0.48
1:D:301:PHE:CE1	1:D:374:ARG:HD3	2.47	0.48
1:E:82:ASP:O	1:E:86:ASN:ND2	2.47	0.48
1:E:164:LEU:HB3	1:E:200:VAL:HG11	1.95	0.48
1:E:400:THR:HG22	1:E:404:LYS:HE3	1.95	0.48
1:E:432:TPO:HG21	1:E:432:TPO:O1P	2.13	0.48
1:F:221:GLU:HB3	4:F:533:HOH:O	2.13	0.48
1:A:126:LEU:O	1:A:130:ILE:HG13	2.13	0.48
1:A:248:PRO:O	1:A:251:ALA:N	2.44	0.48
1:A:347:VAL:O	1:A:348:CYS:HB2	2.12	0.48
1:B:58:GLN:OE1	1:B:243:GLY:HA3	2.13	0.48
1:B:60:LEU:HA	4:B:520:HOH:O	2.13	0.48
1:B:187:GLU:CG	1:B:210:VAL:HG22	2.36	0.48
1:B:473:SER:C	1:B:475:LYS:N	2.66	0.48
1:C:140:ARG:HH11	1:C:140:ARG:HA	1.78	0.48
1:C:379:SER:H	1:C:413:THR:CB	2.07	0.48
1:C:448:GLU:HG2	1:D:466:ALA:CB	2.44	0.48
1:D:315:PHE:CE2	1:D:363:ILE:HG13	2.48	0.48
1:E:60:LEU:HD11	1:E:143:SER:HB2	1.96	0.48
1:E:263:VAL:HG12	1:E:374:ARG:HH21	1.78	0.48
1:E:396:VAL:HG11	1:E:430:ILE:HG23	1.94	0.48
1:F:45:SER:HB2	1:F:182:THR:HB	1.95	0.48
1:F:60:LEU:CD1	1:F:73:PHE:HB2	2.42	0.48
1:F:313:ILE:HG22	1:F:314:LEU:N	2.29	0.48
1:A:124:SER:O	1:A:128:GLU:HG3	2.14	0.48
1:A:408:ILE:CG2	1:A:409:THR:N	2.77	0.48
1:B:25:ILE:HG12	1:B:58:GLN:NE2	2.17	0.48
1:B:164:LEU:HD11	1:B:197:GLU:HG3	1.94	0.48
1:B:307:ALA:C	1:B:309:LYS:H	2.16	0.48
1:C:483:PHE:N	1:C:483:PHE:CD1	2.81	0.48
1:D:49:GLY:O	1:D:218:ARG:NH2	2.45	0.48
1:D:72:VAL:HB	1:D:142:VAL:HG22	1.96	0.48
1:D:262:ARG:HH22	1:D:461:SER:CB	2.26	0.48
1:D:348:CYS:O	1:D:349:ALA:CB	2.59	0.48
1:E:191:ILE:CG2	1:E:198:GLU:HG3	2.43	0.48
1:E:323:GLN:HE21	1:F:459:ARG:HD3	1.76	0.48
1:E:345:LYS:HB2	1:E:370:PHE:CD2	2.48	0.48
1:F:515:LYS:CG	1:F:516:GLY:N	2.75	0.48
1:A:90:PHE:N	1:A:90:PHE:CD1	2.81	0.48
1:B:127:ILE:HG21	1:B:170:ARG:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:387:VAL:CG1	1:C:388:SER:N	2.72	0.48
1:E:191:ILE:HG13	1:E:206:ILE:HD11	1.95	0.48
1:F:198:GLU:HB2	1:F:199:PHE:CE2	2.48	0.48
1:F:246:ILE:HG22	1:F:248:PRO:HD3	1.95	0.48
1:A:188:TYR:HD2	1:A:208:ARG:HH11	1.62	0.48
1:A:278:PHE:CD1	1:A:284:ILE:HG13	2.49	0.48
1:B:337:GLU:OE2	1:B:340:ARG:HD2	2.14	0.48
1:B:385:ARG:HH12	1:C:397:ILE:HD11	1.78	0.48
1:D:79:THR:HG21	1:D:81:GLN:HG2	1.93	0.48
1:D:283:ILE:HD11	1:D:404:LYS:HG3	1.96	0.48
1:E:74:VAL:CG1	1:E:76:PHE:HE1	2.27	0.48
1:A:209:ASN:HD22	1:A:218:ARG:HE	1.62	0.48
1:A:348:CYS:O	1:A:349:ALA:HB2	2.13	0.48
1:B:18:ILE:N	1:B:18:ILE:CD1	2.76	0.48
1:B:184:ARG:HH22	1:B:187:GLU:C	2.17	0.48
1:B:371:LYS:O	1:B:371:LYS:CD	2.62	0.48
1:B:439:LEU:HD12	1:B:439:LEU:O	2.13	0.48
1:C:61:TYR:CE1	1:C:92:TRP:HB3	2.48	0.48
1:C:416:SER:C	1:C:418:GLN:H	2.17	0.48
1:D:64:ILE:HD11	1:D:103:LEU:HB2	1.94	0.48
1:E:194:TYR:O	1:E:196:VAL:HG23	2.14	0.48
1:E:266:GLY:HA3	1:E:300:ARG:HG2	1.95	0.48
1:F:117:VAL:HG22	1:F:154:TYR:CE2	2.48	0.48
1:F:432:TPO:O1P	1:F:432:TPO:CG2	2.62	0.48
1:A:374:ARG:C	1:A:375:ILE:HD12	2.34	0.48
1:A:380:LEU:C	1:A:382:ALA:H	2.17	0.48
1:A:440:LEU:CD2	1:A:453:ILE:HG13	2.42	0.48
1:B:52:LYS:O	1:B:53:THR:C	2.51	0.48
1:B:390:ASN:C	1:B:392:PHE:N	2.66	0.48
1:C:386:GLY:HA2	1:D:390:ASN:OD1	2.14	0.48
1:D:449:MET:CE	1:E:490:ILE:HD11	2.44	0.48
1:E:295:THR:HB	3:E:901:ATP:PA	2.54	0.48
1:E:404:LYS:O	1:E:406:GLU:N	2.46	0.48
1:F:190:PRO:HD2	4:F:524:HOH:O	2.13	0.48
1:F:267:VAL:O	1:F:271:ASP:OD2	2.32	0.48
1:B:299:SER:HB3	1:B:333:MET:HE1	1.95	0.48
1:C:57:ILE:HD11	1:C:83:ILE:CG2	2.44	0.48
1:D:122:ASP:O	1:D:123:LEU:C	2.52	0.48
1:D:299:SER:C	1:D:333:MET:CE	2.82	0.48
1:E:48:SER:HB2	1:F:199:PHE:CD1	2.49	0.48
1:F:38:ILE:HG22	1:F:39:GLY:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:186:GLU:HA	1:F:186:GLU:OE2	2.14	0.48
1:F:279:PHE:CE1	1:F:460:GLY:HA3	2.49	0.48
1:A:254:LEU:HG	1:F:320:SER:HA	1.95	0.48
1:A:294:LYS:HZ1	1:A:415:THR:CA	2.27	0.48
1:B:497:ILE:HD12	1:B:499:VAL:N	2.21	0.48
1:C:31:ILE:O	1:C:231:MET:HG3	2.14	0.48
1:C:36:LEU:HD22	1:C:42:THR:OG1	2.14	0.48
1:C:79:THR:HG23	1:C:82:ASP:H	1.78	0.48
1:C:350:TYR:CE1	1:D:254:LEU:HD12	2.49	0.48
1:C:484:ARG:HB3	1:C:484:ARG:HH11	1.77	0.48
1:D:96:LYS:O	1:D:100:GLU:HG3	2.13	0.48
1:D:142:VAL:HB	1:D:178:THR:CG2	2.41	0.48
1:D:334:ASP:OD2	1:D:336:GLU:HB2	2.14	0.48
1:E:453:ILE:HB	1:E:470:PHE:CD2	2.49	0.48
1:F:270:LEU:O	1:F:272:GLU:N	2.47	0.48
1:F:391:ALA:O	1:F:394:GLN:HB3	2.14	0.48
1:A:36:LEU:HD12	1:A:59:PHE:CE1	2.49	0.47
1:A:247:PHE:CZ	1:A:361:GLN:HB2	2.49	0.47
1:A:256:GLN:HE21	1:A:404:LYS:HB3	1.79	0.47
1:B:43:LEU:HD12	1:B:180:MET:O	2.14	0.47
1:B:186:GLU:OE1	1:B:188:TYR:C	2.52	0.47
1:B:340:ARG:C	1:B:342:ASN:H	2.16	0.47
1:B:360:LEU:C	1:B:360:LEU:HD13	2.34	0.47
1:C:78:GLU:O	1:C:83:ILE:HD11	2.13	0.47
1:D:79:THR:HG22	1:D:82:ASP:HB2	1.96	0.47
1:D:262:ARG:NH1	1:D:275:GLY:C	2.67	0.47
1:E:355:GLY:O	1:E:358:ASP:HB2	2.14	0.47
1:F:352:GLU:OE2	1:F:385:ARG:HD2	2.13	0.47
1:F:429:HIS:CE1	1:F:432:TPO:O3P	2.67	0.47
1:A:79:THR:HG21	1:A:81:GLN:HG2	1.96	0.47
1:A:208:ARG:NH2	1:A:221:GLU:OE2	2.44	0.47
1:A:389:ASN:C	1:A:389:ASN:ND2	2.67	0.47
1:A:425:ILE:HD12	1:A:431:SEP:O1P	2.15	0.47
1:A:443:VAL:CG1	1:A:494:PRO:HG2	2.44	0.47
1:B:486:PHE:CE2	1:B:496:ARG:HB2	2.49	0.47
1:B:497:ILE:CD1	1:B:499:VAL:HG23	2.44	0.47
1:C:90:PHE:N	1:C:90:PHE:CD1	2.82	0.47
1:E:192:ALA:CB	1:E:197:GLU:HB2	2.44	0.47
1:E:223:LEU:HD13	1:E:223:LEU:O	2.14	0.47
1:E:261:VAL:CG1	1:E:262:ARG:N	2.72	0.47
1:F:98:VAL:HA	1:F:103:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:231:MET:CE	1:F:251:ALA:HB2	2.44	0.47
1:F:316:ALA:O	1:F:348:CYS:HA	2.15	0.47
1:F:500:ASP:HB2	1:F:503:SER:HB3	1.96	0.47
1:A:164:LEU:CD1	1:A:197:GLU:HA	2.43	0.47
1:A:287:THR:CG2	1:A:414:ASN:HB3	2.31	0.47
1:A:298:VAL:O	1:A:301:PHE:HB3	2.15	0.47
1:B:356:LEU:N	1:B:356:LEU:CD1	2.78	0.47
1:C:36:LEU:HD22	1:C:42:THR:HG21	1.95	0.47
1:C:97:LEU:HB3	1:C:103:LEU:HB3	1.96	0.47
1:C:130:ILE:O	1:C:134:ILE:HG12	2.15	0.47
1:C:142:VAL:O	1:C:178:THR:HA	2.15	0.47
1:C:484:ARG:HB3	1:C:484:ARG:CZ	2.44	0.47
1:D:284:ILE:HD12	1:D:284:ILE:N	2.30	0.47
1:D:470:PHE:CZ	1:D:472:ILE:HD11	2.49	0.47
1:E:293:GLY:O	1:E:296:LEU:HB3	2.15	0.47
1:B:45:SER:HB3	1:B:182:THR:OG1	2.14	0.47
1:B:116:GLU:O	1:B:118:VAL:HG23	2.13	0.47
1:C:188:TYR:O	1:C:189:GLY:O	2.32	0.47
1:C:248:PRO:O	1:C:250:GLY:N	2.43	0.47
1:C:299:SER:HA	1:C:335:PHE:HZ	1.79	0.47
1:C:338:MET:H	1:C:338:MET:HG2	1.45	0.47
1:D:173:GLN:C	1:D:175:GLY:H	2.16	0.47
1:D:303:GLU:HB2	1:D:333:MET:HE1	1.97	0.47
1:F:151:PHE:CE1	1:F:164:LEU:HD21	2.49	0.47
1:A:344:LEU:HD13	1:A:344:LEU:C	2.35	0.47
1:B:21:MET:HG2	1:B:141:ARG:NH2	2.30	0.47
1:B:88:ARG:HH22	1:B:95:ALA:CB	2.19	0.47
1:B:112:PRO:O	1:C:166:ARG:HG3	2.15	0.47
1:B:502:LYS:HD3	1:B:502:LYS:H	1.78	0.47
1:E:224:LYS:O	1:E:224:LYS:HG3	2.13	0.47
1:A:245:ASN:ND2	1:A:247:PHE:CE1	2.81	0.47
1:B:274:CYS:HB3	1:B:458:MET:SD	2.54	0.47
1:B:452:ALA:HA	1:B:469:GLU:HA	1.95	0.47
1:D:145:ASP:O	1:D:146:SER:OG	2.32	0.47
1:D:191:ILE:HB	1:D:198:GLU:CG	2.44	0.47
1:D:422:ALA:C	1:D:424:SER:H	2.18	0.47
1:E:237:PHE:HB2	1:E:245:ASN:O	2.14	0.47
1:A:20:LYS:HG2	1:A:35:GLY:O	2.15	0.47
1:A:215:ARG:HH22	1:B:233:GLY:C	2.17	0.47
1:A:232:LYS:HD2	1:A:232:LYS:N	2.25	0.47
1:A:462:TRP:O	1:A:463:HIS:O	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:LEU:O	1:B:123:LEU:HD13	2.15	0.47
1:B:274:CYS:HA	1:B:463:HIS:CB	2.45	0.47
1:B:432:TPO:O1P	1:B:432:TPO:CG2	2.62	0.47
1:C:64:ILE:HG21	1:C:102:LYS:O	2.14	0.47
1:C:87:ALA:C	1:C:89:SER:H	2.16	0.47
1:C:140:ARG:HB3	1:C:140:ARG:HH11	1.78	0.47
1:C:348:CYS:O	1:C:349:ALA:HB2	2.14	0.47
1:C:367:ILE:C	1:C:369:ASP:H	2.17	0.47
1:D:186:GLU:OE1	1:D:188:TYR:N	2.48	0.47
1:D:445:ILE:HG22	1:D:446:ARG:HG3	1.97	0.47
1:E:127:ILE:HD12	1:E:167:LEU:HD13	1.96	0.47
1:E:371:LYS:O	1:E:371:LYS:CD	2.61	0.47
1:E:425:ILE:HG22	1:E:426:ASN:H	1.80	0.47
1:E:458:MET:SD	1:E:461:SER:HB3	2.55	0.47
1:F:79:THR:HG22	1:F:82:ASP:CG	2.35	0.47
1:F:182:THR:HG21	1:F:192:ALA:CB	2.44	0.47
1:F:195:GLY:HA2	1:F:198:GLU:CD	2.33	0.47
1:F:345:LYS:HD3	1:F:366:GLU:HG3	1.96	0.47
1:A:188:TYR:CD2	1:A:208:ARG:NH1	2.83	0.47
1:B:197:GLU:H	1:B:197:GLU:CD	2.17	0.47
1:B:437:ILE:HG12	1:B:457:LYS:HE2	1.96	0.47
1:C:121:PHE:CD1	1:C:121:PHE:N	2.83	0.47
1:D:357:GLU:HG2	1:D:358:ASP:N	2.30	0.47
1:E:66:GLU:OE1	1:E:66:GLU:HA	2.15	0.47
1:E:221:GLU:HG2	1:E:222:ILE:N	2.30	0.47
1:F:53:THR:HG23	1:F:145:ASP:OD1	2.15	0.47
1:F:247:PHE:CZ	1:F:361:GLN:HB2	2.50	0.47
1:F:432:TPO:C	1:F:433:ILE:HG23	2.44	0.47
1:A:101:GLY:O	1:A:137:TYR:HD2	1.98	0.47
1:A:146:SER:C	1:A:148:THR:H	2.16	0.47
1:A:313:ILE:HD11	1:A:370:PHE:CD2	2.50	0.47
1:A:331:TRP:O	1:A:475:LYS:O	2.32	0.47
1:A:425:ILE:HG12	1:F:419:PHE:HD2	1.79	0.47
1:A:442:TYR:HB2	4:A:521:HOH:O	2.15	0.47
3:A:903:ATP:O3'	1:B:224:LYS:HA	2.15	0.47
1:B:31:ILE:HG22	1:B:222:ILE:HD12	1.97	0.47
1:B:49:GLY:O	1:B:218:ARG:NH2	2.47	0.47
1:B:146:SER:N	1:B:181:THR:HB	2.26	0.47
1:B:198:GLU:OE1	1:B:198:GLU:N	2.46	0.47
1:B:298:VAL:O	1:B:301:PHE:HB3	2.14	0.47
1:C:111:ASP:C	1:C:113:GLU:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:292:THR:O	1:E:440:LEU:HD13	2.15	0.47
1:F:52:LYS:O	1:F:54:LEU:N	2.47	0.47
1:F:311:ARG:HD2	1:F:370:PHE:O	2.15	0.47
1:F:469:GLU:OE2	1:F:480:LYS:HD2	2.13	0.47
1:A:283:ILE:HD12	1:A:412:PHE:CE1	2.46	0.47
1:B:18:ILE:HD13	1:B:227:GLY:O	2.14	0.47
1:B:75:THR:HG23	1:B:76:PHE:N	2.30	0.47
1:B:320:SER:HB2	1:C:254:LEU:O	2.14	0.47
3:B:903:ATP:O1G	1:C:224:LYS:NZ	2.48	0.47
1:C:28:PHE:CZ	1:C:222:ILE:HD11	2.50	0.47
1:C:191:ILE:HB	1:C:198:GLU:HG2	1.97	0.47
1:C:283:ILE:HD11	1:C:400:THR:O	2.15	0.47
1:D:211:LEU:HG	1:D:211:LEU:O	2.14	0.47
1:D:311:ARG:HD2	1:D:371:LYS:NZ	2.30	0.47
1:D:487:GLU:OE1	1:D:497:ILE:HD13	2.15	0.47
1:E:346:ILE:HG22	1:E:348:CYS:SG	2.55	0.47
1:F:222:ILE:HG21	1:F:225:LEU:HG	1.97	0.47
1:F:320:SER:OG	1:F:323:GLN:HB2	2.15	0.47
1:F:383:LEU:C	1:F:385:ARG:H	2.17	0.47
1:A:88:ARG:HG2	1:A:88:ARG:HH11	1.79	0.46
1:B:50:THR:O	1:B:237:PHE:HZ	1.98	0.46
1:B:246:ILE:HD12	1:B:246:ILE:N	2.30	0.46
1:C:140:ARG:HH11	1:C:140:ARG:CB	2.27	0.46
1:C:387:VAL:CG1	1:C:388:SER:H	2.27	0.46
1:C:413:THR:CG2	1:C:414:ASN:N	2.62	0.46
1:C:426:ASN:HB2	1:C:429:HIS:H	1.80	0.46
1:C:462:TRP:CE3	1:C:463:HIS:N	2.83	0.46
1:D:54:LEU:CD2	1:D:239:ILE:HG23	2.46	0.46
1:E:321:ARG:HG3	1:F:254:LEU:O	2.16	0.46
1:F:31:ILE:HD11	1:F:248:PRO:HG3	1.95	0.46
1:F:130:ILE:O	1:F:134:ILE:HG12	2.15	0.46
1:F:402:TYR:O	1:F:405:GLN:HG2	2.15	0.46
1:A:92:TRP:HD1	1:A:92:TRP:O	1.97	0.46
1:A:152:GLN:HG3	1:B:161:ARG:NH1	2.30	0.46
1:B:125:ALA:O	1:B:128:GLU:N	2.45	0.46
1:B:256:GLN:NE2	1:B:405:GLN:HB3	2.30	0.46
1:C:154:TYR:O	1:C:154:TYR:HD1	1.98	0.46
1:C:204:VAL:HG23	1:C:224:LYS:HG2	1.97	0.46
1:C:370:PHE:O	1:C:371:LYS:HD2	2.15	0.46
1:C:463:HIS:ND1	1:C:463:HIS:C	2.68	0.46
1:D:53:THR:HG23	1:D:57:ILE:HD13	1.90	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:GLN:OE1	1:D:243:GLY:HA3	2.16	0.46
1:D:301:PHE:O	1:D:374:ARG:NH1	2.48	0.46
1:D:308:ASN:O	1:D:309:LYS:HB2	2.16	0.46
1:D:353:SER:O	1:D:354:ALA:HB2	2.15	0.46
1:F:344:LEU:O	1:F:344:LEU:HD13	2.16	0.46
1:A:90:PHE:CZ	3:A:903:ATP:N7	2.83	0.46
1:A:294:LYS:HZ1	1:A:415:THR:HA	1.81	0.46
1:A:299:SER:CB	1:A:333:MET:HE1	2.31	0.46
1:B:21:MET:HE2	1:B:177:THR:HG21	1.96	0.46
1:B:153:GLN:C	1:B:154:TYR:CG	2.88	0.46
1:B:215:ARG:HA	1:B:215:ARG:CZ	2.45	0.46
1:B:341:GLN:O	1:B:342:ASN:C	2.53	0.46
1:B:360:LEU:O	1:B:363:ILE:HB	2.15	0.46
1:C:152:GLN:C	1:D:158:SER:HB3	2.36	0.46
1:C:167:LEU:O	1:C:171:LEU:HG	2.16	0.46
1:D:273:MET:CE	1:D:468:ARG:HD2	2.45	0.46
1:E:318:GLU:HG2	1:F:432:TPO:CG2	2.44	0.46
1:F:121:PHE:O	1:F:125:ALA:N	2.42	0.46
1:A:90:PHE:HB2	1:A:92:TRP:CZ2	2.51	0.46
1:A:238:THR:O	1:A:240:THR:HG23	2.16	0.46
1:A:245:ASN:ND2	1:A:247:PHE:CZ	2.84	0.46
1:A:322:ALA:HB3	1:B:256:GLN:O	2.14	0.46
1:A:444:GLU:C	1:A:445:ILE:HG13	2.34	0.46
1:B:256:GLN:NE2	1:B:405:GLN:N	2.63	0.46
1:C:337:GLU:O	1:C:339:GLU:N	2.49	0.46
1:D:218:ARG:HD3	1:D:237:PHE:CE1	2.49	0.46
1:D:412:PHE:N	1:D:412:PHE:HD1	2.13	0.46
1:E:24:MET:HA	1:E:24:MET:HE3	1.97	0.46
1:E:140:ARG:HA	1:E:140:ARG:HD2	1.80	0.46
1:E:160:VAL:O	1:E:163:GLU:HB2	2.14	0.46
1:E:300:ARG:CA	1:E:333:MET:HE1	2.45	0.46
1:E:447:GLY:O	1:F:467:ILE:HG12	2.15	0.46
1:F:316:ALA:HA	1:F:378:ASP:HB3	1.98	0.46
1:F:492:GLY:O	1:F:494:PRO:HD3	2.15	0.46
1:C:103:LEU:HD12	1:C:104:PHE:N	2.31	0.46
1:D:381:SER:HB3	1:D:414:ASN:OD1	2.15	0.46
3:D:901:ATP:PG	1:E:459:ARG:HH21	2.39	0.46
1:E:153:GLN:HB3	1:E:154:TYR:CE1	2.49	0.46
1:E:294:LYS:HB2	3:E:901:ATP:O1B	2.15	0.46
1:E:447:GLY:O	1:E:448:GLU:HG3	2.15	0.46
1:F:20:LYS:O	1:F:38:ILE:HD11	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:117:VAL:HA	1:F:154:TYR:CZ	2.50	0.46
1:F:286:ALA:N	1:F:412:PHE:O	2.45	0.46
1:F:311:ARG:HD3	1:F:370:PHE:O	2.16	0.46
1:F:469:GLU:HG3	1:F:470:PHE:N	2.29	0.46
1:A:264:SER:HB3	1:A:304:ASN:CG	2.35	0.46
1:C:43:LEU:HB3	1:C:204:VAL:HA	1.96	0.46
1:C:88:ARG:NE	1:D:15:HIS:HA	2.31	0.46
1:C:231:MET:SD	1:C:251:ALA:HB2	2.56	0.46
1:F:380:LEU:O	1:F:383:LEU:N	2.47	0.46
1:A:18:ILE:HG22	1:A:19:ALA:N	2.31	0.46
1:A:110:PRO:HB2	1:B:165:PHE:HE2	1.81	0.46
1:A:203:ASN:OD1	1:A:225:LEU:HA	2.16	0.46
1:A:218:ARG:CZ	1:A:239:ILE:HD12	2.46	0.46
1:A:222:ILE:O	1:A:222:ILE:HG22	2.15	0.46
1:A:435:ASP:HA	1:A:459:ARG:HD2	1.98	0.46
1:B:278:PHE:CD1	1:B:284:ILE:HD13	2.51	0.46
1:B:461:SER:OG	1:B:462:TRP:N	2.49	0.46
1:C:215:ARG:NE	1:C:215:ARG:CA	2.79	0.46
1:D:25:ILE:HG22	1:D:25:ILE:O	2.14	0.46
1:D:271:ASP:OD1	1:D:277:GLY:HA2	2.16	0.46
1:D:347:VAL:O	1:D:348:CYS:CB	2.62	0.46
1:D:356:LEU:O	1:D:358:ASP:N	2.49	0.46
1:D:392:PHE:O	1:D:396:VAL:HG23	2.16	0.46
1:E:20:LYS:HE3	1:E:228:THR:OG1	2.16	0.46
1:E:43:LEU:HD23	1:E:204:VAL:HG13	1.97	0.46
1:E:106:LEU:O	1:E:106:LEU:HG	2.15	0.46
1:E:130:ILE:CG2	1:E:134:ILE:HD11	2.45	0.46
1:E:267:VAL:HG22	1:E:477:PRO:HG3	1.97	0.46
1:E:270:LEU:HD23	1:E:270:LEU:O	2.16	0.46
1:F:426:ASN:N	1:F:426:ASN:ND2	2.62	0.46
1:F:486:PHE:CE2	1:F:496:ARG:HD2	2.47	0.46
1:A:170:ARG:O	1:A:174:ILE:HG12	2.16	0.46
1:A:298:VAL:HA	1:A:411:LEU:HD23	1.96	0.46
1:A:341:GLN:CB	1:A:343:LEU:HG	2.45	0.46
1:A:344:LEU:HD22	1:A:345:LYS:H	1.80	0.46
1:A:467:ILE:HD11	1:F:449:MET:HG2	1.96	0.46
1:B:299:SER:C	1:B:333:MET:HE1	2.36	0.46
1:C:182:THR:HG21	1:C:192:ALA:HB1	1.97	0.46
1:C:252:MET:HG3	1:C:252:MET:O	2.16	0.46
1:C:296:LEU:CD2	1:C:472:ILE:HD12	2.45	0.46
1:D:64:ILE:HG21	1:D:97:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:ARG:O	1:D:174:ILE:HG13	2.16	0.46
1:E:46:GLY:HA2	1:E:184:ARG:HD3	1.98	0.46
1:E:96:LYS:HE2	1:E:100:GLU:OE2	2.15	0.46
1:E:127:ILE:CD1	1:E:167:LEU:HD13	2.45	0.46
1:E:214:GLU:OE2	1:F:217:ARG:NH1	2.49	0.46
1:F:488:ARG:HD3	1:F:495:THR:OG1	2.15	0.46
1:A:52:LYS:O	1:A:53:THR:C	2.55	0.46
1:A:267:VAL:HG12	1:A:270:LEU:H	1.80	0.46
1:A:404:LYS:HE2	1:F:323:GLN:OE1	2.15	0.46
1:B:94:LEU:O	1:B:95:ALA:C	2.54	0.46
1:B:200:VAL:O	1:B:200:VAL:HG12	2.16	0.46
1:B:272:GLU:O	1:B:275:GLY:N	2.47	0.46
1:C:60:LEU:O	1:C:63:GLY:N	2.49	0.46
1:C:134:ILE:CG2	1:C:139:ALA:HB3	2.32	0.46
1:D:21:MET:HE1	1:D:177:THR:HB	1.97	0.46
1:D:70:PRO:HB2	1:D:139:ALA:HA	1.96	0.46
1:D:262:ARG:HH12	1:D:275:GLY:C	2.19	0.46
1:E:325:LEU:CD2	1:E:335:PHE:HB2	2.40	0.46
1:F:183:GLU:H	1:F:183:GLU:HG2	1.40	0.46
1:A:148:THR:CG2	1:A:193:ARG:HD2	2.46	0.46
1:B:421:GLY:O	1:B:423:HIS:N	2.49	0.46
1:C:131:ASN:HA	1:C:134:ILE:HG12	1.98	0.46
1:C:262:ARG:HA	1:C:278:PHE:O	2.16	0.46
1:C:311:ARG:CZ	1:C:371:LYS:HE3	2.46	0.46
1:D:420:MET:HB3	1:D:492:GLY:HA3	1.98	0.46
1:E:153:GLN:O	1:F:158:SER:CB	2.59	0.46
1:F:413:THR:HG22	1:F:414:ASN:N	2.31	0.46
1:A:123:LEU:O	1:A:123:LEU:HD13	2.15	0.45
1:B:502:LYS:HD3	1:B:502:LYS:N	2.31	0.45
1:C:462:TRP:O	1:C:463:HIS:CB	2.63	0.45
1:D:67:PHE:CD2	1:D:67:PHE:N	2.82	0.45
1:D:331:TRP:CD1	4:D:536:HOH:O	2.69	0.45
1:D:486:PHE:HE2	1:D:496:ARG:NH1	2.14	0.45
1:E:267:VAL:CG2	1:E:477:PRO:HG3	2.46	0.45
1:E:273:MET:C	1:E:275:GLY:H	2.19	0.45
1:E:313:ILE:CG1	1:E:372:PRO:HG3	2.46	0.45
1:E:485:ASN:HD22	1:E:496:ARG:CD	2.21	0.45
1:F:21:MET:CE	1:F:59:PHE:CZ	2.99	0.45
1:F:157:SER:O	1:F:196:VAL:HG21	2.16	0.45
1:F:194:TYR:H	1:F:194:TYR:HD1	1.61	0.45
1:F:270:LEU:O	1:F:270:LEU:HD23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:334:ASP:O	1:F:338:MET:HG2	2.15	0.45
1:B:134:ILE:HA	1:B:139:ALA:HB3	1.98	0.45
1:B:416:SER:C	1:B:418:GLN:H	2.19	0.45
1:C:262:ARG:NH2	1:C:461:SER:CB	2.72	0.45
1:C:265:SER:O	1:C:301:PHE:HA	2.16	0.45
1:C:469:GLU:CG	1:C:480:LYS:HE3	2.41	0.45
1:D:113:GLU:HB3	1:D:114:GLY:H	1.51	0.45
1:D:131:ASN:OD1	1:D:174:ILE:HD13	2.16	0.45
1:E:130:ILE:H	1:E:130:ILE:CD1	2.30	0.45
1:E:447:GLY:C	1:F:467:ILE:HG12	2.37	0.45
1:F:509:VAL:CG1	1:F:510:ARG:H	2.28	0.45
1:A:80:PRO:HG2	1:A:107:ASP:HB2	1.98	0.45
1:A:84:ILE:HA	1:A:94:LEU:HD12	1.99	0.45
1:B:67:PHE:HB2	1:B:69:GLU:HG3	1.98	0.45
1:B:187:GLU:HG3	1:B:208:ARG:HG2	1.99	0.45
1:B:445:ILE:HD13	1:B:494:PRO:HG2	1.98	0.45
1:C:149:SER:HA	1:C:152:GLN:HG3	1.98	0.45
1:C:169:ALA:O	1:C:173:GLN:HG3	2.16	0.45
1:C:420:MET:HE3	1:C:492:GLY:CA	2.47	0.45
3:C:903:ATP:HO2'	1:D:230:HIS:CE1	2.32	0.45
1:D:331:TRP:CG	4:D:536:HOH:O	2.69	0.45
1:E:178:THR:CG2	1:E:179:VAL:N	2.76	0.45
1:E:453:ILE:HG12	1:E:454:ASN:H	1.82	0.45
1:E:501:GLU:O	1:E:502:LYS:HG3	2.16	0.45
1:F:269:ARG:HH11	1:F:269:ARG:HG3	1.81	0.45
1:F:453:ILE:HG21	1:F:479:ILE:HD11	1.97	0.45
1:A:303:GLU:O	1:A:306:CYS:N	2.43	0.45
1:A:310:GLU:O	1:A:343:LEU:HB3	2.17	0.45
1:B:119:GLY:C	1:B:121:PHE:H	2.19	0.45
1:B:152:GLN:NE2	1:B:194:TYR:OH	2.50	0.45
1:B:468:ARG:HA	1:B:482:SER:HA	1.98	0.45
1:C:278:PHE:CD2	1:C:278:PHE:N	2.84	0.45
1:D:79:THR:HG23	1:D:81:GLN:N	2.32	0.45
1:D:223:LEU:HA	1:D:223:LEU:HD23	1.69	0.45
1:D:327:ASN:CA	4:D:535:HOH:O	2.61	0.45
1:D:386:GLY:HA2	1:E:390:ASN:ND2	2.32	0.45
1:E:33:HIS:CD2	1:E:230:HIS:HA	2.51	0.45
1:E:45:SER:CB	1:E:182:THR:HG22	2.41	0.45
1:E:70:PRO:HB2	1:E:139:ALA:HA	1.97	0.45
1:E:151:PHE:C	1:E:153:GLN:H	2.20	0.45
1:E:284:ILE:N	1:E:284:ILE:HD12	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:292:THR:HG23	1:E:442:TYR:CE1	2.51	0.45
1:E:295:THR:HG23	1:E:378:ASP:OD2	2.17	0.45
1:E:364:LYS:O	1:E:368:ASN:ND2	2.49	0.45
1:F:453:ILE:HG21	1:F:479:ILE:HD12	1.98	0.45
1:A:492:GLY:C	1:A:494:PRO:HD3	2.36	0.45
1:B:82:ASP:C	1:B:84:ILE:N	2.66	0.45
1:B:311:ARG:HB3	1:B:370:PHE:CD2	2.51	0.45
1:B:432:TPO:O1P	1:B:432:TPO:HG21	2.15	0.45
1:C:21:MET:SD	1:C:141:ARG:NE	2.90	0.45
1:C:375:ILE:O	1:C:410:GLY:HA2	2.17	0.45
1:C:464:ASP:C	1:C:464:ASP:OD1	2.53	0.45
1:D:301:PHE:CZ	1:D:409:THR:HG22	2.52	0.45
1:E:297:LEU:HD11	1:E:440:LEU:HD21	1.98	0.45
1:E:303:GLU:C	1:E:305:ALA:H	2.20	0.45
1:F:53:THR:OG1	1:F:145:ASP:OD1	2.35	0.45
1:F:184:ARG:HH12	1:F:187:GLU:C	2.20	0.45
1:F:230:HIS:HE1	1:F:232:LYS:HG3	1.82	0.45
1:F:261:VAL:O	1:F:279:PHE:HA	2.17	0.45
1:F:514:GLU:O	1:F:515:LYS:CB	2.63	0.45
1:B:151:PHE:HE2	1:B:163:GLU:HB2	1.82	0.45
1:C:370:PHE:HD2	1:C:372:PRO:HG3	1.80	0.45
1:D:57:ILE:O	1:D:58:GLN:C	2.52	0.45
1:D:213:GLY:O	1:D:215:ARG:N	2.49	0.45
1:E:23:THR:C	1:E:25:ILE:H	2.19	0.45
1:F:94:LEU:HB3	1:F:103:LEU:CD2	2.46	0.45
1:F:217:ARG:NH2	1:F:394:GLN:HE22	2.14	0.45
1:F:290:THR:HG23	1:F:290:THR:O	2.16	0.45
1:F:514:GLU:OE1	1:F:515:LYS:N	2.45	0.45
1:A:25:ILE:HG23	1:A:58:GLN:NE2	2.31	0.45
1:A:363:ILE:HG21	1:A:399:VAL:HG13	1.97	0.45
1:A:395:PHE:O	1:A:399:VAL:HG23	2.17	0.45
1:A:451:ARG:HG2	1:A:451:ARG:HH11	1.81	0.45
1:B:298:VAL:HA	1:B:411:LEU:HD23	1.98	0.45
1:B:492:GLY:C	1:B:494:PRO:HD3	2.37	0.45
1:C:53:THR:HG21	1:C:78:GLU:OE2	2.16	0.45
1:C:123:LEU:O	1:C:127:ILE:HG13	2.17	0.45
1:D:126:LEU:HD12	1:D:129:ARG:HD3	1.98	0.45
1:D:164:LEU:O	1:D:168:VAL:HG23	2.16	0.45
1:D:365:SER:O	1:D:369:ASP:N	2.48	0.45
1:D:387:VAL:CG1	1:D:388:SER:N	2.80	0.45
1:E:404:LYS:C	1:E:406:GLU:N	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:191:ILE:CG1	1:F:198:GLU:CG	2.95	0.45
1:F:335:PHE:CD2	1:F:338:MET:HG3	2.52	0.45
1:F:371:LYS:N	1:F:372:PRO:HD3	2.31	0.45
1:B:16:GLN:O	1:B:17:ALA:O	2.34	0.45
1:D:142:VAL:O	1:D:178:THR:HA	2.16	0.45
1:E:293:GLY:HA2	3:E:901:ATP:O5'	2.16	0.45
1:E:383:LEU:O	1:E:385:ARG:N	2.50	0.45
1:F:471:MET:HG2	1:F:478:ASP:HB3	1.99	0.45
1:A:39:GLY:C	1:A:40:ARG:HG3	2.37	0.45
1:A:60:LEU:O	1:A:61:TYR:C	2.55	0.45
1:A:94:LEU:O	1:A:97:LEU:N	2.50	0.45
1:A:445:ILE:O	1:A:447:GLY:N	2.50	0.45
1:B:378:ASP:O	1:B:379:SER:HB3	2.16	0.45
1:C:102:LYS:NZ	1:C:138:ARG:HH12	2.15	0.45
1:D:25:ILE:HG22	1:D:28:PHE:HB2	1.99	0.45
1:D:89:SER:CB	1:E:227:GLY:O	2.65	0.45
1:D:278:PHE:CD1	1:D:284:ILE:HG12	2.52	0.45
1:D:420:MET:HE1	1:E:490:ILE:HD12	1.99	0.45
1:D:495:THR:O	1:D:497:ILE:HG23	2.17	0.45
1:E:121:PHE:O	1:E:125:ALA:CB	2.65	0.45
1:E:191:ILE:HB	1:E:198:GLU:CG	2.42	0.45
1:E:375:ILE:HG22	1:E:408:ILE:CG2	2.47	0.45
1:E:385:ARG:HH12	1:F:397:ILE:HD11	1.81	0.45
1:F:116:GLU:OE1	1:F:117:VAL:HG23	2.17	0.45
1:F:285:LEU:HD12	1:F:285:LEU:C	2.37	0.45
1:F:502:LYS:HG3	1:F:502:LYS:O	2.17	0.45
1:A:79:THR:HG22	1:A:81:GLN:H	1.81	0.45
1:A:230:HIS:ND1	1:A:230:HIS:O	2.50	0.45
1:A:378:ASP:O	1:A:379:SER:HB2	2.17	0.45
1:A:388:SER:HB3	1:A:391:ALA:HB3	1.97	0.45
1:B:20:LYS:HB3	1:B:35:GLY:O	2.17	0.45
1:B:273:MET:HE1	1:B:468:ARG:HD2	1.99	0.45
1:C:36:LEU:HD12	1:C:59:PHE:CZ	2.51	0.45
1:C:295:THR:O	1:C:299:SER:OG	2.33	0.45
1:D:148:THR:HG21	1:D:193:ARG:HD2	1.96	0.45
1:D:362:ILE:O	1:D:366:GLU:HB2	2.17	0.45
1:E:197:GLU:OE2	1:E:197:GLU:N	2.37	0.45
1:E:313:ILE:CD1	1:E:372:PRO:CG	2.95	0.45
1:E:446:ARG:NH2	1:E:496:ARG:NH2	2.57	0.45
1:F:312:ALA:HB2	1:F:374:ARG:HB2	1.99	0.45
1:F:357:GLU:HG3	1:F:358:ASP:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:GLU:HG3	1:A:245:ASN:OD1	2.17	0.44
1:A:106:LEU:HD11	1:A:129:ARG:HE	1.83	0.44
1:A:379:SER:HA	1:A:413:THR:O	2.16	0.44
1:A:444:GLU:N	1:A:492:GLY:O	2.49	0.44
1:B:72:VAL:HG21	1:B:134:ILE:HD13	1.99	0.44
1:B:306:CYS:HB3	1:B:338:MET:SD	2.57	0.44
1:B:435:ASP:O	1:B:458:MET:HA	2.18	0.44
1:C:247:PHE:HZ	1:C:361:GLN:CG	2.28	0.44
1:C:416:SER:O	1:C:418:GLN:N	2.50	0.44
1:D:20:LYS:HE3	1:D:228:THR:CG2	2.42	0.44
1:D:77:GLU:O	1:D:78:GLU:C	2.54	0.44
1:D:315:PHE:HE1	1:D:375:ILE:HG23	1.83	0.44
1:D:318:GLU:OE2	1:E:432:TPO:HB	2.17	0.44
1:D:354:ALA:HB3	1:D:359:HIS:CE1	2.52	0.44
1:E:396:VAL:HG21	1:E:430:ILE:HD11	1.99	0.44
1:F:440:LEU:HD21	1:F:453:ILE:HD12	1.99	0.44
1:A:109:SER:HA	1:A:110:PRO:HD3	1.82	0.44
1:A:387:VAL:CG1	1:A:388:SER:N	2.80	0.44
1:A:406:GLU:HB3	1:A:408:ILE:HG12	1.98	0.44
1:A:451:ARG:HB3	1:A:470:PHE:CZ	2.51	0.44
1:A:471:MET:HE2	1:A:478:ASP:H	1.81	0.44
1:B:103:LEU:HD12	1:B:103:LEU:C	2.37	0.44
1:B:194:TYR:N	1:B:194:TYR:CD1	2.84	0.44
1:B:255:THR:HG22	1:B:255:THR:O	2.17	0.44
1:B:295:THR:HG21	1:B:319:GLU:OE2	2.17	0.44
1:C:44:VAL:O	1:C:44:VAL:HG12	2.17	0.44
1:D:67:PHE:O	1:D:68:ASP:C	2.54	0.44
1:E:61:TYR:CZ	1:E:92:TRP:CD1	3.06	0.44
1:F:429:HIS:ND1	1:F:429:HIS:C	2.70	0.44
1:A:153:GLN:CA	1:B:158:SER:HB2	2.47	0.44
1:B:21:MET:SD	1:B:141:ARG:NE	2.90	0.44
1:B:194:TYR:C	1:B:196:VAL:N	2.67	0.44
1:C:123:LEU:O	1:C:127:ILE:N	2.41	0.44
1:D:222:ILE:CG2	1:D:230:HIS:ND1	2.81	0.44
1:E:211:LEU:O	1:E:215:ARG:O	2.34	0.44
1:E:317:TYR:HB3	1:E:351:PRO:HG3	1.98	0.44
1:E:390:ASN:C	1:E:392:PHE:N	2.69	0.44
1:B:116:GLU:HG2	1:B:117:VAL:N	2.18	0.44
1:B:356:LEU:CD1	1:B:387:VAL:HG21	2.47	0.44
1:B:390:ASN:C	1:B:392:PHE:H	2.21	0.44
1:C:300:ARG:HA	1:C:333:MET:HE1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:ILE:O	1:C:366:GLU:HB2	2.17	0.44
1:C:397:ILE:HD13	1:C:433:ILE:HD13	1.99	0.44
1:D:82:ASP:O	1:D:83:ILE:C	2.54	0.44
1:E:249:LEU:HD12	1:E:394:GLN:HG2	1.98	0.44
1:E:269:ARG:O	1:E:273:MET:HG3	2.16	0.44
1:F:315:PHE:HA	1:F:347:VAL:HB	2.00	0.44
1:A:122:ASP:C	1:A:124:SER:N	2.70	0.44
1:C:79:THR:HG23	1:C:81:GLN:HG2	2.00	0.44
1:C:82:ASP:C	1:C:84:ILE:N	2.70	0.44
1:C:487:GLU:O	1:C:488:ARG:CB	2.65	0.44
1:D:208:ARG:HG2	1:D:208:ARG:NH1	2.32	0.44
1:D:451:ARG:HB3	1:D:470:PHE:CD2	2.52	0.44
1:E:303:GLU:C	1:E:305:ALA:N	2.70	0.44
1:E:504:GLU:HG2	1:E:505:LEU:N	2.32	0.44
1:A:193:ARG:HG2	1:A:193:ARG:HH11	1.83	0.44
1:C:171:LEU:CD1	1:C:178:THR:HG21	2.45	0.44
1:C:420:MET:HE3	1:C:492:GLY:HA3	1.99	0.44
1:D:211:LEU:HD22	1:D:216:ARG:HH11	1.76	0.44
1:E:193:ARG:HB3	1:E:194:TYR:CE1	2.53	0.44
1:E:270:LEU:O	1:E:273:MET:HB2	2.18	0.44
1:E:386:GLY:O	1:E:387:VAL:C	2.56	0.44
1:F:21:MET:CE	1:F:141:ARG:NE	2.81	0.44
1:F:104:PHE:HB2	1:F:137:TYR:CD2	2.52	0.44
1:F:106:LEU:CD1	1:F:129:ARG:CZ	2.95	0.44
1:F:151:PHE:HE1	1:F:164:LEU:HD21	1.80	0.44
1:F:347:VAL:O	1:F:348:CYS:CB	2.66	0.44
1:A:273:MET:O	1:A:464:ASP:N	2.39	0.44
1:B:165:PHE:O	1:B:169:ALA:HB2	2.18	0.44
1:B:261:VAL:HG12	1:B:262:ARG:N	2.33	0.44
1:B:348:CYS:HB3	1:C:254:LEU:HD23	1.99	0.44
1:C:380:LEU:HA	1:C:380:LEU:HD23	1.71	0.44
1:C:420:MET:HE3	1:C:492:GLY:O	2.18	0.44
1:D:42:THR:HG23	1:D:203:ASN:CB	2.42	0.44
1:D:237:PHE:CE1	1:D:244:ILE:HD12	2.51	0.44
1:E:119:GLY:HA2	1:E:122:ASP:CB	2.47	0.44
1:F:52:LYS:O	1:F:53:THR:C	2.56	0.44
1:F:150:VAL:HG13	1:F:151:PHE:N	2.33	0.44
1:F:367:ILE:O	1:F:367:ILE:HG22	2.18	0.44
1:A:79:THR:HG22	1:A:81:GLN:N	2.33	0.44
1:A:266:GLY:O	1:A:300:ARG:NE	2.50	0.44
1:A:284:ILE:HD12	1:A:436:THR:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:LEU:CD1	1:C:59:PHE:CE1	2.99	0.44
1:C:356:LEU:HD12	1:C:356:LEU:N	2.33	0.44
1:C:487:GLU:OE1	1:C:497:ILE:HD13	2.18	0.44
1:D:86:ASN:O	1:D:87:ALA:C	2.56	0.44
1:D:122:ASP:HB3	1:D:123:LEU:H	1.56	0.44
1:E:51:GLY:HA2	3:E:903:ATP:O1A	2.18	0.44
1:E:292:THR:HB	1:E:440:LEU:CB	2.47	0.44
1:F:123:LEU:HG	1:F:163:GLU:HB3	2.00	0.44
1:F:501:GLU:HG3	1:F:502:LYS:N	2.33	0.44
1:A:248:PRO:HB2	1:A:251:ALA:CB	2.48	0.44
1:A:284:ILE:HD12	1:A:436:THR:HG21	2.00	0.44
1:B:80:PRO:HB3	1:B:105:ILE:HG21	1.99	0.44
1:B:149:SER:HB3	1:C:161:ARG:HH21	1.82	0.44
1:B:285:LEU:HD21	1:B:426:ASN:HD21	1.78	0.44
1:C:123:LEU:HD12	1:C:163:GLU:OE2	2.18	0.44
1:C:396:VAL:HG11	1:C:430:ILE:CG2	2.47	0.44
1:E:118:VAL:O	1:E:122:ASP:HB2	2.17	0.44
1:E:160:VAL:HG21	1:E:194:TYR:CD2	2.53	0.44
1:F:164:LEU:O	1:F:167:LEU:N	2.51	0.44
1:F:167:LEU:O	1:F:171:LEU:HD12	2.18	0.44
1:B:205:VAL:CG2	1:B:222:ILE:HG12	2.45	0.43
1:B:428:SER:O	1:B:429:HIS:HB2	2.18	0.43
1:C:252:MET:O	1:C:252:MET:CG	2.65	0.43
1:D:293:GLY:O	1:D:296:LEU:N	2.51	0.43
1:D:330:SER:N	4:D:535:HOH:O	2.33	0.43
1:F:453:ILE:CG2	1:F:479:ILE:HD12	2.47	0.43
1:A:14:GLU:CD	1:A:15:HIS:H	2.21	0.43
1:A:148:THR:OG1	1:A:183:GLU:HG2	2.17	0.43
1:A:385:ARG:HA	1:B:393:ARG:NH1	2.33	0.43
1:B:21:MET:HB2	1:B:38:ILE:HG12	2.00	0.43
1:B:267:VAL:O	1:B:270:LEU:N	2.40	0.43
1:B:291:GLY:O	1:B:442:TYR:OH	2.34	0.43
1:C:51:GLY:O	1:C:52:LYS:C	2.55	0.43
1:C:64:ILE:H	1:C:64:ILE:CD1	2.30	0.43
1:C:191:ILE:HD12	1:C:191:ILE:N	2.33	0.43
1:C:294:LYS:HB3	1:C:413:THR:HG23	1.99	0.43
1:C:353:SER:O	1:C:354:ALA:HB2	2.17	0.43
1:D:173:GLN:C	1:D:175:GLY:N	2.72	0.43
1:D:301:PHE:CZ	1:D:374:ARG:HD3	2.54	0.43
1:D:328:ALA:O	1:D:333:MET:O	2.36	0.43
1:E:184:ARG:NH2	1:E:187:GLU:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:146:SER:N	1:F:181:THR:HG22	2.31	0.43
1:F:223:LEU:HD23	1:F:223:LEU:HA	1.78	0.43
1:F:286:ALA:HB3	1:F:413:THR:HA	2.00	0.43
1:C:111:ASP:O	1:C:113:GLU:N	2.47	0.43
1:D:487:GLU:O	1:D:488:ARG:C	2.56	0.43
1:E:300:ARG:HA	1:E:333:MET:HE1	2.00	0.43
1:E:321:ARG:HG2	1:E:348:CYS:CB	2.47	0.43
1:F:341:GLN:O	1:F:342:ASN:HB2	2.19	0.43
1:A:313:ILE:CG1	1:A:372:PRO:HG2	2.49	0.43
1:A:346:ILE:HG22	1:A:348:CYS:SG	2.59	0.43
1:A:387:VAL:HG12	1:A:388:SER:N	2.33	0.43
1:A:405:GLN:O	1:A:407:GLU:N	2.52	0.43
1:B:79:THR:HG23	1:B:82:ASP:H	1.84	0.43
1:B:111:ASP:O	1:B:113:GLU:N	2.51	0.43
1:C:293:GLY:O	1:C:294:LYS:C	2.56	0.43
1:C:315:PHE:CE2	1:C:347:VAL:HG21	2.54	0.43
1:C:413:THR:O	1:C:414:ASN:CB	2.61	0.43
1:D:126:LEU:O	1:D:129:ARG:N	2.51	0.43
1:D:222:ILE:HG22	1:D:230:HIS:ND1	2.34	0.43
1:D:230:HIS:CD2	1:D:230:HIS:O	2.71	0.43
1:E:219:THR:HA	1:E:235:TYR:O	2.19	0.43
1:E:274:CYS:HB3	1:E:277:GLY:O	2.18	0.43
1:E:379:SER:H	1:E:413:THR:HB	1.83	0.43
1:F:122:ASP:HA	1:F:125:ALA:HB3	1.99	0.43
1:F:299:SER:CB	1:F:333:MET:HE1	2.40	0.43
1:F:345:LYS:NZ	1:F:366:GLU:OE1	2.44	0.43
1:F:377:ILE:CG1	1:F:412:PHE:CE2	3.02	0.43
1:A:230:HIS:NE2	3:F:903:ATP:O2'	2.46	0.43
1:B:121:PHE:H	1:B:121:PHE:HD1	1.66	0.43
1:B:291:GLY:N	3:B:901:ATP:O3G	2.51	0.43
1:C:80:PRO:HG3	1:C:107:ASP:HB2	2.00	0.43
1:F:246:ILE:N	1:F:246:ILE:HD12	2.34	0.43
1:F:247:PHE:HZ	1:F:361:GLN:NE2	2.15	0.43
1:F:249:LEU:HD12	1:F:394:GLN:HG2	1.99	0.43
1:F:319:GLU:HB2	1:F:324:LEU:HG	1.99	0.43
1:F:336:GLU:HA	1:F:336:GLU:OE1	2.19	0.43
1:F:375:ILE:HB	1:F:408:ILE:CG2	2.47	0.43
1:F:484:ARG:HB3	1:F:484:ARG:CZ	2.48	0.43
1:A:326:ARG:CG	1:B:260:ASN:ND2	2.81	0.43
1:A:423:HIS:HE1	1:F:420:MET:O	2.02	0.43
1:B:64:ILE:CG2	1:B:65:ILE:HD13	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ARG:HH11	1:B:88:ARG:CG	2.31	0.43
1:C:52:LYS:HB3	1:C:181:THR:CG2	2.48	0.43
1:C:120:GLY:O	1:C:122:ASP:N	2.51	0.43
1:C:287:THR:HG23	1:C:414:ASN:HD22	1.84	0.43
1:C:325:LEU:CD2	1:C:335:PHE:HB3	2.49	0.43
1:C:385:ARG:HG3	1:C:385:ARG:O	2.18	0.43
1:D:31:ILE:HD11	1:D:248:PRO:HG3	2.01	0.43
1:D:240:THR:C	1:D:242:HIS:N	2.72	0.43
1:E:209:ASN:ND2	1:E:218:ARG:HG2	2.33	0.43
1:E:313:ILE:HG12	1:E:370:PHE:HD2	1.84	0.43
3:E:903:ATP:O3'	1:F:224:LYS:HB2	2.18	0.43
1:F:47:THR:HG22	1:F:184:ARG:O	2.19	0.43
1:F:93:ASP:OD1	1:F:95:ALA:HB3	2.18	0.43
1:F:150:VAL:CG1	1:F:151:PHE:N	2.81	0.43
1:F:248:PRO:C	1:F:250:GLY:N	2.71	0.43
1:F:418:GLN:CG	1:F:422:ALA:HA	2.47	0.43
1:A:220:LEU:HD13	1:A:246:ILE:HD11	2.00	0.43
1:A:278:PHE:CD1	1:A:301:PHE:HE1	2.37	0.43
1:A:489:ILE:HG12	1:F:444:GLU:OE2	2.19	0.43
1:B:294:LYS:HE3	1:B:414:ASN:O	2.19	0.43
1:D:488:ARG:O	1:D:494:PRO:HA	2.19	0.43
1:D:490:ILE:C	1:D:492:GLY:H	2.20	0.43
1:E:20:LYS:HB3	1:E:35:GLY:C	2.38	0.43
1:E:146:SER:C	1:E:148:THR:N	2.70	0.43
1:E:261:VAL:CG1	1:E:262:ARG:H	2.30	0.43
1:E:317:TYR:CD2	1:E:383:LEU:HD21	2.54	0.43
1:E:445:ILE:HG22	1:E:445:ILE:O	2.19	0.43
1:A:148:THR:HG21	1:A:193:ARG:HD2	2.01	0.43
1:A:308:ASN:O	1:A:310:GLU:HG3	2.19	0.43
1:B:21:MET:CG	1:B:141:ARG:HH21	2.32	0.43
1:B:23:THR:HG22	1:B:59:PHE:HD1	1.83	0.43
1:C:261:VAL:CG1	1:C:262:ARG:H	2.24	0.43
1:D:239:ILE:HG12	1:D:244:ILE:CD1	2.49	0.43
1:D:294:LYS:HB2	1:D:294:LYS:HE2	1.78	0.43
1:E:130:ILE:HD12	1:E:130:ILE:H	1.84	0.43
1:E:313:ILE:CD1	1:E:372:PRO:HG3	2.49	0.43
1:F:23:THR:HG1	1:F:25:ILE:HG12	1.78	0.43
1:F:33:HIS:CD2	1:F:229:SER:OG	2.72	0.43
1:F:119:GLY:HA2	1:F:122:ASP:OD1	2.19	0.43
1:F:194:TYR:O	1:F:196:VAL:N	2.51	0.43
1:F:217:ARG:O	1:F:217:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:362:ILE:O	1:F:365:SER:HB3	2.18	0.43
1:F:413:THR:HG22	1:F:414:ASN:H	1.83	0.43
1:F:462:TRP:CE3	1:F:463:HIS:N	2.87	0.43
1:F:467:ILE:O	1:F:467:ILE:HG22	2.19	0.43
1:F:484:ARG:HB3	1:F:484:ARG:HH11	1.83	0.43
1:A:98:VAL:HA	1:A:103:LEU:O	2.17	0.43
1:A:227:GLY:CA	1:F:86:ASN:OD1	2.67	0.43
1:A:371:LYS:O	1:A:371:LYS:CD	2.67	0.43
1:A:490:ILE:HG21	1:F:419:PHE:CE1	2.50	0.43
1:B:127:ILE:CD1	1:B:166:ARG:HG2	2.48	0.43
1:B:375:ILE:HG22	1:B:410:GLY:HA2	2.01	0.43
1:C:370:PHE:C	1:C:372:PRO:HD3	2.38	0.43
1:D:38:ILE:CA	1:D:177:THR:HG23	2.45	0.43
1:D:52:LYS:HE3	3:D:903:ATP:O1B	2.19	0.43
1:D:122:ASP:O	1:D:125:ALA:N	2.50	0.43
1:D:161:ARG:HG3	1:D:200:VAL:CG2	2.49	0.43
1:E:130:ILE:N	1:E:130:ILE:CD1	2.82	0.43
1:F:337:GLU:HA	1:F:340:ARG:HD2	2.01	0.43
1:B:162:ARG:NH1	1:B:162:ARG:CB	2.79	0.43
1:B:273:MET:O	1:B:463:HIS:HA	2.18	0.43
1:D:364:LYS:O	1:D:367:ILE:HB	2.19	0.43
1:D:367:ILE:HG23	1:D:372:PRO:HD2	2.01	0.43
1:D:446:ARG:H	1:D:496:ARG:HH22	1.67	0.43
1:E:72:VAL:CG1	1:E:73:PHE:N	2.81	0.43
1:E:379:SER:HB3	1:E:382:ALA:HB2	2.01	0.43
1:F:109:SER:HA	1:F:110:PRO:HD3	1.79	0.43
1:F:137:TYR:N	1:F:137:TYR:CD1	2.86	0.43
1:A:318:GLU:HB2	1:A:319:GLU:H	1.64	0.42
1:A:370:PHE:C	1:A:372:PRO:HD3	2.39	0.42
1:B:486:PHE:HZ	1:B:496:ARG:HH11	1.67	0.42
1:C:31:ILE:CD1	1:C:246:ILE:HG21	2.49	0.42
1:C:75:THR:OG1	1:C:78:GLU:O	2.29	0.42
1:D:182:THR:HG22	1:D:183:GLU:O	2.18	0.42
1:D:221:GLU:HB2	1:D:234:GLU:HB3	2.00	0.42
1:D:253:ARG:C	1:D:255:THR:H	2.20	0.42
1:D:283:ILE:N	1:D:283:ILE:HD12	2.34	0.42
1:D:315:PHE:HA	1:D:347:VAL:HB	1.99	0.42
1:D:470:PHE:HB2	1:D:478:ASP:O	2.19	0.42
1:F:445:ILE:CD1	1:F:483:PHE:HE2	2.32	0.42
1:B:67:PHE:HB2	1:B:69:GLU:CG	2.49	0.42
1:B:100:GLU:O	1:B:102:LYS:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:PHE:C	1:B:104:PHE:CD1	2.91	0.42
1:C:230:HIS:O	1:C:232:LYS:HD2	2.19	0.42
1:C:384:ALA:HB2	1:C:392:PHE:CZ	2.53	0.42
1:C:437:ILE:HD11	1:C:457:LYS:HE2	2.00	0.42
1:D:191:ILE:CB	1:D:198:GLU:CD	2.81	0.42
1:D:213:GLY:C	1:D:215:ARG:H	2.22	0.42
1:D:359:HIS:O	1:D:362:ILE:N	2.52	0.42
1:D:438:ILE:CG2	1:D:439:LEU:N	2.82	0.42
1:E:309:LYS:HA	1:E:343:LEU:HD13	2.01	0.42
1:E:315:PHE:HB3	1:E:317:TYR:CE1	2.51	0.42
1:F:38:ILE:HA	1:F:177:THR:HG23	2.01	0.42
1:F:95:ALA:O	1:F:99:ASP:HB2	2.19	0.42
1:F:276:GLY:O	1:F:277:GLY:O	2.37	0.42
1:A:52:LYS:O	1:A:55:PHE:N	2.52	0.42
1:A:65:ILE:O	1:A:66:GLU:HG2	2.19	0.42
1:A:379:SER:O	1:A:382:ALA:HB3	2.19	0.42
1:B:468:ARG:HG2	1:B:468:ARG:NH1	2.35	0.42
1:C:62:ASN:O	1:C:66:GLU:HB2	2.19	0.42
1:C:153:GLN:O	1:C:154:TYR:HB3	2.19	0.42
1:D:350:TYR:CD1	1:E:254:LEU:HB2	2.55	0.42
1:D:418:GLN:HB2	1:E:423:HIS:O	2.19	0.42
1:E:104:PHE:CE2	1:E:106:LEU:HB2	2.54	0.42
1:E:152:GLN:CG	1:F:161:ARG:HH11	2.31	0.42
1:E:215:ARG:HD3	1:E:215:ARG:HA	1.73	0.42
1:F:186:GLU:CD	1:F:187:GLU:N	2.72	0.42
1:F:375:ILE:CG2	1:F:408:ILE:HG22	2.49	0.42
1:F:422:ALA:O	1:F:424:SER:N	2.52	0.42
1:F:503:SER:O	1:F:504:GLU:O	2.37	0.42
1:A:134:ILE:O	1:A:138:ARG:N	2.52	0.42
1:A:279:PHE:N	1:A:279:PHE:CD1	2.88	0.42
1:A:380:LEU:C	1:A:382:ALA:N	2.72	0.42
1:A:392:PHE:O	1:A:395:PHE:N	2.51	0.42
1:B:65:ILE:O	1:B:65:ILE:HG22	2.19	0.42
1:B:324:LEU:HA	1:B:324:LEU:HD23	1.77	0.42
1:B:420:MET:HE1	1:C:490:ILE:HD12	2.02	0.42
1:B:448:GLU:HG2	1:C:466:ALA:HA	2.00	0.42
1:B:468:ARG:HG2	1:B:468:ARG:HH11	1.83	0.42
1:B:493:SER:HB3	1:C:488:ARG:CD	2.50	0.42
1:C:106:LEU:O	1:C:107:ASP:C	2.57	0.42
1:C:303:GLU:OE1	1:C:304:ASN:N	2.53	0.42
1:C:351:PRO:HB3	1:C:383:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:ASN:ND2	1:C:402:TYR:OH	2.30	0.42
1:D:148:THR:HA	1:D:151:PHE:CE1	2.54	0.42
1:D:454:ASN:HB2	1:D:466:ALA:O	2.19	0.42
1:D:486:PHE:HB3	1:D:489:ILE:CD1	2.35	0.42
1:E:217:ARG:HH21	1:E:236:PRO:CB	2.33	0.42
1:E:249:LEU:HD12	1:E:394:GLN:CG	2.49	0.42
1:E:306:CYS:SG	1:E:344:LEU:HD23	2.59	0.42
1:E:316:ALA:O	1:E:348:CYS:HA	2.19	0.42
1:E:345:LYS:HE2	1:E:366:GLU:OE1	2.20	0.42
1:F:280:LYS:HA	1:F:409:THR:OG1	2.20	0.42
1:F:327:ASN:HB3	1:F:331:TRP:CZ3	2.53	0.42
1:F:432:TPO:C	1:F:434:THR:N	2.83	0.42
1:A:52:LYS:HD2	1:A:181:THR:CG2	2.49	0.42
1:B:45:SER:HB3	1:B:182:THR:HG1	1.84	0.42
1:B:97:LEU:CB	1:B:103:LEU:HD23	2.39	0.42
1:B:137:TYR:O	1:B:138:ARG:C	2.57	0.42
1:B:445:ILE:HD11	1:B:494:PRO:HG2	2.00	0.42
1:C:64:ILE:CG2	1:C:64:ILE:O	2.67	0.42
1:C:79:THR:CG2	1:C:81:GLN:HG2	2.49	0.42
1:C:301:PHE:HE2	1:C:374:ARG:HB3	1.83	0.42
1:C:448:GLU:HG2	1:D:466:ALA:HB2	2.02	0.42
1:D:358:ASP:O	1:D:359:HIS:C	2.57	0.42
1:E:123:LEU:O	1:E:127:ILE:HG12	2.19	0.42
1:A:209:ASN:ND2	1:A:218:ARG:HG3	2.35	0.42
1:A:283:ILE:HG23	1:A:412:PHE:CD1	2.55	0.42
1:C:325:LEU:HD23	1:C:335:PHE:CB	2.49	0.42
1:C:356:LEU:CD1	1:C:356:LEU:N	2.82	0.42
1:D:198:GLU:HB3	1:D:199:PHE:CD2	2.55	0.42
1:D:333:MET:CG	4:D:538:HOH:O	2.62	0.42
1:D:377:ILE:HG21	1:D:380:LEU:HD23	2.01	0.42
1:D:408:ILE:HG22	1:D:409:THR:N	2.35	0.42
1:D:486:PHE:CD2	1:D:494:PRO:HB3	2.54	0.42
1:E:79:THR:HG23	1:E:82:ASP:OD2	2.19	0.42
1:F:24:MET:HB2	1:F:62:ASN:ND2	2.35	0.42
1:F:193:ARG:O	1:F:195:GLY:N	2.52	0.42
1:A:502:LYS:O	1:A:504:GLU:N	2.53	0.42
1:B:469:GLU:HG3	1:B:470:PHE:N	2.33	0.42
1:C:317:TYR:HD2	1:C:349:ALA:O	2.02	0.42
1:C:349:ALA:N	1:D:254:LEU:HD22	2.34	0.42
1:D:52:LYS:O	1:D:53:THR:C	2.58	0.42
1:D:74:VAL:HA	1:D:106:LEU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:VAL:CG2	1:D:148:THR:N	2.82	0.42
1:D:253:ARG:C	1:D:255:THR:N	2.73	0.42
1:E:130:ILE:HG23	1:E:134:ILE:HD11	2.00	0.42
1:E:490:ILE:H	1:E:490:ILE:HG13	1.65	0.42
1:F:25:ILE:HD13	1:F:62:ASN:ND2	2.34	0.42
1:A:38:ILE:HA	1:A:177:THR:OG1	2.19	0.42
1:A:48:SER:O	1:B:223:LEU:HD22	2.19	0.42
1:A:164:LEU:HD23	1:A:168:VAL:CG2	2.46	0.42
1:A:248:PRO:C	1:A:250:GLY:N	2.73	0.42
1:B:59:PHE:CE2	1:B:141:ARG:HB3	2.55	0.42
1:B:356:LEU:CD1	1:B:356:LEU:H	2.33	0.42
1:C:111:ASP:OD1	1:C:112:PRO:HD2	2.19	0.42
1:C:131:ASN:HA	1:C:134:ILE:CG1	2.50	0.42
1:C:136:LYS:HG2	1:C:136:LYS:O	2.20	0.42
1:C:224:LYS:O	1:C:224:LYS:HG3	2.18	0.42
1:C:265:SER:HB3	1:C:278:PHE:CE2	2.54	0.42
1:D:57:ILE:CD1	1:D:57:ILE:N	2.82	0.42
1:D:439:LEU:C	1:D:439:LEU:HD12	2.39	0.42
1:E:389:ASN:O	1:E:392:PHE:HB3	2.20	0.42
1:F:87:ALA:CB	1:F:94:LEU:HD11	2.50	0.42
1:F:116:GLU:O	1:F:117:VAL:CB	2.67	0.42
1:F:147:VAL:O	1:F:148:THR:C	2.58	0.42
1:F:151:PHE:CD1	1:F:160:VAL:HG22	2.55	0.42
1:F:178:THR:CG2	1:F:179:VAL:N	2.82	0.42
1:F:238:THR:HG22	1:F:239:ILE:N	2.35	0.42
1:F:295:THR:HG21	1:F:319:GLU:OE2	2.19	0.42
1:F:318:GLU:HG3	4:F:537:HOH:O	2.18	0.42
1:A:79:THR:HG23	1:A:80:PRO:CD	2.47	0.42
1:B:72:VAL:O	1:B:142:VAL:HG13	2.19	0.42
1:B:194:TYR:O	1:B:195:GLY:C	2.56	0.42
1:B:244:ILE:HG22	1:B:246:ILE:HD12	2.01	0.42
1:B:467:ILE:HD12	1:B:467:ILE:N	2.34	0.42
1:C:65:ILE:O	1:C:65:ILE:CG2	2.67	0.42
1:C:235:TYR:HD2	1:C:248:PRO:HA	1.85	0.42
1:C:237:PHE:HB2	1:C:246:ILE:HA	2.02	0.42
1:C:325:LEU:HD23	1:C:335:PHE:HB3	2.02	0.42
1:C:462:TRP:O	1:C:463:HIS:CG	2.73	0.42
1:D:267:VAL:CG2	1:D:300:ARG:HG2	2.50	0.42
1:E:64:ILE:O	1:E:64:ILE:HG22	2.19	0.42
1:F:193:ARG:C	1:F:195:GLY:H	2.23	0.42
1:F:212:GLU:O	1:F:212:GLU:HG2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:LEU:HD23	1:A:223:LEU:HA	1.68	0.42
1:A:264:SER:HB3	1:A:304:ASN:OD1	2.20	0.42
1:A:294:LYS:HZ2	1:A:415:THR:HA	1.82	0.42
1:A:296:LEU:CD2	1:A:472:ILE:HD12	2.49	0.42
1:A:317:TYR:O	1:A:318:GLU:HG3	2.19	0.42
1:A:418:GLN:O	1:A:422:ALA:HB2	2.19	0.42
1:B:68:ASP:O	1:B:70:PRO:HD3	2.19	0.42
1:B:289:ALA:CB	1:B:419:PHE:HB3	2.50	0.42
1:C:38:ILE:HG22	1:C:39:GLY:N	2.33	0.42
1:C:389:ASN:HD21	1:C:428:SER:HA	1.84	0.42
1:D:248:PRO:C	1:D:250:GLY:N	2.67	0.42
1:E:503:SER:O	1:E:504:GLU:C	2.58	0.42
1:F:160:VAL:HG21	1:F:194:TYR:CD2	2.55	0.42
1:A:80:PRO:HB2	1:A:81:GLN:HE21	1.85	0.41
1:B:21:MET:HB2	1:B:38:ILE:CD1	2.50	0.41
1:B:196:VAL:O	1:B:200:VAL:HG23	2.20	0.41
1:B:419:PHE:CD1	1:B:419:PHE:C	2.93	0.41
1:B:423:HIS:O	1:B:424:SER:HB3	2.20	0.41
1:C:27:GLY:O	1:C:30:ASP:HB2	2.20	0.41
1:C:219:THR:HB	1:C:234:GLU:HG2	2.02	0.41
1:C:425:ILE:HB	1:C:426:ASN:ND2	2.35	0.41
1:D:21:MET:HE2	1:D:177:THR:CG2	2.40	0.41
1:D:198:GLU:HB3	1:D:199:PHE:CE2	2.55	0.41
1:E:178:THR:HG23	1:E:179:VAL:N	2.35	0.41
1:E:393:ARG:O	1:E:397:ILE:HG13	2.19	0.41
1:E:419:PHE:O	1:E:420:MET:O	2.38	0.41
1:F:257:ARG:NH2	1:F:405:GLN:O	2.47	0.41
1:A:184:ARG:NH1	1:A:187:GLU:O	2.53	0.41
1:A:436:THR:O	1:A:436:THR:HG22	2.20	0.41
1:A:445:ILE:HG22	1:A:446:ARG:HG3	2.03	0.41
1:A:488:ARG:HA	1:F:493:SER:HB2	2.00	0.41
1:B:192:ALA:O	1:B:194:TYR:N	2.53	0.41
1:B:353:SER:HA	1:C:250:GLY:O	2.20	0.41
1:B:360:LEU:CD1	1:B:364:LYS:HE3	2.50	0.41
1:C:185:ILE:HG23	4:D:529:HOH:O	2.20	0.41
1:C:262:ARG:NE	1:C:279:PHE:CE2	2.88	0.41
1:C:315:PHE:HE1	1:C:375:ILE:HD11	1.85	0.41
1:D:67:PHE:O	1:D:69:GLU:N	2.54	0.41
1:D:270:LEU:HD13	1:D:270:LEU:C	2.39	0.41
1:D:445:ILE:HD12	1:D:486:PHE:CE2	2.55	0.41
1:E:303:GLU:OE2	1:E:333:MET:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:425:ILE:HD11	1:E:456:PHE:CE2	2.55	0.41
1:E:469:GLU:HG3	1:E:470:PHE:N	2.35	0.41
1:F:87:ALA:HB3	1:F:94:LEU:HD11	2.03	0.41
1:F:311:ARG:HD3	1:F:370:PHE:CD2	2.55	0.41
1:F:377:ILE:HB	1:F:412:PHE:CD2	2.55	0.41
1:F:451:ARG:HB3	1:F:470:PHE:CE2	2.55	0.41
1:A:38:ILE:CG2	1:A:39:GLY:N	2.82	0.41
1:A:273:MET:SD	1:A:479:ILE:HG21	2.61	0.41
1:B:56:SER:HB2	1:B:143:SER:CB	2.48	0.41
1:C:52:LYS:N	1:C:207:LEU:HD12	2.33	0.41
1:C:161:ARG:HG3	1:C:200:VAL:HG21	2.02	0.41
1:C:371:LYS:O	1:C:371:LYS:CD	2.68	0.41
1:D:52:LYS:HB2	3:D:903:ATP:O1B	2.21	0.41
1:E:313:ILE:HG13	1:E:372:PRO:CG	2.50	0.41
1:F:61:TYR:CE1	1:F:92:TRP:HB3	2.55	0.41
1:F:67:PHE:O	1:F:68:ASP:HB3	2.20	0.41
1:F:80:PRO:HB3	1:F:105:ILE:HG21	2.01	0.41
1:A:78:GLU:CD	1:B:226:ARG:HD3	2.41	0.41
1:A:395:PHE:CE2	1:A:399:VAL:HG21	2.55	0.41
1:B:106:LEU:HD23	1:B:130:ILE:CD1	2.48	0.41
1:B:194:TYR:O	1:B:196:VAL:N	2.53	0.41
1:B:211:LEU:HD12	1:B:212:GLU:H	1.85	0.41
1:B:311:ARG:NH1	1:B:371:LYS:HE3	2.35	0.41
1:B:396:VAL:O	1:B:399:VAL:N	2.52	0.41
1:C:174:ILE:HG22	1:C:174:ILE:O	2.20	0.41
1:C:269:ARG:CG	1:C:479:ILE:HB	2.47	0.41
1:C:356:LEU:HD11	1:C:387:VAL:HG21	2.02	0.41
1:D:264:SER:HB3	1:D:304:ASN:HD21	1.86	0.41
1:D:392:PHE:CE2	1:D:430:ILE:HD11	2.55	0.41
1:E:318:GLU:OE2	1:F:432:TPO:O1P	2.39	0.41
1:F:88:ARG:O	1:F:91:GLY:N	2.43	0.41
1:F:270:LEU:C	1:F:272:GLU:N	2.73	0.41
1:A:21:MET:O	1:A:22:ARG:C	2.57	0.41
1:A:25:ILE:CD1	1:A:58:GLN:HG2	2.51	0.41
1:A:397:ILE:HD13	1:A:433:ILE:HG21	2.03	0.41
1:B:82:ASP:O	1:B:84:ILE:N	2.54	0.41
1:B:145:ASP:HA	1:B:181:THR:CB	2.51	0.41
1:B:244:ILE:HG22	1:B:246:ILE:CD1	2.50	0.41
1:C:150:VAL:CG1	1:C:151:PHE:H	2.33	0.41
1:C:215:ARG:NH2	1:D:234:GLU:O	2.53	0.41
1:C:289:ALA:HB2	1:C:419:PHE:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:TRP:CH2	3:C:901:ATP:O2A	2.68	0.41
1:C:356:LEU:HD13	1:C:387:VAL:HG21	2.01	0.41
1:C:445:ILE:O	1:C:446:ARG:HB2	2.21	0.41
1:D:102:LYS:HA	1:D:102:LYS:HD3	1.81	0.41
1:E:33:HIS:HD2	1:E:230:HIS:HA	1.86	0.41
1:E:110:PRO:HB2	1:F:165:PHE:CE2	2.54	0.41
1:E:248:PRO:O	1:E:250:GLY:N	2.53	0.41
1:F:218:ARG:HH11	1:F:218:ARG:HG2	1.85	0.41
1:F:237:PHE:CD1	1:F:244:ILE:HG23	2.55	0.41
1:F:334:ASP:OD1	1:F:336:GLU:HB2	2.21	0.41
1:A:317:TYR:O	1:A:318:GLU:CG	2.68	0.41
1:B:27:GLY:O	1:B:31:ILE:HG12	2.20	0.41
1:C:154:TYR:O	1:C:154:TYR:CD1	2.73	0.41
1:C:247:PHE:CZ	1:C:361:GLN:HB2	2.55	0.41
1:D:216:ARG:HH21	1:E:223:LEU:HD21	1.84	0.41
1:D:293:GLY:O	1:D:294:LYS:C	2.58	0.41
1:D:295:THR:HG21	1:D:319:GLU:OE2	2.20	0.41
1:D:356:LEU:HD23	1:D:395:PHE:HB2	2.01	0.41
1:E:126:LEU:HD12	1:E:130:ILE:CD1	2.50	0.41
1:E:303:GLU:O	1:E:305:ALA:N	2.53	0.41
1:E:471:MET:HE2	1:E:478:ASP:HB3	2.02	0.41
1:F:61:TYR:O	1:F:64:ILE:N	2.48	0.41
1:F:88:ARG:O	1:F:89:SER:C	2.59	0.41
1:F:198:GLU:HB2	1:F:199:PHE:CD2	2.56	0.41
1:F:311:ARG:HH11	1:F:370:PHE:C	2.24	0.41
1:F:311:ARG:NH1	1:F:370:PHE:HA	2.35	0.41
1:F:356:LEU:HD23	1:F:395:PHE:HB2	2.03	0.41
1:A:154:TYR:O	1:A:154:TYR:CD1	2.74	0.41
1:A:278:PHE:HD1	1:A:301:PHE:HE1	1.67	0.41
1:B:186:GLU:OE1	1:B:188:TYR:N	2.53	0.41
1:B:306:CYS:SG	1:B:344:LEU:CB	3.02	0.41
1:C:80:PRO:HD2	1:C:81:GLN:HE21	1.85	0.41
1:C:191:ILE:HD12	1:C:191:ILE:H	1.85	0.41
1:C:326:ARG:NH1	1:D:259:SER:O	2.46	0.41
1:D:344:LEU:HD13	1:D:344:LEU:C	2.41	0.41
1:D:485:ASN:OD1	1:D:485:ASN:N	2.54	0.41
1:E:269:ARG:NH2	1:E:468:ARG:NH2	2.65	0.41
1:F:60:LEU:O	1:F:61:TYR:C	2.59	0.41
1:F:151:PHE:O	1:F:153:GLN:N	2.47	0.41
1:F:336:GLU:HB3	1:F:340:ARG:CZ	2.48	0.41
1:F:514:GLU:HB2	1:F:518:GLU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:ARG:HD2	1:A:371:LYS:NZ	2.35	0.41
1:A:445:ILE:HG23	1:A:486:PHE:CE2	2.55	0.41
1:B:79:THR:OG1	1:B:81:GLN:HG2	2.21	0.41
1:B:144:ILE:HD12	1:B:144:ILE:H	1.85	0.41
1:B:280:LYS:NZ	1:B:407:GLU:OE2	2.54	0.41
1:B:284:ILE:O	1:B:411:LEU:HD12	2.20	0.41
1:C:21:MET:SD	1:C:141:ARG:HG2	2.60	0.41
1:C:120:GLY:C	1:C:122:ASP:H	2.24	0.41
1:C:437:ILE:CD1	1:C:457:LYS:HE2	2.51	0.41
1:D:216:ARG:HH21	1:E:223:LEU:CD2	2.34	0.41
1:F:59:PHE:CD2	1:F:179:VAL:HG21	2.56	0.41
1:F:121:PHE:HD2	1:F:121:PHE:HA	1.76	0.41
1:F:170:ARG:HB3	1:F:170:ARG:HH11	1.86	0.41
1:F:170:ARG:CB	1:F:170:ARG:HH11	2.33	0.41
1:F:347:VAL:O	1:F:348:CYS:HB2	2.20	0.41
1:F:395:PHE:CE2	1:F:399:VAL:HG21	2.56	0.41
1:A:86:ASN:HB3	1:B:227:GLY:HA2	2.03	0.41
1:A:319:GLU:O	1:A:320:SER:C	2.60	0.41
1:A:408:ILE:HG22	1:A:409:THR:H	1.86	0.41
1:B:164:LEU:C	1:B:166:ARG:N	2.74	0.41
1:B:261:VAL:HG12	1:B:262:ARG:H	1.86	0.41
1:B:332:GLY:O	1:B:333:MET:HG2	2.21	0.41
1:B:364:LYS:HG2	1:B:402:TYR:CD2	2.56	0.41
1:B:471:MET:HG2	1:B:480:LYS:HZ3	1.85	0.41
1:C:36:LEU:CD2	1:C:42:THR:HG21	2.51	0.41
1:C:81:GLN:H	1:C:81:GLN:CD	2.22	0.41
1:C:237:PHE:CD1	1:C:237:PHE:C	2.94	0.41
1:C:375:ILE:O	1:C:375:ILE:CG2	2.68	0.41
1:C:419:PHE:O	1:C:420:MET:CB	2.68	0.41
1:D:147:VAL:HG23	1:D:148:THR:N	2.36	0.41
1:D:311:ARG:HD3	1:D:370:PHE:CD1	2.55	0.41
1:D:425:ILE:H	1:D:425:ILE:CD1	2.31	0.41
1:D:486:PHE:HB2	1:D:489:ILE:HD11	1.99	0.41
1:E:194:TYR:CD1	1:E:194:TYR:N	2.89	0.41
1:E:354:ALA:HB1	1:E:358:ASP:HB2	2.02	0.41
1:F:111:ASP:OD2	1:F:113:GLU:HB2	2.21	0.41
1:F:265:SER:HA	1:F:301:PHE:CD1	2.51	0.41
1:F:306:CYS:SG	1:F:344:LEU:HB2	2.60	0.41
1:F:483:PHE:HD1	1:F:483:PHE:H	1.68	0.41
1:F:509:VAL:CG1	1:F:510:ARG:N	2.84	0.41
1:A:106:LEU:HD11	1:A:129:ARG:NE	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:SER:C	1:A:148:THR:N	2.74	0.41
1:A:251:ALA:O	1:A:252:MET:C	2.58	0.41
1:C:206:ILE:HG22	1:C:208:ARG:HG3	2.02	0.41
1:C:296:LEU:HD13	1:C:331:TRP:CD2	2.56	0.41
1:C:451:ARG:HD2	1:C:472:ILE:HG12	2.03	0.41
1:D:349:ALA:N	1:E:254:LEU:HD23	2.36	0.41
1:D:483:PHE:N	1:D:483:PHE:CD1	2.89	0.41
1:F:197:GLU:O	1:F:199:PHE:N	2.54	0.41
1:F:311:ARG:HA	1:F:343:LEU:O	2.19	0.41
1:A:64:ILE:HG21	1:A:97:LEU:HD22	2.02	0.40
1:A:156:ALA:O	1:A:157:SER:C	2.59	0.40
1:A:295:THR:O	1:A:298:VAL:HB	2.22	0.40
1:B:279:PHE:C	1:B:281:ASP:H	2.25	0.40
1:C:37:PRO:HD2	1:C:203:ASN:ND2	2.36	0.40
1:C:392:PHE:O	1:C:396:VAL:HG23	2.21	0.40
1:D:89:SER:HB2	1:E:227:GLY:O	2.21	0.40
1:D:347:VAL:HG12	1:D:348:CYS:H	1.83	0.40
1:E:18:ILE:HD11	1:E:227:GLY:CA	2.49	0.40
1:E:273:MET:CE	1:E:468:ARG:HD2	2.52	0.40
1:E:467:ILE:HG21	1:E:489:ILE:HG21	2.04	0.40
1:F:162:ARG:CZ	1:F:162:ARG:CB	2.99	0.40
1:F:418:GLN:NE2	1:F:421:GLY:O	2.54	0.40
1:A:213:GLY:O	1:A:214:GLU:CB	2.56	0.40
1:A:401:GLY:O	1:A:404:LYS:N	2.54	0.40
1:B:35:GLY:O	1:B:36:LEU:C	2.59	0.40
1:B:118:VAL:HG12	1:B:121:PHE:HB2	2.02	0.40
1:B:119:GLY:C	1:B:121:PHE:N	2.73	0.40
1:B:334:ASP:OD1	1:B:336:GLU:CB	2.58	0.40
1:B:387:VAL:HG12	1:B:388:SER:N	2.36	0.40
1:C:123:LEU:HD22	1:C:167:LEU:HB2	2.04	0.40
1:C:278:PHE:CD1	1:C:284:ILE:HG13	2.56	0.40
1:C:356:LEU:CD1	1:C:356:LEU:H	2.34	0.40
1:D:54:LEU:HD21	1:D:243:GLY:HA2	2.01	0.40
1:E:42:THR:HA	1:E:203:ASN:HD22	1.85	0.40
1:E:302:VAL:HG12	1:E:303:GLU:N	2.36	0.40
1:E:315:PHE:HE1	1:E:375:ILE:HG13	1.86	0.40
1:E:443:VAL:CG1	1:E:494:PRO:HG2	2.51	0.40
1:F:488:ARG:HB3	1:F:491:SER:OG	2.21	0.40
1:A:169:ALA:O	1:A:173:GLN:HG3	2.21	0.40
1:B:340:ARG:O	1:B:342:ASN:N	2.48	0.40
1:B:483:PHE:HB2	1:B:489:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:GLY:CA	1:C:141:ARG:CZ	3.00	0.40
1:C:199:PHE:O	1:C:226:ARG:NH2	2.54	0.40
1:E:32:SER:O	1:E:33:HIS:C	2.58	0.40
1:E:38:ILE:HG22	1:E:39:GLY:N	2.37	0.40
1:E:79:THR:HA	1:E:80:PRO:HD3	1.88	0.40
1:E:118:VAL:O	1:E:118:VAL:HG12	2.22	0.40
1:E:267:VAL:CG2	1:E:477:PRO:CG	2.99	0.40
1:F:344:LEU:HD13	1:F:344:LEU:C	2.41	0.40
1:F:365:SER:HA	1:F:368:ASN:HD22	1.86	0.40
1:A:43:LEU:HB3	1:A:204:VAL:HG22	2.03	0.40
1:B:437:ILE:HG21	1:B:456:PHE:HD2	1.85	0.40
1:D:473:SER:HA	3:D:901:ATP:C2	2.56	0.40
1:E:24:MET:HB2	1:E:62:ASN:HB3	2.03	0.40
1:E:306:CYS:HB2	1:E:338:MET:SD	2.60	0.40
1:F:36:LEU:N	1:F:36:LEU:HD23	2.36	0.40
1:F:45:SER:CB	1:F:182:THR:HB	2.51	0.40
1:F:104:PHE:CD1	1:F:137:TYR:CZ	3.09	0.40
1:F:153:GLN:O	1:F:154:TYR:CB	2.69	0.40
1:A:321:ARG:HA	1:A:324:LEU:HB2	2.04	0.40
1:B:56:SER:H	1:B:56:SER:HG	1.67	0.40
1:B:287:THR:CG2	1:B:288:GLY:N	2.84	0.40
1:B:392:PHE:O	1:B:393:ARG:C	2.58	0.40
1:D:208:ARG:NH1	1:D:208:ARG:CG	2.85	0.40
1:D:248:PRO:HB2	1:D:251:ALA:HB3	2.03	0.40
1:D:286:ALA:O	1:D:294:LYS:HG2	2.22	0.40
1:D:359:HIS:O	1:D:360:LEU:C	2.59	0.40
1:D:495:THR:O	1:D:495:THR:HG22	2.20	0.40
1:E:186:GLU:HB3	1:E:189:GLY:HA3	2.03	0.40
1:E:470:PHE:CD1	1:E:470:PHE:C	2.94	0.40
1:F:197:GLU:C	1:F:199:PHE:N	2.75	0.40
1:F:299:SER:C	1:F:301:PHE:N	2.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	502/519 (97%)	369 (74%)	97 (19%)	36 (7%)	1	7
1	B	487/519 (94%)	351 (72%)	94 (19%)	42 (9%)	1	4
1	C	484/519 (93%)	361 (75%)	90 (19%)	33 (7%)	1	9
1	D	481/519 (93%)	372 (77%)	77 (16%)	32 (7%)	1	9
1	E	488/519 (94%)	369 (76%)	93 (19%)	26 (5%)	2	15
1	F	502/519 (97%)	363 (72%)	85 (17%)	54 (11%)	0	2
All	All	2944/3114 (94%)	2185 (74%)	536 (18%)	223 (8%)	1	7

All (223) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ALA
1	A	154	TYR
1	A	463	HIS
1	B	17	ALA
1	B	48	SER
1	B	154	TYR
1	B	251	ALA
1	B	252	MET
1	B	333	MET
1	B	342	ASN
1	B	417	ASP
1	B	461	SER
1	C	52	LYS
1	C	117	VAL
1	C	154	TYR
1	C	189	GLY
1	C	193	ARG
1	C	294	LYS
1	C	414	ASN
1	C	429	HIS
1	C	466	ALA
1	D	122	ASP
1	D	249	LEU
1	D	349	ALA
1	D	356	LEU
1	D	463	HIS
1	D	474	ASP

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Mol	Chain	Res	Type
1	E	101	GLY
1	E	117	VAL
1	E	154	TYR
1	E	387	VAL
1	E	425	ILE
1	E	463	HIS
1	E	484	ARG
1	E	504	GLU
1	F	52	LYS
1	F	118	VAL
1	F	154	TYR
1	F	157	SER
1	F	249	LEU
1	F	263	VAL
1	F	333	MET
1	F	417	ASP
1	F	423	HIS
1	F	433	ILE
1	F	463	HIS
1	F	468	ARG
1	F	504	GLU
1	F	507	ARG
1	F	509	VAL
1	A	26	GLU
1	A	65	ILE
1	A	100	GLU
1	A	249	LEU
1	A	289	ALA
1	A	309	LYS
1	A	318	GLU
1	A	355	GLY
1	A	417	ASP
1	A	446	ARG
1	A	500	ASP
1	A	503	SER
1	A	510	ARG
1	B	64	ILE
1	B	100	GLU
1	B	119	GLY
1	B	193	ARG
1	B	212	GLU
1	B	294	LYS

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Mol	Chain	Res	Type
1	B	311	ARG
1	B	347	VAL
1	B	372	PRO
1	B	391	ALA
1	B	422	ALA
1	B	494	PRO
1	C	122	ASP
1	C	174	ILE
1	C	249	LEU
1	C	338	MET
1	C	341	GLN
1	C	405	GLN
1	C	417	ASP
1	C	462	TRP
1	C	488	ARG
1	D	26	GLU
1	D	87	ALA
1	D	123	LEU
1	D	214	GLU
1	D	320	SER
1	D	326	ARG
1	D	333	MET
1	D	420	MET
1	D	422	ALA
1	D	423	HIS
1	D	484	ARG
1	D	485	ASN
1	E	113	GLU
1	E	211	LEU
1	E	333	MET
1	E	379	SER
1	E	385	ARG
1	E	405	GLN
1	E	420	MET
1	F	149	SER
1	F	194	TYR
1	F	211	LEU
1	F	271	ASP
1	F	277	GLY
1	F	369	ASP
1	F	388	SER
1	F	407	GLU

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Mol	Chain	Res	Type
1	F	420	MET
1	F	517	PRO
1	A	198	GLU
1	A	214	GLU
1	A	349	ALA
1	A	420	MET
1	A	511	GLY
1	B	76	PHE
1	B	273	MET
1	B	349	ALA
1	B	389	ASN
1	B	429	HIS
1	B	463	HIS
1	C	107	ASP
1	C	289	ALA
1	C	349	ALA
1	C	368	ASN
1	D	154	TYR
1	D	209	ASN
1	D	357	GLU
1	E	352	GLU
1	E	494	PRO
1	F	53	THR
1	F	117	VAL
1	F	198	GLU
1	F	354	ALA
1	F	483	PHE
1	F	505	LEU
1	F	506	SER
1	F	515	LYS
1	A	33	HIS
1	A	211	LEU
1	A	429	HIS
1	A	454	ASN
1	A	490	ILE
1	A	499	VAL
1	A	502	LYS
1	B	52	LYS
1	B	112	PRO
1	B	373	ALA
1	C	112	PRO
1	C	123	LEU

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Mol	Chain	Res	Type
1	C	454	ASN
1	D	113	GLU
1	D	161	ARG
1	D	289	ALA
1	D	327	ASN
1	D	354	ALA
1	E	52	LYS
1	E	136	LYS
1	E	326	ARG
1	E	348	CYS
1	F	152	GLN
1	F	195	GLY
1	F	257	ARG
1	F	396	VAL
1	F	408	ILE
1	F	429	HIS
1	F	510	ARG
1	A	64	ILE
1	A	117	VAL
1	A	477	PRO
1	A	501	GLU
1	B	87	ALA
1	B	308	ASN
1	B	384	ALA
1	C	106	LEU
1	C	348	CYS
1	C	463	HIS
1	E	304	ASN
1	E	384	ALA
1	F	160	VAL
1	F	161	ARG
1	F	379	SER
1	A	354	ALA
1	A	456	PHE
1	B	341	GLN
1	B	407	GLU
1	B	420	MET
1	B	424	SER
1	C	127	ILE
1	C	379	SER
1	D	254	LEU
1	D	457	LYS

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Mol	Chain	Res	Type
1	F	120	GLY
1	F	193	ARG
1	F	253	ARG
1	F	386	GLY
1	F	427	ASP
1	F	514	GLU
1	A	109	SER
1	B	101	GLY
1	B	117	VAL
1	B	298	VAL
1	D	65	ILE
1	D	268	VAL
1	D	371	LYS
1	F	112	PRO
1	A	494	PRO
1	B	386	GLY
1	C	44	VAL
1	C	261	VAL
1	B	397	ILE
1	C	477	PRO
1	D	118	VAL
1	E	18	ILE
1	E	168	VAL
1	F	65	ILE
1	F	268	VAL
1	F	467	ILE
1	F	508	ILE
1	E	80	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	430/442 (97%)	387 (90%)	43 (10%)	7	30
1	B	417/442 (94%)	375 (90%)	42 (10%)	7	29
1	C	414/442 (94%)	360 (87%)	54 (13%)	4	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	411/442 (93%)	362 (88%)	49 (12%)	5	22
1	E	418/442 (95%)	380 (91%)	38 (9%)	9	34
1	F	430/442 (97%)	388 (90%)	42 (10%)	8	31
All	All	2520/2652 (95%)	2252 (89%)	268 (11%)	6	27

All (268) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	31	ILE
1	A	69	GLU
1	A	75	THR
1	A	90	PHE
1	A	92	TRP
1	A	121	PHE
1	A	123	LEU
1	A	154	TYR
1	A	168	VAL
1	A	185	ILE
1	A	187	GLU
1	A	205	VAL
1	A	212	GLU
1	A	215	ARG
1	A	222	ILE
1	A	223	LEU
1	A	228	THR
1	A	252	MET
1	A	263	VAL
1	A	264	SER
1	A	270	LEU
1	A	290	THR
1	A	303	GLU
1	A	306	CYS
1	A	335	PHE
1	A	337	GLU
1	A	342	ASN
1	A	360	LEU
1	A	371	LYS
1	A	389	ASN
1	A	409	THR
1	A	425	ILE

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Mol	Chain	Res	Type
1	A	426	ASN
1	A	436	THR
1	A	442	TYR
1	A	451	ARG
1	A	456	PHE
1	A	457	LYS
1	A	462	TRP
1	A	471	MET
1	A	485	ASN
1	A	508	ILE
1	B	30	ASP
1	B	42	THR
1	B	67	PHE
1	B	81	GLN
1	B	99	ASP
1	B	103	LEU
1	B	111	ASP
1	B	123	LEU
1	B	140	ARG
1	B	147	VAL
1	B	150	VAL
1	B	154	TYR
1	B	170	ARG
1	B	178	THR
1	B	182	THR
1	B	183	GLU
1	B	185	ILE
1	B	186	GLU
1	B	209	ASN
1	B	212	GLU
1	B	215	ARG
1	B	218	ARG
1	B	223	LEU
1	B	237	PHE
1	B	260	ASN
1	B	263	VAL
1	B	284	ILE
1	B	292	THR
1	B	299	SER
1	B	329	TYR
1	B	336	GLU
1	B	368	ASN

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Mol	Chain	Res	Type
1	B	371	LYS
1	B	427	ASP
1	B	433	ILE
1	B	434	THR
1	B	451	ARG
1	B	454	ASN
1	B	463	HIS
1	B	471	MET
1	B	474	ASP
1	B	502	LYS
1	C	50	THR
1	C	57	ILE
1	C	68	ASP
1	C	75	THR
1	C	81	GLN
1	C	97	LEU
1	C	99	ASP
1	C	121	PHE
1	C	122	ASP
1	C	140	ARG
1	C	148	THR
1	C	151	PHE
1	C	178	THR
1	C	184	ARG
1	C	186	GLU
1	C	204	VAL
1	C	209	ASN
1	C	211	LEU
1	C	223	LEU
1	C	240	THR
1	C	245	ASN
1	C	260	ASN
1	C	263	VAL
1	C	270	LEU
1	C	299	SER
1	C	303	GLU
1	C	323	GLN
1	C	324	LEU
1	C	329	TYR
1	C	333	MET
1	C	336	GLU
1	C	338	MET

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Mol	Chain	Res	Type
1	C	340	ARG
1	C	344	LEU
1	C	369	ASP
1	C	371	LYS
1	C	379	SER
1	C	394	GLN
1	C	400	THR
1	C	405	GLN
1	C	409	THR
1	C	418	GLN
1	C	426	ASN
1	C	427	ASP
1	C	433	ILE
1	C	434	THR
1	C	453	ILE
1	C	458	MET
1	C	461	SER
1	C	463	HIS
1	C	483	PHE
1	C	484	ARG
1	C	498	THR
1	C	501	GLU
1	D	25	ILE
1	D	26	GLU
1	D	30	ASP
1	D	79	THR
1	D	81	GLN
1	D	103	LEU
1	D	106	LEU
1	D	122	ASP
1	D	135	GLN
1	D	140	ARG
1	D	143	SER
1	D	150	VAL
1	D	151	PHE
1	D	152	GLN
1	D	154	TYR
1	D	158	SER
1	D	177	THR
1	D	178	THR
1	D	181	THR
1	D	186	GLU

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Mol	Chain	Res	Type
1	D	198	GLU
1	D	201	SER
1	D	209	ASN
1	D	211	LEU
1	D	212	GLU
1	D	223	LEU
1	D	228	THR
1	D	230	HIS
1	D	231	MET
1	D	245	ASN
1	D	246	ILE
1	D	256	GLN
1	D	287	THR
1	D	303	GLU
1	D	334	ASP
1	D	360	LEU
1	D	366	GLU
1	D	369	ASP
1	D	371	LYS
1	D	399	VAL
1	D	412	PHE
1	D	423	HIS
1	D	434	THR
1	D	451	ARG
1	D	463	HIS
1	D	469	GLU
1	D	470	PHE
1	D	471	MET
1	D	490	ILE
1	E	26	GLU
1	E	32	SER
1	E	79	THR
1	E	100	GLU
1	E	111	ASP
1	E	121	PHE
1	E	132	TYR
1	E	135	GLN
1	E	140	ARG
1	E	151	PHE
1	E	154	TYR
1	E	182	THR
1	E	185	ILE

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Mol	Chain	Res	Type
1	E	186	GLU
1	E	193	ARG
1	E	201	SER
1	E	202	ASP
1	E	203	ASN
1	E	209	ASN
1	E	246	ILE
1	E	255	THR
1	E	256	GLN
1	E	268	VAL
1	E	292	THR
1	E	302	VAL
1	E	330	SER
1	E	336	GLU
1	E	357	GLU
1	E	371	LYS
1	E	375	ILE
1	E	394	GLN
1	E	406	GLU
1	E	426	ASN
1	E	451	ARG
1	E	462	TRP
1	E	465	LYS
1	E	471	MET
1	E	501	GLU
1	F	30	ASP
1	F	33	HIS
1	F	43	LEU
1	F	45	SER
1	F	48	SER
1	F	56	SER
1	F	106	LEU
1	F	121	PHE
1	F	140	ARG
1	F	143	SER
1	F	147	VAL
1	F	154	TYR
1	F	170	ARG
1	F	183	GLU
1	F	184	ARG
1	F	186	GLU
1	F	197	GLU

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Mol	Chain	Res	Type
1	F	198	GLU
1	F	203	ASN
1	F	209	ASN
1	F	211	LEU
1	F	212	GLU
1	F	218	ARG
1	F	220	LEU
1	F	223	LEU
1	F	245	ASN
1	F	263	VAL
1	F	284	ILE
1	F	285	LEU
1	F	344	LEU
1	F	366	GLU
1	F	371	LYS
1	F	406	GLU
1	F	426	ASN
1	F	430	ILE
1	F	451	ARG
1	F	458	MET
1	F	462	TRP
1	F	496	ARG
1	F	497	ILE
1	F	504	GLU
1	F	514	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	62	ASN
1	A	81	GLN
1	A	135	GLN
1	A	209	ASN
1	A	304	ASN
1	A	368	ASN
1	A	389	ASN
1	A	423	HIS
1	B	58	GLN
1	B	62	ASN
1	B	81	GLN
1	B	152	GLN

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Mol	Chain	Res	Type
1	B	209	ASN
1	B	256	GLN
1	B	260	ASN
1	B	361	GLN
1	B	389	ASN
1	B	426	ASN
1	B	441	GLN
1	C	58	GLN
1	C	81	GLN
1	C	135	GLN
1	C	152	GLN
1	C	203	ASN
1	C	209	ASN
1	C	245	ASN
1	C	260	ASN
1	C	389	ASN
1	C	414	ASN
1	C	418	GLN
1	C	426	ASN
1	C	429	HIS
1	D	33	HIS
1	D	209	ASN
1	D	245	ASN
1	D	304	ASN
1	D	308	ASN
1	D	361	GLN
1	D	368	ASN
1	D	414	ASN
1	E	15	HIS
1	E	33	HIS
1	E	62	ASN
1	E	209	ASN
1	E	304	ASN
1	E	323	GLN
1	E	361	GLN
1	E	368	ASN
1	E	390	ASN
1	E	414	ASN
1	E	426	ASN
1	E	485	ASN
1	F	33	HIS
1	F	81	GLN

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Mol	Chain	Res	Type
1	F	153	GLN
1	F	203	ASN
1	F	209	ASN
1	F	245	ASN
1	F	304	ASN
1	F	342	ASN
1	F	368	ASN
1	F	389	ASN
1	F	394	GLN
1	F	418	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPO	D	432	1	8,10,11	0.98	0	10,14,16	1.42	2 (20%)
1	SEP	E	431	1	8,9,10	1.52	1 (12%)	8,12,14	1.31	1 (12%)
1	TPO	A	432	1	8,10,11	1.00	0	10,14,16	1.62	2 (20%)
1	SEP	B	431	1	8,9,10	1.57	1 (12%)	8,12,14	1.03	0
1	TPO	C	432	1	8,10,11	1.07	0	10,14,16	1.29	1 (10%)
1	TPO	F	432	1	8,10,11	1.05	0	10,14,16	1.66	3 (30%)
1	SEP	C	431	1	8,9,10	1.64	1 (12%)	8,12,14	4.21	2 (25%)
1	SEP	F	431	1	8,9,10	1.52	1 (12%)	8,12,14	1.40	1 (12%)
1	SEP	D	431	1	8,9,10	1.52	1 (12%)	8,12,14	0.86	0
1	TPO	E	432	1	8,10,11	0.96	0	10,14,16	1.57	2 (20%)
1	SEP	A	431	1	8,9,10	1.52	1 (12%)	8,12,14	0.94	0

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	1.06	0	10,14,16	1.57	2 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	D	432	1	-	4/9/11/13	-
1	SEP	E	431	1	-	1/5/8/10	-
1	TPO	A	432	1	-	3/9/11/13	-
1	SEP	B	431	1	-	0/5/8/10	-
1	TPO	C	432	1	-	5/9/11/13	-
1	TPO	F	432	1	-	2/9/11/13	-
1	SEP	C	431	1	-	1/5/8/10	-
1	SEP	F	431	1	-	0/5/8/10	-
1	SEP	D	431	1	-	1/5/8/10	-
1	TPO	E	432	1	-	1/9/11/13	-
1	SEP	A	431	1	-	0/5/8/10	-
1	TPO	B	432	1	-	4/9/11/13	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	431	SEP	P-O1P	3.46	1.61	1.50
1	B	431	SEP	P-O1P	3.42	1.61	1.50
1	D	431	SEP	P-O1P	3.33	1.61	1.50
1	E	431	SEP	P-O1P	3.32	1.61	1.50
1	F	431	SEP	P-O1P	3.30	1.61	1.50
1	A	431	SEP	P-O1P	3.26	1.61	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	431	SEP	OG-CB-CA	10.13	118.01	108.14
1	C	431	SEP	P-OG-CB	-5.77	102.40	118.30
1	A	432	TPO	P-OG1-CB	-4.04	111.01	123.21
1	E	432	TPO	P-OG1-CB	-3.91	111.39	123.21
1	F	432	TPO	P-OG1-CB	-3.87	111.52	123.21
1	B	432	TPO	P-OG1-CB	-3.36	113.06	123.21
1	F	431	SEP	P-OG-CB	-3.36	109.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	431	SEP	P-OG-CB	-2.95	110.16	118.30
1	D	432	TPO	P-OG1-CB	-2.92	114.38	123.21
1	B	432	TPO	CG2-CB-CA	-2.73	107.79	113.16
1	C	432	TPO	P-OG1-CB	-2.67	115.13	123.21
1	D	432	TPO	CG2-CB-CA	-2.60	108.03	113.16
1	F	432	TPO	CG2-CB-CA	-2.53	108.16	113.16
1	A	432	TPO	CG2-CB-CA	-2.48	108.28	113.16
1	E	432	TPO	CG2-CB-CA	-2.42	108.40	113.16
1	F	432	TPO	O-C-CA	-2.08	119.33	124.78

There are no chirality outliers.

All (22) torsion outliers are listed below:

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

There are no ring outliers.

9 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	432	TPO	1	0
1	E	431	SEP	2	0
1	A	432	TPO	1	0
1	F	432	TPO	13	0
1	C	431	SEP	1	0
1	D	431	SEP	6	0
1	E	432	TPO	2	0
1	A	431	SEP	3	0
1	B	432	TPO	3	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 20 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	E	903	2	26,33,33	1.26	4 (15%)	31,52,52	1.91	9 (29%)
3	ATP	D	903	2	26,33,33	1.31	2 (7%)	31,52,52	1.82	6 (19%)
3	ATP	A	901	2	26,33,33	1.33	4 (15%)	31,52,52	1.79	7 (22%)
3	ATP	A	903	2	26,33,33	1.35	4 (15%)	31,52,52	1.74	6 (19%)
3	ATP	B	903	2	26,33,33	1.35	4 (15%)	31,52,52	1.71	4 (12%)
3	ATP	B	901	2	26,33,33	1.16	2 (7%)	31,52,52	1.84	5 (16%)
3	ATP	F	903	2	26,33,33	1.21	1 (3%)	31,52,52	1.87	7 (22%)
3	ATP	C	901	2	26,33,33	1.32	4 (15%)	31,52,52	1.72	5 (16%)
3	ATP	C	903	2	26,33,33	1.24	3 (11%)	31,52,52	1.83	5 (16%)
3	ATP	F	901	2	26,33,33	1.32	3 (11%)	31,52,52	1.81	7 (22%)
3	ATP	D	901	2	26,33,33	1.29	2 (7%)	31,52,52	1.75	5 (16%)
3	ATP	E	901	2	26,33,33	1.25	2 (7%)	31,52,52	1.76	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
3	ATP	E	903	2	-	7/18/38/38	0/3/3/3
3	ATP	D	903	2	-	7/18/38/38	0/3/3/3
3	ATP	A	901	2	-	7/18/38/38	0/3/3/3
3	ATP	A	903	2	-	8/18/38/38	0/3/3/3
3	ATP	B	903	2	-	9/18/38/38	0/3/3/3
3	ATP	B	901	2	-	8/18/38/38	0/3/3/3
3	ATP	F	903	2	-	7/18/38/38	0/3/3/3
3	ATP	C	901	2	-	5/18/38/38	0/3/3/3
3	ATP	C	903	2	-	9/18/38/38	0/3/3/3
3	ATP	F	901	2	-	7/18/38/38	0/3/3/3
3	ATP	D	901	2	-	7/18/38/38	0/3/3/3
3	ATP	E	901	2	-	7/18/38/38	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	903	ATP	C2-N3	4.29	1.39	1.32
3	F	901	ATP	C2-N3	4.26	1.39	1.32
3	A	903	ATP	C2-N3	4.23	1.38	1.32
3	E	901	ATP	C2-N3	4.14	1.38	1.32
3	B	903	ATP	C2-N3	4.06	1.38	1.32
3	A	901	ATP	C2-N3	3.98	1.38	1.32
3	F	903	ATP	C2-N3	3.87	1.38	1.32
3	C	903	ATP	C2-N3	3.82	1.38	1.32
3	D	901	ATP	C2-N3	3.82	1.38	1.32
3	B	901	ATP	C2-N3	3.58	1.37	1.32
3	E	903	ATP	C2-N3	3.46	1.37	1.32
3	C	901	ATP	C2-N3	3.39	1.37	1.32
3	F	901	ATP	O4'-C1'	2.60	1.44	1.41
3	C	903	ATP	C2'-C1'	-2.56	1.49	1.53
3	C	901	ATP	C2'-C1'	-2.53	1.49	1.53
3	B	903	ATP	C2'-C1'	-2.52	1.49	1.53
3	A	903	ATP	O4'-C1'	2.47	1.44	1.41
3	B	903	ATP	C2-N1	2.45	1.38	1.33
3	E	903	ATP	O4'-C4'	-2.37	1.39	1.45
3	E	903	ATP	C2-N1	2.34	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	901	ATP	C2'-N1	2.30	1.38	1.33
3	D	903	ATP	C2'-C1'	-2.30	1.50	1.53
3	B	901	ATP	O4'-C1'	2.26	1.44	1.41
3	A	901	ATP	C2'-C1'	-2.24	1.50	1.53
3	F	901	ATP	C2-N1	2.23	1.38	1.33
3	D	901	ATP	C2-N1	2.22	1.38	1.33
3	A	903	ATP	C2-N1	2.21	1.38	1.33
3	B	903	ATP	O4'-C1'	2.20	1.44	1.41
3	A	901	ATP	O4'-C1'	2.19	1.44	1.41
3	A	901	ATP	C2-N1	2.18	1.38	1.33
3	C	901	ATP	O4'-C4'	-2.16	1.40	1.45
3	E	903	ATP	C2'-C1'	-2.12	1.50	1.53
3	C	903	ATP	O4'-C4'	-2.07	1.40	1.45
3	C	901	ATP	C2-N1	2.03	1.37	1.33
3	A	903	ATP	C2'-C1'	-2.00	1.50	1.53

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	903	ATP	N3-C2-N1	-6.14	119.09	128.68
3	D	901	ATP	N3-C2-N1	-5.71	119.75	128.68
3	C	901	ATP	N3-C2-N1	-5.59	119.95	128.68
3	A	903	ATP	N3-C2-N1	-5.55	120.00	128.68
3	B	901	ATP	N3-C2-N1	-5.53	120.03	128.68
3	C	903	ATP	N3-C2-N1	-5.53	120.03	128.68
3	E	901	ATP	N3-C2-N1	-5.49	120.09	128.68
3	F	901	ATP	N3-C2-N1	-5.48	120.11	128.68
3	A	901	ATP	N3-C2-N1	-5.46	120.14	128.68
3	B	903	ATP	N3-C2-N1	-5.44	120.18	128.68
3	E	903	ATP	N3-C2-N1	-5.42	120.21	128.68
3	F	903	ATP	N3-C2-N1	-5.41	120.23	128.68
3	B	901	ATP	C5-C6-N6	4.39	127.03	120.35
3	E	903	ATP	C5-C6-N6	4.18	126.70	120.35
3	C	903	ATP	C5-C6-N6	4.18	126.70	120.35
3	B	901	ATP	C4-C5-N7	-4.17	105.05	109.40
3	F	903	ATP	C5-C6-N6	4.12	126.61	120.35
3	B	903	ATP	C4-C5-N7	-4.11	105.11	109.40
3	E	901	ATP	C4-C5-N7	-4.10	105.13	109.40
3	A	903	ATP	C4-C5-N7	-4.10	105.13	109.40
3	A	901	ATP	C4-C5-N7	-4.10	105.13	109.40
3	C	903	ATP	C4-C5-N7	-4.08	105.15	109.40
3	F	901	ATP	C4-C5-N7	-4.07	105.16	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	903	ATP	C4-C5-N7	-4.07	105.16	109.40
3	D	901	ATP	C4-C5-N7	-4.01	105.22	109.40
3	A	901	ATP	C5-C6-N6	4.00	126.43	120.35
3	B	903	ATP	C5-C6-N6	4.00	126.43	120.35
3	F	903	ATP	C4-C5-N7	-4.00	105.23	109.40
3	E	901	ATP	C5-C6-N6	3.95	126.36	120.35
3	D	903	ATP	C4-C5-N7	-3.88	105.36	109.40
3	F	901	ATP	C5-C6-N6	3.87	126.23	120.35
3	D	901	ATP	C5-C6-N6	3.77	126.09	120.35
3	C	901	ATP	C5-C6-N6	3.67	125.93	120.35
3	D	903	ATP	C5-C6-N6	3.67	125.93	120.35
3	C	901	ATP	C4-C5-N7	-3.58	105.67	109.40
3	A	903	ATP	C5-C6-N6	3.45	125.60	120.35
3	F	903	ATP	PB-O3B-PG	-3.36	121.31	132.83
3	E	903	ATP	PB-O3B-PG	-3.09	122.23	132.83
3	C	903	ATP	C3'-C2'-C1'	2.98	105.47	100.98
3	C	901	ATP	C3'-C2'-C1'	2.67	105.00	100.98
3	D	903	ATP	C3'-C2'-C1'	2.65	104.97	100.98
3	F	903	ATP	O2G-PG-O3B	2.56	113.21	104.64
3	F	903	ATP	N6-C6-N1	-2.50	113.39	118.57
3	A	903	ATP	O2G-PG-O3B	2.49	113.00	104.64
3	F	901	ATP	C3'-C2'-C1'	2.49	104.73	100.98
3	C	903	ATP	N6-C6-N1	-2.37	113.65	118.57
3	E	903	ATP	C3'-C2'-C1'	2.37	104.55	100.98
3	B	901	ATP	N6-C6-N1	-2.36	113.68	118.57
3	A	903	ATP	PB-O3B-PG	-2.34	124.80	132.83
3	E	903	ATP	O2'-C2'-C3'	2.33	119.35	111.82
3	A	901	ATP	PB-O3B-PG	-2.33	124.84	132.83
3	B	901	ATP	C3'-C2'-C1'	2.32	104.47	100.98
3	E	903	ATP	N6-C6-N1	-2.32	113.77	118.57
3	A	901	ATP	C3'-C2'-C1'	2.24	104.36	100.98
3	A	903	ATP	O2'-C2'-C3'	2.24	119.07	111.82
3	D	903	ATP	O2G-PG-O3B	2.24	112.13	104.64
3	E	903	ATP	O2G-PG-O3B	2.19	112.00	104.64
3	F	903	ATP	C3'-C2'-C1'	2.19	104.27	100.98
3	F	901	ATP	N6-C6-N1	-2.16	114.08	118.57
3	D	901	ATP	N6-C6-N1	-2.13	114.14	118.57
3	A	901	ATP	O2G-PG-O3B	2.13	111.77	104.64
3	D	903	ATP	N6-C6-N1	-2.12	114.17	118.57
3	E	901	ATP	N6-C6-N1	-2.12	114.18	118.57
3	F	901	ATP	O2'-C2'-C3'	2.11	118.65	111.82
3	B	903	ATP	O2'-C2'-C3'	2.10	118.60	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	ATP	N6-C6-N1	-2.08	114.25	118.57
3	F	901	ATP	PB-O3B-PG	-2.07	125.71	132.83
3	E	901	ATP	O2'-C2'-C3'	2.06	118.49	111.82
3	E	901	ATP	C3'-C2'-C1'	2.05	104.06	100.98
3	E	903	ATP	O4'-C1'-C2'	2.03	109.90	106.93
3	C	901	ATP	C2'-C3'-C4'	2.03	106.59	102.64
3	D	901	ATP	O2'-C2'-C3'	2.00	118.30	111.82

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	ATP	PB-O3A-PA-O5'
3	A	901	ATP	C5'-O5'-PA-O1A
3	A	901	ATP	O4'-C4'-C5'-O5'
3	A	901	ATP	C3'-C4'-C5'-O5'
3	A	903	ATP	C5'-O5'-PA-O1A
3	A	903	ATP	C3'-C4'-C5'-O5'
3	B	901	ATP	PB-O3B-PG-O3G
3	B	901	ATP	C5'-O5'-PA-O1A
3	B	901	ATP	C5'-O5'-PA-O3A
3	B	901	ATP	O4'-C4'-C5'-O5'
3	B	901	ATP	C3'-C4'-C5'-O5'
3	B	903	ATP	PB-O3B-PG-O3G
3	B	903	ATP	O4'-C4'-C5'-O5'
3	B	903	ATP	C3'-C4'-C5'-O5'
3	C	901	ATP	C3'-C4'-C5'-O5'
3	C	903	ATP	PB-O3B-PG-O3G
3	C	903	ATP	C3'-C4'-C5'-O5'
3	D	901	ATP	C5'-O5'-PA-O3A
3	D	901	ATP	C3'-C4'-C5'-O5'
3	D	903	ATP	PB-O3B-PG-O2G
3	D	903	ATP	PB-O3B-PG-O3G
3	E	901	ATP	C5'-O5'-PA-O1A
3	E	903	ATP	O4'-C4'-C5'-O5'
3	E	903	ATP	C3'-C4'-C5'-O5'
3	F	901	ATP	PB-O3A-PA-O5'
3	F	901	ATP	C5'-O5'-PA-O1A
3	F	901	ATP	C3'-C4'-C5'-O5'
3	F	903	ATP	C5'-O5'-PA-O1A
3	F	903	ATP	O4'-C4'-C5'-O5'
3	F	903	ATP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	C	901	ATP	O4'-C4'-C5'-O5'
3	C	903	ATP	O4'-C4'-C5'-O5'
3	D	903	ATP	O4'-C4'-C5'-O5'
3	D	903	ATP	C3'-C4'-C5'-O5'
3	E	901	ATP	O4'-C4'-C5'-O5'
3	E	901	ATP	C3'-C4'-C5'-O5'
3	F	901	ATP	O4'-C4'-C5'-O5'
3	A	903	ATP	O4'-C4'-C5'-O5'
3	D	901	ATP	O4'-C4'-C5'-O5'
3	B	903	ATP	PB-O3A-PA-O1A
3	E	903	ATP	PB-O3A-PA-O1A
3	C	901	ATP	C4'-C5'-O5'-PA
3	B	901	ATP	C4'-C5'-O5'-PA
3	A	903	ATP	PB-O3A-PA-O5'
3	C	903	ATP	PB-O3A-PA-O5'
3	D	901	ATP	PB-O3A-PA-O5'
3	D	903	ATP	PB-O3A-PA-O5'
3	E	901	ATP	PB-O3A-PA-O5'
3	F	903	ATP	PB-O3A-PA-O5'
3	A	901	ATP	C5'-O5'-PA-O3A
3	A	901	ATP	PA-O3A-PB-O2B
3	A	903	ATP	PA-O3A-PB-O2B
3	B	901	ATP	PA-O3A-PB-O2B
3	B	903	ATP	PA-O3A-PB-O2B
3	C	901	ATP	PA-O3A-PB-O2B
3	C	903	ATP	PA-O3A-PB-O2B
3	D	901	ATP	PA-O3A-PB-O2B
3	D	903	ATP	PA-O3A-PB-O2B
3	E	901	ATP	PA-O3A-PB-O2B
3	E	903	ATP	PA-O3A-PB-O2B
3	F	901	ATP	PA-O3A-PB-O2B
3	F	903	ATP	PA-O3A-PB-O2B
3	D	901	ATP	C5'-O5'-PA-O1A
3	B	903	ATP	PB-O3A-PA-O5'
3	E	903	ATP	PB-O3A-PA-O5'
3	B	901	ATP	PB-O3B-PG-O1G
3	B	903	ATP	PB-O3B-PG-O1G
3	C	903	ATP	PB-O3B-PG-O1G
3	B	903	ATP	PB-O3B-PG-O2G
3	C	903	ATP	PB-O3B-PG-O2G
3	A	903	ATP	C5'-O5'-PA-O3A
3	E	901	ATP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
3	F	901	ATP	C5'-O5'-PA-O3A
3	F	903	ATP	C5'-O5'-PA-O3A
3	A	901	ATP	PA-O3A-PB-O1B
3	A	903	ATP	PA-O3A-PB-O1B
3	A	903	ATP	PB-O3A-PA-O1A
3	B	903	ATP	PA-O3A-PB-O1B
3	C	903	ATP	PA-O3A-PB-O1B
3	D	901	ATP	PB-O3A-PA-O2A
3	E	901	ATP	PB-O3A-PA-O2A
3	E	903	ATP	PA-O3A-PB-O1B
3	F	901	ATP	PB-O3A-PA-O1A
3	F	903	ATP	PA-O3A-PB-O1B
3	C	901	ATP	C5'-O5'-PA-O1A
3	C	903	ATP	C5'-O5'-PA-O1A
3	D	903	ATP	C5'-O5'-PA-O1A
3	E	903	ATP	C5'-O5'-PA-O1A

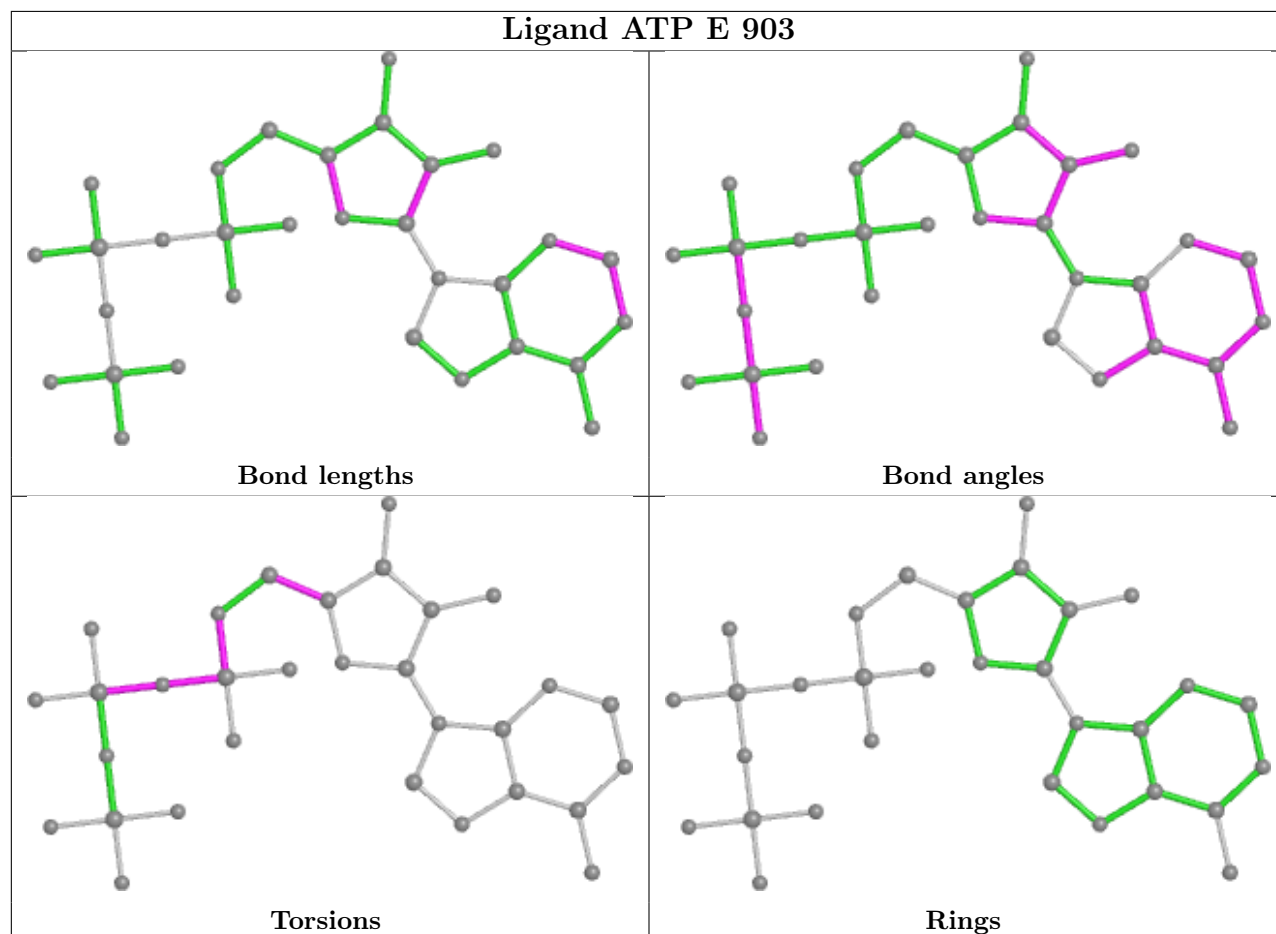
There are no ring outliers.

11 monomers are involved in 35 short contacts:

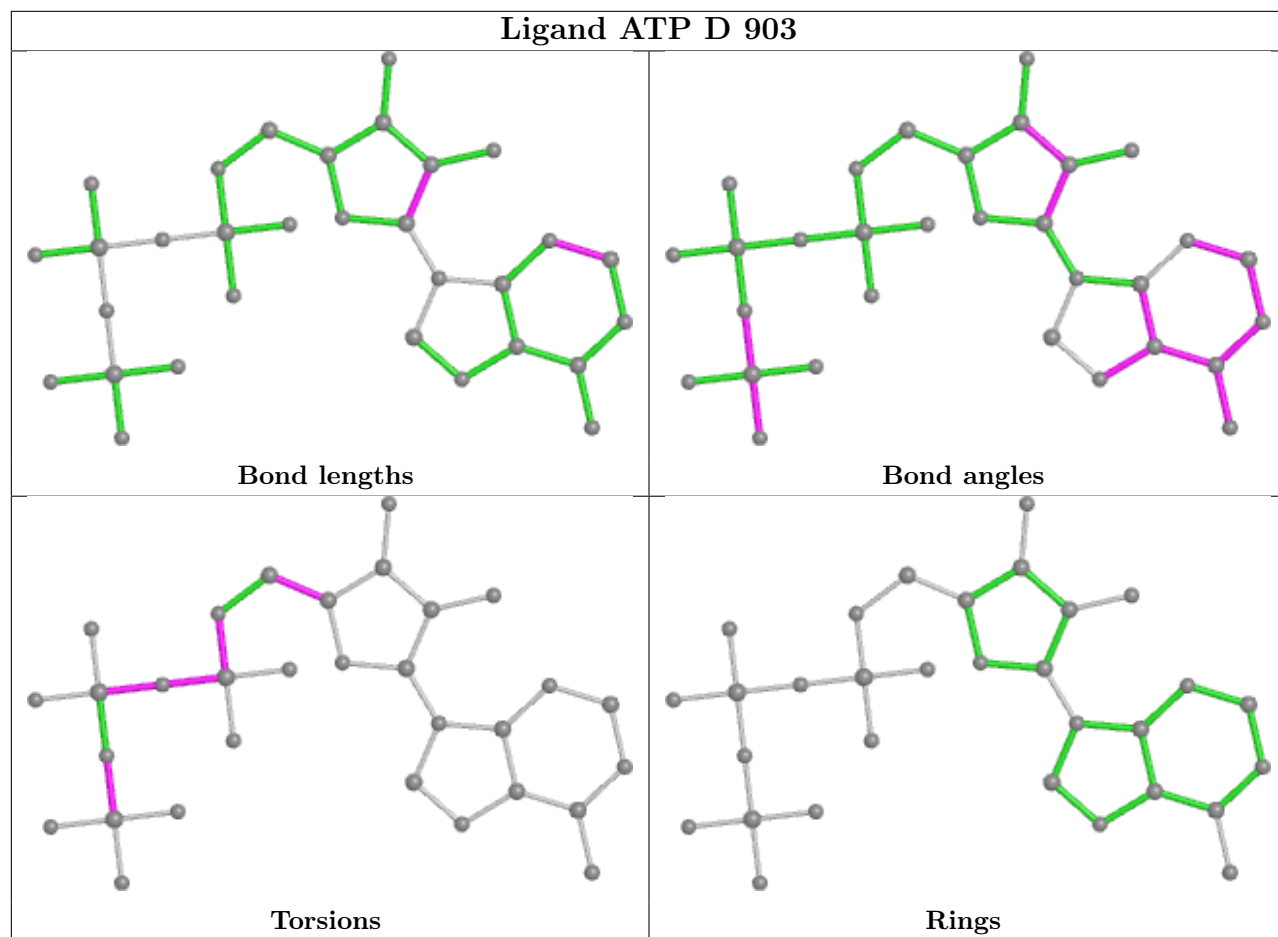
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	903	ATP	3	0
3	D	903	ATP	3	0
3	A	903	ATP	2	0
3	B	903	ATP	4	0
3	B	901	ATP	3	0
3	F	903	ATP	3	0
3	C	901	ATP	3	0
3	C	903	ATP	2	0
3	F	901	ATP	1	0
3	D	901	ATP	5	0
3	E	901	ATP	6	0

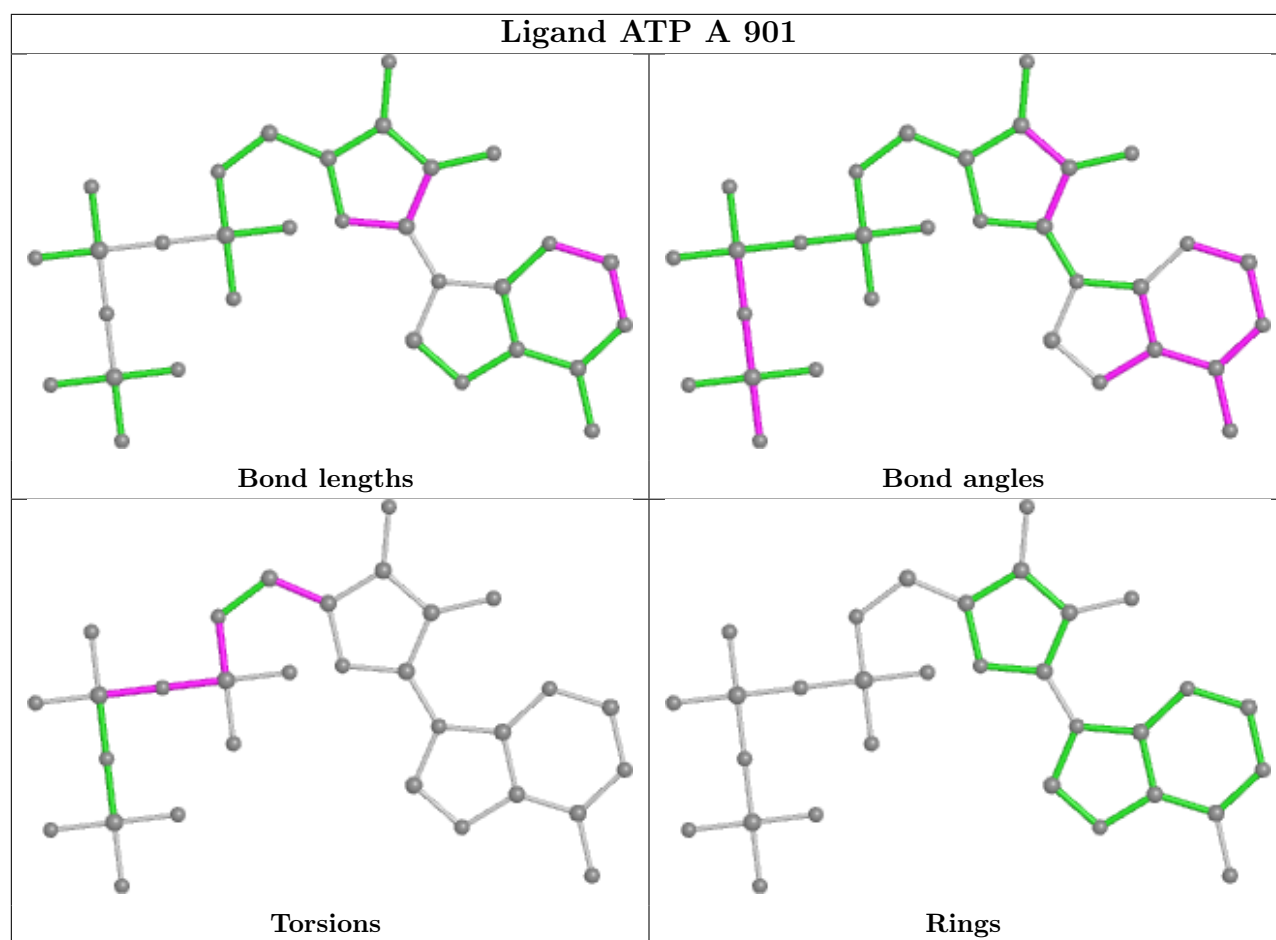
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

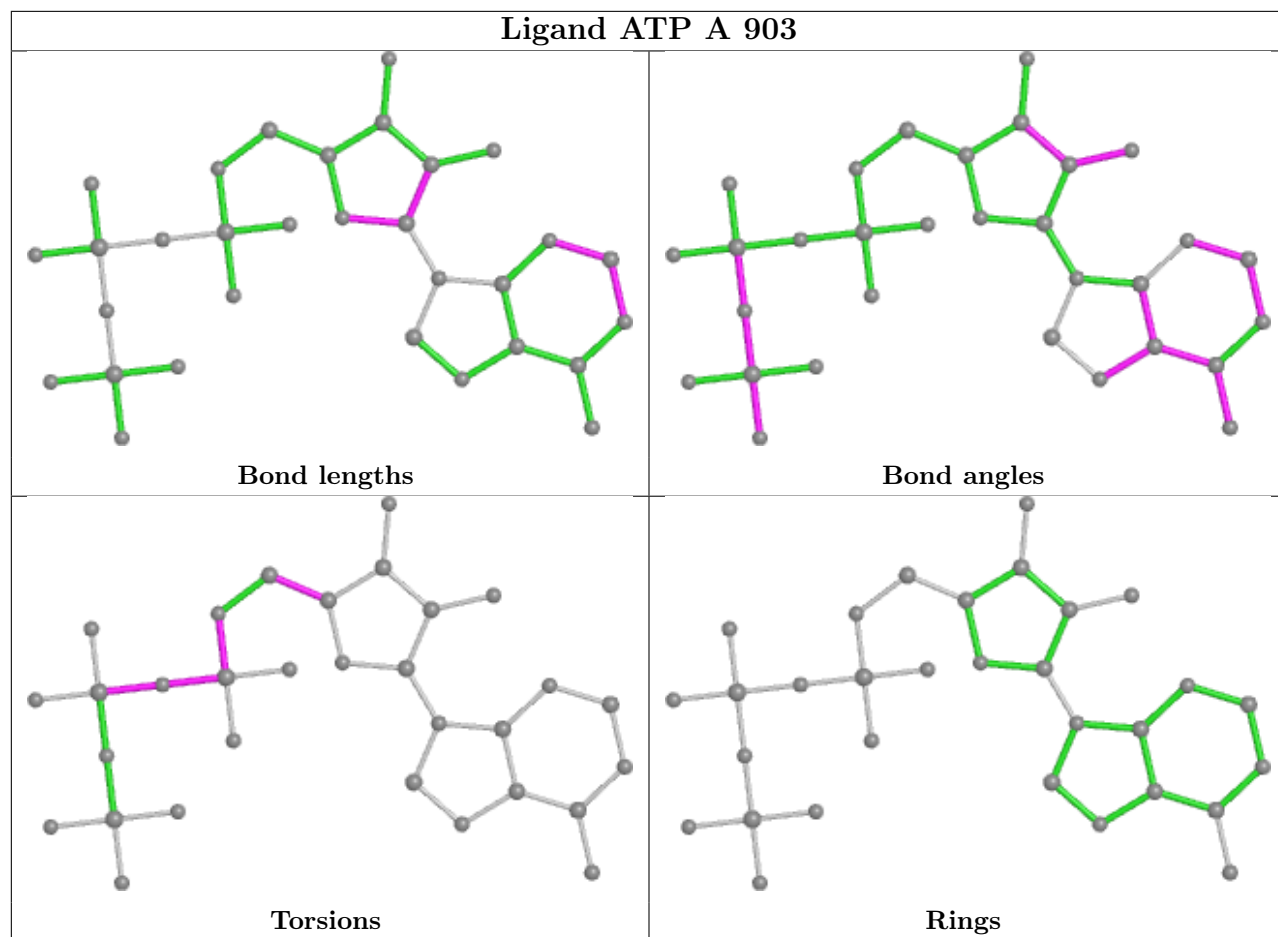


Ligand ATP D 903

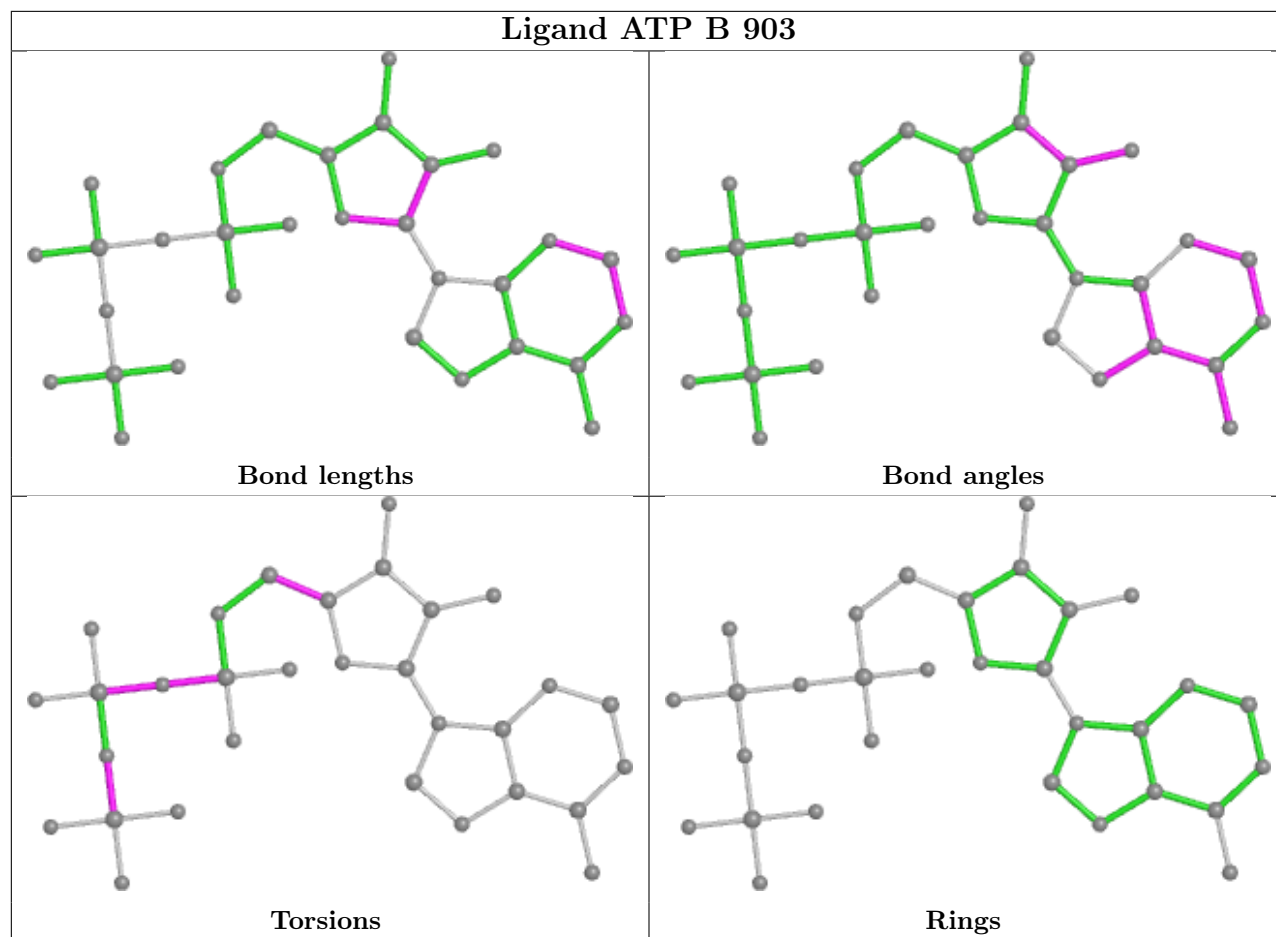




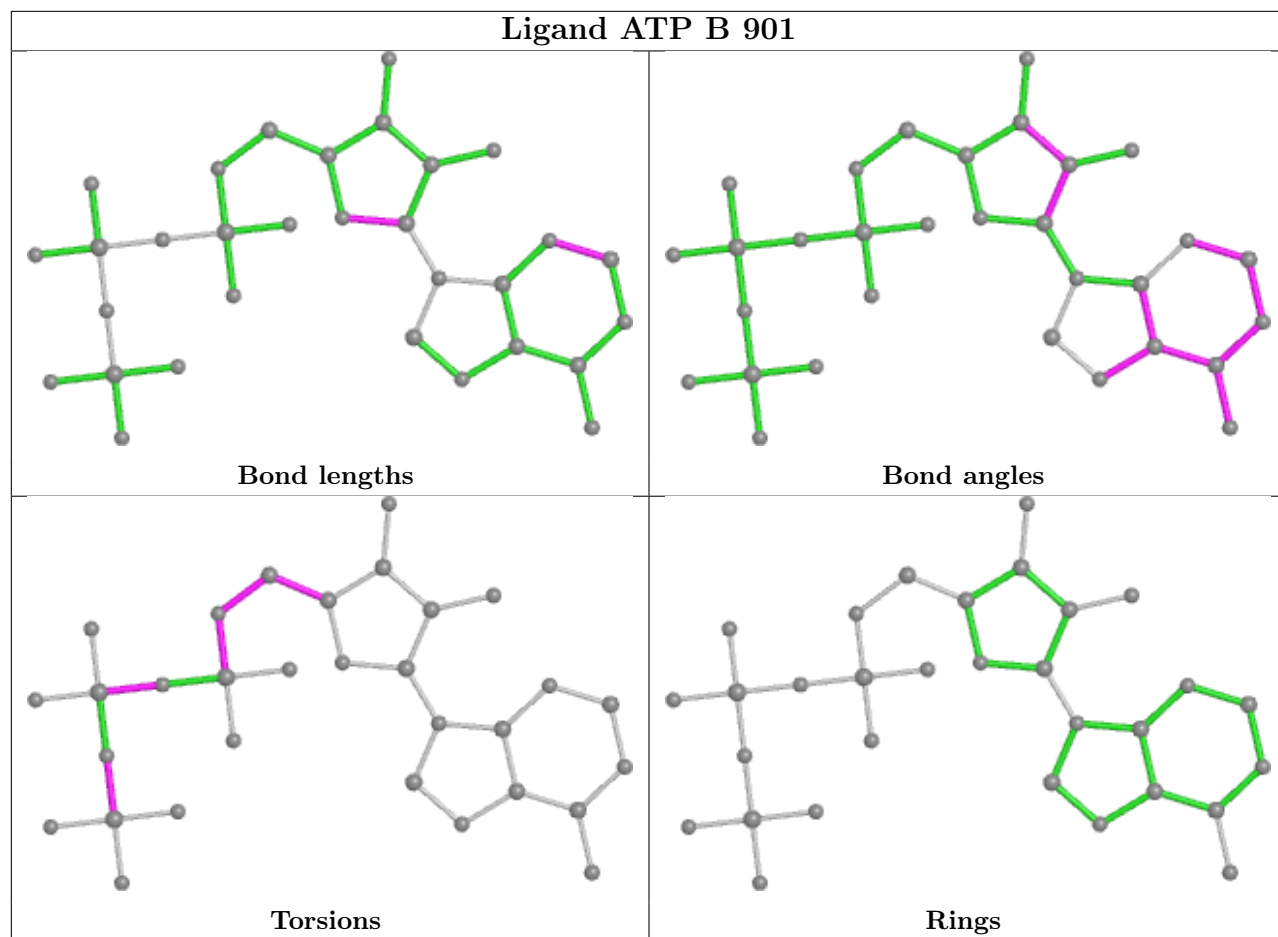
Ligand ATP A 903



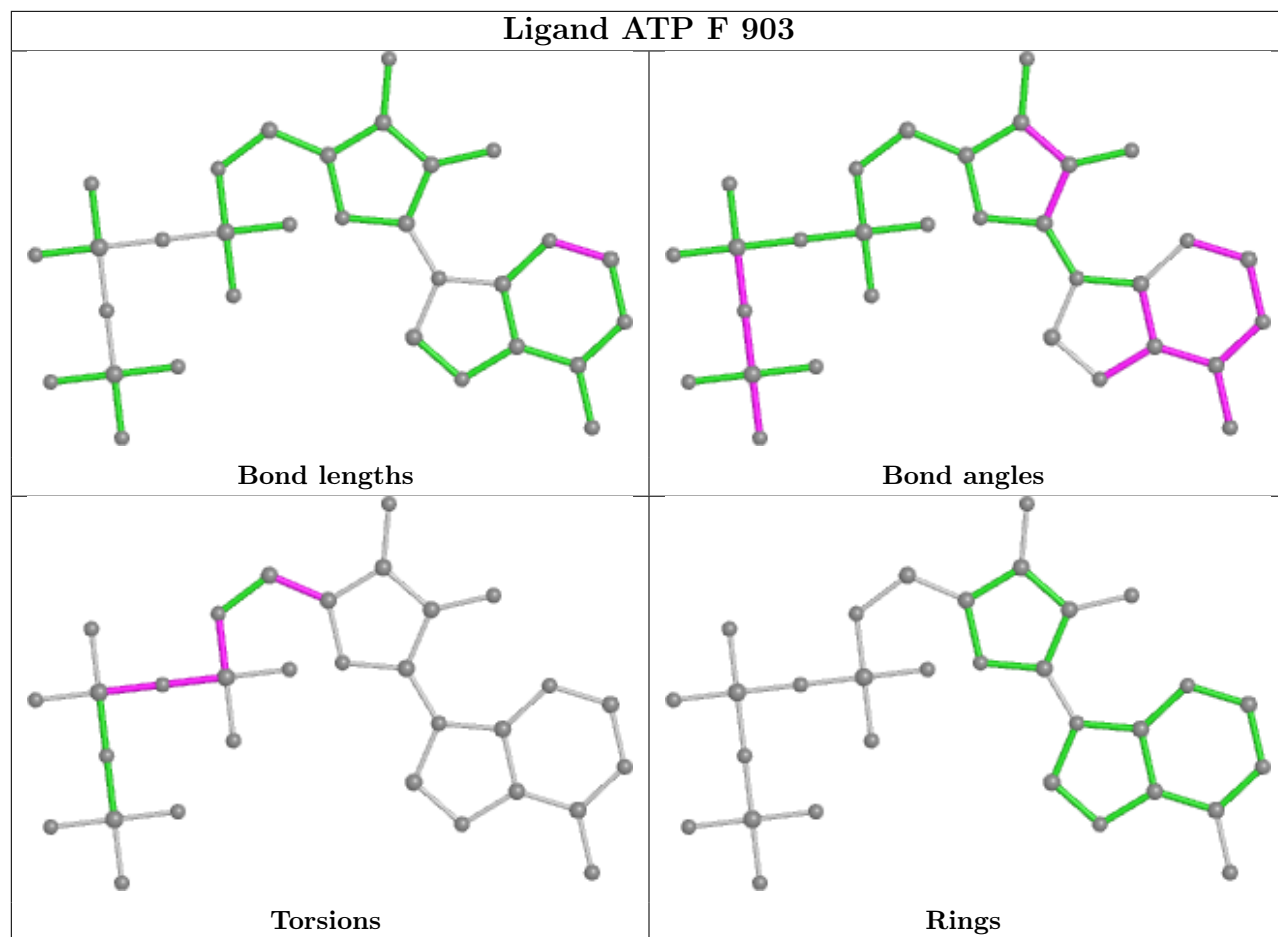
Ligand ATP B 903

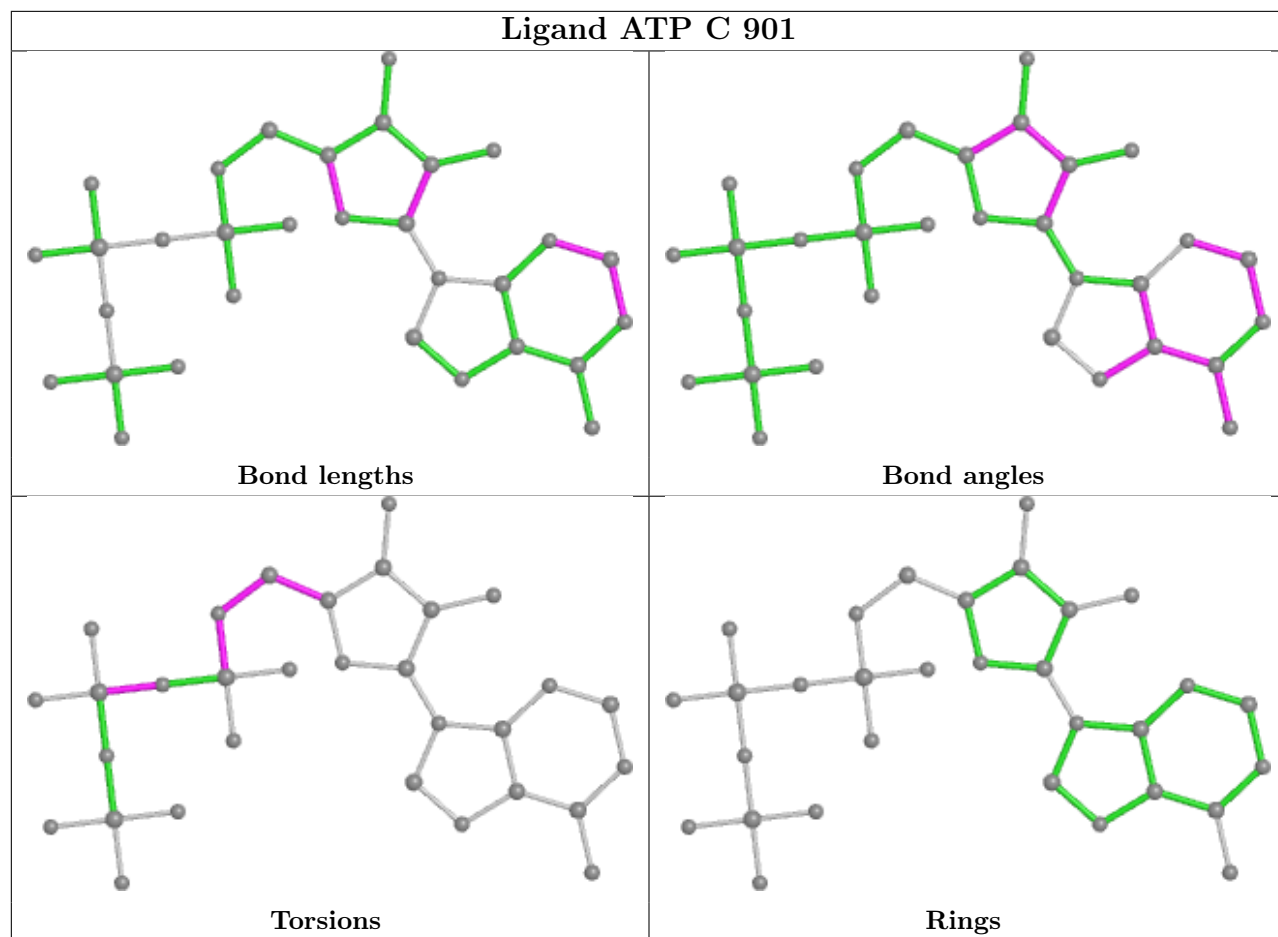


Ligand ATP B 901

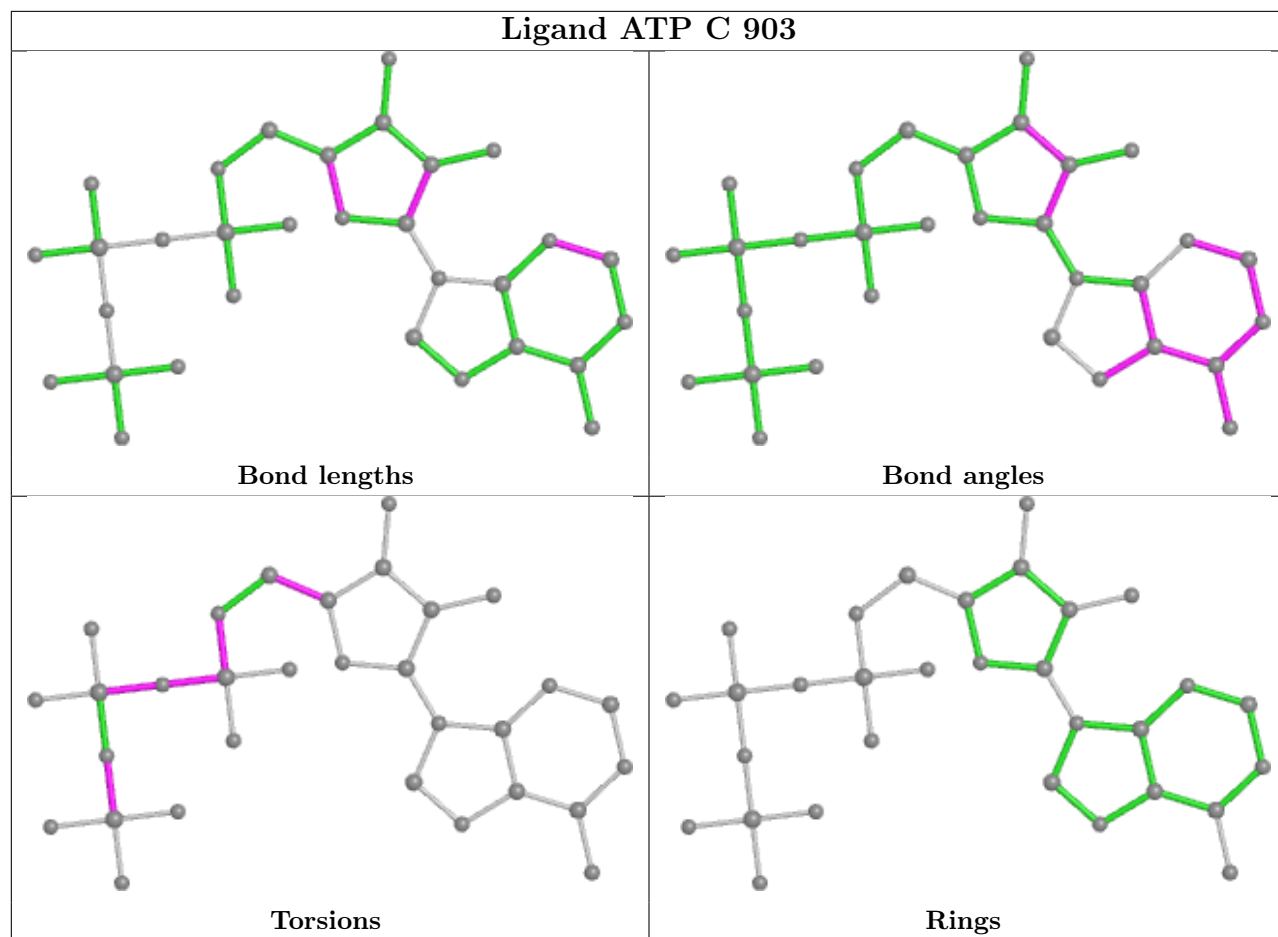


Ligand ATP F 903

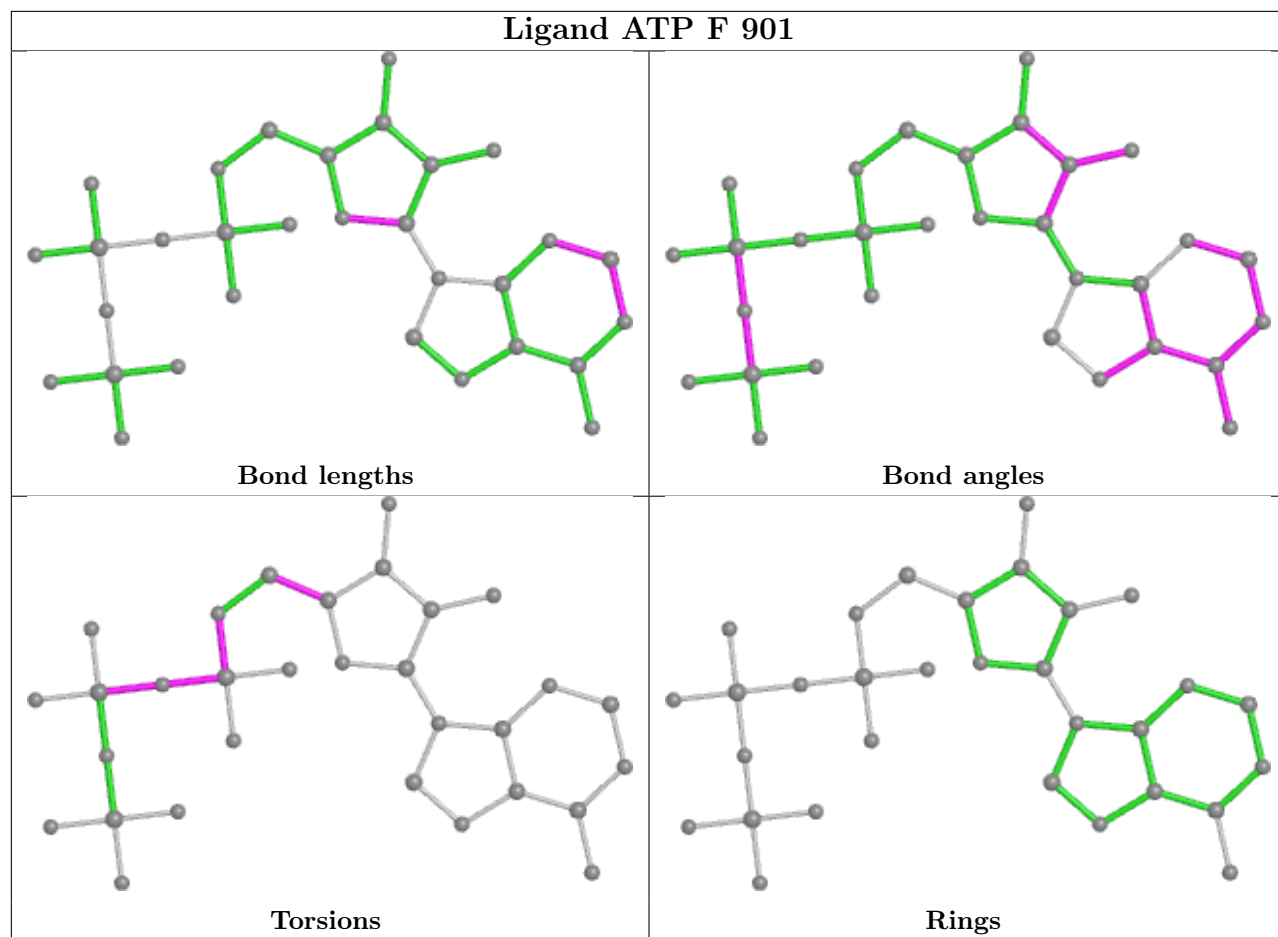


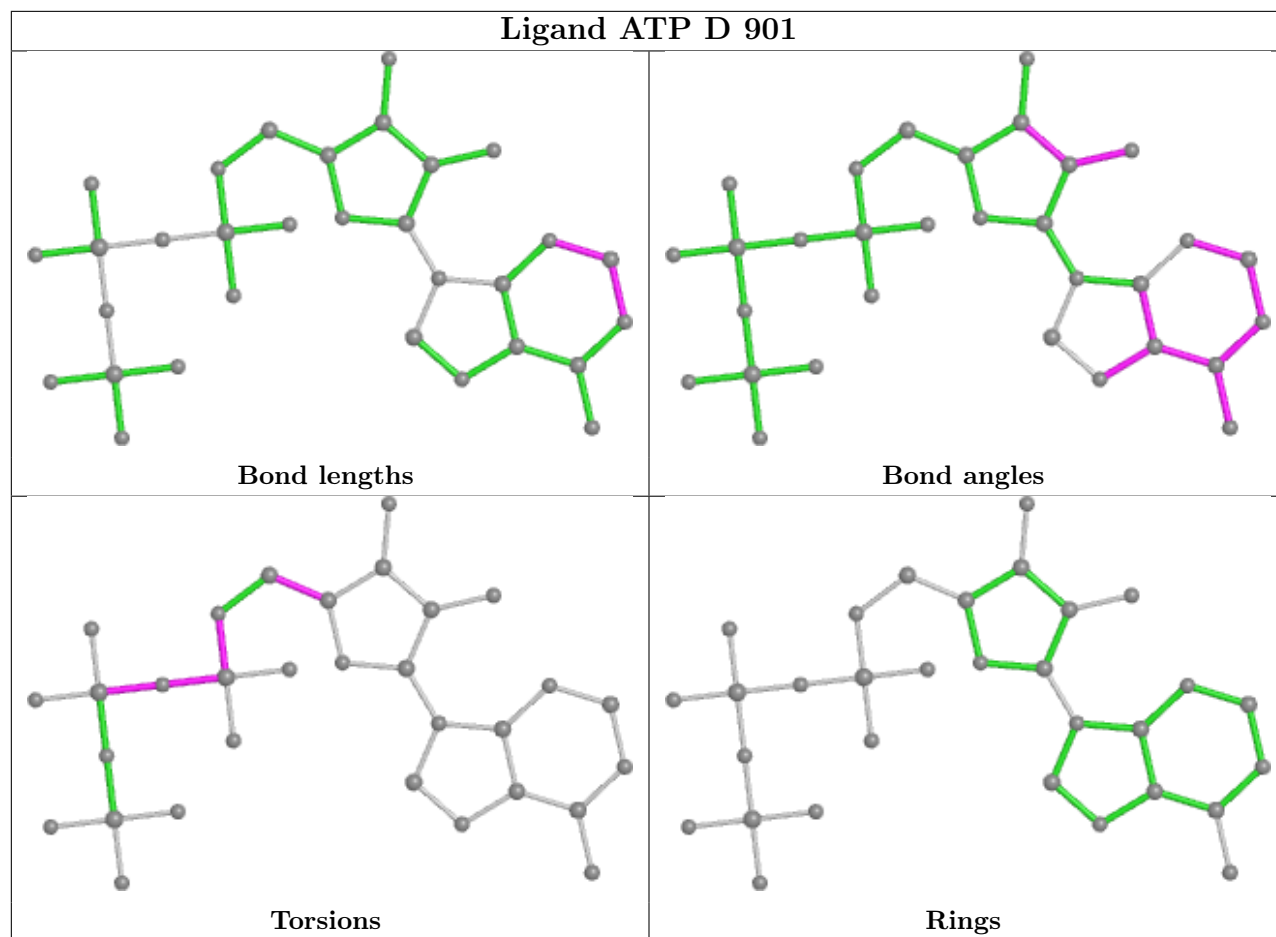


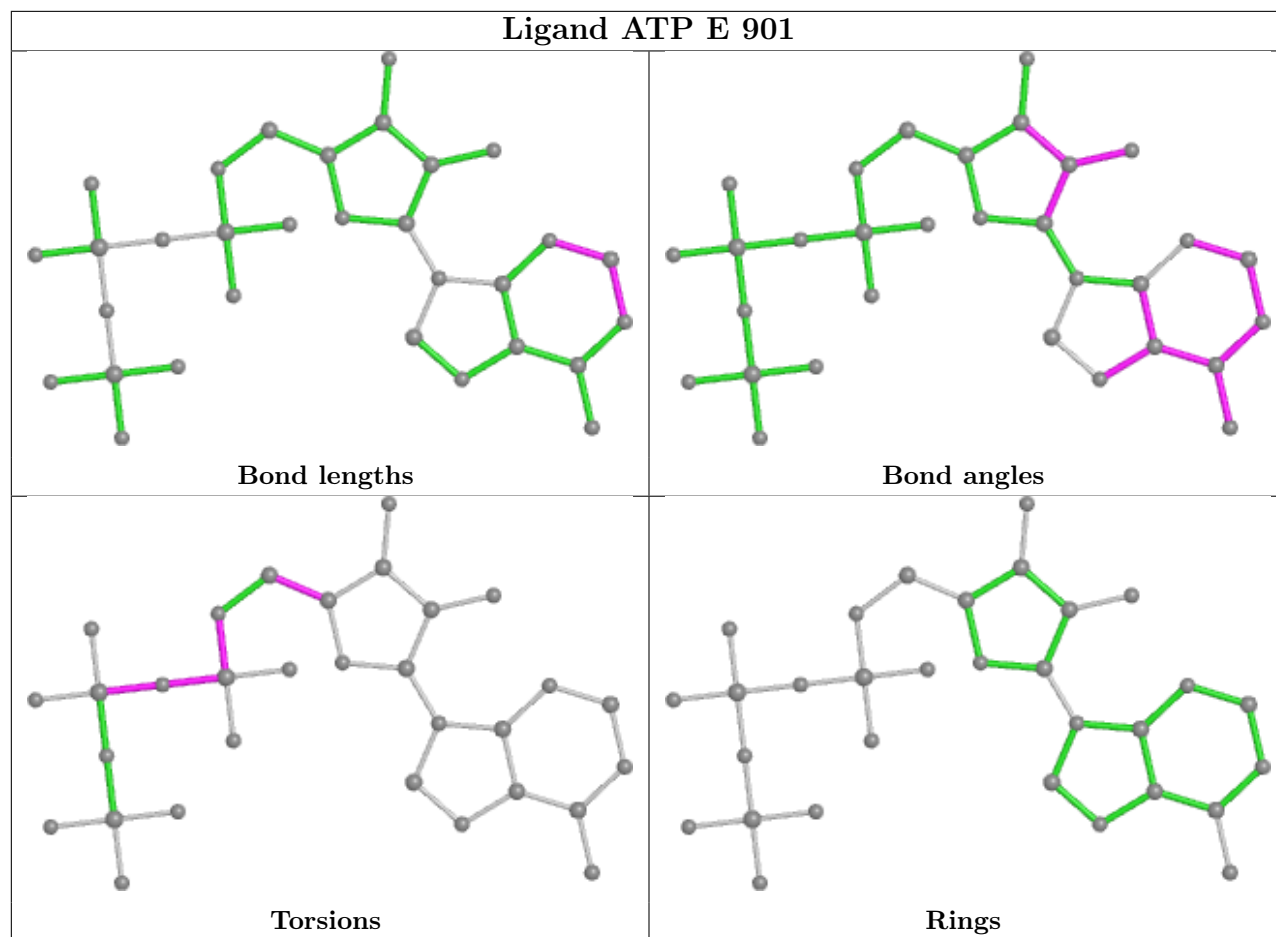
Ligand ATP C 903



Ligand ATP F 901







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	504/519 (97%)	0.46	63 (12%) 3 2	29, 92, 154, 184	0
1	B	489/519 (94%)	0.24	35 (7%) 15 9	47, 95, 151, 185	0
1	C	486/519 (93%)	0.07	28 (5%) 23 13	34, 74, 144, 176	0
1	D	483/519 (93%)	-0.14	21 (4%) 35 22	11, 59, 123, 150	0
1	E	490/519 (94%)	0.04	33 (6%) 17 10	10, 70, 137, 179	0
1	F	504/519 (97%)	0.24	43 (8%) 10 6	15, 84, 154, 175	0
All	All	2956/3114 (94%)	0.16	223 (7%) 14 8	10, 80, 147, 185	0

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	517	PRO	9.0
1	A	519	SER	8.5
1	F	423	HIS	8.1
1	A	503	SER	7.7
1	A	516	GLY	7.5
1	A	517	PRO	7.3
1	F	506	SER	7.2
1	E	500	ASP	7.1
1	A	511	GLY	6.6
1	A	498	THR	6.5
1	A	514	GLU	6.2
1	F	516	GLY	6.1
1	B	500	ASP	5.9
1	C	118	VAL	5.8
1	C	117	VAL	5.8
1	A	257	ARG	5.6
1	F	515	LYS	5.6
1	D	120	GLY	5.5
1	B	501	GLU	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	500	ASP	5.4
1	F	497	ILE	5.3
1	B	503	SER	5.2
1	B	114	GLY	5.1
1	A	506	SER	5.0
1	F	518	GLU	5.0
1	A	499	VAL	4.9
1	B	499	VAL	4.9
1	C	501	GLU	4.9
1	E	121	PHE	4.8
1	C	119	GLY	4.7
1	E	503	SER	4.7
1	A	513	GLN	4.6
1	F	519	SER	4.6
1	A	518	GLU	4.6
1	C	116	GLU	4.6
1	B	121	PHE	4.6
1	E	499	VAL	4.5
1	F	503	SER	4.5
1	C	16	GLN	4.4
1	A	512	VAL	4.4
1	A	339	GLU	4.4
1	F	498	THR	4.4
1	F	507	ARG	4.3
1	F	504	GLU	4.3
1	E	116	GLU	4.3
1	D	157	SER	4.3
1	E	113	GLU	4.3
1	E	118	VAL	4.2
1	F	500	ASP	4.2
1	B	426	ASN	4.2
1	B	498	THR	4.2
1	B	504	GLU	4.2
1	B	117	VAL	4.1
1	C	143	SER	4.1
1	F	156	ALA	4.1
1	A	509	VAL	4.1
1	A	505	LEU	4.1
1	F	343	LEU	4.1
1	A	507	ARG	4.1
1	D	498	THR	4.0
1	F	509	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	423	HIS	4.0
1	A	515	LYS	4.0
1	C	145	ASP	4.0
1	A	427	ASP	4.0
1	E	498	THR	3.9
1	A	508	ILE	3.9
1	F	485	ASN	3.9
1	E	120	GLY	3.8
1	F	496	ARG	3.8
1	C	500	ASP	3.8
1	A	117	VAL	3.8
1	C	499	VAL	3.8
1	F	484	ARG	3.8
1	D	343	LEU	3.8
1	A	116	GLU	3.7
1	A	378	ASP	3.7
1	F	513	GLN	3.6
1	F	154	TYR	3.6
1	C	120	GLY	3.6
1	A	424	SER	3.6
1	A	329	TYR	3.5
1	B	116	GLU	3.4
1	A	504	GLU	3.4
1	F	157	SER	3.4
1	A	115	GLN	3.4
1	A	496	ARG	3.4
1	A	340	ARG	3.3
1	D	15	HIS	3.3
1	C	146	SER	3.2
1	D	119	GLY	3.2
1	E	505	LEU	3.2
1	B	502	LYS	3.2
1	F	342	ASN	3.2
1	A	484	ARG	3.2
1	E	154	TYR	3.2
1	C	189	GLY	3.1
1	A	319	GLU	3.1
1	D	16	GLN	3.1
1	A	154	TYR	3.1
1	B	16	GLN	3.1
1	B	258	SER	3.1
1	F	514	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	119	GLY	3.1
1	B	182	THR	3.1
1	D	158	SER	3.1
1	E	496	ARG	3.1
1	F	505	LEU	3.1
1	D	421	GLY	3.1
1	E	501	GLU	3.0
1	A	413	THR	3.0
1	A	258	SER	3.0
1	B	259	SER	3.0
1	A	501	GLU	2.9
1	B	115	GLN	2.9
1	D	121	PHE	2.9
1	F	153	GLN	2.9
1	A	282	SER	2.9
1	A	492	GLY	2.9
1	A	120	GLY	2.9
1	C	154	TYR	2.9
1	E	417	ASP	2.8
1	A	446	ARG	2.8
1	F	512	VAL	2.8
1	B	321	ARG	2.8
1	A	253	ARG	2.8
1	A	114	GLY	2.8
1	B	497	ILE	2.8
1	D	497	ILE	2.8
1	F	501	GLU	2.7
1	A	483	PHE	2.7
1	C	487	GLU	2.7
1	E	119	GLY	2.7
1	C	140	ARG	2.7
1	A	414	ASN	2.7
1	B	257	ARG	2.7
1	F	295	THR	2.7
1	B	119	GLY	2.7
1	F	424	SER	2.6
1	C	498	THR	2.6
1	E	421	GLY	2.6
1	B	309	LYS	2.6
1	E	502	LYS	2.6
1	C	15	HIS	2.6
1	F	508	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	14	GLU	2.6
1	F	511	GLY	2.6
1	E	485	ASN	2.5
1	A	417	ASP	2.5
1	A	342	ASN	2.5
1	A	423	HIS	2.5
1	A	337	GLU	2.5
1	C	121	PHE	2.5
1	E	504	GLU	2.5
1	D	117	VAL	2.5
1	A	475	LYS	2.5
1	A	428	SER	2.5
1	B	157	SER	2.5
1	F	344	LEU	2.4
1	A	145	ASP	2.4
1	A	255	THR	2.4
1	F	257	ARG	2.4
1	B	162	ARG	2.4
1	A	318	GLU	2.4
1	A	502	LYS	2.4
1	E	497	ILE	2.4
1	C	495	THR	2.4
1	A	485	ASN	2.4
1	B	181	THR	2.4
1	C	417	ASP	2.4
1	D	447	GLY	2.4
1	E	483	PHE	2.4
1	C	181	THR	2.4
1	F	378	ASP	2.4
1	B	15	HIS	2.4
1	A	486	PHE	2.3
1	D	118	VAL	2.3
1	D	156	ALA	2.3
1	C	17	ALA	2.3
1	F	338	MET	2.3
1	E	333	MET	2.3
1	A	510	ARG	2.3
1	B	118	VAL	2.3
1	A	153	GLN	2.2
1	D	295	THR	2.2
1	C	179	VAL	2.2
1	B	280	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	329	TYR	2.2
1	D	14	GLU	2.2
1	A	16	GLN	2.2
1	A	182	THR	2.2
1	E	484	ARG	2.2
1	C	114	GLY	2.2
1	C	423	HIS	2.2
1	F	495	THR	2.2
1	E	418	GLN	2.1
1	E	339	GLU	2.1
1	A	379	SER	2.1
1	B	337	GLU	2.1
1	F	339	GLU	2.1
1	E	112	PRO	2.1
1	B	155	ASP	2.1
1	D	483	PHE	2.1
1	F	502	LYS	2.1
1	B	427	ASP	2.1
1	F	417	ASP	2.1
1	E	422	ALA	2.1
1	E	122	ASP	2.1
1	F	334	ASP	2.1
1	E	486	PHE	2.1
1	B	417	ASP	2.1
1	C	128	GLU	2.0
1	B	261	VAL	2.0
1	A	56	SER	2.0
1	C	153	GLN	2.0
1	F	370	PHE	2.0
1	D	155	ASP	2.0
1	B	180	MET	2.0
1	D	422	ALA	2.0
1	A	268	VAL	2.0
1	E	334	ASP	2.0
1	E	321	ARG	2.0
1	D	485	ASN	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(\AA^2)	Q<0.9
1	SEP	A	431	10/11	0.67	0.26	109,115,120,121	0
1	SEP	C	431	10/11	0.72	0.38	96,106,119,119	0
1	SEP	F	431	10/11	0.76	0.31	104,110,117,117	0
1	SEP	D	431	10/11	0.79	0.24	96,105,117,118	0
1	SEP	B	431	10/11	0.81	0.35	129,136,148,148	0
1	SEP	E	431	10/11	0.88	0.21	89,93,102,104	0
1	TPO	B	432	11/12	0.89	0.35	120,127,130,130	0
1	TPO	A	432	11/12	0.91	0.23	106,109,114,114	0
1	TPO	F	432	11/12	0.92	0.24	97,99,101,103	0
1	TPO	C	432	11/12	0.94	0.24	83,88,91,92	0
1	TPO	E	432	11/12	0.94	0.18	73,80,83,84	0
1	TPO	D	432	11/12	0.95	0.25	77,82,83,89	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
2	MG	A	801	1/1	0.83	0.25	42,42,42,42	0
3	ATP	F	901	31/31	0.85	0.31	103,116,121,121	0
2	MG	C	801	1/1	0.86	0.14	17,17,17,17	0
3	ATP	A	901	31/31	0.89	0.27	83,93,100,100	0
3	ATP	B	903	31/31	0.89	0.24	68,74,79,79	0
2	MG	D	802	1/1	0.89	0.29	15,15,15,15	0
3	ATP	A	903	31/31	0.90	0.23	65,68,74,75	0
2	MG	A	701	1/1	0.90	0.16	27,27,27,27	0
3	ATP	C	903	31/31	0.90	0.29	52,56,76,78	0
3	ATP	E	901	31/31	0.90	0.25	74,92,98,98	0
2	MG	C	701	1/1	0.90	0.68	49,49,49,49	0
2	MG	B	802	1/1	0.91	0.16	57,57,57,57	0
3	ATP	D	903	31/31	0.91	0.30	29,35,62,63	0
3	ATP	C	901	31/31	0.92	0.20	56,59,63,64	0
2	MG	F	802	1/1	0.92	0.67	92,92,92,92	0

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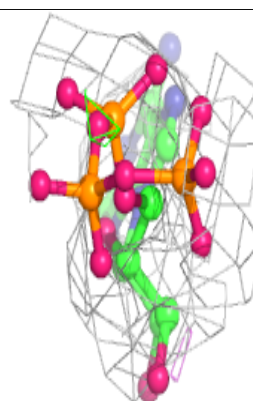
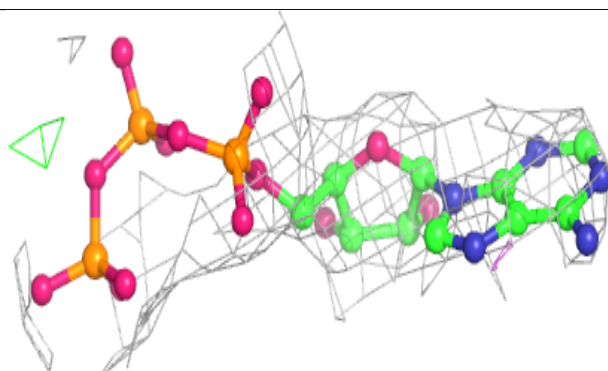
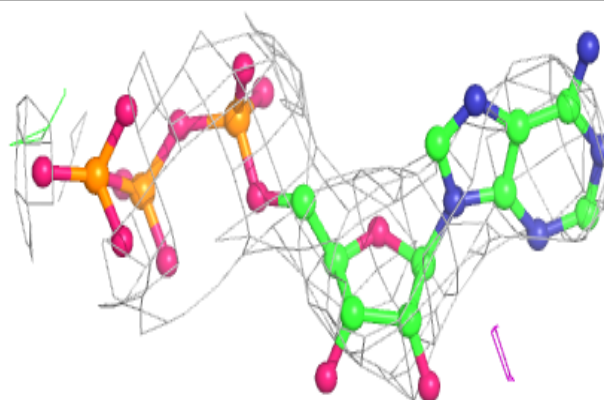
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ATP	D	901	31/31	0.92	0.27	68,73,80,80	0
3	ATP	B	901	31/31	0.93	0.20	69,77,80,82	0
2	MG	B	701	1/1	0.93	0.68	93,93,93,93	0
2	MG	D	520	1/1	0.93	0.54	12,12,12,12	0
2	MG	E	801	1/1	0.93	0.44	44,44,44,44	0
3	ATP	F	903	31/31	0.94	0.23	38,43,47,48	0
2	MG	B	702	1/1	0.95	0.46	61,61,61,61	0
3	ATP	E	903	31/31	0.95	0.21	22,35,50,53	0
2	MG	E	702	1/1	0.96	0.24	56,56,56,56	0
2	MG	B	801	1/1	0.97	0.28	88,88,88,88	0
2	MG	D	801	1/1	0.97	0.11	48,48,48,48	0
2	MG	F	701	1/1	0.97	0.64	67,67,67,67	0
2	MG	C	702	1/1	0.97	0.34	50,50,50,50	0
2	MG	A	802	1/1	0.97	0.21	66,66,66,66	0
2	MG	C	802	1/1	0.98	0.18	105,105,105,105	0
2	MG	F	520	1/1	0.98	0.23	82,82,82,82	0
2	MG	A	702	1/1	0.99	0.23	7,7,7,7	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.

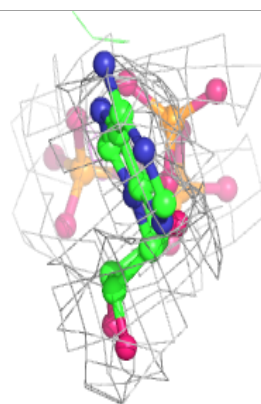
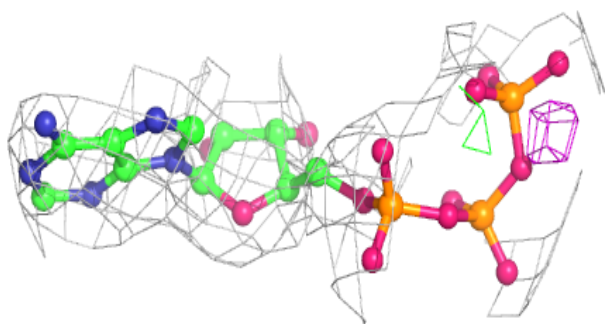
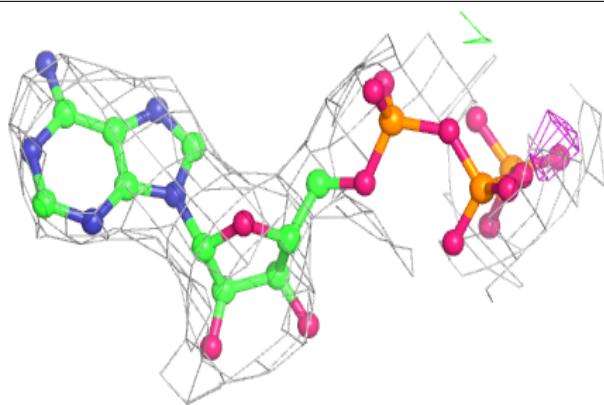
Electron density around ATP F 901:

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

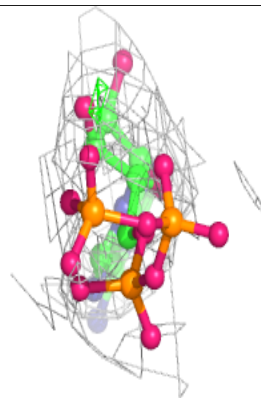
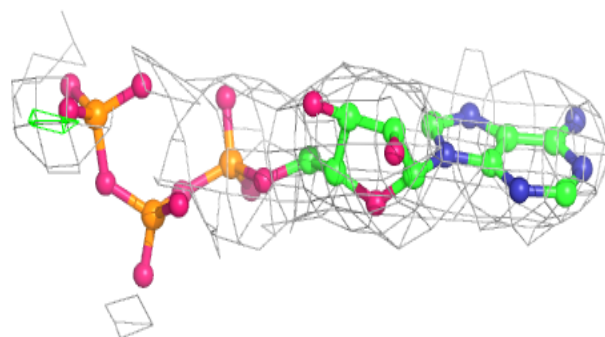
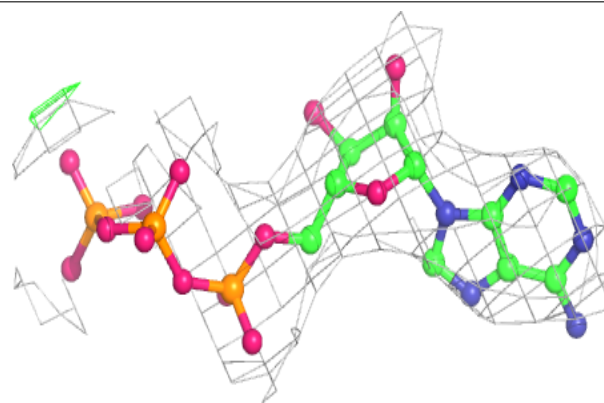


Electron density around ATP A 901:

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

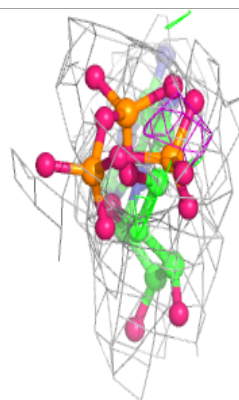
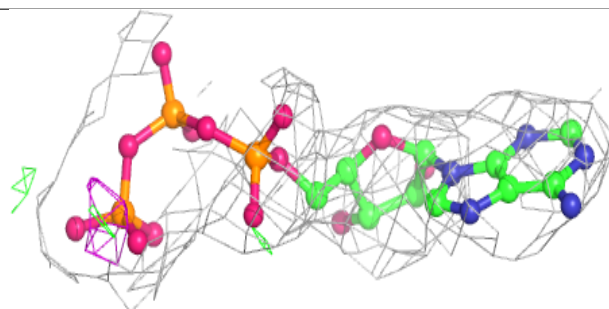
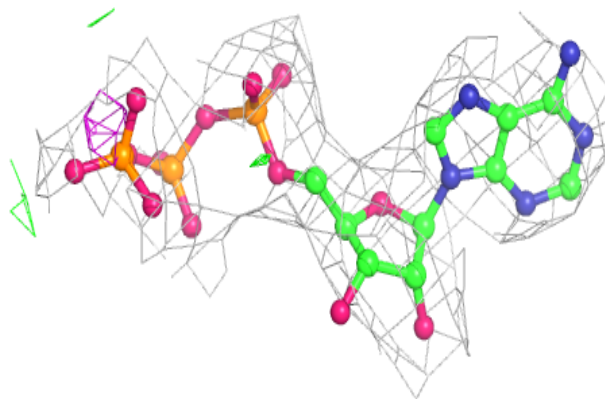
**Electron density around ATP B 903:**

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

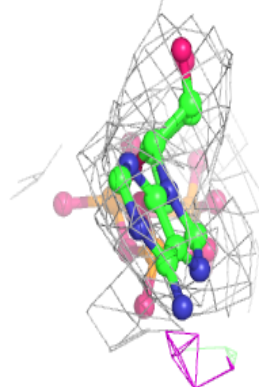
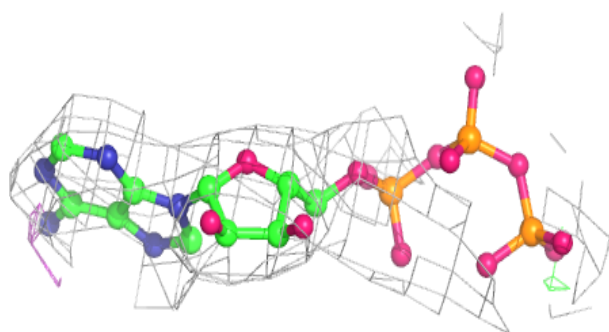
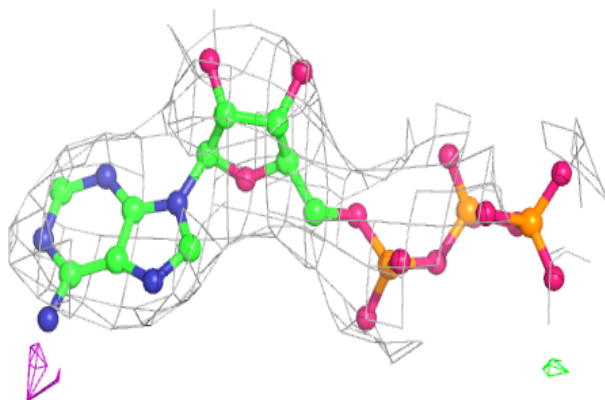


Electron density around ATP A 903:

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

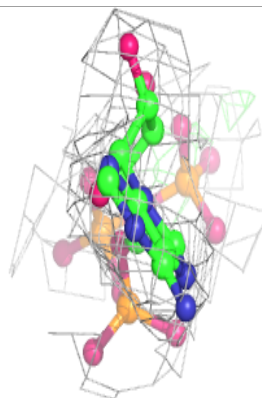
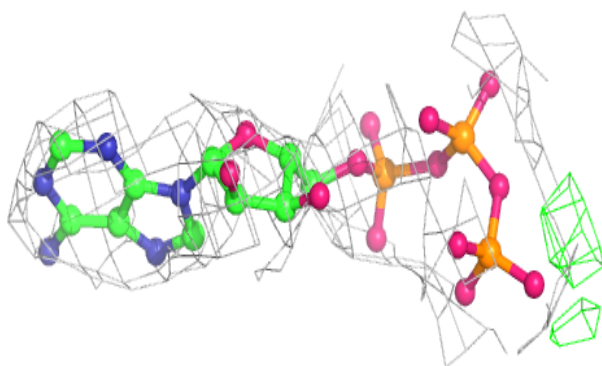
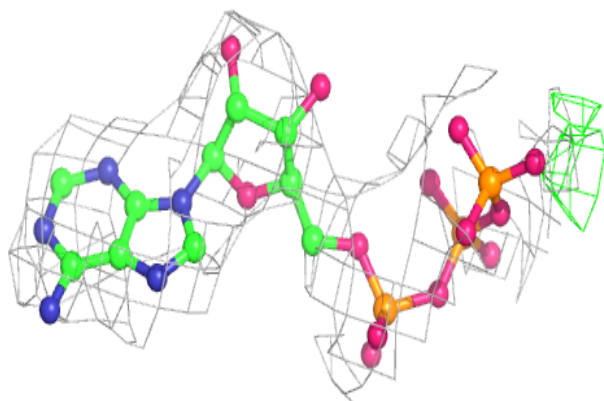
**Electron density around ATP C 903:**

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

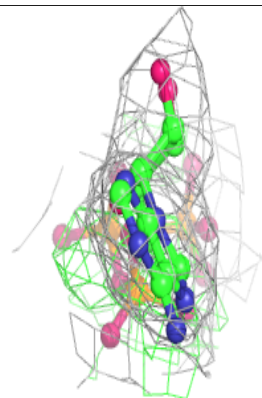
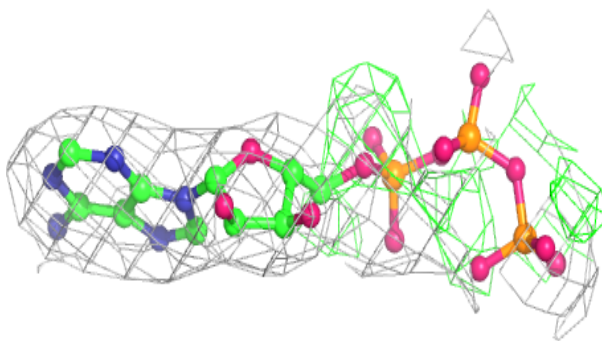
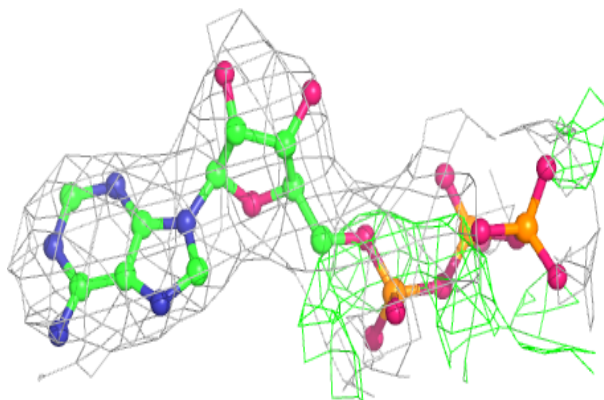


Electron density around ATP E 901:

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

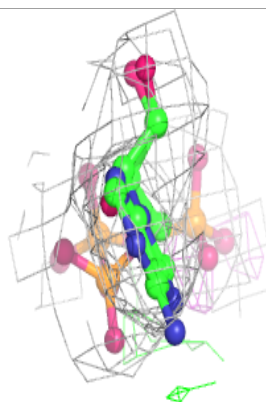
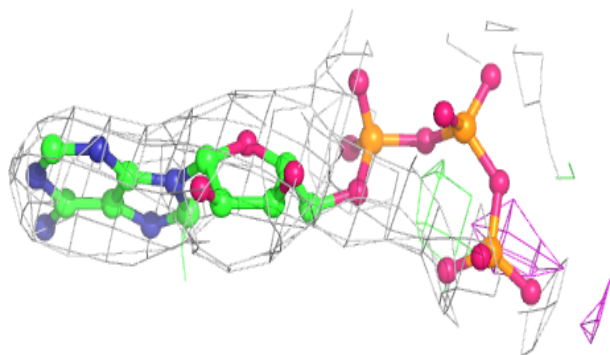
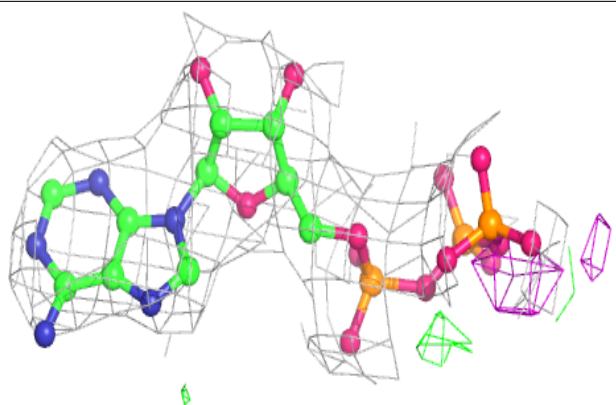
**Electron density around ATP D 903:**

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

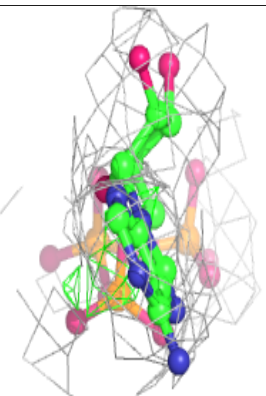
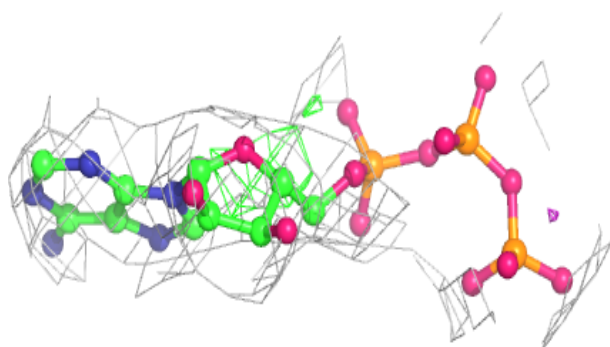
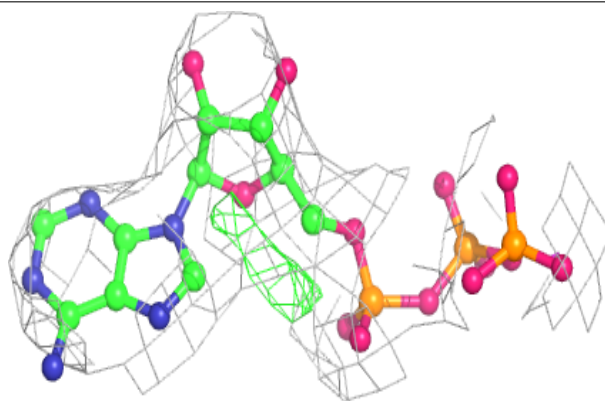


Electron density around ATP C 901:

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

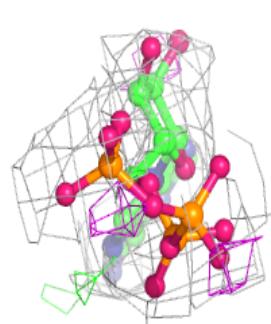
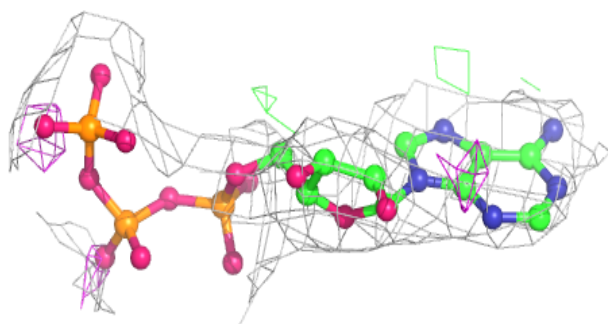
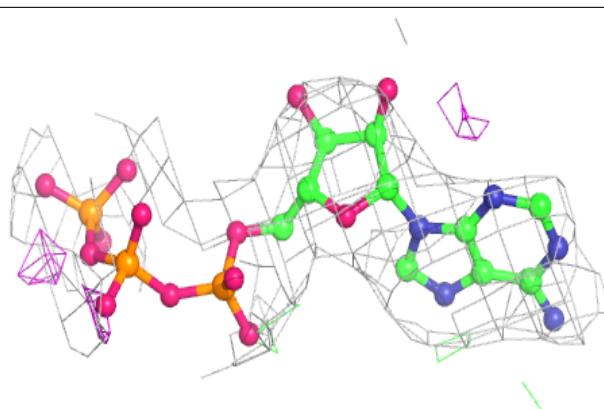
**Electron density around ATP D 901:**

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

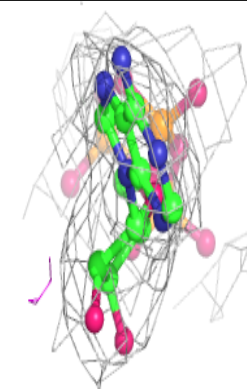
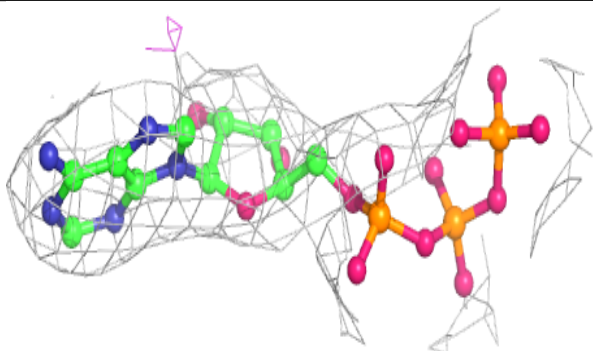
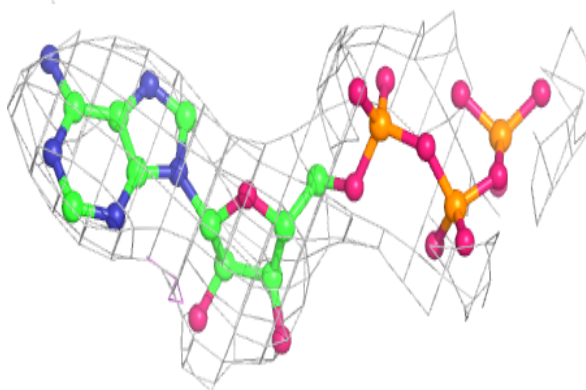


Electron density around ATP B 901:

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

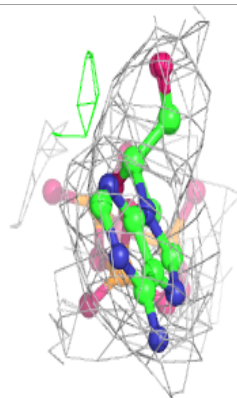
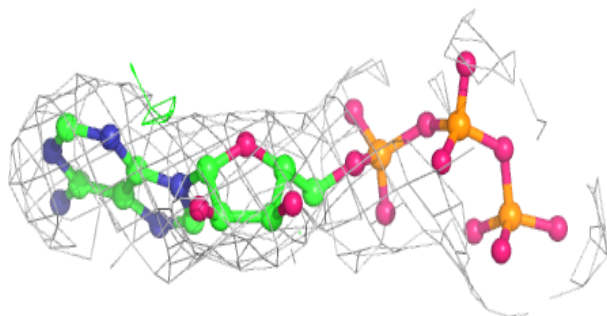
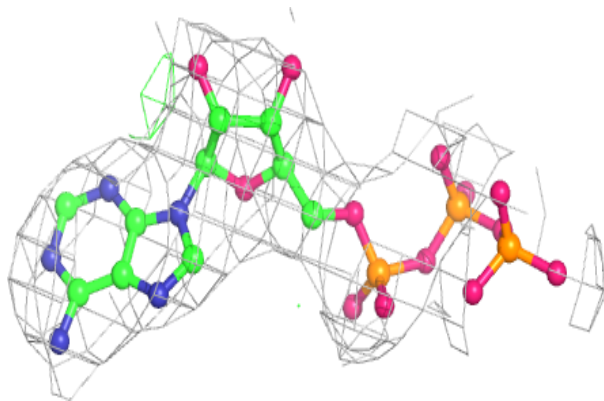
**Electron density around ATP F 903:**

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



Electron density around ATP E 903:

$2mF_o - DF_c$ (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.