



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:56 PM EDT

PDB ID : 3K09 / pdb_00003k09
Title : Crystal structure of the phosphorylation-site mutant S431D 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

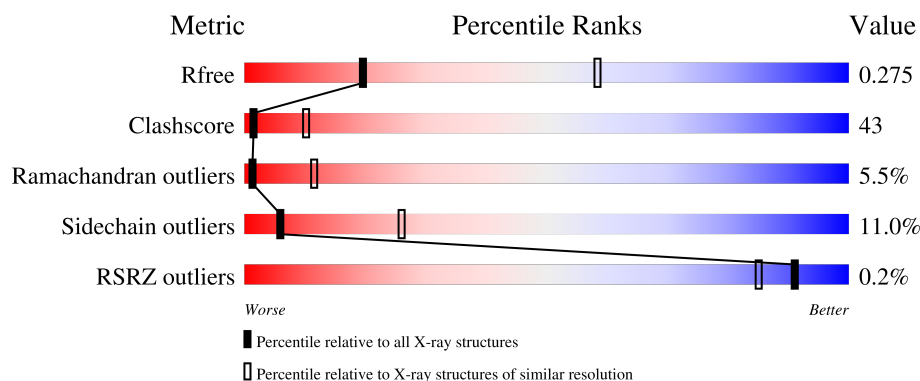
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

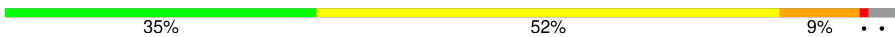
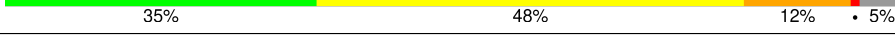
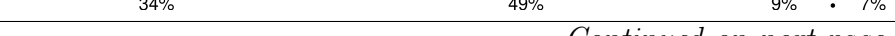
The reported resolution of this entry is 3.20 Å.

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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	
1	B	519	
1	E	519	
2	C	519	
2	D	519	

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Mol	Chain	Length	Quality of chain
2	F	519	35% 49% 12%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23855 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
			3991	2510	701	764	1	15			
1	B	491	Total	C	N	O	P	S	0	0	0
			3876	2440	678	742	1	15			
1	E	492	Total	C	N	O	P	S	0	0	0
			3884	2446	679	743	1	15			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	431	ASP	SER	engineered mutation	UNP Q79PF4
B	431	ASP	SER	engineered mutation	UNP Q79PF4
E	431	ASP	SER	engineered mutation	UNP Q79PF4

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	488	Total	C	N	O	S		0	0	0
			3848	2426	674	733	15				
2	D	485	Total	C	N	O	S		0	0	0
			3824	2412	671	726	15				
2	F	506	Total	C	N	O	S		0	0	0
			3987	2510	701	761	15				

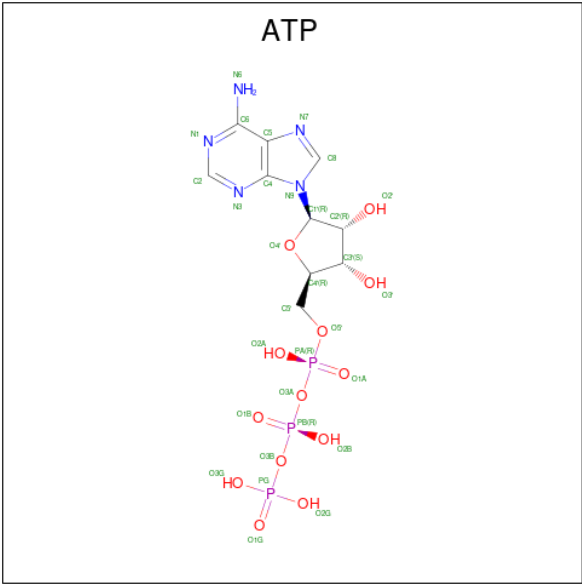
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	431	ASP	SER	engineered mutation	UNP Q79PF4
D	431	ASP	SER	engineered mutation	UNP Q79PF4
F	431	ASP	SER	engineered mutation	UNP Q79PF4

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	Mg	0	0
			5	5		
3	B	1	Total	Mg	0	0
			1	1		
3	C	4	Total	Mg	0	0
			4	4		
3	D	3	Total	Mg	0	0
			3	3		
3	E	4	Total	Mg	0	0
			4	4		
3	F	3	Total	Mg	0	0
			3	3		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

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

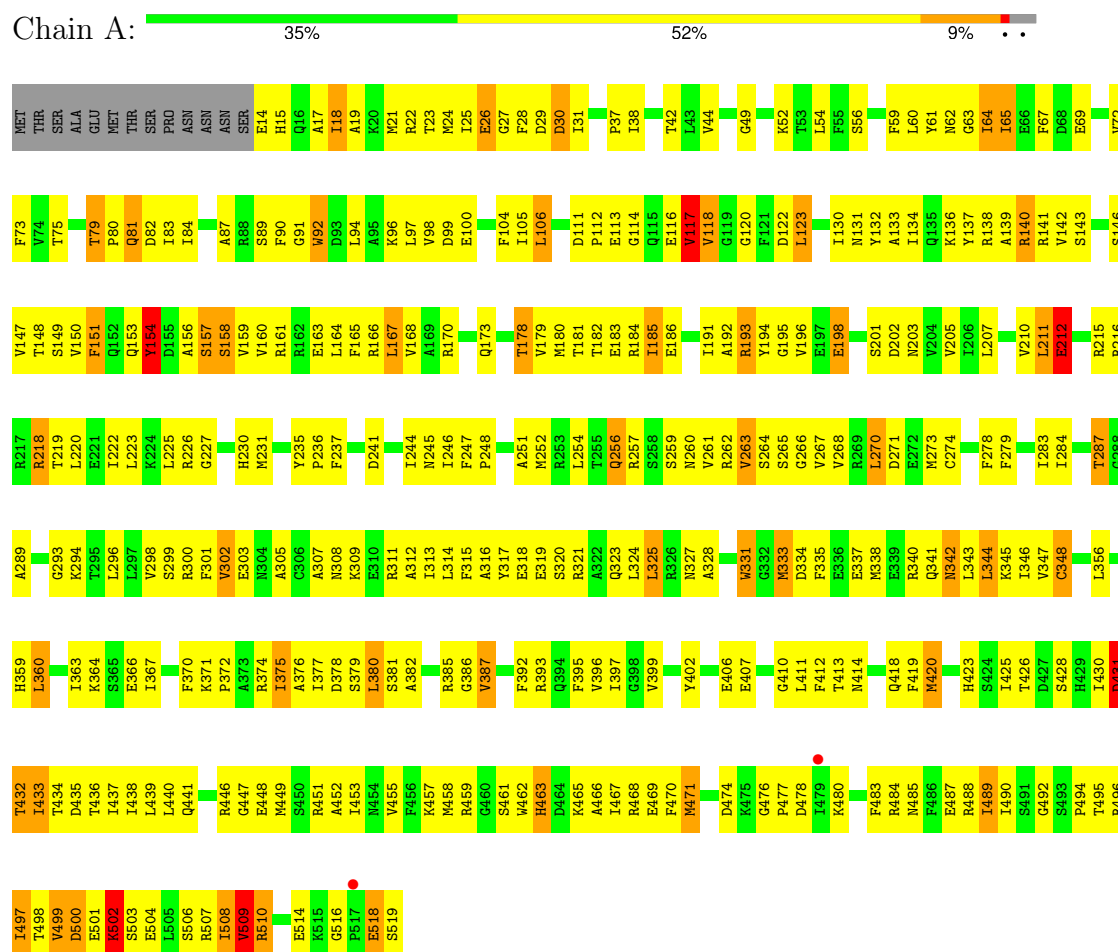
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total	O	0	0
			7	7		
5	B	5	Total	O	0	0
			5	5		
5	C	5	Total	O	0	0
			5	5		
5	D	10	Total	O	0	0
			10	10		
5	E	7	Total	O	0	0
			7	7		
5	F	19	Total	O	0	0
			19	19		

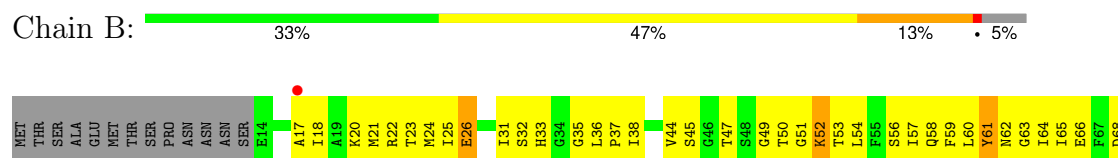
3 Residue-property plots

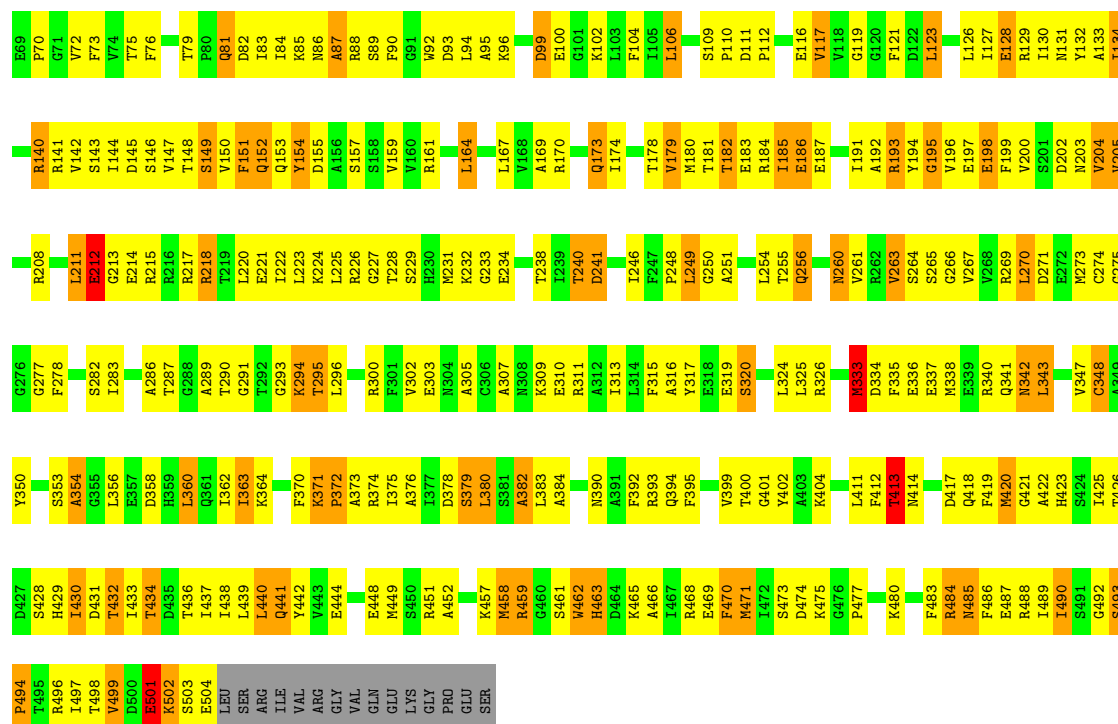
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



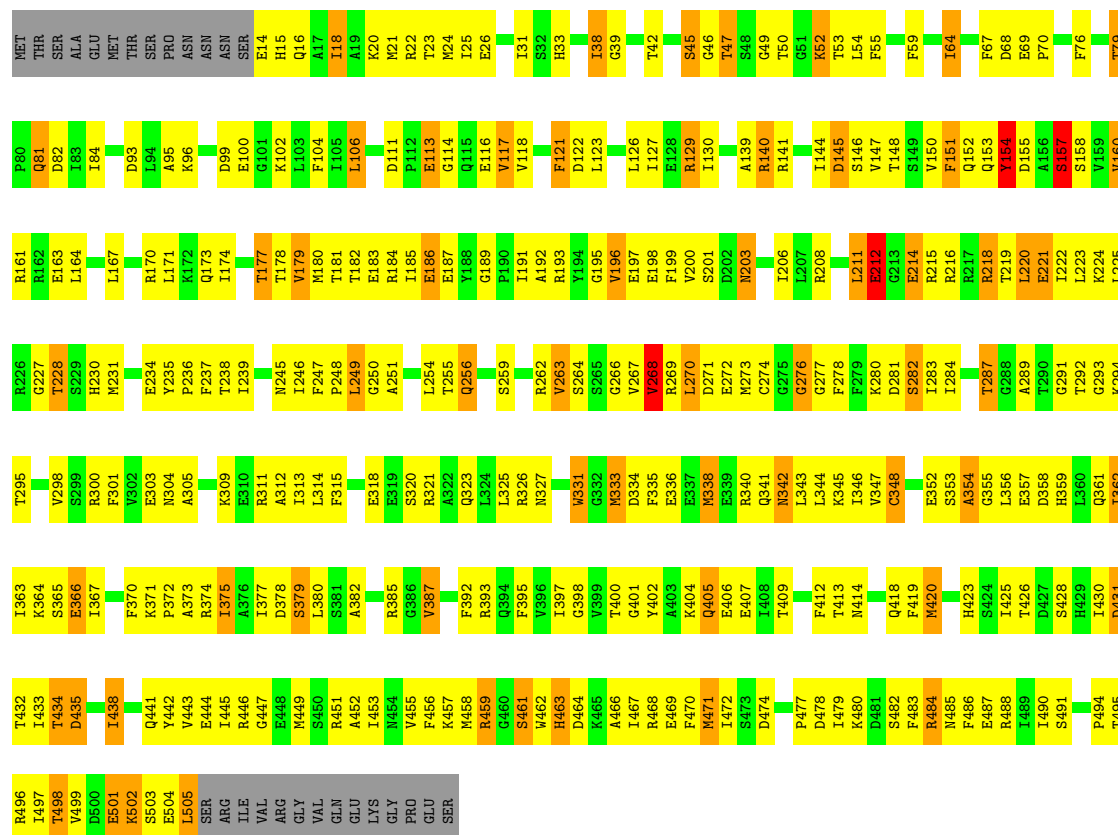
• Molecule 1: Circadian clock protein kinase kaiC



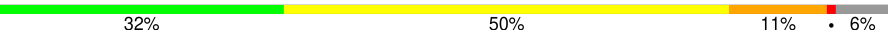


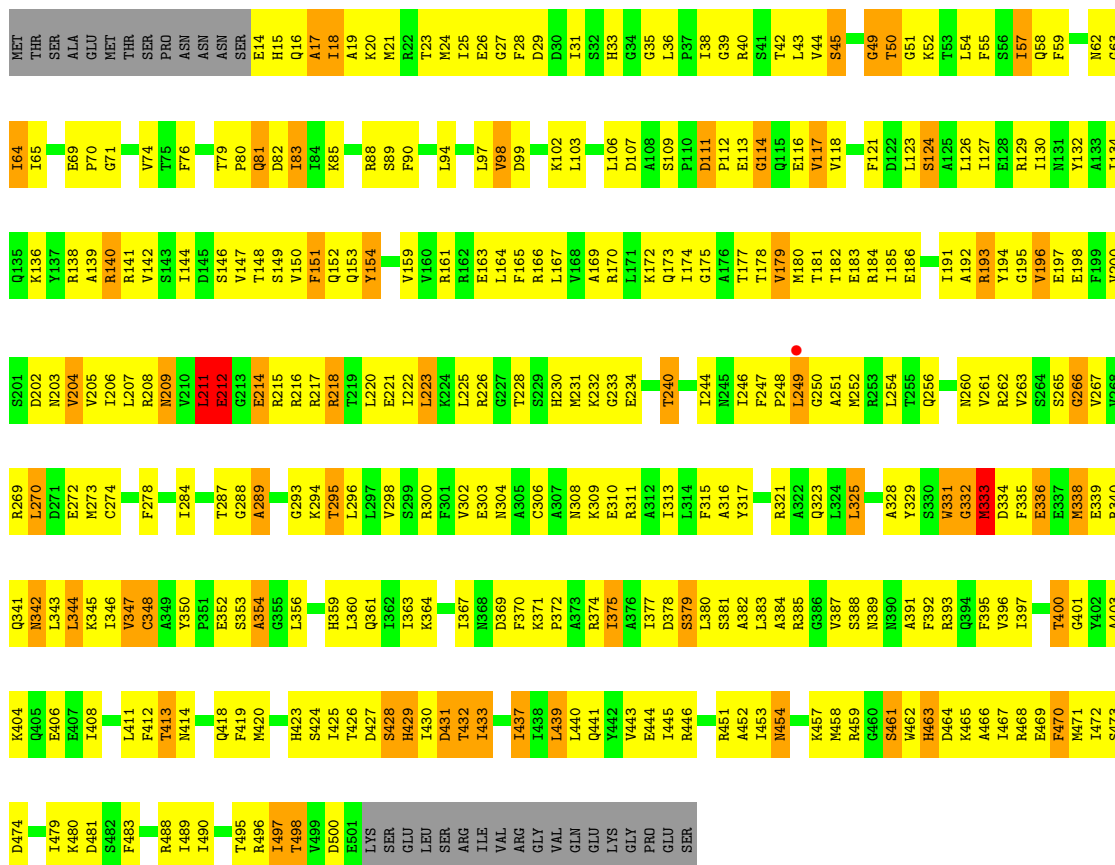
• Molecule 1: Circadian clock protein kinase kaiC

Chain E: 35% 48% 12% 5%

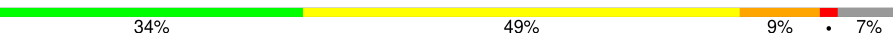


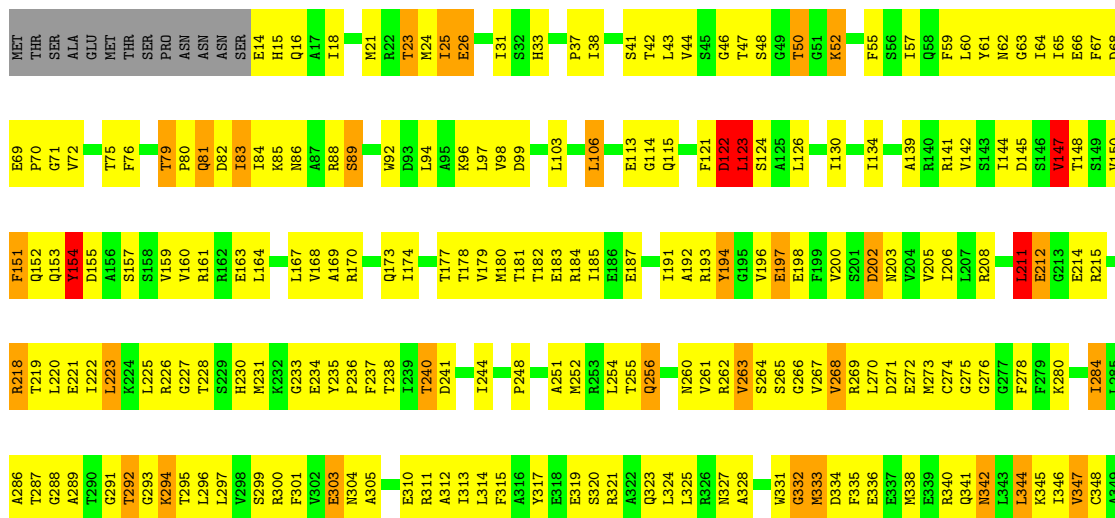
- Molecule 2: Circadian clock protein kinase kaiC

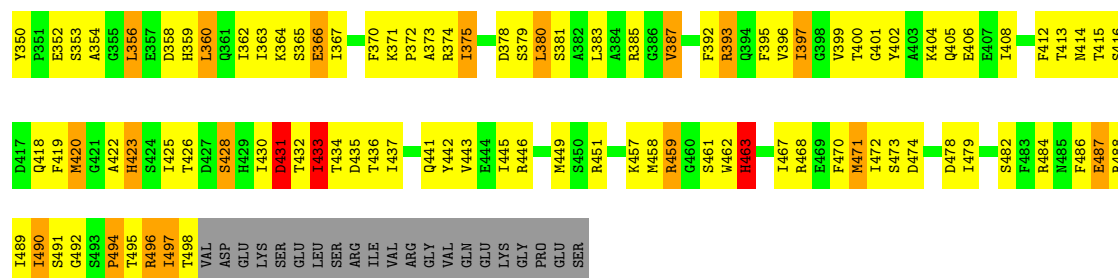
Chain C:  32% 50% 11% 6%



- Molecule 2: Circadian clock protein kinase kaiC

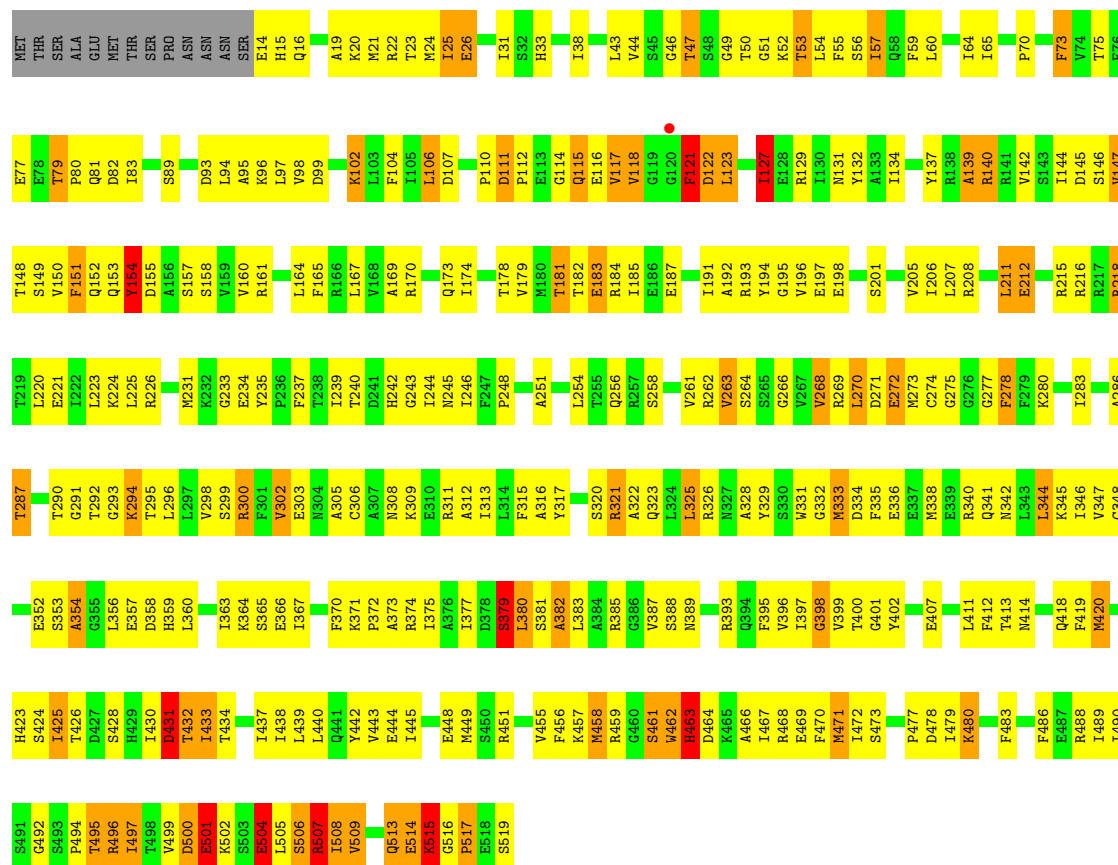
Chain D:  34% 49% 9% 7%





• Molecule 2: Circadian clock protein kinase kaiC

Chain F: 35% 49% 12% • •



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 30.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	81.4 (30.00-3.20) 90.9 (30.00-3.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 3.18Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.233 , 0.296 0.220 , 0.275	Depositor DCC
R_{free} test set	5684 reflections (9.76%)	wwPDB-VP
Wilson B-factor (Å ²)	82.9	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 70.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.028 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23855	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: MG, ATP, TPO

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	0.53	0/4045	1.08	21/5448 (0.4%)
1	B	0.49	0/3929	1.03	25/5293 (0.5%)
1	E	0.61	0/3937	1.09	18/5304 (0.3%)
2	C	0.54	0/3913	1.05	22/5275 (0.4%)
2	D	0.58	0/3889	1.06	17/5242 (0.3%)
2	F	0.59	0/4053	1.12	32/5461 (0.6%)
All	All	0.56	0/23766	1.07	135/32023 (0.4%)

There are no bond length outliers.

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	380	LEU	N-CA-C	-12.57	96.44	112.90
2	D	380	LEU	N-CA-C	-11.43	98.56	111.82
2	C	459	ARG	N-CA-C	10.72	122.54	111.07
1	A	380	LEU	N-CA-C	-10.20	100.10	112.54
1	A	98	VAL	N-CA-C	-9.34	101.46	110.42
1	A	507	ARG	N-CA-C	-9.27	101.73	113.23
1	B	502	LYS	N-CA-C	-8.55	101.99	114.39
2	F	373	ALA	N-CA-C	-8.40	103.47	114.31
1	B	430	ILE	N-CA-C	-8.34	104.89	112.90
1	A	116	GLU	N-CA-C	8.23	123.12	110.36
2	D	459	ARG	N-CA-C	8.13	122.15	111.75
2	D	433	ILE	N-CA-C	-7.86	101.45	113.16
1	E	435	ASP	N-CA-C	7.84	119.73	111.03
2	D	294	LYS	N-CA-C	-7.75	102.77	111.14
1	B	294	LYS	N-CA-C	-7.65	102.54	111.03
1	B	266	GLY	N-CA-C	-7.63	103.95	114.64
1	B	382	ALA	N-CA-C	-7.59	102.67	112.23
2	F	294	LYS	N-CA-C	-7.56	103.11	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	459	ARG	N-CA-C	7.54	121.39	111.75
2	F	382	ALA	N-CA-C	-7.47	101.28	112.04
1	A	194	TYR	N-CA-C	7.37	122.46	113.17
1	E	331	TRP	N-CA-C	-7.29	104.33	112.57
2	D	16	GLN	N-CA-C	7.23	119.91	109.14
2	F	499	VAL	N-CA-C	-7.15	102.51	113.16
1	E	362	ILE	N-CA-C	-7.09	103.87	110.53
1	E	155	ASP	N-CA-C	7.08	120.15	109.95
2	F	235	TYR	CA-C-N	7.06	126.98	119.85
2	F	235	TYR	C-N-CA	7.06	126.98	119.85
2	F	266	GLY	N-CA-C	-7.04	106.70	115.08
2	C	332	GLY	N-CA-C	-6.98	102.87	111.45
1	B	152	GLN	N-CA-C	-6.96	105.59	112.97
2	F	114	GLY	N-CA-C	6.86	121.96	112.57
1	B	380	LEU	N-CA-C	-6.85	103.89	111.36
2	D	373	ALA	N-CA-C	-6.82	105.09	113.41
1	B	173	GLN	N-CA-C	-6.80	103.48	111.03
1	B	413	THR	N-CA-C	6.75	119.74	108.73
1	A	114	GLY	N-CA-C	6.73	121.15	112.54
2	F	25	ILE	N-CA-C	-6.72	100.06	109.21
1	A	459	ARG	N-CA-C	6.66	118.62	111.36
1	E	480	LYS	N-CA-C	6.65	114.23	108.78
2	D	393	ARG	N-CA-C	-6.61	103.18	111.11
1	B	373	ALA	N-CA-C	-6.60	104.95	114.12
2	C	214	GLU	N-CA-C	-6.59	103.84	112.41
2	C	433	ILE	N-CA-C	-6.56	106.07	111.91
1	E	145	ASP	N-CA-C	6.54	118.95	108.41
2	F	380	LEU	N-CA-C	-6.53	104.24	111.82
2	D	266	GLY	N-CA-C	-6.50	106.95	114.69
2	C	206	ILE	N-CA-C	6.45	116.91	107.37
1	A	508	ILE	N-CA-C	-6.43	105.08	111.77
2	D	147	VAL	N-CA-C	-6.32	104.17	110.62
2	F	147	VAL	N-CA-C	-6.25	103.28	111.09
2	F	111	ASP	CA-C-N	6.22	125.91	119.82
2	F	111	ASP	C-N-CA	6.22	125.91	119.82
2	C	433	ILE	CB-CA-C	-6.17	105.10	112.19
2	D	23	THR	N-CA-C	-6.16	105.90	113.41
1	A	514	GLU	N-CA-C	-6.11	104.23	113.89
1	A	502	LYS	N-CA-C	6.07	123.72	110.80
2	D	194	TYR	N-CA-C	6.04	120.27	113.02
1	E	214	GLU	N-CA-C	-6.03	104.74	114.09
2	F	121	PHE	N-CA-C	-5.99	105.93	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	272	GLU	N-CA-C	-5.97	104.69	111.14
2	F	111	ASP	N-CA-C	5.97	118.15	110.39
2	F	123	LEU	N-CA-C	-5.97	104.71	112.23
1	B	459	ARG	N-CA-C	5.96	117.78	111.28
2	D	64	ILE	CB-CA-C	-5.95	104.11	112.14
2	F	432	THR	N-CA-C	5.91	120.10	113.01
2	F	513	GLN	N-CA-C	5.77	118.26	109.95
1	B	439	LEU	N-CA-C	5.76	118.19	107.99
1	A	476	GLY	CA-C-N	5.75	127.03	119.84
1	A	476	GLY	C-N-CA	5.75	127.03	119.84
2	F	155	ASP	N-CA-C	5.71	118.09	109.41
1	B	493	SER	CA-C-N	5.70	126.97	119.84
1	B	493	SER	C-N-CA	5.70	126.97	119.84
2	C	152	GLN	N-CA-C	-5.69	104.98	112.72
2	F	122	ASP	N-CA-C	-5.69	106.17	113.23
1	A	241	ASP	N-CA-C	-5.67	106.36	113.28
2	C	331	TRP	N-CA-C	-5.67	104.94	112.94
2	F	102	LYS	N-CA-C	-5.67	106.53	113.50
2	F	233	GLY	N-CA-C	5.67	119.19	112.33
1	B	343	LEU	N-CA-C	-5.67	107.36	114.56
2	C	222	ILE	N-CA-C	-5.67	98.89	107.73
1	A	308	ASN	N-CA-C	-5.64	104.62	112.30
1	E	64	ILE	N-CA-C	5.64	117.15	111.00
2	C	204	VAL	N-CA-C	5.64	116.25	107.28
1	A	331	TRP	N-CA-C	-5.64	105.74	113.30
1	B	282	SER	N-CA-C	5.64	117.10	108.42
2	D	202	ASP	N-CA-C	-5.62	105.54	112.90
1	B	241	ASP	N-CA-C	-5.62	106.43	113.28
1	B	434	THR	N-CA-C	5.60	118.35	109.50
2	C	461	SER	N-CA-C	5.60	117.13	109.18
2	C	474	ASP	N-CA-C	-5.58	106.64	113.50
2	D	332	GLY	N-CA-C	-5.58	102.11	112.37
2	F	272	GLU	N-CA-C	-5.56	104.24	111.02
2	F	495	THR	N-CA-C	-5.56	99.96	109.24
1	B	307	ALA	N-CA-C	-5.51	105.81	112.54
2	C	369	ASP	N-CA-C	-5.51	106.55	113.72
1	A	164	LEU	N-CA-C	-5.49	104.99	110.97
2	C	413	THR	N-CA-C	5.46	117.32	108.41
1	B	131	ASN	N-CA-C	-5.44	105.45	111.71
2	C	266	GLY	N-CA-C	-5.44	108.21	114.69
1	B	277	GLY	N-CA-C	5.43	118.63	111.52
2	C	209	ASN	N-CA-C	-5.38	101.47	109.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	461	SER	N-CA-C	5.35	116.91	109.31
1	E	373	ALA	N-CA-C	-5.34	105.59	113.61
1	E	220	LEU	N-CA-C	-5.34	100.32	109.24
1	B	371	LYS	CA-C-N	5.34	126.51	119.84
1	B	371	LYS	C-N-CA	5.34	126.51	119.84
1	E	434	THR	N-CA-C	5.32	118.11	109.06
1	A	307	ALA	N-CA-C	-5.32	106.18	113.30
2	F	127	ILE	N-CA-C	-5.31	105.32	110.42
2	D	145	ASP	N-CA-C	5.29	116.88	108.67
1	B	99	ASP	N-CA-C	-5.28	105.60	111.36
2	F	290	THR	N-CA-C	-5.27	103.18	110.35
2	C	272	GLU	N-CA-C	-5.25	104.62	111.02
2	C	380	LEU	N-CA-C	-5.23	105.58	111.28
2	D	25	ILE	N-CA-C	-5.22	102.32	109.37
2	C	437	ILE	N-CA-C	5.22	115.89	106.61
2	F	57	ILE	CB-CA-C	-5.21	105.03	111.70
1	E	158	SER	N-CA-C	5.20	116.64	111.07
2	F	139	ALA	N-CA-C	5.17	118.14	110.48
2	D	482	SER	N-CA-C	5.15	116.74	110.41
1	E	18	ILE	N-CA-C	5.15	116.05	109.30
1	A	516	GLY	N-CA-C	-5.14	101.86	112.34
2	F	22	ARG	N-CA-C	5.13	117.98	109.46
1	A	30	ASP	N-CA-C	-5.12	107.10	113.55
1	E	129	ARG	N-CA-C	-5.12	105.70	111.28
2	C	98	VAL	N-CA-C	-5.10	105.44	111.00
2	C	49	GLY	N-CA-C	5.09	122.35	115.32
2	F	463	HIS	N-CA-C	5.05	121.56	110.80
2	F	395	PHE	N-CA-C	-5.05	105.24	111.40
1	A	178	THR	N-CA-C	5.04	117.55	110.14
2	C	404	LYS	N-CA-C	-5.03	105.99	112.68
1	A	117	VAL	N-CA-C	5.02	119.78	109.34
1	B	204	VAL	N-CA-C	5.02	115.20	107.77
1	E	157	SER	N-CA-C	5.01	121.47	110.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3991	0	3984	355	0
1	B	3876	0	3861	347	0
1	E	3884	0	3873	360	0
2	C	3848	0	3838	355	0
2	D	3824	0	3819	351	0
2	F	3987	0	3984	400	0
3	A	5	0	0	0	0
3	B	1	0	0	0	0
3	C	4	0	0	0	0
3	D	3	0	0	0	0
3	E	4	0	0	0	0
3	F	3	0	0	0	0
4	A	62	0	24	5	0
4	B	62	0	24	7	0
4	C	62	0	24	4	0
4	D	62	0	24	6	0
4	E	62	0	24	6	0
4	F	62	0	24	9	0
5	A	7	0	0	1	0
5	B	5	0	0	2	0
5	C	5	0	0	1	0
5	D	10	0	0	2	0
5	E	7	0	0	1	0
5	F	19	0	0	4	0
All	All	23855	0	23503	2053	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 43.

All (2053) 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:E:305:ALA:HB2	1:E:374:ARG:HD2	1.16	1.14
1:A:14:GLU:HG3	1:A:15:HIS:H	1.13	1.13
2:F:115:GLN:HG2	2:F:116:GLU:N	1.56	1.13
1:B:449:MET:HE3	2:C:467:ILE:HD11	1.26	1.12
2:F:115:GLN:HG2	2:F:116:GLU:H	0.97	1.10
1:A:140:ARG:HB3	1:A:140:ARG:HH11	1.14	1.08
1:B:300:ARG:HA	1:B:333:MET:HE1	1.37	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ALA:HB2	1:A:374:ARG:HD2	1.40	1.04
1:B:140:ARG:HB3	1:B:140:ARG:HH11	1.21	1.03
1:B:147:VAL:HG11	1:B:180:MET:HE3	1.41	1.03
2:C:313:ILE:HG12	2:C:345:LYS:HB3	1.35	1.03
2:F:305:ALA:HB2	2:F:374:ARG:HD2	1.39	1.02
1:A:467:ILE:HD11	2:F:449:MET:HE3	1.43	1.00
1:B:496:ARG:HG2	1:B:498:THR:HG23	1.44	0.99
2:F:263:VAL:HG12	2:F:374:ARG:HH21	1.25	0.98
2:F:127:ILE:HD11	2:F:167:LEU:HA	1.42	0.98
1:B:305:ALA:HB2	1:B:374:ARG:HD2	1.46	0.97
2:D:182:THR:HG21	2:D:192:ALA:HB1	1.46	0.96
2:D:371:LYS:HD2	2:D:371:LYS:O	1.66	0.95
1:A:370:PHE:HD2	1:A:372:PRO:HG3	1.30	0.95
1:E:449:MET:HE3	2:F:467:ILE:HD11	1.47	0.94
2:C:31:ILE:HG23	2:C:231:MET:HB2	1.48	0.94
1:A:140:ARG:HB3	1:A:140:ARG:NH1	1.84	0.92
1:E:79:THR:HG23	1:E:81:GLN:HG2	1.49	0.92
2:D:18:ILE:H	2:D:18:ILE:HD12	1.35	0.92
2:D:70:PRO:HB2	2:D:139:ALA:HA	1.51	0.91
1:E:263:VAL:HG12	1:E:374:ARG:HH21	1.32	0.91
1:E:323:GLN:HE22	2:F:459:ARG:HD3	1.34	0.91
1:A:483:PHE:HB2	1:A:489:ILE:HD11	1.51	0.90
1:B:47:THR:O	1:B:50:THR:HG23	1.72	0.90
1:A:207:LEU:HD21	1:A:220:LEU:HD12	1.53	0.90
1:A:425:ILE:HG21	1:A:431:ASP:HB3	1.54	0.90
1:B:263:VAL:HG12	1:B:374:ARG:HH21	1.36	0.90
1:E:420:MET:HE1	2:F:490:ILE:HG13	1.52	0.90
2:F:191:ILE:HG13	2:F:206:ILE:HD11	1.53	0.90
1:A:147:VAL:HG11	1:A:180:MET:HE3	1.51	0.90
2:F:161:ARG:HB2	2:F:196:VAL:HG11	1.52	0.89
2:F:191:ILE:HB	2:F:198:GLU:HG2	1.54	0.89
1:B:140:ARG:HB3	1:B:140:ARG:NH1	1.88	0.89
1:E:283:ILE:HG13	1:E:400:THR:HG23	1.54	0.89
1:B:191:ILE:HB	1:B:198:GLU:CD	1.97	0.89
2:F:191:ILE:HB	2:F:198:GLU:CG	2.03	0.89
2:C:287:THR:HG23	2:C:414:ASN:HD22	1.37	0.88
2:C:371:LYS:O	2:C:371:LYS:HD2	1.73	0.88
1:A:79:THR:HG23	1:A:81:GLN:HG2	1.53	0.88
1:A:425:ILE:HG22	1:A:426:THR:HG23	1.55	0.88
2:C:323:GLN:HE22	2:D:459:ARG:HD3	1.39	0.88
1:A:24:MET:HB2	1:A:62:ASN:HD22	1.38	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:ARG:HE	2:F:488:ARG:HH12	1.20	0.87
2:D:248:PRO:HB2	2:D:251:ALA:HB3	1.54	0.87
1:E:323:GLN:NE2	2:F:459:ARG:HD3	1.90	0.87
2:C:344:LEU:HD22	2:C:345:LYS:N	1.89	0.87
2:F:140:ARG:HB3	2:F:140:ARG:HH11	1.38	0.87
1:A:379:SER:H	1:A:413:THR:HB	1.39	0.86
1:B:161:ARG:NH2	1:B:199:PHE:HB2	1.91	0.86
2:D:41:SER:HB3	2:D:178:THR:HB	1.57	0.86
2:F:379:SER:H	2:F:413:THR:HB	1.39	0.86
2:D:379:SER:H	2:D:413:THR:HB	1.40	0.86
1:A:318:GLU:OE2	1:B:432:TPO:HG21	1.75	0.86
2:D:449:MET:HE3	1:E:467:ILE:HD11	1.58	0.86
2:F:47:THR:HG23	5:F:522:HOH:O	1.74	0.85
1:B:497:ILE:HD12	1:B:498:THR:N	1.90	0.85
1:A:14:GLU:CG	1:A:15:HIS:H	1.88	0.85
1:B:146:SER:H	1:B:181:THR:HB	1.41	0.85
2:D:431:ASP:HA	2:D:434:THR:HG22	1.58	0.85
2:C:45:SER:HB2	2:C:182:THR:HB	1.59	0.85
2:C:344:LEU:HD22	2:C:345:LYS:H	1.42	0.85
2:D:89:SER:HB2	1:E:227:GLY:O	1.77	0.84
1:E:33:HIS:HD2	1:E:230:HIS:HA	1.42	0.84
1:E:289:ALA:HB2	1:E:419:PHE:HA	1.58	0.84
2:C:287:THR:HG21	2:C:425:ILE:O	1.76	0.84
1:B:170:ARG:O	1:B:174:ILE:HG12	1.78	0.83
1:B:273:MET:HE3	1:B:468:ARG:HD2	1.59	0.83
1:E:371:LYS:HD2	1:E:371:LYS:O	1.78	0.83
1:A:315:PHE:HE1	1:A:375:ILE:HG12	1.44	0.83
2:D:221:GLU:HG3	2:D:233:GLY:O	1.79	0.83
2:D:214:GLU:HB3	1:E:234:GLU:HB2	1.60	0.83
1:E:418:GLN:HB2	2:F:423:HIS:O	1.79	0.83
1:E:163:GLU:HA	1:E:163:GLU:OE2	1.76	0.83
1:B:492:GLY:O	1:B:494:PRO:HD3	1.79	0.82
2:D:147:VAL:O	2:D:150:VAL:HG12	1.79	0.82
1:A:488:ARG:HE	2:F:488:ARG:NH1	1.78	0.82
2:D:161:ARG:HB2	2:D:196:VAL:HG11	1.61	0.82
2:F:50:THR:HA	5:F:534:HOH:O	1.80	0.82
2:D:393:ARG:O	2:D:397:ILE:HG12	1.78	0.82
1:E:263:VAL:CG1	1:E:374:ARG:HH21	1.93	0.81
1:A:140:ARG:HH11	1:A:140:ARG:CB	1.93	0.81
1:B:147:VAL:O	1:B:150:VAL:HG12	1.79	0.81
2:C:94:LEU:O	2:C:98:VAL:HG23	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:79:THR:CG2	1:E:81:GLN:HG2	2.10	0.81
2:F:515:LYS:HG3	2:F:516:GLY:H	1.45	0.81
1:B:379:SER:OG	1:B:382:ALA:HB2	1.81	0.81
1:E:300:ARG:HA	1:E:333:MET:HE1	1.62	0.81
1:E:305:ALA:CB	1:E:374:ARG:HD2	2.08	0.81
2:F:269:ARG:HB3	2:F:479:ILE:HD12	1.60	0.81
2:F:486:PHE:HE2	2:F:496:ARG:HD2	1.45	0.81
2:C:164:LEU:HD11	2:C:197:GLU:HG3	1.62	0.81
2:C:134:ILE:HG23	2:C:139:ALA:HB3	1.63	0.81
1:B:140:ARG:HH11	1:B:140:ARG:CB	1.94	0.80
1:A:441:GLN:HE22	1:A:490:ILE:HD13	1.47	0.80
1:B:287:THR:HG23	1:B:414:ASN:HD22	1.44	0.80
2:F:287:THR:HG21	2:F:425:ILE:O	1.82	0.80
2:D:471:MET:HE2	2:D:478:ASP:HB2	1.65	0.79
2:F:79:THR:HG23	2:F:81:GLN:HG2	1.64	0.79
2:F:115:GLN:CG	2:F:116:GLU:H	1.88	0.79
1:E:425:ILE:HB	1:E:431:ASP:OD2	1.81	0.79
1:B:31:ILE:HG22	1:B:222:ILE:HD12	1.64	0.79
1:E:93:ASP:OD2	1:E:96:LYS:HB2	1.82	0.79
1:A:448:GLU:HG2	1:B:466:ALA:HA	1.62	0.79
1:E:170:ARG:O	1:E:174:ILE:HG12	1.83	0.79
1:B:45:SER:HB3	1:B:182:THR:HB	1.65	0.78
2:F:486:PHE:CE2	2:F:496:ARG:HD2	2.18	0.78
1:B:393:ARG:HH21	1:B:429:HIS:HB2	1.46	0.78
2:D:212:GLU:HG2	2:D:212:GLU:O	1.82	0.78
2:D:496:ARG:HG2	1:E:487:GLU:OE1	1.83	0.78
2:D:379:SER:HA	2:D:413:THR:O	1.82	0.78
2:F:148:THR:HG21	2:F:193:ARG:HD2	1.63	0.78
1:A:14:GLU:HG3	1:A:15:HIS:N	1.94	0.78
2:D:262:ARG:HD2	2:D:276:GLY:O	1.84	0.78
2:C:323:GLN:NE2	2:D:459:ARG:HD3	1.98	0.78
2:C:123:LEU:HD22	2:C:127:ILE:HD11	1.64	0.77
2:F:148:THR:CG2	2:F:193:ARG:HD2	2.14	0.77
2:F:231:MET:HE1	2:F:251:ALA:HB2	1.67	0.77
2:D:471:MET:HG3	2:D:478:ASP:HB3	1.67	0.77
2:F:269:ARG:HG2	2:F:479:ILE:HB	1.66	0.77
2:F:363:ILE:O	2:F:367:ILE:HG13	1.85	0.77
2:C:269:ARG:O	2:C:273:MET:HG3	1.84	0.77
2:C:36:LEU:HD12	2:C:59:PHE:CE1	2.19	0.77
2:C:123:LEU:HD21	2:C:167:LEU:HB2	1.66	0.77
2:F:501:GLU:HG3	2:F:502:LYS:H	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:MET:HB2	1:B:463:HIS:HD2	1.49	0.77
2:D:315:PHE:CZ	2:D:363:ILE:HG23	2.20	0.77
2:C:495:THR:HA	2:D:487:GLU:OE2	1.84	0.76
1:E:441:GLN:HE22	1:E:490:ILE:HD13	1.48	0.76
2:F:263:VAL:CG1	2:F:374:ARG:HH21	1.98	0.76
2:D:332:GLY:O	2:D:333:MET:HG2	1.84	0.76
1:A:433:ILE:HG22	1:A:433:ILE:O	1.85	0.76
1:A:248:PRO:HB2	1:A:251:ALA:HB3	1.66	0.76
1:E:441:GLN:NE2	1:E:490:ILE:HD13	2.00	0.76
2:C:471:MET:HB3	2:C:480:LYS:HZ3	1.48	0.76
2:D:356:LEU:HD22	2:D:387:VAL:HG11	1.67	0.76
1:E:147:VAL:O	1:E:150:VAL:HG12	1.86	0.76
2:C:335:PHE:HA	2:C:338:MET:HG3	1.67	0.76
1:A:18:ILE:H	1:A:18:ILE:HD12	1.50	0.76
1:A:83:ILE:H	1:A:83:ILE:HD12	1.50	0.76
1:B:300:ARG:CA	1:B:333:MET:HE1	2.15	0.76
2:D:345:LYS:HZ3	2:D:366:GLU:HG2	1.50	0.76
1:A:67:PHE:HB2	1:A:69:GLU:HG3	1.66	0.76
2:D:471:MET:HE1	2:D:473:SER:OG	1.86	0.76
2:F:299:SER:C	2:F:333:MET:HE1	2.09	0.75
2:F:146:SER:H	2:F:181:THR:HG22	1.51	0.75
2:D:256:GLN:HG3	2:D:404:LYS:HD3	1.68	0.75
1:E:446:ARG:NH2	1:E:496:ARG:HH22	1.84	0.75
1:E:147:VAL:HG11	1:E:180:MET:HE3	1.67	0.75
2:F:115:GLN:CG	2:F:116:GLU:N	2.43	0.75
2:C:418:GLN:HB2	2:D:423:HIS:O	1.87	0.74
2:F:344:LEU:HD11	2:F:346:ILE:HG13	1.69	0.74
2:C:170:ARG:O	2:C:174:ILE:HG12	1.85	0.74
2:D:130:ILE:O	2:D:134:ILE:HG13	1.87	0.74
1:B:273:MET:O	1:B:463:HIS:HA	1.87	0.74
2:D:114:GLY:O	2:D:115:GLN:HG3	1.87	0.74
1:E:356:LEU:HD11	1:E:387:VAL:HG21	1.68	0.74
1:E:269:ARG:HB3	1:E:479:ILE:HD12	1.68	0.74
2:F:501:GLU:HG3	2:F:502:LYS:N	2.03	0.74
2:C:347:VAL:O	2:C:348:CYS:HB2	1.88	0.74
2:D:44:VAL:HG22	2:D:205:VAL:HB	1.69	0.74
1:E:309:LYS:HA	1:E:343:LEU:HD13	1.68	0.74
2:F:178:THR:HG22	2:F:179:VAL:H	1.53	0.74
1:A:495:THR:HG22	1:A:497:ILE:HG23	1.70	0.74
1:A:21:MET:HE3	1:A:141:ARG:CZ	2.18	0.73
2:D:46:GLY:HA2	5:D:521:HOH:O	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:451:ARG:HB3	2:D:470:PHE:CE2	2.23	0.73
1:E:313:ILE:HG13	1:E:372:PRO:CG	2.16	0.73
2:D:431:ASP:HA	2:D:434:THR:CG2	2.18	0.73
2:F:371:LYS:O	2:F:371:LYS:HD2	1.88	0.73
1:E:216:ARG:NH2	2:F:223:LEU:HD21	2.03	0.73
2:D:293:GLY:HA2	4:D:901:ATP:O1A	1.89	0.73
1:B:147:VAL:HG11	1:B:180:MET:CE	2.16	0.73
1:B:471:MET:HB3	1:B:480:LYS:HZ1	1.54	0.73
2:C:79:THR:HG22	2:C:82:ASP:OD2	1.87	0.73
1:E:81:GLN:NE2	1:E:81:GLN:H	1.87	0.73
1:E:382:ALA:O	1:E:385:ARG:HG3	1.89	0.73
1:A:316:ALA:O	1:A:348:CYS:HA	1.89	0.73
1:A:265:SER:O	1:A:301:PHE:HA	1.89	0.73
1:B:418:GLN:HB2	2:C:423:HIS:O	1.89	0.73
2:D:31:ILE:HA	2:D:231:MET:HG3	1.69	0.73
1:A:183:GLU:HB2	1:B:199:PHE:CE1	2.24	0.72
1:E:287:THR:CG2	1:E:414:ASN:HD22	2.02	0.72
1:A:293:GLY:HA2	4:A:901:ATP:O1A	1.89	0.72
1:E:203:ASN:HB3	1:E:225:LEU:HD23	1.70	0.72
2:F:20:LYS:C	2:F:38:ILE:HD11	2.14	0.72
2:C:159:VAL:O	2:C:163:GLU:HG2	1.90	0.72
2:D:426:THR:HG22	2:D:428:SER:H	1.54	0.72
1:E:325:LEU:CD2	1:E:335:PHE:HB2	2.19	0.72
1:A:488:ARG:NE	2:F:488:ARG:HH12	1.87	0.72
2:D:497:ILE:HD12	2:D:497:ILE:O	1.88	0.72
1:A:21:MET:HE3	1:A:141:ARG:NE	2.04	0.72
1:B:212:GLU:HG2	1:B:212:GLU:O	1.86	0.72
2:C:396:VAL:HG11	2:C:433:ILE:HD11	1.71	0.72
2:D:347:VAL:O	2:D:348:CYS:HB2	1.90	0.72
2:F:382:ALA:O	2:F:385:ARG:HG3	1.89	0.72
2:F:437:ILE:HD12	2:F:457:LYS:HG2	1.69	0.72
1:E:451:ARG:HG2	1:E:451:ARG:HH11	1.54	0.72
1:A:266:GLY:HA3	1:A:300:ARG:O	1.89	0.72
1:A:178:THR:HG22	1:A:179:VAL:N	2.04	0.72
1:B:45:SER:CB	1:B:182:THR:HB	2.19	0.72
1:E:14:GLU:HG3	1:E:16:GLN:H	1.54	0.72
2:D:231:MET:HE1	2:D:251:ALA:HB2	1.70	0.72
1:E:191:ILE:HB	1:E:198:GLU:HG2	1.72	0.72
1:A:147:VAL:O	1:A:150:VAL:HG12	1.90	0.72
1:A:298:VAL:HG22	1:A:411:LEU:HD23	1.71	0.72
2:C:24:MET:HB2	2:C:62:ASN:HD22	1.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:SER:O	1:B:59:PHE:HB3	1.89	0.71
1:E:287:THR:HG23	1:E:414:ASN:HD22	1.55	0.71
2:F:208:ARG:NH2	2:F:221:GLU:OE2	2.22	0.71
2:C:70:PRO:HB2	2:C:139:ALA:HA	1.71	0.71
1:E:294:LYS:HB2	4:E:901:ATP:O1B	1.88	0.71
1:E:313:ILE:HG13	1:E:372:PRO:HG3	1.70	0.71
2:F:393:ARG:O	2:F:397:ILE:HG12	1.90	0.71
1:B:283:ILE:HD12	1:B:412:PHE:HE1	1.55	0.71
2:F:127:ILE:CD1	2:F:167:LEU:HA	2.20	0.71
1:A:79:THR:CG2	1:A:81:GLN:HG2	2.20	0.71
2:D:418:GLN:HB2	1:E:423:HIS:O	1.90	0.71
1:E:212:GLU:O	1:E:212:GLU:HG2	1.89	0.71
2:F:471:MET:HE3	2:F:471:MET:O	1.90	0.71
1:A:61:TYR:CZ	1:A:65:ILE:HG13	2.26	0.71
1:B:25:ILE:HG23	1:B:58:GLN:NE2	2.05	0.71
1:A:211:LEU:HD13	1:A:216:ARG:NE	2.06	0.71
1:A:264:SER:HA	1:A:271:ASP:OD1	1.91	0.71
1:A:305:ALA:CB	1:A:374:ARG:HD2	2.19	0.71
2:F:47:THR:O	2:F:52:LYS:HE2	1.90	0.71
2:D:449:MET:HE2	2:D:449:MET:HA	1.72	0.71
2:D:484:ARG:HB3	2:D:484:ARG:HH11	1.54	0.71
2:F:471:MET:HE2	2:F:478:ASP:HB2	1.72	0.71
1:A:211:LEU:O	1:A:212:GLU:HB3	1.89	0.71
2:D:148:THR:HG21	2:D:193:ARG:HD2	1.73	0.70
2:D:192:ALA:HB3	2:D:197:GLU:OE2	1.90	0.70
1:B:44:VAL:HA	1:B:205:VAL:O	1.90	0.70
2:D:31:ILE:HG22	2:D:222:ILE:HD12	1.73	0.70
1:E:363:ILE:HG22	1:E:367:ILE:HD11	1.72	0.70
2:C:367:ILE:HG12	2:C:375:ILE:HD11	1.72	0.70
2:D:170:ARG:O	2:D:174:ILE:HG12	1.92	0.70
2:F:191:ILE:HG13	2:F:206:ILE:CD1	2.22	0.70
1:A:451:ARG:HD2	1:A:451:ARG:N	2.06	0.70
1:B:360:LEU:O	1:B:360:LEU:HD22	1.91	0.70
1:E:45:SER:HB2	1:E:182:THR:O	1.92	0.70
2:C:393:ARG:HH21	2:C:429:HIS:HB2	1.56	0.69
2:D:197:GLU:H	2:D:197:GLU:CD	2.00	0.69
2:C:25:ILE:HG12	2:C:58:GLN:NE2	2.07	0.69
2:D:264:SER:HA	2:D:271:ASP:OD1	1.92	0.69
2:F:438:ILE:CD1	2:F:455:VAL:HG22	2.21	0.69
1:A:203:ASN:HB3	1:A:225:LEU:HD23	1.74	0.69
2:F:443:VAL:HG12	2:F:445:ILE:HG12	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:SER:O	1:A:333:MET:HE1	1.92	0.69
1:B:263:VAL:HG12	1:B:374:ARG:NH2	2.06	0.69
1:B:31:ILE:HA	1:B:231:MET:SD	2.33	0.69
2:C:45:SER:CB	2:C:182:THR:HB	2.22	0.69
2:D:486:PHE:CE2	2:D:496:ARG:HD3	2.27	0.69
1:B:191:ILE:HB	1:B:198:GLU:CG	2.22	0.69
2:D:218:ARG:HG3	2:D:237:PHE:O	1.93	0.69
2:C:451:ARG:HG2	2:C:451:ARG:HH11	1.57	0.69
2:F:287:THR:CG2	2:F:414:ASN:HD22	2.06	0.69
1:A:22:ARG:HH22	1:A:24:MET:HE1	1.58	0.69
1:A:438:ILE:HD11	1:A:455:VAL:HG22	1.75	0.69
1:B:150:VAL:HG13	1:B:151:PHE:N	2.08	0.69
1:E:140:ARG:HB3	1:E:140:ARG:HH11	1.57	0.69
1:B:286:ALA:HA	1:B:438:ILE:O	1.92	0.69
1:B:358:ASP:O	1:B:362:ILE:HG12	1.93	0.69
1:B:503:SER:O	1:B:504:GLU:HB2	1.94	0.69
2:D:305:ALA:HB2	2:D:374:ARG:HD2	1.73	0.69
2:F:336:GLU:HB3	2:F:340:ARG:NH2	2.08	0.69
2:F:44:VAL:HG22	2:F:205:VAL:HB	1.75	0.68
2:C:88:ARG:CZ	2:D:15:HIS:HA	2.23	0.68
2:C:439:LEU:C	2:C:439:LEU:HD12	2.17	0.68
2:F:283:ILE:HG23	2:F:412:PHE:CE1	2.28	0.68
2:F:79:THR:HG23	2:F:81:GLN:H	1.58	0.68
1:A:347:VAL:O	1:A:348:CYS:HB2	1.93	0.68
2:D:94:LEU:O	2:D:98:VAL:HG23	1.93	0.68
2:D:311:ARG:HD2	2:D:371:LYS:HE3	1.73	0.68
2:F:79:THR:HG22	2:F:82:ASP:H	1.56	0.68
1:E:469:GLU:HB3	1:E:483:PHE:CZ	2.28	0.68
1:B:169:ALA:O	1:B:173:GLN:HG3	1.94	0.68
1:B:202:ASP:HA	1:B:226:ARG:HD2	1.74	0.68
2:C:469:GLU:HG3	2:C:480:LYS:HE3	1.74	0.68
1:A:24:MET:HB2	1:A:62:ASN:ND2	2.09	0.68
2:C:202:ASP:HA	2:C:226:ARG:HD2	1.74	0.68
2:C:221:GLU:HG3	2:C:233:GLY:O	1.93	0.68
1:E:433:ILE:O	1:E:433:ILE:HG22	1.92	0.68
1:A:436:THR:HG23	1:A:458:MET:HG2	1.76	0.68
2:D:148:THR:CG2	2:D:193:ARG:HD2	2.23	0.68
2:D:437:ILE:HD12	2:D:457:LYS:HG2	1.74	0.68
2:F:347:VAL:O	2:F:348:CYS:HB2	1.93	0.68
2:C:218:ARG:HB3	5:C:522:HOH:O	1.94	0.68
2:D:313:ILE:HD12	2:D:372:PRO:HG2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ARG:NH2	1:A:407:GLU:HG2	2.09	0.68
1:A:360:LEU:HD22	1:A:364:LYS:HE3	1.74	0.68
1:A:287:THR:HG21	1:A:425:ILE:O	1.94	0.67
1:A:371:LYS:N	1:A:372:PRO:HD3	2.09	0.67
1:B:311:ARG:HD2	1:B:371:LYS:HE3	1.75	0.67
1:A:370:PHE:CD2	1:A:372:PRO:HG3	2.21	0.67
2:D:61:TYR:HH	2:D:92:TRP:CD1	2.12	0.67
2:D:347:VAL:HG12	2:D:348:CYS:N	2.08	0.67
2:D:383:LEU:HD13	2:D:395:PHE:HE2	1.59	0.67
2:F:492:GLY:O	2:F:494:PRO:HD3	1.95	0.67
1:A:296:LEU:HD13	1:A:331:TRP:CD2	2.29	0.67
1:A:320:SER:HA	1:B:254:LEU:HG	1.75	0.67
2:C:74:VAL:HG22	2:C:106:LEU:HD23	1.76	0.67
2:C:471:MET:HB3	2:C:480:LYS:NZ	2.09	0.67
2:C:182:THR:HG21	2:C:192:ALA:HB1	1.77	0.67
2:C:315:PHE:CE2	2:C:363:ILE:HA	2.29	0.67
2:C:140:ARG:NH1	2:C:140:ARG:HB3	2.10	0.67
2:F:46:GLY:HA2	2:F:184:ARG:HD2	1.77	0.67
2:F:431:ASP:O	2:F:434:THR:HG22	1.94	0.67
1:A:148:THR:HG21	1:A:193:ARG:HD2	1.75	0.67
2:C:308:ASN:O	2:C:310:GLU:HG3	1.94	0.67
2:D:370:PHE:O	2:D:371:LYS:HG3	1.95	0.67
1:E:152:GLN:HG3	2:F:161:ARG:HH11	1.60	0.67
1:A:18:ILE:HD12	1:A:18:ILE:N	2.10	0.67
2:C:18:ILE:HD12	2:C:18:ILE:N	2.10	0.67
2:D:194:TYR:O	2:D:196:VAL:HG23	1.95	0.67
1:A:492:GLY:O	1:A:494:PRO:HD3	1.95	0.66
2:F:311:ARG:HD2	2:F:371:LYS:HE3	1.77	0.66
2:F:514:GLU:HG2	2:F:519:SER:HB3	1.77	0.66
1:B:458:MET:HB2	1:B:463:HIS:CD2	2.29	0.66
2:C:140:ARG:HB3	2:C:140:ARG:HH11	1.61	0.66
2:C:350:TYR:CE1	2:D:252:MET:HE3	2.29	0.66
2:D:446:ARG:HB3	1:E:484:ARG:HG3	1.77	0.66
1:B:248:PRO:HB2	1:B:251:ALA:HB3	1.77	0.66
2:C:444:GLU:OE2	2:D:489:ILE:HG12	1.95	0.66
1:E:148:THR:OG1	1:E:182:THR:HG23	1.95	0.66
2:D:315:PHE:HA	2:D:347:VAL:HB	1.78	0.66
2:D:263:VAL:HG12	2:D:374:ARG:HH21	1.59	0.66
2:D:325:LEU:HD23	2:D:335:PHE:HB2	1.78	0.66
1:E:446:ARG:NH2	1:E:496:ARG:NH2	2.43	0.66
2:F:294:LYS:N	4:F:901:ATP:O1B	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ILE:O	1:A:367:ILE:HG13	1.95	0.66
2:C:21:MET:HE3	2:C:141:ARG:CZ	2.26	0.66
2:D:18:ILE:HD13	2:D:228:THR:HG23	1.76	0.66
2:D:79:THR:HG22	2:D:82:ASP:H	1.59	0.66
1:E:191:ILE:HB	1:E:198:GLU:CG	2.25	0.66
1:E:248:PRO:HB2	1:E:251:ALA:HB3	1.78	0.66
2:F:57:ILE:HD11	2:F:83:ILE:CG2	2.25	0.66
2:C:185:ILE:HD11	2:C:193:ARG:NH1	2.11	0.66
2:C:446:ARG:HA	2:C:496:ARG:NH2	2.11	0.66
2:D:255:THR:O	2:D:255:THR:HG22	1.96	0.66
1:E:214:GLU:HB3	2:F:234:GLU:HB2	1.77	0.66
1:E:504:GLU:OE1	1:E:505:LEU:HD23	1.95	0.66
2:F:293:GLY:HA2	4:F:901:ATP:O1A	1.95	0.66
1:A:299:SER:C	1:A:333:MET:HE1	2.21	0.66
2:D:487:GLU:OE1	2:D:497:ILE:HG12	1.95	0.66
2:F:79:THR:CG2	2:F:81:GLN:HG2	2.26	0.66
2:F:287:THR:HG23	2:F:414:ASN:HD22	1.59	0.66
2:C:123:LEU:HD13	2:C:166:ARG:HD2	1.76	0.66
2:F:325:LEU:CD2	2:F:335:PHE:HB2	2.26	0.66
2:F:377:ILE:HD12	2:F:412:PHE:HE2	1.60	0.66
1:A:287:THR:HG23	1:A:414:ASN:HB3	1.78	0.66
1:E:23:THR:O	1:E:24:MET:HB2	1.97	0.66
1:E:325:LEU:HD23	1:E:335:PHE:HB2	1.77	0.66
2:F:147:VAL:O	2:F:150:VAL:HG12	1.96	0.66
1:B:431:ASP:O	1:B:434:THR:HG22	1.96	0.65
1:E:76:PHE:HZ	1:E:126:LEU:HD21	1.61	0.65
1:A:215:ARG:NH1	1:B:232:LYS:O	2.28	0.65
2:F:215:ARG:HA	2:F:215:ARG:NE	2.10	0.65
2:F:57:ILE:HD11	2:F:83:ILE:HG23	1.77	0.65
2:F:280:LYS:NZ	2:F:407:GLU:HB3	2.11	0.65
2:C:359:HIS:O	2:C:363:ILE:HG13	1.96	0.65
2:C:370:PHE:O	2:C:371:LYS:HG3	1.96	0.65
2:D:340:ARG:C	2:D:342:ASN:H	2.04	0.65
1:A:344:LEU:HD11	1:A:346:ILE:HG13	1.77	0.65
1:B:315:PHE:CE2	1:B:347:VAL:HG21	2.31	0.65
1:E:497:ILE:HG22	1:E:498:THR:H	1.62	0.65
1:E:22:ARG:HD3	5:E:526:HOH:O	1.97	0.65
1:A:438:ILE:CD1	1:A:455:VAL:HG22	2.27	0.65
1:B:178:THR:HG22	1:B:179:VAL:N	2.11	0.65
2:C:406:GLU:O	2:C:408:ILE:HG13	1.97	0.65
2:F:283:ILE:HG23	2:F:412:PHE:HE1	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:430:ILE:O	2:C:432:THR:N	2.28	0.65
2:D:287:THR:HG23	2:D:414:ASN:HD22	1.61	0.65
1:E:426:THR:HG22	1:E:428:SER:H	1.61	0.65
2:F:311:ARG:HD2	2:F:371:LYS:CE	2.27	0.65
1:A:311:ARG:HD2	1:A:371:LYS:CE	2.27	0.65
2:C:54:LEU:HD13	2:C:90:PHE:CZ	2.31	0.65
2:D:151:PHE:C	2:D:153:GLN:H	2.05	0.65
2:F:93:ASP:OD1	2:F:95:ALA:HB3	1.97	0.65
1:A:419:PHE:CD2	1:B:425:ILE:HD12	2.32	0.65
2:C:273:MET:HE3	2:C:468:ARG:HD2	1.77	0.65
2:C:317:TYR:CD2	2:C:383:LEU:HD21	2.32	0.65
2:F:516:GLY:N	2:F:517:PRO:HD2	2.11	0.65
1:E:280:LYS:NZ	1:E:407:GLU:HB3	2.12	0.64
1:E:418:GLN:CB	2:F:423:HIS:O	2.44	0.64
1:E:451:ARG:N	1:E:451:ARG:HD2	2.12	0.64
2:F:178:THR:HG22	2:F:179:VAL:N	2.11	0.64
2:F:300:ARG:NH2	2:F:477:PRO:HD2	2.12	0.64
1:A:24:MET:CB	1:A:62:ASN:HD22	2.07	0.64
2:C:64:ILE:HG22	2:C:65:ILE:N	2.12	0.64
2:D:263:VAL:HG12	2:D:374:ARG:NH2	2.12	0.64
2:D:315:PHE:CD2	2:D:347:VAL:HG21	2.31	0.64
2:F:515:LYS:HG3	2:F:516:GLY:N	2.10	0.64
1:A:106:LEU:C	1:A:106:LEU:HD12	2.23	0.64
2:C:44:VAL:HG22	2:C:205:VAL:HB	1.79	0.64
2:C:64:ILE:HG21	2:C:97:LEU:HD13	1.77	0.64
2:F:377:ILE:CD1	2:F:399:VAL:HG11	2.27	0.64
1:E:225:LEU:HB2	1:E:230:HIS:HD2	1.63	0.64
2:F:20:LYS:C	2:F:38:ILE:CD1	2.71	0.64
2:C:269:ARG:HG2	2:C:479:ILE:HB	1.80	0.64
1:E:289:ALA:O	1:E:292:THR:HG23	1.98	0.64
1:E:320:SER:HA	2:F:254:LEU:HG	1.80	0.64
1:B:263:VAL:CG1	1:B:374:ARG:HH21	2.10	0.64
1:E:335:PHE:HA	1:E:338:MET:HG3	1.79	0.64
1:B:73:PHE:HE2	1:B:83:ILE:HD13	1.63	0.64
1:B:238:THR:HG22	1:B:240:THR:HG22	1.80	0.64
1:A:418:GLN:HB2	1:B:423:HIS:O	1.97	0.64
1:B:287:THR:HG21	1:B:425:ILE:O	1.97	0.64
2:C:396:VAL:HG21	2:C:430:ILE:HD12	1.80	0.64
2:D:41:SER:CB	2:D:178:THR:HB	2.27	0.64
2:D:267:VAL:HG23	2:D:300:ARG:HG2	1.79	0.64
2:D:451:ARG:HG2	2:D:451:ARG:HH11	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:THR:HA	1:A:235:TYR:O	1.98	0.63
2:C:43:LEU:HD11	2:C:182:THR:OG1	1.98	0.63
1:A:311:ARG:HB3	1:A:370:PHE:CE2	2.33	0.63
1:B:283:ILE:HG13	1:B:400:THR:HG23	1.79	0.63
1:E:104:PHE:CE2	1:E:106:LEU:HB2	2.34	0.63
1:E:426:THR:HG21	1:E:430:ILE:HG12	1.79	0.63
2:F:231:MET:CE	2:F:251:ALA:HB2	2.27	0.63
1:A:254:LEU:HG	2:F:320:SER:HA	1.80	0.63
1:A:191:ILE:HB	1:A:198:GLU:CG	2.28	0.63
2:D:495:THR:HG23	1:E:487:GLU:OE2	1.98	0.63
2:F:426:THR:HG22	2:F:428:SER:H	1.63	0.63
1:B:371:LYS:N	1:B:372:PRO:HD3	2.13	0.63
2:C:20:LYS:C	2:C:38:ILE:HD11	2.24	0.63
2:D:286:ALA:O	2:D:294:LYS:HG2	1.98	0.63
1:A:273:MET:O	1:A:463:HIS:HA	1.98	0.63
1:A:458:MET:O	4:F:901:ATP:H3'	1.97	0.63
1:B:73:PHE:CE2	1:B:83:ILE:HD13	2.33	0.63
1:B:338:MET:N	1:B:338:MET:HE2	2.14	0.63
2:C:220:LEU:HD23	2:C:221:GLU:N	2.13	0.63
1:E:59:PHE:CZ	1:E:141:ARG:HD3	2.34	0.63
1:E:185:ILE:HD11	1:E:193:ARG:NH1	2.13	0.63
1:E:344:LEU:C	1:E:344:LEU:HD13	2.23	0.63
1:A:184:ARG:O	1:A:185:ILE:HD13	1.98	0.63
2:C:21:MET:O	2:C:35:GLY:HA3	1.99	0.63
2:D:24:MET:HG3	2:D:66:GLU:HG3	1.80	0.63
1:A:356:LEU:HD13	1:A:387:VAL:HG21	1.81	0.63
1:B:305:ALA:HB2	1:B:374:ARG:CD	2.25	0.63
2:D:269:ARG:HG2	2:D:479:ILE:HB	1.79	0.63
2:F:344:LEU:HD22	2:F:345:LYS:N	2.13	0.63
1:A:451:ARG:HG2	1:A:451:ARG:HH11	1.63	0.62
1:E:451:ARG:HH12	1:E:472:ILE:HD12	1.64	0.62
1:A:313:ILE:HG13	1:A:372:PRO:HG2	1.81	0.62
2:F:298:VAL:HA	2:F:411:LEU:CD2	2.27	0.62
1:B:24:MET:HB2	1:B:62:ASN:HD22	1.64	0.62
1:B:203:ASN:HB3	1:B:225:LEU:HD23	1.81	0.62
1:A:425:ILE:CG2	1:A:431:ASP:HB3	2.27	0.62
2:F:80:PRO:HG2	2:F:107:ASP:HB2	1.81	0.62
2:F:334:ASP:OD1	2:F:336:GLU:HB2	1.99	0.62
2:F:504:GLU:O	2:F:505:LEU:HB2	1.98	0.62
1:B:194:TYR:O	1:B:195:GLY:C	2.41	0.62
2:D:303:GLU:O	2:D:303:GLU:HG2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:471:MET:HE2	2:D:478:ASP:CB	2.28	0.62
1:E:321:ARG:HG2	1:E:348:CYS:SG	2.40	0.62
2:F:140:ARG:HH11	2:F:140:ARG:CB	2.12	0.62
2:C:440:LEU:HD23	2:C:453:ILE:HG13	1.82	0.62
2:F:283:ILE:HG13	2:F:400:THR:HG23	1.82	0.62
2:C:24:MET:CB	2:C:62:ASN:HD22	2.12	0.62
2:C:382:ALA:O	2:C:385:ARG:HG3	1.98	0.62
2:D:430:ILE:O	2:D:433:ILE:HB	2.00	0.62
2:F:451:ARG:HB3	2:F:470:PHE:CE2	2.34	0.62
1:A:311:ARG:HD2	1:A:371:LYS:HE3	1.81	0.62
1:E:435:ASP:HA	1:E:459:ARG:HD2	1.81	0.62
1:E:461:SER:OG	1:E:462:TRP:N	2.28	0.62
1:B:296:LEU:HD21	1:B:477:PRO:HD3	1.81	0.62
1:B:379:SER:H	1:B:413:THR:HB	1.65	0.62
1:B:471:MET:HB3	1:B:480:LYS:NZ	2.15	0.62
2:D:304:ASN:HB3	2:D:374:ARG:HH12	1.64	0.62
1:A:284:ILE:HB	1:A:411:LEU:HD12	1.82	0.62
1:B:76:PHE:CZ	1:B:126:LEU:HD21	2.35	0.62
1:E:33:HIS:HD2	1:E:230:HIS:CA	2.10	0.62
2:F:344:LEU:HD22	2:F:345:LYS:H	1.65	0.61
1:A:311:ARG:HA	1:A:343:LEU:O	1.99	0.61
2:D:164:LEU:HD22	2:D:180:MET:HE1	1.80	0.61
1:E:344:LEU:HD22	1:E:345:LYS:H	1.65	0.61
2:F:371:LYS:O	2:F:371:LYS:CD	2.48	0.61
2:F:377:ILE:HD11	2:F:399:VAL:HG11	1.82	0.61
1:A:24:MET:N	1:A:29:ASP:OD2	2.34	0.61
1:A:274:CYS:HG	1:A:278:PHE:HE2	1.48	0.61
2:C:389:ASN:HD21	2:C:428:SER:HA	1.66	0.61
2:C:182:THR:HG22	2:C:183:GLU:N	2.15	0.61
2:D:155:ASP:OD1	2:D:159:VAL:HG11	1.98	0.61
2:D:269:ARG:O	2:D:272:GLU:HB2	2.00	0.61
1:E:455:VAL:HG11	1:E:463:HIS:HB2	1.82	0.61
1:B:116:GLU:HG2	1:B:117:VAL:H	1.66	0.61
2:D:161:ARG:CB	2:D:196:VAL:HG11	2.31	0.61
1:E:64:ILE:HD13	1:E:102:LYS:HB3	1.81	0.61
1:B:23:THR:O	1:B:24:MET:HB2	2.01	0.61
2:C:262:ARG:NH2	2:C:461:SER:HB2	2.15	0.61
2:F:248:PRO:HB2	2:F:251:ALA:HB3	1.82	0.61
2:F:439:LEU:O	2:F:440:LEU:HD23	1.99	0.61
1:B:418:GLN:HG3	1:B:418:GLN:O	2.01	0.61
2:D:344:LEU:HD13	2:D:344:LEU:C	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:377:ILE:HD12	1:E:412:PHE:CE2	2.35	0.61
1:A:80:PRO:HB2	1:A:81:GLN:NE2	2.16	0.61
1:A:225:LEU:O	1:A:226:ARG:C	2.43	0.61
2:D:287:THR:HG21	2:D:425:ILE:O	2.00	0.61
1:E:33:HIS:CD2	1:E:230:HIS:HA	2.32	0.61
2:F:38:ILE:N	2:F:38:ILE:HD12	2.16	0.61
2:F:296:LEU:HD13	2:F:331:TRP:CD2	2.36	0.61
1:A:319:GLU:O	1:B:254:LEU:HD21	2.01	0.61
1:A:323:GLN:NE2	1:B:459:ARG:HD3	2.15	0.61
2:F:169:ALA:O	2:F:173:GLN:HG3	2.01	0.61
2:F:500:ASP:O	2:F:501:GLU:HB3	2.00	0.61
1:A:360:LEU:CD2	1:A:364:LYS:HE3	2.31	0.60
1:B:436:THR:HG23	1:B:458:MET:HG2	1.83	0.60
2:C:287:THR:HG22	2:C:288:GLY:N	2.16	0.60
2:C:400:THR:HG22	2:C:401:GLY:N	2.16	0.60
2:D:383:LEU:HD13	2:D:395:PHE:CE2	2.35	0.60
1:E:441:GLN:HE22	1:E:490:ILE:HA	1.66	0.60
1:B:32:SER:OG	1:B:35:GLY:HA2	2.01	0.60
2:C:387:VAL:HG12	2:C:391:ALA:HB3	1.83	0.60
2:D:191:ILE:HB	2:D:198:GLU:CG	2.32	0.60
1:E:140:ARG:HB3	1:E:140:ARG:NH1	2.15	0.60
1:A:496:ARG:HG3	1:B:487:GLU:OE1	2.02	0.60
2:C:211:LEU:O	2:C:212:GLU:HB3	1.99	0.60
1:E:283:ILE:HG23	1:E:412:PHE:CE1	2.35	0.60
1:E:425:ILE:HD11	1:E:456:PHE:CE2	2.36	0.60
2:F:16:GLN:HE22	2:F:33:HIS:HB3	1.66	0.60
2:F:191:ILE:CB	2:F:198:GLU:HG2	2.27	0.60
2:F:303:GLU:OE2	2:F:333:MET:HB3	2.01	0.60
2:D:82:ASP:O	2:D:83:ILE:C	2.44	0.60
1:E:46:GLY:O	1:E:52:LYS:HE2	2.02	0.60
1:E:353:SER:O	1:E:354:ALA:HB2	2.00	0.60
1:B:150:VAL:O	1:B:153:GLN:HG3	2.02	0.60
2:D:334:ASP:OD1	2:D:336:GLU:HB2	2.02	0.60
2:C:426:THR:HG21	2:C:430:ILE:HG12	1.84	0.60
2:D:431:ASP:OD1	2:D:431:ASP:N	2.34	0.60
2:D:461:SER:OG	2:D:462:TRP:N	2.34	0.60
2:F:64:ILE:HG21	2:F:97:LEU:HD13	1.83	0.60
2:F:317:TYR:CD2	2:F:383:LEU:HD21	2.37	0.60
1:A:273:MET:SD	1:A:468:ARG:HD2	2.41	0.60
1:B:65:ILE:O	1:B:65:ILE:HG22	2.01	0.60
1:B:493:SER:HB3	2:C:488:ARG:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:350:TYR:CZ	1:E:254:LEU:HD13	2.37	0.60
2:D:371:LYS:N	2:D:372:PRO:HD3	2.16	0.60
1:E:280:LYS:HZ1	1:E:407:GLU:HB3	1.67	0.60
1:E:347:VAL:O	1:E:348:CYS:HB2	2.01	0.60
1:E:363:ILE:HG22	1:E:367:ILE:CD1	2.31	0.60
2:F:483:PHE:HB3	2:F:486:PHE:CD1	2.37	0.60
1:A:344:LEU:HD13	1:A:344:LEU:C	2.27	0.60
2:C:248:PRO:C	2:C:250:GLY:H	2.10	0.60
1:B:337:GLU:HB3	1:B:338:MET:CE	2.31	0.60
2:D:267:VAL:CG2	2:D:300:ARG:HG2	2.32	0.60
1:A:184:ARG:C	1:A:185:ILE:HD13	2.27	0.60
1:A:313:ILE:HG13	1:A:372:PRO:CG	2.32	0.60
2:C:240:THR:HG21	2:C:361:GLN:HE22	1.66	0.60
2:C:353:SER:O	2:C:354:ALA:HB2	2.02	0.60
2:F:53:THR:HG23	2:F:145:ASP:OD1	2.01	0.60
2:C:419:PHE:O	2:C:420:MET:HB2	2.00	0.59
1:E:303:GLU:OE2	1:E:333:MET:HB3	2.02	0.59
1:E:309:LYS:HA	1:E:343:LEU:CD1	2.31	0.59
1:A:22:ARG:NH2	1:A:24:MET:HE1	2.17	0.59
1:A:178:THR:CG2	1:A:179:VAL:N	2.65	0.59
2:F:60:LEU:CD1	2:F:73:PHE:HB2	2.32	0.59
1:B:123:LEU:HD13	1:B:123:LEU:O	2.03	0.59
2:C:191:ILE:HB	2:C:198:GLU:HG2	1.83	0.59
1:E:483:PHE:O	1:E:485:ASN:N	2.36	0.59
2:F:325:LEU:HD21	2:F:335:PHE:HB2	1.84	0.59
1:A:483:PHE:HB2	1:A:489:ILE:CD1	2.27	0.59
1:B:150:VAL:HG13	1:B:151:PHE:H	1.67	0.59
1:B:462:TRP:O	1:B:463:HIS:O	2.20	0.59
2:D:314:LEU:O	2:D:314:LEU:HG	2.02	0.59
2:D:344:LEU:HD11	2:D:346:ILE:HG13	1.83	0.59
1:E:192:ALA:HB3	1:E:197:GLU:OE2	2.02	0.59
1:B:289:ALA:HB2	1:B:419:PHE:HA	1.84	0.59
2:C:38:ILE:HG22	2:C:39:GLY:N	2.16	0.59
2:F:377:ILE:HD12	2:F:412:PHE:CE2	2.37	0.59
1:A:148:THR:CG2	1:A:193:ARG:HD2	2.31	0.59
1:A:457:LYS:HB2	4:F:901:ATP:O3'	2.03	0.59
1:B:104:PHE:HD2	1:B:133:ALA:HB1	1.67	0.59
1:B:274:CYS:HB3	1:B:458:MET:SD	2.43	0.59
1:B:350:TYR:CE1	2:C:252:MET:HE3	2.38	0.59
2:D:396:VAL:HG11	2:D:430:ILE:CG2	2.33	0.59
2:F:471:MET:HE2	2:F:478:ASP:CB	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:ILE:CG2	1:A:426:THR:HG23	2.32	0.59
2:C:147:VAL:O	2:C:150:VAL:HG12	2.02	0.59
1:E:346:ILE:HG22	1:E:347:VAL:N	2.18	0.59
1:A:207:LEU:CD2	1:A:220:LEU:HD12	2.30	0.59
1:B:170:ARG:HH12	1:B:174:ILE:HD11	1.68	0.59
2:D:23:THR:C	2:D:25:ILE:H	2.10	0.59
1:A:136:LYS:HD3	1:A:137:TYR:CE1	2.38	0.59
1:B:79:THR:HG23	1:B:81:GLN:HG2	1.83	0.59
1:E:193:ARG:NH2	2:F:195:GLY:O	2.29	0.59
2:F:80:PRO:CG	2:F:107:ASP:HB2	2.33	0.59
1:A:14:GLU:CG	1:A:15:HIS:N	2.60	0.59
1:B:149:SER:HB3	2:C:161:ARG:NH2	2.18	0.59
2:C:31:ILE:HA	2:C:231:MET:HG3	1.83	0.59
2:C:396:VAL:CG1	2:C:433:ILE:HD11	2.33	0.59
2:D:72:VAL:HB	2:D:142:VAL:HG22	1.85	0.59
2:D:484:ARG:HH11	2:D:484:ARG:CB	2.16	0.59
1:E:334:ASP:OD1	1:E:336:GLU:HB2	2.03	0.59
1:A:471:MET:HE2	1:A:478:ASP:HB3	1.85	0.58
2:D:363:ILE:O	2:D:367:ILE:HG13	2.02	0.58
2:D:419:PHE:CD2	1:E:425:ILE:HD12	2.37	0.58
2:F:299:SER:O	2:F:333:MET:HE1	2.03	0.58
2:C:334:ASP:OD1	2:C:336:GLU:HB2	2.03	0.58
2:D:431:ASP:C	2:D:432:THR:HG23	2.28	0.58
2:F:79:THR:CG2	2:F:82:ASP:H	2.16	0.58
1:B:311:ARG:HD2	1:B:371:LYS:CE	2.34	0.58
1:B:320:SER:HA	2:C:254:LEU:HG	1.84	0.58
2:C:106:LEU:CD2	2:C:130:ILE:HG12	2.33	0.58
2:D:315:PHE:CE1	2:D:363:ILE:HG23	2.38	0.58
1:A:501:GLU:O	1:A:503:SER:N	2.35	0.58
1:B:451:ARG:HH11	1:B:451:ARG:HG2	1.67	0.58
2:D:495:THR:HA	1:E:487:GLU:OE2	2.03	0.58
1:A:159:VAL:O	1:A:163:GLU:HG2	2.03	0.58
1:A:161:ARG:CB	1:A:196:VAL:HG11	2.34	0.58
1:A:227:GLY:O	2:F:89:SER:HB2	2.02	0.58
1:B:293:GLY:HA2	4:B:901:ATP:O1A	2.03	0.58
2:F:111:ASP:OD1	2:F:112:PRO:HD2	2.03	0.58
1:A:165:PHE:CE2	2:F:110:PRO:HG2	2.39	0.58
4:A:903:ATP:C2	1:B:229:SER:HB3	2.38	0.58
2:D:80:PRO:HA	2:D:83:ILE:HD12	1.84	0.58
1:E:123:LEU:O	1:E:127:ILE:HG13	2.03	0.58
2:F:118:VAL:O	2:F:118:VAL:HG13	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:312:ALA:O	2:D:344:LEU:HD22	2.04	0.58
1:E:81:GLN:H	1:E:81:GLN:CD	2.11	0.58
1:B:96:LYS:O	1:B:100:GLU:HG3	2.02	0.58
1:B:305:ALA:CB	1:B:374:ARG:HD2	2.29	0.58
2:C:300:ARG:HA	2:C:333:MET:HE1	1.85	0.58
1:E:264:SER:H	1:E:374:ARG:NH2	2.02	0.58
2:F:73:PHE:C	2:F:73:PHE:CD2	2.82	0.58
2:F:461:SER:OG	2:F:462:TRP:N	2.27	0.58
2:C:317:TYR:HE1	2:C:377:ILE:HG23	1.69	0.58
2:D:345:LYS:NZ	2:D:366:GLU:HG2	2.18	0.58
1:E:191:ILE:HG22	1:E:192:ALA:N	2.19	0.58
1:E:342:ASN:O	1:E:343:LEU:HD23	2.04	0.58
1:A:423:HIS:O	2:F:418:GLN:HB2	2.04	0.58
1:A:448:GLU:HG2	1:B:466:ALA:CA	2.31	0.58
2:F:464:ASP:OD2	2:F:466:ALA:HB3	2.03	0.58
2:C:296:LEU:HD13	2:C:331:TRP:CD2	2.39	0.57
2:C:393:ARG:O	2:C:397:ILE:HG12	2.03	0.57
2:D:182:THR:HG22	2:D:183:GLU:N	2.19	0.57
2:D:362:ILE:O	2:D:365:SER:HB3	2.03	0.57
1:E:151:PHE:C	1:E:153:GLN:H	2.12	0.57
1:A:359:HIS:O	1:A:363:ILE:HG13	2.04	0.57
1:B:184:ARG:HD2	1:B:191:ILE:O	2.04	0.57
1:E:356:LEU:HD12	1:E:356:LEU:N	2.19	0.57
1:E:453:ILE:HG22	1:E:470:PHE:HD2	1.69	0.57
2:F:218:ARG:NH1	2:F:239:ILE:HD12	2.19	0.57
1:A:337:GLU:HG3	1:A:341:GLN:OE1	2.04	0.57
1:B:129:ARG:O	1:B:132:TYR:HB3	2.05	0.57
1:B:337:GLU:HB3	1:B:338:MET:HE3	1.85	0.57
2:D:191:ILE:CG2	2:D:198:GLU:HG3	2.34	0.57
2:F:134:ILE:HD11	2:F:142:VAL:HG21	1.84	0.57
1:B:291:GLY:HA3	1:B:442:TYR:OH	2.05	0.57
2:C:248:PRO:O	2:C:250:GLY:N	2.37	0.57
1:E:262:ARG:HD2	1:E:276:GLY:O	2.03	0.57
1:E:344:LEU:HD22	1:E:345:LYS:N	2.19	0.57
1:E:445:ILE:O	1:E:446:ARG:HB2	2.05	0.57
2:C:63:GLY:HA3	2:C:141:ARG:CZ	2.34	0.57
2:C:317:TYR:CE2	2:C:383:LEU:HD21	2.39	0.57
2:D:443:VAL:HG12	2:D:445:ILE:HG12	1.86	0.57
1:E:266:GLY:HA2	1:E:304:ASN:HD22	1.70	0.57
1:E:268:VAL:O	1:E:271:ASP:HB2	2.05	0.57
2:C:451:ARG:HG2	2:C:451:ARG:NH1	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:117:VAL:HG13	2:F:154:TYR:OH	2.04	0.57
1:B:184:ARG:HH22	1:B:187:GLU:C	2.13	0.57
1:B:437:ILE:HD12	1:B:457:LYS:HG2	1.86	0.57
2:C:483:PHE:HB2	2:C:489:ILE:HD13	1.85	0.57
2:D:31:ILE:HA	2:D:231:MET:CG	2.34	0.57
2:D:178:THR:HG22	2:D:179:VAL:H	1.70	0.57
2:D:379:SER:OG	2:D:381:SER:OG	2.21	0.57
2:F:23:THR:O	2:F:24:MET:HB2	2.03	0.57
2:F:106:LEU:C	2:F:106:LEU:HD12	2.30	0.57
2:F:151:PHE:CZ	2:F:160:VAL:HG13	2.39	0.57
1:A:323:GLN:HE22	1:B:459:ARG:HD3	1.70	0.57
1:B:211:LEU:O	1:B:212:GLU:HB3	2.03	0.57
1:B:457:LYS:O	1:B:457:LYS:HG3	2.05	0.57
4:C:901:ATP:C2	2:D:462:TRP:HA	2.40	0.57
1:E:152:GLN:HG3	2:F:161:ARG:NH1	2.19	0.57
1:E:471:MET:HE2	1:E:478:ASP:CB	2.35	0.57
1:A:80:PRO:HB3	1:A:105:ILE:HG21	1.87	0.57
1:B:289:ALA:CB	1:B:419:PHE:HA	2.34	0.57
2:D:18:ILE:H	2:D:18:ILE:CD1	2.15	0.57
1:E:221:GLU:HG3	1:E:222:ILE:N	2.20	0.57
1:E:499:VAL:O	1:E:499:VAL:HG12	2.02	0.57
1:B:52:LYS:N	4:B:903:ATP:O1B	2.38	0.57
1:B:146:SER:H	1:B:181:THR:CB	2.14	0.57
1:B:294:LYS:N	4:B:901:ATP:O1B	2.33	0.57
2:D:214:GLU:CB	1:E:234:GLU:HB2	2.31	0.57
1:E:38:ILE:HA	1:E:177:THR:HG23	1.86	0.57
1:E:283:ILE:HD12	1:E:412:PHE:HE1	1.70	0.57
2:F:151:PHE:C	2:F:153:GLN:H	2.13	0.57
1:E:259:SER:N	1:E:281:ASP:OD2	2.38	0.56
1:A:130:ILE:O	1:A:134:ILE:HG13	2.05	0.56
1:A:296:LEU:HD13	1:A:331:TRP:CE2	2.40	0.56
2:C:21:MET:HB2	2:C:38:ILE:HG13	1.87	0.56
2:C:89:SER:HB2	2:D:227:GLY:O	2.05	0.56
2:C:446:ARG:HG2	2:C:496:ARG:CZ	2.35	0.56
2:D:484:ARG:CB	2:D:484:ARG:NH1	2.68	0.56
1:E:84:ILE:HG21	1:E:95:ALA:HB2	1.86	0.56
1:E:323:GLN:HE21	1:E:327:ASN:HD21	1.53	0.56
1:B:150:VAL:C	1:B:152:GLN:H	2.12	0.56
1:B:458:MET:SD	1:B:461:SER:HB3	2.46	0.56
1:E:283:ILE:HD12	1:E:412:PHE:CE1	2.40	0.56
1:E:431:ASP:O	1:E:434:THR:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:46:GLY:HA2	2:F:184:ARG:CD	2.35	0.56
2:F:356:LEU:HD11	2:F:387:VAL:HG21	1.87	0.56
2:C:38:ILE:HG23	2:C:177:THR:OG1	2.05	0.56
2:C:54:LEU:HD23	2:C:244:ILE:HG13	1.86	0.56
1:E:76:PHE:CZ	1:E:126:LEU:HD21	2.39	0.56
1:B:127:ILE:HG21	1:B:170:ARG:HG3	1.87	0.56
1:B:360:LEU:HD23	1:B:399:VAL:HG22	1.87	0.56
1:B:469:GLU:HG2	1:B:480:LYS:HE3	1.87	0.56
2:D:31:ILE:HG23	2:D:231:MET:HB2	1.87	0.56
1:A:161:ARG:HA	1:A:196:VAL:HG11	1.88	0.56
1:A:377:ILE:HD12	1:A:412:PHE:CE2	2.40	0.56
2:C:123:LEU:CD2	2:C:167:LEU:HB2	2.36	0.56
2:D:47:THR:O	2:D:50:THR:OG1	2.21	0.56
2:D:211:LEU:O	2:D:215:ARG:O	2.23	0.56
2:D:220:LEU:HD23	2:D:221:GLU:N	2.21	0.56
1:E:362:ILE:O	1:E:365:SER:HB3	2.06	0.56
2:F:164:LEU:O	2:F:165:PHE:C	2.47	0.56
1:A:193:ARG:NH2	1:B:195:GLY:O	2.26	0.56
1:B:87:ALA:C	1:B:89:SER:H	2.13	0.56
1:B:184:ARG:C	1:B:185:ILE:HD13	2.30	0.56
1:E:230:HIS:HD1	1:E:230:HIS:C	2.14	0.56
1:A:161:ARG:HB2	1:A:196:VAL:HG11	1.86	0.56
2:C:85:LYS:HZ3	2:D:14:GLU:HB3	1.71	0.56
2:F:352:GLU:OE2	2:F:385:ARG:HD2	2.06	0.56
1:A:436:THR:CG2	1:A:458:MET:HG2	2.36	0.56
2:C:336:GLU:OE1	2:C:336:GLU:HA	2.05	0.56
1:E:268:VAL:O	1:E:271:ASP:N	2.38	0.56
2:F:54:LEU:HD21	2:F:243:GLY:HA2	1.88	0.56
2:F:439:LEU:HD12	2:F:440:LEU:N	2.21	0.56
2:F:514:GLU:O	2:F:515:LYS:CB	2.54	0.56
1:B:249:LEU:HD12	1:B:394:GLN:HG2	1.88	0.56
1:B:315:PHE:HB3	1:B:317:TYR:HE1	1.71	0.56
1:B:392:PHE:O	1:B:395:PHE:HB3	2.06	0.56
2:C:340:ARG:C	2:C:342:ASN:H	2.13	0.56
2:D:151:PHE:O	2:D:153:GLN:N	2.35	0.56
2:D:161:ARG:HB2	2:D:196:VAL:CG1	2.35	0.56
1:E:191:ILE:CG2	1:E:198:GLU:HG3	2.36	0.56
2:F:49:GLY:HA2	4:F:903:ATP:O2B	2.05	0.56
2:F:451:ARG:HG2	2:F:451:ARG:HH11	1.70	0.56
1:A:379:SER:HA	1:A:413:THR:O	2.06	0.55
2:C:70:PRO:HA	2:C:102:LYS:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:85:LYS:NZ	2:D:14:GLU:HB3	2.21	0.55
2:D:340:ARG:C	2:D:342:ASN:N	2.64	0.55
1:A:31:ILE:HD11	1:A:246:ILE:HG21	1.87	0.55
1:A:220:LEU:HD23	1:A:220:LEU:C	2.31	0.55
1:A:377:ILE:HD11	1:A:399:VAL:HG11	1.89	0.55
2:D:164:LEU:CD2	2:D:180:MET:HE1	2.36	0.55
2:D:431:ASP:O	2:D:432:THR:HG23	2.06	0.55
2:D:436:THR:OG1	2:D:458:MET:HG2	2.06	0.55
1:E:153:GLN:C	2:F:158:SER:HB2	2.32	0.55
1:A:380:LEU:HD21	1:A:412:PHE:HD2	1.72	0.55
1:A:471:MET:HE2	1:A:478:ASP:CB	2.37	0.55
1:B:440:LEU:N	1:B:440:LEU:HD23	2.22	0.55
2:C:425:ILE:CG2	2:C:431:ASP:HB3	2.37	0.55
1:E:126:LEU:O	1:E:130:ILE:HG13	2.07	0.55
1:B:196:VAL:O	1:B:200:VAL:HG23	2.06	0.55
2:C:146:SER:H	2:C:181:THR:HB	1.72	0.55
2:C:392:PHE:O	2:C:395:PHE:HB3	2.07	0.55
2:D:169:ALA:O	2:D:173:GLN:HG3	2.05	0.55
2:D:273:MET:HE3	2:D:468:ARG:HD2	1.88	0.55
2:D:364:LYS:O	2:D:367:ILE:HB	2.05	0.55
2:F:261:VAL:HG12	2:F:262:ARG:N	2.22	0.55
2:F:500:ASP:CG	2:F:501:GLU:H	2.14	0.55
2:F:514:GLU:CD	2:F:515:LYS:H	2.14	0.55
1:A:161:ARG:HD2	1:A:196:VAL:HG13	1.89	0.55
1:A:382:ALA:O	1:A:385:ARG:HG3	2.07	0.55
1:B:433:ILE:O	1:B:433:ILE:HG22	2.07	0.55
2:C:425:ILE:HG21	2:C:431:ASP:HB3	1.89	0.55
2:C:446:ARG:HG2	2:C:496:ARG:NH2	2.21	0.55
2:D:256:GLN:OE1	2:D:256:GLN:N	2.40	0.55
1:E:471:MET:HE2	1:E:478:ASP:HB3	1.89	0.55
1:E:504:GLU:HG2	1:E:505:LEU:N	2.22	0.55
2:F:207:LEU:HD21	2:F:220:LEU:HD12	1.88	0.55
1:A:146:SER:H	1:A:181:THR:HB	1.72	0.55
1:A:325:LEU:HD23	1:A:335:PHE:HB2	1.88	0.55
1:B:44:VAL:HG22	1:B:205:VAL:HB	1.89	0.55
1:B:269:ARG:O	1:B:273:MET:HG3	2.05	0.55
1:B:419:PHE:CD2	2:C:425:ILE:HD12	2.41	0.55
1:E:347:VAL:HG12	1:E:348:CYS:N	2.22	0.55
2:F:52:LYS:HB3	2:F:181:THR:OG1	2.07	0.55
2:F:94:LEU:O	2:F:98:VAL:HG23	2.07	0.55
2:F:192:ALA:HB3	2:F:197:GLU:OE2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:274:CYS:HG	2:F:278:PHE:HE2	1.51	0.55
2:F:311:ARG:HG3	2:F:371:LYS:HZ1	1.70	0.55
2:F:501:GLU:CG	2:F:502:LYS:N	2.70	0.55
1:B:117:VAL:O	1:B:117:VAL:HG12	2.07	0.55
1:B:155:ASP:OD1	1:B:159:VAL:HG11	2.07	0.55
1:B:191:ILE:HB	1:B:198:GLU:OE2	2.05	0.55
2:D:24:MET:HB2	2:D:62:ASN:HD22	1.72	0.55
2:D:122:ASP:O	2:D:123:LEU:C	2.49	0.55
2:D:350:TYR:CE1	1:E:254:LEU:HD13	2.42	0.55
1:A:431:ASP:N	1:A:431:ASP:OD1	2.39	0.55
1:A:446:ARG:HG2	1:A:496:ARG:NH1	2.22	0.55
1:B:56:SER:HB2	1:B:143:SER:HB3	1.88	0.55
2:C:44:VAL:HA	2:C:205:VAL:O	2.07	0.55
2:C:267:VAL:HB	2:C:270:LEU:HB2	1.88	0.55
2:C:325:LEU:HD23	2:C:335:PHE:HB2	1.87	0.55
1:E:300:ARG:CA	1:E:333:MET:HE1	2.35	0.55
2:F:455:VAL:HG11	2:F:463:HIS:HB2	1.88	0.55
1:B:192:ALA:O	1:B:194:TYR:N	2.40	0.55
1:B:441:GLN:HE22	1:B:490:ILE:HA	1.69	0.55
2:C:211:LEU:HA	2:C:216:ARG:HD3	1.89	0.55
2:C:311:ARG:HD2	2:C:371:LYS:CE	2.37	0.55
1:E:255:THR:HG22	1:E:255:THR:O	2.06	0.55
1:A:312:ALA:HA	1:A:374:ARG:O	2.07	0.54
1:A:510:ARG:NE	1:A:510:ARG:HA	2.22	0.54
1:B:150:VAL:CG1	1:B:151:PHE:H	2.21	0.54
2:C:191:ILE:HB	2:C:198:GLU:CG	2.38	0.54
2:C:462:TRP:O	2:C:463:HIS:O	2.25	0.54
1:E:31:ILE:HG22	1:E:222:ILE:CD1	2.37	0.54
1:E:293:GLY:HA2	4:E:901:ATP:O1A	2.07	0.54
1:E:431:ASP:OD1	1:E:431:ASP:N	2.30	0.54
2:F:439:LEU:HD12	2:F:440:LEU:H	1.71	0.54
1:A:419:PHE:HD2	1:B:425:ILE:HD12	1.72	0.54
2:F:458:MET:SD	2:F:461:SER:HB3	2.47	0.54
1:A:191:ILE:HB	1:A:198:GLU:CD	2.32	0.54
1:A:289:ALA:HB2	1:A:419:PHE:HA	1.90	0.54
1:B:164:LEU:HB3	1:B:200:VAL:HG11	1.89	0.54
1:B:340:ARG:C	1:B:342:ASN:H	2.15	0.54
2:D:495:THR:HA	1:E:487:GLU:CD	2.32	0.54
2:C:64:ILE:HD11	2:C:102:LYS:O	2.07	0.54
2:D:182:THR:HG21	2:D:192:ALA:CB	2.30	0.54
1:E:21:MET:HE1	1:E:177:THR:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:163:GLU:OE2	2:C:163:GLU:HA	2.08	0.54
2:C:356:LEU:HD22	2:C:387:VAL:HG11	1.90	0.54
2:D:59:PHE:CE2	2:D:141:ARG:HB3	2.42	0.54
1:E:289:ALA:CB	1:E:419:PHE:HA	2.32	0.54
1:E:393:ARG:O	1:E:397:ILE:HG12	2.07	0.54
2:F:170:ARG:O	2:F:174:ILE:HG12	2.07	0.54
2:F:353:SER:O	2:F:354:ALA:HB2	2.07	0.54
2:F:515:LYS:C	2:F:517:PRO:HD2	2.32	0.54
1:A:137:TYR:O	1:A:138:ARG:HB2	2.07	0.54
1:A:161:ARG:CA	1:A:196:VAL:HG11	2.37	0.54
2:C:389:ASN:O	2:C:392:PHE:HB3	2.07	0.54
2:D:21:MET:HE1	2:D:177:THR:HB	1.90	0.54
2:D:61:TYR:CZ	2:D:92:TRP:CD1	2.96	0.54
2:D:202:ASP:HA	2:D:226:ARG:HD2	1.90	0.54
1:B:255:THR:HG22	1:B:255:THR:O	2.07	0.54
1:B:334:ASP:OD1	1:B:336:GLU:HB2	2.07	0.54
1:B:380:LEU:O	1:B:383:LEU:HB2	2.08	0.54
1:B:492:GLY:C	1:B:494:PRO:HD3	2.32	0.54
2:C:80:PRO:HB2	2:C:81:GLN:NE2	2.22	0.54
2:C:220:LEU:HD23	2:C:220:LEU:C	2.33	0.54
2:C:332:GLY:C	2:C:333:MET:HG2	2.32	0.54
2:D:313:ILE:CD1	2:D:372:PRO:HG2	2.36	0.54
2:D:356:LEU:CD2	2:D:387:VAL:HG11	2.35	0.54
2:D:358:ASP:O	2:D:362:ILE:HG12	2.08	0.54
1:E:248:PRO:O	1:E:251:ALA:N	2.28	0.54
1:E:294:LYS:HG2	1:E:413:THR:HG23	1.89	0.54
2:F:345:LYS:HZ1	2:F:366:GLU:CD	2.15	0.54
1:B:64:ILE:HG22	1:B:65:ILE:HD13	1.90	0.54
2:C:123:LEU:HD12	2:C:163:GLU:OE2	2.08	0.54
1:E:377:ILE:HD12	1:E:412:PHE:HE2	1.71	0.54
1:A:65:ILE:O	1:A:65:ILE:HG22	2.06	0.54
1:B:150:VAL:CG1	1:B:151:PHE:N	2.70	0.54
1:B:249:LEU:CD1	1:B:394:GLN:HG2	2.37	0.54
2:C:295:THR:HB	4:C:901:ATP:PA	2.47	0.54
2:C:325:LEU:CD2	2:C:335:PHE:HB2	2.38	0.54
2:F:455:VAL:HB	5:F:525:HOH:O	2.08	0.54
1:A:318:GLU:OE2	1:B:432:TPO:CG2	2.53	0.53
1:A:406:GLU:O	1:A:407:GLU:HB2	2.07	0.53
1:B:68:ASP:O	1:B:70:PRO:HD3	2.08	0.53
1:B:148:THR:HA	1:B:151:PHE:CE1	2.42	0.53
2:C:464:ASP:OD1	2:C:465:LYS:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:268:VAL:O	2:D:269:ARG:C	2.51	0.53
2:F:269:ARG:HG2	2:F:479:ILE:CB	2.37	0.53
1:A:118:VAL:HG23	1:A:153:GLN:OE1	2.07	0.53
1:B:485:ASN:OD1	1:B:485:ASN:N	2.41	0.53
2:C:182:THR:HG22	2:C:183:GLU:H	1.71	0.53
2:C:313:ILE:HG12	2:C:345:LYS:CB	2.24	0.53
1:A:90:PHE:HB2	1:A:92:TRP:CE2	2.43	0.53
1:A:323:GLN:HG2	1:A:327:ASN:HD21	1.73	0.53
1:A:263:VAL:HG12	1:A:374:ARG:HH21	1.74	0.53
1:A:455:VAL:HG11	1:A:463:HIS:HB2	1.90	0.53
2:C:150:VAL:HG13	2:C:151:PHE:N	2.23	0.53
2:D:467:ILE:HG22	2:D:467:ILE:O	2.08	0.53
1:E:262:ARG:HH12	1:E:461:SER:HB2	1.73	0.53
2:F:262:ARG:HD2	2:F:277:GLY:O	2.08	0.53
2:F:303:GLU:HB2	2:F:333:MET:HE3	1.91	0.53
1:B:53:THR:HB	4:B:903:ATP:O1A	2.08	0.53
2:C:23:THR:O	2:C:24:MET:HB2	2.08	0.53
2:C:81:GLN:NE2	2:C:81:GLN:H	2.06	0.53
1:E:267:VAL:HG21	1:E:477:PRO:HG3	1.89	0.53
4:E:903:ATP:O3G	2:F:224:LYS:NZ	2.41	0.53
1:A:432:TPO:HG21	1:A:432:TPO:O1P	2.08	0.53
2:D:37:PRO:O	2:D:177:THR:HG23	2.08	0.53
2:D:144:ILE:HD12	2:D:180:MET:HG2	1.90	0.53
2:D:231:MET:CE	2:D:251:ALA:HB2	2.37	0.53
1:E:325:LEU:HD21	1:E:335:PHE:HB2	1.89	0.53
2:F:117:VAL:O	2:F:118:VAL:HB	2.07	0.53
2:F:298:VAL:HG22	2:F:411:LEU:CD2	2.39	0.53
1:A:367:ILE:HG12	1:A:375:ILE:HD11	1.90	0.53
1:A:488:ARG:HE	2:F:488:ARG:CZ	2.21	0.53
1:B:325:LEU:HD23	1:B:335:PHE:HB2	1.89	0.53
2:C:164:LEU:HD22	2:C:180:MET:HE1	1.91	0.53
2:C:300:ARG:HD3	2:C:333:MET:HE1	1.91	0.53
2:D:89:SER:CB	1:E:227:GLY:O	2.55	0.53
2:D:123:LEU:HD11	2:D:163:GLU:HB3	1.90	0.53
2:D:178:THR:HG22	2:D:179:VAL:N	2.23	0.53
2:D:301:PHE:CZ	2:D:374:ARG:HD3	2.44	0.53
1:E:67:PHE:HB2	1:E:69:GLU:HG3	1.90	0.53
1:E:363:ILE:O	1:E:367:ILE:HG13	2.09	0.53
1:E:451:ARG:HH12	1:E:472:ILE:CD1	2.21	0.53
1:B:283:ILE:HG22	1:B:434:THR:OG1	2.08	0.53
2:C:379:SER:HA	2:C:413:THR:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:79:THR:CG2	2:D:81:GLN:HG2	2.39	0.53
1:E:273:MET:O	1:E:463:HIS:HA	2.09	0.53
1:A:437:ILE:HD12	1:A:457:LYS:HG2	1.91	0.53
1:B:79:THR:CG2	1:B:81:GLN:HG2	2.39	0.53
2:C:63:GLY:CA	2:C:141:ARG:NH1	2.72	0.53
2:C:161:ARG:HD2	2:C:196:VAL:HG13	1.91	0.53
2:D:273:MET:CE	2:D:468:ARG:HD2	2.39	0.53
2:D:457:LYS:HG3	2:D:457:LYS:O	2.07	0.53
1:E:313:ILE:CD1	1:E:372:PRO:HG2	2.39	0.53
2:F:298:VAL:HG22	2:F:411:LEU:HD23	1.91	0.53
1:A:430:ILE:O	1:A:432:TPO:N	2.42	0.53
1:B:146:SER:N	1:B:181:THR:HB	2.19	0.53
1:B:178:THR:HG22	1:B:179:VAL:H	1.74	0.53
1:B:208:ARG:O	1:B:218:ARG:HA	2.08	0.53
2:C:70:PRO:HG2	2:C:138:ARG:O	2.09	0.53
2:C:340:ARG:O	2:C:342:ASN:N	2.42	0.53
2:D:170:ARG:HH12	2:D:174:ILE:HD11	1.74	0.53
2:D:294:LYS:O	2:D:297:LEU:HB2	2.09	0.53
2:F:127:ILE:HD13	2:F:167:LEU:HD12	1.91	0.53
1:A:104:PHE:HD2	1:A:133:ALA:HB1	1.74	0.52
4:A:903:ATP:N1	1:B:229:SER:HB3	2.25	0.52
1:B:263:VAL:HG23	1:B:278:PHE:O	2.09	0.52
2:C:294:LYS:HG3	2:C:440:LEU:HD12	1.91	0.52
1:E:70:PRO:HB2	1:E:139:ALA:HA	1.92	0.52
1:E:79:THR:HG22	1:E:82:ASP:CG	2.34	0.52
1:E:392:PHE:O	1:E:395:PHE:HB3	2.10	0.52
2:F:302:VAL:HG12	2:F:303:GLU:N	2.23	0.52
1:A:191:ILE:HB	1:A:198:GLU:HG3	1.90	0.52
1:A:470:PHE:CD1	1:A:470:PHE:C	2.87	0.52
1:B:130:ILE:O	1:B:134:ILE:HG13	2.10	0.52
2:C:82:ASP:O	2:C:83:ILE:C	2.52	0.52
2:C:461:SER:OG	2:C:462:TRP:N	2.42	0.52
1:E:49:GLY:O	1:E:218:ARG:NH2	2.43	0.52
1:A:340:ARG:C	1:A:342:ASN:H	2.18	0.52
4:A:903:ATP:O3'	1:B:224:LYS:HB2	2.10	0.52
1:B:347:VAL:O	1:B:348:CYS:HB2	2.10	0.52
1:B:384:ALA:HB2	1:B:392:PHE:CE1	2.44	0.52
2:C:38:ILE:H	2:C:38:ILE:HD12	1.75	0.52
2:C:63:GLY:HA3	2:C:141:ARG:NH1	2.25	0.52
2:D:430:ILE:C	2:D:431:ASP:O	2.52	0.52
1:B:79:THR:HG22	1:B:82:ASP:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:70:PRO:HD2	2:C:140:ARG:HG2	1.91	0.52
2:C:215:ARG:HA	2:C:215:ARG:HE	1.75	0.52
2:D:430:ILE:O	2:D:433:ILE:HD12	2.09	0.52
1:E:116:GLU:O	1:E:118:VAL:HG23	2.09	0.52
2:F:182:THR:CG2	2:F:183:GLU:N	2.73	0.52
2:F:381:SER:HB3	2:F:414:ASN:OD1	2.10	0.52
2:D:221:GLU:HG2	2:D:222:ILE:N	2.23	0.52
2:F:344:LEU:HD11	2:F:346:ILE:CG1	2.38	0.52
1:A:63:GLY:HA3	1:A:141:ARG:HD2	1.91	0.52
1:B:36:LEU:HD12	1:B:59:PHE:CE1	2.45	0.52
2:C:371:LYS:O	2:C:371:LYS:CD	2.53	0.52
2:C:468:ARG:NH1	2:C:468:ARG:HG2	2.25	0.52
2:D:489:ILE:HA	2:D:494:PRO:HG3	1.92	0.52
1:E:140:ARG:HH11	1:E:140:ARG:CB	2.22	0.52
1:E:294:LYS:N	4:E:901:ATP:O1B	2.41	0.52
1:E:497:ILE:HG22	1:E:498:THR:N	2.23	0.52
2:C:151:PHE:C	2:C:153:GLN:H	2.18	0.52
2:D:23:THR:HB	2:D:25:ILE:HD12	1.91	0.52
2:D:291:GLY:C	2:D:442:TYR:OH	2.53	0.52
2:D:293:GLY:HA2	4:D:901:ATP:PA	2.49	0.52
1:E:31:ILE:HG22	1:E:222:ILE:HD12	1.91	0.52
2:F:396:VAL:HG11	2:F:430:ILE:CG2	2.40	0.52
1:A:44:VAL:HG22	1:A:205:VAL:HB	1.91	0.52
1:A:218:ARG:O	1:A:236:PRO:HA	2.10	0.52
2:C:142:VAL:O	2:C:178:THR:HA	2.09	0.52
2:C:317:TYR:CE1	2:C:377:ILE:HG23	2.45	0.52
2:C:471:MET:HE1	2:C:473:SER:HB3	1.90	0.52
2:D:338:MET:HB3	2:D:344:LEU:HB3	1.92	0.52
1:E:104:PHE:HE2	1:E:106:LEU:HB2	1.73	0.52
1:E:313:ILE:HG22	1:E:314:LEU:N	2.23	0.52
2:F:70:PRO:HG2	2:F:139:ALA:HA	1.92	0.52
2:C:413:THR:O	2:C:413:THR:HG22	2.09	0.52
2:D:431:ASP:C	2:D:433:ILE:H	2.17	0.52
1:E:501:GLU:O	1:E:502:LYS:HG3	2.09	0.52
1:A:230:HIS:NE2	4:F:903:ATP:O2'	2.42	0.52
2:C:311:ARG:HA	2:C:343:LEU:O	2.09	0.52
1:E:378:ASP:O	1:E:379:SER:HB3	2.10	0.52
2:F:311:ARG:HG3	2:F:371:LYS:NZ	2.25	0.52
1:B:448:GLU:HG2	2:C:466:ALA:HA	1.93	0.51
2:F:397:ILE:HD13	2:F:433:ILE:HG12	1.91	0.51
1:A:371:LYS:HD2	1:A:371:LYS:C	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ILE:O	1:A:410:GLY:HA2	2.10	0.51
1:B:317:TYR:CE2	1:B:383:LEU:HD21	2.46	0.51
1:E:453:ILE:HG22	1:E:470:PHE:CD2	2.45	0.51
2:F:220:LEU:HD23	2:F:220:LEU:C	2.35	0.51
1:B:79:THR:HG23	1:B:82:ASP:H	1.75	0.51
2:C:79:THR:HG23	2:C:82:ASP:H	1.74	0.51
2:C:88:ARG:NE	2:D:15:HIS:HA	2.25	0.51
2:C:164:LEU:HB3	2:C:200:VAL:HG11	1.91	0.51
2:D:451:ARG:HG2	2:D:451:ARG:NH1	2.26	0.51
1:E:303:GLU:HB2	1:E:333:MET:CE	2.41	0.51
1:B:194:TYR:O	1:B:196:VAL:N	2.43	0.51
2:C:403:ALA:O	2:C:408:ILE:O	2.27	0.51
1:E:263:VAL:HG12	1:E:374:ARG:NH2	2.13	0.51
1:E:264:SER:H	1:E:374:ARG:HH22	1.56	0.51
1:A:28:PHE:HB2	1:A:246:ILE:CD1	2.41	0.51
1:A:60:LEU:HD12	1:A:73:PHE:HD1	1.76	0.51
2:C:126:LEU:O	2:C:129:ARG:N	2.43	0.51
2:D:248:PRO:HB2	2:D:251:ALA:CB	2.33	0.51
2:F:508:ILE:HG22	2:F:508:ILE:O	2.11	0.51
2:D:325:LEU:CD2	2:D:335:PHE:HB2	2.41	0.51
1:E:345:LYS:HE2	1:E:366:GLU:OE1	2.10	0.51
2:F:208:ARG:O	2:F:218:ARG:HA	2.11	0.51
2:F:321:ARG:HG2	2:F:348:CYS:SG	2.51	0.51
1:A:321:ARG:O	1:A:325:LEU:HD12	2.11	0.51
1:A:371:LYS:HD2	1:A:371:LYS:O	2.11	0.51
1:B:421:GLY:O	1:B:422:ALA:C	2.53	0.51
2:C:468:ARG:HG2	2:C:468:ARG:HH11	1.76	0.51
2:D:332:GLY:C	2:D:333:MET:HG2	2.34	0.51
4:E:903:ATP:O3'	2:F:224:LYS:HB2	2.10	0.51
2:F:31:ILE:HD11	2:F:246:ILE:HG21	1.93	0.51
2:F:504:GLU:HA	2:F:507:ARG:HE	1.76	0.51
2:C:20:LYS:HE3	2:C:228:THR:HG21	1.92	0.51
1:E:397:ILE:CD1	1:E:433:ILE:HG12	2.41	0.51
2:F:218:ARG:HG3	2:F:237:PHE:O	2.09	0.51
2:F:471:MET:HG2	2:F:480:LYS:HZ3	1.74	0.51
1:A:117:VAL:HG22	1:A:154:TYR:OH	2.10	0.51
2:C:19:ALA:O	2:C:38:ILE:HD12	2.10	0.51
2:D:67:PHE:HB2	2:D:69:GLU:HG3	1.93	0.51
2:D:323:GLN:HE21	2:D:327:ASN:HD21	1.58	0.51
1:E:451:ARG:HG2	1:E:451:ARG:NH1	2.24	0.51
2:F:451:ARG:HB3	2:F:470:PHE:CZ	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:ILE:O	1:A:433:ILE:CG2	2.56	0.51
1:B:161:ARG:HH22	1:B:199:PHE:HB2	1.74	0.51
2:C:51:GLY:O	2:C:52:LYS:C	2.53	0.51
2:D:167:LEU:O	2:D:170:ARG:N	2.44	0.51
2:D:381:SER:HB3	2:D:414:ASN:OD1	2.11	0.51
2:F:268:VAL:O	2:F:269:ARG:C	2.54	0.51
1:A:18:ILE:HG22	1:A:19:ALA:N	2.25	0.50
2:C:25:ILE:HG12	2:C:58:GLN:HE21	1.76	0.50
2:C:111:ASP:O	2:C:113:GLU:N	2.37	0.50
2:C:214:GLU:C	2:C:215:ARG:HE	2.19	0.50
1:A:356:LEU:CD1	1:A:387:VAL:HG21	2.41	0.50
1:A:370:PHE:C	1:A:372:PRO:HD3	2.37	0.50
2:D:363:ILE:O	2:D:364:LYS:C	2.55	0.50
1:E:146:SER:H	1:E:181:THR:HB	1.77	0.50
1:E:359:HIS:O	1:E:363:ILE:HG13	2.12	0.50
2:F:184:ARG:HG2	2:F:191:ILE:O	2.12	0.50
1:A:397:ILE:HD11	2:F:385:ARG:HH12	1.75	0.50
1:B:60:LEU:O	1:B:61:TYR:C	2.54	0.50
2:C:18:ILE:HB	2:C:228:THR:HG23	1.92	0.50
2:C:178:THR:HG22	2:C:179:VAL:N	2.27	0.50
2:D:311:ARG:CD	2:D:371:LYS:HE3	2.39	0.50
2:F:60:LEU:HD12	2:F:73:PHE:HB2	1.94	0.50
1:A:344:LEU:HD11	1:A:346:ILE:CG1	2.41	0.50
1:A:396:VAL:HG11	1:A:430:ILE:HG23	1.94	0.50
1:A:397:ILE:HD11	2:F:385:ARG:NH1	2.26	0.50
1:B:273:MET:C	1:B:275:GLY:H	2.19	0.50
2:D:420:MET:HE3	2:D:492:GLY:C	2.35	0.50
2:D:430:ILE:O	2:D:431:ASP:C	2.54	0.50
2:F:21:MET:N	2:F:38:ILE:HD11	2.26	0.50
2:F:344:LEU:CD1	2:F:346:ILE:HG13	2.40	0.50
2:C:340:ARG:C	2:C:342:ASN:N	2.67	0.50
2:D:212:GLU:O	2:D:212:GLU:CG	2.55	0.50
1:E:355:GLY:O	1:E:358:ASP:HB2	2.12	0.50
2:C:49:GLY:O	2:C:218:ARG:NH2	2.43	0.50
2:D:437:ILE:CD1	2:D:457:LYS:HE2	2.41	0.50
1:E:312:ALA:HA	1:E:374:ARG:O	2.11	0.50
1:E:449:MET:HA	1:E:449:MET:HE2	1.93	0.50
2:F:150:VAL:HG13	2:F:151:PHE:N	2.26	0.50
1:A:323:GLN:O	1:A:327:ASN:ND2	2.44	0.50
1:B:144:ILE:HG22	1:B:147:VAL:HG12	1.94	0.50
1:B:151:PHE:C	1:B:153:GLN:H	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:269:ARG:HB3	2:D:479:ILE:HD12	1.93	0.50
2:D:304:ASN:HB3	2:D:374:ARG:NH1	2.25	0.50
2:D:441:GLN:HE22	2:D:490:ILE:HD12	1.76	0.50
2:C:185:ILE:HA	5:D:528:HOH:O	2.12	0.50
1:E:230:HIS:C	1:E:230:HIS:ND1	2.69	0.50
1:E:281:ASP:O	1:E:282:SER:HB3	2.11	0.50
1:E:451:ARG:HH11	1:E:451:ARG:CG	2.23	0.50
1:B:18:ILE:HB	1:B:228:THR:HG23	1.94	0.50
2:C:126:LEU:O	2:C:129:ARG:HB2	2.12	0.50
2:D:225:LEU:HB2	2:D:230:HIS:HD2	1.77	0.50
2:D:295:THR:HG23	2:D:378:ASP:OD2	2.11	0.50
1:E:67:PHE:CB	1:E:69:GLU:HG3	2.42	0.50
1:E:237:PHE:HB3	1:E:246:ILE:HG12	1.93	0.50
1:A:79:THR:HG22	1:A:82:ASP:H	1.76	0.49
1:A:344:LEU:HD22	1:A:345:LYS:N	2.27	0.49
1:B:289:ALA:O	1:B:290:THR:C	2.53	0.49
1:B:425:ILE:HD12	1:B:425:ILE:H	1.76	0.49
2:C:107:ASP:C	2:C:107:ASP:OD1	2.55	0.49
1:E:270:LEU:HD11	1:E:438:ILE:HD12	1.94	0.49
1:E:504:GLU:CG	1:E:505:LEU:H	2.25	0.49
2:F:505:LEU:O	2:F:506:SER:CB	2.59	0.49
1:B:232:LYS:N	1:B:232:LYS:HD2	2.27	0.49
2:C:50:THR:HB	2:C:207:LEU:HB3	1.94	0.49
2:C:140:ARG:HH11	2:C:140:ARG:CB	2.23	0.49
2:C:225:LEU:HB2	2:C:230:HIS:HD2	1.77	0.49
2:D:193:ARG:NH2	1:E:195:GLY:O	2.45	0.49
1:E:170:ARG:HD2	1:E:173:GLN:OE1	2.12	0.49
1:E:264:SER:N	1:E:374:ARG:HH22	2.09	0.49
1:E:379:SER:H	1:E:413:THR:HB	1.77	0.49
2:F:122:ASP:OD2	2:F:123:LEU:N	2.45	0.49
2:F:340:ARG:C	2:F:342:ASN:H	2.19	0.49
1:A:266:GLY:HA3	1:A:300:ARG:HG3	1.93	0.49
1:A:344:LEU:HD22	1:A:345:LYS:H	1.75	0.49
1:B:18:ILE:HB	1:B:228:THR:CG2	2.42	0.49
1:B:145:ASP:HA	1:B:181:THR:HB	1.94	0.49
1:B:185:ILE:HD13	1:B:185:ILE:N	2.26	0.49
2:C:164:LEU:CD1	2:C:197:GLU:HG3	2.40	0.49
2:C:389:ASN:HD21	2:C:428:SER:CA	2.25	0.49
2:D:418:GLN:HE21	2:D:422:ALA:HA	1.77	0.49
2:D:486:PHE:HE2	2:D:496:ARG:HD3	1.73	0.49
1:E:364:LYS:HE2	1:E:402:TYR:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ILE:H	1:A:18:ILE:CD1	2.23	0.49
1:A:231:MET:HE1	1:A:251:ALA:HB2	1.94	0.49
1:A:395:PHE:CE2	1:A:399:VAL:HG21	2.47	0.49
1:B:148:THR:HA	1:B:151:PHE:HE1	1.78	0.49
2:C:63:GLY:CA	2:C:141:ARG:CZ	2.90	0.49
2:D:191:ILE:HG21	2:D:198:GLU:HG3	1.94	0.49
2:D:445:ILE:HA	2:D:496:ARG:HH12	1.77	0.49
1:E:281:ASP:OD1	1:E:407:GLU:OE1	2.30	0.49
1:E:295:THR:O	1:E:298:VAL:HB	2.12	0.49
1:E:443:VAL:HG12	1:E:445:ILE:HG12	1.93	0.49
2:F:286:ALA:HA	2:F:438:ILE:O	2.12	0.49
1:A:363:ILE:HG22	1:A:367:ILE:HD11	1.94	0.49
2:C:113:GLU:O	2:C:114:GLY:C	2.56	0.49
2:D:314:LEU:O	2:D:314:LEU:CG	2.60	0.49
2:D:451:ARG:NH1	2:D:472:ILE:CD1	2.75	0.49
1:E:451:ARG:HD2	1:E:451:ARG:H	1.78	0.49
2:F:111:ASP:CG	2:F:112:PRO:HD2	2.38	0.49
2:F:187:GLU:OE2	2:F:208:ARG:HA	2.12	0.49
2:F:312:ALA:HB2	2:F:374:ARG:HB2	1.93	0.49
1:B:221:GLU:HG3	1:B:233:GLY:O	2.12	0.49
2:D:151:PHE:C	2:D:153:GLN:N	2.69	0.49
2:D:458:MET:HB2	2:D:463:HIS:HD2	1.77	0.49
2:F:248:PRO:CB	2:F:251:ALA:HB3	2.43	0.49
2:F:489:ILE:HA	2:F:494:PRO:HG3	1.95	0.49
1:A:131:ASN:O	1:A:132:TYR:C	2.55	0.49
2:C:44:VAL:O	2:C:44:VAL:HG12	2.13	0.49
2:C:116:GLU:O	2:C:117:VAL:HB	2.13	0.49
2:C:381:SER:O	2:C:384:ALA:HB3	2.12	0.49
1:A:437:ILE:HD11	1:A:457:LYS:HE2	1.93	0.49
1:B:45:SER:HB3	1:B:182:THR:CB	2.41	0.49
1:B:51:GLY:O	1:B:52:LYS:C	2.56	0.49
1:B:212:GLU:O	1:B:212:GLU:CG	2.57	0.49
2:D:148:THR:OG1	2:D:182:THR:HG23	2.13	0.49
2:D:451:ARG:NH1	2:D:472:ILE:HD11	2.28	0.49
1:E:121:PHE:CD1	1:E:121:PHE:N	2.80	0.49
1:E:311:ARG:HD3	1:E:370:PHE:CE1	2.48	0.49
1:E:469:GLU:CB	1:E:483:PHE:CZ	2.95	0.49
2:F:184:ARG:HH12	2:F:187:GLU:C	2.20	0.49
1:A:150:VAL:HG13	1:A:151:PHE:N	2.28	0.49
2:C:144:ILE:CG2	2:C:147:VAL:HG12	2.43	0.49
2:C:262:ARG:HH22	2:C:461:SER:HB2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:315:PHE:HE2	2:C:363:ILE:HA	1.75	0.49
1:E:318:GLU:OE2	2:F:432:THR:HB	2.13	0.49
1:E:504:GLU:HG2	1:E:505:LEU:H	1.76	0.49
2:F:500:ASP:O	2:F:501:GLU:CB	2.60	0.49
2:F:515:LYS:CG	2:F:517:PRO:HD2	2.43	0.49
1:A:356:LEU:HD22	1:A:387:VAL:HG11	1.94	0.48
1:A:461:SER:OG	1:A:462:TRP:N	2.46	0.48
1:B:144:ILE:CG2	1:B:147:VAL:HG12	2.43	0.48
1:B:283:ILE:HD12	1:B:412:PHE:CE1	2.43	0.48
1:B:316:ALA:O	1:B:348:CYS:HA	2.12	0.48
2:D:287:THR:HG22	2:D:288:GLY:N	2.27	0.48
1:E:355:GLY:H	1:E:358:ASP:HB2	1.78	0.48
2:F:316:ALA:O	2:F:348:CYS:HA	2.12	0.48
1:A:227:GLY:O	2:F:89:SER:CB	2.61	0.48
1:B:496:ARG:CG	1:B:498:THR:HG23	2.29	0.48
2:D:221:GLU:HG3	2:D:233:GLY:C	2.38	0.48
2:D:305:ALA:HB2	2:D:374:ARG:CD	2.43	0.48
1:E:274:CYS:C	1:E:276:GLY:H	2.21	0.48
1:A:211:LEU:HD13	1:A:216:ARG:HE	1.75	0.48
1:A:263:VAL:CG1	1:A:374:ARG:HH21	2.26	0.48
1:A:311:ARG:HD2	1:A:371:LYS:NZ	2.28	0.48
1:A:313:ILE:CD1	1:A:372:PRO:HG2	2.42	0.48
1:B:72:VAL:HB	1:B:142:VAL:HG13	1.94	0.48
2:C:21:MET:HE3	2:C:141:ARG:NE	2.28	0.48
1:E:231:MET:HE1	1:E:251:ALA:HB2	1.95	0.48
1:E:287:THR:HG23	1:E:414:ASN:HB3	1.95	0.48
2:F:16:GLN:NE2	2:F:33:HIS:HB3	2.27	0.48
2:F:23:THR:HB	2:F:25:ILE:HG13	1.94	0.48
2:F:269:ARG:HG2	2:F:479:ILE:CG2	2.44	0.48
1:A:294:LYS:HD3	1:A:294:LYS:H	1.76	0.48
2:C:64:ILE:HD11	2:C:102:LYS:C	2.38	0.48
2:D:23:THR:HB	2:D:25:ILE:CD1	2.44	0.48
2:D:289:ALA:O	2:D:292:THR:OG1	2.31	0.48
2:D:332:GLY:O	2:D:333:MET:O	2.31	0.48
1:E:325:LEU:HD21	1:E:335:PHE:CB	2.43	0.48
2:F:129:ARG:O	2:F:132:TYR:HB3	2.13	0.48
1:A:83:ILE:HD12	1:A:83:ILE:N	2.25	0.48
2:C:360:LEU:CD2	2:C:364:LYS:HE3	2.43	0.48
2:D:43:LEU:HD11	2:D:182:THR:OG1	2.12	0.48
1:E:47:THR:HG22	1:E:184:ARG:O	2.14	0.48
1:E:47:THR:O	1:E:50:THR:OG1	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:344:LEU:C	2:F:344:LEU:HD13	2.39	0.48
1:A:178:THR:CG2	1:A:179:VAL:H	2.26	0.48
1:A:220:LEU:N	1:A:235:TYR:O	2.43	0.48
1:B:90:PHE:HB2	1:B:92:TRP:CD2	2.48	0.48
2:C:164:LEU:HD11	2:C:197:GLU:CG	2.39	0.48
2:D:400:THR:HG22	2:D:401:GLY:N	2.28	0.48
1:B:240:THR:OG1	1:B:241:ASP:N	2.46	0.48
1:B:461:SER:OG	1:B:462:TRP:N	2.47	0.48
2:D:81:GLN:H	2:D:81:GLN:CD	2.22	0.48
1:E:46:GLY:HA2	1:E:184:ARG:HD3	1.96	0.48
1:E:313:ILE:HG13	1:E:372:PRO:HG2	1.95	0.48
1:A:202:ASP:HA	1:A:226:ARG:HD2	1.96	0.48
1:A:392:PHE:O	1:A:395:PHE:N	2.46	0.48
1:A:488:ARG:HE	2:F:488:ARG:NH2	2.11	0.48
1:B:178:THR:CG2	1:B:179:VAL:N	2.77	0.48
2:C:347:VAL:HG12	2:C:348:CYS:N	2.28	0.48
2:C:426:THR:HG22	2:C:427:ASP:N	2.29	0.48
2:D:311:ARG:HD3	2:D:370:PHE:CE1	2.48	0.48
2:D:334:ASP:OD1	2:D:336:GLU:N	2.46	0.48
2:D:340:ARG:O	2:D:342:ASN:N	2.46	0.48
2:F:73:PHE:HE2	2:F:75:THR:HB	1.79	0.48
2:F:244:ILE:HG22	2:F:245:ASN:N	2.28	0.48
2:F:371:LYS:HD2	2:F:371:LYS:C	2.39	0.48
1:A:436:THR:HG23	1:A:458:MET:CG	2.42	0.48
1:B:24:MET:CB	1:B:62:ASN:HD22	2.27	0.48
1:B:52:LYS:HB2	4:B:903:ATP:O1B	2.14	0.48
1:B:426:THR:HG22	1:B:428:SER:H	1.79	0.48
1:B:499:VAL:O	1:B:501:GLU:N	2.44	0.48
2:C:118:VAL:O	2:C:118:VAL:HG12	2.14	0.48
2:D:79:THR:HG23	2:D:81:GLN:HG2	1.96	0.48
2:D:208:ARG:O	2:D:218:ARG:HA	2.14	0.48
2:D:379:SER:N	2:D:413:THR:HB	2.20	0.48
1:E:256:GLN:HG3	1:E:404:LYS:HD3	1.96	0.48
1:E:291:GLY:HA3	1:E:442:TYR:OH	2.13	0.48
2:F:104:PHE:HE2	2:F:106:LEU:HB2	1.79	0.48
2:F:356:LEU:CD1	2:F:387:VAL:HG21	2.43	0.48
1:A:166:ARG:HG3	2:F:112:PRO:O	2.14	0.48
1:A:265:SER:O	1:A:300:ARG:O	2.32	0.48
1:A:315:PHE:HB3	1:A:317:TYR:HE1	1.78	0.48
1:B:194:TYR:O	1:B:196:VAL:HG23	2.13	0.48
2:C:64:ILE:CD1	2:C:103:LEU:HB2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:232:LYS:HD2	2:C:232:LYS:N	2.27	0.48
2:C:353:SER:O	2:C:354:ALA:CB	2.61	0.48
2:D:147:VAL:CG2	2:D:148:THR:N	2.75	0.48
1:E:195:GLY:C	1:E:198:GLU:OE1	2.57	0.48
2:F:54:LEU:O	2:F:55:PHE:C	2.57	0.48
2:F:142:VAL:HG12	2:F:178:THR:HG23	1.94	0.48
1:A:134:ILE:HG23	1:A:139:ALA:HB3	1.96	0.47
1:A:489:ILE:H	2:F:444:GLU:CD	2.21	0.47
1:B:214:GLU:OE2	2:C:217:ARG:NH1	2.46	0.47
1:B:317:TYR:CD2	1:B:383:LEU:HD21	2.49	0.47
2:C:97:LEU:N	2:C:97:LEU:HD23	2.27	0.47
2:C:335:PHE:O	2:C:339:GLU:HG3	2.14	0.47
2:C:439:LEU:HG	2:C:439:LEU:O	2.13	0.47
1:E:38:ILE:HA	1:E:177:THR:CG2	2.44	0.47
2:F:73:PHE:C	2:F:73:PHE:HD2	2.22	0.47
2:F:79:THR:HG22	2:F:82:ASP:OD2	2.14	0.47
2:F:263:VAL:HG12	2:F:374:ARG:NH2	2.09	0.47
2:F:315:PHE:HE1	2:F:375:ILE:HD11	1.79	0.47
1:A:89:SER:HB2	1:B:227:GLY:O	2.14	0.47
1:A:296:LEU:HD21	1:A:477:PRO:HD3	1.96	0.47
1:B:295:THR:HG21	1:B:319:GLU:OE2	2.13	0.47
1:B:487:GLU:O	1:B:488:ARG:HB2	2.14	0.47
2:C:54:LEU:O	2:C:57:ILE:N	2.47	0.47
2:C:347:VAL:O	2:C:348:CYS:CB	2.58	0.47
2:D:42:THR:HA	2:D:203:ASN:HB2	1.96	0.47
2:D:60:LEU:O	2:D:63:GLY:N	2.47	0.47
2:D:76:PHE:HZ	2:D:126:LEU:CD2	2.27	0.47
2:D:471:MET:CG	2:D:478:ASP:HB3	2.42	0.47
1:E:352:GLU:C	1:E:354:ALA:H	2.22	0.47
2:F:505:LEU:O	2:F:506:SER:HB3	2.13	0.47
1:A:261:VAL:O	1:A:279:PHE:HA	2.14	0.47
1:B:87:ALA:C	1:B:89:SER:N	2.71	0.47
1:B:294:LYS:C	1:B:296:LEU:N	2.70	0.47
2:D:88:ARG:HD3	1:E:15:HIS:C	2.39	0.47
2:D:412:PHE:N	2:D:412:PHE:CD1	2.83	0.47
2:F:44:VAL:O	2:F:181:THR:HA	2.14	0.47
2:F:298:VAL:HA	2:F:411:LEU:HD23	1.94	0.47
1:A:393:ARG:O	1:A:397:ILE:HG12	2.15	0.47
1:A:435:ASP:OD1	2:F:323:GLN:NE2	2.47	0.47
1:A:449:MET:HE2	1:A:449:MET:HA	1.96	0.47
1:B:287:THR:HG23	1:B:414:ASN:ND2	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:164:LEU:CD2	2:C:180:MET:HE1	2.44	0.47
2:C:430:ILE:HG23	2:C:433:ILE:HD11	1.96	0.47
2:D:263:VAL:N	2:D:278:PHE:O	2.47	0.47
1:E:14:GLU:CG	1:E:16:GLN:HB2	2.45	0.47
2:C:441:GLN:HE22	2:C:490:ILE:HD13	1.80	0.47
2:D:370:PHE:C	2:D:372:PRO:HD3	2.39	0.47
1:E:357:GLU:HG3	1:E:358:ASP:N	2.29	0.47
1:A:447:GLY:HA2	1:B:489:ILE:HD12	1.97	0.47
1:A:504:GLU:C	1:A:506:SER:N	2.72	0.47
1:B:220:LEU:HD13	1:B:246:ILE:HD11	1.95	0.47
1:B:294:LYS:O	1:B:296:LEU:N	2.47	0.47
1:B:451:ARG:HB3	1:B:470:PHE:CE2	2.48	0.47
2:C:179:VAL:O	2:C:179:VAL:HG12	2.13	0.47
2:C:293:GLY:HA2	4:C:901:ATP:O1A	2.13	0.47
2:C:387:VAL:CG1	2:C:391:ALA:HB3	2.44	0.47
2:C:440:LEU:HD22	2:C:470:PHE:CZ	2.49	0.47
2:D:406:GLU:HB3	2:D:408:ILE:HD12	1.97	0.47
2:D:437:ILE:HD11	2:D:457:LYS:HE2	1.97	0.47
2:F:211:LEU:HD12	2:F:215:ARG:O	2.15	0.47
1:A:80:PRO:HD2	1:A:81:GLN:HE21	1.79	0.47
1:A:111:ASP:C	1:A:113:GLU:H	2.23	0.47
1:A:419:PHE:O	1:A:420:MET:O	2.32	0.47
1:B:22:ARG:O	1:B:141:ARG:NH2	2.47	0.47
1:B:60:LEU:HA	5:B:521:HOH:O	2.15	0.47
1:B:86:ASN:O	1:B:88:ARG:N	2.47	0.47
1:B:220:LEU:C	1:B:220:LEU:HD23	2.40	0.47
1:B:473:SER:C	1:B:475:LYS:H	2.22	0.47
4:B:901:ATP:H3'	2:C:458:MET:O	2.15	0.47
2:C:52:LYS:N	4:C:903:ATP:O1B	2.48	0.47
2:C:173:GLN:C	2:C:175:GLY:H	2.23	0.47
2:C:300:ARG:HA	2:C:333:MET:CE	2.44	0.47
2:C:311:ARG:HD2	2:C:371:LYS:NZ	2.29	0.47
2:D:23:THR:C	2:D:25:ILE:N	2.73	0.47
2:D:219:THR:HG22	2:D:236:PRO:HA	1.97	0.47
2:D:287:THR:HG23	2:D:414:ASN:ND2	2.26	0.47
1:E:79:THR:CG2	1:E:82:ASP:H	2.27	0.47
1:E:469:GLU:HB3	1:E:483:PHE:CE1	2.49	0.47
2:F:471:MET:HE3	2:F:471:MET:C	2.40	0.47
1:A:27:GLY:O	1:A:30:ASP:N	2.42	0.47
1:A:142:VAL:HG12	1:A:143:SER:N	2.29	0.47
1:A:316:ALA:CB	1:A:324:LEU:HD11	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:121:PHE:HD1	2:C:121:PHE:H	1.62	0.47
2:C:453:ILE:HG12	2:C:454:ASN:N	2.30	0.47
2:D:371:LYS:O	2:D:371:LYS:CD	2.52	0.47
2:D:446:ARG:H	2:D:496:ARG:HH12	1.63	0.47
1:E:353:SER:O	1:E:354:ALA:CB	2.63	0.47
2:F:387:VAL:HG12	2:F:388:SER:N	2.29	0.47
1:A:60:LEU:CD1	1:A:73:PHE:HD1	2.28	0.47
1:A:147:VAL:CG1	1:A:180:MET:HE3	2.35	0.47
1:A:324:LEU:O	1:A:328:ALA:HB2	2.15	0.47
1:A:371:LYS:O	1:A:371:LYS:CD	2.62	0.47
1:B:340:ARG:C	1:B:342:ASN:N	2.73	0.47
1:B:483:PHE:O	1:B:485:ASN:N	2.48	0.47
2:D:44:VAL:HA	2:D:205:VAL:O	2.13	0.47
1:E:67:PHE:O	1:E:68:ASP:C	2.58	0.47
2:F:19:ALA:O	2:F:38:ILE:HD13	2.14	0.47
2:F:269:ARG:O	2:F:273:MET:HG3	2.15	0.47
2:F:492:GLY:C	2:F:494:PRO:HD3	2.40	0.47
2:F:500:ASP:CG	2:F:501:GLU:N	2.73	0.47
1:A:79:THR:O	1:A:82:ASP:N	2.48	0.47
1:A:245:ASN:ND2	1:A:247:PHE:CZ	2.82	0.47
1:A:455:VAL:O	1:A:463:HIS:CE1	2.68	0.47
1:B:340:ARG:O	1:B:342:ASN:N	2.48	0.47
2:C:273:MET:CE	2:C:468:ARG:HD2	2.43	0.47
2:D:261:VAL:HG12	2:D:262:ARG:N	2.30	0.47
2:D:299:SER:C	2:D:333:MET:HE1	2.40	0.47
1:E:123:LEU:HD13	1:E:163:GLU:OE2	2.14	0.47
1:E:145:ASP:O	1:E:146:SER:OG	2.30	0.47
2:F:14:GLU:HG3	2:F:16:GLN:HG3	1.97	0.47
2:F:144:ILE:HD13	2:F:167:LEU:HD21	1.97	0.47
2:F:154:TYR:O	2:F:154:TYR:HD1	1.98	0.47
2:F:313:ILE:HG13	2:F:372:PRO:CG	2.45	0.47
1:A:392:PHE:O	1:A:393:ARG:C	2.58	0.46
1:A:452:ALA:HA	1:A:468:ARG:O	2.14	0.46
1:A:504:GLU:C	1:A:506:SER:H	2.22	0.46
2:C:287:THR:HG22	2:C:288:GLY:H	1.78	0.46
2:D:323:GLN:O	2:D:324:LEU:C	2.58	0.46
2:D:463:HIS:C	2:D:463:HIS:ND1	2.73	0.46
1:E:433:ILE:O	1:E:433:ILE:CG2	2.62	0.46
2:F:396:VAL:HG11	2:F:430:ILE:HG21	1.96	0.46
1:A:161:ARG:NH2	2:F:149:SER:HB3	2.30	0.46
1:A:440:LEU:CD2	1:A:453:ILE:HG13	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:PHE:H	1:B:121:PHE:HD1	1.62	0.46
1:B:294:LYS:HD3	4:B:901:ATP:O1B	2.16	0.46
2:C:328:ALA:O	2:C:329:TYR:C	2.58	0.46
2:F:194:TYR:N	2:F:194:TYR:CD1	2.83	0.46
1:E:18:ILE:HG13	1:E:228:THR:HG23	1.97	0.46
1:A:484:ARG:HB3	1:A:484:ARG:NH1	2.31	0.46
1:B:186:GLU:OE2	1:B:187:GLU:N	2.49	0.46
2:C:106:LEU:HD23	2:C:130:ILE:HG12	1.97	0.46
2:D:296:LEU:HA	2:D:331:TRP:CZ3	2.50	0.46
1:E:111:ASP:C	1:E:113:GLU:H	2.23	0.46
2:F:270:LEU:O	2:F:273:MET:HB2	2.16	0.46
1:B:214:GLU:HA	2:C:234:GLU:HB2	1.98	0.46
2:C:38:ILE:CG2	2:C:39:GLY:N	2.78	0.46
2:C:287:THR:CG2	2:C:414:ASN:HD22	2.18	0.46
2:D:294:LYS:HE3	2:D:414:ASN:O	2.16	0.46
1:E:52:LYS:HD2	1:E:181:THR:HG23	1.97	0.46
1:E:442:TYR:CE1	2:F:456:PHE:CZ	3.03	0.46
2:F:123:LEU:O	2:F:123:LEU:HD13	2.14	0.46
1:A:195:GLY:O	2:F:193:ARG:NH2	2.43	0.46
1:A:441:GLN:HB2	5:A:522:HOH:O	2.15	0.46
1:B:64:ILE:HD11	1:B:102:LYS:O	2.16	0.46
2:D:88:ARG:NE	1:E:15:HIS:HA	2.30	0.46
2:D:338:MET:HB3	2:D:344:LEU:CB	2.46	0.46
1:E:21:MET:HE2	1:E:177:THR:HG21	1.98	0.46
1:E:191:ILE:HG13	1:E:206:ILE:HD11	1.96	0.46
1:E:248:PRO:O	1:E:250:GLY:N	2.48	0.46
2:F:306:CYS:SG	2:F:344:LEU:HB2	2.56	0.46
1:A:178:THR:HG22	1:A:179:VAL:H	1.81	0.46
1:A:259:SER:O	2:F:326:ARG:HD3	2.15	0.46
1:A:433:ILE:HD12	1:A:433:ILE:N	2.30	0.46
1:A:488:ARG:O	1:A:494:PRO:HA	2.15	0.46
1:A:499:VAL:O	1:A:500:ASP:HB2	2.16	0.46
2:C:88:ARG:HD3	2:D:15:HIS:C	2.41	0.46
2:D:163:GLU:HA	2:D:163:GLU:OE2	2.16	0.46
2:D:305:ALA:O	2:D:310:GLU:O	2.34	0.46
2:F:312:ALA:HA	2:F:374:ARG:O	2.16	0.46
1:A:298:VAL:CG2	1:A:411:LEU:HD23	2.42	0.46
1:B:76:PHE:HZ	1:B:126:LEU:HD21	1.78	0.46
1:B:379:SER:OG	1:B:382:ALA:CB	2.57	0.46
2:C:42:THR:HA	2:C:203:ASN:HB2	1.97	0.46
2:C:248:PRO:C	2:C:250:GLY:N	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:192:ALA:HB3	2:D:197:GLU:CD	2.41	0.46
2:D:380:LEU:N	2:D:413:THR:O	2.42	0.46
2:D:385:ARG:HA	1:E:393:ARG:HH12	1.81	0.46
1:E:14:GLU:HG3	1:E:16:GLN:N	2.28	0.46
1:E:157:SER:O	1:E:160:VAL:HB	2.16	0.46
1:E:203:ASN:HB3	1:E:225:LEU:CD2	2.43	0.46
1:E:248:PRO:C	1:E:250:GLY:N	2.72	0.46
1:E:404:LYS:C	1:E:406:GLU:H	2.24	0.46
1:E:484:ARG:HG2	1:E:484:ARG:O	2.15	0.46
2:F:270:LEU:O	2:F:273:MET:N	2.49	0.46
1:B:51:GLY:O	1:B:54:LEU:HB3	2.16	0.46
1:B:106:LEU:C	1:B:106:LEU:HD12	2.41	0.46
1:B:220:LEU:HD13	1:B:246:ILE:CD1	2.46	0.46
1:B:473:SER:C	1:B:475:LYS:N	2.74	0.46
2:C:367:ILE:CD1	2:C:375:ILE:CD1	2.94	0.46
2:C:440:LEU:HA	2:C:452:ALA:O	2.15	0.46
1:E:164:LEU:O	1:E:167:LEU:N	2.49	0.46
1:E:269:ARG:HG2	1:E:479:ILE:HB	1.98	0.46
2:F:269:ARG:O	2:F:272:GLU:HB2	2.16	0.46
2:F:357:GLU:HG3	2:F:358:ASP:N	2.30	0.46
2:F:398:GLY:O	2:F:399:VAL:C	2.58	0.46
1:A:72:VAL:HG23	1:A:139:ALA:CB	2.46	0.46
1:A:299:SER:HB3	1:A:333:MET:HE2	1.98	0.46
1:A:466:ALA:HA	2:F:448:GLU:HG2	1.98	0.46
1:B:21:MET:HB2	1:B:38:ILE:HG12	1.97	0.46
1:B:23:THR:HB	1:B:25:ILE:HG13	1.96	0.46
2:C:443:VAL:HG12	2:C:445:ILE:HG12	1.98	0.46
2:D:419:PHE:O	2:D:420:MET:O	2.34	0.46
1:E:311:ARG:HD2	1:E:371:LYS:HE3	1.97	0.46
1:E:444:GLU:OE1	2:F:490:ILE:HG12	2.15	0.46
2:F:131:ASN:OD1	2:F:174:ILE:HD12	2.16	0.46
2:F:191:ILE:CB	2:F:198:GLU:CG	2.87	0.46
2:F:329:TYR:HA	2:F:332:GLY:O	2.16	0.46
2:F:438:ILE:HD13	2:F:455:VAL:HG22	1.98	0.46
1:B:86:ASN:O	1:B:89:SER:N	2.47	0.45
1:B:313:ILE:HG13	1:B:372:PRO:HG3	1.97	0.45
2:D:320:SER:HB3	1:E:256:GLN:HG2	1.98	0.45
1:E:497:ILE:O	1:E:498:THR:OG1	2.24	0.45
2:F:145:ASP:O	2:F:146:SER:OG	2.31	0.45
2:F:419:PHE:O	2:F:420:MET:O	2.33	0.45
2:F:430:ILE:O	2:F:431:ASP:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:GLY:O	1:B:218:ARG:NH2	2.48	0.45
2:C:497:ILE:C	2:C:498:THR:HG22	2.40	0.45
2:F:154:TYR:O	2:F:154:TYR:CD1	2.69	0.45
2:F:191:ILE:HB	2:F:198:GLU:CD	2.40	0.45
1:A:61:TYR:CE2	1:A:65:ILE:HG13	2.51	0.45
1:B:370:PHE:C	1:B:372:PRO:HD3	2.41	0.45
2:C:338:MET:H	2:C:338:MET:HG2	1.47	0.45
1:E:52:LYS:O	1:E:55:PHE:HB3	2.16	0.45
1:E:294:LYS:O	1:E:295:THR:C	2.59	0.45
1:A:371:LYS:N	1:A:372:PRO:CD	2.78	0.45
1:B:84:ILE:O	1:B:85:LYS:C	2.60	0.45
1:B:264:SER:HA	1:B:271:ASP:OD1	2.17	0.45
2:C:300:ARG:CA	2:C:333:MET:HE1	2.45	0.45
2:C:392:PHE:O	2:C:395:PHE:N	2.42	0.45
1:E:464:ASP:OD2	1:E:466:ALA:HB3	2.16	0.45
2:F:116:GLU:O	2:F:117:VAL:HB	2.16	0.45
2:C:144:ILE:HG21	2:C:147:VAL:HG12	1.98	0.45
2:C:225:LEU:HB2	2:C:230:HIS:CD2	2.52	0.45
1:E:264:SER:N	1:E:374:ARG:NH2	2.64	0.45
1:E:462:TRP:CE3	1:E:463:HIS:N	2.85	0.45
2:F:504:GLU:HA	2:F:507:ARG:NE	2.32	0.45
1:A:313:ILE:CG1	1:A:372:PRO:HG2	2.46	0.45
1:A:334:ASP:O	1:A:338:MET:HG2	2.17	0.45
1:B:213:GLY:O	1:B:214:GLU:HB2	2.16	0.45
1:B:436:THR:CG2	1:B:458:MET:HG2	2.46	0.45
1:B:452:ALA:HA	1:B:468:ARG:O	2.17	0.45
2:D:299:SER:HB3	2:D:333:MET:HE2	1.99	0.45
2:D:468:ARG:HG2	2:D:468:ARG:HH11	1.81	0.45
1:E:118:VAL:O	1:E:118:VAL:HG12	2.16	0.45
1:E:208:ARG:HB2	1:E:219:THR:OG1	2.16	0.45
2:F:49:GLY:CA	4:F:903:ATP:O2B	2.64	0.45
2:F:65:ILE:O	2:F:65:ILE:HG22	2.17	0.45
2:F:142:VAL:O	2:F:178:THR:HA	2.15	0.45
2:F:420:MET:HA	5:F:532:HOH:O	2.16	0.45
2:F:425:ILE:HG22	2:F:426:THR:OG1	2.17	0.45
1:A:356:LEU:CD2	1:A:387:VAL:HG11	2.46	0.45
1:B:315:PHE:HB3	1:B:317:TYR:CE1	2.50	0.45
2:C:215:ARG:HA	2:C:215:ARG:NE	2.30	0.45
2:C:225:LEU:HD12	2:C:230:HIS:HB3	1.98	0.45
2:C:396:VAL:O	2:C:397:ILE:C	2.60	0.45
2:C:437:ILE:CD1	2:C:457:LYS:HE2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:24:MET:HA	1:E:24:MET:HE3	1.98	0.45
1:E:219:THR:HA	1:E:235:TYR:O	2.16	0.45
2:F:308:ASN:O	2:F:309:LYS:HB2	2.16	0.45
1:A:69:GLU:OE1	1:A:141:ARG:NH2	2.48	0.45
1:A:157:SER:O	1:A:160:VAL:N	2.50	0.45
1:A:488:ARG:NE	2:F:488:ARG:HH22	2.15	0.45
1:B:200:VAL:O	1:B:200:VAL:HG12	2.17	0.45
1:B:313:ILE:HG21	1:B:315:PHE:CZ	2.51	0.45
2:C:76:PHE:O	2:C:109:SER:HA	2.16	0.45
2:C:261:VAL:HG12	2:C:262:ARG:N	2.32	0.45
2:C:388:SER:O	2:C:389:ASN:C	2.58	0.45
2:D:353:SER:O	2:D:354:ALA:HB2	2.16	0.45
1:E:20:LYS:HE3	1:E:228:THR:HG21	1.98	0.45
1:E:291:GLY:C	1:E:442:TYR:OH	2.60	0.45
1:E:419:PHE:O	1:E:420:MET:HB2	2.16	0.45
2:F:38:ILE:HD12	2:F:38:ILE:H	1.82	0.45
2:F:79:THR:HG23	2:F:81:GLN:N	2.28	0.45
2:F:215:ARG:NE	2:F:215:ARG:CA	2.77	0.45
2:F:455:VAL:O	2:F:455:VAL:HG12	2.17	0.45
1:A:518:GLU:HB2	1:A:519:SER:H	1.54	0.45
1:B:376:ALA:HA	1:B:411:LEU:O	2.17	0.45
2:C:79:THR:HG22	2:C:82:ASP:CG	2.42	0.45
2:C:262:ARG:HH22	2:C:461:SER:CB	2.30	0.45
2:C:274:CYS:HG	2:C:278:PHE:HE2	1.65	0.45
2:C:308:ASN:O	2:C:310:GLU:N	2.50	0.45
2:D:344:LEU:CD1	2:D:346:ILE:HG13	2.47	0.45
1:E:371:LYS:O	1:E:371:LYS:CD	2.57	0.45
1:A:18:ILE:HG21	1:A:37:PRO:HB3	1.99	0.45
1:A:170:ARG:HD2	1:A:173:GLN:OE1	2.16	0.45
1:A:440:LEU:HD23	1:A:453:ILE:HG13	1.99	0.45
2:C:18:ILE:HB	2:C:228:THR:CG2	2.45	0.45
2:C:33:HIS:CD2	2:C:230:HIS:HA	2.52	0.45
2:C:79:THR:HG23	2:C:81:GLN:HG2	1.99	0.45
2:C:418:GLN:HG3	2:C:418:GLN:O	2.17	0.45
2:D:85:LYS:O	2:D:86:ASN:C	2.59	0.45
2:D:264:SER:OG	2:D:265:SER:N	2.50	0.45
2:D:294:LYS:O	2:D:297:LEU:N	2.50	0.45
2:D:463:HIS:C	2:D:463:HIS:HD1	2.24	0.45
2:F:59:PHE:CD2	2:F:179:VAL:HG21	2.52	0.45
2:F:302:VAL:CG1	2:F:303:GLU:N	2.80	0.45
2:F:325:LEU:HD21	2:F:335:PHE:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:471:MET:HE1	2:F:473:SER:HB3	1.98	0.45
2:F:486:PHE:CB	2:F:489:ILE:HD11	2.47	0.45
1:A:192:ALA:O	1:A:193:ARG:C	2.60	0.44
1:B:273:MET:HE3	1:B:468:ARG:CD	2.41	0.44
1:B:497:ILE:O	1:B:498:THR:C	2.59	0.44
2:C:194:TYR:O	2:C:196:VAL:HG23	2.17	0.44
1:E:203:ASN:HA	1:E:224:LYS:O	2.16	0.44
2:F:347:VAL:O	2:F:348:CYS:CB	2.63	0.44
2:F:504:GLU:HB2	2:F:505:LEU:H	1.48	0.44
1:A:104:PHE:CD2	1:A:133:ALA:HB1	2.52	0.44
1:A:184:ARG:NH2	1:A:186:GLU:O	2.50	0.44
1:A:261:VAL:CG1	1:A:262:ARG:N	2.79	0.44
1:A:364:LYS:O	1:A:367:ILE:HB	2.17	0.44
1:A:496:ARG:O	1:A:497:ILE:HG23	2.17	0.44
2:C:52:LYS:N	2:C:207:LEU:HD12	2.32	0.44
2:C:150:VAL:CG1	2:C:151:PHE:N	2.80	0.44
2:C:348:CYS:HB3	2:D:254:LEU:HB3	1.99	0.44
2:D:79:THR:CG2	2:D:82:ASP:H	2.28	0.44
2:F:145:ASP:OD2	2:F:181:THR:HG21	2.17	0.44
2:F:197:GLU:OE2	2:F:197:GLU:N	2.36	0.44
2:F:329:TYR:O	2:F:332:GLY:N	2.50	0.44
1:A:498:THR:O	1:A:499:VAL:C	2.60	0.44
1:A:502:LYS:HG3	1:A:502:LYS:O	2.17	0.44
1:B:53:THR:O	1:B:54:LEU:C	2.59	0.44
1:B:191:ILE:HD12	1:B:191:ILE:N	2.32	0.44
1:B:238:THR:CG2	1:B:240:THR:HG22	2.47	0.44
2:C:18:ILE:N	2:C:18:ILE:CD1	2.79	0.44
2:C:117:VAL:O	2:C:117:VAL:HG12	2.18	0.44
2:C:164:LEU:O	2:C:165:PHE:C	2.59	0.44
2:C:360:LEU:HD21	2:C:364:LYS:HE3	1.99	0.44
2:D:183:GLU:HB2	1:E:199:PHE:CZ	2.52	0.44
2:D:206:ILE:HD11	2:D:223:LEU:HD12	1.99	0.44
1:E:340:ARG:O	1:E:342:ASN:N	2.51	0.44
2:F:104:PHE:CE2	2:F:106:LEU:HB2	2.51	0.44
1:B:84:ILE:HA	1:B:94:LEU:HD12	1.99	0.44
4:D:903:ATP:O3'	1:E:224:LYS:HB2	2.17	0.44
1:E:164:LEU:HD11	1:E:197:GLU:CG	2.47	0.44
1:E:303:GLU:HB2	1:E:333:MET:HE3	1.98	0.44
2:F:270:LEU:O	2:F:271:ASP:C	2.61	0.44
2:F:379:SER:HB3	2:F:382:ALA:HB2	2.00	0.44
2:F:514:GLU:O	2:F:515:LYS:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:SER:HB2	1:A:143:SER:HB3	1.98	0.44
1:A:79:THR:O	1:A:83:ILE:HD12	2.17	0.44
1:B:185:ILE:HD11	1:B:193:ARG:HG3	1.99	0.44
1:B:401:GLY:O	1:B:402:TYR:C	2.61	0.44
2:C:50:THR:HG23	2:C:209:ASN:HB2	2.00	0.44
2:C:69:GLU:HA	2:C:70:PRO:HD3	1.90	0.44
2:C:148:THR:HG21	2:C:193:ARG:HD2	1.99	0.44
2:C:215:ARG:HE	2:C:215:ARG:CA	2.31	0.44
2:C:344:LEU:HD11	2:C:346:ILE:HG13	1.99	0.44
2:D:262:ARG:NH1	2:D:275:GLY:O	2.51	0.44
2:D:313:ILE:HG13	2:D:372:PRO:HG3	2.00	0.44
1:E:21:MET:HE1	1:E:177:THR:CB	2.48	0.44
1:E:46:GLY:H	1:E:52:LYS:HD3	1.81	0.44
1:E:356:LEU:HD12	1:E:356:LEU:H	1.82	0.44
1:E:446:ARG:HH21	1:E:496:ARG:NH2	2.16	0.44
2:F:115:GLN:HE21	2:F:115:GLN:HB3	1.54	0.44
2:F:264:SER:O	2:F:374:ARG:NH2	2.51	0.44
2:F:516:GLY:N	2:F:517:PRO:CD	2.80	0.44
1:A:65:ILE:O	1:A:65:ILE:CG2	2.65	0.44
1:A:83:ILE:H	1:A:83:ILE:CD1	2.26	0.44
1:A:118:VAL:HG12	1:A:122:ASP:HB3	1.99	0.44
1:B:324:LEU:HD23	1:B:324:LEU:HA	1.89	0.44
1:B:401:GLY:O	1:B:404:LYS:N	2.51	0.44
2:C:123:LEU:O	2:C:124:SER:C	2.61	0.44
2:C:225:LEU:HD23	2:C:225:LEU:HA	1.78	0.44
2:C:419:PHE:O	2:C:420:MET:CB	2.65	0.44
2:D:65:ILE:O	2:D:65:ILE:HG22	2.17	0.44
2:D:98:VAL:HA	2:D:103:LEU:O	2.18	0.44
2:D:225:LEU:HD12	2:D:230:HIS:HB3	2.00	0.44
2:D:419:PHE:O	2:D:420:MET:HB2	2.18	0.44
1:E:346:ILE:CG2	1:E:347:VAL:N	2.80	0.44
1:B:148:THR:C	1:B:150:VAL:H	2.25	0.44
1:B:256:GLN:H	1:B:256:GLN:HG2	1.55	0.44
1:B:291:GLY:HA3	1:B:442:TYR:HH	1.81	0.44
1:E:315:PHE:CD2	1:E:347:VAL:HG21	2.53	0.44
1:E:420:MET:CE	2:F:490:ILE:HG13	2.37	0.44
2:F:292:THR:HB	2:F:440:LEU:HB3	2.00	0.44
2:F:313:ILE:CD1	2:F:372:PRO:HG2	2.48	0.44
1:A:79:THR:O	1:A:82:ASP:HB2	2.17	0.44
1:A:211:LEU:HG	1:A:212:GLU:H	1.82	0.44
1:A:323:GLN:HE21	1:A:327:ASN:HD21	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:TRP:CE3	1:A:463:HIS:N	2.86	0.44
1:B:449:MET:CE	2:C:467:ILE:HD11	2.20	0.44
2:C:42:THR:O	2:C:180:MET:HB2	2.18	0.44
2:D:220:LEU:HD23	2:D:220:LEU:C	2.43	0.44
1:E:340:ARG:C	1:E:342:ASN:H	2.25	0.44
1:E:344:LEU:HD13	1:E:345:LYS:N	2.32	0.44
1:E:420:MET:HE1	2:F:490:ILE:CG1	2.36	0.44
1:B:182:THR:HG21	1:B:192:ALA:HB1	1.99	0.44
1:B:370:PHE:C	1:B:371:LYS:HG3	2.43	0.44
1:B:463:HIS:CE1	1:B:465:LYS:NZ	2.85	0.44
1:B:471:MET:HG2	1:B:480:LYS:HZ3	1.83	0.44
2:C:14:GLU:HG3	2:C:16:GLN:H	1.83	0.44
2:D:359:HIS:O	2:D:363:ILE:HG13	2.17	0.44
1:E:42:THR:HG23	1:E:203:ASN:HB2	1.99	0.44
1:E:401:GLY:O	1:E:405:GLN:HG2	2.18	0.44
2:F:31:ILE:CD1	2:F:246:ILE:HG21	2.47	0.44
2:F:96:LYS:O	2:F:99:ASP:HB2	2.18	0.44
2:F:300:ARG:CZ	2:F:477:PRO:HD2	2.47	0.44
2:F:387:VAL:HG12	2:F:388:SER:O	2.18	0.44
2:F:507:ARG:O	2:F:508:ILE:C	2.61	0.44
1:A:31:ILE:O	1:A:222:ILE:HD12	2.18	0.43
1:A:407:GLU:OE1	1:A:407:GLU:HA	2.18	0.43
1:B:150:VAL:C	1:B:152:GLN:N	2.74	0.43
1:B:197:GLU:O	1:B:200:VAL:N	2.41	0.43
1:B:417:ASP:HB3	2:C:429:HIS:CE1	2.52	0.43
2:C:27:GLY:O	2:C:28:PHE:C	2.61	0.43
2:C:306:CYS:SG	2:C:344:LEU:HB2	2.57	0.43
2:C:457:LYS:O	2:C:457:LYS:HG3	2.17	0.43
2:D:41:SER:HB3	2:D:178:THR:CB	2.39	0.43
2:D:52:LYS:HD2	2:D:182:THR:O	2.18	0.43
2:D:435:ASP:HA	2:D:459:ARG:HD2	1.99	0.43
1:E:167:LEU:O	1:E:171:LEU:HD12	2.18	0.43
1:E:248:PRO:HB2	1:E:251:ALA:CB	2.45	0.43
1:E:367:ILE:HG12	1:E:375:ILE:HD11	2.00	0.43
2:F:150:VAL:CG1	2:F:151:PHE:N	2.80	0.43
2:F:364:LYS:O	2:F:365:SER:C	2.59	0.43
2:F:431:ASP:OD1	2:F:431:ASP:N	2.43	0.43
2:F:483:PHE:CD1	2:F:483:PHE:N	2.86	0.43
1:A:268:VAL:O	1:A:271:ASP:HB2	2.17	0.43
1:B:52:LYS:HB2	1:B:52:LYS:HE3	1.85	0.43
1:B:75:THR:HG23	1:B:75:THR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:GLU:OE2	2:C:489:ILE:HG13	2.18	0.43
2:C:321:ARG:HG2	2:C:348:CYS:SG	2.57	0.43
2:C:360:LEU:HD23	2:C:364:LYS:HG3	2.00	0.43
2:D:76:PHE:HZ	2:D:126:LEU:HD21	1.82	0.43
2:D:197:GLU:OE2	2:D:197:GLU:N	2.43	0.43
2:D:367:ILE:HG12	2:D:375:ILE:HD11	2.00	0.43
1:E:419:PHE:CD2	2:F:425:ILE:HD12	2.53	0.43
1:E:444:GLU:O	1:E:494:PRO:HD2	2.18	0.43
2:F:59:PHE:CE2	2:F:179:VAL:HG23	2.53	0.43
2:F:295:THR:HB	4:F:901:ATP:PA	2.58	0.43
2:C:89:SER:CB	2:D:227:GLY:O	2.66	0.43
2:C:208:ARG:O	2:C:218:ARG:HA	2.18	0.43
2:C:240:THR:HG21	2:C:361:GLN:NE2	2.32	0.43
2:C:247:PHE:HB3	2:C:249:LEU:HD21	2.00	0.43
2:D:61:TYR:OH	2:D:92:TRP:CD1	2.70	0.43
2:D:294:LYS:N	4:D:901:ATP:O1B	2.43	0.43
2:D:401:GLY:O	2:D:405:GLN:HG2	2.18	0.43
1:E:116:GLU:O	1:E:117:VAL:C	2.61	0.43
1:E:356:LEU:N	1:E:356:LEU:CD1	2.81	0.43
2:F:298:VAL:HA	2:F:411:LEU:HD21	1.99	0.43
2:F:401:GLY:O	2:F:402:TYR:C	2.60	0.43
1:A:261:VAL:HG12	1:A:262:ARG:N	2.33	0.43
2:C:412:PHE:N	2:C:412:PHE:CD1	2.87	0.43
2:D:96:LYS:O	2:D:99:ASP:N	2.51	0.43
2:D:396:VAL:HG11	2:D:430:ILE:HG21	2.00	0.43
1:E:140:ARG:HA	1:E:140:ARG:HD2	1.86	0.43
1:E:356:LEU:CD2	1:E:387:VAL:HG11	2.49	0.43
2:F:121:PHE:HD2	2:F:121:PHE:HA	1.73	0.43
2:F:363:ILE:HG22	2:F:367:ILE:HD11	1.99	0.43
2:F:462:TRP:O	2:F:463:HIS:O	2.37	0.43
2:C:123:LEU:HD11	2:C:163:GLU:O	2.18	0.43
1:E:274:CYS:C	1:E:276:GLY:N	2.76	0.43
1:E:363:ILE:O	1:E:364:LYS:C	2.61	0.43
1:E:426:THR:HG21	1:E:430:ILE:CG1	2.47	0.43
1:E:496:ARG:O	1:E:497:ILE:HD13	2.18	0.43
2:F:294:LYS:HE2	2:F:294:LYS:HB2	1.89	0.43
2:F:332:GLY:O	2:F:333:MET:O	2.37	0.43
1:B:161:ARG:NH2	1:B:199:PHE:CB	2.74	0.43
1:B:208:ARG:NE	1:B:234:GLU:OE2	2.45	0.43
1:B:356:LEU:HD23	1:B:395:PHE:HB2	2.01	0.43
2:C:370:PHE:C	2:C:371:LYS:HG3	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:299:SER:HB3	2:D:333:MET:CE	2.49	0.43
1:E:25:ILE:HD12	1:E:55:PHE:CE1	2.53	0.43
1:E:151:PHE:C	1:E:153:GLN:N	2.76	0.43
2:F:164:LEU:HD11	2:F:197:GLU:HG3	2.01	0.43
1:A:153:GLN:O	1:A:154:TYR:CB	2.67	0.43
1:B:126:LEU:C	1:B:128:GLU:N	2.75	0.43
2:C:446:ARG:HG2	2:C:496:ARG:NH1	2.33	0.43
2:D:106:LEU:HD23	2:D:130:ILE:HG12	2.01	0.43
2:D:206:ILE:HG21	2:D:208:ARG:NH1	2.34	0.43
2:D:231:MET:HB3	2:D:235:TYR:OH	2.19	0.43
2:D:240:THR:O	2:D:241:ASP:C	2.62	0.43
1:E:248:PRO:O	1:E:249:LEU:C	2.62	0.43
1:E:264:SER:O	1:E:374:ARG:NH2	2.52	0.43
1:E:326:ARG:HD3	2:F:258:SER:OG	2.19	0.43
2:F:231:MET:SD	2:F:251:ALA:HB2	2.59	0.43
2:F:335:PHE:HA	2:F:338:MET:HG3	2.01	0.43
2:F:445:ILE:HG13	2:F:483:PHE:HE2	1.82	0.43
1:A:84:ILE:O	1:A:87:ALA:HB3	2.19	0.43
1:A:210:VAL:HG12	1:A:211:LEU:O	2.18	0.43
1:A:316:ALA:HB3	1:A:348:CYS:SG	2.59	0.43
1:A:463:HIS:O	1:A:465:LYS:HE2	2.19	0.43
1:B:419:PHE:O	1:B:420:MET:O	2.36	0.43
2:C:471:MET:CE	2:C:473:SER:HB3	2.49	0.43
2:D:41:SER:OG	2:D:168:VAL:HG13	2.18	0.43
2:D:392:PHE:O	2:D:395:PHE:N	2.50	0.43
2:D:415:THR:O	2:D:416:SER:C	2.61	0.43
1:E:356:LEU:H	1:E:356:LEU:CD1	2.31	0.43
1:E:363:ILE:CG2	1:E:367:ILE:HD11	2.44	0.43
2:F:79:THR:CG2	2:F:82:ASP:OD2	2.67	0.43
2:C:184:ARG:C	2:C:185:ILE:HD13	2.44	0.43
2:C:204:VAL:HG11	2:C:223:LEU:HD12	2.00	0.43
2:D:208:ARG:NE	2:D:234:GLU:OE2	2.51	0.43
1:E:178:THR:CG2	1:E:179:VAL:N	2.80	0.43
1:E:392:PHE:O	1:E:395:PHE:N	2.52	0.43
1:E:468:ARG:HA	1:E:482:SER:HA	2.01	0.43
1:E:486:PHE:HA	1:E:495:THR:O	2.19	0.43
2:F:183:GLU:HG3	2:F:193:ARG:HE	1.83	0.43
2:F:340:ARG:C	2:F:342:ASN:N	2.77	0.43
1:A:49:GLY:CA	4:A:903:ATP:O2B	2.66	0.43
1:A:207:LEU:HD22	1:A:237:PHE:CE2	2.53	0.43
1:A:257:ARG:HH22	1:A:407:GLU:HG2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ARG:HG2	1:A:496:ARG:CZ	2.49	0.43
1:B:184:ARG:CD	1:B:191:ILE:O	2.66	0.43
2:C:295:THR:O	2:C:298:VAL:HB	2.18	0.43
2:C:352:GLU:C	2:C:354:ALA:H	2.27	0.43
2:D:153:GLN:O	2:D:154:TYR:CB	2.67	0.43
1:A:402:TYR:O	1:A:406:GLU:HB2	2.18	0.42
1:B:20:LYS:HG2	1:B:35:GLY:O	2.19	0.42
2:C:50:THR:HG21	2:C:207:LEU:C	2.44	0.42
2:C:426:THR:HG22	2:C:428:SER:H	1.84	0.42
2:D:430:ILE:O	2:D:431:ASP:O	2.36	0.42
1:E:313:ILE:CG1	1:E:372:PRO:CG	2.93	0.42
1:E:462:TRP:O	1:E:463:HIS:O	2.37	0.42
2:F:377:ILE:CD1	2:F:412:PHE:HE2	2.31	0.42
2:F:380:LEU:CD1	2:F:412:PHE:HB3	2.49	0.42
2:F:513:GLN:OE1	2:F:513:GLN:HA	2.19	0.42
1:A:28:PHE:C	1:A:28:PHE:CD2	2.96	0.42
1:A:156:ALA:O	1:A:157:SER:C	2.62	0.42
1:A:237:PHE:HA	1:A:245:ASN:O	2.18	0.42
1:B:217:ARG:NH2	1:B:394:GLN:OE1	2.52	0.42
1:B:291:GLY:C	1:B:442:TYR:OH	2.62	0.42
1:B:392:PHE:O	1:B:393:ARG:C	2.61	0.42
2:C:136:LYS:O	2:C:136:LYS:HG2	2.18	0.42
2:D:272:GLU:C	2:D:274:CYS:N	2.77	0.42
2:D:446:ARG:N	2:D:496:ARG:HH12	2.16	0.42
1:E:53:THR:O	1:E:54:LEU:C	2.62	0.42
1:E:164:LEU:HD11	1:E:197:GLU:HG3	2.02	0.42
1:E:451:ARG:NH1	1:E:451:ARG:CG	2.78	0.42
2:F:56:SER:O	2:F:59:PHE:HB3	2.19	0.42
2:F:160:VAL:O	2:F:161:ARG:C	2.62	0.42
2:F:443:VAL:HG12	2:F:445:ILE:CG1	2.47	0.42
1:B:126:LEU:C	1:B:128:GLU:H	2.27	0.42
1:B:334:ASP:O	1:B:338:MET:HG2	2.18	0.42
1:B:371:LYS:N	1:B:372:PRO:CD	2.80	0.42
1:B:392:PHE:O	1:B:395:PHE:N	2.45	0.42
2:C:17:ALA:C	2:C:18:ILE:HD12	2.44	0.42
2:C:54:LEU:O	2:C:55:PHE:C	2.63	0.42
2:C:148:THR:C	2:C:150:VAL:H	2.27	0.42
2:D:200:VAL:O	2:D:200:VAL:HG12	2.19	0.42
1:E:336:GLU:OE1	1:E:336:GLU:HA	2.19	0.42
1:E:452:ALA:HA	1:E:469:GLU:HA	2.00	0.42
2:F:451:ARG:HH11	2:F:451:ARG:CG	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:THR:C	1:A:25:ILE:H	2.26	0.42
1:A:111:ASP:O	1:A:113:GLU:N	2.49	0.42
1:A:211:LEU:CD1	1:A:216:ARG:HG2	2.49	0.42
1:A:287:THR:CG2	1:A:414:ASN:HD22	2.31	0.42
1:A:488:ARG:HE	2:F:488:ARG:HH22	1.65	0.42
1:B:62:ASN:O	1:B:66:GLU:HB2	2.19	0.42
1:B:267:VAL:HB	1:B:270:LEU:HB2	2.01	0.42
1:B:309:LYS:HA	1:B:343:LEU:HD13	2.00	0.42
1:B:483:PHE:HB3	1:B:486:PHE:HD1	1.84	0.42
2:C:437:ILE:HD11	2:C:457:LYS:HE2	2.01	0.42
2:D:193:ARG:NH1	2:D:193:ARG:HG2	2.34	0.42
1:E:301:PHE:HZ	1:E:409:THR:HG22	1.84	0.42
2:F:64:ILE:HD11	2:F:102:LYS:O	2.19	0.42
2:F:451:ARG:NH1	2:F:472:ILE:HD12	2.35	0.42
2:C:211:LEU:O	2:C:212:GLU:CB	2.65	0.42
2:C:378:ASP:O	2:C:379:SER:CB	2.67	0.42
2:D:371:LYS:N	2:D:372:PRO:CD	2.82	0.42
2:D:468:ARG:HG2	2:D:468:ARG:NH1	2.34	0.42
2:F:497:ILE:O	2:F:497:ILE:HG13	2.19	0.42
1:A:150:VAL:CG1	1:A:151:PHE:N	2.81	0.42
1:B:61:TYR:O	1:B:64:ILE:N	2.52	0.42
1:B:178:THR:CG2	1:B:179:VAL:H	2.32	0.42
1:B:248:PRO:HB2	1:B:251:ALA:CB	2.47	0.42
1:B:425:ILE:HD12	1:B:425:ILE:N	2.35	0.42
2:C:433:ILE:O	2:C:433:ILE:HG13	2.19	0.42
2:D:323:GLN:HE22	1:E:459:ARG:HD3	1.84	0.42
1:E:113:GLU:HB3	1:E:114:GLY:H	1.62	0.42
2:F:224:LYS:HZ1	2:F:226:ARG:CZ	2.33	0.42
1:A:52:LYS:HD2	1:A:181:THR:HG23	2.01	0.42
1:A:256:GLN:O	2:F:322:ALA:HB3	2.19	0.42
1:A:323:GLN:HG2	1:A:327:ASN:ND2	2.35	0.42
1:A:487:GLU:OE1	2:F:495:THR:HA	2.19	0.42
1:A:488:ARG:HD3	2:F:488:ARG:HH22	1.85	0.42
1:B:106:LEU:HG	1:B:106:LEU:O	2.20	0.42
1:B:283:ILE:HD13	1:B:283:ILE:HA	1.88	0.42
1:B:311:ARG:HG3	1:B:371:LYS:NZ	2.34	0.42
2:C:28:PHE:O	2:C:31:ILE:N	2.48	0.42
2:C:38:ILE:C	2:C:40:ARG:H	2.26	0.42
2:C:182:THR:CG2	2:C:183:GLU:N	2.82	0.42
2:C:266:GLY:HA3	2:C:300:ARG:HG3	2.00	0.42
2:D:68:ASP:OD1	2:D:68:ASP:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:295:THR:HG21	2:D:319:GLU:OE2	2.20	0.42
2:D:334:ASP:OD1	2:D:334:ASP:C	2.62	0.42
2:D:488:ARG:HB3	2:D:491:SER:HB3	2.02	0.42
2:F:79:THR:HA	2:F:80:PRO:HD3	1.93	0.42
2:F:153:GLN:O	2:F:154:TYR:HB3	2.19	0.42
1:A:146:SER:HA	1:A:181:THR:O	2.20	0.42
1:A:251:ALA:O	1:A:252:MET:C	2.63	0.42
1:A:469:GLU:O	1:A:470:PHE:HB3	2.19	0.42
2:C:129:ARG:O	2:C:132:TYR:HB3	2.20	0.42
2:C:389:ASN:ND2	2:C:428:SER:HA	2.32	0.42
2:D:370:PHE:C	2:D:371:LYS:HG3	2.45	0.42
1:E:96:LYS:O	1:E:100:GLU:HG3	2.19	0.42
1:E:446:ARG:O	1:E:447:GLY:C	2.62	0.42
2:F:287:THR:HG23	2:F:414:ASN:HB3	2.02	0.42
2:F:364:LYS:O	2:F:367:ILE:N	2.51	0.42
1:A:439:LEU:HD12	1:A:440:LEU:N	2.35	0.42
1:B:360:LEU:HD22	1:B:360:LEU:C	2.45	0.42
2:C:174:ILE:HG22	2:C:174:ILE:O	2.19	0.42
2:C:211:LEU:HD12	2:C:215:ARG:O	2.20	0.42
2:C:246:ILE:HG22	2:C:247:PHE:N	2.35	0.42
2:D:96:LYS:O	2:D:97:LEU:C	2.63	0.42
2:D:328:ALA:O	2:D:332:GLY:O	2.38	0.42
1:E:340:ARG:C	1:E:342:ASN:N	2.78	0.42
2:F:379:SER:N	2:F:413:THR:HB	2.20	0.42
1:A:54:LEU:CD2	1:A:244:ILE:HG13	2.50	0.42
1:A:60:LEU:O	1:A:61:TYR:C	2.63	0.42
1:A:167:LEU:O	1:A:168:VAL:C	2.62	0.42
1:B:25:ILE:HG23	1:B:58:GLN:HE21	1.82	0.42
1:B:57:ILE:C	1:B:59:PHE:N	2.76	0.42
1:B:94:LEU:HD23	1:B:94:LEU:HA	1.89	0.42
1:B:104:PHE:HD2	1:B:133:ALA:CB	2.31	0.42
1:B:109:SER:HA	1:B:110:PRO:HD3	1.87	0.42
1:B:220:LEU:HD23	1:B:221:GLU:N	2.35	0.42
1:B:238:THR:HG22	1:B:240:THR:CG2	2.48	0.42
1:B:470:PHE:CD1	1:B:470:PHE:C	2.98	0.42
2:C:148:THR:CG2	2:C:193:ARG:HD2	2.50	0.42
2:C:424:SER:O	2:C:425:ILE:C	2.61	0.42
1:E:79:THR:HG22	1:E:82:ASP:H	1.85	0.42
1:E:153:GLN:C	1:E:154:TYR:CG	2.98	0.42
1:E:284:ILE:O	1:E:412:PHE:HD1	2.02	0.42
2:F:185:ILE:HD11	2:F:193:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:291:GLY:HA3	2:F:442:TYR:OH	2.19	0.42
1:A:84:ILE:HA	1:A:94:LEU:HD12	2.02	0.41
1:A:211:LEU:HD12	1:A:216:ARG:HG2	2.01	0.41
1:B:37:PRO:HG2	5:B:522:HOH:O	2.20	0.41
1:B:213:GLY:O	1:B:214:GLU:CB	2.68	0.41
1:B:294:LYS:C	1:B:296:LEU:H	2.28	0.41
2:C:121:PHE:CD1	2:C:121:PHE:N	2.87	0.41
2:C:287:THR:HG23	2:C:414:ASN:ND2	2.18	0.41
2:D:150:VAL:HG13	2:D:151:PHE:N	2.35	0.41
2:D:167:LEU:O	2:D:168:VAL:C	2.63	0.41
1:E:161:ARG:HB2	1:E:196:VAL:HG11	2.01	0.41
1:E:483:PHE:C	1:E:485:ASN:H	2.28	0.41
2:F:52:LYS:HE3	4:F:903:ATP:O1B	2.20	0.41
2:F:345:LYS:HE2	2:F:366:GLU:OE1	2.19	0.41
2:F:471:MET:HG2	2:F:480:LYS:NZ	2.35	0.41
1:B:70:PRO:HA	1:B:102:LYS:O	2.20	0.41
1:B:146:SER:H	1:B:181:THR:CG2	2.34	0.41
1:B:291:GLY:CA	1:B:442:TYR:OH	2.68	0.41
2:C:451:ARG:NH1	2:C:472:ILE:HD12	2.35	0.41
2:D:313:ILE:CD1	2:D:372:PRO:CG	2.98	0.41
1:E:225:LEU:HD23	1:E:225:LEU:HA	1.90	0.41
1:E:247:PHE:CZ	1:E:361:GLN:HB2	2.55	0.41
2:F:104:PHE:CD1	2:F:137:TYR:CE1	3.08	0.41
2:F:389:ASN:HD21	2:F:428:SER:HA	1.85	0.41
1:A:96:LYS:O	1:A:100:GLU:HG3	2.20	0.41
1:A:148:THR:C	1:A:150:VAL:N	2.78	0.41
1:A:298:VAL:O	1:A:301:PHE:HB3	2.21	0.41
1:B:265:SER:H	1:B:271:ASP:CG	2.27	0.41
1:B:363:ILE:O	1:B:364:LYS:C	2.63	0.41
2:C:59:PHE:O	2:C:141:ARG:NH1	2.51	0.41
2:C:111:ASP:CG	2:C:113:GLU:HG2	2.46	0.41
2:C:289:ALA:HB2	2:C:419:PHE:HA	2.02	0.41
1:E:79:THR:O	1:E:82:ASP:N	2.54	0.41
1:E:200:VAL:O	1:E:200:VAL:HG12	2.19	0.41
1:E:471:MET:HE2	1:E:478:ASP:HB2	1.99	0.41
2:F:151:PHE:C	2:F:153:GLN:N	2.76	0.41
2:F:328:ALA:O	2:F:332:GLY:O	2.38	0.41
1:A:31:ILE:H	1:A:31:ILE:HG13	1.66	0.41
1:A:64:ILE:HG21	1:A:97:LEU:HD22	2.02	0.41
1:A:166:ARG:O	1:A:167:LEU:C	2.63	0.41
1:A:419:PHE:CD2	1:B:425:ILE:CD1	3.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:LEU:O	1:B:63:GLY:N	2.53	0.41
1:B:164:LEU:HD23	1:B:164:LEU:HA	1.86	0.41
1:B:295:THR:HG23	1:B:378:ASP:OD2	2.21	0.41
2:C:265:SER:HB3	2:C:278:PHE:CZ	2.55	0.41
2:C:284:ILE:HB	2:C:411:LEU:HD13	2.02	0.41
2:D:182:THR:CG2	2:D:183:GLU:N	2.82	0.41
1:E:76:PHE:HE1	1:E:144:ILE:HG23	1.85	0.41
1:E:211:LEU:HD12	1:E:215:ARG:O	2.20	0.41
2:F:273:MET:O	2:F:463:HIS:HA	2.20	0.41
2:F:273:MET:O	2:F:463:HIS:HB2	2.21	0.41
1:A:386:GLY:HA2	1:B:390:ASN:OD1	2.19	0.41
1:A:451:ARG:HG2	1:A:451:ARG:NH1	2.34	0.41
1:B:45:SER:HB2	1:B:182:THR:HB	1.98	0.41
1:B:93:ASP:OD2	1:B:96:LYS:HB2	2.20	0.41
1:B:337:GLU:O	1:B:338:MET:C	2.63	0.41
1:B:451:ARG:H	1:B:451:ARG:HD2	1.84	0.41
2:C:371:LYS:N	2:C:372:PRO:HD3	2.35	0.41
2:D:33:HIS:CD2	2:D:230:HIS:HA	2.55	0.41
1:E:54:LEU:CD2	1:E:239:ILE:HG23	2.51	0.41
1:E:378:ASP:O	1:E:379:SER:CB	2.68	0.41
2:F:486:PHE:HB3	2:F:489:ILE:HD11	2.02	0.41
1:A:438:ILE:HD13	1:A:438:ILE:HA	1.89	0.41
1:B:44:VAL:HG13	1:B:205:VAL:HG12	2.01	0.41
1:B:148:THR:C	1:B:150:VAL:N	2.78	0.41
1:B:483:PHE:O	1:B:484:ARG:C	2.64	0.41
2:C:54:LEU:CD1	2:C:90:PHE:CZ	3.03	0.41
2:C:214:GLU:HB3	2:D:234:GLU:HB2	2.01	0.41
2:C:354:ALA:HB3	2:C:359:HIS:CE1	2.56	0.41
2:D:55:PHE:HA	2:D:244:ILE:HD12	2.02	0.41
2:D:83:ILE:O	2:D:84:ILE:C	2.63	0.41
2:D:151:PHE:CE1	2:D:160:VAL:HG13	2.55	0.41
2:D:184:ARG:NH1	2:D:187:GLU:O	2.47	0.41
1:E:230:HIS:ND1	1:E:230:HIS:O	2.54	0.41
1:E:426:THR:HG22	1:E:428:SER:N	2.30	0.41
2:F:79:THR:HG22	2:F:82:ASP:CB	2.51	0.41
2:F:117:VAL:HA	2:F:154:TYR:OH	2.21	0.41
2:F:127:ILE:HD12	2:F:170:ARG:HB2	2.03	0.41
2:F:311:ARG:CG	2:F:371:LYS:NZ	2.83	0.41
2:F:364:LYS:O	2:F:367:ILE:HB	2.20	0.41
1:A:31:ILE:CD1	1:A:246:ILE:HG21	2.51	0.41
1:A:52:LYS:HB3	1:A:181:THR:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ILE:HD12	1:A:412:PHE:HE1	1.85	0.41
1:A:302:VAL:HG21	1:A:314:LEU:HB2	2.02	0.41
1:A:437:ILE:CD1	1:A:457:LYS:HE2	2.51	0.41
1:B:52:LYS:O	1:B:53:THR:C	2.62	0.41
1:B:61:TYR:O	1:B:62:ASN:C	2.63	0.41
1:B:75:THR:HG21	1:B:83:ILE:HD11	2.02	0.41
1:B:426:THR:HG22	1:B:428:SER:N	2.35	0.41
2:C:182:THR:HG21	2:C:192:ALA:CB	2.47	0.41
2:D:274:CYS:SG	2:D:458:MET:SD	3.18	0.41
2:D:360:LEU:HD21	2:D:364:LYS:HE3	2.03	0.41
2:D:399:VAL:O	2:D:400:THR:C	2.62	0.41
1:E:216:ARG:HH21	2:F:223:LEU:HD21	1.84	0.41
2:F:51:GLY:O	2:F:52:LYS:C	2.63	0.41
2:F:332:GLY:O	2:F:333:MET:C	2.63	0.41
1:A:220:LEU:HD23	1:A:220:LEU:O	2.21	0.41
1:A:315:PHE:HD1	1:A:376:ALA:O	2.03	0.41
1:A:379:SER:C	1:A:381:SER:N	2.72	0.41
1:B:213:GLY:C	1:B:215:ARG:H	2.28	0.41
2:C:52:LYS:HE3	2:C:52:LYS:HB2	1.89	0.41
2:C:439:LEU:HD12	2:C:440:LEU:N	2.35	0.41
2:D:48:SER:OG	1:E:224:LYS:HE2	2.21	0.41
2:D:52:LYS:N	4:D:903:ATP:O1B	2.54	0.41
2:D:284:ILE:HG23	2:D:436:THR:CG2	2.51	0.41
2:D:442:TYR:C	2:D:443:VAL:HG23	2.46	0.41
2:F:270:LEU:HD21	2:F:438:ILE:HD12	2.01	0.41
1:A:21:MET:CE	1:A:59:PHE:CZ	3.04	0.41
1:A:130:ILE:HG22	1:A:134:ILE:HD11	2.03	0.41
1:A:420:MET:HE3	1:A:420:MET:HB3	1.99	0.41
1:B:94:LEU:O	1:B:95:ALA:C	2.64	0.41
1:B:204:VAL:HG23	1:B:224:LYS:HG2	2.03	0.41
1:B:305:ALA:O	1:B:310:GLU:O	2.39	0.41
2:C:360:LEU:HD23	2:C:360:LEU:O	2.20	0.41
2:D:46:GLY:O	2:D:183:GLU:HA	2.20	0.41
2:D:60:LEU:HD22	2:D:71:GLY:HA3	2.03	0.41
2:D:278:PHE:N	2:D:278:PHE:CD2	2.86	0.41
2:D:344:LEU:C	2:D:344:LEU:CD1	2.94	0.41
2:D:436:THR:HA	2:D:457:LYS:O	2.20	0.41
1:E:79:THR:HG22	1:E:82:ASP:OD2	2.21	0.41
1:E:267:VAL:O	1:E:268:VAL:C	2.63	0.41
1:E:294:LYS:HB3	1:E:413:THR:HG23	2.03	0.41
1:E:331:TRP:NE1	4:E:901:ATP:N7	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:504:GLU:CD	1:E:505:LEU:HD23	2.45	0.41
2:F:211:LEU:HA	2:F:216:ARG:HD3	2.02	0.41
2:F:283:ILE:CD1	2:F:400:THR:HG23	2.50	0.41
2:F:311:ARG:HD3	2:F:370:PHE:CE2	2.56	0.41
2:F:387:VAL:CG1	2:F:388:SER:N	2.84	0.41
2:F:471:MET:HE1	2:F:473:SER:CB	2.51	0.41
1:A:123:LEU:HD22	1:A:123:LEU:HA	1.97	0.41
1:A:147:VAL:HG21	1:A:180:MET:CE	2.51	0.41
1:B:248:PRO:O	1:B:251:ALA:N	2.53	0.41
1:B:430:ILE:O	1:B:430:ILE:HG22	2.21	0.41
2:C:57:ILE:HD13	2:C:57:ILE:HA	1.88	0.41
2:C:480:LYS:HB3	2:C:481:ASP:H	1.50	0.41
2:D:121:PHE:CD1	2:D:121:PHE:N	2.89	0.41
2:D:402:TYR:O	2:D:405:GLN:HG2	2.20	0.41
1:E:126:LEU:O	1:E:129:ARG:HB2	2.21	0.41
1:E:218:ARG:O	1:E:236:PRO:HA	2.21	0.41
1:E:267:VAL:O	1:E:270:LEU:N	2.52	0.41
1:E:397:ILE:HD11	1:E:433:ILE:HG12	2.03	0.41
1:E:488:ARG:O	1:E:491:SER:OG	2.29	0.41
2:F:43:LEU:HB2	2:F:201:SER:OG	2.21	0.41
2:F:127:ILE:HG21	2:F:170:ARG:HG3	2.03	0.41
1:A:378:ASP:O	1:A:379:SER:HB3	2.21	0.40
1:B:287:THR:CG2	1:B:414:ASN:HD22	2.24	0.40
2:C:147:VAL:HG21	2:C:180:MET:HE2	2.02	0.40
2:C:316:ALA:O	2:C:348:CYS:HA	2.21	0.40
2:D:76:PHE:CZ	2:D:126:LEU:HD21	2.56	0.40
1:E:67:PHE:O	1:E:69:GLU:HG3	2.21	0.40
1:E:163:GLU:OE2	1:E:163:GLU:CA	2.55	0.40
2:F:275:GLY:HA2	2:F:462:TRP:HE3	1.86	0.40
2:F:315:PHE:CZ	2:F:363:ILE:HG23	2.56	0.40
1:A:157:SER:OG	1:A:158:SER:N	2.53	0.40
1:A:331:TRP:C	1:A:474:ASP:O	2.63	0.40
1:A:363:ILE:O	1:A:364:LYS:C	2.64	0.40
1:A:367:ILE:HG12	1:A:375:ILE:CD1	2.51	0.40
1:A:484:ARG:CZ	1:A:484:ARG:CB	2.99	0.40
1:B:86:ASN:O	1:B:87:ALA:C	2.63	0.40
2:C:28:PHE:O	2:C:29:ASP:C	2.63	0.40
2:C:71:GLY:O	2:C:103:LEU:HA	2.21	0.40
2:C:169:ALA:O	2:C:172:LYS:N	2.54	0.40
2:C:287:THR:CG2	2:C:288:GLY:N	2.83	0.40
2:C:294:LYS:HE2	2:C:294:LYS:HB2	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:88:ARG:HH11	2:D:88:ARG:HG2	1.86	0.40
2:F:147:VAL:HG23	2:F:148:THR:N	2.35	0.40
2:F:153:GLN:O	2:F:154:TYR:CB	2.69	0.40
2:F:240:THR:C	2:F:242:HIS:H	2.28	0.40
2:F:261:VAL:CG1	2:F:262:ARG:N	2.84	0.40
1:A:22:ARG:CZ	1:A:24:MET:SD	3.10	0.40
1:A:273:MET:HE1	1:A:453:ILE:HG23	2.04	0.40
1:B:170:ARG:HD2	1:B:173:GLN:OE1	2.21	0.40
1:B:383:LEU:HD13	1:B:395:PHE:CE2	2.56	0.40
2:C:194:TYR:O	2:C:195:GLY:C	2.63	0.40
2:C:240:THR:CG2	2:C:361:GLN:HE22	2.33	0.40
2:C:248:PRO:HB2	2:C:251:ALA:HB3	2.04	0.40
2:D:179:VAL:O	2:D:179:VAL:HG12	2.20	0.40
1:E:435:ASP:O	1:E:457:LYS:HE3	2.21	0.40
2:F:335:PHE:O	2:F:338:MET:HB2	2.21	0.40
1:A:267:VAL:HB	1:A:270:LEU:HB2	2.03	0.40
1:A:344:LEU:HD13	1:A:345:LYS:N	2.36	0.40
1:A:506:SER:HB2	1:A:509:VAL:HA	2.03	0.40
1:B:260:ASN:O	1:B:261:VAL:C	2.64	0.40
1:B:353:SER:O	1:B:354:ALA:HB2	2.21	0.40
2:D:352:GLU:OE1	2:D:385:ARG:NH1	2.54	0.40
1:E:39:GLY:H	1:E:177:THR:HG23	1.86	0.40
1:E:186:GLU:OE2	1:E:187:GLU:N	2.54	0.40
1:E:314:LEU:HD12	1:E:314:LEU:C	2.47	0.40
1:E:483:PHE:C	1:E:485:ASN:N	2.79	0.40
2:F:334:ASP:OD1	2:F:336:GLU:N	2.55	0.40
1:A:82:ASP:O	1:A:83:ILE:C	2.64	0.40
1:B:248:PRO:C	1:B:250:GLY:H	2.28	0.40
2:C:304:ASN:OD1	2:C:374:ARG:NH2	2.54	0.40
2:C:332:GLY:O	2:C:333:MET:O	2.39	0.40
2:D:315:PHE:HB3	2:D:317:TYR:HE1	1.87	0.40
2:D:441:GLN:NE2	2:D:490:ILE:HD12	2.36	0.40
2:D:451:ARG:NH2	4:D:901:ATP:O3'	2.49	0.40
1:E:379:SER:OG	1:E:382:ALA:N	2.53	0.40
2:F:269:ARG:HH22	2:F:468:ARG:NH2	2.19	0.40
2:F:334:ASP:OD1	2:F:334:ASP:C	2.65	0.40
2:F:359:HIS:O	2:F:363:ILE:HG13	2.22	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	503/519 (97%)	389 (77%)	83 (16%)	31 (6%)	1	9
1	B	488/519 (94%)	383 (78%)	71 (14%)	34 (7%)	1	6
1	E	489/519 (94%)	396 (81%)	66 (14%)	27 (6%)	1	11
2	C	486/519 (94%)	394 (81%)	69 (14%)	23 (5%)	2	14
2	D	483/519 (93%)	396 (82%)	68 (14%)	19 (4%)	2	18
2	F	504/519 (97%)	411 (82%)	65 (13%)	28 (6%)	1	11
All	All	2953/3114 (95%)	2369 (80%)	422 (14%)	162 (6%)	1	11

All (162) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	VAL
1	A	154	TYR
1	A	157	SER
1	A	387	VAL
1	A	420	MET
1	A	431	ASP
1	A	463	HIS
1	A	500	ASP
1	A	502	LYS
1	B	17	ALA
1	B	154	TYR
1	B	193	ARG
1	B	420	MET
1	B	463	HIS
1	B	494	PRO
2	C	17	ALA
2	C	117	VAL
2	C	154	TYR
2	C	249	LEU
2	C	309	LYS

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Mol	Chain	Res	Type
2	C	333	MET
2	C	431	ASP
2	C	463	HIS
2	D	122	ASP
2	D	154	TYR
2	D	333	MET
2	D	387	VAL
2	D	463	HIS
1	E	122	ASP
1	E	154	TYR
1	E	157	SER
1	E	333	MET
1	E	354	ALA
1	E	463	HIS
1	E	484	ARG
2	F	118	VAL
2	F	154	TYR
2	F	278	PHE
2	F	333	MET
2	F	420	MET
2	F	463	HIS
2	F	501	GLU
2	F	504	GLU
2	F	506	SER
2	F	507	ARG
2	F	508	ILE
2	F	509	VAL
2	F	515	LYS
1	A	198	GLU
1	A	333	MET
1	A	480	LYS
1	A	499	VAL
1	A	509	VAL
1	B	87	ALA
1	B	119	GLY
1	B	195	GLY
1	B	211	LEU
1	B	341	GLN
1	B	379	SER
1	B	484	ARG
2	C	112	PRO
2	C	289	ALA

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Mol	Chain	Res	Type
2	C	341	GLN
2	C	354	ALA
2	C	379	SER
2	D	113	GLU
2	D	211	LEU
2	D	420	MET
2	D	431	ASP
1	E	117	VAL
1	E	211	LEU
1	E	268	VAL
1	E	277	GLY
1	E	278	PHE
1	E	379	SER
1	E	498	THR
2	F	117	VAL
2	F	157	SER
2	F	211	LEU
2	F	480	LYS
1	A	26	GLU
1	A	65	ILE
1	A	193	ARG
1	A	211	LEU
1	B	61	TYR
1	B	112	PRO
1	B	198	GLU
1	B	295	THR
1	B	501	GLU
2	C	348	CYS
2	C	429	HIS
2	D	26	GLU
2	D	152	GLN
2	D	341	GLN
1	E	341	GLN
1	E	405	GLN
1	E	420	MET
2	F	47	THR
2	F	431	ASP
2	F	500	ASP
1	A	17	ALA
1	A	149	SER
1	B	26	GLU
1	B	33	HIS

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Mol	Chain	Res	Type
1	B	149	SER
1	B	167	LEU
1	B	249	LEU
1	B	326	ARG
1	B	354	ALA
1	B	372	PRO
2	C	211	LEU
1	E	249	LEU
1	E	502	LYS
2	F	212	GLU
2	F	354	ALA
2	F	379	SER
1	A	112	PRO
1	A	120	GLY
1	A	212	GLU
1	A	309	LYS
1	B	333	MET
1	B	348	CYS
2	C	124	SER
2	C	149	SER
2	C	193	ARG
2	C	212	GLU
2	D	123	LEU
2	D	494	PRO
1	E	212	GLU
2	F	26	GLU
2	F	152	GLN
1	A	167	LEU
1	A	348	CYS
1	A	510	ARG
1	B	52	LYS
1	B	157	SER
1	B	212	GLU
2	C	114	GLY
2	C	347	VAL
2	D	52	LYS
2	D	157	SER
1	E	160	VAL
1	E	276	GLY
1	E	282	SER
1	E	348	CYS
1	E	387	VAL

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Mol	Chain	Res	Type
1	E	398	GLY
2	F	341	GLN
1	A	497	ILE
1	B	117	VAL
2	D	83	ILE
2	D	268	VAL
1	E	189	GLY
2	F	398	GLY
1	A	91	GLY
1	A	433	ILE
1	A	64	ILE
2	C	196	VAL
2	F	517	PRO
1	B	134	ILE
1	B	363	ILE
2	D	347	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	431/443 (97%)	387 (90%)	44 (10%)	7	29
1	B	418/443 (94%)	373 (89%)	45 (11%)	6	27
1	E	419/443 (95%)	372 (89%)	47 (11%)	6	25
2	C	416/444 (94%)	372 (89%)	44 (11%)	6	27
2	D	413/444 (93%)	361 (87%)	52 (13%)	4	21
2	F	432/444 (97%)	386 (89%)	46 (11%)	6	27
All	All	2529/2661 (95%)	2251 (89%)	278 (11%)	6	26

All (278) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ILE
1	A	26	GLU

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Mol	Chain	Res	Type
1	A	38	ILE
1	A	42	THR
1	A	75	THR
1	A	79	THR
1	A	81	GLN
1	A	92	TRP
1	A	99	ASP
1	A	106	LEU
1	A	118	VAL
1	A	123	LEU
1	A	140	ARG
1	A	151	PHE
1	A	154	TYR
1	A	158	SER
1	A	182	THR
1	A	185	ILE
1	A	201	SER
1	A	212	GLU
1	A	218	ARG
1	A	223	LEU
1	A	256	GLN
1	A	260	ASN
1	A	263	VAL
1	A	270	LEU
1	A	287	THR
1	A	302	VAL
1	A	303	GLU
1	A	325	LEU
1	A	342	ASN
1	A	344	LEU
1	A	360	LEU
1	A	366	GLU
1	A	375	ILE
1	A	428	SER
1	A	431	ASP
1	A	434	THR
1	A	471	MET
1	A	485	ASN
1	A	489	ILE
1	A	508	ILE
1	A	509	VAL
1	A	518	GLU

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Mol	Chain	Res	Type
1	B	26	GLU
1	B	81	GLN
1	B	99	ASP
1	B	106	LEU
1	B	111	ASP
1	B	123	LEU
1	B	128	GLU
1	B	140	ARG
1	B	151	PHE
1	B	154	TYR
1	B	164	LEU
1	B	179	VAL
1	B	182	THR
1	B	183	GLU
1	B	185	ILE
1	B	186	GLU
1	B	205	VAL
1	B	212	GLU
1	B	218	ARG
1	B	223	LEU
1	B	240	THR
1	B	256	GLN
1	B	260	ASN
1	B	263	VAL
1	B	270	LEU
1	B	302	VAL
1	B	303	GLU
1	B	320	SER
1	B	333	MET
1	B	342	ASN
1	B	360	LEU
1	B	375	ILE
1	B	413	THR
1	B	440	LEU
1	B	441	GLN
1	B	458	MET
1	B	462	TRP
1	B	470	PHE
1	B	471	MET
1	B	474	ASP
1	B	485	ASN
1	B	490	ILE

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Mol	Chain	Res	Type
1	B	499	VAL
1	B	501	GLU
1	B	502	LYS
2	C	15	HIS
2	C	18	ILE
2	C	26	GLU
2	C	45	SER
2	C	50	THR
2	C	57	ILE
2	C	64	ILE
2	C	81	GLN
2	C	83	ILE
2	C	99	ASP
2	C	111	ASP
2	C	140	ARG
2	C	151	PHE
2	C	154	TYR
2	C	179	VAL
2	C	186	GLU
2	C	211	LEU
2	C	212	GLU
2	C	218	ARG
2	C	223	LEU
2	C	240	THR
2	C	256	GLN
2	C	260	ASN
2	C	263	VAL
2	C	270	LEU
2	C	295	THR
2	C	302	VAL
2	C	303	GLU
2	C	325	LEU
2	C	333	MET
2	C	336	GLU
2	C	338	MET
2	C	342	ASN
2	C	344	LEU
2	C	375	ILE
2	C	400	THR
2	C	428	SER
2	C	432	THR
2	C	439	LEU

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Mol	Chain	Res	Type
2	C	454	ASN
2	C	470	PHE
2	C	497	ILE
2	C	498	THR
2	C	500	ASP
2	D	26	GLU
2	D	38	ILE
2	D	50	THR
2	D	57	ILE
2	D	75	THR
2	D	79	THR
2	D	81	GLN
2	D	89	SER
2	D	106	LEU
2	D	122	ASP
2	D	123	LEU
2	D	124	SER
2	D	147	VAL
2	D	151	PHE
2	D	154	TYR
2	D	181	THR
2	D	185	ILE
2	D	197	GLU
2	D	211	LEU
2	D	212	GLU
2	D	218	ARG
2	D	223	LEU
2	D	238	THR
2	D	240	THR
2	D	256	GLN
2	D	260	ASN
2	D	263	VAL
2	D	270	LEU
2	D	280	LYS
2	D	284	ILE
2	D	292	THR
2	D	303	GLU
2	D	321	ARG
2	D	342	ASN
2	D	344	LEU
2	D	356	LEU
2	D	360	LEU

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Mol	Chain	Res	Type
2	D	366	GLU
2	D	375	ILE
2	D	397	ILE
2	D	423	HIS
2	D	428	SER
2	D	431	ASP
2	D	433	ILE
2	D	463	HIS
2	D	471	MET
2	D	474	ASP
2	D	487	GLU
2	D	490	ILE
2	D	496	ARG
2	D	497	ILE
2	D	498	THR
1	E	26	GLU
1	E	38	ILE
1	E	45	SER
1	E	47	THR
1	E	52	LYS
1	E	79	THR
1	E	81	GLN
1	E	99	ASP
1	E	106	LEU
1	E	113	GLU
1	E	121	PHE
1	E	140	ARG
1	E	151	PHE
1	E	154	TYR
1	E	177	THR
1	E	179	VAL
1	E	183	GLU
1	E	186	GLU
1	E	196	VAL
1	E	201	SER
1	E	203	ASN
1	E	212	GLU
1	E	218	ARG
1	E	220	LEU
1	E	221	GLU
1	E	223	LEU
1	E	228	THR

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Mol	Chain	Res	Type
1	E	238	THR
1	E	245	ASN
1	E	256	GLN
1	E	263	VAL
1	E	268	VAL
1	E	270	LEU
1	E	287	THR
1	E	338	MET
1	E	342	ASN
1	E	366	GLU
1	E	375	ILE
1	E	431	ASP
1	E	438	ILE
1	E	458	MET
1	E	461	SER
1	E	471	MET
1	E	474	ASP
1	E	501	GLU
1	E	503	SER
1	E	505	LEU
2	F	15	HIS
2	F	26	GLU
2	F	53	THR
2	F	73	PHE
2	F	77	GLU
2	F	79	THR
2	F	106	LEU
2	F	115	GLN
2	F	121	PHE
2	F	127	ILE
2	F	140	ARG
2	F	151	PHE
2	F	154	TYR
2	F	181	THR
2	F	183	GLU
2	F	212	GLU
2	F	218	ARG
2	F	225	LEU
2	F	256	GLN
2	F	263	VAL
2	F	268	VAL
2	F	270	LEU

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Mol	Chain	Res	Type
2	F	287	THR
2	F	300	ARG
2	F	302	VAL
2	F	321	ARG
2	F	325	LEU
2	F	344	LEU
2	F	360	LEU
2	F	379	SER
2	F	424	SER
2	F	425	ILE
2	F	431	ASP
2	F	433	ILE
2	F	458	MET
2	F	462	TRP
2	F	469	GLU
2	F	471	MET
2	F	496	ARG
2	F	497	ILE
2	F	501	GLU
2	F	504	GLU
2	F	507	ARG
2	F	509	VAL
2	F	514	GLU
2	F	515	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	62	ASN
1	A	81	GLN
1	A	152	GLN
1	A	209	ASN
1	A	323	GLN
1	A	361	GLN
1	A	389	ASN
1	A	414	ASN
1	A	441	GLN
1	B	16	GLN
1	B	62	ASN
1	B	203	ASN
1	B	209	ASN

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Mol	Chain	Res	Type
1	B	260	ASN
1	B	323	GLN
1	B	327	ASN
1	B	341	GLN
1	B	414	ASN
1	B	429	HIS
1	B	441	GLN
2	C	33	HIS
2	C	58	GLN
2	C	62	ASN
2	C	81	GLN
2	C	115	GLN
2	C	152	GLN
2	C	153	GLN
2	C	203	ASN
2	C	209	ASN
2	C	245	ASN
2	C	323	GLN
2	C	342	ASN
2	C	361	GLN
2	C	389	ASN
2	C	414	ASN
2	C	429	HIS
2	C	441	GLN
2	D	33	HIS
2	D	62	ASN
2	D	115	GLN
2	D	209	ASN
2	D	308	ASN
2	D	323	GLN
2	D	418	GLN
2	D	441	GLN
2	D	454	ASN
1	E	15	HIS
1	E	33	HIS
1	E	81	GLN
1	E	135	GLN
1	E	152	GLN
1	E	153	GLN
1	E	260	ASN
1	E	304	ASN
1	E	323	GLN

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Mol	Chain	Res	Type
1	E	327	ASN
1	E	361	GLN
1	E	414	ASN
1	E	418	GLN
1	E	429	HIS
1	E	441	GLN
2	F	16	GLN
2	F	115	GLN
2	F	152	GLN
2	F	153	GLN
2	F	173	GLN
2	F	209	ASN
2	F	256	GLN
2	F	308	ASN
2	F	342	ASN
2	F	389	ASN
2	F	394	GLN
2	F	414	ASN
2	F	454	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	TPO	B	432	1	8,10,11	0.91	0	10,14,16	1.60	2 (20%)
1	TPO	A	432	1	8,10,11	0.98	0	10,14,16	1.91	2 (20%)
1	TPO	E	432	1	8,10,11	1.27	1 (12%)	10,14,16	2.10	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	B	432	1	-	5/9/11/13	-
1	TPO	A	432	1	-	1/9/11/13	-
1	TPO	E	432	1	-	2/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	432	TPO	P-OG1	-2.04	1.55	1.59

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	432	TPO	P-OG1-CB	-5.73	107.75	123.33
1	A	432	TPO	P-OG1-CB	-4.90	110.02	123.33
1	B	432	TPO	CG2-CB-CA	-3.33	106.77	113.26
1	B	432	TPO	P-OG1-CB	-2.92	115.40	123.33
1	A	432	TPO	CG2-CB-CA	-2.88	107.65	113.26
1	E	432	TPO	CG2-CB-CA	-2.40	108.58	113.26

There are no chirality outliers.

All (8) 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	O-C-CA-CB
1	E	432	TPO	C-CA-CB-CG2
1	B	432	TPO	CG2-CB-OG1-P
1	E	432	TPO	N-CA-CB-CG2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	432	TPO	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	432	TPO	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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$
4	ATP	A	901	3	32,33,33	1.20	3 (9%)	48,52,52	1.98	11 (22%)
4	ATP	E	903	3	32,33,33	1.31	4 (12%)	48,52,52	2.16	13 (27%)
4	ATP	F	901	3	32,33,33	1.15	2 (6%)	48,52,52	1.96	12 (25%)
4	ATP	F	903	3	32,33,33	1.24	2 (6%)	48,52,52	2.21	15 (31%)
4	ATP	B	903	3	32,33,33	1.10	3 (9%)	48,52,52	2.09	12 (25%)
4	ATP	C	901	3	32,33,33	1.22	4 (12%)	48,52,52	2.04	11 (22%)
4	ATP	D	903	3	32,33,33	1.38	4 (12%)	48,52,52	2.01	13 (27%)
4	ATP	A	903	3	32,33,33	1.21	4 (12%)	48,52,52	2.16	15 (31%)
4	ATP	C	903	3	32,33,33	1.18	3 (9%)	48,52,52	2.02	12 (25%)
4	ATP	D	901	3	32,33,33	1.14	2 (6%)	48,52,52	2.01	12 (25%)
4	ATP	E	901	3	32,33,33	1.26	3 (9%)	48,52,52	2.11	14 (29%)
4	ATP	B	901	-	32,33,33	1.13	3 (9%)	48,52,52	1.93	12 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	A	901	3	-	8/22/38/38	0/3/3/3
4	ATP	E	903	3	-	8/22/38/38	0/3/3/3
4	ATP	F	901	3	-	7/22/38/38	0/3/3/3
4	ATP	F	903	3	-	6/22/38/38	0/3/3/3
4	ATP	B	903	3	-	8/22/38/38	0/3/3/3
4	ATP	C	901	3	-	8/22/38/38	0/3/3/3
4	ATP	D	903	3	-	10/22/38/38	0/3/3/3
4	ATP	A	903	3	-	10/22/38/38	0/3/3/3
4	ATP	C	903	3	-	8/22/38/38	0/3/3/3
4	ATP	D	901	3	-	7/22/38/38	0/3/3/3
4	ATP	E	901	3	-	6/22/38/38	0/3/3/3
4	ATP	B	901	-	-	5/22/38/38	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	903	ATP	PB-O3B	-4.29	1.54	1.59
4	D	903	ATP	PB-O3B	-3.71	1.55	1.59
4	F	903	ATP	PB-O3B	-3.56	1.55	1.59
4	F	903	ATP	C2-N3	3.49	1.40	1.33
4	E	901	ATP	PB-O3B	-3.12	1.56	1.59
4	F	901	ATP	C2-N3	3.04	1.39	1.33
4	E	903	ATP	C2-N3	2.97	1.39	1.33
4	E	901	ATP	C2-N3	2.89	1.39	1.33
4	D	903	ATP	C2-N3	2.86	1.39	1.33
4	A	901	ATP	C2-N3	2.82	1.38	1.33
4	A	903	ATP	PA-O3A	2.77	1.62	1.59
4	B	901	ATP	C2-N1	2.66	1.38	1.33
4	B	903	ATP	C2-N3	2.60	1.38	1.33
4	D	903	ATP	C4-N3	2.60	1.39	1.34
4	C	901	ATP	C2-N3	2.56	1.38	1.33
4	C	901	ATP	PB-O3A	-2.53	1.56	1.59
4	C	901	ATP	PB-O3B	-2.52	1.56	1.59
4	B	903	ATP	C1'-N9	2.50	1.53	1.46
4	D	901	ATP	C2-N3	2.48	1.38	1.33
4	E	903	ATP	C4-N9	-2.46	1.32	1.37
4	A	903	ATP	C2-N1	2.44	1.38	1.33
4	D	903	ATP	C2-N1	2.43	1.38	1.33
4	D	901	ATP	C2-N1	2.41	1.38	1.33
4	A	901	ATP	PB-O3B	-2.37	1.56	1.59
4	B	901	ATP	C4-N3	2.36	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	903	ATP	C2-N3	2.20	1.37	1.33
4	B	903	ATP	C2-N1	2.19	1.37	1.33
4	E	903	ATP	PB-O3A	2.16	1.61	1.59
4	A	903	ATP	C2-N3	2.15	1.37	1.33
4	C	903	ATP	C2-N1	2.10	1.37	1.33
4	F	901	ATP	C2-N1	2.08	1.37	1.33
4	C	901	ATP	C1'-N9	2.08	1.52	1.46
4	A	903	ATP	PB-O3A	2.08	1.61	1.59
4	C	903	ATP	C5-N7	-2.07	1.35	1.39
4	A	901	ATP	C2-N1	2.02	1.37	1.33
4	E	901	ATP	C2-N1	2.01	1.37	1.33
4	B	901	ATP	C1'-N9	2.01	1.51	1.46

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	903	ATP	N3-C2-N1	-6.00	119.49	128.58
4	E	903	ATP	N3-C2-N1	-5.91	119.63	128.58
4	B	901	ATP	N3-C2-N1	-5.81	119.79	128.58
4	E	901	ATP	N3-C2-N1	-5.80	119.81	128.58
4	C	903	ATP	N3-C2-N1	-5.78	119.84	128.58
4	A	903	ATP	N3-C2-N1	-5.73	119.90	128.58
4	C	901	ATP	N3-C2-N1	-5.68	119.99	128.58
4	A	901	ATP	N3-C2-N1	-5.67	120.00	128.58
4	B	903	ATP	N3-C2-N1	-5.64	120.05	128.58
4	D	901	ATP	N3-C2-N1	-5.57	120.14	128.58
4	F	901	ATP	N3-C2-N1	-5.56	120.16	128.58
4	F	903	ATP	C5-N7-C8	5.53	112.15	103.45
4	F	903	ATP	N3-C2-N1	-5.52	120.23	128.58
4	B	903	ATP	C5-N7-C8	5.50	112.10	103.45
4	E	903	ATP	C4-C5-N7	-5.42	104.38	110.58
4	E	903	ATP	C5-N7-C8	5.32	111.82	103.45
4	F	903	ATP	C4-C5-N7	-5.29	104.54	110.58
4	E	903	ATP	N9-C8-N7	-5.23	106.51	113.94
4	E	901	ATP	C5-N7-C8	5.14	111.53	103.45
4	C	903	ATP	C5-N7-C8	5.06	111.41	103.45
4	B	903	ATP	C4-C5-N7	-5.06	104.80	110.58
4	C	901	ATP	C5-N7-C8	5.04	111.37	103.45
4	C	903	ATP	N9-C8-N7	-5.01	106.83	113.94
4	A	901	ATP	C5-N7-C8	5.00	111.31	103.45
4	F	901	ATP	C5-N7-C8	4.93	111.20	103.45
4	A	903	ATP	C5-N7-C8	4.89	111.13	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	901	ATP	C5-N7-C8	4.87	111.10	103.45
4	F	903	ATP	N9-C8-N7	-4.86	107.03	113.94
4	A	903	ATP	O3A-PB-O1B	4.85	125.29	110.70
4	D	903	ATP	C5-N7-C8	4.83	111.05	103.45
4	B	901	ATP	C5-N7-C8	4.70	110.84	103.45
4	B	903	ATP	N9-C8-N7	-4.68	107.29	113.94
4	C	903	ATP	C4-C5-N7	-4.64	105.28	110.58
4	F	901	ATP	C4-C5-N7	-4.64	105.28	110.58
4	E	901	ATP	C4-C5-N7	-4.60	105.32	110.58
4	A	901	ATP	C4-C5-N7	-4.55	105.38	110.58
4	E	901	ATP	N9-C8-N7	-4.53	107.50	113.94
4	D	903	ATP	C4-C5-N7	-4.52	105.41	110.58
4	A	903	ATP	N9-C8-N7	-4.51	107.54	113.94
4	D	903	ATP	N9-C8-N7	-4.48	107.58	113.94
4	A	903	ATP	C4-C5-N7	-4.48	105.46	110.58
4	C	901	ATP	C4-C5-N7	-4.44	105.51	110.58
4	B	901	ATP	C4-C5-N7	-4.40	105.55	110.58
4	D	901	ATP	C4-C5-N7	-4.39	105.56	110.58
4	D	901	ATP	N9-C8-N7	-4.37	107.73	113.94
4	F	901	ATP	N9-C8-N7	-4.35	107.76	113.94
4	B	901	ATP	N9-C8-N7	-4.35	107.77	113.94
4	C	901	ATP	N9-C8-N7	-4.31	107.81	113.94
4	A	901	ATP	N9-C8-N7	-4.31	107.83	113.94
4	A	903	ATP	O2B-PB-O3A	3.88	117.76	107.27
4	F	903	ATP	C5-C4-N3	-3.61	121.74	126.72
4	B	903	ATP	C5-C4-N3	-3.55	121.83	126.72
4	C	901	ATP	C5-C4-N3	-3.53	121.86	126.72
4	C	901	ATP	C2-N3-C4	3.35	120.02	111.83
4	D	901	ATP	C5-C4-N3	-3.34	122.12	126.72
4	E	903	ATP	C2-N3-C4	3.31	119.92	111.83
4	E	903	ATP	C4-N9-C8	3.27	109.18	105.74
4	B	903	ATP	C2-N3-C4	3.26	119.80	111.83
4	A	901	ATP	C5-C4-N3	-3.19	122.32	126.72
4	E	903	ATP	C6-C5-N7	3.19	138.24	132.09
4	D	903	ATP	C2-N3-C4	3.18	119.61	111.83
4	D	901	ATP	C2-N3-C4	3.14	119.50	111.83
4	F	903	ATP	C2-N3-C4	3.11	119.42	111.83
4	A	901	ATP	C2-N3-C4	3.10	119.40	111.83
4	F	901	ATP	C5-C4-N3	-3.09	122.46	126.72
4	E	901	ATP	C5-C4-N3	-3.08	122.48	126.72
4	E	903	ATP	C5-C4-N3	-3.06	122.51	126.72
4	A	903	ATP	C5-C4-N3	-3.05	122.51	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	901	ATP	C2-N3-C4	3.04	119.25	111.83
4	B	901	ATP	C2-N3-C4	3.02	119.20	111.83
4	F	901	ATP	C2-N3-C4	3.01	119.19	111.83
4	B	901	ATP	O2B-PB-O3B	3.00	115.37	107.27
4	D	903	ATP	C6-C5-N7	2.97	137.82	132.09
4	A	903	ATP	C2-N3-C4	2.96	119.07	111.83
4	B	903	ATP	C6-C5-N7	2.95	137.77	132.09
4	B	901	ATP	C6-C5-N7	2.92	137.72	132.09
4	F	903	ATP	O3A-PB-O1B	-2.92	101.92	110.70
4	C	903	ATP	C6-C5-N7	2.91	137.71	132.09
4	E	901	ATP	O2B-PB-O3B	2.91	115.14	107.27
4	D	903	ATP	C5-C4-N3	-2.91	122.71	126.72
4	C	903	ATP	C4-N9-C8	2.87	108.75	105.74
4	F	903	ATP	C6-C5-N7	2.83	137.55	132.09
4	B	901	ATP	C5-C4-N3	-2.83	122.82	126.72
4	A	901	ATP	C6-C5-N7	2.83	137.54	132.09
4	F	903	ATP	C4-N9-C8	2.83	108.70	105.74
4	F	903	ATP	O2B-PB-O3B	2.79	114.81	107.27
4	C	903	ATP	C2-N3-C4	2.77	118.60	111.83
4	E	901	ATP	C6-C5-N7	2.74	137.37	132.09
4	F	901	ATP	C6-C5-N7	2.71	137.31	132.09
4	C	901	ATP	C2'-C1'-N9	2.70	120.01	113.30
4	A	903	ATP	C6-C5-N7	2.66	137.21	132.09
4	F	901	ATP	O2B-PB-O3B	2.65	114.44	107.27
4	C	901	ATP	O2B-PB-O3B	2.65	114.44	107.27
4	C	901	ATP	C6-C5-N7	2.62	137.15	132.09
4	A	903	ATP	O2G-PG-O3B	-2.60	95.93	104.64
4	E	901	ATP	C2'-C1'-N9	2.59	119.74	113.30
4	D	901	ATP	C6-C5-N7	2.57	137.05	132.09
4	D	901	ATP	O2B-PB-O3B	2.57	114.21	107.27
4	C	903	ATP	O2B-PB-O3B	2.54	114.12	107.27
4	D	903	ATP	C2'-C1'-N9	2.53	119.60	113.30
4	A	903	ATP	C2'-C1'-N9	2.51	119.55	113.30
4	B	903	ATP	C2'-C1'-N9	2.50	119.52	113.30
4	E	903	ATP	C2'-C1'-N9	2.49	119.50	113.30
4	A	901	ATP	O2B-PB-O3B	2.49	114.01	107.27
4	E	901	ATP	O3A-PB-O1B	-2.48	103.25	110.70
4	C	903	ATP	C5-C4-N3	-2.47	123.31	126.72
4	D	903	ATP	C4-N9-C8	2.46	108.32	105.74
4	F	901	ATP	O2'-C2'-C3'	2.44	119.65	111.82
4	E	901	ATP	O3B-PB-O1B	-2.43	103.40	110.70
4	F	903	ATP	O4'-C1'-N9	-2.42	103.44	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	901	ATP	C4-N9-C8	2.41	108.27	105.74
4	D	901	ATP	C4-N9-C8	2.41	108.27	105.74
4	A	901	ATP	C2'-C1'-N9	2.40	119.28	113.30
4	E	901	ATP	O4'-C1'-N9	-2.38	103.52	108.09
4	B	901	ATP	O2'-C2'-C3'	2.37	119.43	111.82
4	E	903	ATP	O2B-PB-O3A	2.36	113.67	107.27
4	F	903	ATP	C2'-C1'-N9	2.36	119.18	113.30
4	F	901	ATP	C4-N9-C8	2.36	108.22	105.74
4	D	901	ATP	O4'-C1'-N9	-2.35	103.58	108.09
4	C	903	ATP	C2'-C1'-N9	2.34	119.12	113.30
4	F	903	ATP	O2B-PB-O3A	2.33	113.58	107.27
4	E	901	ATP	C4-N9-C8	2.33	108.19	105.74
4	F	901	ATP	C2'-C1'-N9	2.31	119.05	113.30
4	A	903	ATP	C4-N9-C8	2.27	108.12	105.74
4	C	901	ATP	O4'-C1'-N9	-2.24	103.80	108.09
4	E	903	ATP	O2'-C2'-C3'	2.22	118.95	111.82
4	A	903	ATP	O2'-C2'-C3'	2.22	118.95	111.82
4	D	901	ATP	C2'-C3'-C4'	2.20	106.86	102.61
4	B	903	ATP	N6-C6-N1	-2.20	113.49	118.38
4	C	901	ATP	O2'-C2'-C3'	2.19	118.85	111.82
4	B	903	ATP	O2'-C2'-C3'	2.19	118.84	111.82
4	A	903	ATP	O3B-PG-O1G	2.19	122.54	111.04
4	A	901	ATP	O2B-PB-O3A	2.15	113.08	107.27
4	D	903	ATP	O2G-PG-O3B	2.15	111.84	104.64
4	D	903	ATP	N6-C6-N1	-2.13	113.64	118.38
4	D	903	ATP	O2B-PB-O3B	2.12	113.01	107.27
4	E	903	ATP	N6-C6-N1	-2.11	113.67	118.38
4	E	903	ATP	C5-C4-N9	2.11	108.11	105.81
4	F	901	ATP	O3B-PB-O1B	-2.10	104.39	110.70
4	B	903	ATP	O2B-PB-O3B	2.09	112.91	107.27
4	E	901	ATP	O2B-PB-O3A	2.07	112.88	107.27
4	B	901	ATP	C2'-C1'-N9	2.07	118.45	113.30
4	F	903	ATP	N3-C4-N9	2.06	130.68	127.17
4	B	901	ATP	O3B-PB-O1B	-2.04	104.57	110.70
4	D	901	ATP	C2'-C1'-N9	2.04	118.36	113.30
4	D	903	ATP	C2-N1-C6	2.03	122.07	118.73
4	C	903	ATP	O3B-PB-O1B	-2.03	104.61	110.70
4	A	901	ATP	C4-N9-C8	2.02	107.86	105.74
4	C	903	ATP	C2-N1-C6	2.02	122.05	118.73
4	B	903	ATP	C5-C4-N9	2.01	108.00	105.81
4	F	903	ATP	O3B-PB-O1B	-2.00	104.68	110.70
4	A	903	ATP	O2B-PB-O1B	-2.00	103.14	112.44

There are no chirality outliers.

All (91) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
4	A	901	ATP	PB-O3A-PA-O5'
4	A	903	ATP	PB-O3A-PA-O5'
4	B	903	ATP	PB-O3A-PA-O5'
4	C	901	ATP	PB-O3A-PA-O5'
4	C	903	ATP	PB-O3A-PA-O5'
4	D	901	ATP	PB-O3A-PA-O5'
4	D	903	ATP	PB-O3A-PA-O5'
4	E	901	ATP	PB-O3A-PA-O5'
4	E	903	ATP	PB-O3A-PA-O5'
4	F	901	ATP	PB-O3A-PA-O5'
4	F	903	ATP	PB-O3A-PA-O5'
4	A	901	ATP	PA-O3A-PB-O2B
4	B	901	ATP	PA-O3A-PB-O2B
4	B	903	ATP	PA-O3A-PB-O2B
4	C	901	ATP	PA-O3A-PB-O2B
4	C	903	ATP	PA-O3A-PB-O2B
4	D	901	ATP	PA-O3A-PB-O2B
4	D	903	ATP	PA-O3A-PB-O2B
4	E	901	ATP	PA-O3A-PB-O2B
4	E	903	ATP	PA-O3A-PB-O2B
4	F	901	ATP	PA-O3A-PB-O2B
4	F	903	ATP	PA-O3A-PB-O2B
4	A	901	ATP	C5'-O5'-PA-O1A
4	A	903	ATP	C5'-O5'-PA-O1A
4	B	903	ATP	C5'-O5'-PA-O1A
4	D	903	ATP	C5'-O5'-PA-O1A
4	E	903	ATP	PB-O3B-PG-O1G
4	F	901	ATP	PB-O3A-PA-O2A
4	F	903	ATP	PB-O3A-PA-O1A
4	B	901	ATP	PB-O3A-PA-O5'
4	B	903	ATP	PB-O3B-PG-O1G
4	A	903	ATP	PB-O3B-PG-O2G
4	D	903	ATP	PB-O3B-PG-O2G
4	A	901	ATP	PA-O3A-PB-O1B
4	A	903	ATP	PG-O3B-PB-O2B
4	A	903	ATP	PA-O3A-PB-O1B
4	A	903	ATP	PB-O3A-PA-O1A
4	B	903	ATP	PA-O3A-PB-O1B
4	C	901	ATP	PA-O3A-PB-O1B
4	C	901	ATP	PB-O3A-PA-O2A
4	C	903	ATP	PB-O3A-PA-O1A
4	D	901	ATP	PB-O3A-PA-O2A

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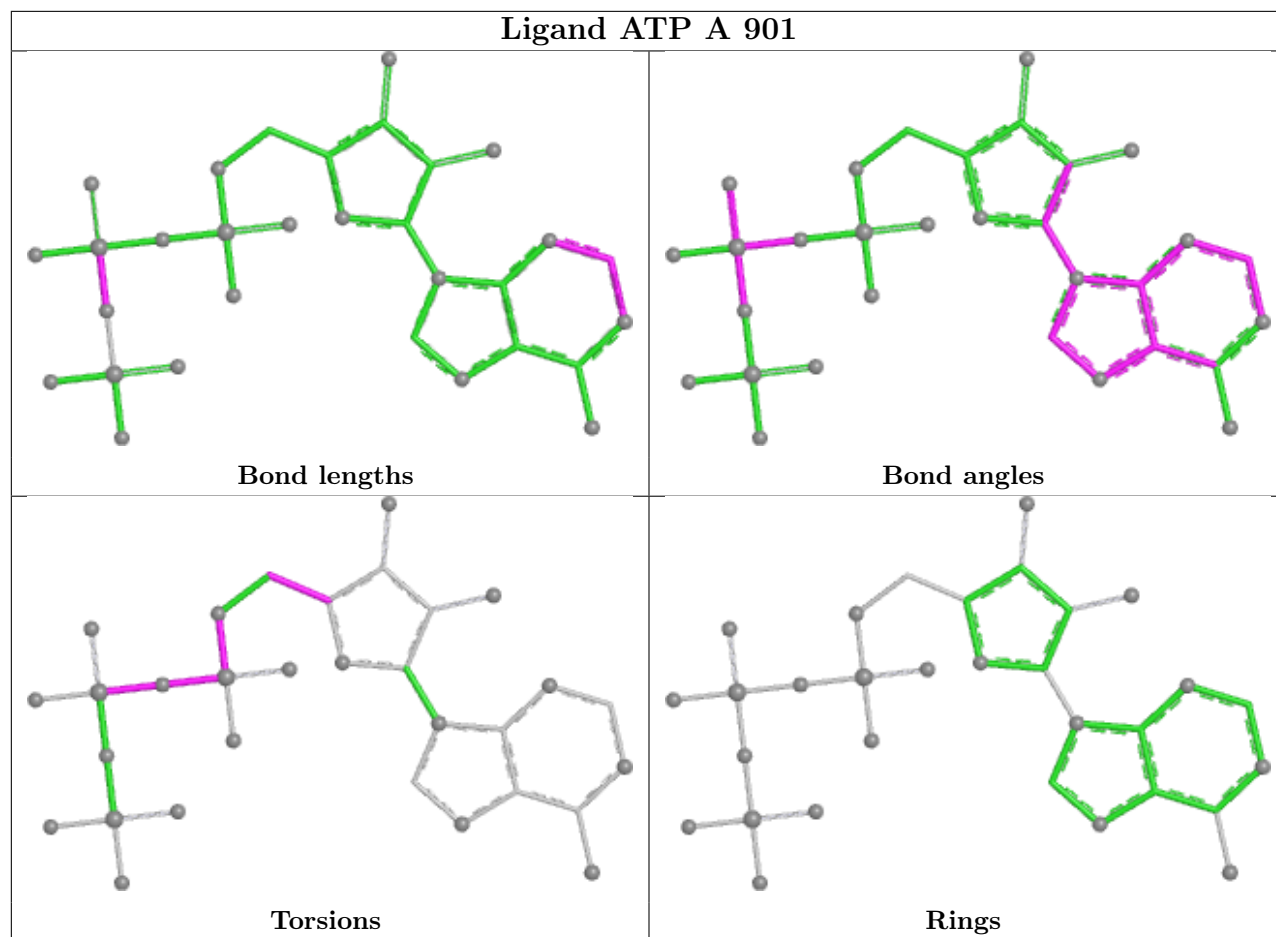
Mol	Chain	Res	Type	Atoms
4	D	903	ATP	PA-O3A-PB-O1B
4	D	903	ATP	PB-O3A-PA-O1A
4	E	903	ATP	PA-O3A-PB-O1B
4	F	901	ATP	PA-O3A-PB-O1B
4	D	903	ATP	PB-O3B-PG-O1G
4	A	901	ATP	PB-O3A-PA-O2A
4	A	903	ATP	PG-O3B-PB-O1B
4	A	903	ATP	PB-O3A-PA-O2A
4	C	903	ATP	PB-O3A-PA-O2A

There are no ring outliers.

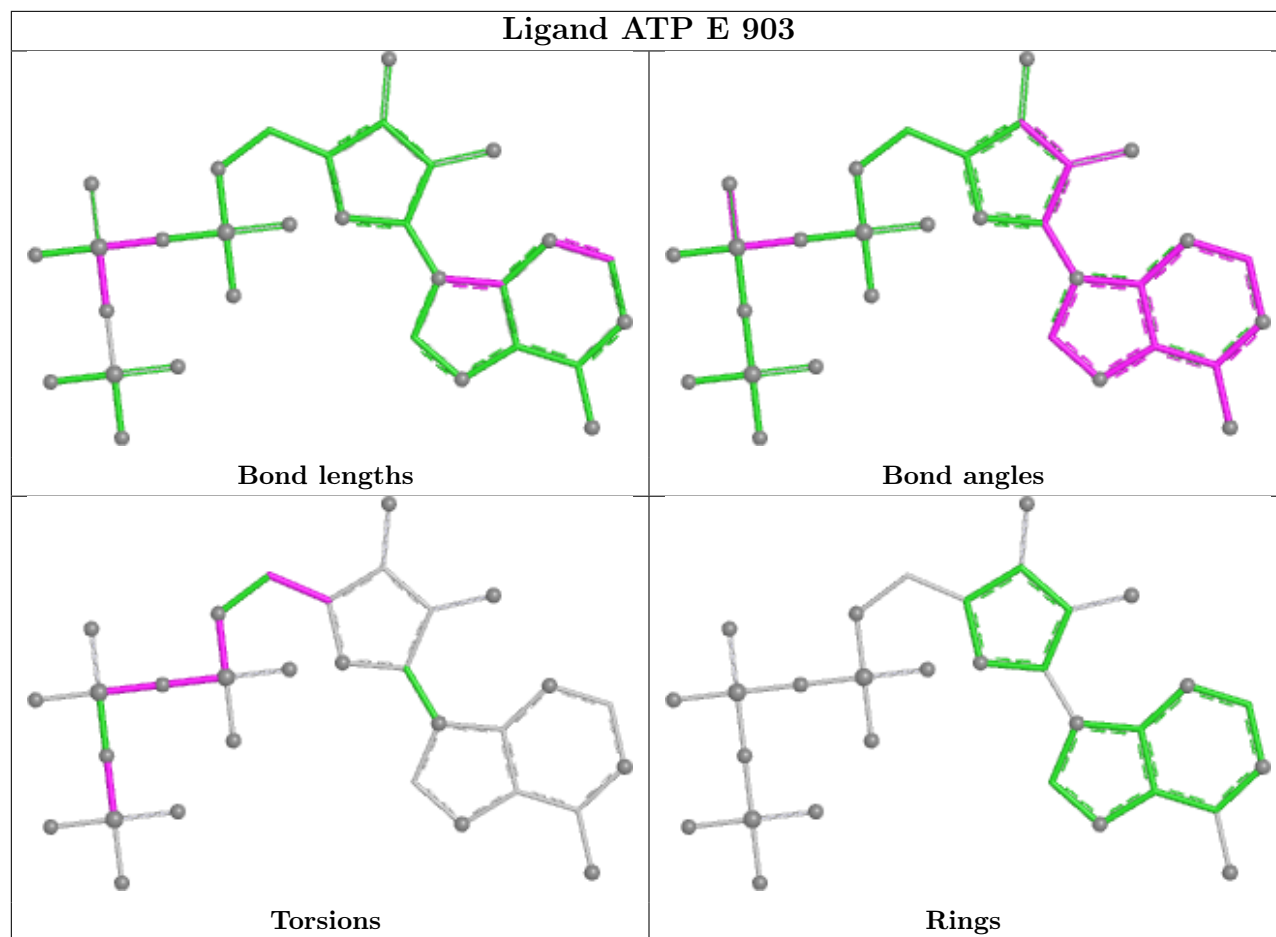
12 monomers are involved in 37 short contacts:

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

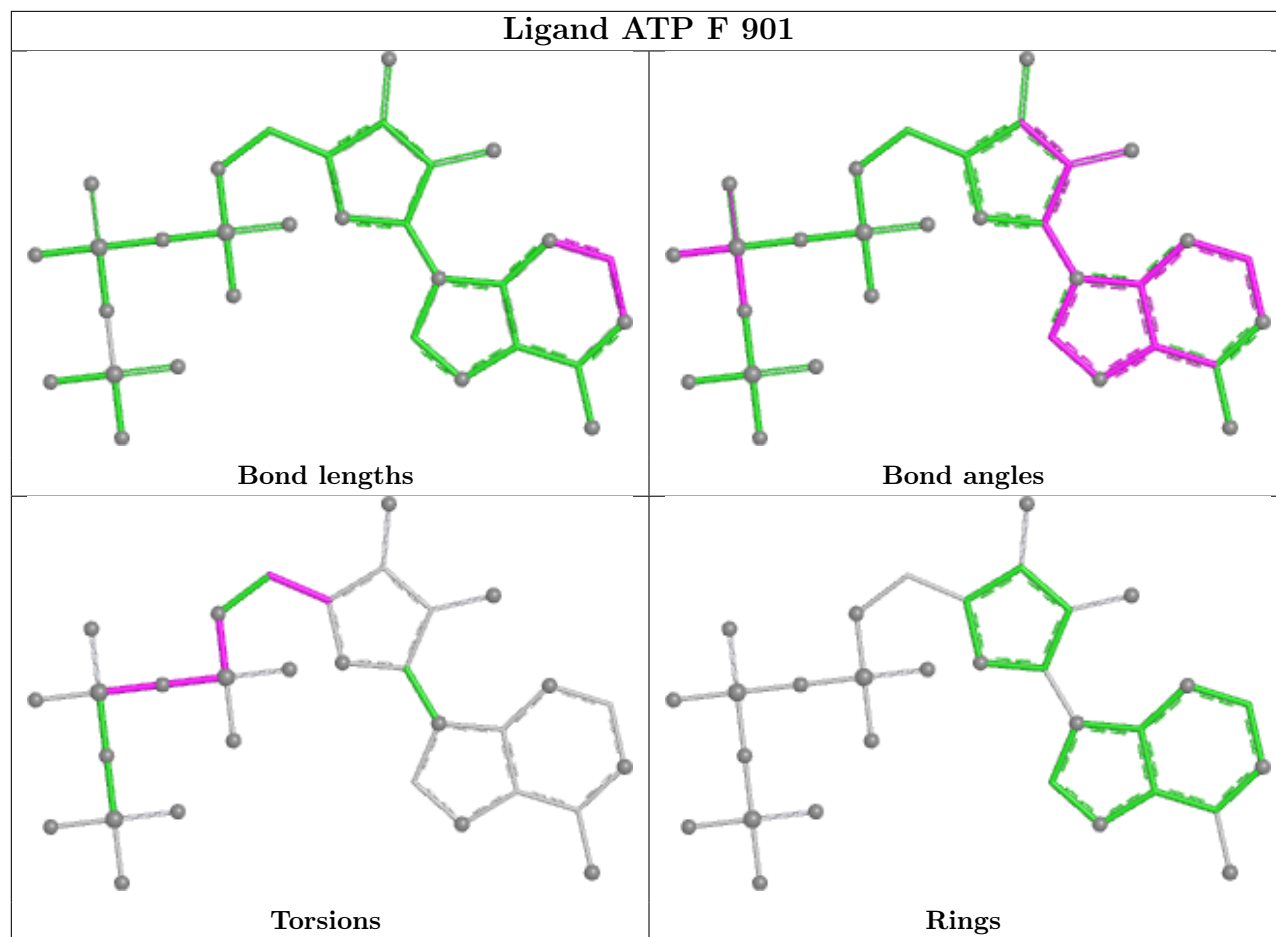
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



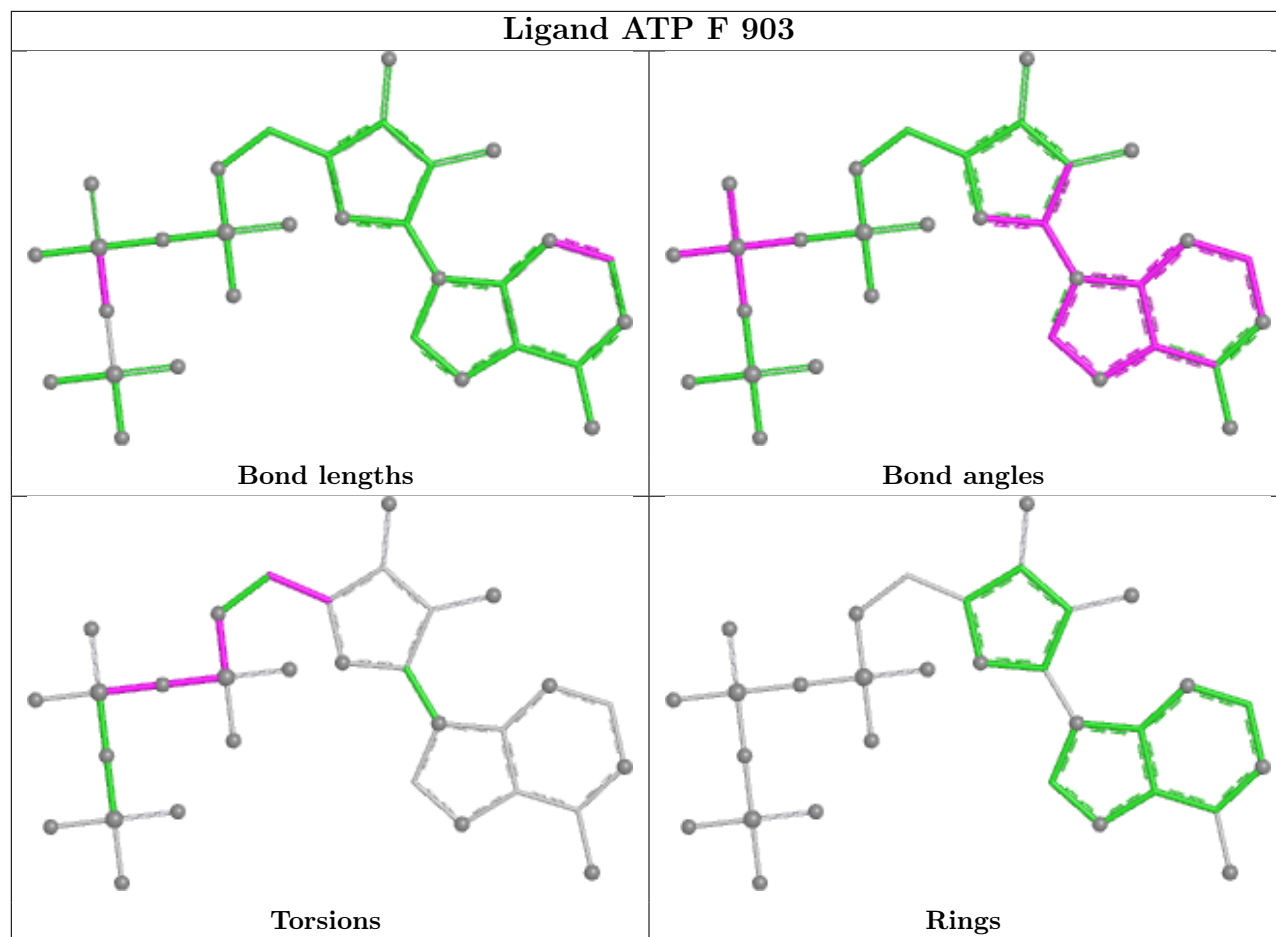
Ligand ATP E 903



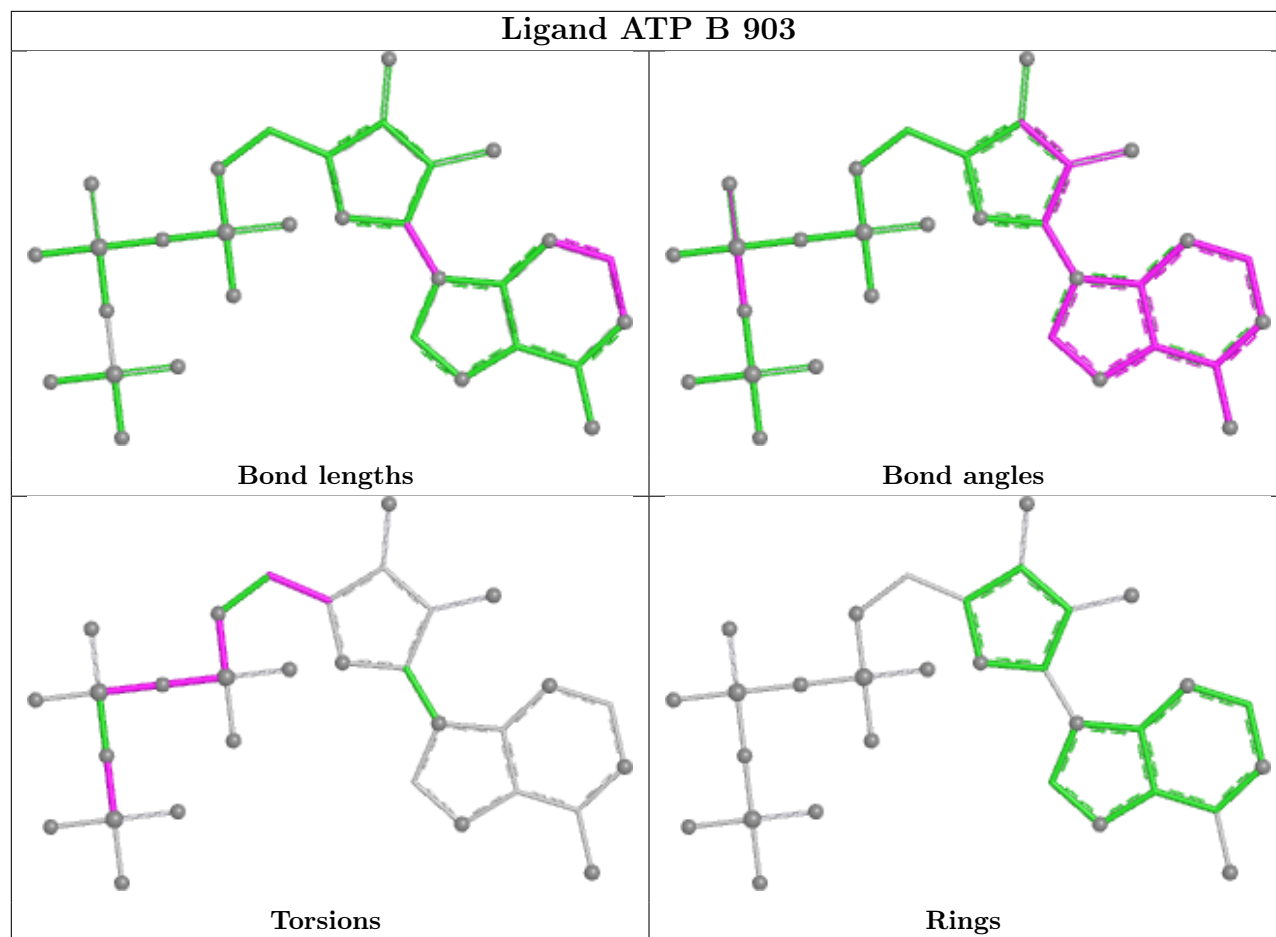
Ligand ATP F 901



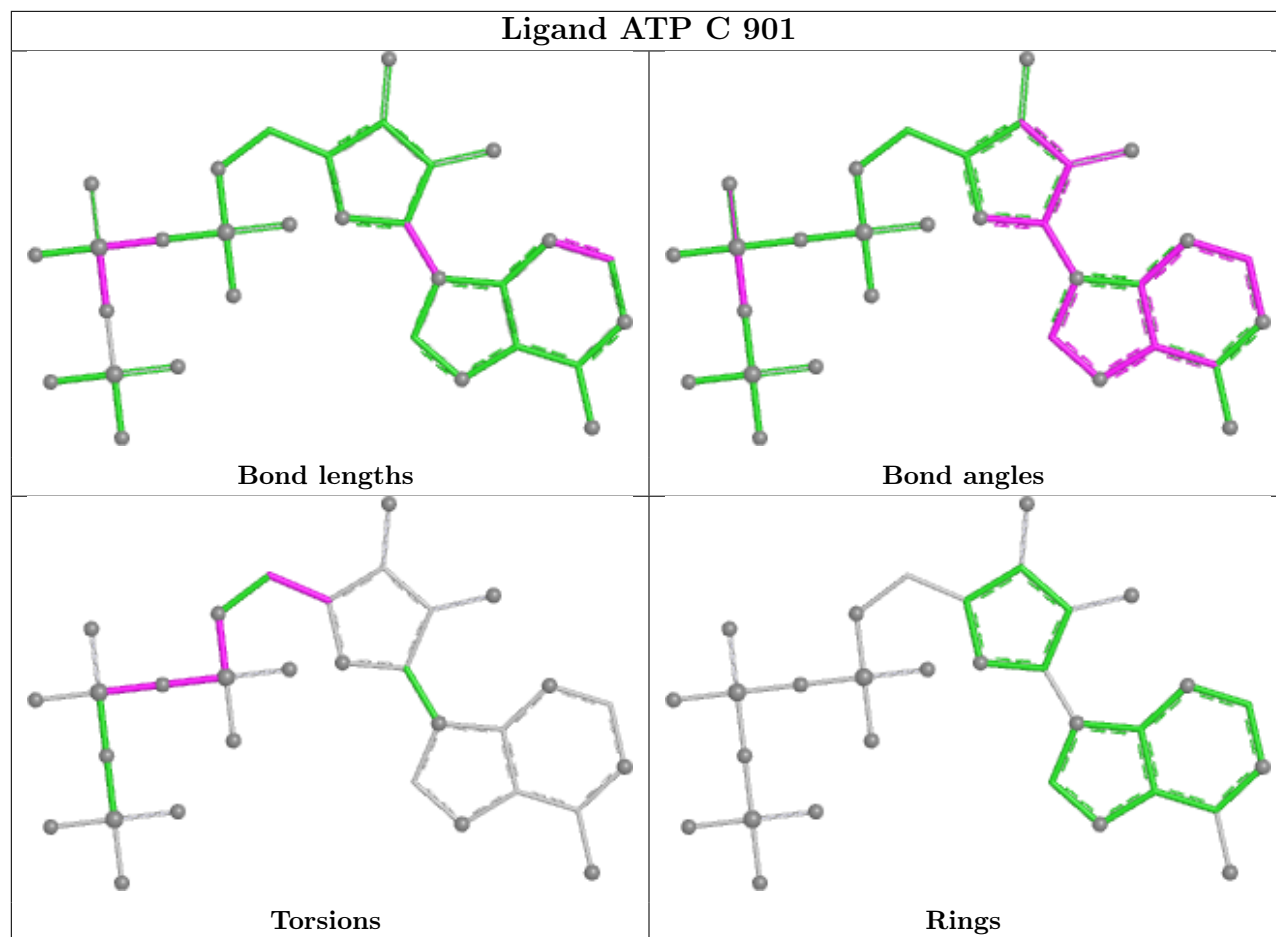
Ligand ATP F 903

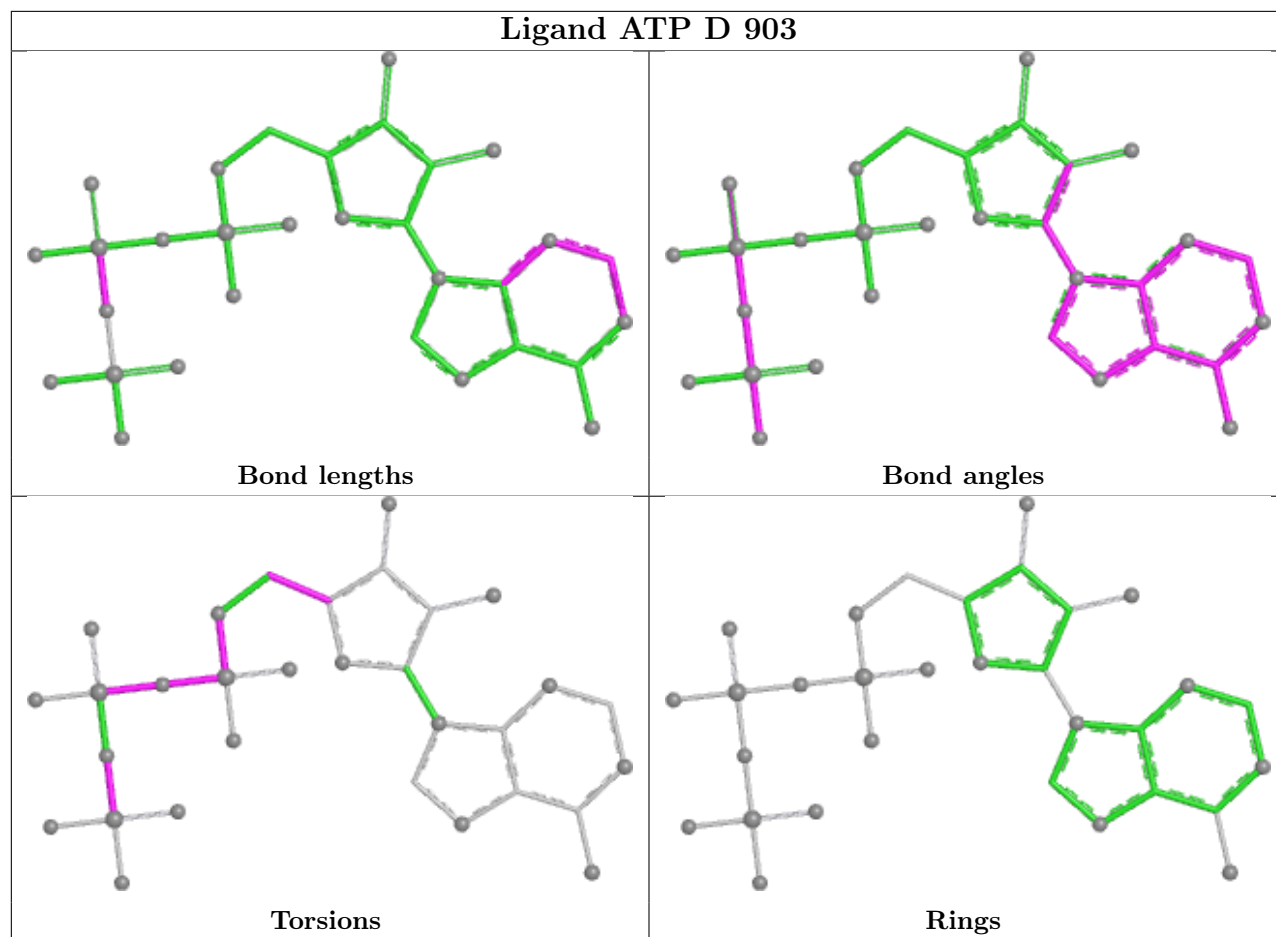


Ligand ATP B 903

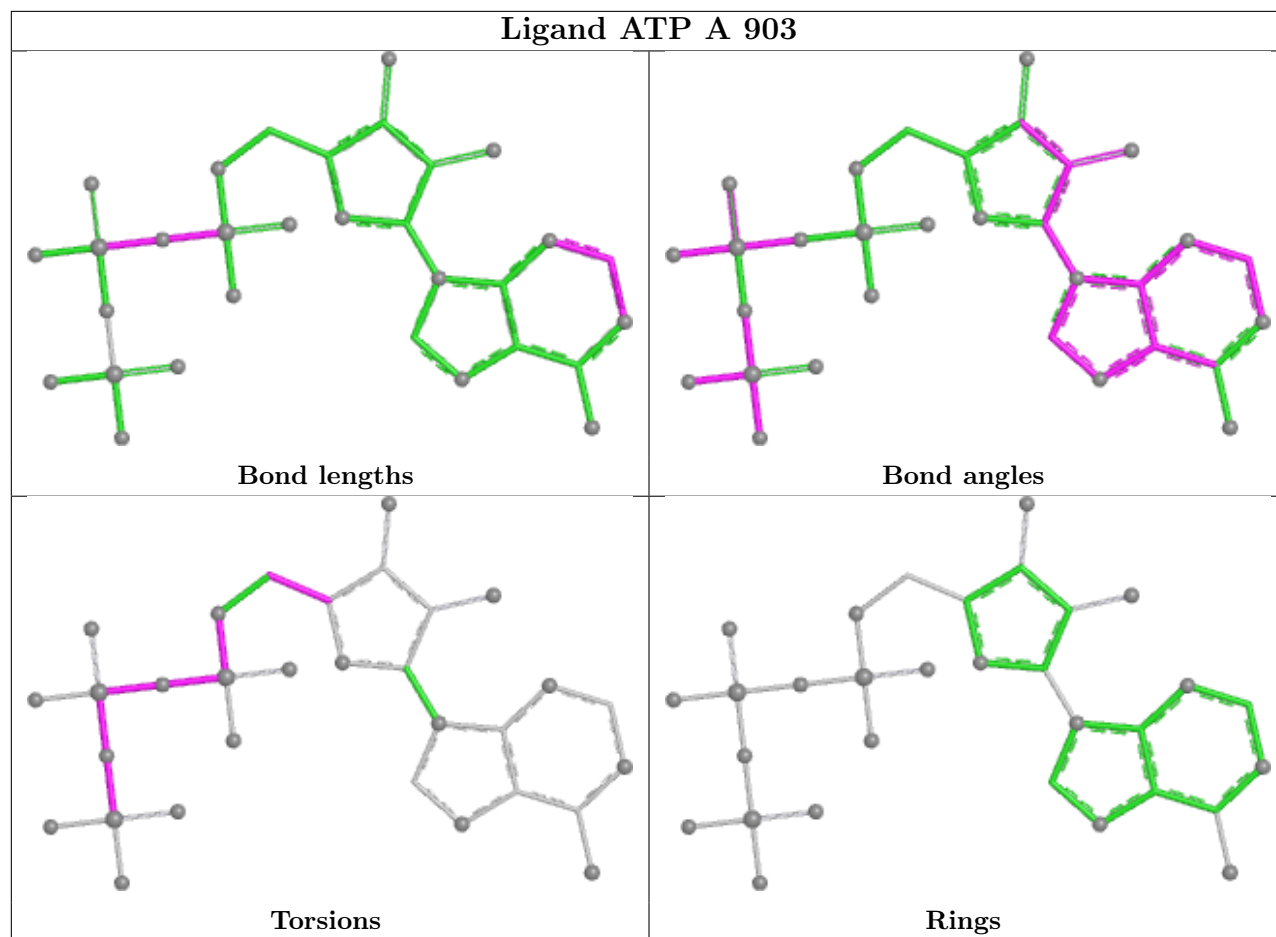


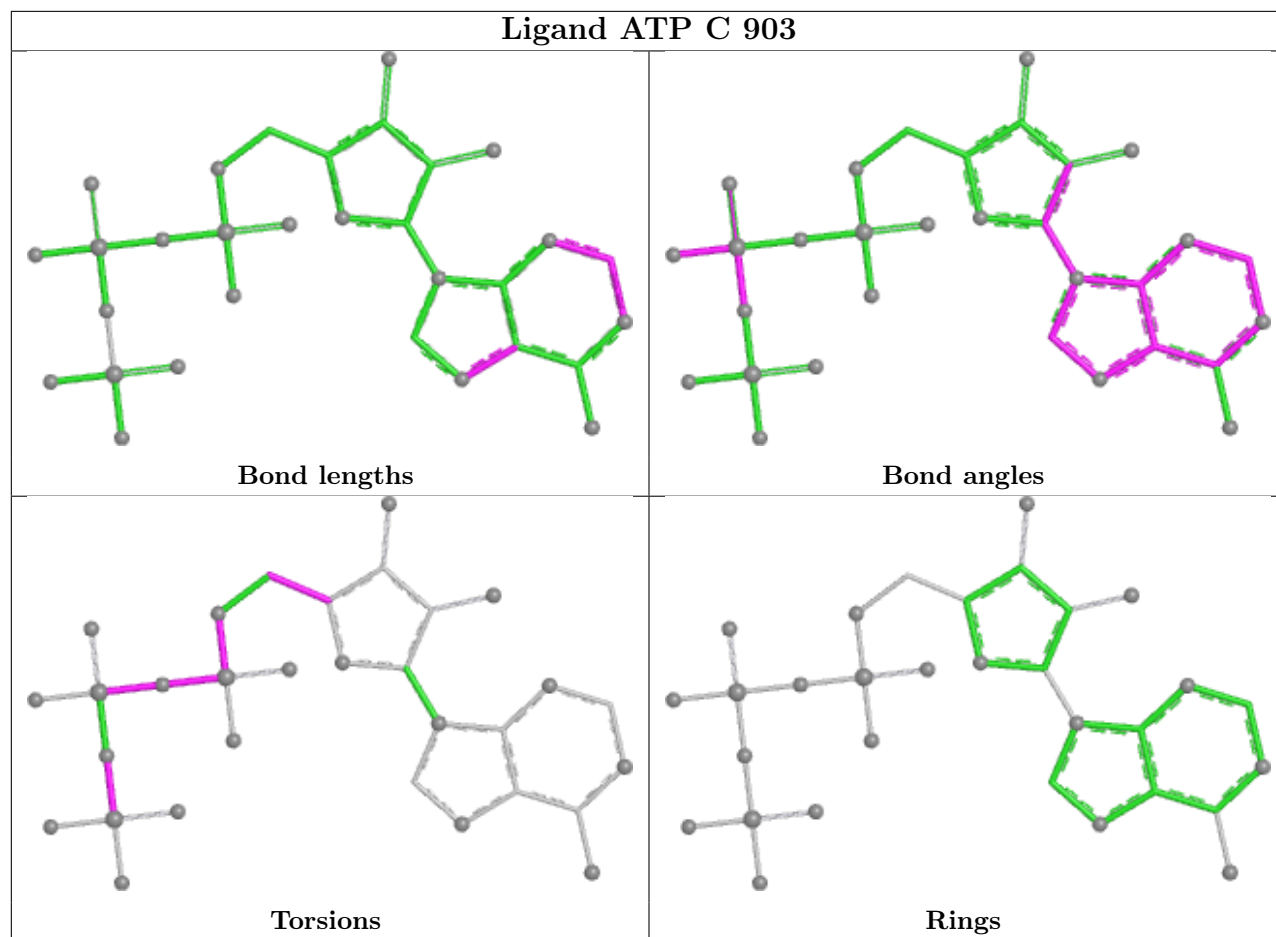
Ligand ATP C 901

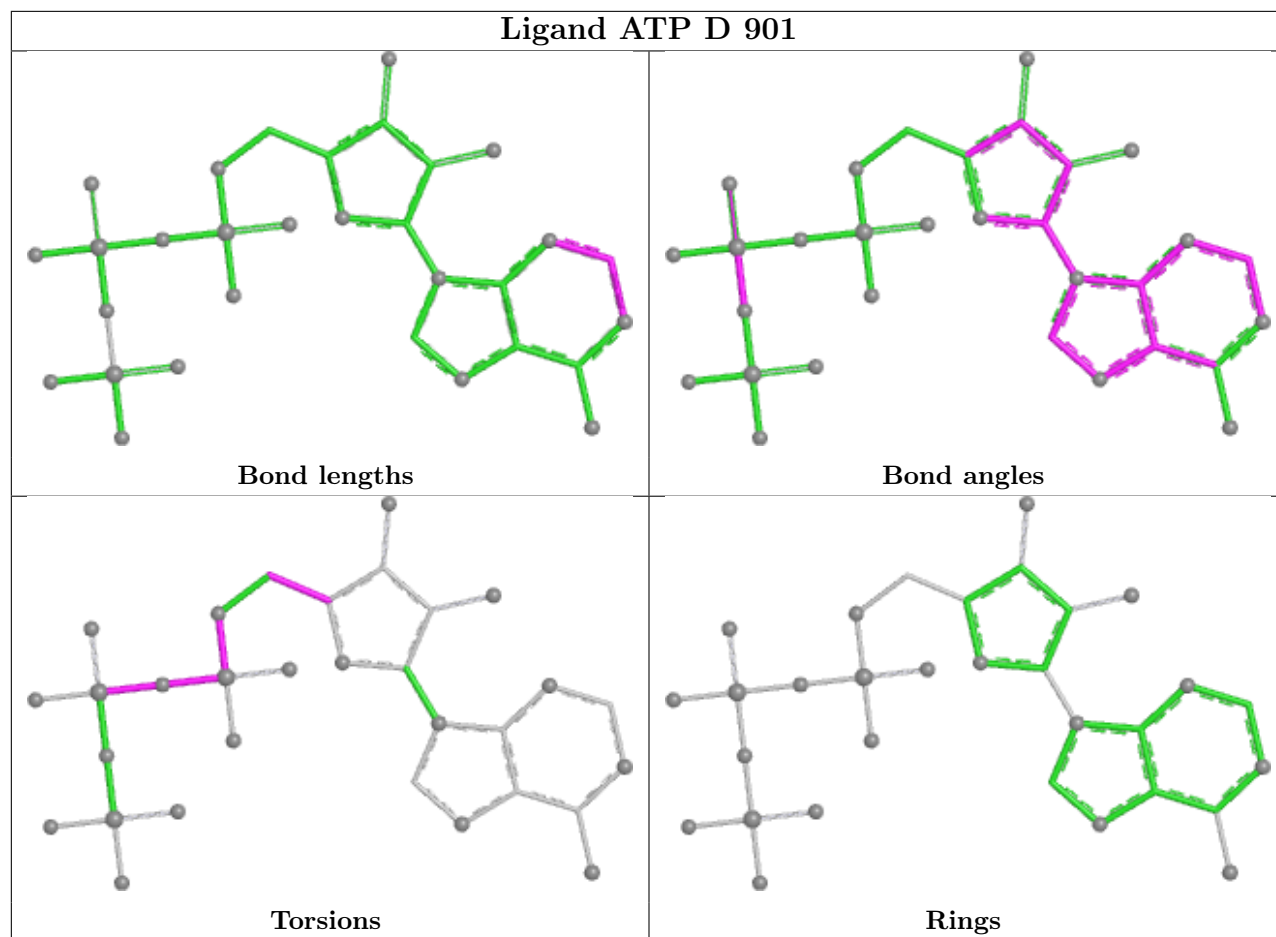




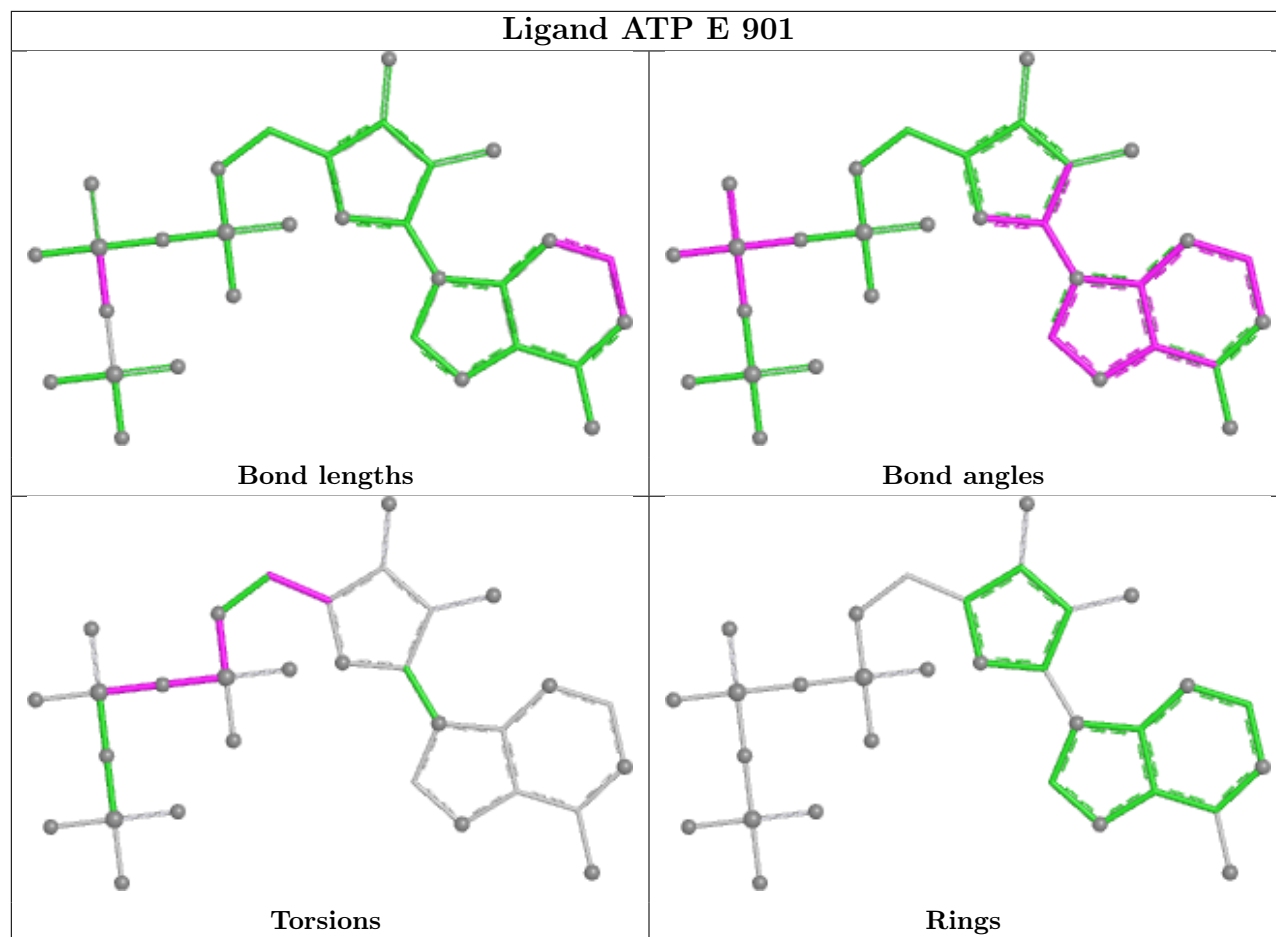
Ligand ATP A 903

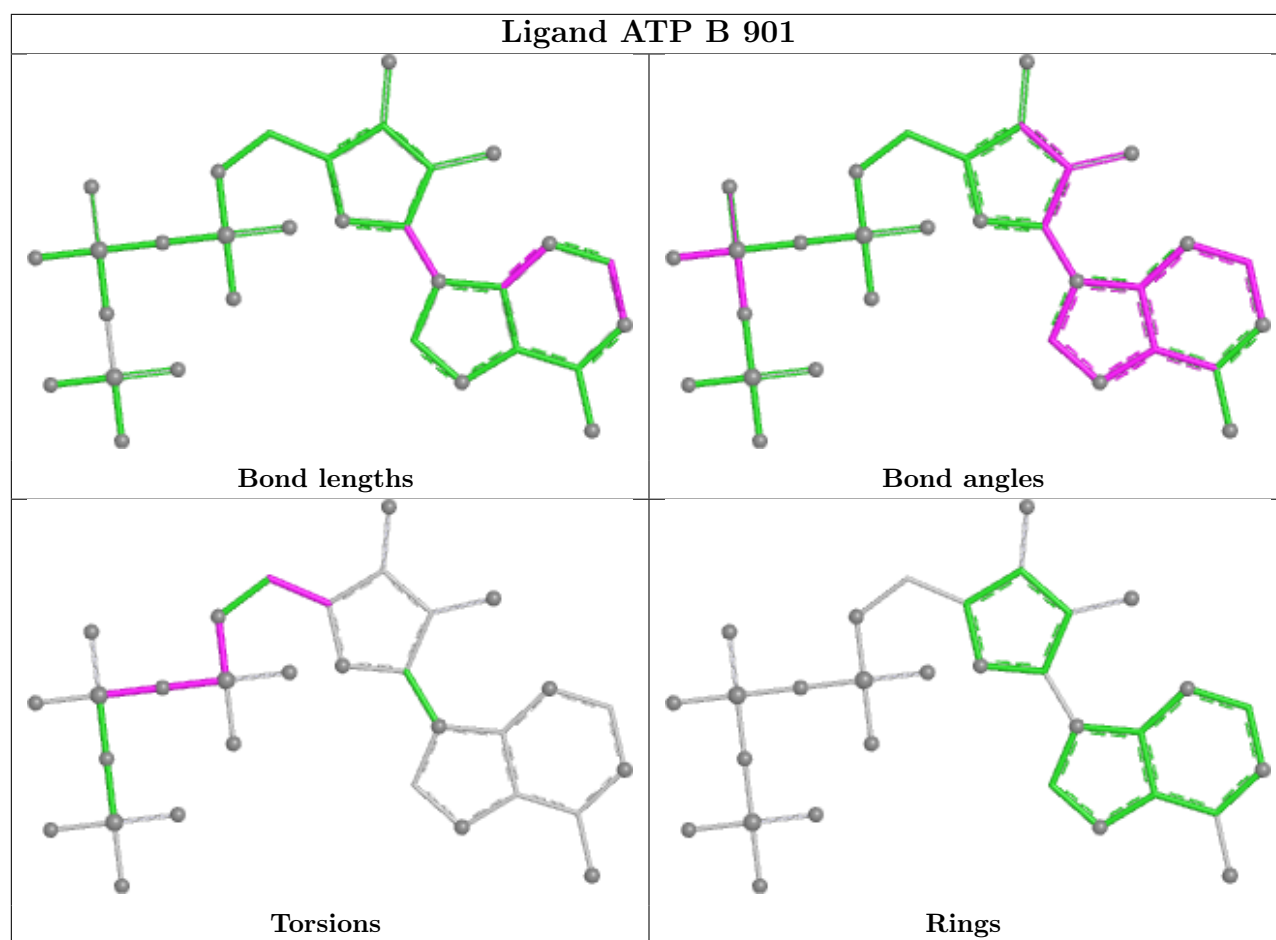






Ligand ATP E 901





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	505/519 (97%)	-0.32	2 (0%) 88 79	30, 83, 129, 159	0
1	B	490/519 (94%)	-0.32	1 (0%) 91 85	43, 85, 130, 165	0
1	E	491/519 (94%)	-0.53	0 100 100	8, 65, 118, 160	0
2	C	488/519 (94%)	-0.42	1 (0%) 91 85	25, 73, 127, 169	0
2	D	485/519 (93%)	-0.52	0 100 100	17, 60, 115, 158	0
2	F	506/519 (97%)	-0.40	1 (0%) 91 85	11, 73, 125, 146	0
All	All	2965/3114 (95%)	-0.42	5 (0%) 91 85	8, 73, 126, 169	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	249	LEU	2.7
1	A	517	PRO	2.2
2	F	120	GLY	2.2
1	A	479	ILE	2.1
1	B	17	ALA	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TPO	B	432	11/12	0.62	0.15	84,94,104,105	0
1	TPO	A	432	11/12	0.85	0.10	82,90,97,97	0
1	TPO	E	432	11/12	0.93	0.08	61,68,76,76	0

6.3 Carbohydrates [i](#)

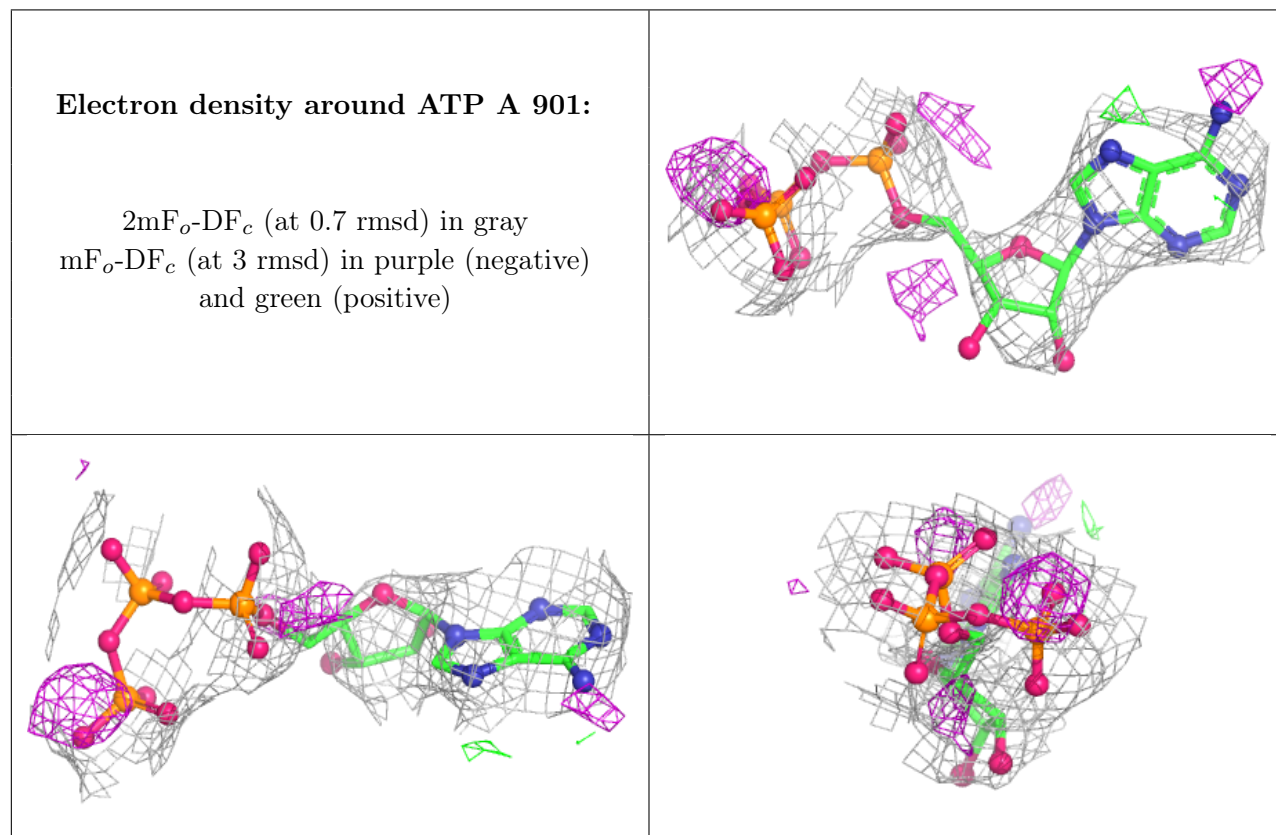
There are no oligosaccharides in this entry.

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.

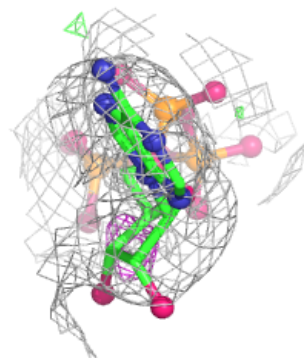
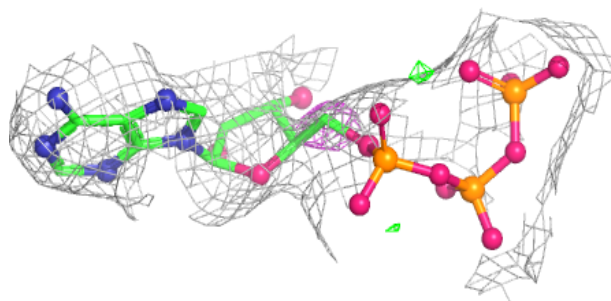
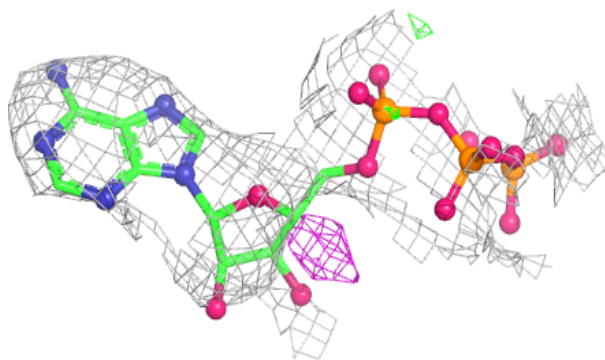
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	E	801	1/1	0.57	0.14	25,25,25,25	0
3	MG	C	701	1/1	0.68	0.29	112,112,112,112	0
3	MG	A	702	1/1	0.74	0.12	90,90,90,90	0
3	MG	A	801	1/1	0.79	0.11	26,26,26,26	0
3	MG	D	520	1/1	0.80	0.09	25,25,25,25	0
3	MG	A	520	1/1	0.80	0.10	113,113,113,113	0
3	MG	C	801	1/1	0.84	0.09	28,28,28,28	0
3	MG	B	701	1/1	0.87	0.12	69,69,69,69	0
3	MG	C	702	1/1	0.89	0.14	104,104,104,104	0
3	MG	E	520	1/1	0.90	0.10	42,42,42,42	0
3	MG	C	802	1/1	0.91	0.09	39,39,39,39	0
3	MG	A	701	1/1	0.91	0.09	75,75,75,75	0
3	MG	E	702	1/1	0.91	0.07	18,18,18,18	0
3	MG	A	802	1/1	0.92	0.11	44,44,44,44	0
4	ATP	A	901	31/31	0.92	0.08	72,82,84,84	0
4	ATP	F	901	31/31	0.92	0.07	93,98,104,104	0
4	ATP	B	903	31/31	0.93	0.07	62,69,79,80	0
3	MG	F	701	1/1	0.93	0.10	60,60,60,60	0
3	MG	F	801	1/1	0.94	0.07	40,40,40,40	0
4	ATP	C	903	31/31	0.94	0.07	45,49,77,80	0
4	ATP	D	901	31/31	0.94	0.07	58,63,70,70	0
4	ATP	E	901	31/31	0.94	0.07	68,74,77,77	0
4	ATP	B	901	31/31	0.94	0.07	62,71,84,84	0
4	ATP	A	903	31/31	0.95	0.07	57,60,67,68	0
3	MG	E	701	1/1	0.95	0.10	91,91,91,91	0
3	MG	D	702	1/1	0.95	0.09	90,90,90,90	0
4	ATP	C	901	31/31	0.95	0.07	47,54,68,69	0
3	MG	F	702	1/1	0.96	0.04	19,19,19,19	0
4	ATP	E	903	31/31	0.96	0.07	24,31,51,52	0
4	ATP	D	903	31/31	0.96	0.07	36,41,61,63	0
4	ATP	F	903	31/31	0.96	0.06	27,33,45,47	0
3	MG	D	801	1/1	0.98	0.09	26,26,26,26	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.

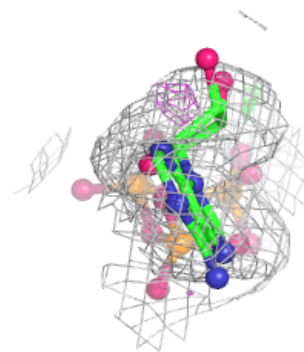
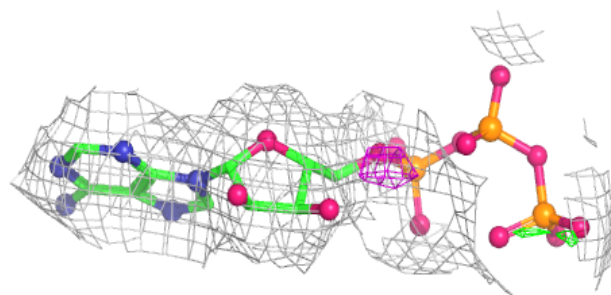
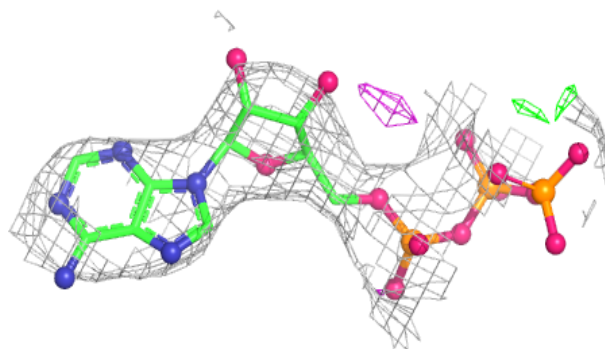


Electron density around ATP F 901:

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

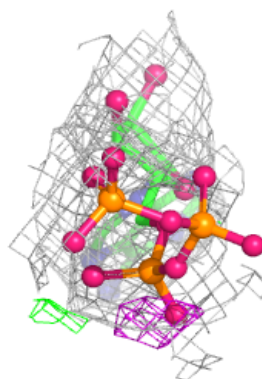
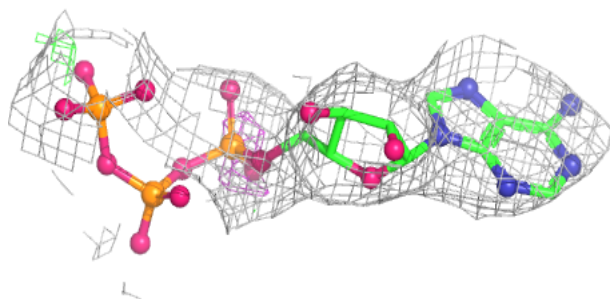
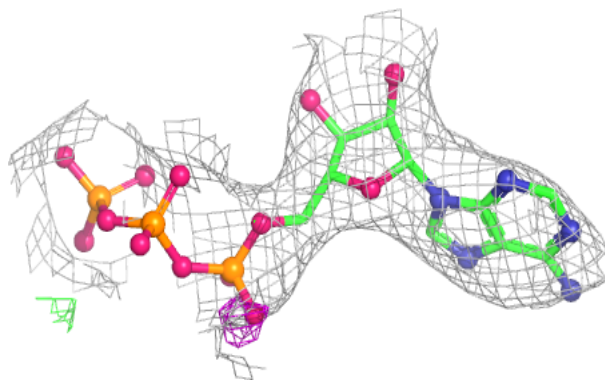
**Electron density around ATP B 903:**

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

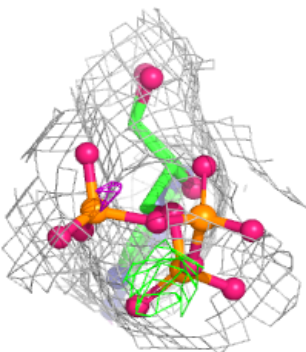
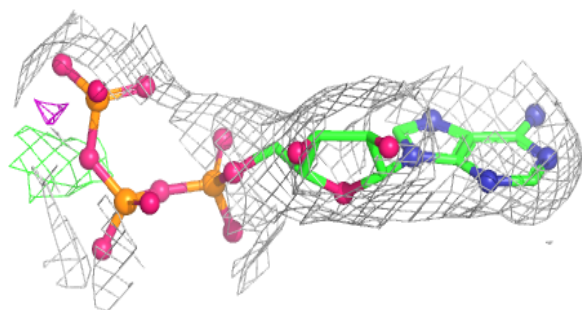
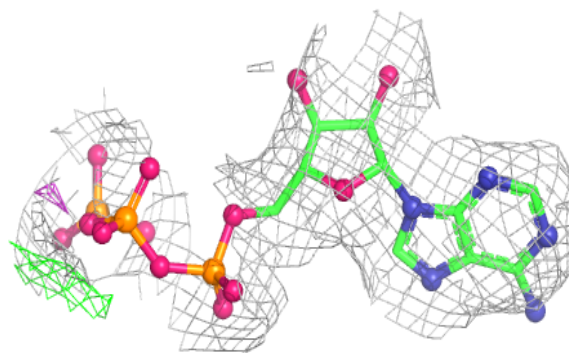


Electron density around ATP C 903:

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

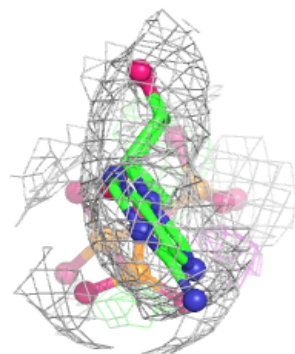
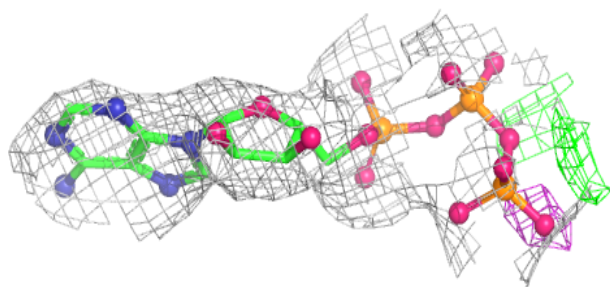
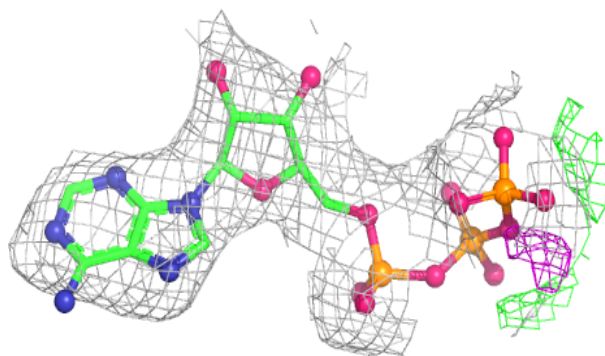
**Electron density around ATP D 901:**

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and green (positive)

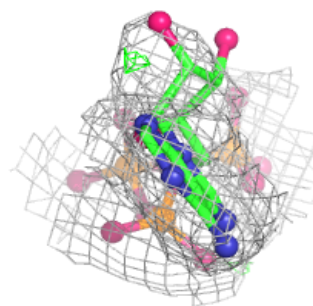
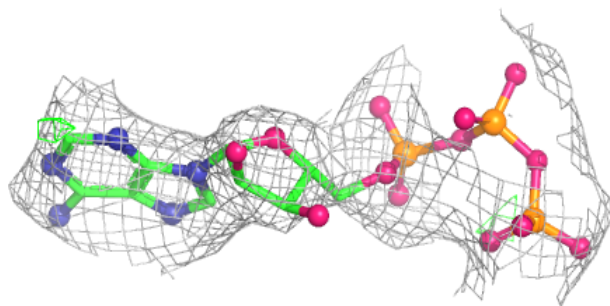
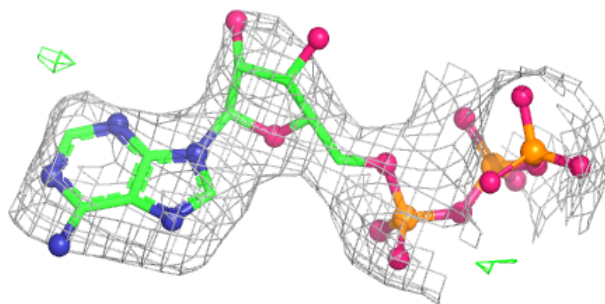


Electron density around ATP E 901:

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

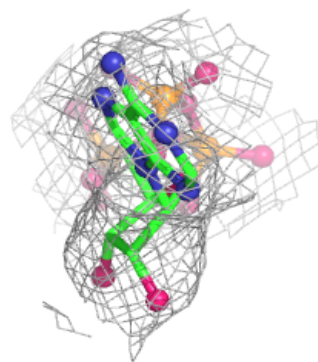
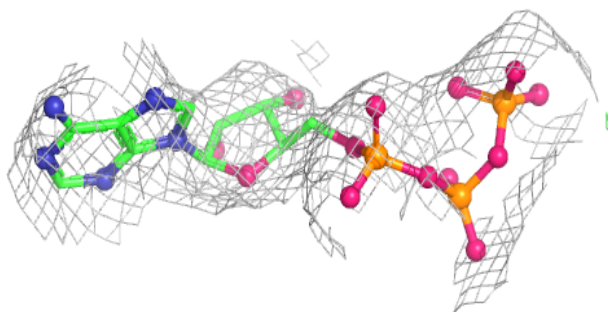
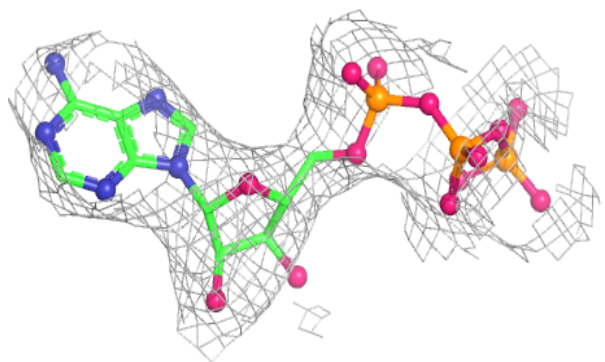
**Electron density around ATP B 901:**

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

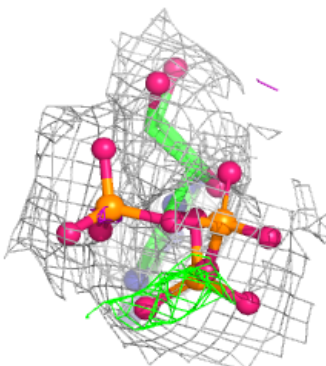
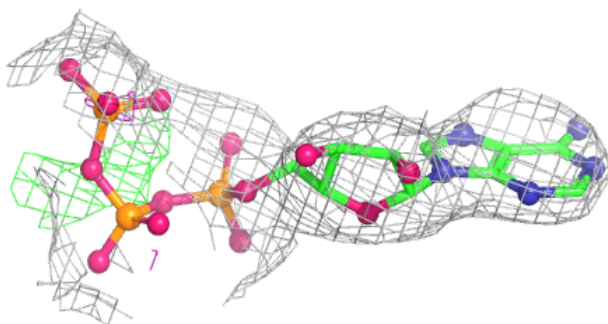
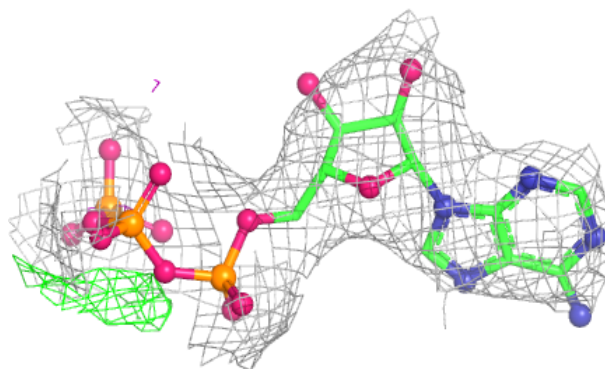


Electron density around ATP A 903:

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

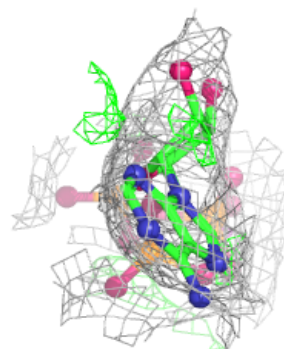
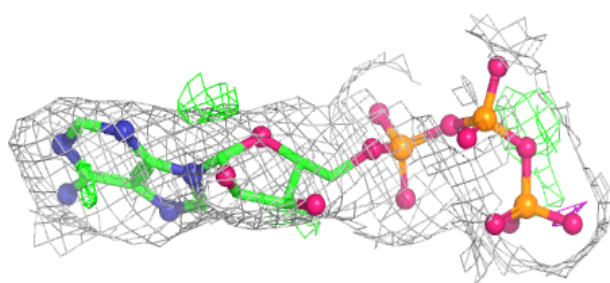
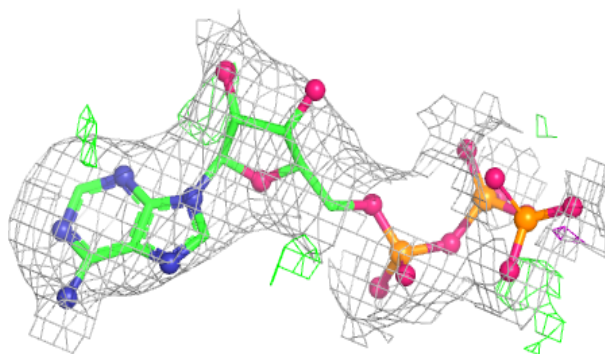
**Electron density around ATP C 901:**

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

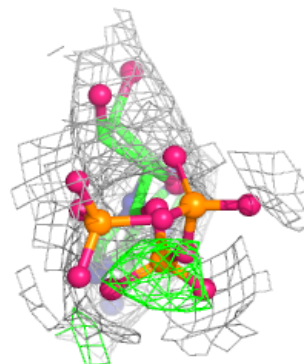
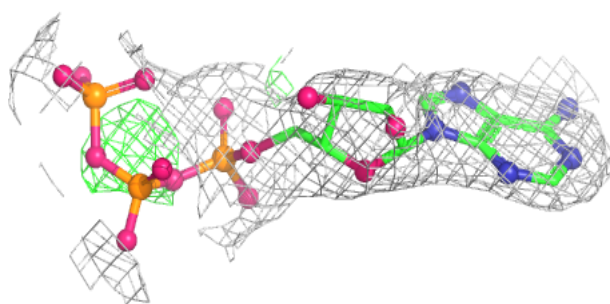
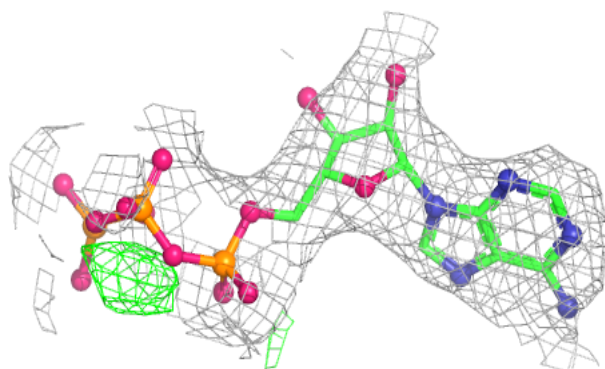


Electron density around ATP E 903:

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

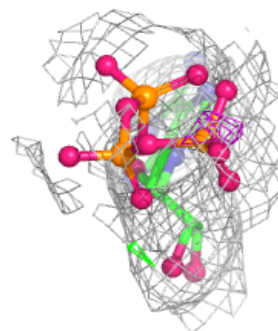
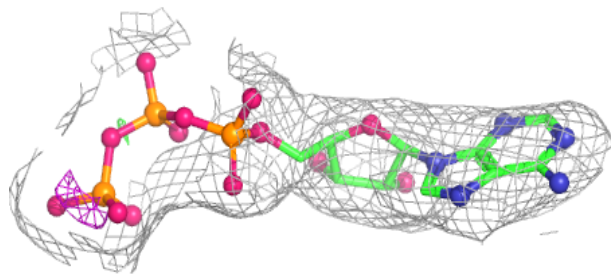
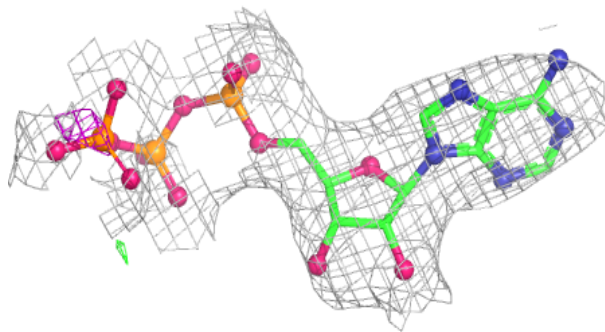
**Electron density around ATP D 903:**

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



Electron density around ATP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.